



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 08:20 PM EST

PDB ID : 8G2D
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with tylosin, mRNA, deacylated A- and E-site tRNA^{phe}, and deacylated P-site tRNA^{met} at 2.70Å resolution
Authors : Aleksandrova, E.V.; Wu, K.J.Y.; Tresco, B.I.C.; Syroegin, E.A.; Killeavy, E.E.; Balasanyants, S.M.; Svetlov, M.S.; Gregory, S.T.; Atkinson, G.C.; Myers, A.G.; Polikanov, Y.S.
Deposited on : 2023-02-03
Resolution : 2.70 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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)

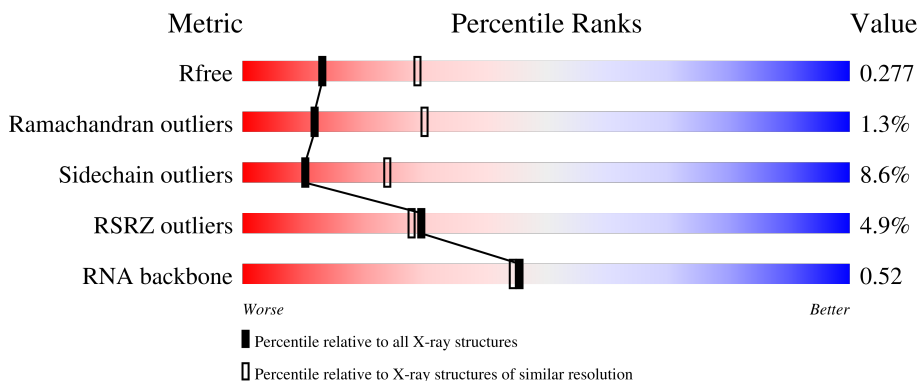
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	
1	2A	2915	
2	1B	121	

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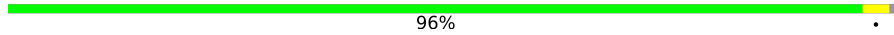
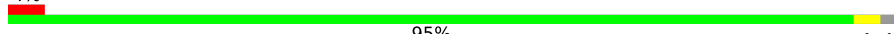
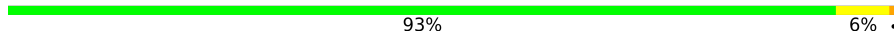

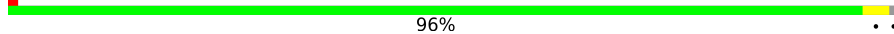
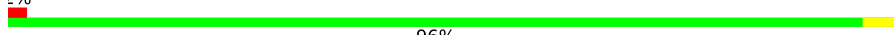
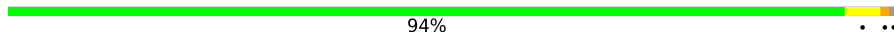
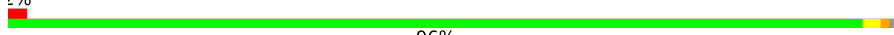





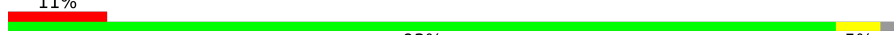


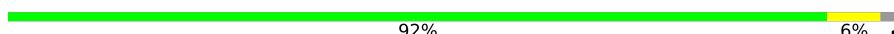






Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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Mol	Chain	Length	Quality of chain
2	2B	121	73% 26%
3	1D	276	95% 5%
3	2D	276	95% 5%
4	1E	206	93% 6%
4	2E	206	93% 6%
5	1F	210	90% 6%
5	2F	210	87% 9%
6	1G	182	91% 8%
6	2G	182	87% 12%
7	1H	180	89% 8%
7	2H	180	88% 8%
8	1I	148	84% 14%
8	2I	148	91% 8%
9	1N	140	95% 5%
9	2N	140	96%
10	1O	122	98%
10	2O	122	94% 6%
11	1P	150	93% 6%
11	2P	150	87% 12%
12	1Q	141	94% 6%
12	2Q	141	91% 9%
13	1R	118	95% 5%
13	2R	118	95% 5%
14	1S	112	92% 6%
14	2S	112	95%

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Mol	Chain	Length	Quality of chain
15	1T	146	 84% 5% 10%
15	2T	146	 86% 10%
16	1U	118	 96% . .
16	2U	118	 95% . .
17	1V	101	 93% 6% .
17	2V	101	 93% 6% .
18	1W	113	 96% . .
18	2W	113	 96% . .
19	1X	96	 94% . . .
19	2X	96	 96% . . .
20	1Y	110	 90% 7% .
20	2Y	110	 88% 9% .
21	1Z	206	 65% 10% 25% 3%
21	2Z	206	 66% 10% 22% 21%
22	10	85	 91% 7% .
22	20	85	 93% 5% .
23	11	98	 90% 9% .
23	21	98	 93% 6% .
24	12	72	 92% 6% .
24	22	72	 89% 8% .
25	13	60	 90% 8% .
25	23	60	 95% . .
26	14	71	 77% 18% . .
26	24	71	 70% 24% . .
27	15	60	 88% 10% .

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Mol	Chain	Length	Quality of chain
27	25	60	90% 8%
28	16	54	89% 9%
28	26	54	2% 89% 9%
29	17	49	6% 92% 6%
29	27	49	10% 92% 6%
30	18	65	95%
30	28	65	3% 94% 5%
31	19	37	100%
31	29	37	16% 89% 11%
32	1a	1521	2% 80% 19%
32	2a	1521	3% 78% 20%
33	1b	256	2% 78% 12% 10%
33	2b	256	25% 77% 12% 10%
34	1c	239	5% 80% 6% 14%
34	2c	239	21% 78% 8% 14%
35	1d	209	7% 90% 9%
35	2d	209	3% 92% 7%
36	1e	162	2% 81% 10% 9%
36	2e	162	11% 85% 6% 9%
37	1f	101	% 94%
37	2f	101	95%
38	1g	156	6% 93% 6%
38	2g	156	12% 88% 11%
39	1h	138	3% 91% 8%
39	2h	138	14% 89% 10%

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Mol	Chain	Length	Quality of chain
40	1i	128	12% 90% 9%
40	2i	128	34% 85% 14%
41	1j	105	6% 82% 10% 8%
41	2j	105	24% 84% 8% 9%
42	1k	129	2% 81% 8% 12%
42	2k	129	2% 81% 7% 12%
43	1l	132	% 85% 8% 8%
43	2l	132	12% 86% 6% 8%
44	1m	126	4% 91% 6%
44	2m	126	17% 87% 10%
45	1n	61	3% 87% 11%
45	2n	61	48% 90% 8%
46	1o	89	4% 91% 8%
46	2o	89	3% 93% ..
47	1p	88	2% 88% 6% 7%
47	2p	88	% 83% 10% 7%
48	1q	105	3% 85% 10% 6%
48	2q	105	10% 87% 8% 6%
49	1r	88	3% 75% 23%
49	2r	88	% 68% 9% 23%
50	1s	93	% 82% 8% 11%
50	2s	93	34% 84% 5% 11%
51	1t	106	5% 83% 7% 9%
51	2t	106	7% 80% 10% 9%
52	1u	27	4% 78% 7% 15%

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

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 299892 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	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
			Total	C	N	O	P			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
5	1F	202	Total 1583	C 1009	N 297	O 275	S 2	0	0	0
5	2F	202	Total 1579	C 1007	N 296	O 274	S 2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
42	2k	114	833	519	156	155	3	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	1106	Total	Mg	0	0
			1106	1106		
56	1B	35	Total	Mg	0	0
			35	35		
56	1D	11	Total	Mg	0	0
			11	11		
56	1E	13	Total	Mg	0	0
			13	13		
56	1F	10	Total	Mg	0	0
			10	10		
56	1G	4	Total	Mg	0	0
			4	4		
56	1I	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1N	5	Total 5	Mg 5	0	0
56	1O	6	Total 6	Mg 6	0	0
56	1P	5	Total 5	Mg 5	0	0
56	1Q	6	Total 6	Mg 6	0	0
56	1R	6	Total 6	Mg 6	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	3	Total 3	Mg 3	0	0
56	1U	12	Total 12	Mg 12	0	0
56	1V	6	Total 6	Mg 6	0	0
56	1W	7	Total 7	Mg 7	0	0
56	1X	7	Total 7	Mg 7	0	0
56	1Y	3	Total 3	Mg 3	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	10	7	Total 7	Mg 7	0	0
56	11	3	Total 3	Mg 3	0	0
56	12	2	Total 2	Mg 2	0	0
56	13	6	Total 6	Mg 6	0	0
56	15	5	Total 5	Mg 5	0	0
56	16	4	Total 4	Mg 4	0	0
56	17	3	Total 3	Mg 3	0	0
56	18	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	19	1	Total Mg 1 1	0	0
56	1a	224	Total Mg 224 224	0	0
56	1b	2	Total Mg 2 2	0	0
56	1d	1	Total Mg 1 1	0	0
56	1e	2	Total Mg 2 2	0	0
56	1f	2	Total Mg 2 2	0	0
56	1h	1	Total Mg 1 1	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	1p	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1v	1	Total Mg 1 1	0	0
56	1w	7	Total Mg 7 7	0	0
56	1x	14	Total Mg 14 14	0	0
56	1y	4	Total Mg 4 4	0	0
56	2A	877	Total Mg 877 877	0	0
56	2B	21	Total Mg 21 21	0	0
56	2D	6	Total Mg 6 6	0	0
56	2E	10	Total Mg 10 10	0	0

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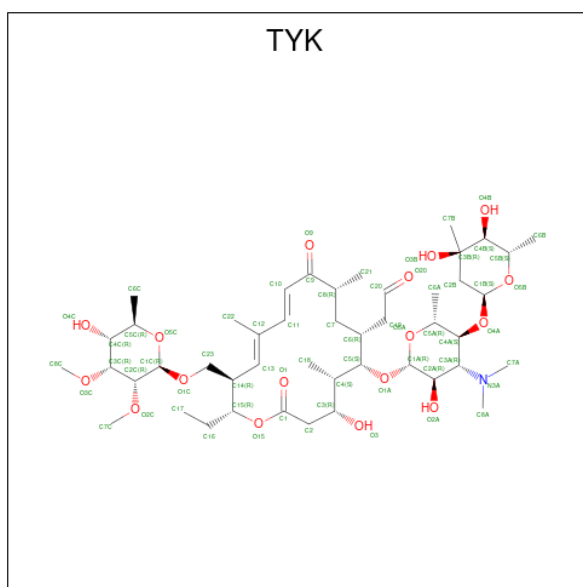
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2F	7	Total Mg 7 7	0	0
56	2G	1	Total Mg 1 1	0	0
56	2N	1	Total Mg 1 1	0	0
56	2O	1	Total Mg 1 1	0	0
56	2P	3	Total Mg 3 3	0	0
56	2Q	3	Total Mg 3 3	0	0
56	2R	2	Total Mg 2 2	0	0
56	2T	3	Total Mg 3 3	0	0
56	2U	1	Total Mg 1 1	0	0
56	2V	2	Total Mg 2 2	0	0
56	2W	3	Total Mg 3 3	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	3	Total Mg 3 3	0	0
56	21	1	Total Mg 1 1	0	0
56	23	4	Total Mg 4 4	0	0
56	25	4	Total Mg 4 4	0	0
56	26	1	Total Mg 1 1	0	0
56	27	1	Total Mg 1 1	0	0
56	28	4	Total Mg 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	29	1	Total Mg 1 1	0	0
56	2a	234	Total Mg 234 234	0	0
56	2d	2	Total Mg 2 2	0	0
56	2e	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0
56	2g	1	Total Mg 1 1	0	0
56	2j	2	Total Mg 2 2	0	0
56	2k	1	Total Mg 1 1	0	0
56	2l	4	Total Mg 4 4	0	0
56	2m	1	Total Mg 1 1	0	0
56	2q	2	Total Mg 2 2	0	0
56	2r	2	Total Mg 2 2	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	2	Total Mg 2 2	0	0
56	2w	7	Total Mg 7 7	0	0
56	2x	4	Total Mg 4 4	0	0
56	2y	6	Total Mg 6 6	0	0

- Molecule 57 is TYLOSIN (three-letter code: TYK) (formula: C₄₆H₇₇NO₁₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
57	1A	1	Total	C	N	O	0	0
			64	46	1	17		
57	2A	1	Total	C	N	O	0	0
			64	46	1	17		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

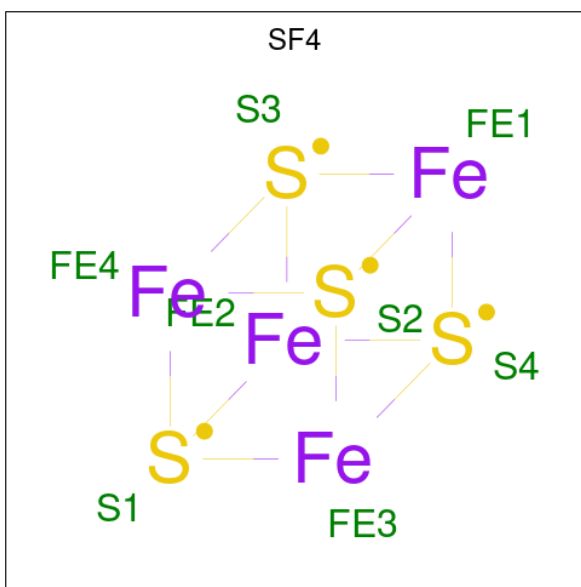
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	2Y	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	29	1	Total Zn 1 1	0	0
58	2n	1	Total Zn 1 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1x	1	Total K 1 1	0	0
60	2A	1	Total K 1 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1864	Total O 1864 1864	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1B	59	Total O 59 59	0	0
61	1D	24	Total O 24 24	0	0
61	1E	26	Total O 26 26	0	0
61	1F	17	Total O 17 17	0	0
61	1G	5	Total O 5 5	0	0
61	1H	1	Total O 1 1	0	0
61	1I	2	Total O 2 2	0	0
61	1N	7	Total O 7 7	0	0
61	1O	9	Total O 9 9	0	0
61	1P	21	Total O 21 21	0	0
61	1Q	10	Total O 10 10	0	0
61	1R	10	Total O 10 10	0	0
61	1S	5	Total O 5 5	0	0
61	1T	7	Total O 7 7	0	0
61	1U	10	Total O 10 10	0	0
61	1V	7	Total O 7 7	0	0
61	1W	8	Total O 8 8	0	0
61	1X	5	Total O 5 5	0	0
61	1Y	3	Total O 3 3	0	0
61	1Z	1	Total O 1 1	0	0
61	10	10	Total O 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	11	9	Total O 9 9	0	0
61	12	4	Total O 4 4	0	0
61	13	4	Total O 4 4	0	0
61	14	1	Total O 1 1	0	0
61	15	5	Total O 5 5	0	0
61	16	2	Total O 2 2	0	0
61	17	10	Total O 10 10	0	0
61	18	13	Total O 13 13	0	0
61	1a	264	Total O 264 264	0	0
61	1b	1	Total O 1 1	0	0
61	1d	1	Total O 1 1	0	0
61	1f	1	Total O 1 1	0	0
61	1g	1	Total O 1 1	0	0
61	1i	2	Total O 2 2	0	0
61	1k	1	Total O 1 1	0	0
61	1l	4	Total O 4 4	0	0
61	1m	1	Total O 1 1	0	0
61	1o	1	Total O 1 1	0	0
61	1p	1	Total O 1 1	0	0
61	1q	5	Total O 5 5	0	0
61	1u	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1v	4	Total O 4 4	0	0
61	1w	13	Total O 13 13	0	0
61	1x	13	Total O 13 13	0	0
61	2A	1086	Total O 1086 1086	0	0
61	2B	21	Total O 21 21	0	0
61	2D	18	Total O 18 18	0	0
61	2E	11	Total O 11 11	0	0
61	2F	13	Total O 13 13	0	0
61	2I	5	Total O 5 5	0	0
61	2N	1	Total O 1 1	0	0
61	2O	1	Total O 1 1	0	0
61	2P	9	Total O 9 9	0	0
61	2Q	3	Total O 3 3	0	0
61	2R	3	Total O 3 3	0	0
61	2T	6	Total O 6 6	0	0
61	2U	1	Total O 1 1	0	0
61	2W	1	Total O 1 1	0	0
61	2X	3	Total O 3 3	0	0
61	2Y	2	Total O 2 2	0	0
61	2Z	1	Total O 1 1	0	0
61	20	5	Total O 5 5	0	0

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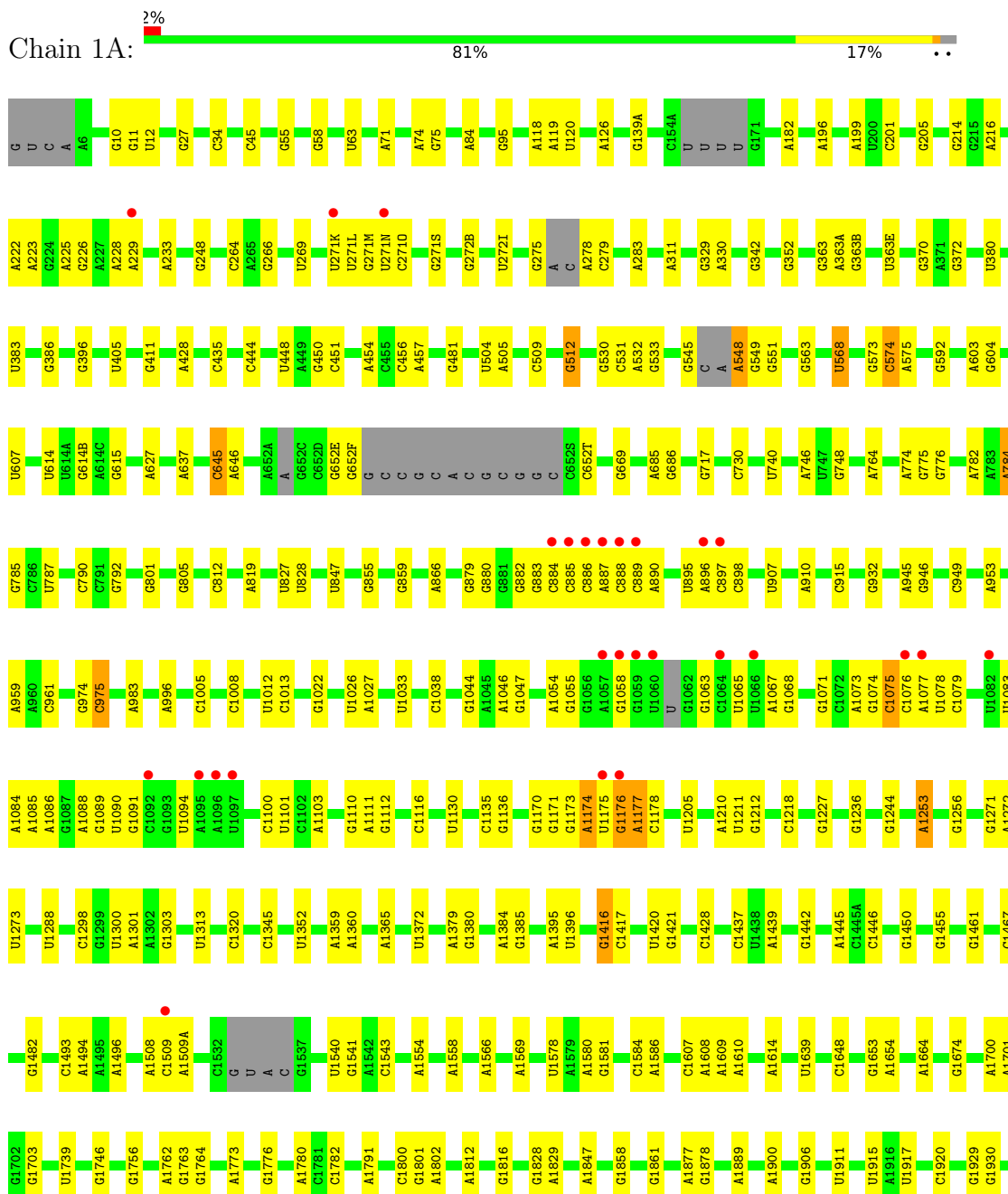
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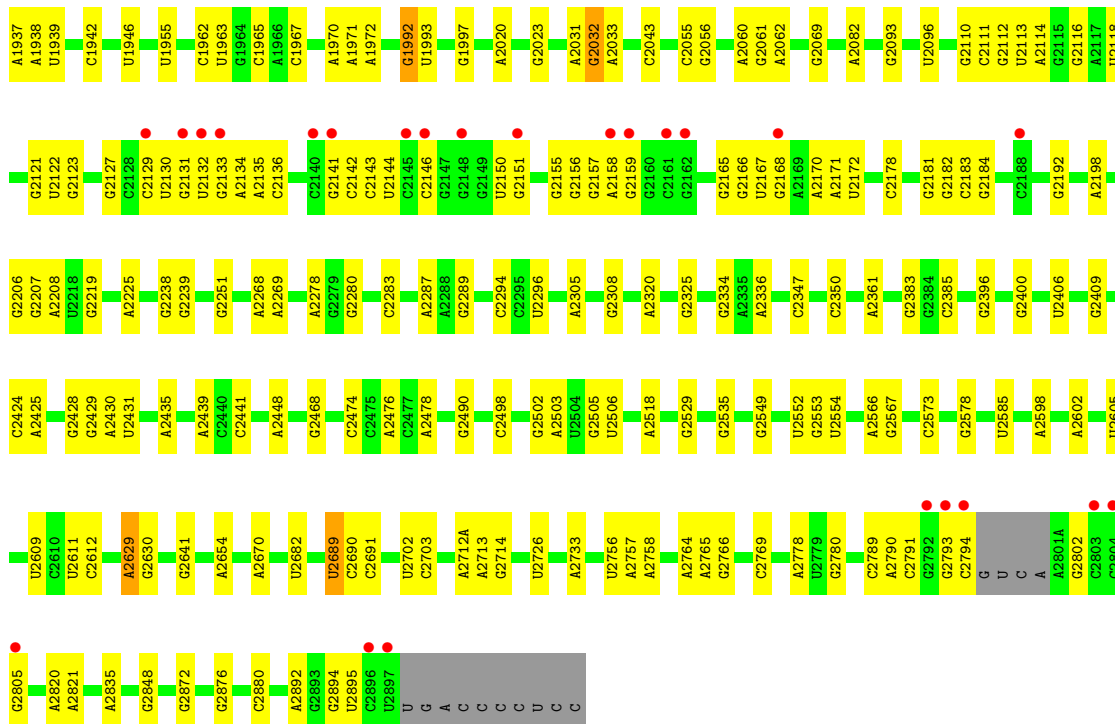
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61	21	9	Total 9	O 9	0	0
61	22	1	Total 1	O 1	0	0
61	23	1	Total 1	O 1	0	0
61	25	3	Total 3	O 3	0	0
61	27	3	Total 3	O 3	0	0
61	28	6	Total 6	O 6	0	0
61	29	1	Total 1	O 1	0	0
61	2a	226	Total 226	O 226	0	0
61	2d	2	Total 2	O 2	0	0
61	2e	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2l	6	Total 6	O 6	0	0
61	2p	3	Total 3	O 3	0	0
61	2q	1	Total 1	O 1	0	0
61	2t	4	Total 4	O 4	0	0
61	2u	1	Total 1	O 1	0	0
61	2v	1	Total 1	O 1	0	0
61	2w	2	Total 2	O 2	0	0
61	2x	7	Total 7	O 7	0	0
61	2y	16	Total 16	O 16	0	0

3 Residue-property plots [i](#)

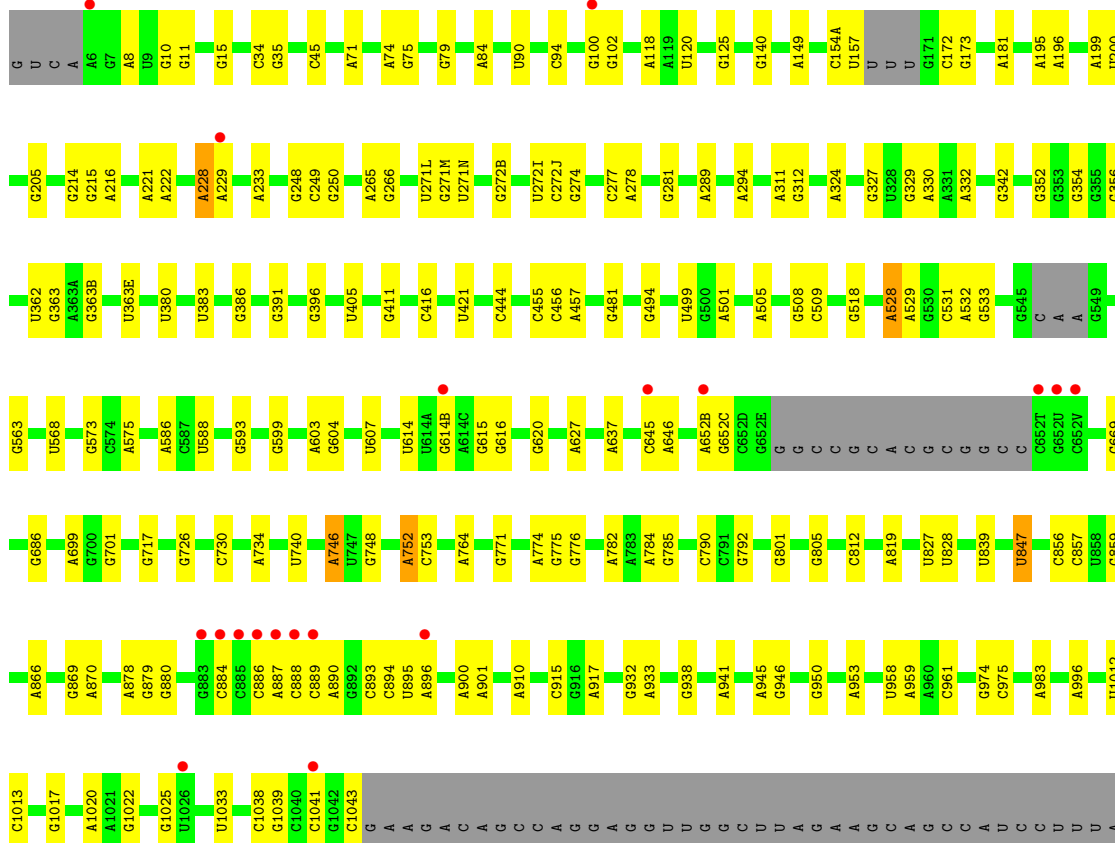
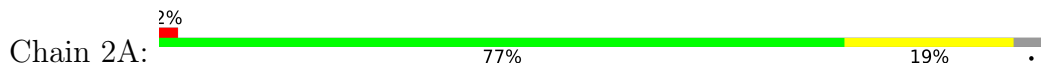
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

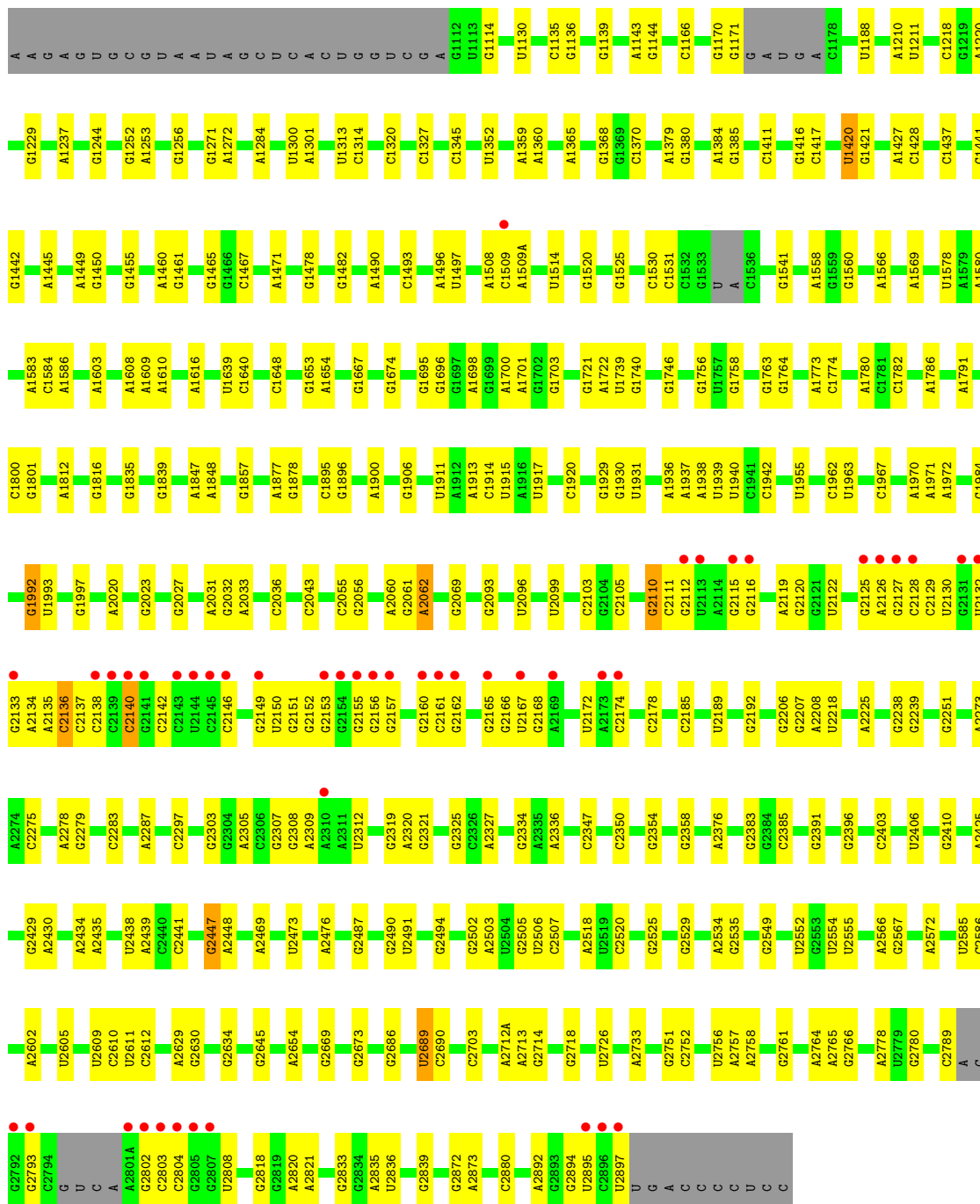
- Molecule 1: 23S Ribosomal RNA



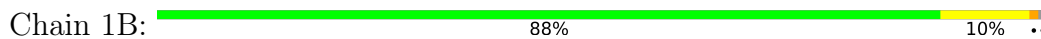


• Molecule 1: 23S Ribosomal RNA





• Molecule 2: 5S Ribosomal RNA



• Molecule 2: 5S Ribosomal RNA





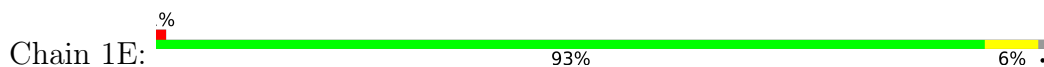
- Molecule 3: 50S ribosomal protein L2



- Molecule 3: 50S ribosomal protein L2



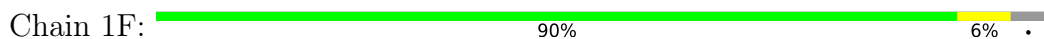
- Molecule 4: 50S ribosomal protein L3



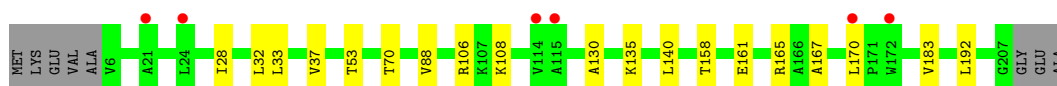
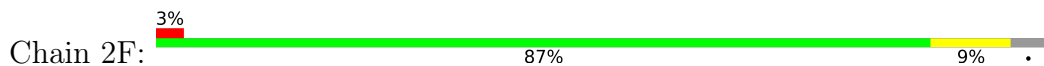
- Molecule 4: 50S ribosomal protein L3



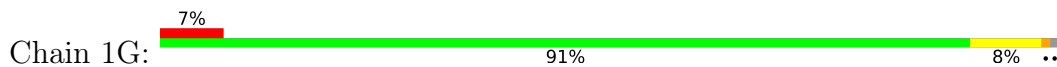
- Molecule 5: 50S ribosomal protein L4

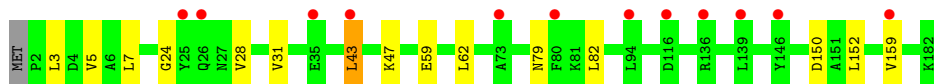


- Molecule 5: 50S ribosomal protein L4

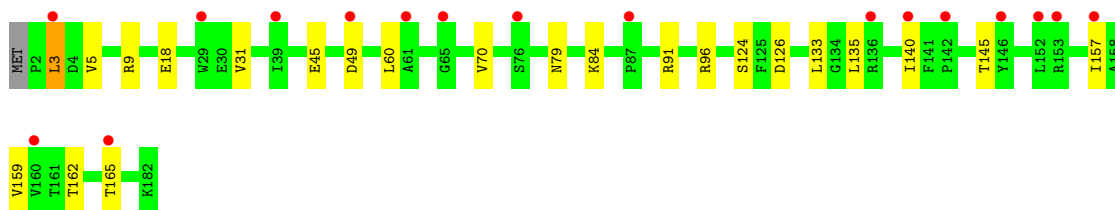
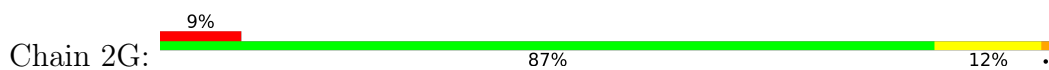


- Molecule 6: 50S ribosomal protein L5

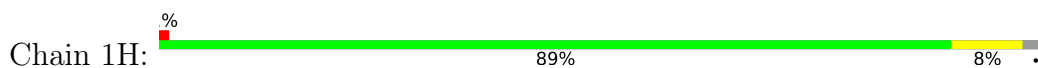




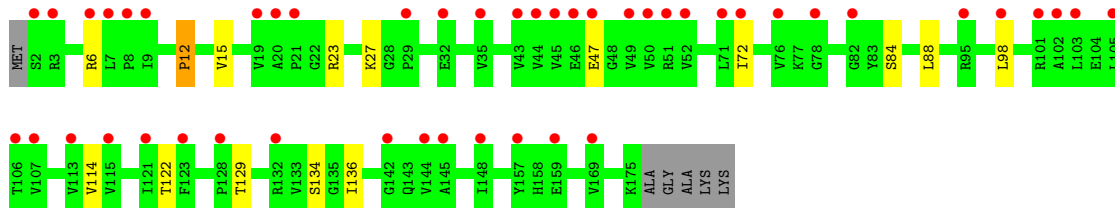
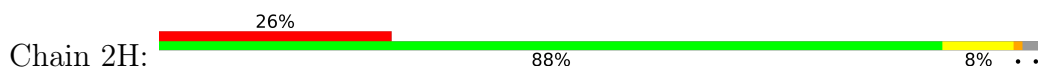
- Molecule 6: 50S ribosomal protein L5



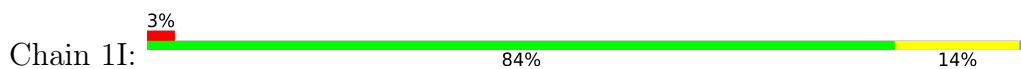
- Molecule 7: 50S ribosomal protein L6



- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9

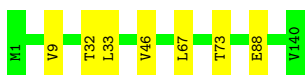


- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13

Chain 1N:  95% 5%



- Molecule 9: 50S ribosomal protein L13

Chain 2N:  3% 96%



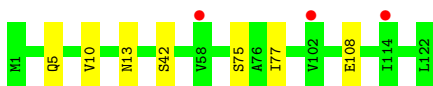
- Molecule 10: 50S ribosomal protein L14

Chain 1O:  98%



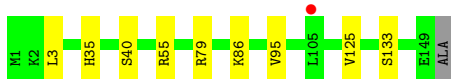
- Molecule 10: 50S ribosomal protein L14

Chain 2O:  2% 94% 6%




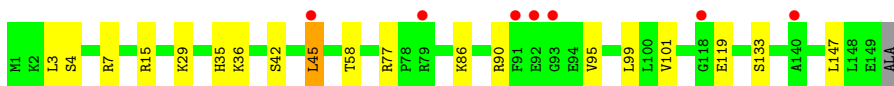
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  0% 93% 6%



- Molecule 11: 50S ribosomal protein L15

Chain 2P:  5% 87% 12% ..

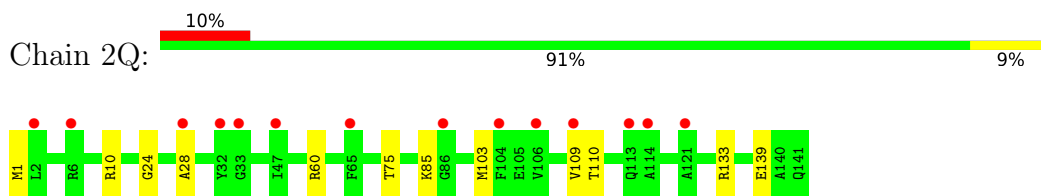


- Molecule 12: 50S ribosomal protein L16

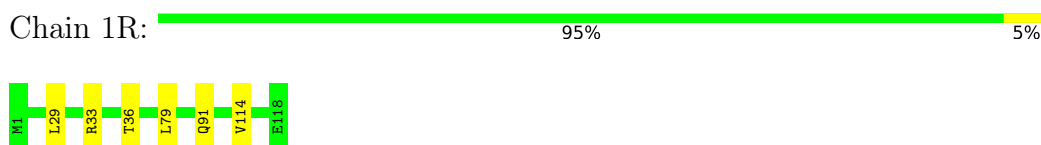
Chain 1Q:  0% 94% 6%



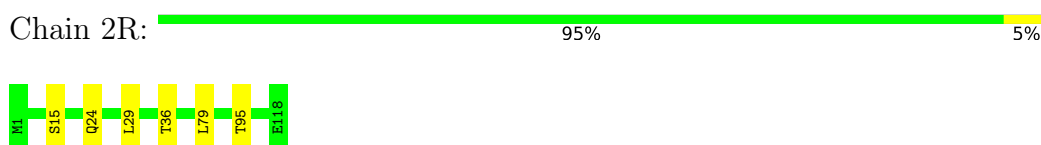
- Molecule 12: 50S ribosomal protein L16



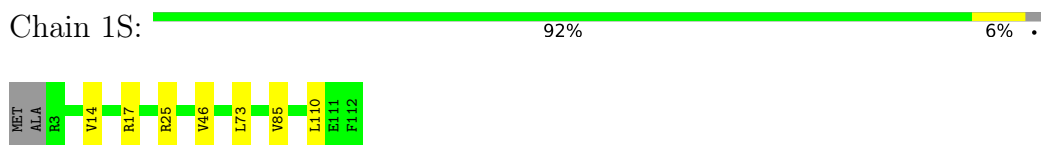
- Molecule 13: 50S ribosomal protein L17



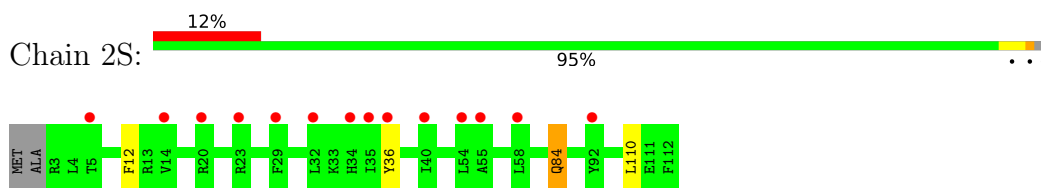
- Molecule 13: 50S ribosomal protein L17



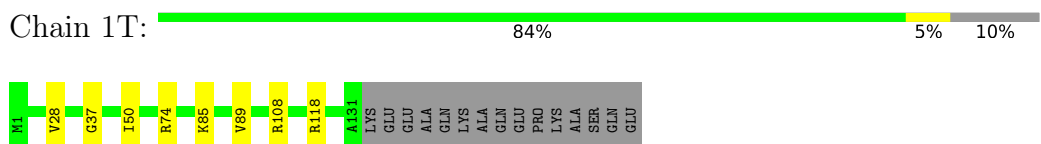
- Molecule 14: 50S ribosomal protein L18



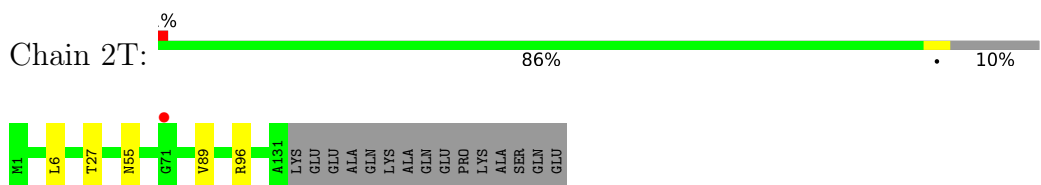
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20

Chain 1U:  96%



- Molecule 16: 50S ribosomal protein L20

Chain 2U:  95%



- Molecule 17: 50S ribosomal protein L21

Chain 1V:  93%



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  93%



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  96%



- Molecule 18: 50S ribosomal protein L22

Chain 2W:  96%

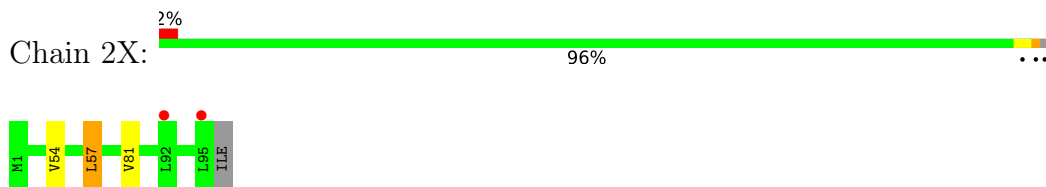


- Molecule 19: 50S ribosomal protein L23

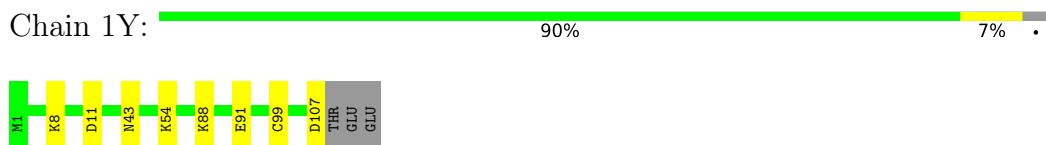
Chain 1X:  94%



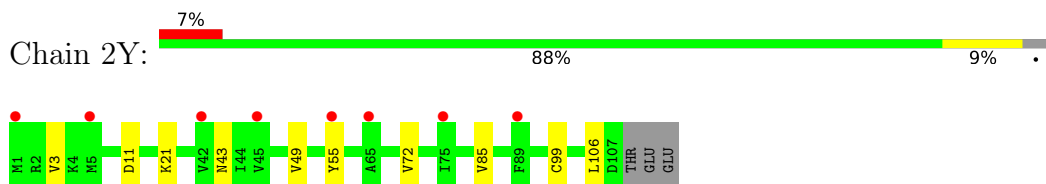
• Molecule 19: 50S ribosomal protein L23



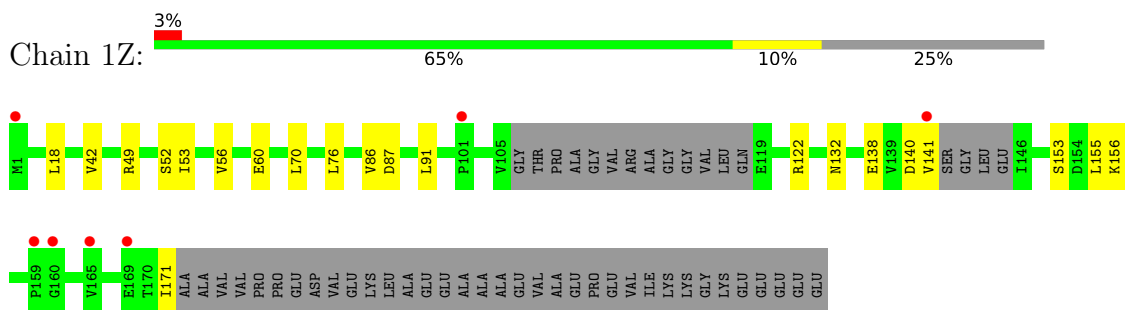
• Molecule 20: 50S ribosomal protein L24



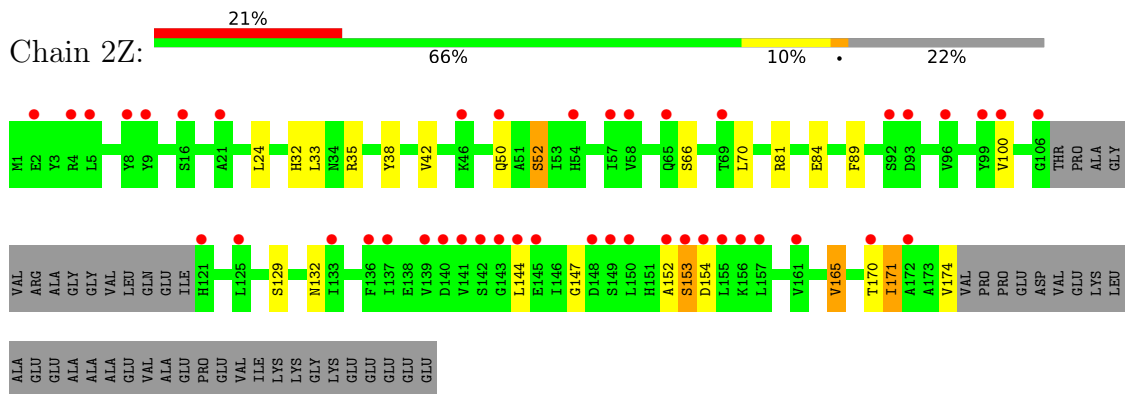
• Molecule 20: 50S ribosomal protein L24



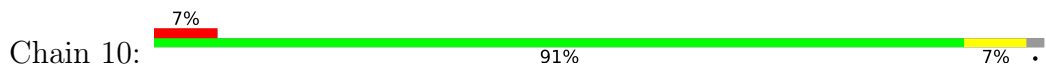
• Molecule 21: 50S ribosomal protein L25

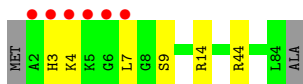


• Molecule 21: 50S ribosomal protein L25



• Molecule 22: 50S ribosomal protein L27

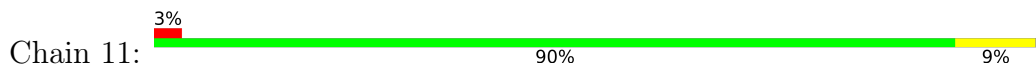




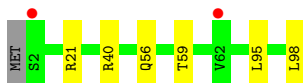
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



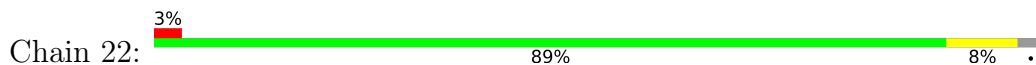
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



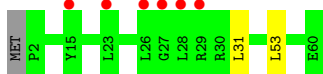
- Molecule 24: 50S ribosomal protein L29



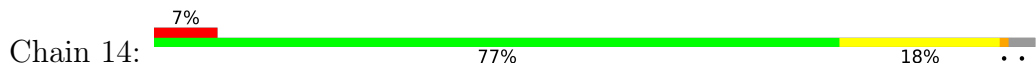
- Molecule 25: 50S ribosomal protein L30



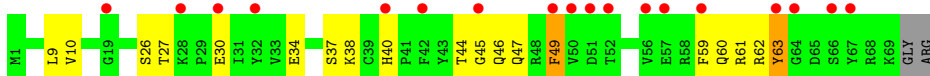
- Molecule 25: 50S ribosomal protein L30



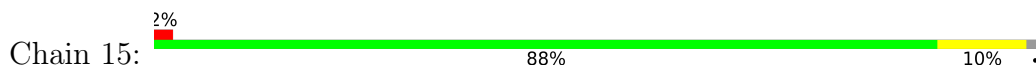
- Molecule 26: 50S ribosomal protein L31



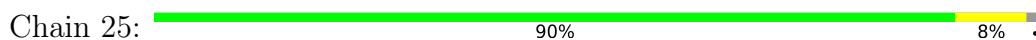
- Molecule 26: 50S ribosomal protein L31



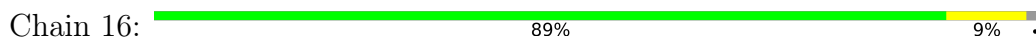
- Molecule 27: 50S ribosomal protein L32



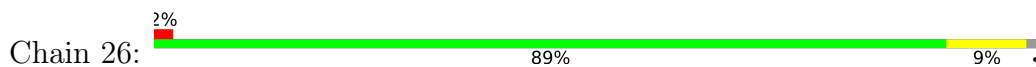
- Molecule 27: 50S ribosomal protein L32



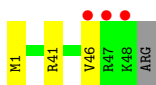
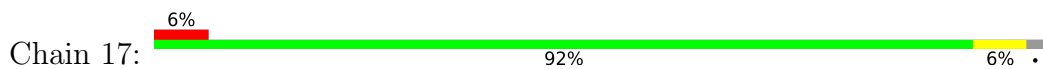
- Molecule 28: 50S ribosomal protein L33



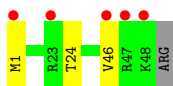
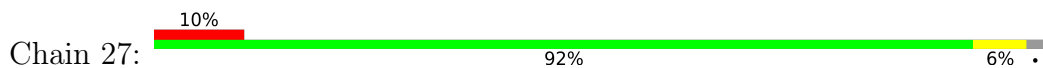
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

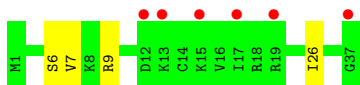
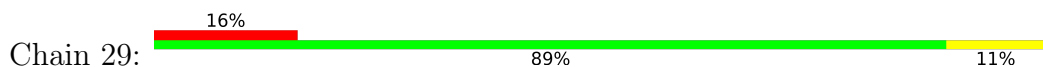


- Molecule 31: 50S ribosomal protein L36

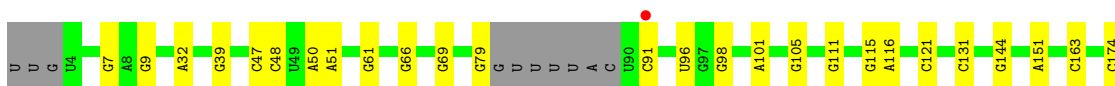
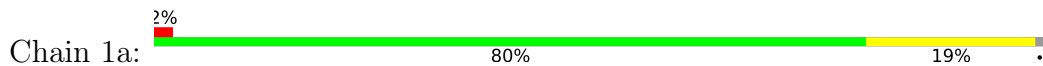


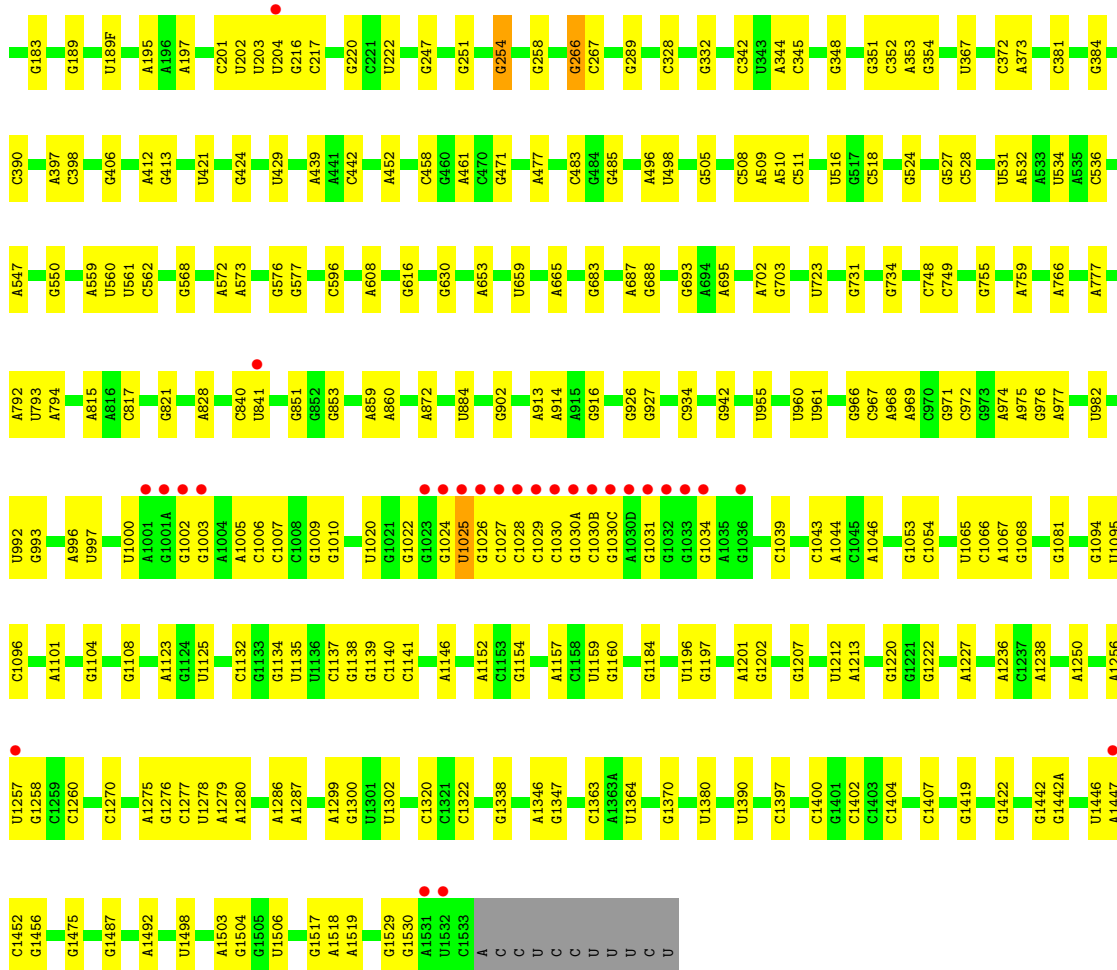
There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L36

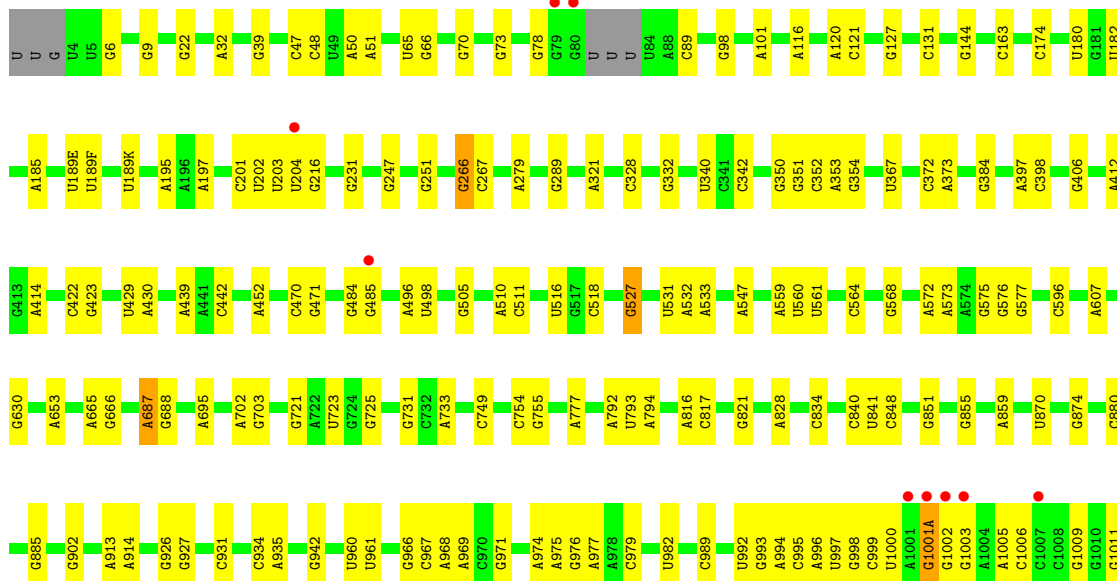
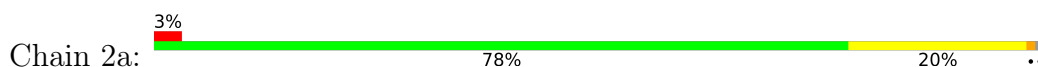


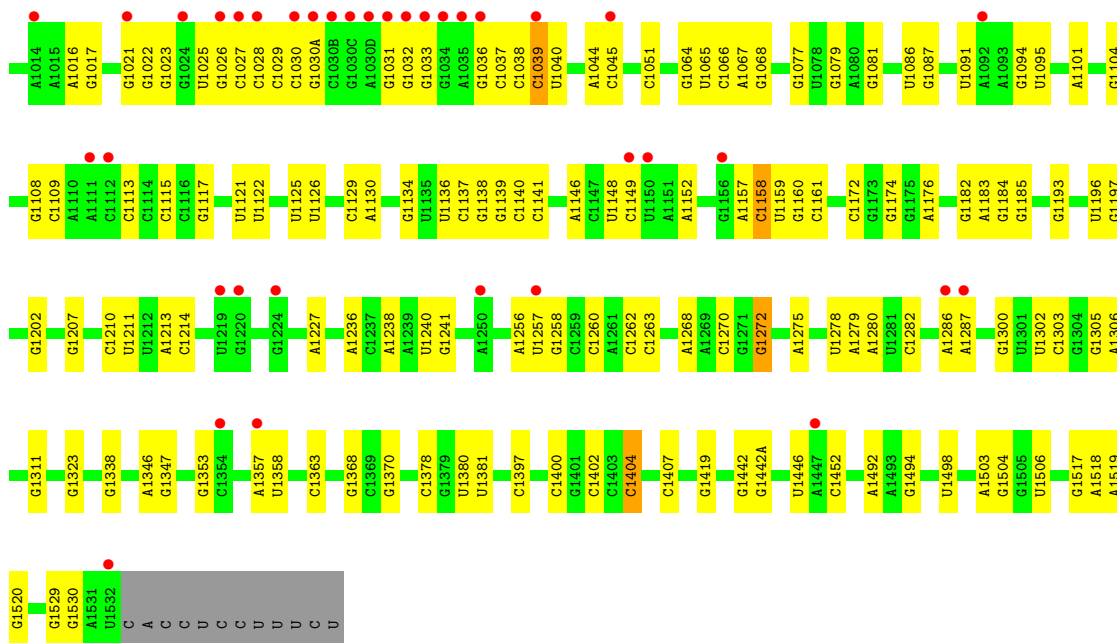
- Molecule 32: 16S Ribosomal RNA



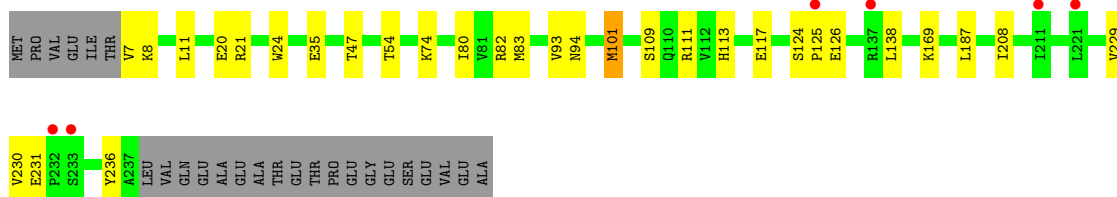
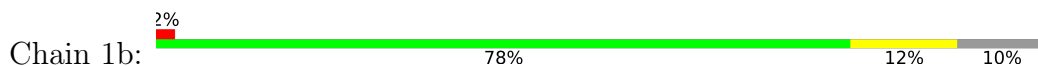


● Molecule 32: 16S Ribosomal RNA

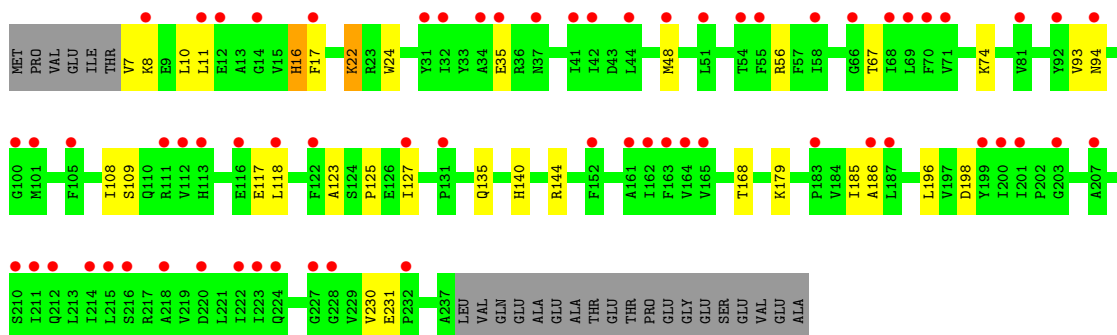
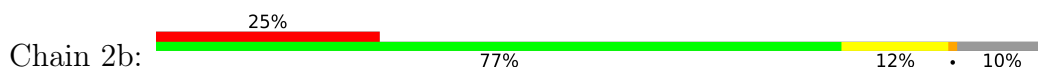




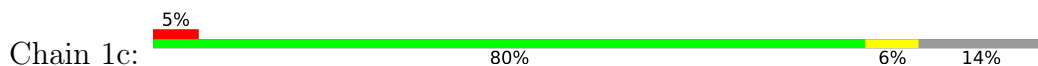
• Molecule 33: 30S ribosomal protein S2

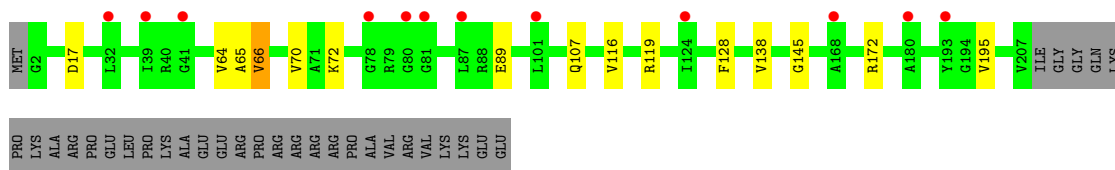


• Molecule 33: 30S ribosomal protein S2

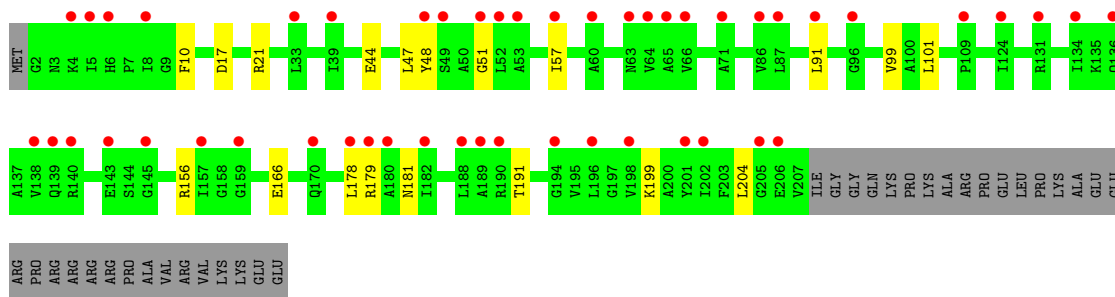
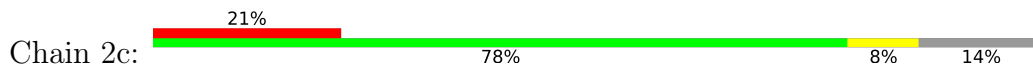


• Molecule 34: 30S ribosomal protein S3

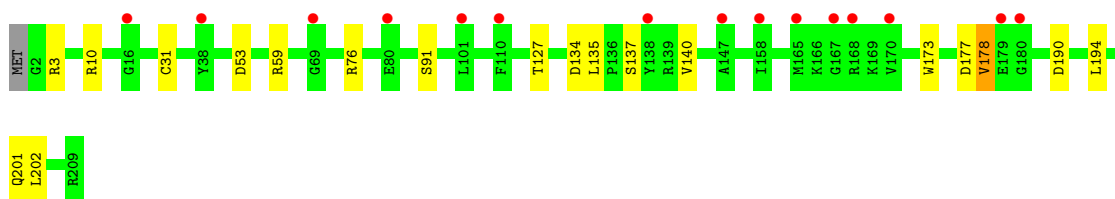




• Molecule 34: 30S ribosomal protein S3



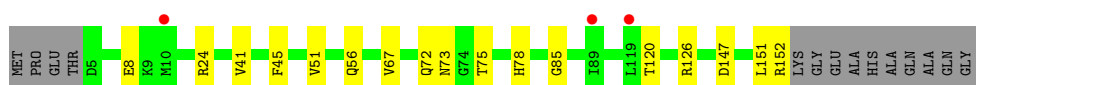
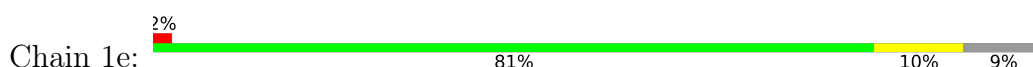
• Molecule 35: 30S ribosomal protein S4



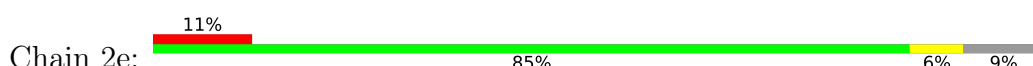
• Molecule 35: 30S ribosomal protein S4

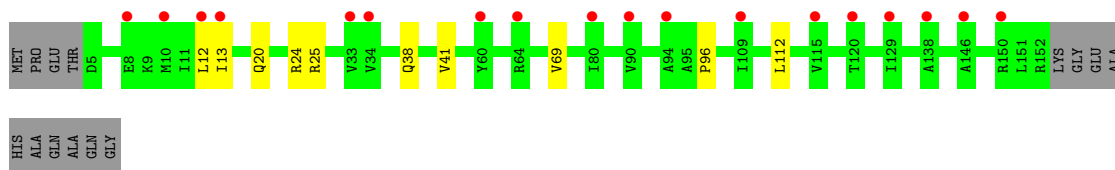


• Molecule 36: 30S ribosomal protein S5

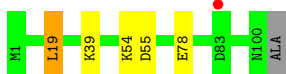


• Molecule 36: 30S ribosomal protein S5





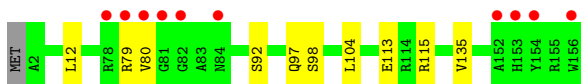
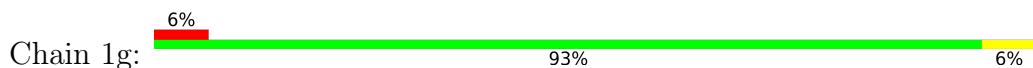
- Molecule 37: 30S ribosomal protein S6



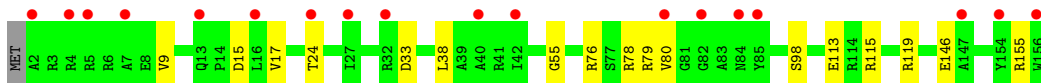
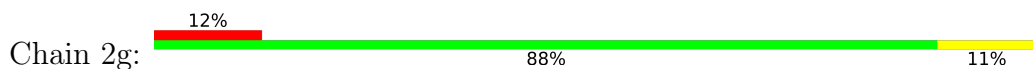
- Molecule 37: 30S ribosomal protein S6



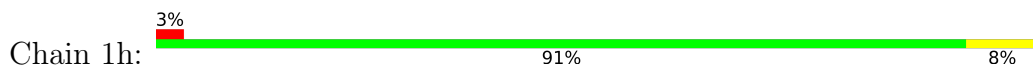
- Molecule 38: 30S ribosomal protein S7



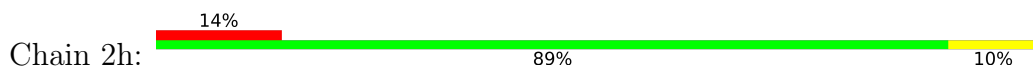
- Molecule 38: 30S ribosomal protein S7



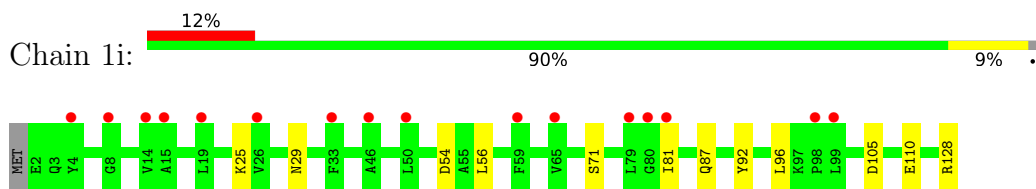
- Molecule 39: 30S ribosomal protein S8



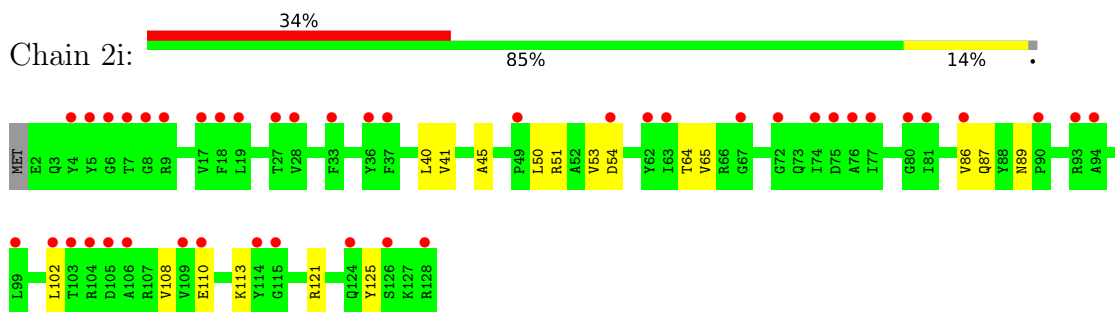
- Molecule 39: 30S ribosomal protein S8



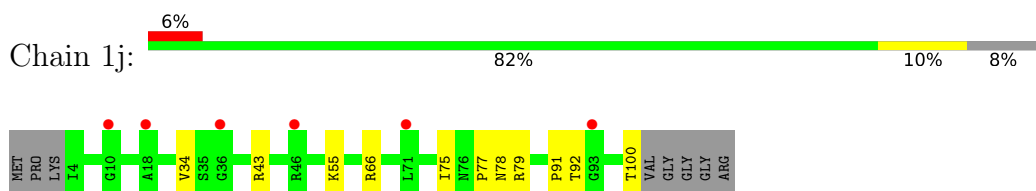
- Molecule 40: 30S ribosomal protein S9



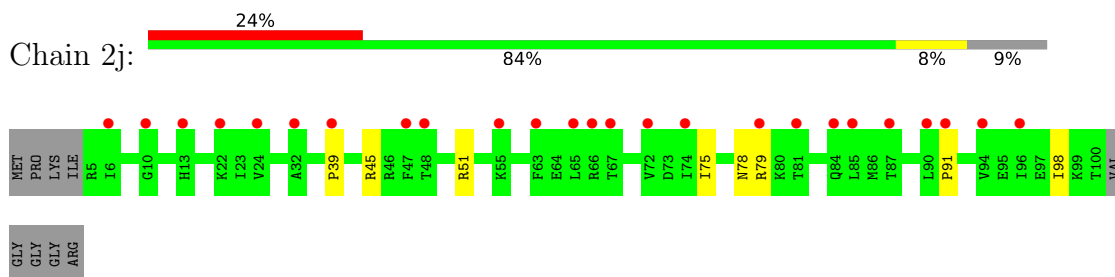
- Molecule 40: 30S ribosomal protein S9



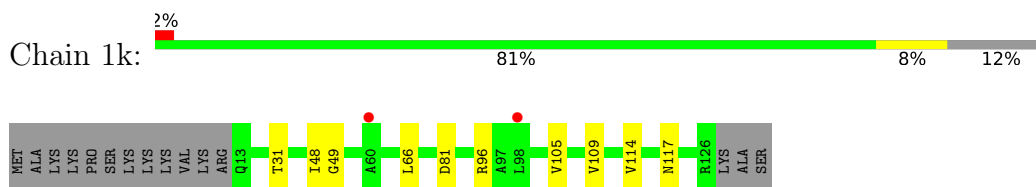
- Molecule 41: 30S ribosomal protein S10



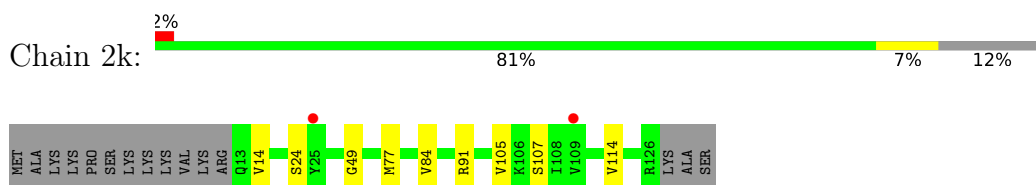
- Molecule 41: 30S ribosomal protein S10



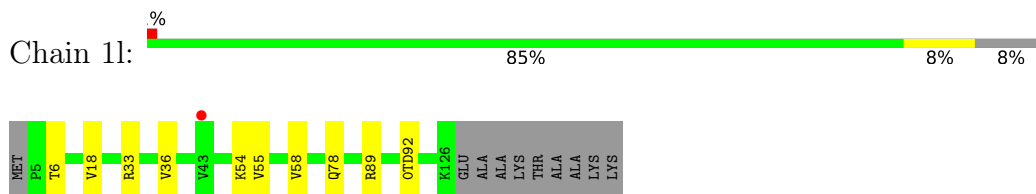
- Molecule 42: 30S ribosomal protein S11



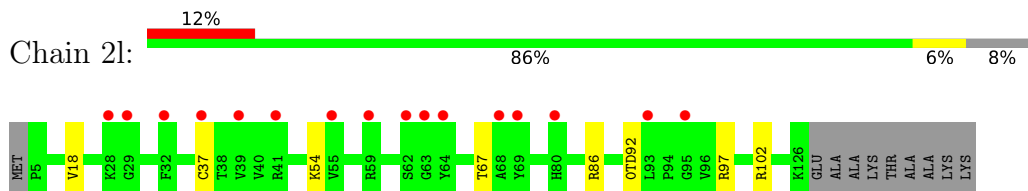
- Molecule 42: 30S ribosomal protein S11



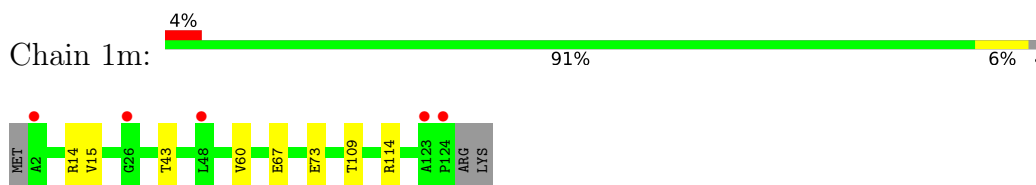
- Molecule 43: 30S ribosomal protein S12



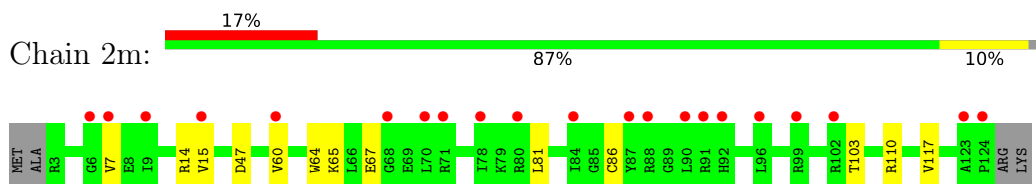
- Molecule 43: 30S ribosomal protein S12



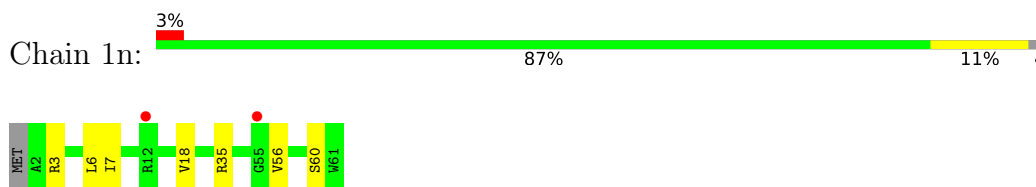
- Molecule 44: 30S ribosomal protein S13



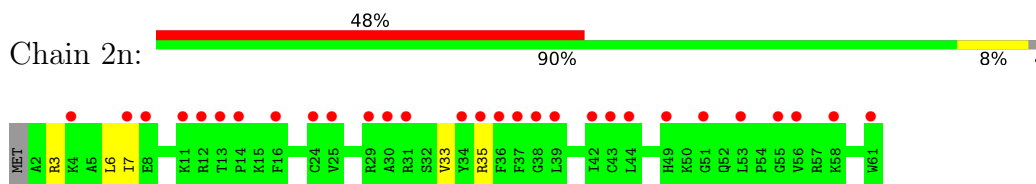
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z

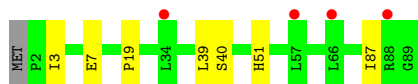


- Molecule 45: 30S ribosomal protein S14 type Z

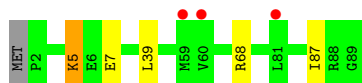


- Molecule 46: 30S ribosomal protein S15

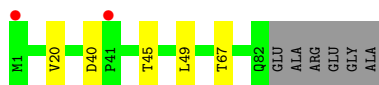
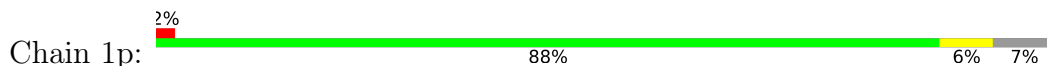




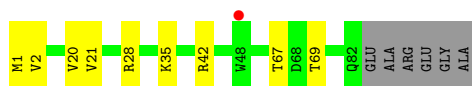
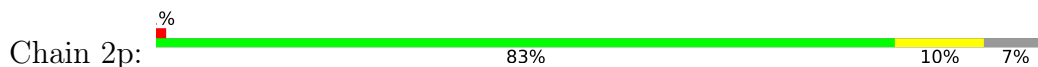
- Molecule 46: 30S ribosomal protein S15



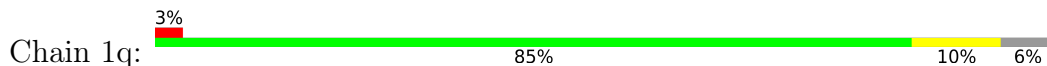
- Molecule 47: 30S ribosomal protein S16



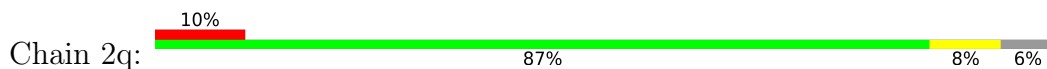
- Molecule 47: 30S ribosomal protein S16



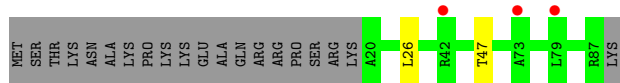
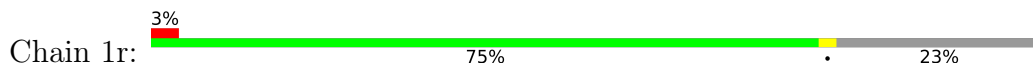
- Molecule 48: 30S ribosomal protein S17



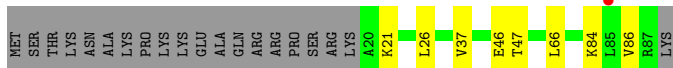
- Molecule 48: 30S ribosomal protein S17



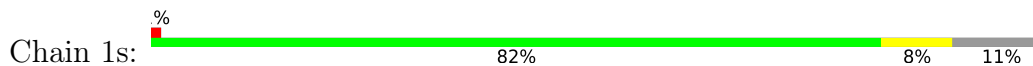
- Molecule 49: 30S ribosomal protein S18



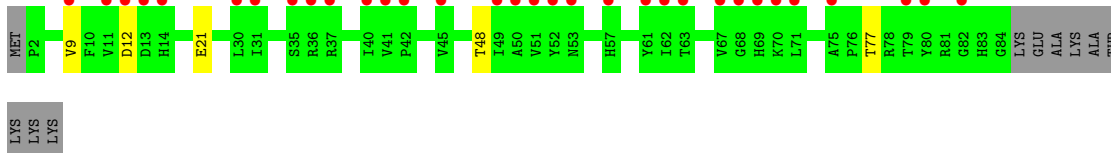
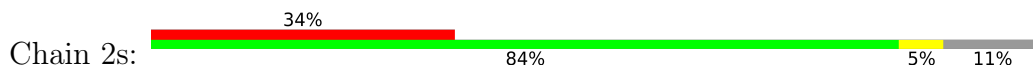
- Molecule 49: 30S ribosomal protein S18



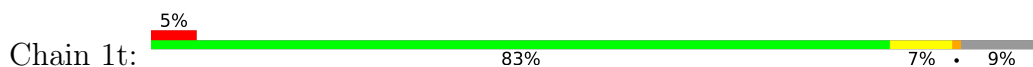
- Molecule 50: 30S ribosomal protein S19



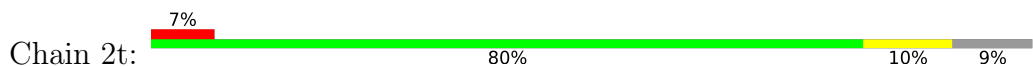
- Molecule 50: 30S ribosomal protein S19



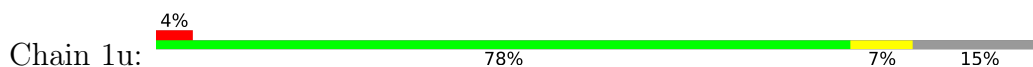
- Molecule 51: 30S ribosomal protein S20



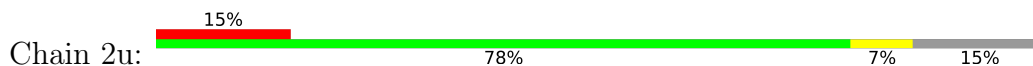
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx





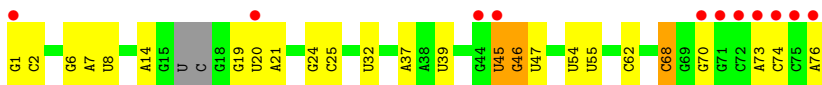
- Molecule 53: MF-mRNA



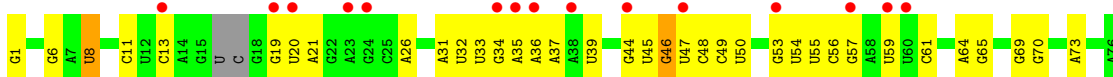
- Molecule 53: MF-mRNA



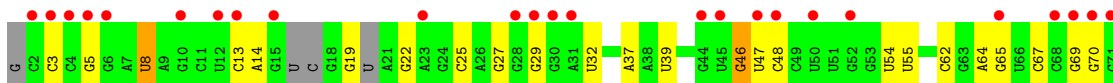
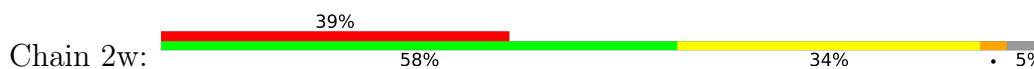
- Molecule 54: A-site and E-site Deacylated tRNAphe



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

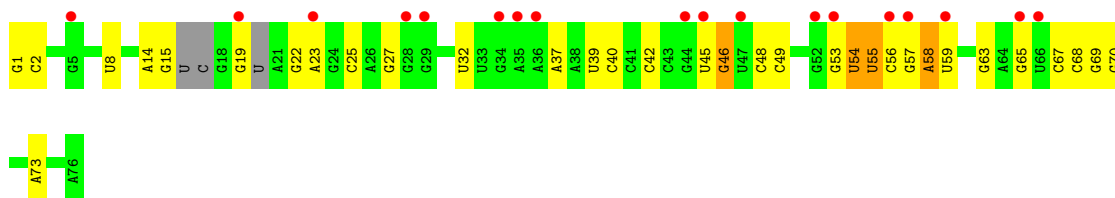


- Molecule 54: A-site and E-site Deacylated tRNAphe



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





- Molecule 55: P-site Deacylated tRNA^{Met}

Chain 1x: 75% 21%



- Molecule 55: P-site Deacylated tRNA^{Met}

Chain 2x: 70% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.36Å 449.77Å 616.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	254.37 – 2.70 254.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.1 (254.37-2.70) 97.1 (254.37-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.224 , 0.277 0.224 , 0.277	Depositor DCC
R_{free} test set	76639 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtrriage
Anisotropy	0.166	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	299892	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.51	0/69010	0.95	56/107716 (0.1%)
1	2A	0.39	0/67294	0.87	34/105038 (0.0%)
2	1B	0.44	1/2882 (0.0%)	0.84	0/4494
2	2B	0.39	1/2879 (0.0%)	0.86	4/4487 (0.1%)
3	1D	0.35	0/2186	0.54	0/2944
3	2D	0.32	0/2186	0.51	0/2944
4	1E	0.35	0/1592	0.53	0/2149
4	2E	0.31	0/1592	0.51	0/2149
5	1F	0.33	0/1618	0.52	0/2191
5	2F	0.31	0/1614	0.49	0/2186
6	1G	0.31	0/1448	0.49	0/1957
6	2G	0.29	0/1453	0.48	0/1963
7	1H	0.33	0/1356	0.51	0/1834
7	2H	0.28	0/1356	0.49	0/1834
8	1I	0.29	0/1112	0.50	0/1514
8	2I	0.29	0/1079	0.47	0/1475
9	1N	0.34	0/1144	0.50	0/1543
9	2N	0.28	0/1144	0.45	0/1543
10	1O	0.35	0/943	0.53	0/1269
10	2O	0.32	0/943	0.52	0/1269
11	1P	0.33	0/1152	0.58	0/1533
11	2P	0.31	0/1152	0.52	0/1533
12	1Q	0.35	0/1143	0.51	0/1527
12	2Q	0.29	0/1143	0.48	0/1527
13	1R	0.32	0/982	0.52	0/1312
13	2R	0.28	0/982	0.51	0/1312
14	1S	0.32	0/883	0.52	0/1176
14	2S	0.28	0/880	0.48	0/1172
15	1T	0.34	0/1105	0.51	0/1477
15	2T	0.30	0/1097	0.49	0/1468
16	1U	0.36	0/977	0.51	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.30	0/977	0.45	0/1301
17	1V	0.33	0/782	0.56	0/1049
17	2V	0.30	0/782	0.50	0/1049
18	1W	0.36	0/897	0.54	0/1205
18	2W	0.30	0/897	0.48	0/1205
19	1X	0.35	0/764	0.60	1/1025 (0.1%)
19	2X	0.31	0/764	0.58	1/1025 (0.1%)
20	1Y	0.35	0/819	0.54	0/1095
20	2Y	0.31	0/819	0.49	0/1095
21	1Z	0.30	0/1267	0.47	0/1717
21	2Z	0.30	0/1299	0.53	1/1763 (0.1%)
22	10	0.34	0/662	0.51	0/881
22	20	0.31	0/662	0.48	0/881
23	11	0.36	0/762	0.50	0/1014
23	21	0.32	0/762	0.52	0/1014
24	12	0.32	0/590	0.48	0/781
24	22	0.27	0/590	0.41	0/781
25	13	0.34	0/474	0.51	0/635
25	23	0.29	0/469	0.48	0/630
26	14	0.35	0/565	0.61	0/761
26	24	0.31	0/545	0.54	0/737
27	15	0.32	0/469	0.53	0/635
27	25	0.31	0/469	0.50	0/635
28	16	0.37	0/460	0.52	0/613
28	26	0.29	0/456	0.48	0/608
29	17	0.35	0/426	0.55	0/561
29	27	0.30	0/426	0.50	0/561
30	18	0.34	0/525	0.53	0/691
30	28	0.30	0/525	0.49	0/691
31	19	0.37	0/310	0.55	0/407
31	29	0.28	0/310	0.52	0/407
32	1a	0.37	0/35795	0.87	27/55864 (0.0%)
32	2a	0.36	3/35886 (0.0%)	0.89	37/56005 (0.1%)
33	1b	0.30	0/1881	0.49	0/2542
33	2b	0.30	0/1860	0.49	0/2518
34	1c	0.28	0/1572	0.47	0/2126
34	2c	0.28	0/1566	0.48	0/2119
35	1d	0.28	0/1685	0.47	0/2262
35	2d	0.29	0/1704	0.46	0/2284
36	1e	0.30	0/1145	0.51	0/1543
36	2e	0.30	0/1149	0.53	0/1548
37	1f	0.29	0/823	0.51	1/1115 (0.1%)
37	2f	0.29	0/829	0.50	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.27	0/1250	0.46	0/1679
38	2g	0.27	0/1254	0.44	0/1683
39	1h	0.28	0/1108	0.47	0/1494
39	2h	0.27	0/1108	0.48	0/1494
40	1i	0.29	0/1002	0.51	0/1346
40	2i	0.29	0/997	0.51	0/1343
41	1j	0.28	0/722	0.48	0/982
41	2j	0.28	0/727	0.51	0/988
42	1k	0.28	0/844	0.48	0/1145
42	2k	0.29	0/848	0.47	0/1149
43	1l	0.30	0/937	0.51	0/1260
43	2l	0.28	0/937	0.49	0/1260
44	1m	0.29	0/969	0.49	0/1302
44	2m	0.28	0/961	0.47	0/1291
45	1n	0.29	0/501	0.48	0/664
45	2n	0.30	0/501	0.48	0/664
46	1o	0.27	0/739	0.44	0/985
46	2o	0.27	0/739	0.42	0/985
47	1p	0.28	0/697	0.49	0/939
47	2p	0.28	0/693	0.51	0/935
48	1q	0.30	0/836	0.51	0/1117
48	2q	0.29	0/836	0.49	0/1117
49	1r	0.30	0/560	0.46	0/746
49	2r	0.27	0/560	0.42	0/746
50	1s	0.28	0/667	0.54	0/900
50	2s	0.30	0/661	0.57	0/893
51	1t	0.28	0/730	0.46	0/965
51	2t	0.27	0/729	0.45	0/965
52	1u	0.28	0/203	0.48	0/266
52	2u	0.30	0/203	0.48	0/266
53	1v	0.36	0/310	0.86	0/480
53	2v	0.39	0/310	0.85	0/480
54	1w	0.49	1/1606 (0.1%)	1.01	2/2497 (0.1%)
54	1y	0.49	1/1606 (0.1%)	1.05	7/2497 (0.3%)
54	2w	0.45	0/1556	1.03	2/2418 (0.1%)
54	2y	0.51	1/1583 (0.1%)	1.03	3/2459 (0.1%)
55	1x	0.50	1/1725 (0.1%)	1.08	13/2689 (0.5%)
55	2x	0.42	0/1725	0.96	3/2689 (0.1%)
All	All	0.40	9/316686 (0.0%)	0.82	192/474117 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	0	1
33	2b	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	1	G	OP3-P	-10.35	1.48	1.61
54	1w	1	G	OP3-P	-10.31	1.48	1.61
2	2B	1	U	OP3-P	-10.17	1.49	1.61
54	2y	1	G	OP3-P	-10.16	1.49	1.61
2	1B	1	U	OP3-P	-10.13	1.49	1.61
32	2a	1272	G	C6-N1	-9.45	1.32	1.39
32	2a	1272	G	N1-C2	-8.75	1.30	1.37
32	2a	1263	C	N3-C4	-5.57	1.30	1.33
55	1x	14	A	C8-N7	-5.52	1.27	1.31

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C5-C6-O6	20.69	141.02	128.60
32	2a	1263	C	N1-C2-O2	20.56	131.24	118.90
32	2a	1272	G	N3-C2-N2	17.07	131.85	119.90
32	2a	1272	G	N1-C2-N2	-16.20	101.62	116.20
32	2a	1272	G	N1-C6-O6	-15.22	110.77	119.90
32	2a	1263	C	C2-N3-C4	13.12	126.46	119.90
32	2a	1263	C	N3-C2-O2	-12.98	112.81	121.90
1	1A	1063	G	C5-C6-O6	10.51	134.91	128.60
1	1A	2682	U	O5'-P-OP2	-9.66	97.01	105.70
1	1A	1075	C	N1-C2-O2	9.62	124.67	118.90
32	1a	1027	C	C5-C4-N4	9.53	126.87	120.20
1	1A	1086	A	N1-C6-N6	-9.33	113.00	118.60
32	2a	1263	C	C5-C4-N4	9.26	126.68	120.20
55	1x	14	A	C4-C5-C6	9.17	121.59	117.00
1	1A	1614	A	O5'-P-OP1	-8.97	97.63	105.70
1	1A	1063	G	C6-N1-C2	8.96	130.47	125.10
1	1A	1075	C	C2-N3-C4	8.73	124.27	119.90
1	2A	2136	C	N1-C2-O2	8.69	124.11	118.90
32	2a	1263	C	C5-C6-N1	8.39	125.20	121.00
55	1x	14	A	C5-N7-C8	8.35	108.08	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C6-N1-C2	8.19	130.01	125.10
32	2a	1263	C	C6-N1-C2	-8.13	117.05	120.30
32	1a	1025	U	N1-C2-O2	8.13	128.49	122.80
32	1a	1027	C	N3-C2-O2	-8.11	116.22	121.90
32	2a	1001(A)	G	N3-C4-N9	8.06	130.84	126.00
1	1A	512	G	O4'-C1'-N9	7.99	114.59	108.20
32	2a	754	C	C2-N1-C1'	7.98	127.58	118.80
1	2A	2128	C	C2-N3-C4	7.89	123.85	119.90
2	2B	80	U	O4'-C1'-N1	7.89	114.51	108.20
32	2a	1263	C	N3-C4-N4	-7.67	112.63	118.00
54	1y	33	U	C2-N1-C1'	7.67	126.90	117.70
1	1A	2167	U	C2-N1-C1'	7.51	126.71	117.70
1	1A	226	G	O4'-C1'-N9	7.41	114.13	108.20
32	1a	1034	G	N9-C4-C5	-7.40	102.44	105.40
32	2a	754	C	N1-C2-O2	7.34	123.30	118.90
55	2x	14	A	C4-C5-C6	7.28	120.64	117.00
55	1x	46	G	C6-N1-C2	-7.26	120.74	125.10
1	1A	2553	G	N3-C4-N9	7.19	130.32	126.00
1	2A	2473	U	C2-N1-C1'	7.17	126.31	117.70
2	2B	1	U	N1-C2-O2	7.10	127.77	122.80
55	1x	14	A	C5-C6-N1	-7.07	114.16	117.70
2	2B	1	U	C2-N1-C1'	7.06	126.17	117.70
32	1a	1027	C	N3-C4-C5	-6.95	119.12	121.90
1	1A	2553	G	N3-C4-C5	-6.94	125.13	128.60
1	1A	975	C	N1-C2-O2	-6.87	114.78	118.90
1	1A	2598	A	O5'-P-OP1	-6.87	99.52	105.70
32	2a	1272	G	C2-N3-C4	-6.83	108.48	111.90
1	1A	1063	G	N3-C2-N2	6.82	124.68	119.90
32	2a	1028	C	C2-N3-C4	6.77	123.29	119.90
32	1a	1034	G	N3-C4-N9	6.72	130.03	126.00
1	1A	1176	G	OP1-P-O3'	6.71	119.95	105.20
1	2A	2136	C	N3-C2-O2	-6.69	117.22	121.90
32	2a	1272	G	C5-C6-N1	-6.66	108.17	111.50
55	2x	14	A	C5-N7-C8	6.65	107.23	103.90
1	2A	2062	A	N1-C6-N6	6.65	122.59	118.60
32	2a	754	C	C6-N1-C1'	-6.51	112.99	120.80
32	1a	1034	G	C4-C5-N7	6.47	113.39	110.80
32	1a	1034	G	N3-C2-N2	6.44	124.41	119.90
1	1A	847	U	C2-N1-C1'	6.44	125.43	117.70
1	1A	372	G	O4'-C1'-N9	6.41	113.33	108.20
1	1A	1063	G	C5-C6-N1	-6.32	108.34	111.50
1	1A	2167	U	N1-C2-O2	6.29	127.20	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	64	A	C5-C6-N6	6.28	128.73	123.70
32	1a	1027	C	N1-C2-O2	6.27	122.66	118.90
1	1A	748	G	O4'-C1'-N9	6.26	113.20	108.20
32	1a	1030	C	C2-N3-C4	6.26	123.03	119.90
2	2B	1	U	N3-C2-O2	-6.21	117.86	122.20
1	1A	801	G	O5'-P-OP2	-6.19	100.12	105.70
32	1a	1025	U	N3-C2-O2	-6.18	117.87	122.20
54	2y	22	G	N1-C6-O6	6.13	123.58	119.90
1	1A	2629	A	P-O3'-C3'	6.11	127.03	119.70
1	2A	2160	G	C6-N1-C2	6.08	128.75	125.10
32	2a	1001(A)	G	C4-N9-C1'	6.08	134.40	126.50
1	1A	1416	G	O4'-C1'-N9	6.08	113.06	108.20
32	2a	1001(A)	G	C8-N9-C1'	-6.07	119.10	127.00
19	2X	57	LEU	CA-CB-CG	6.02	129.15	115.30
1	1A	1776	G	O5'-P-OP2	-5.99	100.31	105.70
32	1a	1030	C	C5-C4-N4	5.99	124.39	120.20
32	1a	1034	G	C8-N9-C1'	-5.96	119.25	127.00
1	1A	1639	U	O5'-P-OP2	-5.95	100.35	105.70
32	2a	1272	G	C4-N9-C1'	5.93	134.21	126.50
1	2A	748	G	C4-N9-C1'	-5.93	118.79	126.50
1	2A	2096	U	N1-C2-O2	5.88	126.92	122.80
1	1A	383	U	C2-N1-C1'	-5.83	110.70	117.70
1	2A	2473	U	N3-C2-O2	-5.82	118.13	122.20
55	2x	14	A	C5-C6-N1	-5.81	114.80	117.70
1	1A	2848	G	O4'-C1'-N9	5.79	112.83	108.20
1	1A	847	U	N1-C2-O2	5.77	126.84	122.80
1	2A	2473	U	N1-C2-O2	5.77	126.84	122.80
1	2A	2140	C	C2-N1-C1'	5.77	125.14	118.80
32	1a	1025	U	C2-N1-C1'	5.76	124.61	117.70
32	2a	1263	C	C2-N1-C1'	5.76	125.14	118.80
32	1a	560	U	C2-N1-C1'	5.75	124.61	117.70
1	2A	746	A	O4'-C1'-N9	5.74	112.79	108.20
1	1A	2167	U	N3-C2-O2	-5.73	118.19	122.20
1	1A	2032	G	C5-N7-C8	5.73	107.16	104.30
32	1a	1027	C	N3-C4-N4	-5.70	114.01	118.00
54	1w	68	C	N1-C2-O2	5.68	122.31	118.90
1	1A	548	A	P-O3'-C3'	5.65	126.48	119.70
1	1A	774	A	C8-N9-C4	-5.64	103.55	105.80
1	2A	748	G	C8-N9-C1'	5.63	134.32	127.00
32	1a	1034	G	C4-N9-C1'	5.62	133.81	126.50
32	1a	266	G	P-O3'-C3'	5.62	126.44	119.70
1	2A	1992	G	P-O3'-C3'	5.62	126.44	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1313	U	C2-N1-C1'	5.60	124.42	117.70
1	2A	801	G	O5'-P-OP2	-5.59	100.67	105.70
54	2y	58	A	OP1-P-O3'	5.59	117.50	105.20
1	1A	1992	G	P-O3'-C3'	5.58	126.40	119.70
55	1x	22	G	C8-N9-C1'	5.58	134.26	127.00
55	1x	22	G	C4-C5-C6	-5.57	115.46	118.80
54	1y	33	U	C6-N1-C1'	-5.55	113.44	121.20
1	2A	2629	A	O4'-C1'-N9	5.55	112.64	108.20
32	2a	1158	C	C2-N1-C1'	5.55	124.90	118.80
32	1a	254	G	O5'-P-OP1	-5.54	100.71	105.70
32	2a	1001(A)	G	N9-C4-C5	-5.54	103.18	105.40
1	1A	1075	C	N3-C2-O2	-5.52	118.04	121.90
32	2a	1263	C	C4-C5-C6	-5.49	114.65	117.40
1	1A	1174	A	P-O3'-C3'	5.48	126.28	119.70
1	2A	2149	G	N3-C4-N9	5.48	129.29	126.00
54	1y	50	U	C2-N3-C4	5.45	130.27	127.00
1	1A	1075	C	C5-C4-N4	5.44	124.01	120.20
32	1a	1067	A	P-O3'-C3'	5.41	126.20	119.70
54	2y	58	A	P-O3'-C3'	5.41	126.19	119.70
1	1A	574	C	N1-C2-O2	-5.41	115.66	118.90
1	2A	1420	U	P-O3'-C3'	5.41	126.19	119.70
1	2A	2128	C	C5-C6-N1	5.40	123.70	121.00
1	2A	1313	U	C2-N1-C1'	5.40	124.18	117.70
54	1y	64	A	C6-N1-C2	5.38	121.83	118.60
32	2a	1039	C	C5-C4-N4	-5.36	116.45	120.20
1	2A	528	A	P-O3'-C3'	5.35	126.12	119.70
32	1a	1027	C	C6-N1-C1'	5.35	127.22	120.80
1	2A	2689	U	N3-C2-O2	-5.35	118.45	122.20
1	2A	2149	G	N9-C4-C5	-5.35	103.26	105.40
54	1w	45	U	N1-C2-O2	5.34	126.54	122.80
54	1y	64	A	N1-C6-N6	-5.34	115.39	118.60
1	2A	383	U	O4'-C1'-N1	5.32	112.46	108.20
32	2a	687	A	P-O3'-C3'	5.32	126.08	119.70
1	2A	2447	G	C4-N9-C1'	-5.31	119.60	126.50
1	1A	1253	A	C8-N9-C4	5.30	107.92	105.80
32	1a	1002	G	C4-N9-C1'	5.30	133.38	126.50
1	1A	568	U	C5-C4-O4	-5.29	122.72	125.90
1	1A	847	U	N3-C2-O2	-5.29	118.50	122.20
1	2A	847	U	C2-N1-C1'	5.27	124.02	117.70
1	1A	1174	A	OP1-P-O3'	5.27	116.79	105.20
1	1A	1063	G	N1-C6-O6	-5.25	116.75	119.90
32	1a	1027	C	C6-N1-C2	-5.25	118.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	787	U	O5'-P-OP1	-5.25	100.98	105.70
32	2a	1001(A)	G	N3-C4-C5	-5.25	125.97	128.60
32	2a	1272	G	C8-N9-C1'	-5.25	120.18	127.00
37	1f	19	LEU	CA-CB-CG	5.24	127.35	115.30
1	1A	2689	U	N3-C2-O2	-5.23	118.54	122.20
32	2a	1039	C	C2-N1-C1'	5.23	124.55	118.80
55	1x	14	A	C4-N9-C1'	5.21	135.69	126.30
54	2w	3	C	N1-C2-O2	5.21	122.03	118.90
55	1x	22	G	N3-C4-N9	-5.21	122.88	126.00
32	2a	266	G	P-O3'-C3'	5.21	125.95	119.70
32	1a	1034	G	C6-C5-N7	-5.20	127.28	130.40
1	2A	2149	G	C4-C5-N7	5.20	112.88	110.80
1	1A	1176	G	P-O3'-C3'	5.20	125.93	119.70
1	1A	784	A	O4'-C1'-N9	5.18	112.34	108.20
32	2a	913	A	P-O3'-C3'	5.18	125.92	119.70
55	1x	14	A	C4-C5-N7	-5.17	108.11	110.70
32	1a	1201	A	P-O3'-C3'	5.17	125.91	119.70
1	2A	752	A	P-O3'-C3'	5.17	125.90	119.70
54	2w	3	C	C2-N1-C1'	5.16	124.47	118.80
1	2A	2321	G	C4-N9-C1'	5.15	133.20	126.50
32	2a	1039	C	N1-C2-O2	5.15	121.99	118.90
1	2A	228	A	P-O3'-C3'	5.14	125.87	119.70
1	1A	645	C	C2-N1-C1'	5.14	124.45	118.80
54	1y	33	U	N1-C2-O2	5.14	126.39	122.80
55	1x	70	G	N3-C4-N9	-5.13	122.92	126.00
1	2A	614	U	N3-C2-O2	-5.13	118.61	122.20
1	2A	1698	A	O4'-C1'-N9	5.12	112.30	108.20
55	1x	14	A	C8-N9-C1'	-5.12	118.49	127.70
32	2a	1001(A)	G	C6-C5-N7	-5.12	127.33	130.40
1	2A	2110	G	C4-N9-C1'	-5.12	119.85	126.50
1	1A	1177	A	O5'-P-OP1	-5.11	101.10	105.70
1	1A	1086	A	C5-C6-N6	5.11	127.79	123.70
32	1a	748	C	P-O3'-C3'	5.10	125.83	119.70
1	1A	1313	U	N1-C2-O2	5.10	126.37	122.80
1	1A	383	U	O4'-C1'-N1	5.09	112.27	108.20
19	1X	57	LEU	CA-CB-CG	5.09	127.00	115.30
32	1a	1027	C	C2-N3-C4	5.07	122.44	119.90
32	2a	1033	G	C6-N1-C2	5.06	128.13	125.10
1	1A	975	C	C2-N1-C1'	-5.05	113.25	118.80
1	2A	1411	C	C2-N1-C1'	5.05	124.35	118.80
1	1A	450	G	C5-C6-N1	5.04	114.02	111.50
1	1A	614	U	C2-N1-C1'	5.03	123.73	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2Z	81	ARG	C-N-CA	5.02	134.26	121.70
32	2a	1158	C	N1-C2-O2	5.01	121.91	118.90
55	1x	22	G	C4-N9-C1'	-5.00	119.99	126.50
55	1x	22	G	C5-N7-C8	-5.00	101.80	104.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
11	2P	35	HIS	Peptide
33	2b	186	ALA	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	252 (92%)	21 (8%)	0	100	100
4	1E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	29	54
4	2E	202/206 (98%)	186 (92%)	13 (6%)	3 (2%)	10	26
5	1F	200/210 (95%)	194 (97%)	5 (2%)	1 (0%)	29	54
5	2F	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	15	37
6	1G	179/182 (98%)	160 (89%)	16 (9%)	3 (2%)	9	23
6	2G	179/182 (98%)	153 (86%)	20 (11%)	6 (3%)	3	8
7	1H	172/180 (96%)	157 (91%)	15 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	2H	172/180 (96%)	152 (88%)	18 (10%)	2 (1%)	13	32
8	1I	144/148 (97%)	131 (91%)	12 (8%)	1 (1%)	22	46
8	2I	144/148 (97%)	120 (83%)	23 (16%)	1 (1%)	22	46
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
10	1O	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	19	43
11	1P	147/150 (98%)	130 (88%)	17 (12%)	0	100	100
11	2P	147/150 (98%)	130 (88%)	16 (11%)	1 (1%)	22	46
12	1Q	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
12	2Q	139/141 (99%)	129 (93%)	8 (6%)	2 (1%)	11	28
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	100 (93%)	8 (7%)	0	100	100
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	17	40
15	1T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	19	43
15	2T	129/146 (88%)	122 (95%)	6 (5%)	1 (1%)	19	43
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	7	19
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	37
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	86 (92%)	5 (5%)	2 (2%)	6	17
19	2X	93/96 (97%)	83 (89%)	10 (11%)	0	100	100
20	1Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	15	37
20	2Y	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	15	37
21	1Z	148/206 (72%)	126 (85%)	17 (12%)	5 (3%)	3	8
21	2Z	156/206 (76%)	124 (80%)	25 (16%)	7 (4%)	2	5
22	10	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13	32
22	20	81/85 (95%)	73 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	34
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	14	67/71 (94%)	52 (78%)	8 (12%)	7 (10%)	0	0
26	24	67/71 (94%)	43 (64%)	18 (27%)	6 (9%)	1	1
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
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%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	184 (80%)	38 (17%)	7 (3%)	4	9
33	2b	229/256 (90%)	189 (82%)	32 (14%)	8 (4%)	3	8
34	1c	204/239 (85%)	184 (90%)	16 (8%)	4 (2%)	7	19
34	2c	204/239 (85%)	167 (82%)	31 (15%)	6 (3%)	4	10
35	1d	206/209 (99%)	185 (90%)	19 (9%)	2 (1%)	15	37
35	2d	206/209 (99%)	186 (90%)	19 (9%)	1 (0%)	29	54
36	1e	146/162 (90%)	123 (84%)	20 (14%)	3 (2%)	7	18
36	2e	146/162 (90%)	132 (90%)	12 (8%)	2 (1%)	11	28
37	1f	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
37	2f	98/101 (97%)	91 (93%)	6 (6%)	1 (1%)	15	37
38	1g	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	22	46
38	2g	153/156 (98%)	135 (88%)	15 (10%)	3 (2%)	7	19
39	1h	135/138 (98%)	121 (90%)	12 (9%)	2 (2%)	10	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	2h	135/138 (98%)	118 (87%)	15 (11%)	2 (2%)	10	26
40	1i	125/128 (98%)	105 (84%)	18 (14%)	2 (2%)	9	24
40	2i	125/128 (98%)	104 (83%)	18 (14%)	3 (2%)	6	15
41	1j	95/105 (90%)	81 (85%)	8 (8%)	6 (6%)	1	2
41	2j	94/105 (90%)	76 (81%)	12 (13%)	6 (6%)	1	2
42	1k	112/129 (87%)	93 (83%)	16 (14%)	3 (3%)	5	12
42	2k	112/129 (87%)	97 (87%)	12 (11%)	3 (3%)	5	12
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
44	1m	121/126 (96%)	104 (86%)	16 (13%)	1 (1%)	19	43
44	2m	120/126 (95%)	96 (80%)	22 (18%)	2 (2%)	9	23
45	1n	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9	23
45	2n	58/61 (95%)	48 (83%)	10 (17%)	0	100	100
46	1o	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	13	32
46	2o	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	13	32
47	1p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
47	2p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	5 (5%)	2 (2%)	7	18
48	2q	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	7	18
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
50	1s	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	13	32
50	2s	81/93 (87%)	63 (78%)	16 (20%)	2 (2%)	5	14
51	1t	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	2	3
51	2t	94/106 (89%)	81 (86%)	9 (10%)	4 (4%)	2	5
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11368/12128 (94%)	10247 (90%)	973 (9%)	148 (1%)	12	30

All (148) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA

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Mol	Chain	Res	Type
23	11	3	LYS
26	14	58	ARG
26	14	62	ARG
34	1c	66	VAL
38	1g	80	VAL
40	1i	54	ASP
41	1j	79	ARG
44	1m	67	GLU
5	2F	130	ALA
6	2G	96	ARG
6	2G	126	ASP
26	24	49	PHE
33	2b	16	HIS
33	2b	17	PHE
33	2b	123	ALA
38	2g	80	VAL
40	2i	54	ASP
50	2s	12	ASP
15	1T	37	GLY
17	1V	43	GLU
19	1X	93	GLU
20	1Y	54	LYS
21	1Z	53	ILE
21	1Z	153	SER
21	1Z	156	LYS
26	14	45	GLY
26	14	49	PHE
26	14	53	GLU
33	1b	101	MET
33	1b	126	GLU
36	1e	72	GLN
39	1h	54	ASP
41	1j	55	LYS
48	1q	33	GLY
48	1q	81	ARG
50	1s	81	ARG
51	1t	10	LEU
6	2G	45	GLU
6	2G	84	LYS
11	2P	45	LEU
17	2V	79	VAL
21	2Z	153	SER

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Mol	Chain	Res	Type
26	24	30	GLU
33	2b	74	LYS
34	2c	51	GLY
34	2c	91	LEU
34	2c	156	ARG
38	2g	55	GLY
40	2i	121	ARG
41	2j	79	ARG
42	2k	49	GLY
42	2k	77	MET
51	2t	95	ALA
4	1E	52	LEU
8	1I	11	ASN
21	1Z	52	SER
21	1Z	60	GLU
22	10	4	LYS
33	1b	20	GLU
33	1b	230	VAL
33	1b	231	GLU
34	1c	107	GLN
35	1d	173	TRP
36	1e	85	GLY
45	1n	60	SER
51	1t	100	ILE
4	2E	52	LEU
6	2G	124	SER
7	2H	47	GLU
8	2I	10	GLU
10	2O	5	GLN
12	2Q	24	GLY
12	2Q	28	ALA
15	2T	55	ASN
21	2Z	66	SER
26	24	45	GLY
34	2c	181	ASN
34	2c	204	LEU
39	2h	34	GLU
40	2i	45	ALA
44	2m	67	GLU
46	2o	5	LYS
48	2q	68	ARG
51	2t	47	GLY

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Mol	Chain	Res	Type
51	2t	99	LEU
6	1G	43	LEU
33	1b	124	SER
33	1b	125	PRO
34	1c	65	ALA
40	1i	29	ASN
42	1k	105	VAL
51	1t	95	ALA
51	1t	102	GLY
5	2F	167	ALA
14	2S	84	GLN
20	2Y	21	LYS
21	2Z	52	SER
26	24	38	LYS
26	24	63	TYR
37	2f	71	ARG
41	2j	51	ARG
41	2j	78	ASN
42	2k	91	ARG
6	1G	47	LYS
17	1V	79	VAL
26	14	48	ARG
36	1e	126	ARG
39	1h	133	LEU
41	1j	75	ILE
41	1j	78	ASN
42	1k	117	ASN
4	2E	113	PHE
4	2E	144	ARG
6	2G	3	LEU
21	2Z	152	ALA
21	2Z	165	VAL
33	2b	22	LYS
39	2h	68	ARG
41	2j	39	PRO
46	1o	19	PRO
26	24	47	GLN
51	2t	10	LEU
6	1G	24	GLY
41	1j	91	PRO
7	2H	12	PRO
33	2b	125	PRO

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Mol	Chain	Res	Type
36	2e	96	PRO
41	2j	91	PRO
44	2m	7	VAL
19	1X	94	GLY
42	1k	49	GLY
21	2Z	147	GLY
38	2g	17	VAL
51	1t	47	GLY
34	2c	99	VAL
35	2d	37	PRO
36	2e	69	VAL
41	2j	75	ILE
50	2s	9	VAL
26	14	56	VAL
34	1c	145	GLY
41	1j	77	PRO
33	2b	108	ILE
33	2b	231	GLU
48	2q	30	PRO
35	1d	178	VAL
21	2Z	171	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	202 (94%)	13 (6%)	19	42
3	2D	215/218 (99%)	202 (94%)	13 (6%)	19	42
4	1E	164/166 (99%)	153 (93%)	11 (7%)	16	37
4	2E	164/166 (99%)	154 (94%)	10 (6%)	18	41
5	1F	160/166 (96%)	148 (92%)	12 (8%)	13	31
5	2F	159/166 (96%)	142 (89%)	17 (11%)	6	15
6	1G	143/156 (92%)	130 (91%)	13 (9%)	9	21
6	2G	143/156 (92%)	125 (87%)	18 (13%)	4	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	1H	144/148 (97%)	130 (90%)	14 (10%)	8	19
7	2H	144/148 (97%)	130 (90%)	14 (10%)	8	19
8	1I	113/124 (91%)	93 (82%)	20 (18%)	2	4
8	2I	105/124 (85%)	94 (90%)	11 (10%)	7	16
9	1N	118/119 (99%)	111 (94%)	7 (6%)	19	43
9	2N	118/119 (99%)	112 (95%)	6 (5%)	24	50
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	70
10	2O	100/100 (100%)	94 (94%)	6 (6%)	19	42
11	1P	115/116 (99%)	107 (93%)	8 (7%)	15	35
11	2P	115/116 (99%)	97 (84%)	18 (16%)	2	6
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11	27
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	9	22
13	1R	101/101 (100%)	95 (94%)	6 (6%)	19	43
13	2R	101/101 (100%)	95 (94%)	6 (6%)	19	43
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11	27
14	2S	85/88 (97%)	81 (95%)	4 (5%)	26	54
15	1T	115/127 (91%)	108 (94%)	7 (6%)	18	41
15	2T	113/127 (89%)	109 (96%)	4 (4%)	36	65
16	1U	93/94 (99%)	90 (97%)	3 (3%)	39	68
16	2U	93/94 (99%)	89 (96%)	4 (4%)	29	57
17	1V	80/82 (98%)	75 (94%)	5 (6%)	18	40
17	2V	80/82 (98%)	73 (91%)	7 (9%)	10	23
18	1W	90/92 (98%)	87 (97%)	3 (3%)	38	67
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28	56
19	1X	77/78 (99%)	74 (96%)	3 (4%)	32	61
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	61
20	1Y	85/91 (93%)	78 (92%)	7 (8%)	11	26
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6	15
21	1Z	135/179 (75%)	119 (88%)	16 (12%)	5	12
21	2Z	137/179 (76%)	116 (85%)	21 (15%)	2	7
22	10	65/67 (97%)	60 (92%)	5 (8%)	13	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	20	65/67 (97%)	61 (94%)	4 (6%)	18	40
23	11	80/83 (96%)	72 (90%)	8 (10%)	7	18
23	21	80/83 (96%)	74 (92%)	6 (8%)	13	31
24	12	65/67 (97%)	61 (94%)	4 (6%)	18	40
24	22	65/67 (97%)	59 (91%)	6 (9%)	9	21
25	13	51/52 (98%)	46 (90%)	5 (10%)	8	18
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	60
26	14	59/63 (94%)	51 (86%)	8 (14%)	3	8
26	24	53/63 (84%)	38 (72%)	15 (28%)	0	1
27	15	50/52 (96%)	45 (90%)	5 (10%)	7	18
27	25	50/52 (96%)	45 (90%)	5 (10%)	7	18
28	16	51/52 (98%)	46 (90%)	5 (10%)	8	18
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	18
29	17	41/42 (98%)	38 (93%)	3 (7%)	14	33
29	27	41/42 (98%)	38 (93%)	3 (7%)	14	33
30	18	54/55 (98%)	52 (96%)	2 (4%)	34	63
30	28	54/55 (98%)	51 (94%)	3 (6%)	21	45
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	30 (88%)	4 (12%)	5	12
33	1b	192/220 (87%)	167 (87%)	25 (13%)	4	10
33	2b	187/220 (85%)	161 (86%)	26 (14%)	3	8
34	1c	142/188 (76%)	130 (92%)	12 (8%)	10	24
34	2c	140/188 (74%)	127 (91%)	13 (9%)	9	21
35	1d	169/181 (93%)	151 (89%)	18 (11%)	6	15
35	2d	173/181 (96%)	159 (92%)	14 (8%)	11	27
36	1e	113/123 (92%)	99 (88%)	14 (12%)	4	11
36	2e	114/123 (93%)	106 (93%)	8 (7%)	15	35
37	1f	84/90 (93%)	79 (94%)	5 (6%)	19	42
37	2f	85/90 (94%)	82 (96%)	3 (4%)	36	65
38	1g	119/127 (94%)	110 (92%)	9 (8%)	13	30
38	2g	120/127 (94%)	106 (88%)	14 (12%)	5	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	1h	114/119 (96%)	103 (90%)	11 (10%)	8	19
39	2h	114/119 (96%)	102 (90%)	12 (10%)	7	16
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	14
40	2i	89/99 (90%)	74 (83%)	15 (17%)	2	5
41	1j	66/92 (72%)	61 (92%)	5 (8%)	13	30
41	2j	69/92 (75%)	67 (97%)	2 (3%)	42	71
42	1k	82/99 (83%)	75 (92%)	7 (8%)	10	24
42	2k	83/99 (84%)	77 (93%)	6 (7%)	14	34
43	1l	96/108 (89%)	87 (91%)	9 (9%)	8	20
43	2l	96/108 (89%)	89 (93%)	7 (7%)	14	33
44	1m	93/101 (92%)	86 (92%)	7 (8%)	13	31
44	2m	92/101 (91%)	81 (88%)	11 (12%)	5	11
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	11
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	17
46	1o	78/80 (98%)	72 (92%)	6 (8%)	13	30
46	2o	78/80 (98%)	73 (94%)	5 (6%)	17	39
47	1p	69/74 (93%)	64 (93%)	5 (7%)	14	34
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	9
48	1q	94/97 (97%)	86 (92%)	8 (8%)	10	24
48	2q	94/97 (97%)	88 (94%)	6 (6%)	17	39
49	1r	59/77 (77%)	57 (97%)	2 (3%)	37	66
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	8
50	1s	69/80 (86%)	63 (91%)	6 (9%)	10	23
50	2s	67/80 (84%)	64 (96%)	3 (4%)	27	55
51	1t	70/82 (85%)	66 (94%)	4 (6%)	20	44
51	2t	70/82 (85%)	63 (90%)	7 (10%)	7	18
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	14
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	14
All	All	9303/10064 (92%)	8506 (91%)	797 (9%)	10	24

All (797) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	12	SER
3	1D	32	SER
3	1D	37	LEU
3	1D	68	LYS
3	1D	88	ARG
3	1D	99	ASP
3	1D	140	THR
3	1D	193	VAL
3	1D	211	ARG
3	1D	217	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	253	GLN
4	1E	21	VAL
4	1E	73	GLU
4	1E	75	VAL
4	1E	89	ASP
4	1E	113	PHE
4	1E	116	VAL
4	1E	154	LYS
4	1E	175	VAL
4	1E	178	GLU
4	1E	185	LYS
4	1E	195	LEU
5	1F	18	ARG
5	1F	19	GLU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	88	VAL
5	1F	95	ARG
5	1F	106	ARG
5	1F	175	THR
5	1F	192	LEU
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	28	VAL
6	1G	31	VAL
6	1G	43	LEU
6	1G	59	GLU

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Mol	Chain	Res	Type
6	1G	62	LEU
6	1G	79	ASN
6	1G	82	LEU
6	1G	150	ASP
6	1G	152	LEU
6	1G	159	VAL
7	1H	15	VAL
7	1H	23	ARG
7	1H	33	LEU
7	1H	44	VAL
7	1H	50	VAL
7	1H	59	ARG
7	1H	67	LEU
7	1H	76	VAL
7	1H	88	LEU
7	1H	95	ARG
7	1H	107	VAL
7	1H	119	GLU
7	1H	125	VAL
7	1H	129	THR
8	1I	5	LEU
8	1I	9	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	20	ASP
8	1I	38	LEU
8	1I	43	ASN
8	1I	61	ARG
8	1I	77	LEU
8	1I	86	THR
8	1I	99	GLU
8	1I	108	THR
8	1I	109	ILE
8	1I	114	LEU
8	1I	116	LEU
8	1I	123	LEU
8	1I	127	VAL
8	1I	129	THR
8	1I	140	LEU
8	1I	144	VAL
9	1N	9	VAL
9	1N	32	THR

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Mol	Chain	Res	Type
9	1N	33	LEU
9	1N	46	VAL
9	1N	67	LEU
9	1N	73	THR
9	1N	88	GLU
10	1O	80	ASP
10	1O	89	ASN
10	1O	106	LEU
11	1P	3	LEU
11	1P	40	SER
11	1P	55	ARG
11	1P	79	ARG
11	1P	86	LYS
11	1P	95	VAL
11	1P	125	VAL
11	1P	133	SER
12	1Q	1	MET
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	35	VAL
12	1Q	55	VAL
12	1Q	106	VAL
12	1Q	109	VAL
12	1Q	110	THR
12	1Q	130	LYS
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	79	LEU
13	1R	91	GLN
13	1R	114	VAL
14	1S	14	VAL
14	1S	17	ARG
14	1S	25	ARG
14	1S	46	VAL
14	1S	73	LEU
14	1S	85	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	50	ILE
15	1T	74	ARG
15	1T	85	LYS

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Mol	Chain	Res	Type
15	1T	89	VAL
15	1T	108	ARG
15	1T	118	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	95	LEU
17	1V	46	VAL
17	1V	52	VAL
17	1V	56	SER
17	1V	79	VAL
17	1V	85	LYS
18	1W	11	ARG
18	1W	17	VAL
18	1W	67	ASP
19	1X	23	GLU
19	1X	57	LEU
19	1X	82	GLN
20	1Y	8	LYS
20	1Y	11	ASP
20	1Y	43	ASN
20	1Y	88	LYS
20	1Y	91	GLU
20	1Y	99	CYS
20	1Y	107	ASP
21	1Z	18	LEU
21	1Z	42	VAL
21	1Z	49	ARG
21	1Z	56	VAL
21	1Z	70	LEU
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	87	ASP
21	1Z	91	LEU
21	1Z	122	ARG
21	1Z	132	ASN
21	1Z	138	GLU
21	1Z	140	ASP
21	1Z	141	VAL
21	1Z	155	LEU
21	1Z	171	ILE
22	10	3	HIS
22	10	7	LEU

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Mol	Chain	Res	Type
22	10	9	SER
22	10	14	ARG
22	10	44	ARG
23	11	46	LEU
23	11	52	ARG
23	11	56	GLN
23	11	59	THR
23	11	78	LYS
23	11	83	GLU
23	11	86	SER
23	11	95	LEU
24	12	3	LEU
24	12	19	VAL
24	12	45	SER
24	12	70	GLN
25	13	23	LEU
25	13	30	ARG
25	13	55	ARG
25	13	56	VAL
25	13	60	GLU
26	14	16	CYS
26	14	37	SER
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	60	GLN
26	14	63	TYR
26	14	65	ASP
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	40	LYS
27	15	58	LEU
28	16	6	ARG
28	16	14	THR
28	16	19	ARG
28	16	44	ARG
28	16	48	VAL
29	17	1	MET
29	17	41	ARG
29	17	46	VAL
30	18	31	HIS

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Mol	Chain	Res	Type
30	18	34	TRP
33	1b	7	VAL
33	1b	8	LYS
33	1b	11	LEU
33	1b	21	ARG
33	1b	24	TRP
33	1b	35	GLU
33	1b	47	THR
33	1b	54	THR
33	1b	74	LYS
33	1b	80	ILE
33	1b	82	ARG
33	1b	83	MET
33	1b	93	VAL
33	1b	94	ASN
33	1b	101	MET
33	1b	109	SER
33	1b	111	ARG
33	1b	113	HIS
33	1b	117	GLU
33	1b	138	LEU
33	1b	169	LYS
33	1b	187	LEU
33	1b	208	ILE
33	1b	229	VAL
33	1b	236	TYR
34	1c	17	ASP
34	1c	64	VAL
34	1c	66	VAL
34	1c	70	VAL
34	1c	72	LYS
34	1c	89	GLU
34	1c	116	VAL
34	1c	119	ARG
34	1c	128	PHE
34	1c	138	VAL
34	1c	172	ARG
34	1c	195	VAL
35	1d	3	ARG
35	1d	10	ARG
35	1d	31	CYS
35	1d	53	ASP

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Mol	Chain	Res	Type
35	1d	59	ARG
35	1d	76	ARG
35	1d	91	SER
35	1d	127	THR
35	1d	134	ASP
35	1d	135	LEU
35	1d	137	SER
35	1d	140	VAL
35	1d	177	ASP
35	1d	178	VAL
35	1d	190	ASP
35	1d	194	LEU
35	1d	201	GLN
35	1d	202	LEU
36	1e	8	GLU
36	1e	24	ARG
36	1e	41	VAL
36	1e	45	PHE
36	1e	51	VAL
36	1e	56	GLN
36	1e	67	VAL
36	1e	73	ASN
36	1e	75	THR
36	1e	78	HIS
36	1e	120	THR
36	1e	147	ASP
36	1e	151	LEU
36	1e	152	ARG
37	1f	19	LEU
37	1f	39	LYS
37	1f	54	LYS
37	1f	55	ASP
37	1f	78	GLU
38	1g	12	LEU
38	1g	79	ARG
38	1g	92	SER
38	1g	97	GLN
38	1g	98	SER
38	1g	104	LEU
38	1g	113	GLU
38	1g	115	ARG
38	1g	135	VAL

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Mol	Chain	Res	Type
39	1h	2	LEU
39	1h	29	SER
39	1h	32	LYS
39	1h	52	ASP
39	1h	54	ASP
39	1h	60	ARG
39	1h	77	GLU
39	1h	85	ARG
39	1h	112	LEU
39	1h	122	ARG
39	1h	127	LEU
40	1i	25	LYS
40	1i	56	LEU
40	1i	71	SER
40	1i	81	ILE
40	1i	87	GLN
40	1i	92	TYR
40	1i	96	LEU
40	1i	105	ASP
40	1i	110	GLU
40	1i	128	ARG
41	1j	34	VAL
41	1j	43	ARG
41	1j	66	ARG
41	1j	92	THR
41	1j	100	THR
42	1k	31	THR
42	1k	48	ILE
42	1k	66	LEU
42	1k	81	ASP
42	1k	96	ARG
42	1k	109	VAL
42	1k	114	VAL
43	1l	6	THR
43	1l	18	VAL
43	1l	33	ARG
43	1l	36	VAL
43	1l	54	LYS
43	1l	55	VAL
43	1l	58	VAL
43	1l	78	GLN
43	1l	89	ARG

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Mol	Chain	Res	Type
44	1m	14	ARG
44	1m	15	VAL
44	1m	43	THR
44	1m	60	VAL
44	1m	73	GLU
44	1m	109	THR
44	1m	114	ARG
45	1n	3	ARG
45	1n	6	LEU
45	1n	7	ILE
45	1n	18	VAL
45	1n	35	ARG
45	1n	56	VAL
46	1o	3	ILE
46	1o	7	GLU
46	1o	39	LEU
46	1o	40	SER
46	1o	51	HIS
46	1o	87	ILE
47	1p	20	VAL
47	1p	40	ASP
47	1p	45	THR
47	1p	49	LEU
47	1p	67	THR
48	1q	12	SER
48	1q	19	VAL
48	1q	35	VAL
48	1q	52	LYS
48	1q	53	LEU
48	1q	62	SER
48	1q	63	ARG
48	1q	72	ARG
49	1r	26	LEU
49	1r	47	THR
50	1s	12	ASP
50	1s	14	HIS
50	1s	17	GLU
50	1s	37	ARG
50	1s	49	ILE
50	1s	66	MET
51	1t	10	LEU
51	1t	25	ARG

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Mol	Chain	Res	Type
51	1t	56	MET
51	1t	62	LEU
52	1u	7	ARG
52	1u	17	THR
3	2D	3	VAL
3	2D	34	VAL
3	2D	37	LEU
3	2D	38	LYS
3	2D	106	ILE
3	2D	111	LEU
3	2D	113	VAL
3	2D	142	VAL
3	2D	171	ASP
3	2D	217	ARG
3	2D	242	ARG
3	2D	271	ILE
3	2D	276	LYS
4	2E	12	THR
4	2E	14	ILE
4	2E	21	VAL
4	2E	38	THR
4	2E	49	LEU
4	2E	73	GLU
4	2E	75	VAL
4	2E	89	ASP
4	2E	116	VAL
4	2E	195	LEU
5	2F	28	ILE
5	2F	32	LEU
5	2F	33	LEU
5	2F	37	VAL
5	2F	53	THR
5	2F	70	THR
5	2F	88	VAL
5	2F	106	ARG
5	2F	108	LYS
5	2F	135	LYS
5	2F	140	LEU
5	2F	158	THR
5	2F	161	GLU
5	2F	165	ARG
5	2F	170	LEU

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Mol	Chain	Res	Type
5	2F	183	VAL
5	2F	192	LEU
6	2G	3	LEU
6	2G	5	VAL
6	2G	9	ARG
6	2G	18	GLU
6	2G	31	VAL
6	2G	49	ASP
6	2G	60	LEU
6	2G	70	VAL
6	2G	79	ASN
6	2G	91	ARG
6	2G	133	LEU
6	2G	135	LEU
6	2G	140	ILE
6	2G	145	THR
6	2G	157	ILE
6	2G	159	VAL
6	2G	162	THR
6	2G	165	THR
7	2H	6	ARG
7	2H	12	PRO
7	2H	15	VAL
7	2H	23	ARG
7	2H	27	LYS
7	2H	72	ILE
7	2H	84	SER
7	2H	88	LEU
7	2H	98	LEU
7	2H	114	VAL
7	2H	122	THR
7	2H	129	THR
7	2H	134	SER
7	2H	136	ILE
8	2I	15	VAL
8	2I	38	LEU
8	2I	40	THR
8	2I	43	ASN
8	2I	58	LEU
8	2I	74	ASN
8	2I	92	VAL
8	2I	125	GLU

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Mol	Chain	Res	Type
8	2I	127	VAL
8	2I	144	VAL
8	2I	145	VAL
9	2N	38	HIS
9	2N	46	VAL
9	2N	62	VAL
9	2N	68	GLU
9	2N	85	ILE
9	2N	118	LYS
10	2O	10	VAL
10	2O	13	ASN
10	2O	42	SER
10	2O	75	SER
10	2O	77	ILE
10	2O	108	GLU
11	2P	3	LEU
11	2P	4	SER
11	2P	7	ARG
11	2P	15	ARG
11	2P	29	LYS
11	2P	36	LYS
11	2P	42	SER
11	2P	45	LEU
11	2P	58	THR
11	2P	77	ARG
11	2P	86	LYS
11	2P	90	ARG
11	2P	95	VAL
11	2P	99	LEU
11	2P	101	VAL
11	2P	119	GLU
11	2P	133	SER
11	2P	147	LEU
12	2Q	1	MET
12	2Q	10	ARG
12	2Q	60	ARG
12	2Q	75	THR
12	2Q	85	LYS
12	2Q	103	MET
12	2Q	109	VAL
12	2Q	110	THR
12	2Q	133	ARG

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Mol	Chain	Res	Type
12	2Q	139	GLU
13	2R	15	SER
13	2R	24	GLN
13	2R	29	LEU
13	2R	36	THR
13	2R	79	LEU
13	2R	95	THR
14	2S	12	PHE
14	2S	36	TYR
14	2S	84	GLN
14	2S	110	LEU
15	2T	6	LEU
15	2T	27	THR
15	2T	89	VAL
15	2T	96	ARG
16	2U	6	THR
16	2U	53	ARG
16	2U	55	ARG
16	2U	74	LEU
17	2V	7	THR
17	2V	14	VAL
17	2V	33	VAL
17	2V	52	VAL
17	2V	79	VAL
17	2V	98	GLU
17	2V	100	ARG
18	2W	11	ARG
18	2W	17	VAL
18	2W	67	ASP
18	2W	68	ARG
19	2X	54	VAL
19	2X	57	LEU
19	2X	81	VAL
20	2Y	3	VAL
20	2Y	11	ASP
20	2Y	43	ASN
20	2Y	49	VAL
20	2Y	55	TYR
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	99	CYS
20	2Y	106	LEU

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Mol	Chain	Res	Type
21	2Z	24	LEU
21	2Z	32	HIS
21	2Z	33	LEU
21	2Z	35	ARG
21	2Z	38	TYR
21	2Z	42	VAL
21	2Z	50	GLN
21	2Z	52	SER
21	2Z	70	LEU
21	2Z	84	GLU
21	2Z	89	PHE
21	2Z	100	VAL
21	2Z	129	SER
21	2Z	132	ASN
21	2Z	144	LEU
21	2Z	153	SER
21	2Z	154	ASP
21	2Z	165	VAL
21	2Z	170	THR
21	2Z	171	ILE
21	2Z	174	VAL
22	20	7	LEU
22	20	14	ARG
22	20	30	VAL
22	20	68	GLU
23	21	21	ARG
23	21	40	ARG
23	21	56	GLN
23	21	59	THR
23	21	95	LEU
23	21	98	LEU
24	22	35	LEU
24	22	49	LYS
24	22	55	ARG
24	22	60	LEU
24	22	64	LEU
24	22	70	GLN
25	23	31	LEU
25	23	53	LEU
26	24	9	LEU
26	24	10	VAL
26	24	26	SER

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Mol	Chain	Res	Type
26	24	27	THR
26	24	34	GLU
26	24	37	SER
26	24	40	HIS
26	24	44	THR
26	24	46	GLN
26	24	49	PHE
26	24	59	PHE
26	24	60	GLN
26	24	61	ARG
26	24	62	ARG
26	24	63	TYR
27	25	6	VAL
27	25	15	ARG
27	25	16	ARG
27	25	29	THR
27	25	58	LEU
28	26	5	VAL
28	26	6	ARG
28	26	19	ARG
28	26	30	THR
28	26	48	VAL
29	27	1	MET
29	27	24	THR
29	27	46	VAL
30	28	23	VAL
30	28	31	HIS
30	28	46	ARG
31	29	6	SER
31	29	7	VAL
31	29	9	ARG
31	29	26	ILE
33	2b	7	VAL
33	2b	8	LYS
33	2b	10	LEU
33	2b	11	LEU
33	2b	16	HIS
33	2b	22	LYS
33	2b	24	TRP
33	2b	35	GLU
33	2b	48	MET
33	2b	56	ARG

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Mol	Chain	Res	Type
33	2b	67	THR
33	2b	93	VAL
33	2b	94	ASN
33	2b	109	SER
33	2b	117	GLU
33	2b	118	LEU
33	2b	127	ILE
33	2b	135	GLN
33	2b	140	HIS
33	2b	144	ARG
33	2b	168	THR
33	2b	179	LYS
33	2b	185	ILE
33	2b	196	LEU
33	2b	198	ASP
33	2b	230	VAL
34	2c	10	PHE
34	2c	17	ASP
34	2c	21	ARG
34	2c	44	GLU
34	2c	47	LEU
34	2c	48	TYR
34	2c	57	ILE
34	2c	101	LEU
34	2c	166	GLU
34	2c	178	LEU
34	2c	179	ARG
34	2c	191	THR
34	2c	199	LYS
35	2d	5	ILE
35	2d	10	ARG
35	2d	17	VAL
35	2d	31	CYS
35	2d	47	ARG
35	2d	76	ARG
35	2d	118	ARG
35	2d	135	LEU
35	2d	150	GLU
35	2d	156	GLU
35	2d	166	LYS
35	2d	168	ARG
35	2d	175	SER

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Mol	Chain	Res	Type
35	2d	205	GLU
36	2e	12	LEU
36	2e	13	ILE
36	2e	20	GLN
36	2e	24	ARG
36	2e	25	ARG
36	2e	38	GLN
36	2e	41	VAL
36	2e	112	LEU
37	2f	23	LYS
37	2f	63	TYR
37	2f	70	ASP
38	2g	9	VAL
38	2g	15	ASP
38	2g	24	THR
38	2g	33	ASP
38	2g	38	LEU
38	2g	76	ARG
38	2g	78	ARG
38	2g	79	ARG
38	2g	98	SER
38	2g	113	GLU
38	2g	115	ARG
38	2g	119	ARG
38	2g	146	GLU
38	2g	155	ARG
39	2h	10	LEU
39	2h	24	THR
39	2h	51	VAL
39	2h	52	ASP
39	2h	77	GLU
39	2h	88	LYS
39	2h	98	LYS
39	2h	99	GLU
39	2h	122	ARG
39	2h	127	LEU
39	2h	133	LEU
39	2h	137	VAL
40	2i	40	LEU
40	2i	41	VAL
40	2i	50	LEU
40	2i	51	ARG

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Mol	Chain	Res	Type
40	2i	53	VAL
40	2i	64	THR
40	2i	65	VAL
40	2i	86	VAL
40	2i	87	GLN
40	2i	89	ASN
40	2i	102	LEU
40	2i	108	VAL
40	2i	110	GLU
40	2i	113	LYS
40	2i	125	TYR
41	2j	45	ARG
41	2j	98	ILE
42	2k	14	VAL
42	2k	24	SER
42	2k	84	VAL
42	2k	105	VAL
42	2k	107	SER
42	2k	114	VAL
43	2l	18	VAL
43	2l	37	CYS
43	2l	54	LYS
43	2l	67	THR
43	2l	86	ARG
43	2l	97	ARG
43	2l	102	ARG
44	2m	14	ARG
44	2m	15	VAL
44	2m	47	ASP
44	2m	60	VAL
44	2m	64	TRP
44	2m	65	LYS
44	2m	81	LEU
44	2m	86	CYS
44	2m	103	THR
44	2m	110	ARG
44	2m	117	VAL
45	2n	3	ARG
45	2n	6	LEU
45	2n	7	ILE
45	2n	33	VAL
45	2n	35	ARG

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Mol	Chain	Res	Type
46	2o	5	LYS
46	2o	7	GLU
46	2o	39	LEU
46	2o	68	ARG
46	2o	87	ILE
47	2p	1	MET
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	28	ARG
47	2p	35	LYS
47	2p	42	ARG
47	2p	67	THR
47	2p	69	THR
48	2q	5	VAL
48	2q	14	LYS
48	2q	41	LYS
48	2q	63	ARG
48	2q	83	ASP
48	2q	93	GLN
49	2r	21	LYS
49	2r	26	LEU
49	2r	37	VAL
49	2r	46	GLU
49	2r	47	THR
49	2r	66	LEU
49	2r	84	LYS
49	2r	86	VAL
50	2s	21	GLU
50	2s	48	THR
50	2s	77	THR
51	2t	15	ARG
51	2t	24	LEU
51	2t	37	SER
51	2t	51	GLU
51	2t	62	LEU
51	2t	71	THR
51	2t	100	ILE
52	2u	7	ARG
52	2u	22	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
4	1E	85	ASN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
6	1G	108	ASN
8	1I	105	HIS
10	1O	3	GLN
10	1O	89	ASN
12	1Q	12	GLN
12	1Q	57	HIS
16	1U	94	ASN
19	1X	31	HIS
20	1Y	6	HIS
21	1Z	34	ASN
21	1Z	55	HIS
21	1Z	73	GLN
23	11	56	GLN
24	12	38	GLN
24	12	70	GLN
26	14	46	GLN
33	1b	40	HIS
33	1b	78	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	162	GLN
35	1d	42	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
35	1d	201	GLN
36	1e	73	ASN
37	1f	32	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	96	GLN
39	1h	15	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	58	HIS
40	1i	89	ASN

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Mol	Chain	Res	Type
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
45	1n	49	HIS
46	1o	46	HIS
46	1o	62	GLN
48	1q	16	GLN
48	1q	26	GLN
50	1s	23	ASN
50	1s	47	HIS
50	1s	83	HIS
51	1t	73	HIS
51	1t	75	ASN
3	2D	112	GLN
4	2E	48	GLN
5	2F	69	HIS
6	2G	66	GLN
6	2G	132	ASN
7	2H	139	GLN
10	2O	13	ASN
10	2O	89	ASN
10	2O	90	GLN
12	2Q	57	HIS
12	2Q	89	ASN
12	2Q	113	GLN
14	2S	34	HIS
14	2S	38	GLN
15	2T	55	ASN
16	2U	81	HIS
17	2V	80	GLN
18	2W	60	ASN
19	2X	31	HIS
20	2Y	43	ASN
21	2Z	34	ASN
21	2Z	50	GLN
21	2Z	55	HIS
21	2Z	73	GLN
21	2Z	151	HIS
22	20	70	GLN
23	21	56	GLN
24	22	38	GLN
24	22	70	GLN

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Mol	Chain	Res	Type
25	23	32	GLN
31	29	20	HIS
33	2b	25	ASN
33	2b	40	HIS
33	2b	78	GLN
33	2b	95	GLN
33	2b	212	GLN
34	2c	6	HIS
34	2c	98	ASN
34	2c	102	ASN
34	2c	123	GLN
35	2d	45	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	161	ASN
36	2e	72	GLN
36	2e	73	ASN
36	2e	130	ASN
37	2f	73	ASN
38	2g	28	ASN
38	2g	37	ASN
38	2g	68	ASN
39	2h	15	ASN
40	2i	89	ASN
41	2j	13	HIS
43	2l	99	HIS
44	2m	77	ASN
46	2o	62	GLN
48	2q	16	GLN
50	2s	23	ASN
50	2s	69	HIS
50	2s	83	HIS
51	2t	45	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	470 (16%)	36 (1%)
1	2A	2789/2915 (95%)	518 (18%)	25 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1B	120/121 (99%)	12 (10%)	1 (0%)
2	2B	118/121 (97%)	30 (25%)	0
32	1a	1494/1521 (98%)	270 (18%)	0
32	2a	1498/1521 (98%)	301 (20%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	18 (25%)	0
54	1y	71/76 (93%)	27 (38%)	0
54	2w	68/76 (89%)	22 (32%)	0
54	2y	69/76 (90%)	27 (39%)	0
55	1x	75/77 (97%)	12 (16%)	0
55	2x	75/77 (97%)	17 (22%)	0
All	All	9334/9620 (97%)	1729 (18%)	62 (0%)

All (1729) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	11	G
1	1A	12	U
1	1A	27	G
1	1A	34	C
1	1A	45	C
1	1A	55	G
1	1A	58	G
1	1A	63	U
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	126	A
1	1A	139(A)	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

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Mol	Chain	Res	Type
1	1A	216	A
1	1A	222	A
1	1A	223	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	264	C
1	1A	269	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	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	283	A
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	342	G
1	1A	352	G
1	1A	363	G
1	1A	363(A)	A
1	1A	363(B)	G
1	1A	363(E)	U
1	1A	370	G
1	1A	380	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	435	C
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	454	A
1	1A	456	C

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Mol	Chain	Res	Type
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	512	G
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	551	G
1	1A	563	G
1	1A	568	U
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	740	U
1	1A	746	A
1	1A	764	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A

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Mol	Chain	Res	Type
1	1A	785	G
1	1A	790	C
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	855	G
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	915	C
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	949	C
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1005	C
1	1A	1008	C

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Mol	Chain	Res	Type
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1038	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1083	U
1	1A	1084	A
1	1A	1085	A
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1094	U
1	1A	1100	C
1	1A	1101	U
1	1A	1103	A
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1170	G
1	1A	1171	G

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Mol	Chain	Res	Type
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	1205	U
1	1A	1211	U
1	1A	1212	G
1	1A	1218	C
1	1A	1227	G
1	1A	1236	G
1	1A	1244	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1288	U
1	1A	1298	C
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1320	C
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1372	U
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
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	1437	C
1	1A	1439	A

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Mol	Chain	Res	Type
1	1A	1445	A
1	1A	1446	C
1	1A	1450	G
1	1A	1455	G
1	1A	1461	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1496	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1540	U
1	1A	1541	G
1	1A	1543	C
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1607	C
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1674	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1739	U
1	1A	1746	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A

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Mol	Chain	Res	Type
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1802	A
1	1A	1812	A
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
1	1A	1847	A
1	1A	1858	G
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1946	U
1	1A	1955	U
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	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A

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Mol	Chain	Res	Type
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2082	A
1	1A	2093	G
1	1A	2096	U
1	1A	2110	G
1	1A	2111	C
1	1A	2112	G
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2118	U
1	1A	2121	G
1	1A	2122	U
1	1A	2123	G
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2141	G
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2178	C

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Mol	Chain	Res	Type
1	1A	2181	G
1	1A	2182	G
1	1A	2183	C
1	1A	2184	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2278	A
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2294	C
1	1A	2296	U
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2396	G
1	1A	2400	G
1	1A	2406	U
1	1A	2409	G
1	1A	2424	C
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A

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Mol	Chain	Res	Type
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2474	C
1	1A	2476	A
1	1A	2478	A
1	1A	2490	G
1	1A	2498	C
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2578	G
1	1A	2585	U
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2641	G
1	1A	2654	A
1	1A	2670	A
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U

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Mol	Chain	Res	Type
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2769	C
1	1A	2778	A
1	1A	2780	G
1	1A	2789	C
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2805	G
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2872	G
1	1A	2876	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	5	C
2	1B	15	A
2	1B	24	G
2	1B	35	U
2	1B	52	A
2	1B	56	G
2	1B	73	A
2	1B	85	G
2	1B	106	G
2	1B	110	G
2	1B	118	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C

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Mol	Chain	Res	Type
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	66	G
32	1a	69	G
32	1a	79	G
32	1a	91	C
32	1a	96	U
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	111	G
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	151	A
32	1a	163	C
32	1a	174	C
32	1a	183	G
32	1a	189	G
32	1a	189(F)	U
32	1a	195	A
32	1a	197	A
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	220	G
32	1a	222	U
32	1a	247	G
32	1a	251	G
32	1a	254	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	328	C

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Mol	Chain	Res	Type
32	1a	332	G
32	1a	342	C
32	1a	344	A
32	1a	345	C
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	381	C
32	1a	384	G
32	1a	390	C
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	421	U
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	458	C
32	1a	461	A
32	1a	471	G
32	1a	477	A
32	1a	483	C
32	1a	485	G
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	524	G
32	1a	528	C

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Mol	Chain	Res	Type
32	1a	531	U
32	1a	532	A
32	1a	534	U
32	1a	536	C
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	608	A
32	1a	616	G
32	1a	630	G
32	1a	653	A
32	1a	659	U
32	1a	665	A
32	1a	683	G
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	695	A
32	1a	702	A
32	1a	703	G
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	749	C
32	1a	755	G
32	1a	759	A
32	1a	766	A
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G

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Mol	Chain	Res	Type
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	853	G
32	1a	859	A
32	1a	860	A
32	1a	872	A
32	1a	884	U
32	1a	902	G
32	1a	913	A
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	942	G
32	1a	955	U
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	982	U
32	1a	992	U
32	1a	993	G
32	1a	996	A
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1007	C
32	1a	1009	G
32	1a	1010	G
32	1a	1020	U
32	1a	1022	G

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Mol	Chain	Res	Type
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1028	C
32	1a	1029	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1039	C
32	1a	1043	C
32	1a	1044	A
32	1a	1046	A
32	1a	1053	G
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1096	C
32	1a	1101	A
32	1a	1104	G
32	1a	1108	G
32	1a	1123	A
32	1a	1125	U
32	1a	1132	C
32	1a	1134	G
32	1a	1135	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1157	A
32	1a	1159	U
32	1a	1160	G
32	1a	1184	G

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Mol	Chain	Res	Type
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1220	G
32	1a	1222	G
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1276	G
32	1a	1277	C
32	1a	1278	U
32	1a	1279	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	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1380	U
32	1a	1390	U
32	1a	1397	C
32	1a	1419	G
32	1a	1422	G
32	1a	1442	G
32	1a	1442(A)	G

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Mol	Chain	Res	Type
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1475	G
32	1a	1487	G
32	1a	1492	A
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	24	A
54	1w	2	C
54	1w	6	G
54	1w	7	A
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	24	G
54	1w	25	C
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	62	C
54	1w	68	C
54	1w	70	G
54	1w	73	A
54	1w	74	C
54	1w	76	A
55	1x	3	C
55	1x	9	G
55	1x	13	C
55	1x	14	A
55	1x	18	G
55	1x	19	G
55	1x	21	A
55	1x	46	G
55	1x	47	U

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Mol	Chain	Res	Type
55	1x	61	C
55	1x	69	C
55	1x	76	A
54	1y	6	G
54	1y	8	4SU
54	1y	11	C
54	1y	13	C
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	26	A
54	1y	31	A
54	1y	34	G
54	1y	35	A
54	1y	36	A
54	1y	44	G
54	1y	45	U
54	1y	46	G7M
54	1y	47	U
54	1y	48	C
54	1y	49	C
54	1y	53	G
54	1y	56	C
54	1y	57	G
54	1y	59	U
54	1y	61	C
54	1y	65	G
54	1y	69	G
54	1y	70	G
54	1y	73	A
1	2A	8	A
1	2A	10	G
1	2A	11	G
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A

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Mol	Chain	Res	Type
1	2A	90	U
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	125	G
1	2A	140	G
1	2A	149	A
1	2A	154(A)	C
1	2A	157	U
1	2A	172	C
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	200	U
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	265	A
1	2A	266	G
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	272(I)	U
1	2A	272(J)	C
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	281	G
1	2A	289	A

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Mol	Chain	Res	Type
1	2A	294	A
1	2A	311	A
1	2A	312	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	332	A
1	2A	342	G
1	2A	352	G
1	2A	354	G
1	2A	356	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	363(E)	U
1	2A	380	U
1	2A	386	G
1	2A	391	G
1	2A	396	G
1	2A	405	U
1	2A	411	G
1	2A	416	C
1	2A	421	U
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	494	G
1	2A	499	U
1	2A	501	A
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	518	G
1	2A	529	A
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	568	U

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Mol	Chain	Res	Type
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	593	G
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	620	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	699	A
1	2A	701	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	734	A
1	2A	740	U
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A

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Mol	Chain	Res	Type
1	2A	827	U
1	2A	828	U
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	870	A
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	950	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1012	U

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Mol	Chain	Res	Type
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1114	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1143	A
1	2A	1144	G
1	2A	1166	C
1	2A	1170	G
1	2A	1171	G
1	2A	1188	U
1	2A	1211	U
1	2A	1218	C
1	2A	1220	A
1	2A	1229	G
1	2A	1237	A
1	2A	1244	G
1	2A	1252	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1320	C
1	2A	1327	C
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A

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Mol	Chain	Res	Type
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1379	A
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1441	G
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1465	G
1	2A	1467	C
1	2A	1471	A
1	2A	1478	G
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1514	U
1	2A	1520	G
1	2A	1525	G
1	2A	1531	C
1	2A	1541	G
1	2A	1558	A
1	2A	1560	G
1	2A	1566	A
1	2A	1569	A

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Mol	Chain	Res	Type
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1639	U
1	2A	1640	C
1	2A	1648	C
1	2A	1653	G
1	2A	1654	A
1	2A	1667	G
1	2A	1674	G
1	2A	1695	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1774	C
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1835	G

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Mol	Chain	Res	Type
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1857	G
1	2A	1877	A
1	2A	1878	G
1	2A	1895	C
1	2A	1896	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1937	A
1	2A	1938	A
1	2A	1940	U
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2027	G
1	2A	2031	A
1	2A	2032	G
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	2062	A

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Mol	Chain	Res	Type
1	2A	2069	G
1	2A	2093	G
1	2A	2099	U
1	2A	2103	C
1	2A	2105	C
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2115	G
1	2A	2116	G
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	2129	C
1	2A	2130	U
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2151	G
1	2A	2152	G
1	2A	2153	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2161	C
1	2A	2162	G
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U

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Mol	Chain	Res	Type
1	2A	2174	C
1	2A	2178	C
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2273	A
1	2A	2275	C
1	2A	2278	A
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2297	C
1	2A	2303	G
1	2A	2305	A
1	2A	2307	G
1	2A	2308	G
1	2A	2309	A
1	2A	2312	U
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	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2358	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2391	G
1	2A	2396	G
1	2A	2403	C
1	2A	2406	U

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Mol	Chain	Res	Type
1	2A	2410	G
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2438	U
1	2A	2439	A
1	2A	2441	C
1	2A	2447	G
1	2A	2448	A
1	2A	2469	A
1	2A	2476	A
1	2A	2487	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	2525	G
1	2A	2529	G
1	2A	2534	A
1	2A	2535	G
1	2A	2549	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2572	A
1	2A	2585	U
1	2A	2586	C
1	2A	2602	A
1	2A	2609	U
1	2A	2610	C
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G

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Mol	Chain	Res	Type
1	2A	2645	G
1	2A	2654	A
1	2A	2669	G
1	2A	2673	G
1	2A	2686	G
1	2A	2689	U
1	2A	2690	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2752	C
1	2A	2757	A
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2780	G
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2804	C
1	2A	2808	U
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2839	G
1	2A	2872	G
1	2A	2873	A
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G

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Mol	Chain	Res	Type
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	9	G
2	2B	10	C
2	2B	13	A
2	2B	19	G
2	2B	31	C
2	2B	34	U
2	2B	40	U
2	2B	41	U
2	2B	42	C
2	2B	45	A
2	2B	53	A
2	2B	56	G
2	2B	63	G
2	2B	65	C
2	2B	67	G
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	89	G
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	114	C
2	2B	116	G
2	2B	120	A
32	2a	6	G
32	2a	9	G
32	2a	22	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	65	U

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Mol	Chain	Res	Type
32	2a	66	G
32	2a	70	G
32	2a	73	G
32	2a	78	G
32	2a	89	C
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	120	A
32	2a	121	C
32	2a	127	G
32	2a	131	C
32	2a	144	G
32	2a	163	C
32	2a	174	C
32	2a	180	U
32	2a	182	U
32	2a	185	A
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	189(K)	U
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	231	G
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	279	A
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	340	U
32	2a	342	C
32	2a	350	G
32	2a	351	G

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Mol	Chain	Res	Type
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	414	A
32	2a	422	C
32	2a	423	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	471	G
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	575	G

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Mol	Chain	Res	Type
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	607	A
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	703	G
32	2a	721	G
32	2a	723	U
32	2a	725	G
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	855	G
32	2a	859	A
32	2a	870	U
32	2a	874	G
32	2a	880	C
32	2a	885	G
32	2a	902	G
32	2a	914	A
32	2a	926	G

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Mol	Chain	Res	Type
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	979	C
32	2a	982	U
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	996	A
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1017	G
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1029	C
32	2a	1030	C

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Mol	Chain	Res	Type
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1036	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1044	A
32	2a	1045	C
32	2a	1051	C
32	2a	1064	G
32	2a	1065	U
32	2a	1066	C
32	2a	1067	A
32	2a	1068	G
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1086	U
32	2a	1087	G
32	2a	1091	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1104	G
32	2a	1108	G
32	2a	1109	C
32	2a	1113	C
32	2a	1115	C
32	2a	1117	G
32	2a	1121	U
32	2a	1122	U
32	2a	1125	U
32	2a	1126	U
32	2a	1129	C
32	2a	1130	A
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G

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Mol	Chain	Res	Type
32	2a	1140	C
32	2a	1141	C
32	2a	1146	A
32	2a	1148	U
32	2a	1149	C
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1160	G
32	2a	1161	C
32	2a	1172	C
32	2a	1174	G
32	2a	1176	A
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1185	G
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1210	C
32	2a	1211	U
32	2a	1213	A
32	2a	1214	C
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1262	C
32	2a	1268	A
32	2a	1270	C
32	2a	1272	G
32	2a	1275	A
32	2a	1278	U
32	2a	1279	A

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Mol	Chain	Res	Type
32	2a	1280	A
32	2a	1282	C
32	2a	1286	A
32	2a	1287	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1311	G
32	2a	1323	G
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1357	A
32	2a	1358	U
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1378	C
32	2a	1380	U
32	2a	1381	U
32	2a	1397	C
32	2a	1404	5MC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1452	C
32	2a	1492	A
32	2a	1494	G
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
53	2v	13	A
53	2v	14	A
53	2v	24	A

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Mol	Chain	Res	Type
54	2w	5	G
54	2w	8	4SU
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	25	C
54	2w	27	G
54	2w	29	G
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	62	C
54	2w	64	A
54	2w	65	G
54	2w	67	C
54	2w	69	G
54	2w	70	G
54	2w	73	A
54	2w	74	C
54	2w	75	C
54	2w	76	A
55	2x	9	G
55	2x	10	G
55	2x	13	C
55	2x	18	G
55	2x	19	G
55	2x	20	U
55	2x	21	A
55	2x	22	G
55	2x	28	C
55	2x	46	G
55	2x	47	U
55	2x	51	C
55	2x	52	G
55	2x	56	C
55	2x	61	C
55	2x	63	G
55	2x	76	A
54	2y	2	C
54	2y	14	A
54	2y	15	G

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Mol	Chain	Res	Type
54	2y	19	G
54	2y	23	A
54	2y	25	C
54	2y	27	G
54	2y	40	C
54	2y	42	C
54	2y	45	U
54	2y	46	G7M
54	2y	48	C
54	2y	49	C
54	2y	53	G
54	2y	54	5MU
54	2y	55	PSU
54	2y	56	C
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	63	G
54	2y	65	G
54	2y	67	C
54	2y	68	C
54	2y	69	G
54	2y	70	G
54	2y	73	A

All (62) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	573	G
1	1A	685	A
1	1A	746	A
1	1A	764	A
1	1A	895	U
1	1A	974	G
1	1A	1065	U
1	1A	1067	A
1	1A	1078	U

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Mol	Chain	Res	Type
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1379	A
1	1A	1420	U
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1653	G
1	1A	1929	G
1	1A	1992	G
1	1A	2134	A
1	1A	2170	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
2	1B	1	U
1	2A	195	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	746	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	839	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G

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Mol	Chain	Res	Type
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	U
1	2A	2756	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
43	0TD	1l	92	43	7,9,10	4.75	1 (14%)	6,11,13	7.42	2 (33%)
1	PSU	1A	1917	1	18,21,22	1.31	2 (11%)	22,30,33	1.76	4 (18%)
54	MIA	2y	37	54	18,24,32	1.09	2 (11%)	18,35,47	1.31	3 (16%)
32	2MG	2a	1207	32	18,26,27	0.91	1 (5%)	16,38,41	1.10	2 (12%)
54	PSU	2w	32	54	18,21,22	1.34	3 (16%)	22,30,33	1.75	3 (13%)
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	22,30,33	1.86	4 (18%)
54	5MU	1y	54	54	19,22,23	1.50	6 (31%)	28,32,35	2.22	8 (28%)
32	4OC	1a	1402	32	20,23,24	0.78	0	26,32,35	0.99	1 (3%)
32	M2G	2a	966	32	20,27,28	1.35	3 (15%)	22,40,43	1.12	2 (9%)
32	UR3	2a	1498	32	19,22,23	1.00	1 (5%)	26,32,35	1.41	2 (7%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
1	PSU	1A	2605	1,56	18,21,22	1.42	4 (22%)	22,30,33	1.89	3 (13%)
54	MIA	1w	37	54	24,31,32	2.30	4 (16%)	26,44,47	2.47	9 (34%)
32	5MC	1a	1400	32	18,22,23	0.98	2 (11%)	26,32,35	1.14	2 (7%)
32	5MC	2a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.11	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.84	0	26,31,34	0.95	1 (3%)
55	4SU	2x	8	55	18,21,22	1.96	6 (33%)	26,30,33	1.36	3 (11%)
1	5MC	1A	1942	1,56	18,22,23	0.97	2 (11%)	26,32,35	1.16	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	2A	1915	1	19,22,23	1.47	5 (26%)	28,32,35	2.14	5 (17%)
32	MA6	1a	1518	32	19,26,27	0.84	0	18,38,41	1.44	2 (11%)
54	G7M	2y	46	54	20,26,27	1.39	2 (10%)	17,39,42	0.65	0
54	5MU	2w	54	54	19,22,23	1.35	4 (21%)	28,32,35	1.69	6 (21%)
1	5MC	2A	1942	1	18,22,23	0.96	1 (5%)	26,32,35	1.06	2 (7%)
32	MA6	1a	1519	32	19,26,27	0.84	0	18,38,41	1.64	3 (16%)
55	4SU	1x	8	55	18,21,22	2.09	4 (22%)	26,30,33	1.56	5 (19%)
55	5MU	2x	54	55	19,22,23	1.36	5 (26%)	28,32,35	1.98	6 (21%)
1	5MU	1A	1915	1	19,22,23	1.46	5 (26%)	28,32,35	2.03	8 (28%)
32	5MC	1a	967	32	18,22,23	0.95	2 (11%)	26,32,35	1.15	2 (7%)
55	5MC	1x	32	55	18,22,23	0.99	2 (11%)	26,32,35	1.19	2 (7%)
32	M2G	1a	966	32	20,27,28	1.45	3 (15%)	22,40,43	0.92	2 (9%)
32	G7M	2a	527	56,32	20,26,27	1.24	2 (10%)	17,39,42	0.54	0
43	0TD	2l	92	43	7,9,10	4.81	1 (14%)	6,11,13	2.41	3 (50%)
54	PSU	2y	32	54	18,21,22	1.33	2 (11%)	22,30,33	1.77	3 (13%)
1	2MA	2A	2503	1,56	17,25,26	1.01	1 (5%)	17,37,40	1.02	2 (11%)
32	4OC	2a	1402	56,32	20,23,24	0.79	1 (5%)	26,32,35	0.90	1 (3%)
54	PSU	2w	39	54	18,21,22	1.38	2 (11%)	22,30,33	1.62	3 (13%)
1	5MC	1A	1962	1	18,22,23	0.97	2 (11%)	26,32,35	1.16	2 (7%)
55	PSU	1x	55	56,55	18,21,22	1.34	2 (11%)	22,30,33	1.80	3 (13%)
1	OMG	1A	2251	1,56,55	18,26,27	1.03	1 (5%)	19,38,41	1.02	2 (10%)
32	2MG	1a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	1.11	2 (12%)
54	5MU	1w	54	54	19,22,23	1.41	5 (26%)	28,32,35	1.99	7 (25%)
55	5MU	1x	54	56,55	19,22,23	1.43	5 (26%)	28,32,35	1.89	6 (21%)
54	PSU	2w	55	54	18,21,22	1.38	2 (11%)	22,30,33	1.85	3 (13%)
54	4SU	1y	8	56,54	18,21,22	1.63	4 (22%)	26,30,33	2.11	4 (15%)
32	MA6	2a	1518	32	19,26,27	0.79	0	18,38,41	1.43	2 (11%)
1	PSU	2A	2605	1	18,21,22	1.29	3 (16%)	22,30,33	1.91	4 (18%)
54	MIA	1y	37	54	18,24,32	1.16	2 (11%)	18,35,47	1.24	2 (11%)
54	4SU	1w	8	54	18,21,22	1.72	4 (22%)	26,30,33	1.86	6 (23%)
54	5MU	2y	54	54	19,22,23	1.50	4 (21%)	28,32,35	1.97	8 (28%)
1	2MA	1A	2503	1,56	17,25,26	0.99	0	17,37,40	1.00	1 (5%)
1	OMC	1A	1920	1	19,22,23	0.86	0	26,31,34	0.89	1 (3%)
1	PSU	1A	1911	1	18,21,22	1.31	2 (11%)	22,30,33	1.96	4 (18%)
54	PSU	2y	39	54	18,21,22	1.35	2 (11%)	22,30,33	1.76	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	2A	1962	1,56	18,22,23	0.96	2 (11%)	26,32,35	1.13	2 (7%)
32	5MC	2a	1407	32	18,22,23	1.00	2 (11%)	26,32,35	1.30	3 (11%)
1	5MU	2A	1939	1,56	19,22,23	1.37	5 (26%)	28,32,35	2.23	6 (21%)
32	G7M	1a	527	32	20,26,27	1.20	2 (10%)	17,39,42	0.58	0
54	PSU	1y	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
54	PSU	1y	32	54	18,21,22	1.36	2 (11%)	22,30,33	1.69	3 (13%)
1	2MU	2A	2552	1,56	19,22,24	1.30	2 (10%)	26,31,36	1.75	5 (19%)
32	MA6	2a	1519	32	19,26,27	0.79	0	18,38,41	1.50	2 (11%)
32	5MC	2a	1404	32	18,22,23	0.99	2 (11%)	26,32,35	1.22	3 (11%)
54	MIA	2w	37	54	20,27,32	1.81	4 (20%)	22,39,47	1.77	7 (31%)
32	5MC	2a	1400	32	18,22,23	0.98	2 (11%)	26,32,35	1.24	3 (11%)
54	4SU	2w	8	54	18,21,22	1.65	4 (22%)	26,30,33	2.22	5 (19%)
55	5MC	2x	32	55	18,22,23	1.02	2 (11%)	26,32,35	1.18	3 (11%)
32	PSU	1a	516	56,32	18,21,22	1.37	2 (11%)	22,30,33	1.82	4 (18%)
1	5MU	1A	1939	1,56	19,22,23	1.48	6 (31%)	28,32,35	2.23	6 (21%)
32	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.56	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.31	2 (11%)	22,30,33	1.82	3 (13%)
54	G7M	1y	46	54	20,26,27	1.30	2 (10%)	17,39,42	0.58	0
54	G7M	1w	46	54	20,26,27	1.24	2 (10%)	17,39,42	0.59	0
54	PSU	2y	55	54	18,21,22	1.35	2 (11%)	22,30,33	1.77	4 (18%)
32	5MC	1a	1407	32	18,22,23	0.92	2 (11%)	26,32,35	1.17	4 (15%)
1	OMG	2A	2251	1,55	18,26,27	0.95	1 (5%)	19,38,41	1.09	2 (10%)
54	PSU	1y	39	54	18,21,22	1.38	2 (11%)	22,30,33	1.70	4 (18%)
32	5MC	1a	1404	32	18,22,23	1.04	2 (11%)	26,32,35	1.15	2 (7%)
54	PSU	1w	39	54	18,21,22	1.32	2 (11%)	22,30,33	1.80	3 (13%)
1	2MU	1A	2552	1,56	19,22,24	1.30	3 (15%)	26,31,36	1.75	5 (19%)
54	G7M	2w	46	54	20,26,27	1.24	1 (5%)	17,39,42	0.61	0
54	4SU	2y	8	54	18,21,22	1.77	5 (27%)	26,30,33	2.11	5 (19%)
54	PSU	1w	32	56,54	18,21,22	1.32	2 (11%)	22,30,33	1.82	3 (13%)
1	PSU	2A	1911	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
54	PSU	1w	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)

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
43	0TD	1l	92	43	-	2/7/12/14	-
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/3/25/34	0/3/3/3
32	2MG	2a	1207	32	-	1/5/27/28	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	2/11/33/34	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,56	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	1/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
54	G7M	2y	46	54	-	0/3/25/26	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	G7M	2a	527	56,32	-	2/3/25/26	0/3/3/3
43	0TD	2l	92	43	-	1/7/12/14	-
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	2/3/25/26	0/3/3/3
32	4OC	2a	1402	56,32	-	2/9/29/30	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	2/7/25/26	0/2/2/2
55	PSU	1x	55	56,55	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,56,55	-	0/5/27/28	0/3/3/3
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	1x	54	56,55	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	56,54	-	3/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	4/7/25/26	0/2/2/2
1	2MA	1A	2503	1,56	-	2/3/25/26	0/3/3/3
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	2/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32	-	3/3/25/26	0/3/3/3
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	3/7/29/34	0/3/3/3
32	5MC	2a	1400	32	-	3/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	56,32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	2/7/25/26	0/2/2/2
54	G7M	1y	46	54	-	1/3/25/26	0/3/3/3
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
54	PSU	2y	55	54	-	3/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	1,56	-	0/9/27/28	0/2/2/2
54	G7M	2w	46	54	-	3/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	56,54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	2/7/25/26	0/2/2/2

All (196) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.41	1.69	1.82
43	1l	92	0TD	CB-SB	-12.17	1.69	1.82
54	1w	37	MIA	C13-C14	7.42	1.53	1.32
54	1w	37	MIA	C2-S10	-6.99	1.69	1.75
54	2w	37	MIA	C2-S10	-6.54	1.70	1.75
55	1x	8	4SU	C4-N3	-4.71	1.32	1.37
55	2x	8	4SU	C4-N3	-4.67	1.32	1.37
32	1a	966	M2G	C2-N3	4.66	1.36	1.30
54	2y	8	4SU	C4-S4	-4.47	1.59	1.68
54	2w	8	4SU	C4-S4	-4.33	1.60	1.68
32	2a	966	M2G	C2-N3	4.33	1.36	1.30
54	1w	8	4SU	C4-S4	-4.30	1.60	1.68
55	1x	8	4SU	C4-S4	-4.27	1.60	1.68
54	2y	46	G7M	C5-C4	4.21	1.47	1.39
54	1y	8	4SU	C4-S4	-4.15	1.60	1.68
55	2x	8	4SU	C4-S4	-4.09	1.60	1.68
54	1y	46	G7M	C5-C4	4.01	1.47	1.39
54	1y	32	PSU	C6-C5	3.90	1.39	1.35
55	1x	8	4SU	C2-N3	-3.87	1.31	1.38
54	2w	55	PSU	C6-C5	3.87	1.39	1.35
54	2w	46	G7M	C5-C4	3.83	1.46	1.39
54	1w	46	G7M	C5-C4	3.81	1.46	1.39
32	2a	527	G7M	C5-C4	3.78	1.46	1.39
54	1y	39	PSU	C6-C5	3.77	1.39	1.35
54	1w	55	PSU	C6-C5	3.72	1.39	1.35
54	2w	39	PSU	C6-C5	3.69	1.39	1.35
55	2x	55	PSU	C6-C5	3.67	1.39	1.35
32	1a	527	G7M	C5-C4	3.64	1.46	1.39
54	2y	32	PSU	C6-C5	3.59	1.39	1.35
32	1a	516	PSU	C6-C5	3.54	1.39	1.35
54	2y	39	PSU	C6-C5	3.48	1.39	1.35
32	2a	516	PSU	C6-C5	3.47	1.39	1.35
54	2w	32	PSU	C6-C5	3.37	1.39	1.35
1	2A	1911	PSU	C6-C5	3.35	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	54	5MU	C2-N1	3.30	1.43	1.38
54	1y	55	PSU	C6-C5	3.25	1.39	1.35
55	1x	55	PSU	C6-C5	3.18	1.39	1.35
55	1x	8	4SU	C5-C4	-3.16	1.38	1.42
54	1w	39	PSU	C6-C5	3.15	1.39	1.35
54	2y	8	4SU	C4-N3	-3.15	1.34	1.37
54	1w	32	PSU	C6-C5	3.15	1.39	1.35
32	2a	1404	5MC	C6-C5	3.12	1.39	1.34
1	2A	1917	PSU	C6-C5	3.07	1.38	1.35
1	1A	1939	5MU	C6-C5	3.05	1.39	1.34
32	1a	1404	5MC	C6-C5	3.02	1.39	1.34
54	1w	8	4SU	C4-N3	-3.01	1.34	1.37
1	2A	1915	5MU	C6-C5	3.01	1.39	1.34
54	2y	55	PSU	C6-C5	2.99	1.38	1.35
1	1A	2251	OMG	C6-N1	-2.97	1.33	1.37
55	1x	54	5MU	C6-C5	2.93	1.39	1.34
54	1y	8	4SU	C4-N3	-2.92	1.34	1.37
55	2x	32	5MC	C6-C5	2.92	1.39	1.34
54	1y	54	5MU	C4-C5	2.91	1.49	1.44
1	1A	1942	5MC	C6-C5	2.91	1.39	1.34
1	1A	1939	5MU	C4-N3	-2.91	1.33	1.38
32	1a	1400	5MC	C6-C5	2.89	1.39	1.34
1	1A	1911	PSU	C6-C5	2.89	1.38	1.35
54	2y	54	5MU	C6-C5	2.88	1.39	1.34
1	2A	1942	5MC	C6-C5	2.87	1.39	1.34
1	1A	1915	5MU	C2-N1	2.87	1.43	1.38
54	2w	8	4SU	C4-N3	-2.83	1.34	1.37
1	1A	2552	2MU	C4-N3	-2.82	1.33	1.38
54	1y	37	MIA	C5-C4	2.82	1.48	1.40
1	2A	1939	5MU	C4-N3	-2.82	1.33	1.38
55	1x	32	5MC	C6-C5	2.81	1.39	1.34
54	2w	54	5MU	C6-C5	2.81	1.39	1.34
54	1y	54	5MU	C6-C5	2.81	1.39	1.34
1	1A	1917	PSU	C6-C5	2.79	1.38	1.35
32	2a	1407	5MC	C6-C5	2.79	1.39	1.34
55	2x	8	4SU	C5-C4	-2.79	1.39	1.42
55	2x	8	4SU	C2-N3	-2.76	1.33	1.38
1	1A	1915	5MU	C6-C5	2.76	1.39	1.34
32	1a	966	M2G	C2-N2	2.76	1.40	1.35
32	2a	1400	5MC	C6-C5	2.75	1.39	1.34
1	2A	1939	5MU	C6-C5	2.74	1.39	1.34
1	2A	1962	5MC	C6-C5	2.74	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2605	PSU	C6-C5	2.72	1.38	1.35
32	2a	967	5MC	C6-C5	2.72	1.39	1.34
54	1w	8	4SU	C5-C4	-2.72	1.39	1.42
1	1A	2605	PSU	C4-N3	-2.71	1.33	1.38
1	2A	2251	OMG	C6-N1	-2.71	1.33	1.37
54	1y	54	5MU	C4-N3	-2.68	1.33	1.38
32	1a	967	5MC	C6-C5	2.68	1.39	1.34
54	1y	37	MIA	C2-N3	2.68	1.36	1.32
54	1y	55	PSU	C4-N3	-2.68	1.33	1.38
54	2y	37	MIA	C5-C4	2.67	1.48	1.40
54	1w	54	5MU	C6-C5	2.66	1.39	1.34
54	2w	37	MIA	C5-C4	2.66	1.48	1.40
54	2y	54	5MU	C4-N3	-2.65	1.33	1.38
55	2x	54	5MU	C6-C5	2.64	1.38	1.34
1	2A	1915	5MU	C4-C5	2.63	1.49	1.44
1	1A	1962	5MC	C6-N1	-2.63	1.33	1.38
54	2y	8	4SU	C2-N1	2.62	1.42	1.38
54	2y	39	PSU	C4-N3	-2.62	1.34	1.38
1	2A	1915	5MU	C2-N1	2.62	1.42	1.38
54	2w	39	PSU	C4-N3	-2.61	1.34	1.38
54	1y	39	PSU	C4-N3	-2.61	1.34	1.38
54	1w	32	PSU	C4-N3	-2.61	1.34	1.38
54	2w	54	5MU	C4-N3	-2.60	1.34	1.38
54	2y	55	PSU	C4-N3	-2.60	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.58	1.34	1.37
1	1A	2605	PSU	C6-C5	2.58	1.38	1.35
54	1w	39	PSU	C4-N3	-2.58	1.34	1.38
1	1A	1911	PSU	C4-N3	-2.57	1.34	1.38
54	1w	37	MIA	C5-C4	2.57	1.47	1.40
54	2y	46	G7M	C6-N1	-2.57	1.34	1.37
55	2x	54	5MU	C4-N3	-2.55	1.34	1.38
55	1x	54	5MU	C4-N3	-2.54	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.51	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.51	1.34	1.38
54	1w	54	5MU	C4-N3	-2.50	1.34	1.38
1	1A	2605	PSU	C2-N1	-2.50	1.33	1.36
1	2A	2605	PSU	C4-N3	-2.50	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.49	1.34	1.38
32	2a	966	M2G	C2-N2	2.49	1.39	1.35
55	1x	54	5MU	C4-C5	2.49	1.48	1.44
1	2A	1911	PSU	C4-N3	-2.49	1.34	1.38
1	1A	1915	5MU	C4-C5	2.48	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	2MU	C5-C4	2.47	1.49	1.43
1	1A	1917	PSU	C4-N3	-2.47	1.34	1.38
54	2y	37	MIA	C2-N3	2.47	1.36	1.32
1	1A	1962	5MC	C6-C5	2.47	1.38	1.34
54	2y	8	4SU	C5-C4	-2.46	1.39	1.42
32	1a	516	PSU	C4-N3	-2.45	1.34	1.38
54	1y	54	5MU	C2-N1	2.44	1.42	1.38
55	1x	55	PSU	C4-N3	-2.44	1.34	1.38
54	1w	54	5MU	C4-C5	2.42	1.48	1.44
32	1a	1407	5MC	C6-C5	2.41	1.38	1.34
1	1A	2552	2MU	C5-C4	2.41	1.49	1.43
54	2w	32	PSU	C4-N3	-2.39	1.34	1.38
54	1w	46	G7M	C6-N1	-2.39	1.34	1.37
32	1a	1404	5MC	C6-N1	-2.38	1.34	1.38
32	2a	516	PSU	C4-N3	-2.38	1.34	1.38
54	2w	37	MIA	C6-N1	2.38	1.36	1.32
54	1w	8	4SU	C2-N1	2.37	1.42	1.38
54	2w	8	4SU	C2-N1	2.37	1.42	1.38
54	2w	55	PSU	C4-N3	-2.37	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.36	1.34	1.38
54	2y	32	PSU	C4-N3	-2.35	1.34	1.38
55	2x	55	PSU	C4-N3	-2.35	1.34	1.38
54	2y	54	5MU	C4-C5	2.34	1.48	1.44
1	1A	1939	5MU	C2-N3	-2.34	1.33	1.38
55	1x	32	5MC	C6-N1	-2.33	1.34	1.38
1	1A	1939	5MU	C6-N1	-2.33	1.34	1.38
32	1a	1498	UR3	C2-N1	2.33	1.41	1.38
1	2A	1939	5MU	C6-N1	-2.32	1.34	1.38
54	1y	54	5MU	C6-N1	-2.32	1.34	1.38
54	1w	54	5MU	C2-N1	2.32	1.42	1.38
1	2A	2503	2MA	C2-N3	2.32	1.36	1.31
1	2A	2552	2MU	C4-N3	-2.31	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.31	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.31	1.34	1.37
32	2a	527	G7M	C6-N1	-2.31	1.34	1.37
32	1a	527	G7M	C6-N1	-2.29	1.34	1.37
32	2a	1407	5MC	C6-N1	-2.29	1.34	1.38
1	1A	1939	5MU	C4-C5	2.28	1.48	1.44
54	2w	8	4SU	C5-C4	-2.28	1.39	1.42
1	2A	1962	5MC	C6-N1	-2.27	1.34	1.38
54	1w	55	PSU	C4-N3	-2.27	1.34	1.38
32	1a	967	5MC	C6-N1	-2.24	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1400	5MC	C6-N1	-2.24	1.34	1.38
32	1a	966	M2G	C6-N1	-2.23	1.34	1.37
1	1A	1939	5MU	C2-N1	2.23	1.42	1.38
54	1y	8	4SU	C5-C4	-2.19	1.39	1.42
54	1y	8	4SU	C2-N1	2.19	1.42	1.38
55	1x	54	5MU	C2-N1	2.17	1.41	1.38
1	2A	2605	PSU	C2-N3	-2.17	1.33	1.37
55	2x	54	5MU	C2-N1	2.16	1.41	1.38
54	1y	32	PSU	C4-N3	-2.14	1.34	1.38
55	2x	54	5MU	C4-C5	2.14	1.48	1.44
55	2x	8	4SU	O2-C2	2.13	1.26	1.23
1	1A	1942	5MC	C6-N1	-2.12	1.34	1.38
55	2x	54	5MU	C6-N1	-2.11	1.34	1.38
32	2a	966	M2G	C6-N1	-2.11	1.34	1.37
1	2A	1939	5MU	C2-N3	-2.10	1.34	1.38
32	2a	967	5MC	C6-N1	-2.10	1.34	1.38
55	2x	8	4SU	C2-N1	2.09	1.41	1.38
54	1y	54	5MU	C2-N3	-2.09	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.08	1.33	1.37
1	1A	1915	5MU	C6-N1	-2.08	1.34	1.38
54	1w	54	5MU	C6-N1	-2.07	1.34	1.38
32	2a	1498	UR3	C6-C5	2.07	1.39	1.35
54	2w	54	5MU	C4-C5	2.07	1.48	1.44
1	2A	1915	5MU	C6-N1	-2.06	1.34	1.38
54	2w	32	PSU	C4-C5	2.06	1.50	1.44
1	2A	1939	5MU	C4-C5	2.05	1.48	1.44
54	2w	54	5MU	C2-N3	-2.05	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.05	1.34	1.38
55	1x	54	5MU	C6-N1	-2.04	1.34	1.38
54	1y	46	G7M	C6-N1	-2.04	1.34	1.37
54	1w	37	MIA	C6-N1	2.03	1.35	1.32
54	2y	8	4SU	C2-N3	-2.03	1.34	1.38
54	2w	37	MIA	C2-N1	2.02	1.37	1.34
55	2x	32	5MC	C6-N1	-2.02	1.34	1.38
1	1A	2552	2MU	C2-N3	-2.01	1.34	1.38
32	2a	1402	4OC	C6-C5	2.00	1.39	1.35

All (269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-17.70	70.41	102.44
54	1w	37	MIA	C12-C13-C14	-7.77	112.02	127.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	8	4SU	C4-N3-C2	-6.64	120.89	127.34
54	1y	8	4SU	C4-N3-C2	-6.63	120.90	127.34
32	1a	1498	UR3	C4-N3-C2	-6.42	118.52	124.56
1	2A	1911	PSU	N1-C2-N3	6.17	122.12	115.13
54	1y	55	PSU	N1-C2-N3	6.04	121.98	115.13
54	2y	8	4SU	C4-N3-C2	-5.98	121.53	127.34
1	1A	1911	PSU	N1-C2-N3	5.96	121.89	115.13
54	2w	8	4SU	C5-C4-N3	5.96	120.22	114.69
32	2a	516	PSU	N1-C2-N3	5.93	121.85	115.13
54	1w	32	PSU	N1-C2-N3	5.87	121.78	115.13
55	2x	55	PSU	N1-C2-N3	5.82	121.72	115.13
1	1A	2605	PSU	N1-C2-N3	5.82	121.72	115.13
32	2a	1498	UR3	C4-N3-C2	-5.78	119.12	124.56
54	2w	55	PSU	N1-C2-N3	5.76	121.66	115.13
1	2A	1917	PSU	N1-C2-N3	5.72	121.62	115.13
1	2A	2605	PSU	N1-C2-N3	5.72	121.62	115.13
54	1y	54	5MU	N3-C2-N1	5.70	122.45	114.89
54	1y	54	5MU	C4-N3-C2	-5.68	120.00	127.35
54	2y	8	4SU	C5-C4-N3	5.68	119.96	114.69
54	1w	39	PSU	N1-C2-N3	5.66	121.55	115.13
32	1a	516	PSU	N1-C2-N3	5.65	121.53	115.13
1	1A	2552	2MU	N3-C2-N1	5.62	122.35	114.89
54	1w	55	PSU	N1-C2-N3	5.60	121.48	115.13
1	2A	1939	5MU	C4-N3-C2	-5.60	120.11	127.35
55	1x	55	PSU	N1-C2-N3	5.57	121.44	115.13
1	1A	1939	5MU	C4-N3-C2	-5.55	120.16	127.35
54	2y	32	PSU	N1-C2-N3	5.55	121.42	115.13
54	2y	39	PSU	N1-C2-N3	5.48	121.34	115.13
54	2w	32	PSU	N1-C2-N3	5.45	121.31	115.13
54	1y	8	4SU	C5-C4-N3	5.43	119.73	114.69
1	1A	1917	PSU	N1-C2-N3	5.38	121.22	115.13
1	2A	1915	5MU	C4-N3-C2	-5.37	120.40	127.35
54	1y	32	PSU	N1-C2-N3	5.28	121.11	115.13
54	1y	39	PSU	N1-C2-N3	5.22	121.05	115.13
1	2A	1939	5MU	N3-C2-N1	5.18	121.77	114.89
1	1A	1939	5MU	C5-C4-N3	5.11	119.67	115.31
54	2y	55	PSU	N1-C2-N3	5.11	120.92	115.13
54	2w	39	PSU	N1-C2-N3	5.10	120.91	115.13
54	1w	8	4SU	C5-C4-N3	5.08	119.40	114.69
1	1A	1939	5MU	N3-C2-N1	5.05	121.60	114.89
1	1A	1915	5MU	N3-C2-N1	5.03	121.56	114.89
1	2A	1915	5MU	C5-C4-N3	5.01	119.59	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1518	MA6	N3-C2-N1	-4.96	120.92	128.68
32	1a	1519	MA6	N3-C2-N1	-4.96	120.93	128.68
32	2a	1518	MA6	N3-C2-N1	-4.93	120.98	128.68
54	1w	54	5MU	C4-N3-C2	-4.91	120.99	127.35
55	1x	54	5MU	N3-C2-N1	4.89	121.38	114.89
1	1A	1915	5MU	C4-N3-C2	-4.87	121.05	127.35
1	2A	1915	5MU	N3-C2-N1	4.86	121.33	114.89
1	2A	2552	2MU	N3-C2-N1	4.84	121.31	114.89
1	2A	1939	5MU	C5-C4-N3	4.79	119.40	115.31
32	2a	1519	MA6	N3-C2-N1	-4.78	121.20	128.68
55	2x	54	5MU	N3-C2-N1	4.78	121.23	114.89
55	2x	54	5MU	C4-N3-C2	-4.77	121.18	127.35
1	1A	1939	5MU	C5-C6-N1	-4.70	118.51	123.34
54	1w	8	4SU	C4-N3-C2	-4.61	122.87	127.34
54	1w	54	5MU	N3-C2-N1	4.58	120.97	114.89
55	1x	54	5MU	C4-N3-C2	-4.57	121.44	127.35
1	1A	2552	2MU	C4-N3-C2	-4.49	120.66	126.58
1	2A	1939	5MU	O4-C4-C5	-4.45	119.74	124.90
54	1w	54	5MU	C5-C4-N3	4.45	119.11	115.31
1	2A	1939	5MU	C5-C6-N1	-4.35	118.86	123.34
1	1A	1911	PSU	C4-N3-C2	-4.32	120.12	126.34
54	2y	54	5MU	N3-C2-N1	4.29	120.59	114.89
54	1y	54	5MU	C5-C4-N3	4.25	118.94	115.31
1	1A	1939	5MU	O4-C4-C5	-4.25	119.98	124.90
1	2A	2605	PSU	C4-N3-C2	-4.22	120.26	126.34
1	1A	1962	5MC	C5-C6-N1	-4.16	119.06	123.34
54	1y	8	4SU	N3-C2-N1	4.16	120.41	114.89
54	2y	54	5MU	C4-N3-C2	-4.15	121.97	127.35
54	1y	54	5MU	C5-C6-N1	-4.13	119.08	123.34
55	2x	54	5MU	C5-C4-N3	4.13	118.83	115.31
54	1w	37	MIA	C2-N3-C4	4.13	121.01	115.32
1	2A	1915	5MU	O4-C4-C5	-4.09	120.16	124.90
1	1A	1915	5MU	C5-C4-N3	4.08	118.80	115.31
1	2A	2552	2MU	C4-N3-C2	-4.04	121.25	126.58
54	2w	37	MIA	C5-C6-N1	-4.04	117.45	120.81
32	1a	967	5MC	C5-C6-N1	-4.04	119.19	123.34
54	2w	37	MIA	C2-N3-C4	4.03	120.88	115.32
54	2y	54	5MU	C5-C4-N3	4.01	118.73	115.31
55	1x	32	5MC	C5-C6-N1	-3.99	119.23	123.34
1	2A	1915	5MU	C5-C6-N1	-3.98	119.25	123.34
55	2x	54	5MU	O4-C4-C5	-3.96	120.32	124.90
54	1y	55	PSU	C4-N3-C2	-3.96	120.64	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	37	MIA	C5-C6-N1	-3.92	117.55	120.81
54	2w	8	4SU	N3-C2-N1	3.92	120.09	114.89
32	2a	1404	5MC	C5-C6-N1	-3.89	119.34	123.34
54	2w	54	5MU	N3-C2-N1	3.88	120.04	114.89
32	1a	1404	5MC	C5-C6-N1	-3.88	119.35	123.34
54	1w	55	PSU	O2-C2-N1	-3.87	118.53	122.79
32	2a	516	PSU	C4-N3-C2	-3.84	120.81	126.34
54	2y	55	PSU	C4-N3-C2	-3.83	120.81	126.34
1	2A	1911	PSU	C4-N3-C2	-3.83	120.82	126.34
54	2y	8	4SU	N3-C2-N1	3.80	119.93	114.89
32	2a	1400	5MC	C5-C6-N1	-3.79	119.44	123.34
54	2w	54	5MU	C4-N3-C2	-3.78	122.45	127.35
55	2x	55	PSU	C4-N3-C2	-3.78	120.90	126.34
54	2w	54	5MU	O4-C4-C5	-3.77	120.53	124.90
54	2w	54	5MU	C5-C4-N3	3.76	118.52	115.31
54	1w	54	5MU	O4-C4-C5	-3.75	120.55	124.90
55	1x	55	PSU	C4-N3-C2	-3.74	120.94	126.34
1	1A	2605	PSU	C4-N3-C2	-3.74	120.96	126.34
32	1a	1400	5MC	C5-C6-N1	-3.73	119.50	123.34
1	2A	1917	PSU	C4-N3-C2	-3.72	120.98	126.34
32	2a	967	5MC	C5-C6-N1	-3.71	119.52	123.34
1	1A	2605	PSU	O2-C2-N1	-3.71	118.71	122.79
54	1w	37	MIA	C15-C14-C13	-3.70	111.95	122.65
54	1w	39	PSU	C4-N3-C2	-3.70	121.01	126.34
1	1A	1911	PSU	O2-C2-N1	-3.69	118.73	122.79
54	1w	37	MIA	C16-C14-C13	-3.67	112.05	122.65
54	2y	54	5MU	O4-C4-C5	-3.67	120.65	124.90
32	1a	516	PSU	C4-N3-C2	-3.66	121.07	126.34
43	2l	92	0TD	CSB-SB-CB	-3.65	95.84	102.44
54	1w	32	PSU	C4-N3-C2	-3.63	121.11	126.34
1	1A	1917	PSU	C4-N3-C2	-3.63	121.11	126.34
54	2w	8	4SU	C5-C4-S4	-3.62	119.80	124.47
55	1x	54	5MU	C5-C4-N3	3.62	118.40	115.31
55	1x	8	4SU	C5-C4-N3	3.61	118.04	114.69
54	2w	55	PSU	C4-N3-C2	-3.60	121.15	126.34
54	2y	37	MIA	N3-C2-N1	-3.58	123.09	128.68
54	1w	55	PSU	C4-N3-C2	-3.57	121.19	126.34
1	2A	1962	5MC	C5-C6-N1	-3.57	119.66	123.34
55	1x	8	4SU	O2-C2-N1	3.57	127.53	122.79
1	1A	1915	5MU	O4-C4-C5	-3.57	120.76	124.90
54	2y	39	PSU	C4-N3-C2	-3.57	121.20	126.34
54	2w	32	PSU	C4-N3-C2	-3.56	121.20	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	8	4SU	C5-C4-S4	-3.56	119.88	124.47
54	2y	32	PSU	C4-N3-C2	-3.55	121.22	126.34
43	2l	92	0TD	OD2-CG-CB	3.51	120.73	113.15
54	1w	54	5MU	C5-C6-N1	-3.50	119.74	123.34
54	2y	54	5MU	C1'-N1-C2	3.49	123.88	117.57
55	1x	8	4SU	C6-C5-C4	-3.47	116.95	119.95
55	2x	8	4SU	C5-C4-N3	3.44	117.88	114.69
54	1y	37	MIA	N3-C2-N1	-3.44	123.30	128.68
54	2w	55	PSU	O2-C2-N1	-3.44	119.01	122.79
55	2x	55	PSU	O2-C2-N1	-3.44	119.01	122.79
1	2A	1917	PSU	O2-C2-N1	-3.43	119.01	122.79
32	1a	1407	5MC	C5-C6-N1	-3.40	119.84	123.34
54	1y	39	PSU	C4-N3-C2	-3.40	121.44	126.34
55	2x	8	4SU	C1'-N1-C2	3.39	123.71	117.57
55	1x	54	5MU	O4-C4-C5	-3.35	121.01	124.90
54	1w	8	4SU	C5-C4-S4	-3.35	120.15	124.47
54	1y	55	PSU	O2-C2-N1	-3.33	119.12	122.79
32	2a	1519	MA6	C4-C5-N7	-3.32	105.94	109.40
1	1A	1942	5MC	C5-C4-N3	-3.31	118.11	121.67
1	2A	1911	PSU	O2-C2-N1	-3.30	119.15	122.79
1	2A	1942	5MC	C5-C6-N1	-3.30	119.94	123.34
54	1w	32	PSU	O2-C2-N1	-3.25	119.21	122.79
1	2A	2552	2MU	O2-C2-N1	-3.25	118.47	122.79
55	2x	32	5MC	C5-C6-N1	-3.23	120.01	123.34
54	1y	32	PSU	C4-N3-C2	-3.20	121.72	126.34
54	1y	8	4SU	C5-C4-S4	-3.20	120.35	124.47
32	1a	1519	MA6	C4-C5-N7	-3.19	106.07	109.40
1	2A	1939	5MU	O2-C2-N1	-3.18	118.56	122.79
54	2w	39	PSU	C4-N3-C2	-3.16	121.78	126.34
32	2a	516	PSU	O2-C2-N1	-3.16	119.32	122.79
54	1y	54	5MU	O4-C4-C5	-3.15	121.25	124.90
43	1l	92	0TD	OD2-CG-CB	3.14	119.94	113.15
32	2a	1407	5MC	C5-C4-N3	-3.12	118.31	121.67
1	1A	1917	PSU	O2-C2-N1	-3.11	119.36	122.79
54	1w	8	4SU	N3-C2-N1	3.10	119.00	114.89
55	1x	54	5MU	C5-C6-N1	-3.09	120.16	123.34
54	2w	37	MIA	N6-C6-N1	3.07	122.33	118.50
54	1w	8	4SU	C1'-N1-C2	3.06	123.10	117.57
32	1a	516	PSU	O2-C2-N1	-3.04	119.44	122.79
54	1w	39	PSU	O2-C2-N1	-3.02	119.46	122.79
54	1y	32	PSU	O2-C2-N1	-3.01	119.47	122.79
1	1A	2552	2MU	O2-C2-N1	-3.00	118.80	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	54	5MU	C5-C6-N1	-3.00	120.25	123.34
1	2A	2605	PSU	O2-C2-N1	-2.99	119.50	122.79
55	1x	8	4SU	C1'-N1-C2	2.97	122.94	117.57
54	1w	37	MIA	C4-C5-N7	-2.94	106.34	109.40
54	1w	37	MIA	C2-N1-C6	2.92	122.42	117.19
54	2y	54	5MU	C1'-N1-C6	-2.90	116.29	121.12
1	1A	1942	5MC	C5-C6-N1	-2.90	120.35	123.34
32	2a	1407	5MC	O2-C2-N3	-2.90	117.62	122.33
54	2w	8	4SU	C1'-N1-C2	2.88	122.79	117.57
54	2y	39	PSU	O2-C2-N1	-2.86	119.64	122.79
55	1x	55	PSU	O2-C2-N1	-2.86	119.64	122.79
32	2a	1407	5MC	C5-C6-N1	-2.83	120.43	123.34
54	2w	54	5MU	C5-C6-N1	-2.80	120.46	123.34
54	2y	55	PSU	O2-C2-N1	-2.78	119.73	122.79
54	2y	32	PSU	O2-C2-N1	-2.78	119.73	122.79
32	1a	1404	5MC	C5-C4-N3	-2.78	118.68	121.67
54	2y	54	5MU	C5-C6-N1	-2.77	120.49	123.34
55	2x	32	5MC	C5-C4-N3	-2.76	118.70	121.67
1	2A	2503	2MA	C5-C6-N1	2.73	118.74	114.02
55	1x	54	5MU	O2-C2-N1	-2.71	119.19	122.79
55	1x	32	5MC	C5-C4-N3	-2.70	118.76	121.67
54	2w	37	MIA	C2-N1-C6	2.68	121.99	117.19
54	2w	32	PSU	O2-C2-N1	-2.68	119.84	122.79
54	2y	37	MIA	C4-C5-N7	-2.66	106.63	109.40
32	1a	1402	4OC	C6-C5-C4	2.65	120.20	116.96
54	2w	37	MIA	C4-C5-N7	-2.64	106.65	109.40
54	1y	37	MIA	C4-C5-N7	-2.63	106.66	109.40
1	1A	1939	5MU	O2-C2-N1	-2.62	119.30	122.79
32	1a	1207	2MG	C8-N7-C5	2.62	107.98	102.99
54	1y	54	5MU	O2-C2-N1	-2.61	119.32	122.79
43	2l	92	0TD	OD1-CG-CB	-2.59	117.01	122.44
32	2a	1404	5MC	C5-C4-N3	-2.57	118.90	121.67
1	1A	1915	5MU	C5M-C5-C4	2.56	121.59	118.77
32	1a	1407	5MC	C5-C4-N3	-2.56	118.91	121.67
32	1a	1400	5MC	C5-C4-N3	-2.55	118.92	121.67
1	2A	1942	5MC	C5-C4-N3	-2.55	118.93	121.67
1	1A	1915	5MU	C5-C6-N1	-2.54	120.72	123.34
54	2y	54	5MU	O2-C2-N3	-2.53	116.79	121.50
55	2x	32	5MC	O2-C2-N3	-2.51	118.24	122.33
32	1a	1518	MA6	C4-C5-N7	-2.51	106.78	109.40
55	1x	8	4SU	O2-C2-N3	-2.48	116.89	121.50
32	2a	1400	5MC	O2-C2-N3	-2.47	118.31	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1518	MA6	C4-C5-N7	-2.47	106.83	109.40
32	2a	1400	5MC	C5-C4-N3	-2.46	119.02	121.67
32	2a	1207	2MG	C8-N7-C5	2.41	107.58	102.99
32	2a	966	M2G	C8-N7-C5	2.39	107.55	102.99
1	2A	2552	2MU	C5-C4-N3	2.38	118.41	114.84
1	2A	2251	OMG	C5-C6-N1	2.38	118.15	113.95
1	2A	1962	5MC	C5-C4-N3	-2.37	119.11	121.67
54	1w	37	MIA	N3-C2-N1	-2.37	122.63	126.98
32	1a	1207	2MG	CM2-N2-C2	-2.35	118.67	123.86
54	1y	54	5MU	C5M-C5-C6	-2.35	119.71	122.85
1	2A	1920	OMC	O2-C2-N3	-2.34	118.53	122.33
32	2a	966	M2G	C5-C6-N1	2.33	118.07	113.95
1	1A	1962	5MC	C5-C4-N3	-2.32	119.17	121.67
32	1a	1407	5MC	CM5-C5-C6	-2.32	119.75	122.85
1	1A	2552	2MU	C5-C4-N3	2.31	118.30	114.84
1	2A	2552	2MU	O4-C4-C5	-2.31	121.09	125.16
54	1w	37	MIA	C12-N6-C6	-2.30	119.14	122.55
54	2y	8	4SU	C1'-N1-C2	2.30	121.74	117.57
32	2a	967	5MC	C5-C4-N3	-2.30	119.19	121.67
54	2w	39	PSU	O2-C2-N1	-2.30	120.26	122.79
32	2a	1404	5MC	O2-C2-N3	-2.29	118.61	122.33
55	2x	8	4SU	C6-C5-C4	-2.28	117.97	119.95
1	2A	2503	2MA	C8-N7-C5	2.27	107.31	102.99
1	2A	2251	OMG	C8-N7-C5	2.26	107.31	102.99
1	1A	2251	OMG	C5-C6-N1	2.25	117.92	113.95
54	1y	39	PSU	O2-C2-N1	-2.21	120.36	122.79
54	2w	37	MIA	N3-C2-N1	-2.20	122.94	126.98
1	1A	2552	2MU	O4-C4-C5	-2.18	121.32	125.16
1	1A	2251	OMG	C8-N7-C5	2.18	107.15	102.99
32	1a	967	5MC	C5-C4-N3	-2.18	119.32	121.67
32	1a	1498	UR3	C3U-N3-C2	2.18	121.14	117.31
32	1a	516	PSU	O4'-C1'-C2'	2.17	108.21	105.14
54	1y	54	5MU	C5M-C5-C4	2.17	121.15	118.77
54	1y	39	PSU	C6-C5-C4	-2.17	116.68	118.20
55	2x	54	5MU	O2-C2-N1	-2.16	119.92	122.79
1	1A	1911	PSU	C5-C6-N1	-2.15	118.89	122.11
1	1A	1915	5MU	C5M-C5-C6	-2.14	119.99	122.85
54	2y	55	PSU	C6-C5-C4	-2.14	116.70	118.20
32	2a	1207	2MG	C5-C6-N1	2.14	117.72	113.95
32	2a	516	PSU	O4'-C1'-C2'	2.13	108.15	105.14
32	2a	1402	4OC	C6-C5-C4	2.12	119.56	116.96
32	1a	1407	5MC	O2-C2-N3	-2.12	118.88	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2503	2MA	C8-N7-C5	2.11	107.02	102.99
32	2a	1498	UR3	C3U-N3-C4	2.11	120.91	117.89
32	1a	966	M2G	C8-N7-C5	2.10	107.00	102.99
32	1a	1519	MA6	C1'-N9-C4	-2.10	122.94	126.64
1	2A	2605	PSU	C5-C6-N1	-2.09	118.98	122.11
32	1a	966	M2G	C5-C6-N1	2.09	117.64	113.95
1	1A	1917	PSU	C5-C6-N1	-2.04	119.05	122.11
54	2y	37	MIA	C2-N1-C6	2.03	122.23	118.75
1	1A	1915	5MU	C1'-N1-C2	2.02	121.23	117.57
54	1w	54	5MU	C5M-C5-C4	2.02	120.99	118.77
54	2w	54	5MU	O2-C2-N1	-2.02	120.10	122.79
54	1w	8	4SU	C6-N1-C2	-2.01	118.42	120.99
54	2w	37	MIA	C12-N6-C6	-2.01	121.14	122.87
54	1w	54	5MU	O2-C2-N1	-2.01	120.11	122.79
1	1A	1920	OMC	O2-C2-N3	-2.01	119.06	122.33

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	O-C-CA-CB
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
54	1y	8	4SU	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	2w	37	MIA	N1-C6-N6-C12
54	2w	37	MIA	N1-C2-S10-C11
54	2w	37	MIA	N3-C2-S10-C11
54	2y	54	5MU	C3'-C4'-C5'-O5'
54	2y	54	5MU	O4'-C4'-C5'-O5'
54	1w	46	G7M	C4'-C5'-O5'-P
32	1a	1519	MA6	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
1	2A	2503	2MA	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
54	1y	54	5MU	O4'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
32	2a	1404	5MC	O4'-C4'-C5'-O5'
32	2a	1404	5MC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
54	2y	55	PSU	O4'-C4'-C5'-O5'
54	2w	46	G7M	C4'-C5'-O5'-P
32	1a	1402	4OC	C3'-C4'-C5'-O5'
1	2A	1917	PSU	C3'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
1	2A	1915	5MU	O4'-C4'-C5'-O5'
54	2w	46	G7M	C3'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
54	1y	8	4SU	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
54	2y	54	5MU	C2'-C1'-N1-C6
32	1a	527	G7M	C4'-C5'-O5'-P
54	1y	46	G7M	C4'-C5'-O5'-P
54	1w	55	PSU	O4'-C1'-C5-C4
54	1y	55	PSU	O4'-C1'-C5-C4
32	2a	1400	5MC	O4'-C1'-N1-C6
54	2y	54	5MU	C2'-C1'-N1-C2
1	1A	1962	5MC	C2'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6
1	2A	1962	5MC	O4'-C4'-C5'-O5'
54	2w	46	G7M	O4'-C4'-C5'-O5'
54	1y	54	5MU	C3'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
54	2y	55	PSU	C3'-C4'-C5'-O5'
1	1A	1962	5MC	O4'-C1'-N1-C6
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	55	PSU	O4'-C1'-C5-C6
43	2l	92	0TD	CG-CB-SB-CSB
54	2y	55	PSU	O4'-C1'-C5-C6
32	1a	1519	MA6	C4'-C5'-O5'-P
1	1A	2503	2MA	O4'-C4'-C5'-O5'
1	2A	1962	5MC	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2807 ligands modelled in this entry, 2803 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	SF4	2d	303	35	0,12,12	-	-	-		
57	TYK	1A	4107	1	67,67,67	1.74	8 (11%)	83,97,97	1.24	9 (10%)
57	TYK	2A	3879	1	67,67,67	1.81	5 (7%)	83,97,97	1.36	10 (12%)
59	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
59	SF4	2d	303	35	-	-	0/6/5/5
57	TYK	1A	4107	1	-	2/67/126/126	0/3/4/4
57	TYK	2A	3879	1	-	4/67/126/126	0/3/4/4
59	SF4	1d	302	35	-	-	0/6/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3879	TYK	C14-C13	-8.27	1.37	1.50
57	1A	4107	TYK	C14-C13	-8.06	1.38	1.50
57	2A	3879	TYK	C8-C9	-7.90	1.37	1.51
57	1A	4107	TYK	C8-C9	-6.86	1.39	1.51
57	2A	3879	TYK	C2-C1	-4.79	1.41	1.50
57	1A	4107	TYK	C2-C1	-4.05	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3879	TYK	C11-C12	-3.39	1.38	1.45
57	1A	4107	TYK	O1C-C1C	3.25	1.45	1.40
57	1A	4107	TYK	C11-C12	-2.81	1.39	1.45
57	1A	4107	TYK	O1A-C1A	2.44	1.48	1.41
57	2A	3879	TYK	O4A-C1B	2.22	1.47	1.41
57	1A	4107	TYK	C2A-C3A	-2.12	1.50	1.53
57	1A	4107	TYK	C11-C10	2.09	1.39	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2A	3879	TYK	C23-O1C-C1C	-4.00	105.93	113.74
57	2A	3879	TYK	C10-C11-C12	-3.93	120.30	126.23
57	2A	3879	TYK	C18-C4-C3	-3.41	105.84	111.17
57	2A	3879	TYK	C3B-C2B-C1B	-3.39	108.32	114.82
57	2A	3879	TYK	C6B-C5B-C4B	-2.66	108.04	112.57
57	1A	4107	TYK	O20-C20-C19	-2.56	117.96	125.43
57	1A	4107	TYK	C3B-C2B-C1B	-2.55	109.94	114.82
57	1A	4107	TYK	O15-C15-C16	-2.53	102.89	106.92
57	1A	4107	TYK	C1A-O5A-C5A	-2.41	109.52	113.67
57	2A	3879	TYK	O20-C20-C19	-2.39	118.48	125.43
57	1A	4107	TYK	C22-C12-C11	2.37	121.81	118.08
57	1A	4107	TYK	C6-C5-C4	-2.32	108.61	114.14
57	1A	4107	TYK	C2A-C3A-N3A	-2.30	104.38	113.39
57	2A	3879	TYK	C1A-O5A-C5A	-2.26	109.78	113.67
57	1A	4107	TYK	C15-O15-C1	2.24	122.19	117.83
57	2A	3879	TYK	C8C-O3C-C3C	-2.16	108.86	114.52
57	2A	3879	TYK	O4A-C1B-O5B	2.13	116.73	109.86
57	2A	3879	TYK	C2A-C3A-N3A	-2.11	105.15	113.39
57	1A	4107	TYK	C10-C11-C12	-2.05	123.14	126.23

There are no chirality outliers.

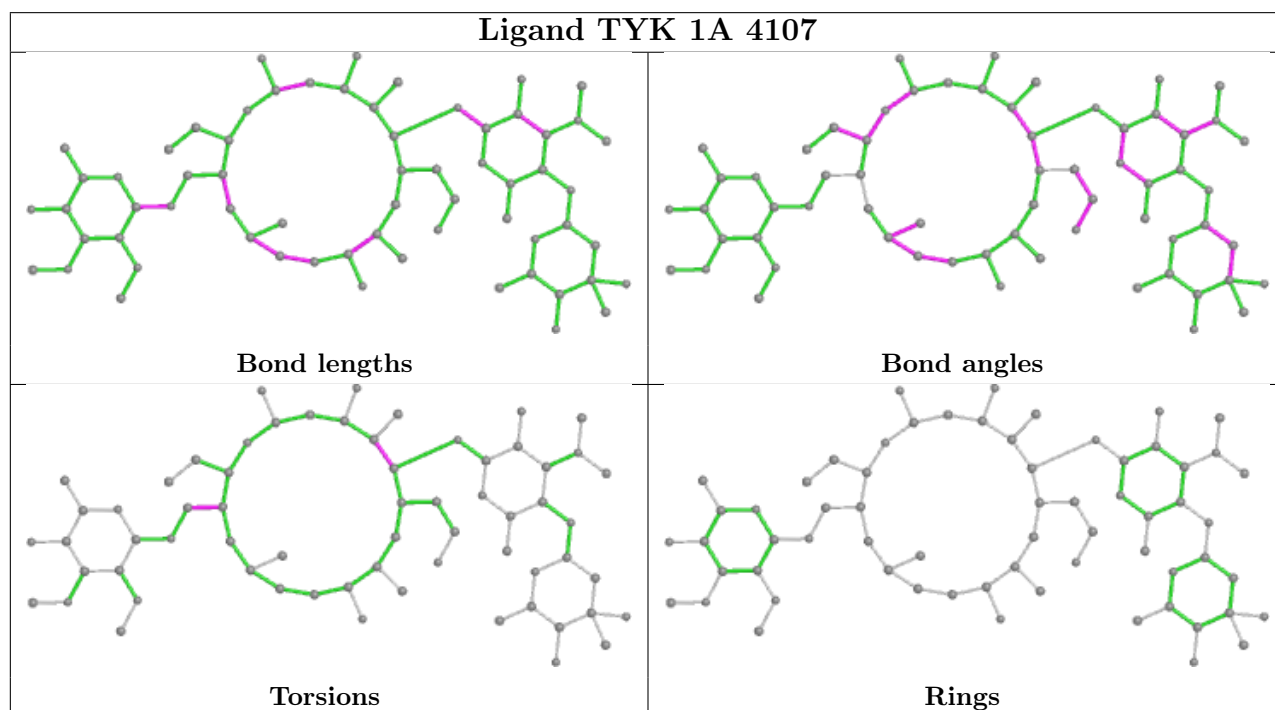
All (6) torsion outliers are listed below:

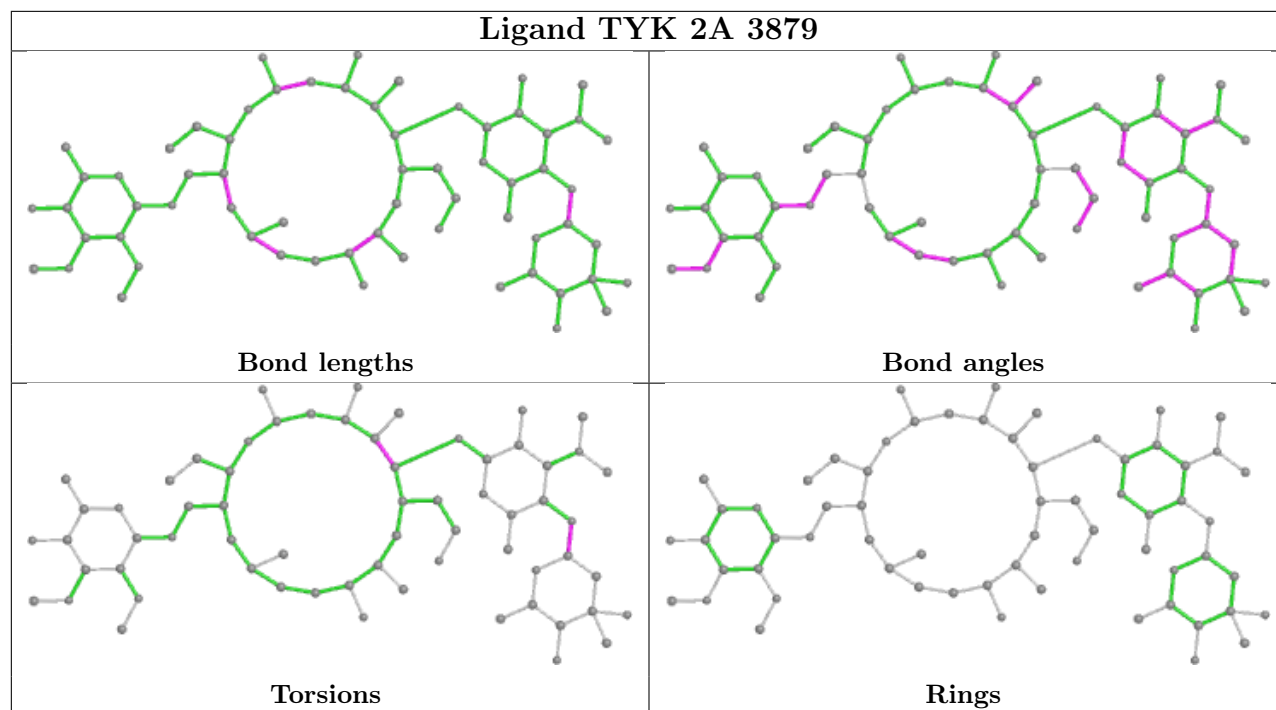
Mol	Chain	Res	Type	Atoms
57	1A	4107	TYK	C15-C14-C23-O1C
57	2A	3879	TYK	C2B-C1B-O4A-C4A
57	2A	3879	TYK	C18-C4-C5-C6
57	1A	4107	TYK	C18-C4-C5-C6
57	2A	3879	TYK	O5B-C1B-O4A-C4A
57	2A	3879	TYK	C3-C4-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.54	51 (1%) 68 70	14, 32, 85, 95	0
1	2A	2789/2915 (95%)	0.30	65 (2%) 60 62	30, 51, 84, 99	0
2	1B	120/121 (99%)	0.25	0 100 100	27, 46, 59, 76	0
2	2B	120/121 (99%)	0.19	0 100 100	55, 71, 78, 84	0
3	1D	275/276 (99%)	0.43	0 100 100	17, 32, 45, 65	0
3	2D	275/276 (99%)	0.49	3 (1%) 80 82	29, 45, 56, 75	0
4	1E	204/206 (99%)	0.48	2 (0%) 82 83	14, 34, 54, 69	0
4	2E	204/206 (99%)	0.34	1 (0%) 91 92	31, 51, 64, 72	0
5	1F	202/210 (96%)	0.49	0 100 100	15, 37, 59, 77	0
5	2F	202/210 (96%)	0.57	6 (2%) 50 51	29, 59, 70, 77	0
6	1G	181/182 (99%)	0.60	12 (6%) 18 16	39, 53, 66, 78	0
6	2G	181/182 (99%)	0.93	17 (9%) 8 6	61, 70, 75, 86	0
7	1H	174/180 (96%)	0.35	1 (0%) 89 91	35, 46, 58, 68	0
7	2H	174/180 (96%)	1.47	47 (27%) 0 0	58, 73, 81, 88	0
8	1I	146/148 (98%)	0.53	5 (3%) 45 45	38, 64, 74, 78	0
8	2I	146/148 (98%)	0.22	1 (0%) 87 89	46, 62, 71, 77	0
9	1N	140/140 (100%)	0.45	0 100 100	20, 34, 53, 65	0
9	2N	140/140 (100%)	0.45	4 (2%) 51 52	40, 57, 68, 76	0
10	1O	122/122 (100%)	0.29	0 100 100	24, 36, 50, 53	0
10	2O	122/122 (100%)	0.45	3 (2%) 57 59	42, 52, 64, 68	0
11	1P	149/150 (99%)	0.44	1 (0%) 87 89	17, 40, 62, 70	0
11	2P	149/150 (99%)	0.74	7 (4%) 31 30	37, 58, 74, 81	0
12	1Q	141/141 (100%)	0.47	1 (0%) 87 89	24, 38, 52, 68	0
12	2Q	141/141 (100%)	0.88	14 (9%) 7 5	46, 61, 70, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.42	0 100 100	18, 32, 43, 53	0
13	2R	118/118 (100%)	0.30	0 100 100	37, 47, 55, 62	0
14	1S	110/112 (98%)	0.45	0 100 100	34, 46, 55, 63	0
14	2S	110/112 (98%)	0.85	14 (12%) 3 3	55, 65, 74, 79	0
15	1T	131/146 (89%)	0.27	0 100 100	25, 39, 60, 65	0
15	2T	131/146 (89%)	0.26	1 (0%) 86 87	45, 54, 67, 74	0
16	1U	116/118 (98%)	0.50	0 100 100	18, 25, 40, 59	0
16	2U	116/118 (98%)	0.72	5 (4%) 35 33	39, 56, 67, 74	0
17	1V	101/101 (100%)	0.30	0 100 100	18, 34, 51, 65	0
17	2V	101/101 (100%)	0.69	5 (4%) 28 27	39, 62, 69, 83	0
18	1W	112/113 (99%)	0.46	1 (0%) 84 85	19, 27, 43, 69	0
18	2W	112/113 (99%)	0.48	2 (1%) 68 70	35, 43, 58, 82	0
19	1X	95/96 (98%)	0.45	0 100 100	22, 34, 55, 64	0
19	2X	95/96 (98%)	0.67	2 (2%) 63 65	42, 54, 66, 78	0
20	1Y	107/110 (97%)	0.38	0 100 100	31, 44, 58, 70	0
20	2Y	107/110 (97%)	0.89	8 (7%) 14 12	51, 62, 73, 77	0
21	1Z	154/206 (74%)	0.52	7 (4%) 33 31	32, 58, 76, 82	0
21	2Z	160/206 (77%)	1.44	44 (27%) 0 0	63, 72, 79, 86	0
22	10	83/85 (97%)	0.66	6 (7%) 15 13	26, 33, 59, 73	0
22	20	83/85 (97%)	0.90	9 (10%) 5 4	38, 59, 74, 83	0
23	11	97/98 (98%)	0.49	3 (3%) 49 49	23, 38, 62, 68	0
23	21	97/98 (98%)	0.36	2 (2%) 63 65	34, 47, 65, 67	0
24	12	70/72 (97%)	0.35	0 100 100	30, 42, 55, 59	0
24	22	70/72 (97%)	0.57	2 (2%) 51 52	50, 60, 67, 73	0
25	13	59/60 (98%)	0.37	0 100 100	19, 32, 55, 63	0
25	23	59/60 (98%)	1.02	6 (10%) 6 5	48, 59, 69, 74	0
26	14	69/71 (97%)	0.65	5 (7%) 15 13	48, 67, 77, 81	0
26	24	69/71 (97%)	1.29	18 (26%) 0 0	64, 77, 84, 87	0
27	15	59/60 (98%)	0.42	1 (1%) 70 72	17, 29, 52, 59	0
27	25	59/60 (98%)	0.30	0 100 100	33, 46, 64, 76	0
28	16	53/54 (98%)	0.42	0 100 100	29, 37, 50, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.45	1 (1%) 66 69	46, 55, 61, 62	0
29	17	48/49 (97%)	0.64	3 (6%) 20 19	17, 24, 52, 60	0
29	27	48/49 (97%)	0.79	5 (10%) 6 4	29, 36, 58, 68	0
30	18	64/65 (98%)	0.28	0 100 100	23, 29, 36, 48	0
30	28	64/65 (98%)	0.55	2 (3%) 49 49	42, 50, 55, 59	0
31	19	37/37 (100%)	0.52	0 100 100	22, 32, 52, 59	0
31	29	37/37 (100%)	1.25	6 (16%) 1 1	54, 61, 68, 72	0
32	1a	1488/1521 (97%)	0.21	28 (1%) 66 69	31, 60, 83, 97	0
32	2a	1491/1521 (98%)	0.30	45 (3%) 50 51	43, 68, 86, 96	0
33	1b	231/256 (90%)	0.51	6 (2%) 56 57	50, 69, 78, 85	0
33	2b	231/256 (90%)	1.52	65 (28%) 0 0	59, 75, 81, 84	0
34	1c	206/239 (86%)	0.67	12 (5%) 23 22	48, 66, 75, 82	0
34	2c	206/239 (86%)	1.38	49 (23%) 0 0	65, 74, 80, 84	0
35	1d	208/209 (99%)	0.75	15 (7%) 15 13	45, 63, 72, 80	0
35	2d	208/209 (99%)	0.70	6 (2%) 51 52	50, 61, 70, 75	0
36	1e	148/162 (91%)	0.49	3 (2%) 65 67	42, 57, 66, 71	0
36	2e	148/162 (91%)	0.94	18 (12%) 4 3	57, 68, 74, 80	0
37	1f	100/101 (99%)	0.34	1 (1%) 82 83	51, 60, 67, 73	0
37	2f	100/101 (99%)	0.31	0 100 100	51, 62, 69, 75	0
38	1g	155/156 (99%)	0.60	10 (6%) 18 17	52, 62, 73, 82	0
38	2g	155/156 (99%)	0.71	18 (11%) 4 3	61, 70, 78, 85	0
39	1h	137/138 (99%)	0.47	4 (2%) 51 52	47, 58, 64, 71	0
39	2h	137/138 (99%)	1.06	19 (13%) 2 2	60, 67, 74, 78	0
40	1i	127/128 (99%)	0.98	16 (12%) 3 3	50, 67, 75, 78	0
40	2i	127/128 (99%)	1.59	43 (33%) 0 0	63, 74, 79, 82	0
41	1j	97/105 (92%)	0.65	6 (6%) 20 19	53, 70, 79, 86	0
41	2j	96/105 (91%)	1.40	25 (26%) 0 0	67, 76, 83, 85	0
42	1k	114/129 (88%)	0.58	2 (1%) 68 70	38, 57, 67, 71	0
42	2k	114/129 (88%)	0.44	2 (1%) 68 70	50, 65, 71, 74	0
43	1l	121/132 (91%)	0.20	1 (0%) 86 87	36, 49, 58, 65	0
43	2l	121/132 (91%)	0.89	16 (13%) 3 2	49, 63, 70, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.47	5 (4%) 37 36	47, 62, 69, 73	0
44	2m	122/126 (96%)	0.87	21 (17%) 1 1	64, 73, 77, 81	0
45	1n	60/61 (98%)	0.83	2 (3%) 46 46	53, 61, 67, 71	0
45	2n	60/61 (98%)	2.07	29 (48%) 0 0	70, 76, 82, 85	0
46	1o	88/89 (98%)	0.48	4 (4%) 33 31	42, 57, 70, 77	0
46	2o	88/89 (98%)	0.58	3 (3%) 45 45	53, 64, 73, 76	0
47	1p	82/88 (93%)	0.68	2 (2%) 59 60	47, 62, 70, 77	0
47	2p	82/88 (93%)	0.53	1 (1%) 79 80	50, 59, 67, 72	0
48	1q	99/105 (94%)	0.30	3 (3%) 50 51	45, 58, 69, 72	0
48	2q	99/105 (94%)	0.91	10 (10%) 7 5	51, 64, 71, 75	0
49	1r	68/88 (77%)	0.59	3 (4%) 34 33	46, 58, 67, 69	0
49	2r	68/88 (77%)	0.41	1 (1%) 73 76	51, 63, 71, 75	0
50	1s	83/93 (89%)	0.36	1 (1%) 79 80	49, 64, 73, 79	0
50	2s	83/93 (89%)	1.70	32 (38%) 0 0	70, 77, 81, 86	0
51	1t	96/106 (90%)	0.43	5 (5%) 27 25	51, 63, 69, 72	0
51	2t	96/106 (90%)	0.89	7 (7%) 15 13	51, 62, 72, 80	0
52	1u	23/27 (85%)	0.72	1 (4%) 35 33	57, 59, 64, 67	0
52	2u	23/27 (85%)	1.22	4 (17%) 1 1	64, 71, 75, 78	0
53	1v	13/24 (54%)	0.96	3 (23%) 0 0	42, 55, 75, 87	0
53	2v	13/24 (54%)	1.47	4 (30%) 0 0	63, 74, 87, 91	0
54	1w	67/76 (88%)	0.97	11 (16%) 1 1	55, 79, 89, 95	0
54	1y	67/76 (88%)	1.20	15 (22%) 0 0	33, 83, 90, 93	0
54	2w	65/76 (85%)	2.18	30 (46%) 0 0	74, 85, 92, 97	0
54	2y	66/76 (86%)	1.44	18 (27%) 0 0	49, 87, 92, 95	0
55	1x	72/77 (93%)	0.23	0 100 100	26, 55, 74, 83	0
55	2x	72/77 (93%)	0.35	1 (1%) 75 77	44, 71, 80, 89	0
All	All	20873/21748 (95%)	0.54	1025 (4%) 29 28	14, 57, 80, 99	0

All (1025) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	2Z	141	VAL	9.8
54	2w	76	A	8.7

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Mol	Chain	Res	Type	RSRZ
32	2a	1030(B)	C	7.1
21	2Z	139	VAL	6.5
34	2c	157	ILE	6.3
26	24	59	PHE	6.2
44	1m	2	ALA	6.0
41	2j	72	VAL	5.9
26	24	49	PHE	5.8
1	1A	2131	G	5.8
45	2n	39	LEU	5.7
1	2A	888	C	5.7
32	2a	1033	G	5.7
54	1w	71	G	5.6
21	2Z	144	LEU	5.6
1	2A	2133	G	5.6
7	2H	52	VAL	5.5
33	2b	48	MET	5.5
54	1y	20	U	5.5
22	20	5	LYS	5.4
1	2A	2793	G	5.4
54	2y	36	A	5.4
54	2w	71	G	5.3
21	2Z	149	SER	5.3
7	2H	44	VAL	5.3
1	2A	2155	G	5.2
39	2h	128	GLY	5.2
50	2s	79	THR	5.1
1	2A	2154	G	5.1
45	2n	25	VAL	5.1
33	2b	34	ALA	5.1
54	1y	35	A	5.1
21	2Z	106	GLY	5.1
34	2c	198	VAL	5.1
21	2Z	153	SER	5.1
1	2A	2802	G	5.1
33	2b	220	ASP	5.1
54	1w	76	A	5.1
41	2j	85	LEU	5.1
54	2w	4	C	5.0
40	2i	7	THR	5.0
32	1a	1030(C)	G	5.0
34	2c	53	ALA	4.9
7	2H	159	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
50	2s	50	ALA	4.9
33	2b	207	ALA	4.9
48	2q	9	VAL	4.8
40	2i	76	ALA	4.8
33	2b	118	LEU	4.8
54	2w	75	C	4.8
6	1G	139	LEU	4.8
1	2A	229	A	4.7
21	2Z	155	LEU	4.7
22	20	3	HIS	4.7
54	2w	72	C	4.7
18	2W	112	GLY	4.7
50	2s	40	ILE	4.7
45	2n	37	PHE	4.7
33	2b	228	GLY	4.7
33	2b	165	VAL	4.6
34	2c	87	LEU	4.6
36	2e	10	MET	4.6
33	2b	101	MET	4.5
33	2b	187	LEU	4.5
6	1G	146	TYR	4.5
26	24	63	TYR	4.5
7	2H	35	VAL	4.5
32	1a	1001(A)	G	4.5
34	1c	39	ILE	4.5
22	10	3	HIS	4.4
33	2b	81	VAL	4.4
1	2A	887	A	4.4
54	2w	31	A	4.4
32	1a	1030(B)	C	4.4
7	2H	113	VAL	4.4
7	2H	2	SER	4.3
54	1w	20	U	4.3
1	1A	2159	G	4.3
54	2w	70	G	4.3
38	1g	80	VAL	4.3
19	2X	92	LEU	4.3
33	2b	200	ILE	4.3
26	24	51	ASP	4.3
50	2s	14	HIS	4.3
7	2H	19	VAL	4.2
33	2b	92	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
45	2n	38	GLY	4.2
1	2A	885	C	4.2
1	2A	2139	C	4.2
40	2i	27	THR	4.2
7	2H	72	ILE	4.1
34	2c	86	VAL	4.1
53	2v	24	A	4.1
29	27	47	ARG	4.1
43	2l	39	VAL	4.1
38	1g	153	HIS	4.1
6	2G	49	ASP	4.1
33	2b	201	ILE	4.1
40	2i	109	VAL	4.1
1	1A	2140	C	4.1
32	2a	1030(A)	G	4.1
54	1w	75	C	4.0
20	2Y	65	ALA	4.0
34	2c	124	ILE	4.0
41	2j	47	PHE	4.0
1	2A	884	C	4.0
40	2i	103	THR	4.0
40	1i	8	GLY	4.0
33	1b	233	SER	4.0
34	2c	145	GLY	3.9
45	2n	34	TYR	3.9
32	1a	1028	C	3.9
54	2w	28	G	3.9
41	2j	32	ALA	3.9
1	2A	2128	C	3.9
1	2A	2804	C	3.9
27	15	60	VAL	3.9
34	2c	182	ILE	3.9
33	2b	218	ALA	3.9
33	2b	51	LEU	3.9
1	2A	2153	G	3.9
54	1w	70	G	3.9
26	14	17	GLY	3.9
38	2g	84	ASN	3.9
20	2Y	5	MET	3.9
12	2Q	109	VAL	3.9
51	2t	59	ALA	3.9
33	2b	227	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
22	20	4	LYS	3.8
33	2b	71	VAL	3.8
54	2y	34	G	3.8
33	2b	211	ILE	3.8
3	2D	2	ALA	3.8
21	2Z	157	LEU	3.8
54	2w	3	C	3.8
11	2P	92	GLU	3.8
50	2s	80	TYR	3.8
33	2b	164	VAL	3.8
33	2b	152	PHE	3.7
22	20	7	LEU	3.7
1	1A	884	C	3.7
54	2y	56	C	3.7
7	2H	102	ALA	3.7
40	2i	17	VAL	3.7
32	1a	1030(A)	G	3.7
44	2m	123	ALA	3.7
43	2l	55	VAL	3.7
21	2Z	140	ASP	3.7
22	20	45	PHE	3.7
1	2A	886	C	3.7
1	2A	2145	C	3.7
34	1c	193	TYR	3.7
45	2n	13	THR	3.7
54	1y	47	U	3.7
1	2A	2132	U	3.7
41	2j	10	GLY	3.7
32	2a	1030(C)	G	3.7
36	2e	12	LEU	3.6
1	2A	2146	C	3.6
7	2H	105	LEU	3.6
40	1i	15	ALA	3.6
40	2i	72	GLY	3.6
45	2n	8	GLU	3.6
40	2i	86	VAL	3.6
45	2n	14	PRO	3.6
7	2H	47	GLU	3.6
1	1A	896	A	3.6
34	1c	87	LEU	3.6
45	2n	56	VAL	3.6
50	2s	45	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
54	2w	45	U	3.6
1	1A	271(K)	U	3.5
1	1A	1077	A	3.5
1	1A	897	C	3.5
1	2A	2113	U	3.5
6	2G	39	ILE	3.5
1	2A	2792	G	3.5
40	2i	54	ASP	3.5
12	2Q	6	ARG	3.5
26	14	50	VAL	3.5
44	2m	70	LEU	3.5
45	2n	36	PHE	3.5
1	1A	1059	G	3.5
32	2a	1030(D)	A	3.5
54	1y	36	A	3.5
31	29	37	GLY	3.5
34	2c	138	VAL	3.5
1	2A	2127	G	3.5
54	1w	44	G	3.5
32	1a	1257	U	3.5
33	2b	70	PHE	3.5
26	24	66	SER	3.5
35	1d	180	GLY	3.5
11	1P	105	LEU	3.5
14	2S	58	LEU	3.5
33	2b	55	PHE	3.5
21	1Z	1	MET	3.5
40	2i	49	PRO	3.5
50	2s	12	ASP	3.5
1	2A	883	G	3.4
1	1A	2129	C	3.4
1	2A	2140	C	3.4
21	2Z	50	GLN	3.4
17	2V	72	VAL	3.4
23	11	2	SER	3.4
33	2b	127	ILE	3.4
43	2l	28	LYS	3.4
54	1w	73	A	3.4
12	2Q	33	GLY	3.4
34	2c	64	VAL	3.4
34	2c	205	GLY	3.4
46	2o	60	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
6	2G	140	ILE	3.4
50	2s	52	TYR	3.4
32	2a	1034	G	3.3
33	2b	68	ILE	3.3
1	1A	2132	U	3.3
49	1r	73	ALA	3.3
6	2G	146	TYR	3.3
45	2n	51	GLY	3.3
54	1w	74	C	3.3
54	2w	74	C	3.3
7	2H	7	LEU	3.3
7	2H	82	GLY	3.3
39	2h	104	ARG	3.3
1	1A	887	A	3.3
20	2Y	55	TYR	3.3
35	1d	38	TYR	3.3
32	1a	1029	C	3.3
34	2c	51	GLY	3.3
35	2d	164	ALA	3.3
26	14	18	CYS	3.3
54	1y	59	U	3.3
43	2l	64	TYR	3.3
54	2y	29	G	3.3
44	2m	124	PRO	3.3
35	1d	167	GLY	3.3
44	2m	87	TYR	3.2
50	2s	63	THR	3.2
40	2i	6	GLY	3.2
53	2v	12	A	3.2
38	2g	4	ARG	3.2
39	2h	112	LEU	3.2
23	2l	2	SER	3.2
1	2A	2896	C	3.2
21	1Z	160	GLY	3.2
32	1a	1030	C	3.2
32	2a	1030	C	3.2
35	2d	23	GLY	3.2
40	2i	62	TYR	3.2
6	2G	136	ARG	3.2
7	2H	51	ARG	3.2
33	2b	44	LEU	3.2
40	1i	80	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
41	1j	10	GLY	3.2
50	2s	30	LEU	3.2
1	2A	896	A	3.2
7	2H	128	PRO	3.2
1	2A	2805	G	3.2
38	2g	80	VAL	3.2
40	1i	33	PHE	3.2
7	2H	20	ALA	3.2
33	2b	203	GLY	3.2
36	2e	109	ILE	3.2
34	2c	33	LEU	3.2
1	1A	1509	C	3.2
21	2Z	170	THR	3.1
1	1A	889	C	3.1
45	2n	12	ARG	3.1
38	1g	156	TRP	3.1
33	2b	112	VAL	3.1
1	1A	885	C	3.1
21	2Z	152	ALA	3.1
26	24	50	VAL	3.1
33	2b	17	PHE	3.1
33	2b	66	GLY	3.1
34	2c	139	GLN	3.1
6	2G	142	PRO	3.1
45	2n	58	LYS	3.1
34	2c	6	HIS	3.1
39	1h	53	VAL	3.1
1	1A	2793	G	3.1
1	2A	2156	G	3.1
1	2A	2157	G	3.1
22	10	2	ALA	3.1
25	23	26	LEU	3.1
33	2b	214	ILE	3.1
21	2Z	69	THR	3.1
44	2m	60	VAL	3.1
5	2F	115	ALA	3.1
22	20	2	ALA	3.1
34	2c	65	ALA	3.1
32	2a	1257	U	3.1
1	2A	2138	C	3.1
11	2P	91	PHE	3.1
7	2H	95	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
7	2H	101	ARG	3.1
44	2m	68	GLY	3.1
38	2g	156	TRP	3.1
50	2s	41	VAL	3.1
1	1A	886	C	3.1
12	2Q	114	ALA	3.1
14	2S	32	LEU	3.1
33	2b	215	LEU	3.1
44	1m	124	PRO	3.1
1	2A	2116	G	3.0
32	1a	1002	G	3.0
34	2c	39	ILE	3.0
40	2i	63	ILE	3.0
32	2a	1014	A	3.0
54	2w	73	A	3.0
50	2s	36	ARG	3.0
1	2A	6	A	3.0
6	2G	29	TRP	3.0
32	2a	1150	U	3.0
50	2s	35	SER	3.0
35	1d	101	LEU	3.0
1	1A	2792	G	3.0
54	1y	24	G	3.0
1	2A	1509	C	3.0
35	1d	168	ARG	3.0
21	2Z	148	ASP	3.0
45	2n	53	LEU	3.0
50	2s	71	LEU	3.0
53	1v	12	A	3.0
1	1A	271(N)	U	3.0
21	2Z	46	LYS	3.0
38	2g	154	TYR	3.0
1	2A	2125	G	3.0
54	2w	5	G	3.0
34	2c	180	ALA	3.0
42	1k	60	ALA	3.0
41	1j	36	GLY	3.0
54	2y	45	U	3.0
40	1i	4	TYR	3.0
45	2n	11	LYS	3.0
1	1A	2162	G	3.0
32	1a	1023	G	3.0

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Mol	Chain	Res	Type	RSRZ
40	2i	90	PRO	3.0
39	2h	134	ILE	3.0
50	2s	62	ILE	3.0
1	2A	2801(A)	A	3.0
3	2D	38	LYS	3.0
26	24	42	PHE	3.0
50	2s	13	ASP	3.0
21	2Z	5	LEU	3.0
32	2a	1001(A)	G	2.9
48	2q	80	GLY	2.9
36	2e	146	ALA	2.9
38	2g	5	ARG	2.9
40	2i	114	TYR	2.9
54	2y	65	G	2.9
7	2H	76	VAL	2.9
29	17	48	LYS	2.9
39	2h	45	ILE	2.9
1	1A	888	C	2.9
1	2A	1041	C	2.9
44	1m	26	GLY	2.9
6	2G	152	LEU	2.9
14	2S	36	TYR	2.9
25	23	15	TYR	2.9
41	2j	48	THR	2.9
32	1a	1036	G	2.9
41	1j	18	ALA	2.9
54	2y	5	G	2.9
40	1i	81	ILE	2.9
40	2i	9	ARG	2.9
1	1A	1097	U	2.9
22	10	7	LEU	2.9
43	2l	69	TYR	2.9
14	2S	55	ALA	2.9
44	2m	92	HIS	2.9
54	2w	44	G	2.9
34	2c	188	LEU	2.9
35	1d	179	GLU	2.9
21	2Z	21	ALA	2.9
32	1a	204	U	2.9
32	1a	1532	U	2.9
54	1y	13	C	2.9
32	1a	1032	G	2.9

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Mol	Chain	Res	Type	RSRZ
54	2w	15	G	2.9
38	2g	7	ALA	2.9
1	1A	2897	U	2.9
55	2x	47	U	2.9
39	2h	136	GLU	2.9
7	2H	106	THR	2.9
7	2H	115	VAL	2.9
32	1a	1031	G	2.9
32	2a	1024	G	2.9
35	2d	168	ARG	2.9
50	2s	11	VAL	2.9
6	1G	26	GLN	2.8
32	1a	1001	A	2.8
53	2v	23	A	2.8
39	2h	35	ILE	2.8
12	2Q	2	LEU	2.8
33	2b	94	ASN	2.8
33	2b	183	PRO	2.8
41	2j	55	LYS	2.8
44	2m	6	GLY	2.8
1	2A	2160	G	2.8
1	1A	1175	U	2.8
32	2a	1286	A	2.8
12	2Q	65	PHE	2.8
7	2H	71	LEU	2.8
44	2m	99	ARG	2.8
21	2Z	156	LYS	2.8
36	2e	34	VAL	2.8
38	2g	2	ALA	2.8
40	2i	36	TYR	2.8
14	2S	29	PHE	2.8
45	2n	44	LEU	2.8
3	2D	276	LYS	2.8
20	2Y	45	VAL	2.8
44	1m	123	ALA	2.8
44	2m	15	VAL	2.8
48	2q	12	SER	2.8
7	2H	46	GLU	2.8
33	2b	11	LEU	2.8
40	2i	115	GLY	2.8
48	2q	23	VAL	2.8
38	2g	32	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
7	2H	98	LEU	2.8
7	2H	148	ILE	2.8
23	11	98	LEU	2.8
21	1Z	165	VAL	2.8
34	2c	60	ALA	2.8
32	2a	1036	G	2.8
41	2j	13	HIS	2.8
39	2h	65	TYR	2.8
40	2i	80	GLY	2.8
14	2S	20	ARG	2.8
33	1b	137	ARG	2.8
21	2Z	145	GLU	2.8
34	2c	170	GLN	2.8
34	1c	101	LEU	2.8
44	1m	48	LEU	2.8
54	1y	19	G	2.8
54	2y	35	A	2.8
45	2n	43	CYS	2.8
33	2b	105	PHE	2.7
38	2g	16	LEU	2.7
34	2c	8	ILE	2.7
38	2g	82	GLY	2.7
50	2s	82	GLY	2.7
1	1A	1095	A	2.7
7	2H	45	VAL	2.7
35	1d	170	VAL	2.7
7	2H	6	ARG	2.7
1	1A	2146	C	2.7
32	2a	1287	A	2.7
32	1a	1034	G	2.7
32	2a	1003	G	2.7
21	2Z	99	TYR	2.7
40	2i	33	PHE	2.7
35	2d	146	ILE	2.7
40	1i	14	VAL	2.7
1	1A	1076	C	2.7
33	2b	14	GLY	2.7
6	1G	80	PHE	2.7
1	2A	2897	U	2.7
26	24	32	TYR	2.7
16	2U	17	ILE	2.7
21	2Z	137	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
40	2i	106	ALA	2.7
43	2l	68	ALA	2.7
20	2Y	42	VAL	2.7
36	2e	33	VAL	2.7
26	24	40	HIS	2.7
38	2g	85	TYR	2.7
39	1h	35	ILE	2.7
1	2A	2112	G	2.7
32	2a	1026	G	2.7
7	2H	43	VAL	2.7
43	1l	43	VAL	2.7
17	2V	39	LEU	2.7
40	2i	102	LEU	2.7
21	2Z	154	ASP	2.7
34	2c	140	ARG	2.7
38	2g	24	THR	2.7
41	2j	81	THR	2.7
21	1Z	159	PRO	2.7
32	2a	1220	G	2.7
35	1d	165	MET	2.7
8	1I	41	GLU	2.7
33	1b	232	PRO	2.6
7	2H	107	VAL	2.6
54	2w	6	G	2.6
38	1g	79	ARG	2.6
41	1j	46	ARG	2.6
33	2b	58	ILE	2.6
41	2j	6	ILE	2.6
26	24	52	THR	2.6
1	1A	2896	C	2.6
1	1A	229	A	2.6
32	1a	1003	G	2.6
33	2b	199	TYR	2.6
34	2c	57	ILE	2.6
54	2w	29	G	2.6
21	2Z	4	ARG	2.6
32	2a	1001	A	2.6
33	2b	222	ILE	2.6
40	2i	81	ILE	2.6
22	10	4	LYS	2.6
44	2m	90	LEU	2.6
49	2r	85	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
32	2a	1532	U	2.6
1	1A	2145	C	2.6
1	1A	2803	C	2.6
33	2b	210	SER	2.6
21	2Z	57	ILE	2.6
32	2a	1035	A	2.6
38	1g	84	ASN	2.6
53	1v	13	A	2.6
43	2l	37	CYS	2.6
40	2i	99	LEU	2.6
54	2y	19	G	2.6
17	2V	42	GLY	2.6
22	20	76	GLY	2.6
1	2A	2174	C	2.6
7	2H	21	PRO	2.6
33	2b	162	ILE	2.6
34	2c	202	ILE	2.6
38	2g	27	ILE	2.6
40	2i	77	ILE	2.6
34	2c	201	TYR	2.6
32	1a	1030(D)	A	2.6
42	1k	98	LEU	2.6
1	1A	2133	G	2.6
32	1a	1024	G	2.6
32	2a	1156	G	2.6
36	2e	150	ARG	2.6
54	2y	57	G	2.6
14	2S	5	THR	2.6
33	2b	37	ASN	2.6
33	2b	113	HIS	2.6
48	2q	10	VAL	2.6
6	2G	3	LEU	2.6
48	1q	98	LEU	2.6
40	2i	37	PHE	2.6
33	2b	216	SER	2.6
17	2V	70	ILE	2.5
21	2Z	8	TYR	2.5
7	2H	103	LEU	2.5
21	2Z	125	LEU	2.5
21	2Z	161	VAL	2.5
40	2i	28	VAL	2.5
50	2s	9	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
32	2a	1354	C	2.5
34	1c	78	GLY	2.5
7	2H	123	PHE	2.5
12	2Q	28	ALA	2.5
41	2j	67	THR	2.5
50	2s	31	ILE	2.5
54	2w	47	U	2.5
12	2Q	32	TYR	2.5
21	1Z	141	VAL	2.5
33	1b	221	LEU	2.5
34	1c	32	LEU	2.5
50	2s	67	VAL	2.5
44	2m	88	ARG	2.5
36	1e	10	MET	2.5
54	1y	53	G	2.5
6	1G	116	ASP	2.5
21	2Z	93	ASP	2.5
21	2Z	133	ILE	2.5
51	2t	55	ILE	2.5
11	2P	118	GLY	2.5
14	2S	92	TYR	2.5
40	1i	19	LEU	2.5
40	1i	50	LEU	2.5
33	2b	212	GLN	2.5
45	2n	16	PHE	2.5
34	1c	124	ILE	2.5
22	10	6	GLY	2.5
35	1d	16	GLY	2.5
36	2e	115	VAL	2.5
1	2A	2310	A	2.5
50	2s	53	ASN	2.5
34	1c	180	ALA	2.5
43	2l	41	ARG	2.5
1	2A	889	C	2.5
1	2A	2803	C	2.5
30	28	41	ILE	2.5
38	1g	81	GLY	2.5
48	2q	59	ILE	2.5
33	2b	69	LEU	2.5
41	2j	65	LEU	2.5
21	2Z	143	GLY	2.5
41	2j	74	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
43	2l	93	LEU	2.5
1	1A	2141	G	2.5
33	2b	122	PHE	2.5
40	2i	18	PHE	2.5
51	1t	69	GLY	2.5
1	1A	2158	A	2.5
6	2G	157	ILE	2.5
52	2u	13	ILE	2.5
34	2c	4	LYS	2.5
42	2k	25	TYR	2.5
40	2i	93	ARG	2.5
54	1y	57	G	2.5
54	2y	53	G	2.5
34	1c	80	GLY	2.4
39	2h	124	ALA	2.4
23	11	97	LEU	2.4
50	2s	49	ILE	2.4
14	2S	14	VAL	2.4
29	27	46	VAL	2.4
40	1i	65	VAL	2.4
34	2c	131	ARG	2.4
49	1r	42	ARG	2.4
40	2i	4	TYR	2.4
36	2e	90	VAL	2.4
1	2A	2126	A	2.4
34	1c	168	ALA	2.4
45	2n	30	ALA	2.4
50	2s	57	HIS	2.4
34	2c	52	LEU	2.4
34	2c	196	LEU	2.4
6	1G	159	VAL	2.4
7	2H	49	VAL	2.4
26	24	57	GLU	2.4
34	2c	143	GLU	2.4
33	2b	163	PHE	2.4
35	1d	110	PHE	2.4
7	2H	157	TYR	2.4
8	1I	89	TYR	2.4
51	1t	47	GLY	2.4
47	1p	1	MET	2.4
41	2j	39	PRO	2.4
5	2F	24	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
6	1G	73	ALA	2.4
1	1A	2794	C	2.4
1	2A	645	C	2.4
14	2S	35	ILE	2.4
41	2j	96	ILE	2.4
54	2w	68	C	2.4
1	1A	2168	G	2.4
54	2y	44	G	2.4
5	2F	21	ALA	2.4
34	2c	71	ALA	2.4
40	2i	94	ALA	2.4
31	29	12	ASP	2.4
1	1A	1066	U	2.4
1	2A	2161	C	2.4
12	2Q	86	GLY	2.4
21	2Z	136	PHE	2.4
45	2n	61	TRP	2.4
51	2t	47	GLY	2.4
12	1Q	59	ARG	2.4
14	2S	34	HIS	2.4
4	1E	195	LEU	2.4
21	2Z	150	LEU	2.4
39	2h	36	LEU	2.4
46	1o	57	LEU	2.4
54	1w	1	G	2.4
34	2c	49	SER	2.4
14	2S	40	ILE	2.4
26	24	19	GLY	2.4
21	2Z	100	VAL	2.4
21	2Z	2	GLU	2.4
33	2b	116	GLU	2.4
36	2e	60	TYR	2.4
12	2Q	113	GLN	2.4
36	2e	138	ALA	2.4
40	2i	105	ASP	2.4
26	24	45	GLY	2.4
40	2i	8	GLY	2.4
45	2n	42	ILE	2.4
43	2l	32	PHE	2.4
1	1A	1060	U	2.3
32	2a	1007	C	2.3
32	2a	1092	A	2.3

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Mol	Chain	Res	Type	RSRZ
32	2a	1250	A	2.3
50	2s	42	PRO	2.3
22	10	5	LYS	2.3
35	1d	80	GLU	2.3
36	2e	8	GLU	2.3
44	2m	78	ILE	2.3
45	2n	35	ARG	2.3
21	2Z	96	VAL	2.3
39	1h	93	VAL	2.3
1	2A	2807	G	2.3
16	2U	2	PRO	2.3
32	2a	1219	U	2.3
33	2b	232	PRO	2.3
52	2u	23	PRO	2.3
11	2P	140	ALA	2.3
17	2V	101	GLY	2.3
32	2a	1149	C	2.3
38	1g	152	ALA	2.3
43	2l	95	GLY	2.3
33	2b	111	ARG	2.3
33	2b	41	ILE	2.3
36	1e	89	ILE	2.3
41	2j	63	PHE	2.3
41	2j	94	VAL	2.3
50	2s	51	VAL	2.3
29	27	48	LYS	2.3
33	2b	8	LYS	2.3
1	2A	2144	U	2.3
6	2G	76	SER	2.3
11	2P	79	ARG	2.3
21	2Z	142	SER	2.3
31	29	19	ARG	2.3
34	2c	190	ARG	2.3
46	1o	34	LEU	2.3
9	2N	8	GLN	2.3
34	2c	136	GLN	2.3
6	2G	65	GLY	2.3
34	2c	194	GLY	2.3
48	2q	18	THR	2.3
32	2a	204	U	2.3
1	2A	652(U)	G	2.3
1	2A	2162	G	2.3

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Mol	Chain	Res	Type	RSRZ
31	29	15	LYS	2.3
32	2a	485	G	2.3
29	17	46	VAL	2.3
44	2m	7	VAL	2.3
1	1A	1057	A	2.3
1	2A	652(B)	A	2.3
39	2h	122	ARG	2.3
48	2q	92	ARG	2.3
33	2b	100	GLY	2.3
33	2b	131	PRO	2.3
50	2s	69	HIS	2.3
33	2b	161	ALA	2.3
7	2H	121	ILE	2.3
10	2O	114	ILE	2.3
12	2Q	104	PHE	2.3
33	1b	211	ILE	2.3
1	1A	2805	G	2.3
1	2A	2115	G	2.3
6	1G	136	ARG	2.3
48	2q	91	ARG	2.3
45	2n	4	LYS	2.3
25	23	23	LEU	2.3
39	2h	133	LEU	2.3
54	1y	38	A	2.3
8	1I	94	ALA	2.3
16	2U	21	ALA	2.3
40	2i	110	GLU	2.3
36	2e	129	ILE	2.3
39	2h	86	ILE	2.3
48	1q	36	ILE	2.3
39	2h	137	VAL	2.3
41	2j	24	VAL	2.3
1	1A	2148	G	2.3
7	2H	29	PRO	2.3
34	2c	178	LEU	2.3
54	1y	34	G	2.3
54	2w	65	G	2.3
7	2H	145	ALA	2.3
26	14	32	TYR	2.3
45	2n	24	CYS	2.3
46	1o	88	ARG	2.3
41	2j	22	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
21	2Z	58	VAL	2.3
1	2A	2167	U	2.2
9	2N	105	GLY	2.2
32	1a	841	U	2.2
34	2c	159	GLY	2.2
52	1u	16	GLY	2.2
33	2b	224	GLN	2.2
11	2P	45	LEU	2.2
47	1p	41	PRO	2.2
20	2Y	1	MET	2.2
51	1t	13	LEU	2.2
1	2A	2149	G	2.2
32	2a	1027	C	2.2
40	2i	104	ARG	2.2
1	1A	1096	A	2.2
26	24	64	GLY	2.2
34	1c	41	GLY	2.2
29	27	1	MET	2.2
34	2c	179	ARG	2.2
45	2n	29	ARG	2.2
37	1f	83	ASP	2.2
34	2c	134	ILE	2.2
35	2d	183	GLY	2.2
54	2w	13	C	2.2
32	2a	79	G	2.2
32	2a	1032	G	2.2
54	2w	10	G	2.2
54	2w	30	G	2.2
21	1Z	169	GLU	2.2
7	1H	2	SER	2.2
16	2U	44	ASN	2.2
43	2l	62	SER	2.2
22	20	37	LEU	2.2
34	2c	109	PRO	2.2
40	1i	98	PRO	2.2
7	2H	3	ARG	2.2
6	2G	61	ALA	2.2
50	2s	75	ALA	2.2
21	2Z	9	TYR	2.2
4	1E	87	GLU	2.2
12	2Q	106	VAL	2.2
28	26	52	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
31	29	13	LYS	2.2
1	1A	1064	C	2.2
1	1A	2161	C	2.2
1	2A	652(V)	C	2.2
32	1a	1027	C	2.2
39	2h	135	CYS	2.2
54	1y	44	G	2.2
54	2w	52	G	2.2
1	2A	2173	A	2.2
22	20	33	ALA	2.2
6	2G	165	THR	2.2
32	2a	1357	A	2.2
54	2y	66	U	2.2
45	2n	55	GLY	2.2
50	2s	61	TYR	2.2
33	2b	223	ILE	2.2
40	1i	26	VAL	2.2
34	2c	63	ASN	2.2
38	1g	78	ARG	2.2
16	2U	18	LEU	2.2
18	2W	14	PRO	2.2
34	2c	91	LEU	2.2
1	1A	1058	G	2.2
7	2H	142	GLY	2.2
40	1i	59	PHE	2.2
40	2i	5	TYR	2.2
53	1v	14	A	2.2
7	2H	169	VAL	2.2
36	2e	64	ARG	2.2
38	2g	42	ILE	2.2
44	2m	91	ARG	2.2
45	1n	12	ARG	2.2
7	2H	8	PRO	2.2
40	1i	99	LEU	2.2
50	1s	71	LEU	2.2
38	2g	13	GLN	2.2
25	23	27	GLY	2.2
35	2d	69	GLY	2.2
36	2e	120	THR	2.2
54	1w	72	C	2.2
32	1a	1025	U	2.2
39	2h	37	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
45	2n	31	ARG	2.2
1	2A	100	G	2.2
32	2a	1031	G	2.2
10	2O	102	VAL	2.2
54	1y	23	A	2.2
26	24	30	GLU	2.2
40	2i	75	ASP	2.2
41	1j	93	GLY	2.2
46	2o	59	MET	2.2
54	1w	45	U	2.1
7	2H	32	GLU	2.1
10	2O	58	VAL	2.1
24	22	12	GLU	2.1
26	24	56	VAL	2.1
32	2a	1021	G	2.1
43	2l	80	HIS	2.1
54	2w	69	G	2.1
32	1a	1531	A	2.1
34	1c	81	GLY	2.1
35	1d	69	GLY	2.1
24	22	1	MET	2.1
25	23	29	ARG	2.1
34	2c	189	ALA	2.1
38	2g	147	ALA	2.1
20	2Y	89	PHE	2.1
32	2a	1039	C	2.1
7	2H	144	VAL	2.1
20	2Y	75	ILE	2.1
44	2m	84	ILE	2.1
4	2E	52	LEU	2.1
5	2F	170	LEU	2.1
25	23	28	LEU	2.1
41	1j	71	LEU	2.1
41	2j	91	PRO	2.1
45	1n	55	GLY	2.1
48	1q	28	PRO	2.1
7	2H	132	ARG	2.1
1	2A	614(B)	G	2.1
1	2A	2141	G	2.1
54	2y	28	G	2.1
21	2Z	65	GLN	2.1
38	1g	154	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
6	1G	94	LEU	2.1
1	1A	1082	U	2.1
1	2A	2143	C	2.1
7	2H	78	GLY	2.1
36	1e	119	LEU	2.1
38	1g	82	GLY	2.1
40	2i	128	ARG	2.1
33	2b	186	ALA	2.1
51	2t	44	ALA	2.1
47	2p	48	TRP	2.1
40	2i	124	GLN	2.1
1	2A	2169	A	2.1
6	2G	160	VAL	2.1
8	1I	136	VAL	2.1
14	2S	23	ARG	2.1
19	2X	95	LEU	2.1
23	2I	62	VAL	2.1
26	14	55	ARG	2.1
29	27	23	ARG	2.1
34	2c	48	TYR	2.1
40	1i	79	LEU	2.1
41	2j	66	ARG	2.1
41	2j	79	ARG	2.1
41	2j	90	LEU	2.1
44	2m	96	LEU	2.1
51	2t	36	LEU	2.1
51	2t	57	ARG	2.1
21	2Z	172	ALA	2.1
32	2a	1045	C	2.1
36	2e	94	ALA	2.1
40	1i	46	ALA	2.1
51	1t	76	ALA	2.1
41	2j	87	THR	2.1
40	2i	126	SER	2.1
50	2s	70	LYS	2.1
1	1A	2151	G	2.1
26	24	67	TYR	2.1
35	1d	158	ILE	2.1
36	2e	80	ILE	2.1
45	2n	7	ILE	2.1
49	1r	79	LEU	2.1
32	1a	1033	G	2.1

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Mol	Chain	Res	Type	RSRZ
32	1a	1447	A	2.1
32	2a	1002	G	2.1
32	2a	1447	A	2.1
54	2y	52	G	2.1
1	2A	2895	U	2.1
35	1d	147	ALA	2.1
1	1A	2188	C	2.1
43	2l	59	ARG	2.1
11	2P	93	GLY	2.1
15	2T	71	GLY	2.1
33	2b	12	GLU	2.1
21	2Z	54	HIS	2.1
34	2c	66	VAL	2.1
42	2k	109	VAL	2.1
45	2n	49	HIS	2.1
46	2o	81	LEU	2.1
35	1d	138	TYR	2.1
1	1A	1176	G	2.1
1	2A	2165	G	2.1
32	2a	1224	G	2.1
38	2g	40	ALA	2.1
53	2v	14	A	2.1
52	2u	8	THR	2.1
54	1y	60	U	2.1
54	2w	12	U	2.1
54	2w	50	U	2.1
54	2y	59	U	2.1
1	1A	1092	C	2.1
8	1I	106	GLY	2.1
6	1G	43	LEU	2.1
7	2H	50	VAL	2.1
46	1o	66	LEU	2.1
33	2b	42	ILE	2.1
51	1t	55	ILE	2.1
44	2m	102	ARG	2.1
8	2I	1	MET	2.1
32	2a	80	G	2.0
40	2i	67	GLY	2.1
54	2w	23	A	2.1
1	1A	2804	C	2.0
5	2F	114	VAL	2.0
18	1W	111	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
12	2Q	47	ILE	2.0
33	1b	125	PRO	2.0
33	2b	32	ILE	2.0
36	2e	13	ILE	2.0
29	17	47	ARG	2.0
44	2m	80	ARG	2.0
9	2N	45	ASN	2.0
33	2b	35	GLU	2.0
48	2q	33	GLY	2.0
5	2F	172	TRP	2.0
1	2A	1026	U	2.0
1	2A	2131	G	2.0
32	1a	1026	G	2.0
44	2m	9	ILE	2.0
6	1G	25	TYR	2.0
32	1a	91	C	2.0
32	2a	1028	C	2.0
50	2s	37	ARG	2.0
33	2b	31	TYR	2.0
39	1h	58	TYR	2.0
39	2h	58	TYR	2.0
54	2w	2	C	2.0
39	2h	28	ALA	2.0
21	2Z	92	SER	2.0
26	24	28	LYS	2.0
33	2b	54	THR	2.0
43	2l	29	GLY	2.0
50	2s	68	GLY	2.0
41	2j	84	GLN	2.0
51	2t	72	LEU	2.0
34	2c	5	ILE	2.0
34	2c	206	GLU	2.0
44	2m	71	ARG	2.0
54	2y	47	U	2.0
7	2H	9	ILE	2.0
31	29	17	ILE	2.0
40	2i	74	ILE	2.0
32	2a	1111	A	2.0
54	2y	23	A	2.0
1	2A	652(T)	C	2.0
12	2Q	121	ALA	2.0
9	2N	76	SER	2.0

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Mol	Chain	Res	Type	RSRZ
21	2Z	16	SER	2.0
32	2a	1112	C	2.0
34	2c	96	GLY	2.0
43	2l	63	GLY	2.0
54	2w	48	C	2.0
52	2u	17	THR	2.0
6	1G	35	GLU	2.0
6	2G	153	ARG	2.0
14	2S	54	LEU	2.0
40	2i	19	LEU	2.0
21	2Z	121	HIS	2.0
30	28	7	HIS	2.0
6	2G	87	PRO	2.0
21	1Z	101	PRO	2.0
39	2h	61	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	4SU	2w	8	20/21	0.73	0.31	83,90,102,110	0
54	5MU	1y	54	21/22	0.76	0.27	75,79,90,97	0
54	G7M	2y	46	24/25	0.77	0.22	77,86,90,100	0
54	PSU	2w	55	20/21	0.78	0.26	74,85,94,95	0
54	PSU	2y	55	20/21	0.78	0.31	83,90,100,105	0
54	5MU	2y	54	21/22	0.79	0.32	82,87,95,111	0
54	G7M	1w	46	24/25	0.80	0.20	69,79,94,113	0
54	G7M	2w	46	24/25	0.80	0.31	80,90,96,109	0
54	4SU	1y	8	20/21	0.81	0.21	79,86,92,95	0
54	PSU	2y	32	20/21	0.81	0.25	61,76,85,89	0
54	PSU	1y	55	20/21	0.81	0.34	79,86,93,101	0
54	PSU	1y	32	20/21	0.81	0.23	67,75,82,83	0
54	G7M	1y	46	24/25	0.81	0.24	77,87,100,106	0
54	MIA	2y	37	22/30	0.83	0.29	69,78,85,91	0
54	PSU	2y	39	20/21	0.84	0.33	72,75,93,95	0
32	2MG	2a	1207	24/25	0.86	0.20	70,78,84,88	0
54	MIA	1y	37	22/30	0.86	0.29	70,76,80,89	0
54	PSU	1w	55	20/21	0.88	0.22	62,73,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	5MU	2w	54	21/22	0.88	0.22	68,77,83,89	0
54	MIA	2w	37	25/30	0.88	0.22	60,73,79,85	0
43	0TD	2l	92	10/11	0.89	0.17	56,61,65,71	0
54	PSU	2w	32	20/21	0.89	0.33	68,80,86,87	0
55	5MU	2x	54	21/22	0.90	0.27	67,75,80,83	0
54	4SU	2y	8	20/21	0.90	0.17	79,87,100,106	0
54	PSU	1y	39	20/21	0.91	0.22	68,74,83,84	0
54	PSU	1w	32	20/21	0.91	0.19	60,66,72,75	0
32	M2G	2a	966	25/26	0.91	0.22	61,67,77,80	0
32	5MC	2a	967	21/22	0.91	0.17	61,66,74,79	0
32	PSU	2a	516	20/21	0.92	0.16	62,73,80,82	0
55	PSU	1x	55	20/21	0.92	0.21	55,61,66,68	0
55	4SU	2x	8	20/21	0.92	0.15	74,78,83,87	0
54	PSU	2w	39	20/21	0.92	0.29	67,76,80,81	0
55	PSU	2x	55	20/21	0.92	0.22	68,74,78,81	0
1	5MU	2A	1915	21/22	0.92	0.16	62,69,73,75	0
1	PSU	2A	1911	20/21	0.93	0.16	56,59,63,64	0
55	4SU	1x	8	20/21	0.93	0.18	54,60,65,66	0
55	5MC	2x	32	21/22	0.93	0.17	64,70,72,79	0
32	5MC	2a	1404	21/22	0.93	0.20	45,51,54,57	0
54	4SU	1w	8	20/21	0.93	0.20	71,76,84,85	0
43	0TD	1l	92	10/11	0.93	0.20	46,50,51,59	0
1	5MU	1A	1915	21/22	0.94	0.17	36,48,59,64	0
54	MIA	1w	37	29/30	0.94	0.20	48,56,62,68	0
32	2MG	1a	1207	24/25	0.94	0.17	59,62,66,70	0
1	PSU	2A	1917	20/21	0.94	0.14	56,63,69,70	0
32	4OC	2a	1402	22/23	0.94	0.18	48,59,62,71	0
32	G7M	2a	527	24/25	0.95	0.15	56,61,66,71	0
32	5MC	1a	967	21/22	0.95	0.19	45,49,55,56	0
54	5MU	1w	54	21/22	0.95	0.16	60,67,71,74	0
32	M2G	1a	966	25/26	0.95	0.20	43,48,58,60	0
32	5MC	2a	1400	21/22	0.95	0.23	57,65,70,74	0
1	OMC	2A	1920	21/22	0.95	0.20	49,58,62,67	0
1	2MU	2A	2552	21/23	0.95	0.19	31,40,44,50	0
32	5MC	2a	1407	21/22	0.95	0.20	42,52,56,57	0
54	PSU	1w	39	20/21	0.95	0.18	37,57,64,66	0
32	UR3	2a	1498	21/22	0.96	0.21	41,55,58,63	0
32	MA6	2a	1518	24/25	0.96	0.19	51,59,64,66	0
32	MA6	2a	1519	24/25	0.96	0.22	44,59,64,67	0
55	5MU	1x	54	21/22	0.96	0.15	59,62,66,72	0
1	PSU	1A	1911	20/21	0.96	0.19	33,44,52,54	0
1	PSU	1A	1917	20/21	0.96	0.18	38,46,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	5MC	2A	1942	21/22	0.96	0.16	48,53,57,58	0
1	5MC	2A	1962	21/22	0.96	0.19	33,45,51,56	0
32	PSU	1a	516	20/21	0.96	0.15	50,55,59,60	0
1	PSU	2A	2605	20/21	0.96	0.21	28,37,43,53	0
32	G7M	1a	527	24/25	0.96	0.17	42,46,50,54	0
1	5MC	1A	1942	21/22	0.97	0.23	32,40,46,48	0
55	5MC	1x	32	21/22	0.97	0.20	46,48,53,62	0
32	5MC	1a	1400	21/22	0.97	0.18	40,44,46,50	0
32	5MC	1a	1404	21/22	0.97	0.18	32,33,38,41	0
32	MA6	1a	1519	24/25	0.97	0.20	30,37,40,54	0
32	UR3	1a	1498	21/22	0.98	0.23	30,37,41,44	0
32	MA6	1a	1518	24/25	0.98	0.22	27,37,42,42	0
1	5MU	1A	1939	21/22	0.98	0.20	20,28,30,33	0
1	OMC	1A	1920	21/22	0.98	0.20	31,39,46,47	0
1	5MU	2A	1939	21/22	0.98	0.19	33,36,40,42	0
1	5MC	1A	1962	21/22	0.98	0.19	25,30,35,41	0
1	OMG	1A	2251	24/25	0.98	0.22	17,19,22,29	0
1	OMG	2A	2251	24/25	0.98	0.20	35,40,44,45	0
1	2MA	2A	2503	23/24	0.98	0.18	25,31,35,36	0
1	2MA	1A	2503	23/24	0.98	0.23	13,17,19,23	0
1	2MU	1A	2552	21/23	0.98	0.23	19,22,28,30	0
32	4OC	1a	1402	22/23	0.98	0.20	33,39,41,45	0
1	PSU	1A	2605	20/21	0.98	0.22	17,20,31,34	0
32	5MC	1a	1407	21/22	0.98	0.20	31,38,41,42	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(\AA^2)	Q<0.9
56	MG	2A	3403	1/1	0.53	0.23	59,59,59,59	0
56	MG	2A	3463	1/1	0.53	0.27	65,65,65,65	0
56	MG	1a	1634	1/1	0.54	0.21	65,65,65,65	0
56	MG	1A	4029	1/1	0.55	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	ZN	24	501	1/1	0.55	0.19	134,134,134,134	0
56	MG	2w	107	1/1	0.56	0.17	74,74,74,74	0
56	MG	2A	3661	1/1	0.56	0.21	68,68,68,68	0
56	MG	1A	3365	1/1	0.57	0.29	50,50,50,50	0
56	MG	2A	3635	1/1	0.58	0.14	76,76,76,76	0
56	MG	2A	3090	1/1	0.59	0.18	60,60,60,60	0
56	MG	2A	3268	1/1	0.59	0.19	77,77,77,77	0
56	MG	2A	3783	1/1	0.60	0.07	53,53,53,53	0
56	MG	1A	3571	1/1	0.62	0.20	49,49,49,49	0
56	MG	1A	3413	1/1	0.62	0.23	64,64,64,64	0
56	MG	2A	3192	1/1	0.63	0.19	53,53,53,53	0
56	MG	1A	4100	1/1	0.64	0.16	76,76,76,76	0
56	MG	2a	3001	1/1	0.64	0.21	60,60,60,60	0
56	MG	1a	1645	1/1	0.65	0.18	55,55,55,55	0
56	MG	1A	4060	1/1	0.66	0.17	31,31,31,31	0
56	MG	2A	3294	1/1	0.66	0.16	50,50,50,50	0
56	MG	1A	3931	1/1	0.67	0.16	53,53,53,53	0
56	MG	2a	3020	1/1	0.67	0.14	71,71,71,71	0
56	MG	1A	3511	1/1	0.67	0.23	62,62,62,62	0
56	MG	1w	102	1/1	0.67	0.27	68,68,68,68	0
56	MG	1A	3833	1/1	0.68	0.12	58,58,58,58	0
56	MG	1B	212	1/1	0.68	0.20	62,62,62,62	0
56	MG	2a	3226	1/1	0.69	0.16	62,62,62,62	0
56	MG	2A	3306	1/1	0.69	0.14	71,71,71,71	0
56	MG	1A	3386	1/1	0.69	0.24	51,51,51,51	0
56	MG	1a	1680	1/1	0.70	0.17	59,59,59,59	0
56	MG	1A	3080	1/1	0.70	0.25	49,49,49,49	0
56	MG	2a	3124	1/1	0.70	0.17	49,49,49,49	0
56	MG	1Y	202	1/1	0.71	0.17	58,58,58,58	0
56	MG	2A	3744	1/1	0.71	0.10	55,55,55,55	0
56	MG	1a	1715	1/1	0.71	0.19	45,45,45,45	0
56	MG	2A	3871	1/1	0.71	0.10	52,52,52,52	0
56	MG	1A	3875	1/1	0.71	0.11	68,68,68,68	0
56	MG	2A	3357	1/1	0.71	0.17	65,65,65,65	0
56	MG	2a	3060	1/1	0.71	0.17	70,70,70,70	0
56	MG	2A	3070	1/1	0.71	0.15	46,46,46,46	0
56	MG	1a	1635	1/1	0.71	0.15	66,66,66,66	0
56	MG	2A	3475	1/1	0.71	0.14	51,51,51,51	0
56	MG	1A	3470	1/1	0.71	0.18	62,62,62,62	0
56	MG	1A	4007	1/1	0.72	0.27	57,57,57,57	0
56	MG	2a	3008	1/1	0.72	0.23	57,57,57,57	0
56	MG	1A	3695	1/1	0.72	0.16	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3968	1/1	0.72	0.12	58,58,58,58	0
56	MG	1A	3232	1/1	0.73	0.27	53,53,53,53	0
56	MG	1A	4045	1/1	0.73	0.13	69,69,69,69	0
56	MG	2a	3146	1/1	0.73	0.12	65,65,65,65	0
56	MG	1A	3529	1/1	0.74	0.29	44,44,44,44	0
56	MG	2A	3435	1/1	0.74	0.22	56,56,56,56	0
56	MG	1a	1693	1/1	0.74	0.14	60,60,60,60	0
56	MG	1A	3834	1/1	0.74	0.10	43,43,43,43	0
56	MG	1a	1777	1/1	0.74	0.15	64,64,64,64	0
56	MG	1a	1641	1/1	0.74	0.12	64,64,64,64	0
56	MG	2a	3140	1/1	0.74	0.11	56,56,56,56	0
56	MG	2A	3669	1/1	0.74	0.16	79,79,79,79	0
56	MG	2A	3685	1/1	0.74	0.11	58,58,58,58	0
56	MG	2A	3335	1/1	0.74	0.19	43,43,43,43	0
56	MG	1a	1623	1/1	0.74	0.17	50,50,50,50	0
56	MG	2A	3821	1/1	0.75	0.11	58,58,58,58	0
56	MG	1A	3426	1/1	0.75	0.15	55,55,55,55	0
56	MG	1A	3590	1/1	0.75	0.23	53,53,53,53	0
56	MG	1w	104	1/1	0.75	0.19	70,70,70,70	0
56	MG	1A	3383	1/1	0.75	0.21	47,47,47,47	0
56	MG	1A	3831	1/1	0.75	0.14	41,41,41,41	0
56	MG	2a	3076	1/1	0.75	0.28	56,56,56,56	0
56	MG	1A	3509	1/1	0.75	0.16	46,46,46,46	0
56	MG	2A	3221	1/1	0.75	0.15	55,55,55,55	0
56	MG	1A	3351	1/1	0.75	0.22	39,39,39,39	0
56	MG	1A	3350	1/1	0.75	0.20	45,45,45,45	0
56	MG	1a	1713	1/1	0.75	0.11	74,74,74,74	0
56	MG	1A	3569	1/1	0.75	0.17	57,57,57,57	0
56	MG	2A	3816	1/1	0.76	0.10	48,48,48,48	0
56	MG	2a	3065	1/1	0.76	0.16	55,55,55,55	0
56	MG	1A	3367	1/1	0.76	0.18	54,54,54,54	0
56	MG	1A	3368	1/1	0.76	0.23	58,58,58,58	0
56	MG	2B	214	1/1	0.76	0.13	73,73,73,73	0
56	MG	2A	3164	1/1	0.76	0.18	43,43,43,43	0
56	MG	1A	3573	1/1	0.76	0.25	33,33,33,33	0
56	MG	2A	3787	1/1	0.76	0.12	64,64,64,64	0
56	MG	2a	3058	1/1	0.76	0.15	56,56,56,56	0
56	MG	1A	3880	1/1	0.77	0.19	45,45,45,45	0
56	MG	2A	3867	1/1	0.77	0.23	33,33,33,33	0
56	MG	1A	4086	1/1	0.77	0.10	43,43,43,43	0
56	MG	1A	4096	1/1	0.77	0.20	46,46,46,46	0
56	MG	1a	1661	1/1	0.77	0.15	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	3715	1/1	0.77	0.14	40,40,40,40	0
56	MG	2A	3569	1/1	0.77	0.13	31,31,31,31	0
56	MG	2A	3630	1/1	0.77	0.14	47,47,47,47	0
56	MG	1A	3120	1/1	0.77	0.24	55,55,55,55	0
56	MG	2A	3200	1/1	0.77	0.20	63,63,63,63	0
56	MG	1A	3187	1/1	0.77	0.18	53,53,53,53	0
56	MG	2A	3265	1/1	0.77	0.16	43,43,43,43	0
56	MG	2A	3700	1/1	0.77	0.14	65,65,65,65	0
56	MG	1A	3564	1/1	0.77	0.23	40,40,40,40	0
56	MG	1A	3203	1/1	0.77	0.34	59,59,59,59	0
56	MG	2t	201	1/1	0.77	0.14	47,47,47,47	0
56	MG	1a	1810	1/1	0.77	0.13	66,66,66,66	0
56	MG	2y	106	1/1	0.77	0.24	81,81,81,81	0
56	MG	1d	301	1/1	0.77	0.31	58,58,58,58	0
56	MG	1A	3624	1/1	0.78	0.23	54,54,54,54	0
56	MG	2A	3346	1/1	0.78	0.24	54,54,54,54	0
56	MG	2a	3021	1/1	0.78	0.17	58,58,58,58	0
56	MG	2A	3348	1/1	0.78	0.14	61,61,61,61	0
56	MG	1A	3409	1/1	0.78	0.27	35,35,35,35	0
56	MG	2A	3212	1/1	0.78	0.15	60,60,60,60	0
56	MG	2A	3409	1/1	0.78	0.21	66,66,66,66	0
56	MG	2A	3064	1/1	0.78	0.20	58,58,58,58	0
56	MG	1B	233	1/1	0.78	0.26	63,63,63,63	0
56	MG	1A	3980	1/1	0.78	0.11	59,59,59,59	0
56	MG	2a	3167	1/1	0.78	0.17	75,75,75,75	0
56	MG	2a	3188	1/1	0.78	0.08	65,65,65,65	0
56	MG	2A	3132	1/1	0.78	0.15	71,71,71,71	0
56	MG	1a	1710	1/1	0.78	0.29	61,61,61,61	0
56	MG	2A	3333	1/1	0.78	0.21	62,62,62,62	0
56	MG	2F	304	1/1	0.78	0.20	49,49,49,49	0
56	MG	2A	3650	1/1	0.78	0.13	53,53,53,53	0
56	MG	1A	3265	1/1	0.79	0.15	31,31,31,31	0
56	MG	1a	1779	1/1	0.79	0.20	65,65,65,65	0
56	MG	1A	3585	1/1	0.79	0.19	50,50,50,50	0
56	MG	2A	3246	1/1	0.79	0.18	56,56,56,56	0
56	MG	1a	1822	1/1	0.79	0.12	59,59,59,59	0
56	MG	2a	3027	1/1	0.79	0.34	61,61,61,61	0
56	MG	2a	3049	1/1	0.79	0.12	63,63,63,63	0
56	MG	1A	3166	1/1	0.79	0.24	59,59,59,59	0
56	MG	1A	3225	1/1	0.79	0.23	32,32,32,32	0
56	MG	2a	3061	1/1	0.79	0.12	59,59,59,59	0
56	MG	1A	3912	1/1	0.79	0.16	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3465	1/1	0.79	0.21	56,56,56,56	0
56	MG	2a	3099	1/1	0.79	0.23	58,58,58,58	0
56	MG	1A	3192	1/1	0.79	0.18	35,35,35,35	0
56	MG	2a	3130	1/1	0.79	0.19	60,60,60,60	0
56	MG	2a	3135	1/1	0.79	0.25	67,67,67,67	0
56	MG	2A	3345	1/1	0.79	0.12	64,64,64,64	0
56	MG	2A	3773	1/1	0.79	0.33	60,60,60,60	0
56	MG	1a	1696	1/1	0.79	0.27	61,61,61,61	0
56	MG	1A	3737	1/1	0.79	0.22	32,32,32,32	0
56	MG	2A	3351	1/1	0.79	0.12	49,49,49,49	0
56	MG	1A	4004	1/1	0.79	0.18	74,74,74,74	0
56	MG	2A	3178	1/1	0.79	0.13	48,48,48,48	0
56	MG	2x	101	1/1	0.79	0.17	66,66,66,66	0
56	MG	2A	3179	1/1	0.79	0.14	59,59,59,59	0
56	MG	1A	3479	1/1	0.79	0.19	48,48,48,48	0
56	MG	1A	3877	1/1	0.80	0.12	48,48,48,48	0
56	MG	2A	3209	1/1	0.80	0.33	62,62,62,62	0
56	MG	2A	3458	1/1	0.80	0.19	64,64,64,64	0
56	MG	1a	1824	1/1	0.80	0.17	54,54,54,54	0
56	MG	2A	3219	1/1	0.80	0.16	57,57,57,57	0
56	MG	2A	3494	1/1	0.80	0.19	50,50,50,50	0
56	MG	1a	1691	1/1	0.80	0.12	55,55,55,55	0
56	MG	2a	3050	1/1	0.80	0.19	56,56,56,56	0
56	MG	2A	3242	1/1	0.80	0.14	43,43,43,43	0
56	MG	1F	302	1/1	0.80	0.25	33,33,33,33	0
56	MG	2A	3645	1/1	0.80	0.14	43,43,43,43	0
56	MG	1A	3489	1/1	0.80	0.30	51,51,51,51	0
56	MG	2A	3018	1/1	0.80	0.13	53,53,53,53	0
56	MG	2a	3094	1/1	0.80	0.11	61,61,61,61	0
56	MG	2a	3096	1/1	0.80	0.19	61,61,61,61	0
56	MG	2A	3275	1/1	0.80	0.14	58,58,58,58	0
56	MG	1a	1707	1/1	0.80	0.19	50,50,50,50	0
56	MG	1A	3185	1/1	0.80	0.18	45,45,45,45	0
56	MG	1A	3610	1/1	0.80	0.27	34,34,34,34	0
56	MG	2A	3334	1/1	0.80	0.14	53,53,53,53	0
56	MG	2A	3104	1/1	0.80	0.17	54,54,54,54	0
56	MG	1A	3622	1/1	0.80	0.24	53,53,53,53	0
56	MG	2A	3807	1/1	0.80	0.23	70,70,70,70	0
56	MG	1a	1720	1/1	0.80	0.18	50,50,50,50	0
56	MG	2a	3227	1/1	0.80	0.11	66,66,66,66	0
56	MG	1A	3979	1/1	0.80	0.15	64,64,64,64	0
56	MG	2A	3831	1/1	0.80	0.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3359	1/1	0.80	0.28	50,50,50,50	0
56	MG	2A	3185	1/1	0.80	0.19	50,50,50,50	0
56	MG	1A	3448	1/1	0.80	0.22	39,39,39,39	0
60	K	2A	3473	1/1	0.80	0.25	75,75,75,75	0
56	MG	1A	3306	1/1	0.81	0.27	32,32,32,32	0
56	MG	2F	307	1/1	0.81	0.29	52,52,52,52	0
56	MG	25	102	1/1	0.81	0.21	45,45,45,45	0
56	MG	2A	3461	1/1	0.81	0.10	75,75,75,75	0
56	MG	2a	3005	1/1	0.81	0.15	54,54,54,54	0
56	MG	1A	3613	1/1	0.81	0.37	56,56,56,56	0
56	MG	1A	3550	1/1	0.81	0.14	64,64,64,64	0
56	MG	2A	3492	1/1	0.81	0.37	57,57,57,57	0
56	MG	1y	103	1/1	0.81	0.20	66,66,66,66	0
56	MG	2A	3496	1/1	0.81	0.18	61,61,61,61	0
56	MG	2A	3500	1/1	0.81	0.19	49,49,49,49	0
56	MG	2A	3545	1/1	0.81	0.12	68,68,68,68	0
56	MG	2A	3263	1/1	0.81	0.31	57,57,57,57	0
56	MG	1A	3312	1/1	0.81	0.39	64,64,64,64	0
56	MG	1A	3670	1/1	0.81	0.25	48,48,48,48	0
56	MG	2a	3069	1/1	0.81	0.17	60,60,60,60	0
56	MG	1A	3390	1/1	0.81	0.19	36,36,36,36	0
56	MG	1A	3189	1/1	0.81	0.15	41,41,41,41	0
56	MG	1A	3075	1/1	0.81	0.16	22,22,22,22	0
56	MG	2A	3320	1/1	0.81	0.13	39,39,39,39	0
56	MG	2A	3111	1/1	0.81	0.17	55,55,55,55	0
56	MG	1F	309	1/1	0.81	0.18	44,44,44,44	0
56	MG	1A	3740	1/1	0.81	0.11	37,37,37,37	0
56	MG	16	105	1/1	0.81	0.17	51,51,51,51	0
56	MG	1a	1721	1/1	0.81	0.17	59,59,59,59	0
56	MG	1A	3780	1/1	0.81	0.18	39,39,39,39	0
56	MG	2A	3802	1/1	0.81	0.17	41,41,41,41	0
56	MG	1a	1628	1/1	0.81	0.15	59,59,59,59	0
56	MG	1A	3381	1/1	0.81	0.21	50,50,50,50	0
56	MG	2A	3364	1/1	0.81	0.16	56,56,56,56	0
56	MG	2A	3203	1/1	0.81	0.15	49,49,49,49	0
56	MG	2A	3851	1/1	0.81	0.09	55,55,55,55	0
56	MG	1A	3432	1/1	0.81	0.13	52,52,52,52	0
56	MG	2A	3410	1/1	0.81	0.13	60,60,60,60	0
56	MG	1A	4039	1/1	0.81	0.13	65,65,65,65	0
56	MG	1A	3054	1/1	0.82	0.26	38,38,38,38	0
56	MG	2A	3180	1/1	0.82	0.19	58,58,58,58	0
56	MG	1A	3819	1/1	0.82	0.08	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3675	1/1	0.82	0.13	61,61,61,61	0
56	MG	1a	1718	1/1	0.82	0.25	56,56,56,56	0
56	MG	1a	1670	1/1	0.82	0.17	49,49,49,49	0
56	MG	1a	1604	1/1	0.82	0.12	55,55,55,55	0
56	MG	1a	1739	1/1	0.82	0.35	59,59,59,59	0
56	MG	2A	3491	1/1	0.82	0.18	43,43,43,43	0
56	MG	1a	1757	1/1	0.82	0.19	66,66,66,66	0
56	MG	1A	3355	1/1	0.82	0.19	49,49,49,49	0
56	MG	1B	214	1/1	0.82	0.13	54,54,54,54	0
56	MG	1a	1805	1/1	0.82	0.15	57,57,57,57	0
56	MG	1A	4059	1/1	0.82	0.21	58,58,58,58	0
56	MG	1A	3876	1/1	0.82	0.17	53,53,53,53	0
56	MG	2y	104	1/1	0.82	0.10	80,80,80,80	0
56	MG	1A	3938	1/1	0.82	0.25	51,51,51,51	0
56	MG	2A	3401	1/1	0.82	0.12	55,55,55,55	0
56	MG	2A	3267	1/1	0.82	0.16	49,49,49,49	0
56	MG	2a	3010	1/1	0.83	0.09	67,67,67,67	0
56	MG	1A	3380	1/1	0.83	0.67	63,63,63,63	0
56	MG	2A	3350	1/1	0.83	0.16	66,66,66,66	0
56	MG	1x	103	1/1	0.83	0.18	58,58,58,58	0
56	MG	2a	3039	1/1	0.83	0.20	65,65,65,65	0
56	MG	2a	3040	1/1	0.83	0.11	58,58,58,58	0
56	MG	1a	1626	1/1	0.83	0.23	53,53,53,53	0
56	MG	1A	3190	1/1	0.83	0.22	56,56,56,56	0
56	MG	2A	3367	1/1	0.83	0.13	59,59,59,59	0
56	MG	2A	3400	1/1	0.83	0.14	68,68,68,68	0
56	MG	2A	3238	1/1	0.83	0.12	64,64,64,64	0
56	MG	1A	3188	1/1	0.83	0.13	67,67,67,67	0
56	MG	2A	3756	1/1	0.83	0.09	53,53,53,53	0
56	MG	1A	3326	1/1	0.83	0.18	33,33,33,33	0
56	MG	2a	3086	1/1	0.83	0.20	44,44,44,44	0
56	MG	1a	1725	1/1	0.83	0.14	47,47,47,47	0
56	MG	1A	3093	1/1	0.83	0.15	44,44,44,44	0
56	MG	1A	3476	1/1	0.83	0.26	42,42,42,42	0
56	MG	2a	3108	1/1	0.83	0.21	63,63,63,63	0
56	MG	2a	3123	1/1	0.83	0.25	59,59,59,59	0
56	MG	1A	3405	1/1	0.83	0.26	17,17,17,17	0
56	MG	2A	3809	1/1	0.83	0.13	47,47,47,47	0
56	MG	2A	3159	1/1	0.83	0.10	58,58,58,58	0
56	MG	1A	3770	1/1	0.83	0.25	47,47,47,47	0
56	MG	2A	3477	1/1	0.83	0.24	48,48,48,48	0
56	MG	2a	3154	1/1	0.83	0.08	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3489	1/1	0.83	0.20	56,56,56,56	0
56	MG	2A	3296	1/1	0.83	0.13	69,69,69,69	0
56	MG	2a	3217	1/1	0.83	0.12	72,72,72,72	0
56	MG	1A	3485	1/1	0.83	0.26	49,49,49,49	0
56	MG	1A	3814	1/1	0.83	0.20	48,48,48,48	0
56	MG	1A	3287	1/1	0.83	0.18	39,39,39,39	0
56	MG	1A	3605	1/1	0.83	0.20	42,42,42,42	0
56	MG	2G	201	1/1	0.83	0.18	69,69,69,69	0
56	MG	2y	102	1/1	0.83	0.12	73,73,73,73	0
56	MG	2A	3502	1/1	0.83	0.22	45,45,45,45	0
56	MG	1A	3493	1/1	0.83	0.29	52,52,52,52	0
56	MG	1n	102	1/1	0.83	0.20	62,62,62,62	0
56	MG	1A	3373	1/1	0.83	0.23	54,54,54,54	0
56	MG	2F	303	1/1	0.84	0.14	39,39,39,39	0
56	MG	2A	3414	1/1	0.84	0.36	57,57,57,57	0
56	MG	2A	3428	1/1	0.84	0.25	49,49,49,49	0
56	MG	1A	3379	1/1	0.84	0.19	39,39,39,39	0
56	MG	2A	3231	1/1	0.84	0.25	36,36,36,36	0
56	MG	2A	3235	1/1	0.84	0.22	42,42,42,42	0
56	MG	1x	102	1/1	0.84	0.28	57,57,57,57	0
56	MG	1A	3504	1/1	0.84	0.21	47,47,47,47	0
56	MG	1A	3169	1/1	0.84	0.19	26,26,26,26	0
56	MG	2A	3255	1/1	0.84	0.10	60,60,60,60	0
56	MG	2A	3008	1/1	0.84	0.12	55,55,55,55	0
56	MG	2a	3025	1/1	0.84	0.14	56,56,56,56	0
56	MG	1A	3510	1/1	0.84	0.22	33,33,33,33	0
56	MG	2A	3043	1/1	0.84	0.14	45,45,45,45	0
56	MG	1A	3347	1/1	0.84	0.15	53,53,53,53	0
56	MG	1A	3842	1/1	0.84	0.18	37,37,37,37	0
56	MG	2A	3088	1/1	0.84	0.17	41,41,41,41	0
56	MG	1B	211	1/1	0.84	0.23	57,57,57,57	0
56	MG	2A	3554	1/1	0.84	0.12	42,42,42,42	0
56	MG	2A	3300	1/1	0.84	0.16	53,53,53,53	0
56	MG	1a	1740	1/1	0.84	0.13	55,55,55,55	0
56	MG	2A	3312	1/1	0.84	0.21	53,53,53,53	0
56	MG	1A	3983	1/1	0.84	0.09	39,39,39,39	0
56	MG	2a	3083	1/1	0.84	0.08	55,55,55,55	0
56	MG	2A	3332	1/1	0.84	0.18	52,52,52,52	0
56	MG	2A	3113	1/1	0.84	0.15	50,50,50,50	0
56	MG	1a	1762	1/1	0.84	0.21	52,52,52,52	0
56	MG	1a	1763	1/1	0.84	0.15	68,68,68,68	0
56	MG	1A	4003	1/1	0.84	0.08	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	3112	1/1	0.84	0.21	60,60,60,60	0
56	MG	2A	3173	1/1	0.84	0.17	74,74,74,74	0
56	MG	2A	3708	1/1	0.84	0.14	58,58,58,58	0
56	MG	2A	3720	1/1	0.84	0.14	38,38,38,38	0
56	MG	1a	1665	1/1	0.84	0.19	55,55,55,55	0
56	MG	2A	3746	1/1	0.84	0.10	43,43,43,43	0
56	MG	1a	1797	1/1	0.84	0.25	53,53,53,53	0
56	MG	2a	3153	1/1	0.84	0.08	73,73,73,73	0
56	MG	1a	1799	1/1	0.84	0.16	60,60,60,60	0
56	MG	2a	3158	1/1	0.84	0.09	68,68,68,68	0
56	MG	2A	3781	1/1	0.84	0.12	70,70,70,70	0
56	MG	2A	3356	1/1	0.84	0.17	48,48,48,48	0
56	MG	2a	3190	1/1	0.84	0.19	63,63,63,63	0
56	MG	2a	3196	1/1	0.84	0.12	68,68,68,68	0
56	MG	1A	3229	1/1	0.84	0.17	41,41,41,41	0
56	MG	2A	3186	1/1	0.84	0.16	50,50,50,50	0
56	MG	1A	3230	1/1	0.84	0.22	44,44,44,44	0
56	MG	2l	204	1/1	0.84	0.10	59,59,59,59	0
56	MG	2A	3383	1/1	0.84	0.10	57,57,57,57	0
56	MG	2A	3388	1/1	0.84	0.19	41,41,41,41	0
56	MG	2A	3390	1/1	0.84	0.21	63,63,63,63	0
56	MG	1A	4012	1/1	0.84	0.22	26,26,26,26	0
56	MG	1I	201	1/1	0.84	0.14	63,63,63,63	0
56	MG	1N	203	1/1	0.84	0.21	45,45,45,45	0
56	MG	1A	3153	1/1	0.84	0.32	31,31,31,31	0
56	MG	1A	3615	1/1	0.84	0.26	33,33,33,33	0
56	MG	1T	203	1/1	0.85	0.23	55,55,55,55	0
56	MG	1X	106	1/1	0.85	0.16	51,51,51,51	0
56	MG	1A	3799	1/1	0.85	0.23	27,27,27,27	0
56	MG	10	104	1/1	0.85	0.20	51,51,51,51	0
56	MG	1A	3600	1/1	0.85	0.20	33,33,33,33	0
56	MG	1A	3227	1/1	0.85	0.15	46,46,46,46	0
56	MG	1a	1611	1/1	0.85	0.09	57,57,57,57	0
56	MG	2A	3201	1/1	0.85	0.17	59,59,59,59	0
56	MG	1a	1782	1/1	0.85	0.17	55,55,55,55	0
56	MG	1a	1786	1/1	0.85	0.13	74,74,74,74	0
56	MG	2A	3438	1/1	0.85	0.19	53,53,53,53	0
56	MG	1a	1614	1/1	0.85	0.12	55,55,55,55	0
56	MG	2A	3213	1/1	0.85	0.17	61,61,61,61	0
56	MG	1A	3607	1/1	0.85	0.15	31,31,31,31	0
56	MG	2A	3470	1/1	0.85	0.31	60,60,60,60	0
56	MG	1A	3329	1/1	0.85	0.17	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4030	1/1	0.85	0.24	36,36,36,36	0
56	MG	1A	3519	1/1	0.85	0.24	57,57,57,57	0
56	MG	1A	3487	1/1	0.85	0.13	59,59,59,59	0
56	MG	1A	4057	1/1	0.85	0.17	40,40,40,40	0
56	MG	2A	3243	1/1	0.85	0.12	52,52,52,52	0
56	MG	1e	201	1/1	0.85	0.11	59,59,59,59	0
56	MG	1A	4058	1/1	0.85	0.15	49,49,49,49	0
56	MG	1A	3186	1/1	0.85	0.15	41,41,41,41	0
56	MG	2a	3073	1/1	0.85	0.08	50,50,50,50	0
56	MG	2A	3538	1/1	0.85	0.16	61,61,61,61	0
56	MG	1A	3490	1/1	0.85	0.21	40,40,40,40	0
56	MG	1A	3491	1/1	0.85	0.14	48,48,48,48	0
56	MG	1A	3213	1/1	0.85	0.17	37,37,37,37	0
56	MG	2A	3271	1/1	0.85	0.14	55,55,55,55	0
56	MG	1A	3901	1/1	0.85	0.12	33,33,33,33	0
56	MG	1B	207	1/1	0.85	0.23	41,41,41,41	0
56	MG	1A	3498	1/1	0.85	0.27	41,41,41,41	0
56	MG	2a	3119	1/1	0.85	0.23	59,59,59,59	0
56	MG	2a	3121	1/1	0.85	0.11	66,66,66,66	0
56	MG	1a	1705	1/1	0.85	0.23	45,45,45,45	0
56	MG	1a	1706	1/1	0.85	0.32	48,48,48,48	0
56	MG	2a	3128	1/1	0.85	0.19	63,63,63,63	0
56	MG	1A	3581	1/1	0.85	0.24	64,64,64,64	0
56	MG	2A	3680	1/1	0.85	0.15	43,43,43,43	0
56	MG	2A	3682	1/1	0.85	0.23	44,44,44,44	0
56	MG	2A	3072	1/1	0.85	0.13	41,41,41,41	0
56	MG	2A	3696	1/1	0.85	0.17	50,50,50,50	0
56	MG	2A	3331	1/1	0.85	0.39	63,63,63,63	0
56	MG	2a	3157	1/1	0.85	0.10	57,57,57,57	0
56	MG	2A	3084	1/1	0.85	0.14	60,60,60,60	0
56	MG	2a	3166	1/1	0.85	0.15	50,50,50,50	0
56	MG	2A	3086	1/1	0.85	0.12	40,40,40,40	0
56	MG	2a	3174	1/1	0.85	0.14	58,58,58,58	0
56	MG	2a	3186	1/1	0.85	0.13	66,66,66,66	0
56	MG	1A	3410	1/1	0.85	0.18	43,43,43,43	0
56	MG	1A	3955	1/1	0.85	0.12	35,35,35,35	0
56	MG	1A	3755	1/1	0.85	0.16	40,40,40,40	0
56	MG	2A	3108	1/1	0.85	0.17	68,68,68,68	0
56	MG	1a	1717	1/1	0.85	0.17	57,57,57,57	0
56	MG	1A	3756	1/1	0.85	0.16	45,45,45,45	0
56	MG	2j	201	1/1	0.85	0.24	69,69,69,69	0
56	MG	2A	3116	1/1	0.85	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3172	1/1	0.85	0.15	53,53,53,53	0
56	MG	1A	3593	1/1	0.85	0.15	32,32,32,32	0
56	MG	2A	3363	1/1	0.85	0.15	50,50,50,50	0
56	MG	2A	3163	1/1	0.85	0.16	53,53,53,53	0
56	MG	1R	203	1/1	0.85	0.25	42,42,42,42	0
56	MG	2A	3371	1/1	0.85	0.12	60,60,60,60	0
56	MG	2A	3374	1/1	0.85	0.18	47,47,47,47	0
56	MG	1a	1735	1/1	0.85	0.17	60,60,60,60	0
56	MG	2Q	203	1/1	0.86	0.23	49,49,49,49	0
56	MG	2V	202	1/1	0.86	0.13	49,49,49,49	0
56	MG	1Z	3701	1/1	0.86	0.12	51,51,51,51	0
56	MG	2A	3317	1/1	0.86	0.19	40,40,40,40	0
56	MG	1A	4082	1/1	0.86	0.13	36,36,36,36	0
56	MG	2A	3327	1/1	0.86	0.32	52,52,52,52	0
56	MG	2A	3328	1/1	0.86	0.13	47,47,47,47	0
56	MG	1A	3835	1/1	0.86	0.15	58,58,58,58	0
56	MG	1A	3838	1/1	0.86	0.14	43,43,43,43	0
56	MG	1A	3309	1/1	0.86	0.16	39,39,39,39	0
56	MG	1A	3988	1/1	0.86	0.14	18,18,18,18	0
56	MG	2a	3038	1/1	0.86	0.12	69,69,69,69	0
56	MG	1a	1616	1/1	0.86	0.12	46,46,46,46	0
56	MG	1w	106	1/1	0.86	0.12	75,75,75,75	0
56	MG	2A	3557	1/1	0.86	0.14	46,46,46,46	0
56	MG	2A	3190	1/1	0.86	0.21	60,60,60,60	0
56	MG	2A	3608	1/1	0.86	0.16	28,28,28,28	0
56	MG	1A	3348	1/1	0.86	0.27	36,36,36,36	0
56	MG	2A	3349	1/1	0.86	0.37	64,64,64,64	0
56	MG	2A	3639	1/1	0.86	0.14	36,36,36,36	0
56	MG	1A	3175	1/1	0.86	0.33	42,42,42,42	0
56	MG	1x	110	1/1	0.86	0.09	66,66,66,66	0
56	MG	1A	3516	1/1	0.86	0.22	37,37,37,37	0
56	MG	2A	3005	1/1	0.86	0.27	55,55,55,55	0
56	MG	1a	1632	1/1	0.86	0.09	55,55,55,55	0
56	MG	1A	3291	1/1	0.86	0.18	40,40,40,40	0
56	MG	2A	3366	1/1	0.86	0.18	55,55,55,55	0
56	MG	1A	3272	1/1	0.86	0.17	54,54,54,54	0
56	MG	2A	3689	1/1	0.86	0.12	63,63,63,63	0
56	MG	2A	3050	1/1	0.86	0.15	55,55,55,55	0
56	MG	1A	3537	1/1	0.86	0.20	36,36,36,36	0
56	MG	1A	3830	1/1	0.86	0.15	10,10,10,10	0
56	MG	2A	3386	1/1	0.86	0.20	46,46,46,46	0
56	MG	2A	3731	1/1	0.86	0.12	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3071	1/1	0.86	0.14	60,60,60,60	0
56	MG	1A	3540	1/1	0.86	0.13	46,46,46,46	0
56	MG	2A	3391	1/1	0.86	0.17	47,47,47,47	0
56	MG	2A	3760	1/1	0.86	0.12	58,58,58,58	0
56	MG	2A	3770	1/1	0.86	0.17	47,47,47,47	0
56	MG	1a	1768	1/1	0.86	0.14	61,61,61,61	0
56	MG	1a	1664	1/1	0.86	0.16	45,45,45,45	0
56	MG	1O	206	1/1	0.86	0.22	57,57,57,57	0
56	MG	2A	3408	1/1	0.86	0.23	66,66,66,66	0
56	MG	1P	204	1/1	0.86	0.12	33,33,33,33	0
56	MG	2A	3805	1/1	0.86	0.20	75,75,75,75	0
56	MG	1a	1785	1/1	0.86	0.12	63,63,63,63	0
56	MG	2A	3412	1/1	0.86	0.17	57,57,57,57	0
56	MG	2a	3187	1/1	0.86	0.15	61,61,61,61	0
56	MG	1A	3340	1/1	0.86	0.19	46,46,46,46	0
56	MG	1A	3960	1/1	0.86	0.19	46,46,46,46	0
56	MG	1U	207	1/1	0.86	0.23	34,34,34,34	0
56	MG	2A	3274	1/1	0.86	0.15	54,54,54,54	0
56	MG	2A	3863	1/1	0.86	0.10	42,42,42,42	0
56	MG	2A	3441	1/1	0.86	0.19	47,47,47,47	0
56	MG	2A	3451	1/1	0.86	0.17	37,37,37,37	0
56	MG	2A	3878	1/1	0.86	0.14	63,63,63,63	0
56	MG	1A	3967	1/1	0.86	0.18	29,29,29,29	0
56	MG	2w	105	1/1	0.86	0.11	67,67,67,67	0
56	MG	2B	216	1/1	0.86	0.11	58,58,58,58	0
56	MG	2D	302	1/1	0.86	0.27	42,42,42,42	0
56	MG	2A	3117	1/1	0.86	0.17	50,50,50,50	0
56	MG	1a	1806	1/1	0.86	0.20	70,70,70,70	0
56	MG	2A	3137	1/1	0.86	0.19	36,36,36,36	0
56	MG	1A	3342	1/1	0.86	0.34	49,49,49,49	0
60	K	1x	101	1/1	0.86	0.17	62,62,62,62	0
56	MG	2P	203	1/1	0.86	0.11	53,53,53,53	0
56	MG	12	102	1/1	0.87	0.27	39,39,39,39	0
56	MG	25	103	1/1	0.87	0.14	42,42,42,42	0
56	MG	1A	3061	1/1	0.87	0.16	47,47,47,47	0
56	MG	18	102	1/1	0.87	0.32	38,38,38,38	0
56	MG	2A	3196	1/1	0.87	0.15	48,48,48,48	0
56	MG	2A	3587	1/1	0.87	0.14	70,70,70,70	0
56	MG	1a	1602	1/1	0.87	0.14	48,48,48,48	0
56	MG	1A	3823	1/1	0.87	0.16	81,81,81,81	0
56	MG	1A	3152	1/1	0.87	0.28	33,33,33,33	0
56	MG	2A	3362	1/1	0.87	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3034	1/1	0.87	0.12	67,67,67,67	0
56	MG	1A	3633	1/1	0.87	0.15	23,23,23,23	0
56	MG	1A	3832	1/1	0.87	0.12	29,29,29,29	0
56	MG	2A	3012	1/1	0.87	0.12	34,34,34,34	0
56	MG	1a	1618	1/1	0.87	0.19	53,53,53,53	0
56	MG	2A	3671	1/1	0.87	0.19	49,49,49,49	0
56	MG	2A	3020	1/1	0.87	0.20	55,55,55,55	0
56	MG	2A	3223	1/1	0.87	0.12	52,52,52,52	0
56	MG	2A	3021	1/1	0.87	0.13	37,37,37,37	0
56	MG	1a	1619	1/1	0.87	0.15	40,40,40,40	0
56	MG	1B	209	1/1	0.87	0.17	31,31,31,31	0
56	MG	2A	3695	1/1	0.87	0.15	52,52,52,52	0
56	MG	2A	3052	1/1	0.87	0.12	66,66,66,66	0
56	MG	2A	3055	1/1	0.87	0.10	60,60,60,60	0
56	MG	2A	3703	1/1	0.87	0.13	52,52,52,52	0
56	MG	1a	1753	1/1	0.87	0.12	46,46,46,46	0
56	MG	1A	3576	1/1	0.87	0.23	28,28,28,28	0
56	MG	1A	3019	1/1	0.87	0.25	43,43,43,43	0
56	MG	2A	3740	1/1	0.87	0.10	54,54,54,54	0
56	MG	2A	3743	1/1	0.87	0.14	51,51,51,51	0
56	MG	2a	3117	1/1	0.87	0.12	73,73,73,73	0
56	MG	1A	3400	1/1	0.87	0.22	38,38,38,38	0
56	MG	2a	3120	1/1	0.87	0.23	67,67,67,67	0
56	MG	1A	3995	1/1	0.87	0.11	39,39,39,39	0
56	MG	2A	3748	1/1	0.87	0.16	57,57,57,57	0
56	MG	1A	4000	1/1	0.87	0.21	62,62,62,62	0
56	MG	1A	3729	1/1	0.87	0.15	36,36,36,36	0
56	MG	1A	3525	1/1	0.87	0.22	42,42,42,42	0
56	MG	2A	3415	1/1	0.87	0.17	67,67,67,67	0
56	MG	2a	3138	1/1	0.87	0.12	64,64,64,64	0
56	MG	2A	3424	1/1	0.87	0.25	36,36,36,36	0
56	MG	1A	3851	1/1	0.87	0.14	35,35,35,35	0
56	MG	2a	3151	1/1	0.87	0.15	44,44,44,44	0
56	MG	2A	3430	1/1	0.87	0.15	44,44,44,44	0
56	MG	1a	1663	1/1	0.87	0.15	53,53,53,53	0
56	MG	1O	201	1/1	0.87	0.36	62,62,62,62	0
56	MG	1A	3739	1/1	0.87	0.16	34,34,34,34	0
56	MG	1A	3453	1/1	0.87	0.25	35,35,35,35	0
56	MG	2A	3455	1/1	0.87	0.19	50,50,50,50	0
56	MG	2A	3817	1/1	0.87	0.12	53,53,53,53	0
56	MG	2A	3819	1/1	0.87	0.09	61,61,61,61	0
56	MG	2A	3457	1/1	0.87	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3311	1/1	0.87	0.21	53,53,53,53	0
56	MG	1A	3251	1/1	0.87	0.21	50,50,50,50	0
56	MG	2A	3852	1/1	0.87	0.10	55,55,55,55	0
56	MG	2A	3314	1/1	0.87	0.11	53,53,53,53	0
56	MG	2a	3221	1/1	0.87	0.14	74,74,74,74	0
56	MG	2A	3464	1/1	0.87	0.21	46,46,46,46	0
56	MG	1a	1682	1/1	0.87	0.38	56,56,56,56	0
56	MG	1a	1817	1/1	0.87	0.12	40,40,40,40	0
56	MG	2l	202	1/1	0.87	0.10	56,56,56,56	0
56	MG	1A	3407	1/1	0.87	0.18	37,37,37,37	0
56	MG	1A	3252	1/1	0.87	0.27	49,49,49,49	0
56	MG	2A	3329	1/1	0.87	0.11	56,56,56,56	0
56	MG	1A	3505	1/1	0.87	0.14	48,48,48,48	0
56	MG	1A	3930	1/1	0.87	0.16	45,45,45,45	0
56	MG	1A	3565	1/1	0.87	0.16	53,53,53,53	0
56	MG	1t	201	1/1	0.87	0.17	50,50,50,50	0
56	MG	1v	101	1/1	0.87	0.20	58,58,58,58	0
56	MG	2A	3528	1/1	0.87	0.14	33,33,33,33	0
56	MG	1A	3255	1/1	0.87	0.17	23,23,23,23	0
56	MG	23	101	1/1	0.87	0.28	54,54,54,54	0
56	MG	2A	3031	1/1	0.88	0.15	62,62,62,62	0
56	MG	2A	3250	1/1	0.88	0.28	56,56,56,56	0
56	MG	1A	3580	1/1	0.88	0.21	33,33,33,33	0
56	MG	2E	304	1/1	0.88	0.11	58,58,58,58	0
56	MG	2A	3259	1/1	0.88	0.24	49,49,49,49	0
56	MG	1A	4052	1/1	0.88	0.14	38,38,38,38	0
56	MG	1a	1730	1/1	0.88	0.14	46,46,46,46	0
56	MG	2A	3053	1/1	0.88	0.26	54,54,54,54	0
56	MG	1A	3468	1/1	0.88	0.15	60,60,60,60	0
56	MG	1A	3165	1/1	0.88	0.23	34,34,34,34	0
56	MG	2T	201	1/1	0.88	0.15	49,49,49,49	0
56	MG	2A	3476	1/1	0.88	0.10	52,52,52,52	0
56	MG	1A	3754	1/1	0.88	0.08	45,45,45,45	0
56	MG	2A	3479	1/1	0.88	0.17	52,52,52,52	0
56	MG	1A	3920	1/1	0.88	0.14	26,26,26,26	0
56	MG	2A	3289	1/1	0.88	0.16	41,41,41,41	0
56	MG	2a	3003	1/1	0.88	0.12	62,62,62,62	0
56	MG	2A	3292	1/1	0.88	0.30	67,67,67,67	0
56	MG	1A	3927	1/1	0.88	0.13	46,46,46,46	0
56	MG	2A	3295	1/1	0.88	0.18	56,56,56,56	0
56	MG	2a	3012	1/1	0.88	0.28	62,62,62,62	0
56	MG	2a	3014	1/1	0.88	0.18	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3018	1/1	0.88	0.17	66,66,66,66	0
56	MG	1A	3535	1/1	0.88	0.15	50,50,50,50	0
56	MG	1A	3473	1/1	0.88	0.14	54,54,54,54	0
56	MG	2A	3503	1/1	0.88	0.17	62,62,62,62	0
56	MG	2A	3305	1/1	0.88	0.17	53,53,53,53	0
56	MG	2A	3529	1/1	0.88	0.12	62,62,62,62	0
56	MG	1A	3597	1/1	0.88	0.13	30,30,30,30	0
56	MG	2A	3089	1/1	0.88	0.12	60,60,60,60	0
56	MG	1A	4104	1/1	0.88	0.11	46,46,46,46	0
56	MG	2A	3097	1/1	0.88	0.13	50,50,50,50	0
56	MG	2A	3567	1/1	0.88	0.12	69,69,69,69	0
56	MG	2A	3099	1/1	0.88	0.15	58,58,58,58	0
56	MG	2A	3318	1/1	0.88	0.47	55,55,55,55	0
56	MG	2A	3607	1/1	0.88	0.19	53,53,53,53	0
56	MG	2a	3062	1/1	0.88	0.12	64,64,64,64	0
56	MG	2a	3064	1/1	0.88	0.13	70,70,70,70	0
56	MG	2A	3100	1/1	0.88	0.20	64,64,64,64	0
56	MG	2a	3067	1/1	0.88	0.08	63,63,63,63	0
56	MG	2A	3103	1/1	0.88	0.15	50,50,50,50	0
56	MG	1A	3940	1/1	0.88	0.22	46,46,46,46	0
56	MG	1A	3952	1/1	0.88	0.13	50,50,50,50	0
56	MG	2a	3079	1/1	0.88	0.22	52,52,52,52	0
56	MG	2A	3330	1/1	0.88	0.14	60,60,60,60	0
56	MG	1A	3538	1/1	0.88	0.30	59,59,59,59	0
56	MG	1A	3298	1/1	0.88	0.16	38,38,38,38	0
56	MG	2a	3095	1/1	0.88	0.16	40,40,40,40	0
56	MG	2A	3114	1/1	0.88	0.20	60,60,60,60	0
56	MG	1a	1796	1/1	0.88	0.18	47,47,47,47	0
56	MG	2a	3101	1/1	0.88	0.16	55,55,55,55	0
56	MG	1A	3541	1/1	0.88	0.14	60,60,60,60	0
56	MG	2a	3110	1/1	0.88	0.17	65,65,65,65	0
56	MG	1A	3542	1/1	0.88	0.19	56,56,56,56	0
56	MG	1a	1650	1/1	0.88	0.19	55,55,55,55	0
56	MG	2A	3684	1/1	0.88	0.10	63,63,63,63	0
56	MG	2A	3145	1/1	0.88	0.20	56,56,56,56	0
56	MG	2A	3149	1/1	0.88	0.11	40,40,40,40	0
56	MG	2A	3154	1/1	0.88	0.25	51,51,51,51	0
56	MG	1a	1655	1/1	0.88	0.15	50,50,50,50	0
56	MG	1D	310	1/1	0.88	0.21	49,49,49,49	0
56	MG	1A	3442	1/1	0.88	0.18	31,31,31,31	0
56	MG	2A	3358	1/1	0.88	0.27	42,42,42,42	0
56	MG	2A	3169	1/1	0.88	0.12	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3725	1/1	0.88	0.11	59,59,59,59	0
56	MG	1A	3447	1/1	0.88	0.26	39,39,39,39	0
56	MG	1A	3982	1/1	0.88	0.12	37,37,37,37	0
56	MG	1A	3401	1/1	0.88	0.21	42,42,42,42	0
56	MG	1a	1671	1/1	0.88	0.12	56,56,56,56	0
56	MG	1n	101	1/1	0.88	0.24	44,44,44,44	0
56	MG	1N	205	1/1	0.88	0.24	48,48,48,48	0
56	MG	2A	3375	1/1	0.88	0.14	49,49,49,49	0
56	MG	2A	3381	1/1	0.88	0.10	59,59,59,59	0
56	MG	2A	3767	1/1	0.88	0.14	40,40,40,40	0
56	MG	1A	3566	1/1	0.88	0.32	50,50,50,50	0
56	MG	1A	3568	1/1	0.88	0.20	52,52,52,52	0
56	MG	2A	3779	1/1	0.88	0.16	65,65,65,65	0
56	MG	1a	1692	1/1	0.88	0.16	62,62,62,62	0
56	MG	1A	3997	1/1	0.88	0.24	55,55,55,55	0
56	MG	1A	3654	1/1	0.88	0.15	35,35,35,35	0
56	MG	2A	3793	1/1	0.88	0.10	63,63,63,63	0
56	MG	1R	205	1/1	0.88	0.18	34,34,34,34	0
56	MG	1A	3488	1/1	0.88	0.22	52,52,52,52	0
56	MG	1x	105	1/1	0.88	0.21	56,56,56,56	0
56	MG	1x	108	1/1	0.88	0.14	49,49,49,49	0
56	MG	1A	3674	1/1	0.88	0.16	52,52,52,52	0
56	MG	1X	102	1/1	0.88	0.15	28,28,28,28	0
56	MG	2v	102	1/1	0.88	0.14	64,64,64,64	0
56	MG	1A	3411	1/1	0.88	0.21	45,45,45,45	0
56	MG	2A	3225	1/1	0.88	0.57	44,44,44,44	0
56	MG	1A	3699	1/1	0.88	0.15	26,26,26,26	0
56	MG	1a	1716	1/1	0.88	0.19	49,49,49,49	0
56	MG	2y	103	1/1	0.88	0.12	56,56,56,56	0
56	MG	2A	3237	1/1	0.88	0.17	55,55,55,55	0
56	MG	1A	3869	1/1	0.88	0.16	42,42,42,42	0
56	MG	2A	3239	1/1	0.88	0.23	54,54,54,54	0
56	MG	1A	3518	1/1	0.88	0.18	51,51,51,51	0
56	MG	1A	3234	1/1	0.88	0.18	26,26,26,26	0
56	MG	1a	1607	1/1	0.89	0.23	51,51,51,51	0
56	MG	2A	3176	1/1	0.89	0.14	47,47,47,47	0
56	MG	1A	4021	1/1	0.89	0.12	36,36,36,36	0
56	MG	1A	3060	1/1	0.89	0.15	25,25,25,25	0
56	MG	1A	3353	1/1	0.89	0.20	38,38,38,38	0
56	MG	1A	3103	1/1	0.89	0.17	56,56,56,56	0
56	MG	2A	3811	1/1	0.89	0.23	57,57,57,57	0
56	MG	1A	3053	1/1	0.89	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3187	1/1	0.89	0.26	49,49,49,49	0
56	MG	2A	3392	1/1	0.89	0.19	43,43,43,43	0
56	MG	2A	3393	1/1	0.89	0.16	55,55,55,55	0
56	MG	2A	3398	1/1	0.89	0.28	60,60,60,60	0
56	MG	1A	4047	1/1	0.89	0.09	52,52,52,52	0
56	MG	1f	202	1/1	0.89	0.22	58,58,58,58	0
56	MG	2A	3853	1/1	0.89	0.20	66,66,66,66	0
56	MG	1l	201	1/1	0.89	0.15	59,59,59,59	0
56	MG	2A	3404	1/1	0.89	0.18	65,65,65,65	0
56	MG	1a	1625	1/1	0.89	0.10	55,55,55,55	0
56	MG	1A	3128	1/1	0.89	0.44	36,36,36,36	0
56	MG	1A	3366	1/1	0.89	0.15	38,38,38,38	0
56	MG	2A	3204	1/1	0.89	0.18	54,54,54,54	0
56	MG	2B	221	1/1	0.89	0.13	59,59,59,59	0
56	MG	1A	3422	1/1	0.89	0.14	42,42,42,42	0
56	MG	1A	3133	1/1	0.89	0.29	31,31,31,31	0
56	MG	2E	308	1/1	0.89	0.14	52,52,52,52	0
56	MG	1A	3430	1/1	0.89	0.15	48,48,48,48	0
56	MG	2A	3426	1/1	0.89	0.24	35,35,35,35	0
56	MG	1A	3431	1/1	0.89	0.24	33,33,33,33	0
56	MG	1A	3241	1/1	0.89	0.35	62,62,62,62	0
56	MG	1A	3436	1/1	0.89	0.22	38,38,38,38	0
56	MG	2A	3436	1/1	0.89	0.27	47,47,47,47	0
56	MG	1A	3322	1/1	0.89	0.17	36,36,36,36	0
56	MG	1A	3443	1/1	0.89	0.19	32,32,32,32	0
56	MG	20	103	1/1	0.89	0.15	54,54,54,54	0
56	MG	2A	3443	1/1	0.89	0.17	43,43,43,43	0
56	MG	1A	3618	1/1	0.89	0.28	49,49,49,49	0
56	MG	1B	208	1/1	0.89	0.10	56,56,56,56	0
56	MG	28	102	1/1	0.89	0.14	47,47,47,47	0
56	MG	1A	3520	1/1	0.89	0.11	56,56,56,56	0
56	MG	2a	3002	1/1	0.89	0.13	63,63,63,63	0
56	MG	2A	3006	1/1	0.89	0.18	50,50,50,50	0
56	MG	2a	3004	1/1	0.89	0.21	57,57,57,57	0
56	MG	1A	3137	1/1	0.89	0.13	39,39,39,39	0
56	MG	2a	3007	1/1	0.89	0.14	54,54,54,54	0
56	MG	1A	3628	1/1	0.89	0.21	32,32,32,32	0
56	MG	1A	3204	1/1	0.89	0.20	35,35,35,35	0
56	MG	2A	3468	1/1	0.89	0.20	36,36,36,36	0
56	MG	2A	3469	1/1	0.89	0.20	42,42,42,42	0
56	MG	2a	3015	1/1	0.89	0.20	51,51,51,51	0
56	MG	2A	3019	1/1	0.89	0.15	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3472	1/1	0.89	0.14	45,45,45,45	0
56	MG	2A	3252	1/1	0.89	0.09	55,55,55,55	0
56	MG	2A	3253	1/1	0.89	0.12	58,58,58,58	0
56	MG	1B	230	1/1	0.89	0.23	60,60,60,60	0
56	MG	2A	3258	1/1	0.89	0.12	62,62,62,62	0
56	MG	1a	1689	1/1	0.89	0.15	48,48,48,48	0
56	MG	1A	3646	1/1	0.89	0.15	31,31,31,31	0
56	MG	2A	3035	1/1	0.89	0.18	42,42,42,42	0
56	MG	2a	3042	1/1	0.89	0.20	65,65,65,65	0
56	MG	1D	306	1/1	0.89	0.19	29,29,29,29	0
56	MG	1A	3530	1/1	0.89	0.27	52,52,52,52	0
56	MG	2a	3053	1/1	0.89	0.12	62,62,62,62	0
56	MG	2a	3057	1/1	0.89	0.33	59,59,59,59	0
56	MG	1E	305	1/1	0.89	0.26	35,35,35,35	0
56	MG	1A	3655	1/1	0.89	0.17	45,45,45,45	0
56	MG	1A	3661	1/1	0.89	0.13	21,21,21,21	0
56	MG	2A	3526	1/1	0.89	0.20	40,40,40,40	0
56	MG	2A	3282	1/1	0.89	0.18	53,53,53,53	0
56	MG	2A	3283	1/1	0.89	0.29	54,54,54,54	0
56	MG	2A	3532	1/1	0.89	0.21	32,32,32,32	0
56	MG	2A	3056	1/1	0.89	0.17	56,56,56,56	0
56	MG	1A	3669	1/1	0.89	0.15	39,39,39,39	0
56	MG	2A	3551	1/1	0.89	0.15	39,39,39,39	0
56	MG	1A	3533	1/1	0.89	0.24	33,33,33,33	0
56	MG	1A	3150	1/1	0.89	0.32	40,40,40,40	0
56	MG	2A	3558	1/1	0.89	0.12	34,34,34,34	0
56	MG	2A	3563	1/1	0.89	0.18	41,41,41,41	0
56	MG	1A	3455	1/1	0.89	0.22	48,48,48,48	0
56	MG	2A	3074	1/1	0.89	0.28	43,43,43,43	0
56	MG	2A	3302	1/1	0.89	0.12	49,49,49,49	0
56	MG	2A	3598	1/1	0.89	0.10	51,51,51,51	0
56	MG	1A	3457	1/1	0.89	0.19	39,39,39,39	0
56	MG	1A	3708	1/1	0.89	0.17	15,15,15,15	0
56	MG	2A	3620	1/1	0.89	0.17	39,39,39,39	0
56	MG	2a	3115	1/1	0.89	0.18	67,67,67,67	0
56	MG	1P	205	1/1	0.89	0.12	34,34,34,34	0
56	MG	2A	3631	1/1	0.89	0.13	37,37,37,37	0
56	MG	2A	3632	1/1	0.89	0.10	68,68,68,68	0
56	MG	2A	3633	1/1	0.89	0.17	46,46,46,46	0
56	MG	1A	3459	1/1	0.89	0.13	40,40,40,40	0
56	MG	1R	204	1/1	0.89	0.33	49,49,49,49	0
56	MG	2a	3127	1/1	0.89	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3640	1/1	0.89	0.23	46,46,46,46	0
56	MG	2A	3315	1/1	0.89	0.26	57,57,57,57	0
56	MG	2A	3091	1/1	0.89	0.24	40,40,40,40	0
56	MG	2A	3093	1/1	0.89	0.19	41,41,41,41	0
56	MG	2A	3663	1/1	0.89	0.09	50,50,50,50	0
56	MG	1A	3460	1/1	0.89	0.18	32,32,32,32	0
56	MG	2A	3326	1/1	0.89	0.15	51,51,51,51	0
56	MG	1S	203	1/1	0.89	0.30	70,70,70,70	0
56	MG	1A	3216	1/1	0.89	0.17	36,36,36,36	0
56	MG	1U	206	1/1	0.89	0.19	29,29,29,29	0
56	MG	1A	3543	1/1	0.89	0.18	44,44,44,44	0
56	MG	1A	3266	1/1	0.89	0.18	31,31,31,31	0
56	MG	1A	3090	1/1	0.89	0.24	29,29,29,29	0
56	MG	1A	3394	1/1	0.89	0.18	28,28,28,28	0
56	MG	2a	3178	1/1	0.89	0.11	69,69,69,69	0
56	MG	1A	3398	1/1	0.89	0.16	37,37,37,37	0
56	MG	10	103	1/1	0.89	0.27	32,32,32,32	0
56	MG	1A	3764	1/1	0.89	0.18	54,54,54,54	0
56	MG	2A	3125	1/1	0.89	0.10	52,52,52,52	0
56	MG	2A	3719	1/1	0.89	0.14	29,29,29,29	0
56	MG	2a	3197	1/1	0.89	0.15	67,67,67,67	0
56	MG	2a	3199	1/1	0.89	0.09	50,50,50,50	0
56	MG	2a	3201	1/1	0.89	0.12	68,68,68,68	0
56	MG	2a	3209	1/1	0.89	0.10	58,58,58,58	0
56	MG	10	106	1/1	0.89	0.13	40,40,40,40	0
56	MG	2A	3135	1/1	0.89	0.15	36,36,36,36	0
56	MG	11	102	1/1	0.89	0.12	47,47,47,47	0
56	MG	2A	3733	1/1	0.89	0.11	35,35,35,35	0
56	MG	2a	3228	1/1	0.89	0.14	77,77,77,77	0
56	MG	1A	3399	1/1	0.89	0.17	62,62,62,62	0
56	MG	2A	3742	1/1	0.89	0.09	56,56,56,56	0
56	MG	2A	3354	1/1	0.89	0.17	60,60,60,60	0
56	MG	2A	3146	1/1	0.89	0.12	51,51,51,51	0
56	MG	1A	3349	1/1	0.89	0.18	55,55,55,55	0
56	MG	2A	3150	1/1	0.89	0.19	52,52,52,52	0
56	MG	2A	3755	1/1	0.89	0.17	39,39,39,39	0
56	MG	2A	3359	1/1	0.89	0.15	38,38,38,38	0
56	MG	2y	101	1/1	0.89	0.11	59,59,59,59	0
56	MG	2A	3153	1/1	0.89	0.12	60,60,60,60	0
56	MG	1A	3285	1/1	0.89	0.20	54,54,54,54	0
56	MG	18	103	1/1	0.89	0.13	48,48,48,48	0
56	MG	2y	105	1/1	0.89	0.10	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3805	1/1	0.89	0.19	12,12,12,12	0
56	MG	1a	1803	1/1	0.89	0.10	56,56,56,56	0
56	MG	1A	4018	1/1	0.89	0.19	53,53,53,53	0
56	MG	2A	3372	1/1	0.89	0.15	47,47,47,47	0
56	MG	2A	3316	1/1	0.90	0.16	53,53,53,53	0
56	MG	2A	3508	1/1	0.90	0.15	46,46,46,46	0
56	MG	2A	3510	1/1	0.90	0.09	54,54,54,54	0
56	MG	2A	3525	1/1	0.90	0.15	47,47,47,47	0
56	MG	1A	3623	1/1	0.90	0.38	37,37,37,37	0
56	MG	2A	3127	1/1	0.90	0.21	46,46,46,46	0
56	MG	2W	203	1/1	0.90	0.38	57,57,57,57	0
56	MG	1A	3539	1/1	0.90	0.13	42,42,42,42	0
56	MG	2A	3321	1/1	0.90	0.16	57,57,57,57	0
56	MG	25	101	1/1	0.90	0.21	53,53,53,53	0
56	MG	1A	3246	1/1	0.90	0.23	26,26,26,26	0
56	MG	1A	3417	1/1	0.90	0.18	45,45,45,45	0
56	MG	1A	4071	1/1	0.90	0.07	38,38,38,38	0
56	MG	2A	3553	1/1	0.90	0.10	60,60,60,60	0
56	MG	1A	3645	1/1	0.90	0.19	12,12,12,12	0
56	MG	1a	1807	1/1	0.90	0.13	36,36,36,36	0
56	MG	1A	3064	1/1	0.90	0.23	29,29,29,29	0
56	MG	1A	3123	1/1	0.90	0.29	32,32,32,32	0
56	MG	1A	4099	1/1	0.90	0.22	35,35,35,35	0
56	MG	1a	1627	1/1	0.90	0.32	36,36,36,36	0
56	MG	1A	3374	1/1	0.90	0.23	41,41,41,41	0
56	MG	2A	3597	1/1	0.90	0.10	54,54,54,54	0
56	MG	2a	3013	1/1	0.90	0.14	62,62,62,62	0
56	MG	1a	1629	1/1	0.90	0.10	56,56,56,56	0
56	MG	2A	3166	1/1	0.90	0.15	51,51,51,51	0
56	MG	1A	4102	1/1	0.90	0.15	54,54,54,54	0
56	MG	1A	3561	1/1	0.90	0.28	38,38,38,38	0
56	MG	2A	3621	1/1	0.90	0.12	41,41,41,41	0
56	MG	2A	3629	1/1	0.90	0.21	54,54,54,54	0
56	MG	1A	3562	1/1	0.90	0.11	39,39,39,39	0
56	MG	1A	3254	1/1	0.90	0.16	53,53,53,53	0
56	MG	1A	3334	1/1	0.90	0.17	22,22,22,22	0
56	MG	1A	3433	1/1	0.90	0.11	47,47,47,47	0
56	MG	1A	3074	1/1	0.90	0.29	36,36,36,36	0
56	MG	1A	3494	1/1	0.90	0.21	38,38,38,38	0
56	MG	2a	3048	1/1	0.90	0.17	59,59,59,59	0
56	MG	1B	226	1/1	0.90	0.22	36,36,36,36	0
56	MG	1B	229	1/1	0.90	0.08	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3341	1/1	0.90	0.26	52,52,52,52	0
56	MG	2A	3656	1/1	0.90	0.12	39,39,39,39	0
56	MG	2A	3193	1/1	0.90	0.11	53,53,53,53	0
56	MG	1a	1666	1/1	0.90	0.13	50,50,50,50	0
56	MG	1A	3264	1/1	0.90	0.21	53,53,53,53	0
56	MG	1A	3947	1/1	0.90	0.21	34,34,34,34	0
56	MG	1a	1676	1/1	0.90	0.15	45,45,45,45	0
56	MG	1a	1677	1/1	0.90	0.18	47,47,47,47	0
56	MG	2A	3206	1/1	0.90	0.15	45,45,45,45	0
56	MG	1A	3735	1/1	0.90	0.13	42,42,42,42	0
56	MG	2A	3211	1/1	0.90	0.16	51,51,51,51	0
56	MG	2A	3686	1/1	0.90	0.06	66,66,66,66	0
56	MG	1A	3343	1/1	0.90	0.20	35,35,35,35	0
56	MG	1A	3577	1/1	0.90	0.28	35,35,35,35	0
56	MG	2a	3084	1/1	0.90	0.08	62,62,62,62	0
56	MG	2A	3214	1/1	0.90	0.25	43,43,43,43	0
56	MG	1A	3966	1/1	0.90	0.14	23,23,23,23	0
56	MG	1A	3214	1/1	0.90	0.10	61,61,61,61	0
56	MG	1A	3449	1/1	0.90	0.10	42,42,42,42	0
56	MG	1A	3973	1/1	0.90	0.22	27,27,27,27	0
56	MG	2A	3399	1/1	0.90	0.23	54,54,54,54	0
56	MG	2a	3104	1/1	0.90	0.13	62,62,62,62	0
56	MG	2A	3722	1/1	0.90	0.12	50,50,50,50	0
56	MG	2A	3029	1/1	0.90	0.24	54,54,54,54	0
56	MG	1A	3130	1/1	0.90	0.21	44,44,44,44	0
56	MG	2A	3032	1/1	0.90	0.14	45,45,45,45	0
56	MG	2A	3735	1/1	0.90	0.11	52,52,52,52	0
56	MG	2A	3737	1/1	0.90	0.11	55,55,55,55	0
56	MG	1A	3039	1/1	0.90	0.22	29,29,29,29	0
56	MG	2A	3406	1/1	0.90	0.16	48,48,48,48	0
56	MG	1A	3007	1/1	0.90	0.17	30,30,30,30	0
56	MG	2A	3240	1/1	0.90	0.25	38,38,38,38	0
56	MG	2a	3126	1/1	0.90	0.14	62,62,62,62	0
56	MG	1A	3146	1/1	0.90	0.18	39,39,39,39	0
56	MG	1A	3774	1/1	0.90	0.28	12,12,12,12	0
56	MG	2A	3753	1/1	0.90	0.10	55,55,55,55	0
56	MG	1A	3599	1/1	0.90	0.09	57,57,57,57	0
56	MG	2A	3249	1/1	0.90	0.17	60,60,60,60	0
56	MG	1A	3794	1/1	0.90	0.19	18,18,18,18	0
56	MG	1A	3999	1/1	0.90	0.07	60,60,60,60	0
56	MG	2a	3147	1/1	0.90	0.14	64,64,64,64	0
56	MG	1A	3795	1/1	0.90	0.19	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3152	1/1	0.90	0.15	46,46,46,46	0
56	MG	1A	3022	1/1	0.90	0.24	36,36,36,36	0
56	MG	2A	3433	1/1	0.90	0.23	49,49,49,49	0
56	MG	1A	3462	1/1	0.90	0.33	34,34,34,34	0
56	MG	1A	4006	1/1	0.90	0.11	43,43,43,43	0
56	MG	2A	3786	1/1	0.90	0.16	56,56,56,56	0
56	MG	1A	3026	1/1	0.90	0.17	45,45,45,45	0
56	MG	2A	3791	1/1	0.90	0.08	66,66,66,66	0
56	MG	2A	3076	1/1	0.90	0.23	50,50,50,50	0
56	MG	2a	3184	1/1	0.90	0.18	50,50,50,50	0
56	MG	2a	3185	1/1	0.90	0.11	65,65,65,65	0
56	MG	1a	1733	1/1	0.90	0.23	55,55,55,55	0
56	MG	1A	4008	1/1	0.90	0.08	67,67,67,67	0
56	MG	2A	3454	1/1	0.90	0.15	45,45,45,45	0
56	MG	2A	3087	1/1	0.90	0.14	49,49,49,49	0
56	MG	2a	3191	1/1	0.90	0.07	64,64,64,64	0
56	MG	1A	4009	1/1	0.90	0.10	50,50,50,50	0
56	MG	1A	3816	1/1	0.90	0.09	77,77,77,77	0
56	MG	2A	3460	1/1	0.90	0.17	50,50,50,50	0
56	MG	2A	3818	1/1	0.90	0.05	45,45,45,45	0
56	MG	2a	3207	1/1	0.90	0.15	60,60,60,60	0
56	MG	2A	3276	1/1	0.90	0.28	50,50,50,50	0
56	MG	2a	3216	1/1	0.90	0.14	58,58,58,58	0
56	MG	1A	3609	1/1	0.90	0.20	31,31,31,31	0
56	MG	1A	3821	1/1	0.90	0.09	42,42,42,42	0
56	MG	2A	3284	1/1	0.90	0.15	56,56,56,56	0
56	MG	1a	1761	1/1	0.90	0.14	44,44,44,44	0
56	MG	1A	3466	1/1	0.90	0.17	25,25,25,25	0
56	MG	2a	3234	1/1	0.90	0.19	58,58,58,58	0
56	MG	2A	3862	1/1	0.90	0.12	50,50,50,50	0
56	MG	2j	202	1/1	0.90	0.09	58,58,58,58	0
56	MG	2A	3293	1/1	0.90	0.10	62,62,62,62	0
56	MG	1A	3611	1/1	0.90	0.29	40,40,40,40	0
56	MG	1A	3029	1/1	0.90	0.15	28,28,28,28	0
56	MG	1a	1769	1/1	0.90	0.15	63,63,63,63	0
56	MG	2w	103	1/1	0.90	0.07	54,54,54,54	0
56	MG	1a	1772	1/1	0.90	0.14	43,43,43,43	0
56	MG	2B	215	1/1	0.90	0.15	52,52,52,52	0
56	MG	2A	3107	1/1	0.90	0.12	33,33,33,33	0
56	MG	1a	1776	1/1	0.90	0.13	57,57,57,57	0
56	MG	2D	301	1/1	0.90	0.27	41,41,41,41	0
56	MG	1A	3308	1/1	0.90	0.12	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2D	306	1/1	0.90	0.10	52,52,52,52	0
56	MG	1A	3117	1/1	0.90	0.20	31,31,31,31	0
56	MG	1A	3474	1/1	0.90	0.17	56,56,56,56	0
56	MG	2E	309	1/1	0.90	0.11	42,42,42,42	0
56	MG	1a	1603	1/1	0.90	0.13	43,43,43,43	0
56	MG	1A	4053	1/1	0.90	0.11	48,48,48,48	0
56	MG	1A	3957	1/1	0.91	0.13	30,30,30,30	0
56	MG	1a	1699	1/1	0.91	0.23	35,35,35,35	0
56	MG	2A	3478	1/1	0.91	0.21	71,71,71,71	0
56	MG	2E	303	1/1	0.91	0.10	41,41,41,41	0
56	MG	1F	306	1/1	0.91	0.15	39,39,39,39	0
56	MG	2A	3485	1/1	0.91	0.17	56,56,56,56	0
56	MG	1A	3727	1/1	0.91	0.13	28,28,28,28	0
56	MG	2A	3278	1/1	0.91	0.10	55,55,55,55	0
56	MG	2A	3280	1/1	0.91	0.21	34,34,34,34	0
56	MG	2A	3281	1/1	0.91	0.08	36,36,36,36	0
56	MG	1A	3962	1/1	0.91	0.11	32,32,32,32	0
56	MG	2N	201	1/1	0.91	0.18	40,40,40,40	0
56	MG	2A	3497	1/1	0.91	0.20	61,61,61,61	0
56	MG	1a	1709	1/1	0.91	0.17	43,43,43,43	0
56	MG	2R	202	1/1	0.91	0.11	46,46,46,46	0
56	MG	1N	202	1/1	0.91	0.15	46,46,46,46	0
56	MG	1a	1712	1/1	0.91	0.15	51,51,51,51	0
56	MG	1A	3492	1/1	0.91	0.36	40,40,40,40	0
56	MG	1A	3570	1/1	0.91	0.15	54,54,54,54	0
56	MG	2A	3517	1/1	0.91	0.12	55,55,55,55	0
56	MG	1A	3437	1/1	0.91	0.20	50,50,50,50	0
56	MG	1A	3438	1/1	0.91	0.27	44,44,44,44	0
56	MG	1P	203	1/1	0.91	0.32	29,29,29,29	0
56	MG	1A	3974	1/1	0.91	0.07	41,41,41,41	0
56	MG	2A	3301	1/1	0.91	0.21	58,58,58,58	0
56	MG	1A	3574	1/1	0.91	0.24	42,42,42,42	0
56	MG	1R	202	1/1	0.91	0.21	38,38,38,38	0
56	MG	2A	3549	1/1	0.91	0.12	37,37,37,37	0
56	MG	1a	1726	1/1	0.91	0.26	44,44,44,44	0
56	MG	1A	3496	1/1	0.91	0.17	35,35,35,35	0
56	MG	1A	3497	1/1	0.91	0.26	38,38,38,38	0
56	MG	2A	3101	1/1	0.91	0.19	49,49,49,49	0
56	MG	1A	3104	1/1	0.91	0.18	33,33,33,33	0
56	MG	1A	3393	1/1	0.91	0.19	28,28,28,28	0
56	MG	1A	3768	1/1	0.91	0.18	44,44,44,44	0
56	MG	1A	3584	1/1	0.91	0.23	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3017	1/1	0.91	0.13	51,51,51,51	0
56	MG	2A	3575	1/1	0.91	0.10	40,40,40,40	0
56	MG	1A	3233	1/1	0.91	0.19	31,31,31,31	0
56	MG	1V	204	1/1	0.91	0.21	39,39,39,39	0
56	MG	1A	3396	1/1	0.91	0.18	48,48,48,48	0
56	MG	2a	3026	1/1	0.91	0.18	50,50,50,50	0
56	MG	1A	3208	1/1	0.91	0.15	42,42,42,42	0
56	MG	2a	3030	1/1	0.91	0.14	46,46,46,46	0
56	MG	1A	3209	1/1	0.91	0.18	19,19,19,19	0
56	MG	2A	3617	1/1	0.91	0.17	48,48,48,48	0
56	MG	2A	3619	1/1	0.91	0.14	58,58,58,58	0
56	MG	2A	3121	1/1	0.91	0.14	56,56,56,56	0
56	MG	1A	3512	1/1	0.91	0.19	54,54,54,54	0
56	MG	2a	3044	1/1	0.91	0.09	54,54,54,54	0
56	MG	1A	3301	1/1	0.91	0.27	48,48,48,48	0
56	MG	1a	1773	1/1	0.91	0.11	58,58,58,58	0
56	MG	2A	3133	1/1	0.91	0.13	35,35,35,35	0
56	MG	1A	3105	1/1	0.91	0.19	30,30,30,30	0
56	MG	1A	3135	1/1	0.91	0.21	35,35,35,35	0
56	MG	2A	3338	1/1	0.91	0.18	46,46,46,46	0
56	MG	1A	3358	1/1	0.91	0.12	45,45,45,45	0
56	MG	1A	4015	1/1	0.91	0.10	29,29,29,29	0
56	MG	2A	3347	1/1	0.91	0.12	54,54,54,54	0
56	MG	16	102	1/1	0.91	0.51	51,51,51,51	0
56	MG	1A	3024	1/1	0.91	0.19	44,44,44,44	0
56	MG	1a	1792	1/1	0.91	0.27	36,36,36,36	0
56	MG	1A	4019	1/1	0.91	0.10	45,45,45,45	0
56	MG	2a	3072	1/1	0.91	0.23	42,42,42,42	0
56	MG	2A	3353	1/1	0.91	0.10	66,66,66,66	0
56	MG	2a	3074	1/1	0.91	0.09	67,67,67,67	0
56	MG	1A	3463	1/1	0.91	0.57	43,43,43,43	0
56	MG	2A	3355	1/1	0.91	0.23	41,41,41,41	0
56	MG	1A	4026	1/1	0.91	0.16	26,26,26,26	0
56	MG	1A	3218	1/1	0.91	0.13	36,36,36,36	0
56	MG	2A	3683	1/1	0.91	0.14	47,47,47,47	0
56	MG	2a	3087	1/1	0.91	0.12	55,55,55,55	0
56	MG	1A	3532	1/1	0.91	0.27	37,37,37,37	0
56	MG	2A	3167	1/1	0.91	0.22	34,34,34,34	0
56	MG	1A	3616	1/1	0.91	0.21	50,50,50,50	0
56	MG	2A	3687	1/1	0.91	0.11	61,61,61,61	0
56	MG	2A	3171	1/1	0.91	0.12	72,72,72,72	0
56	MG	1A	3315	1/1	0.91	0.17	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3412	1/1	0.91	0.26	38,38,38,38	0
56	MG	2A	3699	1/1	0.91	0.10	54,54,54,54	0
56	MG	1a	1816	1/1	0.91	0.12	51,51,51,51	0
56	MG	1A	3469	1/1	0.91	0.28	33,33,33,33	0
56	MG	1A	3224	1/1	0.91	0.20	40,40,40,40	0
56	MG	1A	3625	1/1	0.91	0.27	39,39,39,39	0
56	MG	1A	3471	1/1	0.91	0.23	40,40,40,40	0
56	MG	1A	3853	1/1	0.91	0.10	19,19,19,19	0
56	MG	2A	3188	1/1	0.91	0.14	41,41,41,41	0
56	MG	2A	3189	1/1	0.91	0.16	58,58,58,58	0
56	MG	1f	201	1/1	0.91	0.16	42,42,42,42	0
56	MG	1A	3002	1/1	0.91	0.16	52,52,52,52	0
56	MG	2A	3736	1/1	0.91	0.12	50,50,50,50	0
56	MG	1A	3418	1/1	0.91	0.15	44,44,44,44	0
56	MG	2a	3132	1/1	0.91	0.16	58,58,58,58	0
56	MG	2a	3134	1/1	0.91	0.23	49,49,49,49	0
56	MG	1A	4075	1/1	0.91	0.15	33,33,33,33	0
56	MG	2a	3136	1/1	0.91	0.09	60,60,60,60	0
56	MG	2A	3197	1/1	0.91	0.13	48,48,48,48	0
56	MG	1A	3100	1/1	0.91	0.15	34,34,34,34	0
56	MG	1a	1630	1/1	0.91	0.28	51,51,51,51	0
56	MG	1A	3423	1/1	0.91	0.26	39,39,39,39	0
56	MG	1A	3544	1/1	0.91	0.26	41,41,41,41	0
56	MG	1A	4097	1/1	0.91	0.14	49,49,49,49	0
56	MG	2A	3207	1/1	0.91	0.13	54,54,54,54	0
56	MG	1a	1637	1/1	0.91	0.16	43,43,43,43	0
56	MG	1A	3886	1/1	0.91	0.15	57,57,57,57	0
56	MG	2A	3762	1/1	0.91	0.22	60,60,60,60	0
56	MG	2a	3163	1/1	0.91	0.18	66,66,66,66	0
56	MG	2A	3766	1/1	0.91	0.17	48,48,48,48	0
56	MG	1A	3892	1/1	0.91	0.14	37,37,37,37	0
56	MG	2A	3769	1/1	0.91	0.17	56,56,56,56	0
56	MG	1A	3897	1/1	0.91	0.11	34,34,34,34	0
56	MG	2A	3772	1/1	0.91	0.12	40,40,40,40	0
56	MG	1a	1651	1/1	0.91	0.15	49,49,49,49	0
56	MG	1A	3658	1/1	0.91	0.13	33,33,33,33	0
56	MG	1x	111	1/1	0.91	0.12	36,36,36,36	0
56	MG	2A	3416	1/1	0.91	0.13	50,50,50,50	0
56	MG	1A	3906	1/1	0.91	0.26	41,41,41,41	0
56	MG	1y	104	1/1	0.91	0.29	72,72,72,72	0
56	MG	2A	3228	1/1	0.91	0.16	42,42,42,42	0
56	MG	2A	3001	1/1	0.91	0.36	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3484	1/1	0.91	0.17	47,47,47,47	0
56	MG	1A	3913	1/1	0.91	0.15	18,18,18,18	0
56	MG	2a	3206	1/1	0.91	0.22	58,58,58,58	0
56	MG	1B	210	1/1	0.91	0.31	41,41,41,41	0
56	MG	1A	3914	1/1	0.91	0.23	29,29,29,29	0
56	MG	2a	3214	1/1	0.91	0.12	64,64,64,64	0
56	MG	2A	3013	1/1	0.91	0.20	50,50,50,50	0
56	MG	2A	3442	1/1	0.91	0.13	46,46,46,46	0
56	MG	2A	3014	1/1	0.91	0.26	49,49,49,49	0
56	MG	2A	3447	1/1	0.91	0.17	45,45,45,45	0
56	MG	2A	3016	1/1	0.91	0.18	60,60,60,60	0
56	MG	1a	1667	1/1	0.91	0.13	62,62,62,62	0
56	MG	1A	3665	1/1	0.91	0.20	23,23,23,23	0
56	MG	2e	201	1/1	0.91	0.07	52,52,52,52	0
56	MG	1A	3556	1/1	0.91	0.19	52,52,52,52	0
56	MG	1A	3193	1/1	0.91	0.20	29,29,29,29	0
56	MG	2l	201	1/1	0.91	0.11	59,59,59,59	0
56	MG	1B	228	1/1	0.91	0.07	59,59,59,59	0
56	MG	2A	3254	1/1	0.91	0.19	61,61,61,61	0
56	MG	2q	202	1/1	0.91	0.17	60,60,60,60	0
56	MG	1A	3269	1/1	0.91	0.18	44,44,44,44	0
56	MG	2A	3865	1/1	0.91	0.09	46,46,46,46	0
56	MG	1A	3679	1/1	0.91	0.16	33,33,33,33	0
56	MG	1a	1687	1/1	0.91	0.21	32,32,32,32	0
56	MG	2w	106	1/1	0.91	0.25	72,72,72,72	0
56	MG	2A	3876	1/1	0.91	0.10	66,66,66,66	0
56	MG	1A	3082	1/1	0.91	0.16	23,23,23,23	0
56	MG	2x	104	1/1	0.91	0.17	48,48,48,48	0
56	MG	2B	202	1/1	0.91	0.16	53,53,53,53	0
56	MG	2B	203	1/1	0.91	0.16	63,63,63,63	0
56	MG	2B	208	1/1	0.91	0.18	52,52,52,52	0
56	MG	2B	209	1/1	0.91	0.15	53,53,53,53	0
56	MG	2B	213	1/1	0.91	0.23	55,55,55,55	0
56	MG	1A	3279	1/1	0.91	0.23	44,44,44,44	0
56	MG	2A	3471	1/1	0.91	0.19	47,47,47,47	0
56	MG	1A	3281	1/1	0.91	0.23	49,49,49,49	0
56	MG	1A	3345	1/1	0.91	0.14	51,51,51,51	0
56	MG	1a	1631	1/1	0.92	0.20	43,43,43,43	0
56	MG	2A	3448	1/1	0.92	0.16	48,48,48,48	0
56	MG	2A	3224	1/1	0.92	0.12	62,62,62,62	0
56	MG	2B	201	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	4095	1/1	0.92	0.21	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1x	107	1/1	0.92	0.19	51,51,51,51	0
56	MG	2B	206	1/1	0.92	0.16	50,50,50,50	0
56	MG	2A	3230	1/1	0.92	0.20	46,46,46,46	0
56	MG	1A	3899	1/1	0.92	0.23	43,43,43,43	0
56	MG	2B	210	1/1	0.92	0.10	57,57,57,57	0
56	MG	2A	3459	1/1	0.92	0.23	43,43,43,43	0
56	MG	1A	3900	1/1	0.92	0.21	28,28,28,28	0
56	MG	1A	3692	1/1	0.92	0.22	28,28,28,28	0
56	MG	1x	113	1/1	0.92	0.29	51,51,51,51	0
56	MG	2B	219	1/1	0.92	0.17	49,49,49,49	0
56	MG	1x	114	1/1	0.92	0.13	60,60,60,60	0
56	MG	2A	3466	1/1	0.92	0.12	40,40,40,40	0
56	MG	1y	102	1/1	0.92	0.13	45,45,45,45	0
56	MG	1A	3006	1/1	0.92	0.20	42,42,42,42	0
56	MG	1A	3696	1/1	0.92	0.14	28,28,28,28	0
56	MG	1A	3454	1/1	0.92	0.13	41,41,41,41	0
56	MG	2A	3248	1/1	0.92	0.19	48,48,48,48	0
56	MG	2A	3002	1/1	0.92	0.29	45,45,45,45	0
56	MG	1A	3702	1/1	0.92	0.13	28,28,28,28	0
56	MG	1A	3915	1/1	0.92	0.25	21,21,21,21	0
56	MG	1A	3704	1/1	0.92	0.17	18,18,18,18	0
56	MG	1A	3706	1/1	0.92	0.19	12,12,12,12	0
56	MG	1A	3156	1/1	0.92	0.50	35,35,35,35	0
56	MG	1A	3710	1/1	0.92	0.19	47,47,47,47	0
56	MG	2Q	202	1/1	0.92	0.17	44,44,44,44	0
56	MG	1B	213	1/1	0.92	0.19	50,50,50,50	0
56	MG	1A	3244	1/1	0.92	0.14	44,44,44,44	0
56	MG	1A	3160	1/1	0.92	0.14	42,42,42,42	0
56	MG	2A	3266	1/1	0.92	0.11	42,42,42,42	0
56	MG	1A	3946	1/1	0.92	0.17	38,38,38,38	0
56	MG	1A	3416	1/1	0.92	0.26	41,41,41,41	0
56	MG	2A	3027	1/1	0.92	0.10	35,35,35,35	0
56	MG	2A	3272	1/1	0.92	0.16	54,54,54,54	0
56	MG	2A	3505	1/1	0.92	0.18	41,41,41,41	0
56	MG	1A	3951	1/1	0.92	0.13	54,54,54,54	0
56	MG	25	104	1/1	0.92	0.20	46,46,46,46	0
56	MG	28	101	1/1	0.92	0.26	59,59,59,59	0
56	MG	2A	3509	1/1	0.92	0.20	58,58,58,58	0
56	MG	28	104	1/1	0.92	0.21	53,53,53,53	0
56	MG	1A	3295	1/1	0.92	0.18	33,33,33,33	0
56	MG	1a	1681	1/1	0.92	0.13	66,66,66,66	0
56	MG	1A	3517	1/1	0.92	0.20	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3039	1/1	0.92	0.18	46,46,46,46	0
56	MG	2A	3041	1/1	0.92	0.20	54,54,54,54	0
56	MG	1a	1685	1/1	0.92	0.22	47,47,47,47	0
56	MG	2A	3530	1/1	0.92	0.09	36,36,36,36	0
56	MG	1A	3587	1/1	0.92	0.25	18,18,18,18	0
56	MG	1A	3959	1/1	0.92	0.09	35,35,35,35	0
56	MG	1E	307	1/1	0.92	0.23	41,41,41,41	0
56	MG	2A	3054	1/1	0.92	0.11	42,42,42,42	0
56	MG	1A	3346	1/1	0.92	0.21	36,36,36,36	0
56	MG	2a	3016	1/1	0.92	0.14	55,55,55,55	0
56	MG	1A	3745	1/1	0.92	0.24	50,50,50,50	0
56	MG	1a	1695	1/1	0.92	0.23	47,47,47,47	0
56	MG	2A	3065	1/1	0.92	0.20	49,49,49,49	0
56	MG	2A	3297	1/1	0.92	0.16	68,68,68,68	0
56	MG	2A	3299	1/1	0.92	0.21	52,52,52,52	0
56	MG	1A	3964	1/1	0.92	0.08	45,45,45,45	0
56	MG	1G	204	1/1	0.92	0.12	54,54,54,54	0
56	MG	1a	1702	1/1	0.92	0.30	57,57,57,57	0
56	MG	2A	3577	1/1	0.92	0.07	67,67,67,67	0
56	MG	2A	3579	1/1	0.92	0.14	53,53,53,53	0
56	MG	2A	3586	1/1	0.92	0.14	62,62,62,62	0
56	MG	2A	3304	1/1	0.92	0.22	52,52,52,52	0
56	MG	2A	3591	1/1	0.92	0.16	33,33,33,33	0
56	MG	2a	3043	1/1	0.92	0.15	62,62,62,62	0
56	MG	1a	1703	1/1	0.92	0.28	41,41,41,41	0
56	MG	2a	3047	1/1	0.92	0.11	51,51,51,51	0
56	MG	1a	1704	1/1	0.92	0.21	53,53,53,53	0
56	MG	2A	3078	1/1	0.92	0.12	45,45,45,45	0
56	MG	1A	3420	1/1	0.92	0.17	34,34,34,34	0
56	MG	2A	3610	1/1	0.92	0.13	49,49,49,49	0
56	MG	1A	3421	1/1	0.92	0.11	39,39,39,39	0
56	MG	1A	3249	1/1	0.92	0.30	35,35,35,35	0
56	MG	2a	3059	1/1	0.92	0.20	46,46,46,46	0
56	MG	1A	3526	1/1	0.92	0.27	47,47,47,47	0
56	MG	1A	3766	1/1	0.92	0.12	57,57,57,57	0
56	MG	2A	3626	1/1	0.92	0.11	37,37,37,37	0
56	MG	1a	1711	1/1	0.92	0.21	48,48,48,48	0
56	MG	2A	3319	1/1	0.92	0.10	55,55,55,55	0
56	MG	1A	3976	1/1	0.92	0.14	34,34,34,34	0
56	MG	1P	202	1/1	0.92	0.16	23,23,23,23	0
56	MG	2A	3322	1/1	0.92	0.21	57,57,57,57	0
56	MG	1A	3601	1/1	0.92	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3769	1/1	0.92	0.10	43,43,43,43	0
56	MG	1A	3981	1/1	0.92	0.15	33,33,33,33	0
56	MG	1A	3384	1/1	0.92	0.17	31,31,31,31	0
56	MG	2A	3647	1/1	0.92	0.19	49,49,49,49	0
56	MG	1A	3425	1/1	0.92	0.20	36,36,36,36	0
56	MG	2a	3085	1/1	0.92	0.15	49,49,49,49	0
56	MG	1A	3164	1/1	0.92	0.38	35,35,35,35	0
56	MG	2A	3659	1/1	0.92	0.21	46,46,46,46	0
56	MG	2a	3089	1/1	0.92	0.21	53,53,53,53	0
56	MG	2a	3090	1/1	0.92	0.13	59,59,59,59	0
56	MG	1A	3990	1/1	0.92	0.11	38,38,38,38	0
56	MG	1A	3428	1/1	0.92	0.27	38,38,38,38	0
56	MG	2A	3666	1/1	0.92	0.12	58,58,58,58	0
56	MG	1a	1727	1/1	0.92	0.21	37,37,37,37	0
56	MG	1T	202	1/1	0.92	0.15	46,46,46,46	0
56	MG	2a	3102	1/1	0.92	0.11	48,48,48,48	0
56	MG	1a	1732	1/1	0.92	0.28	43,43,43,43	0
56	MG	2A	3678	1/1	0.92	0.16	50,50,50,50	0
56	MG	2A	3343	1/1	0.92	0.29	55,55,55,55	0
56	MG	1A	3304	1/1	0.92	0.27	12,12,12,12	0
56	MG	1U	202	1/1	0.92	0.23	31,31,31,31	0
56	MG	2A	3118	1/1	0.92	0.15	66,66,66,66	0
56	MG	2a	3118	1/1	0.92	0.28	61,61,61,61	0
56	MG	1a	1738	1/1	0.92	0.29	47,47,47,47	0
56	MG	1A	3219	1/1	0.92	0.17	35,35,35,35	0
56	MG	1A	3800	1/1	0.92	0.14	38,38,38,38	0
56	MG	1U	210	1/1	0.92	0.23	49,49,49,49	0
56	MG	2A	3352	1/1	0.92	0.13	48,48,48,48	0
56	MG	1A	3134	1/1	0.92	0.10	25,25,25,25	0
56	MG	1A	3480	1/1	0.92	0.21	45,45,45,45	0
56	MG	1X	104	1/1	0.92	0.38	34,34,34,34	0
56	MG	2A	3702	1/1	0.92	0.12	44,44,44,44	0
56	MG	2A	3138	1/1	0.92	0.28	38,38,38,38	0
56	MG	2A	3142	1/1	0.92	0.27	38,38,38,38	0
56	MG	1A	3041	1/1	0.92	0.16	38,38,38,38	0
56	MG	1a	1767	1/1	0.92	0.07	57,57,57,57	0
56	MG	2A	3721	1/1	0.92	0.15	49,49,49,49	0
56	MG	2A	3360	1/1	0.92	0.23	66,66,66,66	0
56	MG	2a	3141	1/1	0.92	0.17	64,64,64,64	0
56	MG	1Y	201	1/1	0.92	0.21	44,44,44,44	0
56	MG	2A	3729	1/1	0.92	0.11	55,55,55,55	0
56	MG	1A	3226	1/1	0.92	0.22	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3046	1/1	0.92	0.18	33,33,33,33	0
56	MG	10	102	1/1	0.92	0.14	40,40,40,40	0
56	MG	1A	3030	1/1	0.92	0.23	33,33,33,33	0
56	MG	2a	3155	1/1	0.92	0.08	67,67,67,67	0
56	MG	1A	3440	1/1	0.92	0.34	51,51,51,51	0
56	MG	1A	3360	1/1	0.92	0.19	40,40,40,40	0
56	MG	1A	3552	1/1	0.92	0.20	37,37,37,37	0
56	MG	1A	3634	1/1	0.92	0.10	29,29,29,29	0
56	MG	2A	3376	1/1	0.92	0.11	46,46,46,46	0
56	MG	2A	3377	1/1	0.92	0.15	57,57,57,57	0
56	MG	2A	3168	1/1	0.92	0.10	55,55,55,55	0
56	MG	2a	3179	1/1	0.92	0.12	60,60,60,60	0
56	MG	2A	3750	1/1	0.92	0.13	56,56,56,56	0
56	MG	1A	3638	1/1	0.92	0.15	17,17,17,17	0
56	MG	1a	1788	1/1	0.92	0.23	67,67,67,67	0
56	MG	16	103	1/1	0.92	0.18	46,46,46,46	0
56	MG	1A	4023	1/1	0.92	0.17	39,39,39,39	0
56	MG	2a	3189	1/1	0.92	0.16	49,49,49,49	0
56	MG	1A	3553	1/1	0.92	0.32	55,55,55,55	0
56	MG	2A	3763	1/1	0.92	0.12	43,43,43,43	0
56	MG	2a	3195	1/1	0.92	0.11	62,62,62,62	0
56	MG	1a	1798	1/1	0.92	0.10	42,42,42,42	0
56	MG	1A	3402	1/1	0.92	0.27	42,42,42,42	0
56	MG	2A	3397	1/1	0.92	0.08	58,58,58,58	0
56	MG	2A	3181	1/1	0.92	0.08	36,36,36,36	0
56	MG	1A	3841	1/1	0.92	0.14	42,42,42,42	0
56	MG	1A	3446	1/1	0.92	0.10	55,55,55,55	0
56	MG	2a	3208	1/1	0.92	0.12	51,51,51,51	0
56	MG	1A	4040	1/1	0.92	0.11	41,41,41,41	0
56	MG	2a	3212	1/1	0.92	0.13	59,59,59,59	0
56	MG	2a	3213	1/1	0.92	0.15	56,56,56,56	0
56	MG	2A	3780	1/1	0.92	0.08	48,48,48,48	0
56	MG	2A	3402	1/1	0.92	0.12	38,38,38,38	0
56	MG	2A	3782	1/1	0.92	0.17	55,55,55,55	0
56	MG	1a	1606	1/1	0.92	0.18	51,51,51,51	0
56	MG	1A	3068	1/1	0.92	0.21	43,43,43,43	0
56	MG	2A	3405	1/1	0.92	0.17	48,48,48,48	0
56	MG	2A	3788	1/1	0.92	0.10	33,33,33,33	0
56	MG	1a	1609	1/1	0.92	0.14	50,50,50,50	0
56	MG	1A	3183	1/1	0.92	0.16	25,25,25,25	0
56	MG	2f	201	1/1	0.92	0.16	40,40,40,40	0
56	MG	2g	201	1/1	0.92	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3798	1/1	0.92	0.17	54,54,54,54	0
56	MG	2A	3801	1/1	0.92	0.13	66,66,66,66	0
56	MG	1a	1613	1/1	0.92	0.21	48,48,48,48	0
56	MG	1A	3855	1/1	0.92	0.19	31,31,31,31	0
56	MG	2l	203	1/1	0.92	0.10	62,62,62,62	0
56	MG	1A	3132	1/1	0.92	0.12	59,59,59,59	0
56	MG	1a	1617	1/1	0.92	0.20	36,36,36,36	0
56	MG	1A	3450	1/1	0.92	0.16	49,49,49,49	0
56	MG	2A	3815	1/1	0.92	0.24	41,41,41,41	0
56	MG	1A	3452	1/1	0.92	0.14	34,34,34,34	0
56	MG	2A	3421	1/1	0.92	0.24	43,43,43,43	0
56	MG	1a	1620	1/1	0.92	0.14	44,44,44,44	0
56	MG	1a	1622	1/1	0.92	0.21	52,52,52,52	0
56	MG	1A	3499	1/1	0.92	0.16	47,47,47,47	0
56	MG	2A	3830	1/1	0.92	0.10	66,66,66,66	0
56	MG	1p	101	1/1	0.92	0.19	38,38,38,38	0
56	MG	2A	3850	1/1	0.92	0.10	58,58,58,58	0
56	MG	1A	3671	1/1	0.92	0.16	20,20,20,20	0
56	MG	1A	4061	1/1	0.92	0.18	38,38,38,38	0
56	MG	1A	3501	1/1	0.92	0.15	41,41,41,41	0
56	MG	1A	3503	1/1	0.92	0.25	51,51,51,51	0
56	MG	1A	3683	1/1	0.92	0.18	31,31,31,31	0
56	MG	1A	3898	1/1	0.92	0.13	41,41,41,41	0
56	MG	2A	3222	1/1	0.92	0.57	53,53,53,53	0
56	MG	1A	3534	1/1	0.93	0.20	29,29,29,29	0
56	MG	2A	3877	1/1	0.93	0.07	45,45,45,45	0
56	MG	2A	3449	1/1	0.93	0.06	65,65,65,65	0
56	MG	2A	3450	1/1	0.93	0.15	51,51,51,51	0
56	MG	1a	1608	1/1	0.93	0.18	42,42,42,42	0
56	MG	2A	3453	1/1	0.93	0.19	43,43,43,43	0
56	MG	1A	4048	1/1	0.93	0.09	38,38,38,38	0
56	MG	1A	3642	1/1	0.93	0.16	33,33,33,33	0
56	MG	2A	3210	1/1	0.93	0.17	40,40,40,40	0
56	MG	1m	3001	1/1	0.93	0.09	53,53,53,53	0
56	MG	1A	3867	1/1	0.93	0.11	32,32,32,32	0
56	MG	1A	3868	1/1	0.93	0.12	41,41,41,41	0
56	MG	1A	3145	1/1	0.93	0.24	37,37,37,37	0
56	MG	2A	3462	1/1	0.93	0.29	51,51,51,51	0
56	MG	2A	3218	1/1	0.93	0.20	45,45,45,45	0
56	MG	1A	3324	1/1	0.93	0.20	54,54,54,54	0
56	MG	1A	3325	1/1	0.93	0.25	42,42,42,42	0
56	MG	2A	3467	1/1	0.93	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1w	101	1/1	0.93	0.09	60,60,60,60	0
56	MG	2E	302	1/1	0.93	0.14	52,52,52,52	0
56	MG	1A	3048	1/1	0.93	0.21	22,22,22,22	0
56	MG	1A	4069	1/1	0.93	0.26	32,32,32,32	0
56	MG	1A	3327	1/1	0.93	0.28	43,43,43,43	0
56	MG	1A	3467	1/1	0.93	0.14	63,63,63,63	0
56	MG	2F	302	1/1	0.93	0.25	58,58,58,58	0
56	MG	1A	4080	1/1	0.93	0.19	59,59,59,59	0
56	MG	1A	3149	1/1	0.93	0.17	28,28,28,28	0
56	MG	1A	4083	1/1	0.93	0.19	37,37,37,37	0
56	MG	1A	4084	1/1	0.93	0.11	44,44,44,44	0
56	MG	1A	3332	1/1	0.93	0.31	52,52,52,52	0
56	MG	2A	3482	1/1	0.93	0.38	56,56,56,56	0
56	MG	1A	3250	1/1	0.93	0.13	48,48,48,48	0
56	MG	1A	3546	1/1	0.93	0.12	37,37,37,37	0
56	MG	1A	3549	1/1	0.93	0.21	31,31,31,31	0
56	MG	1y	101	1/1	0.93	0.24	41,41,41,41	0
56	MG	2A	3245	1/1	0.93	0.22	59,59,59,59	0
56	MG	1A	3201	1/1	0.93	0.10	48,48,48,48	0
56	MG	20	101	1/1	0.93	0.20	45,45,45,45	0
56	MG	1A	3076	1/1	0.93	0.15	23,23,23,23	0
56	MG	2A	3499	1/1	0.93	0.22	54,54,54,54	0
56	MG	23	103	1/1	0.93	0.20	53,53,53,53	0
56	MG	1A	3005	1/1	0.93	0.21	36,36,36,36	0
56	MG	1A	3113	1/1	0.93	0.20	39,39,39,39	0
56	MG	1B	201	1/1	0.93	0.17	38,38,38,38	0
56	MG	1B	202	1/1	0.93	0.32	38,38,38,38	0
56	MG	27	101	1/1	0.93	0.36	44,44,44,44	0
56	MG	1B	203	1/1	0.93	0.31	52,52,52,52	0
56	MG	1A	3560	1/1	0.93	0.18	24,24,24,24	0
56	MG	2A	3256	1/1	0.93	0.20	66,66,66,66	0
56	MG	2A	3009	1/1	0.93	0.16	44,44,44,44	0
56	MG	1a	1660	1/1	0.93	0.22	63,63,63,63	0
56	MG	1A	3344	1/1	0.93	0.21	35,35,35,35	0
56	MG	1A	3917	1/1	0.93	0.16	36,36,36,36	0
56	MG	1A	3262	1/1	0.93	0.17	31,31,31,31	0
56	MG	1A	3922	1/1	0.93	0.15	22,22,22,22	0
56	MG	1A	3924	1/1	0.93	0.22	55,55,55,55	0
56	MG	1A	3481	1/1	0.93	0.17	27,27,27,27	0
56	MG	1a	1668	1/1	0.93	0.12	44,44,44,44	0
56	MG	2A	3022	1/1	0.93	0.26	46,46,46,46	0
56	MG	2A	3023	1/1	0.93	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3114	1/1	0.93	0.19	35,35,35,35	0
56	MG	1B	215	1/1	0.93	0.11	46,46,46,46	0
56	MG	2A	3279	1/1	0.93	0.21	48,48,48,48	0
56	MG	2A	3030	1/1	0.93	0.14	43,43,43,43	0
56	MG	2a	3019	1/1	0.93	0.08	59,59,59,59	0
56	MG	2A	3562	1/1	0.93	0.13	42,42,42,42	0
56	MG	1a	1672	1/1	0.93	0.27	48,48,48,48	0
56	MG	2A	3565	1/1	0.93	0.16	33,33,33,33	0
56	MG	1B	221	1/1	0.93	0.19	43,43,43,43	0
56	MG	1B	223	1/1	0.93	0.12	51,51,51,51	0
56	MG	2a	3028	1/1	0.93	0.10	59,59,59,59	0
56	MG	2A	3037	1/1	0.93	0.13	37,37,37,37	0
56	MG	2a	3031	1/1	0.93	0.18	46,46,46,46	0
56	MG	2A	3038	1/1	0.93	0.15	29,29,29,29	0
56	MG	2a	3037	1/1	0.93	0.22	46,46,46,46	0
56	MG	2A	3290	1/1	0.93	0.10	48,48,48,48	0
56	MG	2A	3291	1/1	0.93	0.06	62,62,62,62	0
56	MG	1a	1679	1/1	0.93	0.16	46,46,46,46	0
56	MG	2a	3041	1/1	0.93	0.29	56,56,56,56	0
56	MG	2A	3040	1/1	0.93	0.18	47,47,47,47	0
56	MG	1A	3065	1/1	0.93	0.29	41,41,41,41	0
56	MG	2A	3042	1/1	0.93	0.24	59,59,59,59	0
56	MG	2a	3045	1/1	0.93	0.08	46,46,46,46	0
56	MG	2a	3046	1/1	0.93	0.26	55,55,55,55	0
56	MG	1A	3486	1/1	0.93	0.17	38,38,38,38	0
56	MG	2A	3044	1/1	0.93	0.11	44,44,44,44	0
56	MG	1A	3939	1/1	0.93	0.18	34,34,34,34	0
56	MG	2A	3051	1/1	0.93	0.08	41,41,41,41	0
56	MG	1A	3713	1/1	0.93	0.18	45,45,45,45	0
56	MG	1B	231	1/1	0.93	0.22	53,53,53,53	0
56	MG	1A	3084	1/1	0.93	0.20	22,22,22,22	0
56	MG	2A	3623	1/1	0.93	0.16	35,35,35,35	0
56	MG	1D	303	1/1	0.93	0.20	10,10,10,10	0
56	MG	1D	304	1/1	0.93	0.16	28,28,28,28	0
56	MG	2A	3061	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	3717	1/1	0.93	0.15	39,39,39,39	0
56	MG	2A	3313	1/1	0.93	0.14	59,59,59,59	0
56	MG	1A	3950	1/1	0.93	0.16	34,34,34,34	0
56	MG	2A	3066	1/1	0.93	0.25	47,47,47,47	0
56	MG	2A	3638	1/1	0.93	0.14	30,30,30,30	0
56	MG	2A	3069	1/1	0.93	0.36	55,55,55,55	0
56	MG	1E	303	1/1	0.93	0.14	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3643	1/1	0.93	0.18	47,47,47,47	0
56	MG	2a	3078	1/1	0.93	0.12	55,55,55,55	0
56	MG	1a	1697	1/1	0.93	0.21	36,36,36,36	0
56	MG	2a	3081	1/1	0.93	0.17	60,60,60,60	0
56	MG	1A	3722	1/1	0.93	0.16	16,16,16,16	0
56	MG	1a	1701	1/1	0.93	0.24	45,45,45,45	0
56	MG	1A	3067	1/1	0.93	0.18	31,31,31,31	0
56	MG	1E	308	1/1	0.93	0.17	16,16,16,16	0
56	MG	2A	3324	1/1	0.93	0.13	44,44,44,44	0
56	MG	2A	3079	1/1	0.93	0.14	51,51,51,51	0
56	MG	2A	3081	1/1	0.93	0.18	46,46,46,46	0
56	MG	2A	3668	1/1	0.93	0.15	59,59,59,59	0
56	MG	1E	312	1/1	0.93	0.24	45,45,45,45	0
56	MG	1E	313	1/1	0.93	0.12	23,23,23,23	0
56	MG	1A	3271	1/1	0.93	0.15	57,57,57,57	0
56	MG	1A	3124	1/1	0.93	0.22	32,32,32,32	0
56	MG	1a	1708	1/1	0.93	0.27	48,48,48,48	0
56	MG	2a	3103	1/1	0.93	0.11	54,54,54,54	0
56	MG	1F	308	1/1	0.93	0.24	40,40,40,40	0
56	MG	2a	3105	1/1	0.93	0.15	53,53,53,53	0
56	MG	1A	3277	1/1	0.93	0.17	28,28,28,28	0
56	MG	1F	310	1/1	0.93	0.21	31,31,31,31	0
56	MG	2A	3337	1/1	0.93	0.36	52,52,52,52	0
56	MG	1A	3167	1/1	0.93	0.20	36,36,36,36	0
56	MG	2A	3341	1/1	0.93	0.13	57,57,57,57	0
56	MG	2A	3098	1/1	0.93	0.17	47,47,47,47	0
56	MG	2A	3690	1/1	0.93	0.11	67,67,67,67	0
56	MG	2A	3344	1/1	0.93	0.15	37,37,37,37	0
56	MG	1A	3125	1/1	0.93	0.19	23,23,23,23	0
56	MG	1A	3578	1/1	0.93	0.20	31,31,31,31	0
56	MG	1A	3427	1/1	0.93	0.14	37,37,37,37	0
56	MG	1A	3091	1/1	0.93	0.18	32,32,32,32	0
56	MG	1A	3583	1/1	0.93	0.34	40,40,40,40	0
56	MG	1A	3972	1/1	0.93	0.18	31,31,31,31	0
56	MG	2A	3713	1/1	0.93	0.10	56,56,56,56	0
56	MG	2a	3131	1/1	0.93	0.27	58,58,58,58	0
56	MG	1P	201	1/1	0.93	0.21	26,26,26,26	0
56	MG	1A	3009	1/1	0.93	0.19	23,23,23,23	0
56	MG	1A	3288	1/1	0.93	0.20	30,30,30,30	0
56	MG	1A	3176	1/1	0.93	0.14	33,33,33,33	0
56	MG	1A	3228	1/1	0.93	0.15	37,37,37,37	0
56	MG	1A	3297	1/1	0.93	0.19	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3773	1/1	0.93	0.12	40,40,40,40	0
56	MG	2A	3119	1/1	0.93	0.17	31,31,31,31	0
56	MG	2A	3734	1/1	0.93	0.20	38,38,38,38	0
56	MG	1A	3369	1/1	0.93	0.23	52,52,52,52	0
56	MG	2A	3123	1/1	0.93	0.25	59,59,59,59	0
56	MG	2A	3124	1/1	0.93	0.16	50,50,50,50	0
56	MG	1a	1737	1/1	0.93	0.21	55,55,55,55	0
56	MG	1A	3370	1/1	0.93	0.11	37,37,37,37	0
56	MG	2a	3156	1/1	0.93	0.12	58,58,58,58	0
56	MG	2A	3128	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	3782	1/1	0.93	0.18	33,33,33,33	0
56	MG	2A	3370	1/1	0.93	0.13	50,50,50,50	0
56	MG	1A	3506	1/1	0.93	0.23	33,33,33,33	0
56	MG	1a	1748	1/1	0.93	0.17	34,34,34,34	0
56	MG	2a	3168	1/1	0.93	0.10	62,62,62,62	0
56	MG	2A	3136	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3991	1/1	0.93	0.24	37,37,37,37	0
56	MG	1A	3439	1/1	0.93	0.14	39,39,39,39	0
56	MG	1a	1758	1/1	0.93	0.13	53,53,53,53	0
56	MG	1U	205	1/1	0.93	0.39	38,38,38,38	0
56	MG	1A	3094	1/1	0.93	0.21	18,18,18,18	0
56	MG	2A	3148	1/1	0.93	0.23	37,37,37,37	0
56	MG	1A	3998	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3300	1/1	0.93	0.21	37,37,37,37	0
56	MG	2A	3151	1/1	0.93	0.12	55,55,55,55	0
56	MG	1A	3375	1/1	0.93	0.12	46,46,46,46	0
56	MG	1W	207	1/1	0.93	0.20	18,18,18,18	0
56	MG	2A	3155	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3809	1/1	0.93	0.15	32,32,32,32	0
56	MG	2a	3198	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3515	1/1	0.93	0.20	31,31,31,31	0
56	MG	1X	105	1/1	0.93	0.12	40,40,40,40	0
56	MG	2a	3203	1/1	0.93	0.10	71,71,71,71	0
56	MG	1A	3377	1/1	0.93	0.23	41,41,41,41	0
56	MG	1A	3096	1/1	0.93	0.23	49,49,49,49	0
56	MG	1A	3614	1/1	0.93	0.23	34,34,34,34	0
56	MG	1A	3098	1/1	0.93	0.17	29,29,29,29	0
56	MG	2a	3211	1/1	0.93	0.22	68,68,68,68	0
56	MG	2A	3790	1/1	0.93	0.20	58,58,58,58	0
56	MG	1A	4010	1/1	0.93	0.18	11,11,11,11	0
56	MG	1A	4011	1/1	0.93	0.15	21,21,21,21	0
56	MG	2A	3796	1/1	0.93	0.27	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3407	1/1	0.93	0.13	62,62,62,62	0
56	MG	1a	1790	1/1	0.93	0.26	77,77,77,77	0
56	MG	2a	3225	1/1	0.93	0.16	57,57,57,57	0
56	MG	1A	3010	1/1	0.93	0.20	32,32,32,32	0
56	MG	2A	3803	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	4014	1/1	0.93	0.17	34,34,34,34	0
56	MG	2A	3806	1/1	0.93	0.16	64,64,64,64	0
56	MG	1A	3102	1/1	0.93	0.10	41,41,41,41	0
56	MG	1l	103	1/1	0.93	0.14	43,43,43,43	0
56	MG	1A	3521	1/1	0.93	0.12	50,50,50,50	0
56	MG	1a	1800	1/1	0.93	0.21	38,38,38,38	0
56	MG	2A	3419	1/1	0.93	0.22	41,41,41,41	0
56	MG	2k	201	1/1	0.93	0.17	49,49,49,49	0
56	MG	1A	3240	1/1	0.93	0.24	35,35,35,35	0
56	MG	1A	3140	1/1	0.93	0.16	28,28,28,28	0
56	MG	1A	3388	1/1	0.93	0.15	46,46,46,46	0
56	MG	2A	3427	1/1	0.93	0.22	36,36,36,36	0
56	MG	2m	201	1/1	0.93	0.15	61,61,61,61	0
56	MG	2A	3827	1/1	0.93	0.14	35,35,35,35	0
56	MG	2r	102	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3389	1/1	0.93	0.10	38,38,38,38	0
56	MG	2v	101	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3629	1/1	0.93	0.26	38,38,38,38	0
56	MG	2w	101	1/1	0.93	0.18	61,61,61,61	0
56	MG	2w	102	1/1	0.93	0.15	59,59,59,59	0
56	MG	2A	3843	1/1	0.93	0.11	41,41,41,41	0
56	MG	2A	3846	1/1	0.93	0.11	40,40,40,40	0
56	MG	1a	1601	1/1	0.93	0.21	60,60,60,60	0
56	MG	2A	3194	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3242	1/1	0.93	0.32	24,24,24,24	0
56	MG	2x	103	1/1	0.93	0.21	59,59,59,59	0
56	MG	1a	1821	1/1	0.93	0.24	55,55,55,55	0
56	MG	2A	3856	1/1	0.93	0.12	37,37,37,37	0
56	MG	2A	3861	1/1	0.93	0.13	51,51,51,51	0
56	MG	2A	3440	1/1	0.93	0.23	56,56,56,56	0
56	MG	1A	3844	1/1	0.93	0.13	35,35,35,35	0
56	MG	1A	3849	1/1	0.93	0.14	40,40,40,40	0
56	MG	2A	3202	1/1	0.93	0.15	39,39,39,39	0
58	ZN	14	501	1/1	0.93	0.14	110,110,110,110	0
56	MG	2A	3870	1/1	0.93	0.12	48,48,48,48	0
56	MG	1A	3317	1/1	0.93	0.27	33,33,33,33	0
56	MG	2A	3874	1/1	0.93	0.25	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3823	1/1	0.94	0.12	61,61,61,61	0
56	MG	1a	1780	1/1	0.94	0.13	51,51,51,51	0
56	MG	1a	1781	1/1	0.94	0.07	76,76,76,76	0
56	MG	1X	101	1/1	0.94	0.34	25,25,25,25	0
56	MG	2A	3841	1/1	0.94	0.06	65,65,65,65	0
56	MG	1A	4005	1/1	0.94	0.17	68,68,68,68	0
56	MG	2A	3845	1/1	0.94	0.14	38,38,38,38	0
56	MG	1A	3220	1/1	0.94	0.19	42,42,42,42	0
56	MG	2A	3847	1/1	0.94	0.12	48,48,48,48	0
56	MG	2A	3175	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3545	1/1	0.94	0.13	42,42,42,42	0
56	MG	1A	3811	1/1	0.94	0.16	21,21,21,21	0
56	MG	1A	3812	1/1	0.94	0.15	36,36,36,36	0
56	MG	2A	3855	1/1	0.94	0.11	64,64,64,64	0
56	MG	1a	1795	1/1	0.94	0.13	58,58,58,58	0
56	MG	2A	3432	1/1	0.94	0.24	45,45,45,45	0
56	MG	1A	3221	1/1	0.94	0.16	33,33,33,33	0
56	MG	2A	3434	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	3406	1/1	0.94	0.14	17,17,17,17	0
56	MG	1A	3818	1/1	0.94	0.12	26,26,26,26	0
56	MG	1A	3636	1/1	0.94	0.19	23,23,23,23	0
56	MG	1A	3637	1/1	0.94	0.14	30,30,30,30	0
56	MG	1a	1801	1/1	0.94	0.08	46,46,46,46	0
56	MG	2A	3875	1/1	0.94	0.22	57,57,57,57	0
56	MG	1A	3495	1/1	0.94	0.19	31,31,31,31	0
56	MG	2A	3191	1/1	0.94	0.18	55,55,55,55	0
56	MG	2A	3444	1/1	0.94	0.30	31,31,31,31	0
56	MG	10	107	1/1	0.94	0.21	63,63,63,63	0
56	MG	1A	3824	1/1	0.94	0.16	34,34,34,34	0
56	MG	1A	4020	1/1	0.94	0.17	38,38,38,38	0
56	MG	2B	205	1/1	0.94	0.14	52,52,52,52	0
56	MG	12	101	1/1	0.94	0.17	44,44,44,44	0
56	MG	1a	1815	1/1	0.94	0.12	48,48,48,48	0
56	MG	2A	3452	1/1	0.94	0.16	32,32,32,32	0
56	MG	1A	3639	1/1	0.94	0.23	50,50,50,50	0
56	MG	2B	212	1/1	0.94	0.12	52,52,52,52	0
56	MG	13	101	1/1	0.94	0.16	25,25,25,25	0
56	MG	15	105	1/1	0.94	0.11	48,48,48,48	0
56	MG	1A	3052	1/1	0.94	0.33	42,42,42,42	0
56	MG	1A	3089	1/1	0.94	0.15	41,41,41,41	0
56	MG	2B	218	1/1	0.94	0.11	62,62,62,62	0
56	MG	2A	3205	1/1	0.94	0.13	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	1b	301	1/1	0.94	0.23	70,70,70,70	0
56	MG	1A	3363	1/1	0.94	0.18	23,23,23,23	0
56	MG	1A	3653	1/1	0.94	0.15	23,23,23,23	0
56	MG	2D	304	1/1	0.94	0.13	28,28,28,28	0
56	MG	1A	4032	1/1	0.94	0.14	22,22,22,22	0
56	MG	18	104	1/1	0.94	0.26	34,34,34,34	0
56	MG	1A	4033	1/1	0.94	0.20	27,27,27,27	0
56	MG	1l	202	1/1	0.94	0.13	66,66,66,66	0
56	MG	1A	3558	1/1	0.94	0.35	41,41,41,41	0
56	MG	2A	3216	1/1	0.94	0.16	48,48,48,48	0
56	MG	2F	301	1/1	0.94	0.23	41,41,41,41	0
56	MG	2A	3217	1/1	0.94	0.10	51,51,51,51	0
56	MG	1A	3836	1/1	0.94	0.17	19,19,19,19	0
56	MG	1A	4042	1/1	0.94	0.13	60,60,60,60	0
56	MG	1A	3314	1/1	0.94	0.34	40,40,40,40	0
56	MG	1A	3839	1/1	0.94	0.17	17,17,17,17	0
56	MG	1A	3656	1/1	0.94	0.16	58,58,58,58	0
56	MG	2P	202	1/1	0.94	0.10	52,52,52,52	0
56	MG	1A	4050	1/1	0.94	0.10	49,49,49,49	0
56	MG	1A	3500	1/1	0.94	0.23	33,33,33,33	0
56	MG	1w	103	1/1	0.94	0.09	50,50,50,50	0
56	MG	2R	201	1/1	0.94	0.22	56,56,56,56	0
56	MG	2A	3229	1/1	0.94	0.12	31,31,31,31	0
56	MG	1A	3660	1/1	0.94	0.15	19,19,19,19	0
56	MG	2T	202	1/1	0.94	0.16	54,54,54,54	0
56	MG	2V	201	1/1	0.94	0.53	49,49,49,49	0
56	MG	2A	3490	1/1	0.94	0.14	49,49,49,49	0
56	MG	2W	201	1/1	0.94	0.38	40,40,40,40	0
56	MG	2W	202	1/1	0.94	0.22	44,44,44,44	0
56	MG	1A	4056	1/1	0.94	0.14	36,36,36,36	0
56	MG	2X	101	1/1	0.94	0.40	60,60,60,60	0
56	MG	1a	1615	1/1	0.94	0.12	51,51,51,51	0
56	MG	20	102	1/1	0.94	0.15	52,52,52,52	0
56	MG	2A	3236	1/1	0.94	0.12	35,35,35,35	0
56	MG	1A	3154	1/1	0.94	0.33	37,37,37,37	0
56	MG	1A	3662	1/1	0.94	0.18	24,24,24,24	0
56	MG	1A	3563	1/1	0.94	0.27	53,53,53,53	0
56	MG	1A	3668	1/1	0.94	0.09	36,36,36,36	0
56	MG	1x	109	1/1	0.94	0.21	65,65,65,65	0
56	MG	1A	3864	1/1	0.94	0.10	40,40,40,40	0
56	MG	1A	4063	1/1	0.94	0.15	34,34,34,34	0
56	MG	2A	3506	1/1	0.94	0.16	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1x	112	1/1	0.94	0.19	50,50,50,50	0
56	MG	2A	3247	1/1	0.94	0.16	42,42,42,42	0
56	MG	1A	4066	1/1	0.94	0.20	24,24,24,24	0
56	MG	1A	4067	1/1	0.94	0.36	45,45,45,45	0
56	MG	2A	3524	1/1	0.94	0.18	54,54,54,54	0
56	MG	1A	3865	1/1	0.94	0.16	49,49,49,49	0
56	MG	1A	4070	1/1	0.94	0.23	23,23,23,23	0
56	MG	1A	3456	1/1	0.94	0.21	44,44,44,44	0
56	MG	1A	3023	1/1	0.94	0.13	21,21,21,21	0
56	MG	1A	3415	1/1	0.94	0.25	36,36,36,36	0
56	MG	1A	3042	1/1	0.94	0.27	22,22,22,22	0
56	MG	2A	3533	1/1	0.94	0.14	44,44,44,44	0
56	MG	2A	3535	1/1	0.94	0.10	43,43,43,43	0
56	MG	2A	3536	1/1	0.94	0.17	38,38,38,38	0
56	MG	2A	3004	1/1	0.94	0.22	38,38,38,38	0
56	MG	2A	3539	1/1	0.94	0.11	31,31,31,31	0
56	MG	1A	3677	1/1	0.94	0.18	28,28,28,28	0
56	MG	2A	3260	1/1	0.94	0.17	49,49,49,49	0
56	MG	2A	3262	1/1	0.94	0.19	57,57,57,57	0
56	MG	1a	1633	1/1	0.94	0.20	19,19,19,19	0
56	MG	2a	3022	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	3678	1/1	0.94	0.12	27,27,27,27	0
56	MG	1A	4085	1/1	0.94	0.12	35,35,35,35	0
56	MG	2A	3011	1/1	0.94	0.15	48,48,48,48	0
56	MG	1A	3507	1/1	0.94	0.21	35,35,35,35	0
56	MG	2A	3270	1/1	0.94	0.12	44,44,44,44	0
56	MG	1a	1639	1/1	0.94	0.13	52,52,52,52	0
56	MG	1a	1640	1/1	0.94	0.28	32,32,32,32	0
56	MG	1A	4094	1/1	0.94	0.27	45,45,45,45	0
56	MG	2A	3573	1/1	0.94	0.10	31,31,31,31	0
56	MG	1a	1642	1/1	0.94	0.25	42,42,42,42	0
56	MG	1a	1644	1/1	0.94	0.12	61,61,61,61	0
56	MG	2A	3277	1/1	0.94	0.13	40,40,40,40	0
56	MG	2A	3580	1/1	0.94	0.13	37,37,37,37	0
56	MG	2A	3583	1/1	0.94	0.14	35,35,35,35	0
56	MG	2A	3584	1/1	0.94	0.18	44,44,44,44	0
56	MG	1A	3881	1/1	0.94	0.14	50,50,50,50	0
56	MG	1a	1646	1/1	0.94	0.22	53,53,53,53	0
56	MG	2A	3590	1/1	0.94	0.23	40,40,40,40	0
56	MG	1A	3883	1/1	0.94	0.19	13,13,13,13	0
56	MG	2A	3592	1/1	0.94	0.22	44,44,44,44	0
56	MG	2A	3594	1/1	0.94	0.18	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3051	1/1	0.94	0.10	52,52,52,52	0
56	MG	1A	3681	1/1	0.94	0.11	41,41,41,41	0
56	MG	2a	3055	1/1	0.94	0.12	70,70,70,70	0
56	MG	1A	3891	1/1	0.94	0.17	59,59,59,59	0
56	MG	2A	3599	1/1	0.94	0.17	63,63,63,63	0
56	MG	2A	3605	1/1	0.94	0.17	41,41,41,41	0
56	MG	1a	1657	1/1	0.94	0.20	45,45,45,45	0
56	MG	1A	3323	1/1	0.94	0.24	36,36,36,36	0
56	MG	2A	3609	1/1	0.94	0.14	56,56,56,56	0
56	MG	1A	3108	1/1	0.94	0.28	44,44,44,44	0
56	MG	1a	1662	1/1	0.94	0.17	54,54,54,54	0
56	MG	2A	3033	1/1	0.94	0.14	39,39,39,39	0
56	MG	1A	3109	1/1	0.94	0.21	28,28,28,28	0
56	MG	1A	3276	1/1	0.94	0.14	26,26,26,26	0
56	MG	2A	3622	1/1	0.94	0.09	39,39,39,39	0
56	MG	1A	3514	1/1	0.94	0.11	22,22,22,22	0
56	MG	2A	3624	1/1	0.94	0.19	43,43,43,43	0
56	MG	2a	3077	1/1	0.94	0.14	45,45,45,45	0
56	MG	2A	3625	1/1	0.94	0.14	37,37,37,37	0
56	MG	1A	3701	1/1	0.94	0.17	17,17,17,17	0
56	MG	1A	3903	1/1	0.94	0.19	29,29,29,29	0
56	MG	1A	3194	1/1	0.94	0.19	27,27,27,27	0
56	MG	2A	3298	1/1	0.94	0.11	48,48,48,48	0
56	MG	1a	1669	1/1	0.94	0.08	56,56,56,56	0
56	MG	1A	3196	1/1	0.94	0.18	44,44,44,44	0
56	MG	1A	3331	1/1	0.94	0.26	40,40,40,40	0
56	MG	2A	3046	1/1	0.94	0.14	49,49,49,49	0
56	MG	1A	3280	1/1	0.94	0.22	43,43,43,43	0
56	MG	2a	3092	1/1	0.94	0.18	51,51,51,51	0
56	MG	1a	1673	1/1	0.94	0.20	34,34,34,34	0
56	MG	1a	1675	1/1	0.94	0.14	56,56,56,56	0
56	MG	1A	3092	1/1	0.94	0.12	28,28,28,28	0
56	MG	2a	3097	1/1	0.94	0.09	59,59,59,59	0
56	MG	2a	3098	1/1	0.94	0.09	67,67,67,67	0
56	MG	1A	3916	1/1	0.94	0.21	37,37,37,37	0
56	MG	2A	3648	1/1	0.94	0.18	33,33,33,33	0
56	MG	2A	3649	1/1	0.94	0.20	44,44,44,44	0
56	MG	1a	1678	1/1	0.94	0.18	54,54,54,54	0
56	MG	1A	3711	1/1	0.94	0.10	45,45,45,45	0
56	MG	2A	3657	1/1	0.94	0.10	51,51,51,51	0
56	MG	2A	3658	1/1	0.94	0.14	61,61,61,61	0
56	MG	2a	3109	1/1	0.94	0.19	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3059	1/1	0.94	0.15	41,41,41,41	0
56	MG	2A	3060	1/1	0.94	0.11	53,53,53,53	0
56	MG	1A	3472	1/1	0.94	0.19	43,43,43,43	0
56	MG	2A	3665	1/1	0.94	0.14	56,56,56,56	0
56	MG	2A	3062	1/1	0.94	0.24	50,50,50,50	0
56	MG	2A	3667	1/1	0.94	0.16	42,42,42,42	0
56	MG	1A	3283	1/1	0.94	0.18	34,34,34,34	0
56	MG	1A	3522	1/1	0.94	0.14	31,31,31,31	0
56	MG	2A	3670	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	3588	1/1	0.94	0.13	49,49,49,49	0
56	MG	1A	3929	1/1	0.94	0.11	41,41,41,41	0
56	MG	2A	3323	1/1	0.94	0.16	51,51,51,51	0
56	MG	1a	1688	1/1	0.94	0.17	53,53,53,53	0
56	MG	1A	3723	1/1	0.94	0.20	21,21,21,21	0
56	MG	1a	1690	1/1	0.94	0.11	58,58,58,58	0
56	MG	1A	3726	1/1	0.94	0.17	25,25,25,25	0
56	MG	2a	3133	1/1	0.94	0.24	45,45,45,45	0
56	MG	1A	3523	1/1	0.94	0.20	30,30,30,30	0
56	MG	1A	3591	1/1	0.94	0.25	38,38,38,38	0
56	MG	1D	301	1/1	0.94	0.33	55,55,55,55	0
56	MG	1A	3730	1/1	0.94	0.19	25,25,25,25	0
56	MG	2A	3082	1/1	0.94	0.42	45,45,45,45	0
56	MG	2A	3694	1/1	0.94	0.13	46,46,46,46	0
56	MG	2a	3144	1/1	0.94	0.13	76,76,76,76	0
56	MG	2A	3083	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3731	1/1	0.94	0.15	31,31,31,31	0
56	MG	2a	3148	1/1	0.94	0.14	56,56,56,56	0
56	MG	2a	3149	1/1	0.94	0.14	42,42,42,42	0
56	MG	2A	3697	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3524	1/1	0.94	0.11	55,55,55,55	0
56	MG	1A	3949	1/1	0.94	0.22	44,44,44,44	0
56	MG	1A	3429	1/1	0.94	0.17	29,29,29,29	0
56	MG	2A	3342	1/1	0.94	0.15	56,56,56,56	0
56	MG	2A	3704	1/1	0.94	0.14	62,62,62,62	0
56	MG	2A	3706	1/1	0.94	0.14	47,47,47,47	0
56	MG	2A	3707	1/1	0.94	0.19	67,67,67,67	0
56	MG	1A	3738	1/1	0.94	0.21	28,28,28,28	0
56	MG	1A	3284	1/1	0.94	0.19	27,27,27,27	0
56	MG	2A	3715	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	3953	1/1	0.94	0.21	46,46,46,46	0
56	MG	2a	3169	1/1	0.94	0.07	55,55,55,55	0
56	MG	2a	3171	1/1	0.94	0.17	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1E	310	1/1	0.94	0.11	58,58,58,58	0
56	MG	2a	3176	1/1	0.94	0.17	40,40,40,40	0
56	MG	2A	3095	1/1	0.94	0.20	50,50,50,50	0
56	MG	2A	3096	1/1	0.94	0.13	59,59,59,59	0
56	MG	2a	3183	1/1	0.94	0.19	40,40,40,40	0
56	MG	1A	3527	1/1	0.94	0.16	44,44,44,44	0
56	MG	1A	3477	1/1	0.94	0.15	40,40,40,40	0
56	MG	1A	3958	1/1	0.94	0.14	22,22,22,22	0
56	MG	2A	3732	1/1	0.94	0.18	54,54,54,54	0
56	MG	1F	303	1/1	0.94	0.09	33,33,33,33	0
56	MG	1A	3746	1/1	0.94	0.26	13,13,13,13	0
56	MG	1A	3750	1/1	0.94	0.23	34,34,34,34	0
56	MG	1A	3752	1/1	0.94	0.17	29,29,29,29	0
56	MG	1a	1714	1/1	0.94	0.24	52,52,52,52	0
56	MG	1A	3603	1/1	0.94	0.14	37,37,37,37	0
56	MG	2A	3110	1/1	0.94	0.09	49,49,49,49	0
56	MG	1G	201	1/1	0.94	0.13	36,36,36,36	0
56	MG	1A	3021	1/1	0.94	0.21	15,15,15,15	0
56	MG	2a	3200	1/1	0.94	0.16	63,63,63,63	0
56	MG	1A	3531	1/1	0.94	0.16	25,25,25,25	0
56	MG	2A	3747	1/1	0.94	0.10	59,59,59,59	0
56	MG	1a	1719	1/1	0.94	0.21	41,41,41,41	0
56	MG	1A	3763	1/1	0.94	0.16	21,21,21,21	0
56	MG	2A	3752	1/1	0.94	0.13	53,53,53,53	0
56	MG	2A	3365	1/1	0.94	0.19	56,56,56,56	0
56	MG	1A	3286	1/1	0.94	0.16	33,33,33,33	0
56	MG	1N	204	1/1	0.94	0.43	39,39,39,39	0
56	MG	2A	3759	1/1	0.94	0.14	47,47,47,47	0
56	MG	2A	3368	1/1	0.94	0.14	58,58,58,58	0
56	MG	2A	3369	1/1	0.94	0.11	57,57,57,57	0
56	MG	2A	3120	1/1	0.94	0.20	41,41,41,41	0
56	MG	2a	3220	1/1	0.94	0.15	54,54,54,54	0
56	MG	1A	3765	1/1	0.94	0.14	43,43,43,43	0
56	MG	2a	3224	1/1	0.94	0.12	62,62,62,62	0
56	MG	1A	3168	1/1	0.94	0.17	23,23,23,23	0
56	MG	2A	3768	1/1	0.94	0.08	60,60,60,60	0
56	MG	1a	1728	1/1	0.94	0.21	35,35,35,35	0
56	MG	1A	3483	1/1	0.94	0.11	34,34,34,34	0
56	MG	2a	3229	1/1	0.94	0.12	66,66,66,66	0
56	MG	2a	3231	1/1	0.94	0.21	58,58,58,58	0
56	MG	2a	3232	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3115	1/1	0.94	0.17	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2d	301	1/1	0.94	0.20	46,46,46,46	0
56	MG	1A	3536	1/1	0.94	0.17	20,20,20,20	0
56	MG	2A	3775	1/1	0.94	0.11	55,55,55,55	0
56	MG	2A	3777	1/1	0.94	0.11	64,64,64,64	0
56	MG	2A	3378	1/1	0.94	0.15	50,50,50,50	0
56	MG	2A	3130	1/1	0.94	0.15	36,36,36,36	0
56	MG	1A	3772	1/1	0.94	0.20	32,32,32,32	0
56	MG	2A	3384	1/1	0.94	0.23	30,30,30,30	0
56	MG	1A	3144	1/1	0.94	0.10	32,32,32,32	0
56	MG	2A	3785	1/1	0.94	0.33	64,64,64,64	0
56	MG	2A	3387	1/1	0.94	0.11	48,48,48,48	0
56	MG	2A	3134	1/1	0.94	0.14	41,41,41,41	0
56	MG	1A	3173	1/1	0.94	0.25	49,49,49,49	0
56	MG	1Q	204	1/1	0.94	0.22	44,44,44,44	0
56	MG	1A	3986	1/1	0.94	0.07	32,32,32,32	0
56	MG	1A	3987	1/1	0.94	0.15	34,34,34,34	0
56	MG	2A	3794	1/1	0.94	0.05	46,46,46,46	0
56	MG	2A	3395	1/1	0.94	0.17	46,46,46,46	0
56	MG	1A	3004	1/1	0.94	0.23	19,19,19,19	0
56	MG	2A	3799	1/1	0.94	0.10	68,68,68,68	0
56	MG	2w	104	1/1	0.94	0.48	73,73,73,73	0
56	MG	1A	3989	1/1	0.94	0.17	43,43,43,43	0
56	MG	1A	3049	1/1	0.94	0.29	35,35,35,35	0
56	MG	1A	3788	1/1	0.94	0.16	55,55,55,55	0
56	MG	1A	3789	1/1	0.94	0.18	49,49,49,49	0
56	MG	2x	102	1/1	0.94	0.07	52,52,52,52	0
56	MG	1U	201	1/1	0.94	0.13	26,26,26,26	0
56	MG	1A	3050	1/1	0.94	0.26	25,25,25,25	0
56	MG	2A	3808	1/1	0.94	0.12	58,58,58,58	0
56	MG	1A	3083	1/1	0.94	0.24	28,28,28,28	0
56	MG	1A	3796	1/1	0.94	0.18	19,19,19,19	0
56	MG	1A	3253	1/1	0.94	0.21	43,43,43,43	0
56	MG	1A	4002	1/1	0.94	0.13	58,58,58,58	0
56	MG	2A	3160	1/1	0.94	0.09	53,53,53,53	0
58	ZN	1Y	204	1/1	0.94	0.13	67,67,67,67	0
56	MG	1A	3626	1/1	0.94	0.28	52,52,52,52	0
56	MG	1W	203	1/1	0.94	0.32	44,44,44,44	0
58	ZN	2n	501	1/1	0.94	0.06	86,86,86,86	0
56	MG	2A	3820	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3802	1/1	0.94	0.21	20,20,20,20	0
56	MG	1A	3157	1/1	0.95	0.23	33,33,33,33	0
56	MG	2A	3518	1/1	0.95	0.13	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3519	1/1	0.95	0.16	42,42,42,42	0
56	MG	1a	1656	1/1	0.95	0.16	61,61,61,61	0
56	MG	1A	3612	1/1	0.95	0.42	38,38,38,38	0
56	MG	2B	220	1/1	0.95	0.16	70,70,70,70	0
56	MG	2A	3261	1/1	0.95	0.14	55,55,55,55	0
56	MG	1A	3158	1/1	0.95	0.21	25,25,25,25	0
56	MG	1A	3475	1/1	0.95	0.29	38,38,38,38	0
56	MG	2D	303	1/1	0.95	0.39	41,41,41,41	0
56	MG	2A	3264	1/1	0.95	0.19	46,46,46,46	0
56	MG	1A	3744	1/1	0.95	0.18	32,32,32,32	0
56	MG	2E	301	1/1	0.95	0.11	50,50,50,50	0
56	MG	1A	3926	1/1	0.95	0.18	27,27,27,27	0
56	MG	1B	217	1/1	0.95	0.14	43,43,43,43	0
56	MG	1B	218	1/1	0.95	0.21	36,36,36,36	0
56	MG	2A	3537	1/1	0.95	0.15	53,53,53,53	0
56	MG	2A	3269	1/1	0.95	0.26	48,48,48,48	0
56	MG	1B	220	1/1	0.95	0.21	50,50,50,50	0
56	MG	2A	3544	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3282	1/1	0.95	0.17	36,36,36,36	0
56	MG	1B	222	1/1	0.95	0.23	41,41,41,41	0
56	MG	2F	305	1/1	0.95	0.16	37,37,37,37	0
56	MG	1A	3231	1/1	0.95	0.14	37,37,37,37	0
56	MG	1B	225	1/1	0.95	0.16	52,52,52,52	0
56	MG	1A	3617	1/1	0.95	0.36	40,40,40,40	0
56	MG	1B	227	1/1	0.95	0.13	39,39,39,39	0
56	MG	1A	3751	1/1	0.95	0.13	42,42,42,42	0
56	MG	1A	3933	1/1	0.95	0.24	39,39,39,39	0
56	MG	1A	3936	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3564	1/1	0.95	0.19	46,46,46,46	0
56	MG	1A	3478	1/1	0.95	0.20	31,31,31,31	0
56	MG	2A	3566	1/1	0.95	0.17	42,42,42,42	0
56	MG	1A	3619	1/1	0.95	0.21	32,32,32,32	0
56	MG	1A	3620	1/1	0.95	0.11	46,46,46,46	0
56	MG	2A	3045	1/1	0.95	0.14	65,65,65,65	0
56	MG	2A	3285	1/1	0.95	0.09	45,45,45,45	0
56	MG	2A	3286	1/1	0.95	0.18	46,46,46,46	0
56	MG	2A	3287	1/1	0.95	0.10	42,42,42,42	0
56	MG	2A	3288	1/1	0.95	0.13	40,40,40,40	0
56	MG	2X	102	1/1	0.95	0.12	44,44,44,44	0
56	MG	1A	3414	1/1	0.95	0.24	44,44,44,44	0
56	MG	2A	3047	1/1	0.95	0.23	41,41,41,41	0
56	MG	2A	3585	1/1	0.95	0.05	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3757	1/1	0.95	0.10	47,47,47,47	0
56	MG	23	102	1/1	0.95	0.21	59,59,59,59	0
56	MG	1A	3079	1/1	0.95	0.19	26,26,26,26	0
56	MG	2A	3588	1/1	0.95	0.14	29,29,29,29	0
56	MG	1D	307	1/1	0.95	0.28	37,37,37,37	0
56	MG	1a	1686	1/1	0.95	0.20	31,31,31,31	0
56	MG	1D	308	1/1	0.95	0.17	35,35,35,35	0
56	MG	26	101	1/1	0.95	0.27	52,52,52,52	0
56	MG	1D	309	1/1	0.95	0.35	22,22,22,22	0
56	MG	2A	3595	1/1	0.95	0.23	58,58,58,58	0
56	MG	2A	3596	1/1	0.95	0.23	53,53,53,53	0
56	MG	1A	3008	1/1	0.95	0.19	19,19,19,19	0
56	MG	2A	3057	1/1	0.95	0.24	38,38,38,38	0
56	MG	2A	3058	1/1	0.95	0.18	53,53,53,53	0
56	MG	2A	3600	1/1	0.95	0.13	26,26,26,26	0
56	MG	1D	311	1/1	0.95	0.20	29,29,29,29	0
56	MG	1E	302	1/1	0.95	0.12	28,28,28,28	0
56	MG	1A	3198	1/1	0.95	0.46	30,30,30,30	0
56	MG	1A	3235	1/1	0.95	0.30	25,25,25,25	0
56	MG	1A	3767	1/1	0.95	0.13	41,41,41,41	0
56	MG	2A	3612	1/1	0.95	0.12	57,57,57,57	0
56	MG	2A	3613	1/1	0.95	0.17	57,57,57,57	0
56	MG	2A	3614	1/1	0.95	0.18	57,57,57,57	0
56	MG	1A	3200	1/1	0.95	0.16	26,26,26,26	0
56	MG	1A	3956	1/1	0.95	0.16	66,66,66,66	0
56	MG	1A	3081	1/1	0.95	0.17	30,30,30,30	0
56	MG	1A	3631	1/1	0.95	0.26	49,49,49,49	0
56	MG	1A	3202	1/1	0.95	0.14	28,28,28,28	0
56	MG	1A	3031	1/1	0.95	0.19	22,22,22,22	0
56	MG	1F	304	1/1	0.95	0.18	25,25,25,25	0
56	MG	1F	305	1/1	0.95	0.19	22,22,22,22	0
56	MG	1A	3635	1/1	0.95	0.21	39,39,39,39	0
56	MG	1F	307	1/1	0.95	0.19	39,39,39,39	0
56	MG	1A	3777	1/1	0.95	0.22	12,12,12,12	0
56	MG	1A	3062	1/1	0.95	0.21	44,44,44,44	0
56	MG	1A	3551	1/1	0.95	0.23	36,36,36,36	0
56	MG	1A	3783	1/1	0.95	0.24	46,46,46,46	0
56	MG	2a	3032	1/1	0.95	0.20	51,51,51,51	0
56	MG	2a	3033	1/1	0.95	0.11	59,59,59,59	0
56	MG	1G	203	1/1	0.95	0.11	41,41,41,41	0
56	MG	2a	3035	1/1	0.95	0.12	38,38,38,38	0
56	MG	2a	3036	1/1	0.95	0.25	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3785	1/1	0.95	0.14	34,34,34,34	0
56	MG	1A	3786	1/1	0.95	0.21	25,25,25,25	0
56	MG	1A	3787	1/1	0.95	0.12	42,42,42,42	0
56	MG	1A	3248	1/1	0.95	0.18	19,19,19,19	0
56	MG	1A	3205	1/1	0.95	0.20	18,18,18,18	0
56	MG	2A	3646	1/1	0.95	0.17	35,35,35,35	0
56	MG	1A	3791	1/1	0.95	0.21	11,11,11,11	0
56	MG	1A	3554	1/1	0.95	0.24	26,26,26,26	0
56	MG	1A	3302	1/1	0.95	0.17	44,44,44,44	0
56	MG	1A	3303	1/1	0.95	0.13	35,35,35,35	0
56	MG	2A	3651	1/1	0.95	0.16	41,41,41,41	0
56	MG	2A	3655	1/1	0.95	0.30	44,44,44,44	0
56	MG	1a	1724	1/1	0.95	0.19	31,31,31,31	0
56	MG	2A	3336	1/1	0.95	0.09	38,38,38,38	0
56	MG	1A	3797	1/1	0.95	0.22	36,36,36,36	0
56	MG	1A	3647	1/1	0.95	0.15	11,11,11,11	0
56	MG	1A	3648	1/1	0.95	0.22	30,30,30,30	0
56	MG	2a	3056	1/1	0.95	0.05	69,69,69,69	0
56	MG	2A	3662	1/1	0.95	0.20	43,43,43,43	0
56	MG	1A	3801	1/1	0.95	0.19	23,23,23,23	0
56	MG	2A	3664	1/1	0.95	0.28	67,67,67,67	0
56	MG	1A	3651	1/1	0.95	0.22	29,29,29,29	0
56	MG	1a	1731	1/1	0.95	0.17	33,33,33,33	0
56	MG	1Q	206	1/1	0.95	0.23	36,36,36,36	0
56	MG	1A	3559	1/1	0.95	0.32	36,36,36,36	0
56	MG	1A	3808	1/1	0.95	0.13	51,51,51,51	0
56	MG	1A	3207	1/1	0.95	0.14	26,26,26,26	0
56	MG	2a	3068	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3810	1/1	0.95	0.12	21,21,21,21	0
56	MG	2A	3115	1/1	0.95	0.19	53,53,53,53	0
56	MG	2A	3676	1/1	0.95	0.11	45,45,45,45	0
56	MG	1A	3020	1/1	0.95	0.19	30,30,30,30	0
56	MG	2A	3679	1/1	0.95	0.14	40,40,40,40	0
56	MG	1T	201	1/1	0.95	0.23	44,44,44,44	0
56	MG	2A	3681	1/1	0.95	0.17	46,46,46,46	0
56	MG	1a	1742	1/1	0.95	0.18	58,58,58,58	0
56	MG	1a	1744	1/1	0.95	0.12	52,52,52,52	0
56	MG	2a	3082	1/1	0.95	0.13	50,50,50,50	0
56	MG	1A	3371	1/1	0.95	0.14	44,44,44,44	0
56	MG	1a	1752	1/1	0.95	0.14	41,41,41,41	0
56	MG	1A	3307	1/1	0.95	0.20	54,54,54,54	0
56	MG	1a	1754	1/1	0.95	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1755	1/1	0.95	0.24	61,61,61,61	0
56	MG	1A	3659	1/1	0.95	0.16	15,15,15,15	0
56	MG	2A	3692	1/1	0.95	0.16	43,43,43,43	0
56	MG	1A	3435	1/1	0.95	0.24	43,43,43,43	0
56	MG	2A	3129	1/1	0.95	0.45	46,46,46,46	0
56	MG	1A	3088	1/1	0.95	0.24	37,37,37,37	0
56	MG	1A	3138	1/1	0.95	0.17	23,23,23,23	0
56	MG	1A	3663	1/1	0.95	0.17	16,16,16,16	0
56	MG	1a	1766	1/1	0.95	0.17	46,46,46,46	0
56	MG	1A	3376	1/1	0.95	0.18	41,41,41,41	0
56	MG	1U	211	1/1	0.95	0.49	52,52,52,52	0
56	MG	1U	212	1/1	0.95	0.14	36,36,36,36	0
56	MG	2A	3705	1/1	0.95	0.15	47,47,47,47	0
56	MG	1A	3825	1/1	0.95	0.16	46,46,46,46	0
56	MG	2A	3139	1/1	0.95	0.15	46,46,46,46	0
56	MG	2a	3106	1/1	0.95	0.13	48,48,48,48	0
56	MG	1V	206	1/1	0.95	0.17	39,39,39,39	0
56	MG	2A	3709	1/1	0.95	0.12	59,59,59,59	0
56	MG	2A	3143	1/1	0.95	0.14	37,37,37,37	0
56	MG	2A	3144	1/1	0.95	0.23	33,33,33,33	0
56	MG	1a	1774	1/1	0.95	0.12	55,55,55,55	0
56	MG	2a	3116	1/1	0.95	0.22	48,48,48,48	0
56	MG	1A	3826	1/1	0.95	0.16	41,41,41,41	0
56	MG	2A	3379	1/1	0.95	0.24	68,68,68,68	0
56	MG	1A	3667	1/1	0.95	0.08	44,44,44,44	0
56	MG	2A	3723	1/1	0.95	0.08	59,59,59,59	0
56	MG	1A	3110	1/1	0.95	0.16	24,24,24,24	0
56	MG	2a	3122	1/1	0.95	0.20	53,53,53,53	0
56	MG	2A	3727	1/1	0.95	0.08	58,58,58,58	0
56	MG	1A	4013	1/1	0.95	0.12	17,17,17,17	0
56	MG	2A	3730	1/1	0.95	0.13	35,35,35,35	0
56	MG	2A	3385	1/1	0.95	0.20	51,51,51,51	0
56	MG	1A	3378	1/1	0.95	0.16	42,42,42,42	0
56	MG	1A	3313	1/1	0.95	0.36	22,22,22,22	0
56	MG	1a	1783	1/1	0.95	0.17	49,49,49,49	0
56	MG	1A	3572	1/1	0.95	0.15	22,22,22,22	0
56	MG	2A	3157	1/1	0.95	0.12	42,42,42,42	0
56	MG	1A	3215	1/1	0.95	0.18	30,30,30,30	0
56	MG	1a	1787	1/1	0.95	0.12	70,70,70,70	0
56	MG	2A	3162	1/1	0.95	0.17	60,60,60,60	0
56	MG	1A	3257	1/1	0.95	0.24	31,31,31,31	0
56	MG	2a	3139	1/1	0.95	0.17	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3261	1/1	0.95	0.41	46,46,46,46	0
56	MG	2A	3745	1/1	0.95	0.17	58,58,58,58	0
56	MG	2A	3165	1/1	0.95	0.24	46,46,46,46	0
56	MG	1A	4022	1/1	0.95	0.13	45,45,45,45	0
56	MG	1A	3111	1/1	0.95	0.20	21,21,21,21	0
56	MG	1A	3385	1/1	0.95	0.21	34,34,34,34	0
56	MG	1A	3025	1/1	0.95	0.24	32,32,32,32	0
56	MG	2A	3170	1/1	0.95	0.08	45,45,45,45	0
56	MG	2A	3754	1/1	0.95	0.12	52,52,52,52	0
56	MG	1A	3843	1/1	0.95	0.14	28,28,28,28	0
56	MG	1A	4031	1/1	0.95	0.24	27,27,27,27	0
56	MG	2A	3757	1/1	0.95	0.13	54,54,54,54	0
56	MG	2A	3174	1/1	0.95	0.23	36,36,36,36	0
56	MG	1A	3686	1/1	0.95	0.19	48,48,48,48	0
56	MG	1A	3846	1/1	0.95	0.16	44,44,44,44	0
56	MG	2a	3162	1/1	0.95	0.19	53,53,53,53	0
56	MG	1A	4037	1/1	0.95	0.14	32,32,32,32	0
56	MG	2a	3164	1/1	0.95	0.10	65,65,65,65	0
56	MG	2a	3165	1/1	0.95	0.15	60,60,60,60	0
56	MG	1a	1804	1/1	0.95	0.16	47,47,47,47	0
56	MG	1A	3848	1/1	0.95	0.18	17,17,17,17	0
56	MG	13	104	1/1	0.95	0.15	53,53,53,53	0
56	MG	2A	3182	1/1	0.95	0.14	43,43,43,43	0
56	MG	2A	3183	1/1	0.95	0.18	48,48,48,48	0
56	MG	2A	3771	1/1	0.95	0.13	28,28,28,28	0
56	MG	2A	3420	1/1	0.95	0.22	35,35,35,35	0
56	MG	2a	3177	1/1	0.95	0.12	48,48,48,48	0
56	MG	15	101	1/1	0.95	0.20	29,29,29,29	0
56	MG	1A	3687	1/1	0.95	0.21	41,41,41,41	0
56	MG	2A	3776	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3850	1/1	0.95	0.18	29,29,29,29	0
56	MG	2A	3778	1/1	0.95	0.15	38,38,38,38	0
56	MG	1A	3688	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3690	1/1	0.95	0.19	24,24,24,24	0
56	MG	2A	3429	1/1	0.95	0.20	30,30,30,30	0
56	MG	1a	1819	1/1	0.95	0.23	43,43,43,43	0
56	MG	2A	3431	1/1	0.95	0.17	54,54,54,54	0
56	MG	2A	3784	1/1	0.95	0.07	48,48,48,48	0
56	MG	2a	3194	1/1	0.95	0.18	58,58,58,58	0
56	MG	17	101	1/1	0.95	0.14	25,25,25,25	0
56	MG	1A	3387	1/1	0.95	0.19	47,47,47,47	0
56	MG	1a	1823	1/1	0.95	0.17	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3582	1/1	0.95	0.19	42,42,42,42	0
56	MG	1A	3180	1/1	0.95	0.19	23,23,23,23	0
56	MG	19	101	1/1	0.95	0.14	41,41,41,41	0
56	MG	2A	3199	1/1	0.95	0.09	45,45,45,45	0
56	MG	2a	3202	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	3066	1/1	0.95	0.28	29,29,29,29	0
56	MG	1e	202	1/1	0.95	0.15	51,51,51,51	0
56	MG	1A	3267	1/1	0.95	0.16	37,37,37,37	0
56	MG	1A	3268	1/1	0.95	0.17	36,36,36,36	0
56	MG	2A	3800	1/1	0.95	0.17	37,37,37,37	0
56	MG	2A	3446	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	3871	1/1	0.95	0.11	38,38,38,38	0
56	MG	1a	1605	1/1	0.95	0.21	50,50,50,50	0
56	MG	1A	3872	1/1	0.95	0.10	40,40,40,40	0
56	MG	1A	3873	1/1	0.95	0.25	39,39,39,39	0
56	MG	1A	3328	1/1	0.95	0.32	42,42,42,42	0
56	MG	2a	3219	1/1	0.95	0.12	71,71,71,71	0
56	MG	1A	3395	1/1	0.95	0.33	51,51,51,51	0
56	MG	1A	3015	1/1	0.95	0.33	32,32,32,32	0
56	MG	1A	3879	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	4068	1/1	0.95	0.17	31,31,31,31	0
56	MG	2A	3456	1/1	0.95	0.23	52,52,52,52	0
56	MG	1A	3709	1/1	0.95	0.13	24,24,24,24	0
56	MG	1A	3397	1/1	0.95	0.19	18,18,18,18	0
56	MG	1A	3882	1/1	0.95	0.09	36,36,36,36	0
56	MG	2a	3230	1/1	0.95	0.12	60,60,60,60	0
56	MG	1w	105	1/1	0.95	0.18	58,58,58,58	0
56	MG	1A	3595	1/1	0.95	0.23	33,33,33,33	0
56	MG	2a	3233	1/1	0.95	0.17	61,61,61,61	0
56	MG	1A	4076	1/1	0.95	0.31	63,63,63,63	0
56	MG	2A	3824	1/1	0.95	0.18	34,34,34,34	0
56	MG	2d	302	1/1	0.95	0.08	59,59,59,59	0
56	MG	1A	3018	1/1	0.95	0.11	32,32,32,32	0
56	MG	2A	3828	1/1	0.95	0.12	32,32,32,32	0
56	MG	1A	3069	1/1	0.95	0.23	28,28,28,28	0
56	MG	1A	3273	1/1	0.95	0.23	28,28,28,28	0
56	MG	1A	3893	1/1	0.95	0.11	27,27,27,27	0
56	MG	1A	3894	1/1	0.95	0.18	35,35,35,35	0
56	MG	1A	3895	1/1	0.95	0.14	46,46,46,46	0
56	MG	1A	4088	1/1	0.95	0.13	36,36,36,36	0
56	MG	1A	3896	1/1	0.95	0.12	33,33,33,33	0
56	MG	2A	3849	1/1	0.95	0.14	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3232	1/1	0.95	0.13	37,37,37,37	0
56	MG	2q	201	1/1	0.95	0.14	58,58,58,58	0
56	MG	2A	3234	1/1	0.95	0.13	35,35,35,35	0
56	MG	1A	3720	1/1	0.95	0.13	33,33,33,33	0
56	MG	1A	3336	1/1	0.95	0.17	21,21,21,21	0
56	MG	1A	3274	1/1	0.95	0.18	51,51,51,51	0
56	MG	1A	3724	1/1	0.95	0.11	49,49,49,49	0
56	MG	2A	3480	1/1	0.95	0.33	28,28,28,28	0
56	MG	2A	3481	1/1	0.95	0.23	35,35,35,35	0
56	MG	1A	3604	1/1	0.95	0.25	30,30,30,30	0
56	MG	1A	4101	1/1	0.95	0.20	56,56,56,56	0
56	MG	2A	3241	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3902	1/1	0.95	0.19	30,30,30,30	0
56	MG	1A	3275	1/1	0.95	0.15	28,28,28,28	0
56	MG	1A	4105	1/1	0.95	0.27	50,50,50,50	0
56	MG	1A	3728	1/1	0.95	0.18	20,20,20,20	0
56	MG	1A	3908	1/1	0.95	0.21	41,41,41,41	0
56	MG	1a	1643	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3055	1/1	0.95	0.28	27,27,27,27	0
56	MG	2A	3010	1/1	0.95	0.18	45,45,45,45	0
56	MG	2A	3251	1/1	0.95	0.14	55,55,55,55	0
56	MG	1B	205	1/1	0.95	0.12	37,37,37,37	0
56	MG	2A	3504	1/1	0.95	0.26	52,52,52,52	0
56	MG	1A	3608	1/1	0.95	0.20	42,42,42,42	0
56	MG	1A	3057	1/1	0.95	0.23	19,19,19,19	0
56	MG	1A	3059	1/1	0.95	0.28	40,40,40,40	0
56	MG	2A	3015	1/1	0.95	0.19	34,34,34,34	0
56	MG	2B	211	1/1	0.95	0.17	52,52,52,52	0
56	MG	2A	3257	1/1	0.95	0.17	42,42,42,42	0
56	MG	2A	3511	1/1	0.95	0.14	34,34,34,34	0
56	MG	1A	3263	1/1	0.96	0.14	36,36,36,36	0
56	MG	2A	3413	1/1	0.96	0.10	59,59,59,59	0
56	MG	1A	3806	1/1	0.96	0.19	20,20,20,20	0
56	MG	2A	3672	1/1	0.96	0.07	28,28,28,28	0
56	MG	1A	4074	1/1	0.96	0.05	42,42,42,42	0
56	MG	2A	3226	1/1	0.96	0.12	58,58,58,58	0
56	MG	2A	3418	1/1	0.96	0.18	43,43,43,43	0
56	MG	28	103	1/1	0.96	0.15	37,37,37,37	0
56	MG	2A	3227	1/1	0.96	0.18	59,59,59,59	0
56	MG	29	101	1/1	0.96	0.14	59,59,59,59	0
56	MG	1A	3502	1/1	0.96	0.24	26,26,26,26	0
56	MG	1A	3621	1/1	0.96	0.33	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3423	1/1	0.96	0.23	42,42,42,42	0
56	MG	1A	4079	1/1	0.96	0.22	35,35,35,35	0
56	MG	1A	3932	1/1	0.96	0.14	34,34,34,34	0
56	MG	1A	3047	1/1	0.96	0.17	30,30,30,30	0
56	MG	2A	3233	1/1	0.96	0.59	43,43,43,43	0
56	MG	1A	3027	1/1	0.96	0.12	65,65,65,65	0
56	MG	2a	3011	1/1	0.96	0.16	49,49,49,49	0
56	MG	1Z	3702	1/1	0.96	0.20	53,53,53,53	0
56	MG	2A	3049	1/1	0.96	0.17	20,20,20,20	0
56	MG	10	101	1/1	0.96	0.36	43,43,43,43	0
56	MG	1A	3129	1/1	0.96	0.18	32,32,32,32	0
56	MG	1a	1729	1/1	0.96	0.25	46,46,46,46	0
56	MG	1A	3813	1/1	0.96	0.20	35,35,35,35	0
56	MG	1A	3712	1/1	0.96	0.13	18,18,18,18	0
56	MG	1A	3944	1/1	0.96	0.15	22,22,22,22	0
56	MG	1A	4092	1/1	0.96	0.12	35,35,35,35	0
56	MG	2A	3701	1/1	0.96	0.14	54,54,54,54	0
56	MG	1a	1734	1/1	0.96	0.13	51,51,51,51	0
56	MG	2a	3024	1/1	0.96	0.20	38,38,38,38	0
56	MG	1A	3085	1/1	0.96	0.14	30,30,30,30	0
56	MG	1A	3178	1/1	0.96	0.32	28,28,28,28	0
56	MG	1A	3354	1/1	0.96	0.23	38,38,38,38	0
56	MG	1A	3206	1/1	0.96	0.27	24,24,24,24	0
56	MG	1A	3630	1/1	0.96	0.22	12,12,12,12	0
56	MG	1A	3408	1/1	0.96	0.47	32,32,32,32	0
56	MG	1A	3632	1/1	0.96	0.23	38,38,38,38	0
56	MG	2A	3710	1/1	0.96	0.13	56,56,56,56	0
56	MG	2A	3712	1/1	0.96	0.17	69,69,69,69	0
56	MG	15	103	1/1	0.96	0.36	32,32,32,32	0
56	MG	2A	3714	1/1	0.96	0.12	50,50,50,50	0
56	MG	2A	3068	1/1	0.96	0.16	28,28,28,28	0
56	MG	2A	3717	1/1	0.96	0.14	27,27,27,27	0
56	MG	1a	1749	1/1	0.96	0.12	32,32,32,32	0
56	MG	1a	1751	1/1	0.96	0.11	34,34,34,34	0
56	MG	1A	3954	1/1	0.96	0.20	41,41,41,41	0
56	MG	1A	3461	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3829	1/1	0.96	0.15	18,18,18,18	0
56	MG	1A	4106	1/1	0.96	0.11	45,45,45,45	0
56	MG	2A	3077	1/1	0.96	0.23	26,26,26,26	0
56	MG	1A	3513	1/1	0.96	0.18	38,38,38,38	0
56	MG	1A	3310	1/1	0.96	0.17	28,28,28,28	0
56	MG	1a	1759	1/1	0.96	0.26	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3179	1/1	0.96	0.25	33,33,33,33	0
56	MG	1A	3464	1/1	0.96	0.22	27,27,27,27	0
56	MG	1A	3236	1/1	0.96	0.18	40,40,40,40	0
56	MG	2a	3052	1/1	0.96	0.16	54,54,54,54	0
56	MG	2A	3085	1/1	0.96	0.08	37,37,37,37	0
56	MG	2a	3054	1/1	0.96	0.12	55,55,55,55	0
56	MG	1A	3963	1/1	0.96	0.21	14,14,14,14	0
56	MG	1A	3732	1/1	0.96	0.21	17,17,17,17	0
56	MG	2A	3738	1/1	0.96	0.21	48,48,48,48	0
56	MG	2A	3739	1/1	0.96	0.10	62,62,62,62	0
56	MG	1A	3965	1/1	0.96	0.24	17,17,17,17	0
56	MG	1A	3734	1/1	0.96	0.16	17,17,17,17	0
56	MG	2A	3273	1/1	0.96	0.10	59,59,59,59	0
56	MG	1A	3361	1/1	0.96	0.21	26,26,26,26	0
56	MG	1A	3237	1/1	0.96	0.15	45,45,45,45	0
56	MG	1A	3644	1/1	0.96	0.16	30,30,30,30	0
56	MG	2A	3094	1/1	0.96	0.19	33,33,33,33	0
56	MG	1A	3131	1/1	0.96	0.18	20,20,20,20	0
56	MG	1A	3316	1/1	0.96	0.23	23,23,23,23	0
56	MG	2a	3071	1/1	0.96	0.14	45,45,45,45	0
56	MG	2A	3751	1/1	0.96	0.12	54,54,54,54	0
56	MG	1A	3742	1/1	0.96	0.21	40,40,40,40	0
56	MG	1A	3978	1/1	0.96	0.12	42,42,42,42	0
56	MG	1A	3743	1/1	0.96	0.14	37,37,37,37	0
56	MG	1A	3847	1/1	0.96	0.18	49,49,49,49	0
56	MG	1A	3086	1/1	0.96	0.24	22,22,22,22	0
56	MG	2A	3102	1/1	0.96	0.11	37,37,37,37	0
56	MG	2A	3758	1/1	0.96	0.09	35,35,35,35	0
56	MG	1a	1784	1/1	0.96	0.16	43,43,43,43	0
56	MG	1A	3319	1/1	0.96	0.26	46,46,46,46	0
56	MG	2A	3493	1/1	0.96	0.14	25,25,25,25	0
56	MG	2A	3105	1/1	0.96	0.13	48,48,48,48	0
56	MG	2A	3764	1/1	0.96	0.10	48,48,48,48	0
56	MG	2A	3765	1/1	0.96	0.07	54,54,54,54	0
56	MG	2A	3106	1/1	0.96	0.13	39,39,39,39	0
56	MG	1A	3320	1/1	0.96	0.20	41,41,41,41	0
56	MG	2A	3498	1/1	0.96	0.17	38,38,38,38	0
56	MG	1A	3747	1/1	0.96	0.12	55,55,55,55	0
56	MG	2A	3109	1/1	0.96	0.18	55,55,55,55	0
56	MG	1A	3852	1/1	0.96	0.16	45,45,45,45	0
56	MG	1A	3749	1/1	0.96	0.14	52,52,52,52	0
56	MG	1A	3321	1/1	0.96	0.16	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3774	1/1	0.96	0.19	45,45,45,45	0
56	MG	2a	3100	1/1	0.96	0.11	58,58,58,58	0
56	MG	1a	1624	1/1	0.96	0.24	47,47,47,47	0
56	MG	1A	3860	1/1	0.96	0.14	41,41,41,41	0
56	MG	1A	3861	1/1	0.96	0.27	27,27,27,27	0
56	MG	1A	3994	1/1	0.96	0.14	38,38,38,38	0
56	MG	1A	3210	1/1	0.96	0.18	28,28,28,28	0
56	MG	1A	3372	1/1	0.96	0.17	47,47,47,47	0
56	MG	2A	3513	1/1	0.96	0.09	47,47,47,47	0
56	MG	2A	3514	1/1	0.96	0.11	47,47,47,47	0
56	MG	2A	3515	1/1	0.96	0.18	35,35,35,35	0
56	MG	2A	3516	1/1	0.96	0.22	48,48,48,48	0
56	MG	2a	3113	1/1	0.96	0.11	58,58,58,58	0
56	MG	1A	3528	1/1	0.96	0.20	41,41,41,41	0
56	MG	2A	3303	1/1	0.96	0.15	46,46,46,46	0
56	MG	1a	1802	1/1	0.96	0.06	52,52,52,52	0
56	MG	2A	3521	1/1	0.96	0.13	57,57,57,57	0
56	MG	2A	3789	1/1	0.96	0.21	52,52,52,52	0
56	MG	2A	3122	1/1	0.96	0.16	51,51,51,51	0
56	MG	1A	3243	1/1	0.96	0.17	18,18,18,18	0
56	MG	1A	3087	1/1	0.96	0.24	21,21,21,21	0
56	MG	1A	3870	1/1	0.96	0.09	61,61,61,61	0
56	MG	2A	3126	1/1	0.96	0.13	61,61,61,61	0
56	MG	2A	3797	1/1	0.96	0.09	52,52,52,52	0
56	MG	1A	3245	1/1	0.96	0.33	34,34,34,34	0
56	MG	1A	3759	1/1	0.96	0.18	45,45,45,45	0
56	MG	2a	3129	1/1	0.96	0.26	46,46,46,46	0
56	MG	1A	3078	1/1	0.96	0.17	27,27,27,27	0
56	MG	1a	1813	1/1	0.96	0.10	52,52,52,52	0
56	MG	1a	1638	1/1	0.96	0.34	38,38,38,38	0
56	MG	1A	3874	1/1	0.96	0.14	32,32,32,32	0
56	MG	2A	3804	1/1	0.96	0.09	49,49,49,49	0
56	MG	1E	304	1/1	0.96	0.15	26,26,26,26	0
56	MG	1A	3594	1/1	0.96	0.15	23,23,23,23	0
56	MG	2A	3540	1/1	0.96	0.17	48,48,48,48	0
56	MG	2A	3541	1/1	0.96	0.16	47,47,47,47	0
56	MG	2A	3542	1/1	0.96	0.20	44,44,44,44	0
56	MG	2A	3810	1/1	0.96	0.05	77,77,77,77	0
56	MG	1A	3247	1/1	0.96	0.29	31,31,31,31	0
56	MG	1A	3596	1/1	0.96	0.19	37,37,37,37	0
56	MG	2A	3547	1/1	0.96	0.19	43,43,43,43	0
56	MG	2A	3548	1/1	0.96	0.13	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3878	1/1	0.96	0.13	41,41,41,41	0
56	MG	2A	3325	1/1	0.96	0.25	49,49,49,49	0
56	MG	1E	311	1/1	0.96	0.35	37,37,37,37	0
56	MG	2A	3141	1/1	0.96	0.10	50,50,50,50	0
56	MG	1A	3116	1/1	0.96	0.19	33,33,33,33	0
56	MG	1b	302	1/1	0.96	0.17	58,58,58,58	0
56	MG	2A	3826	1/1	0.96	0.11	35,35,35,35	0
56	MG	2A	3560	1/1	0.96	0.17	51,51,51,51	0
56	MG	1a	1648	1/1	0.96	0.06	45,45,45,45	0
56	MG	2a	3159	1/1	0.96	0.10	39,39,39,39	0
56	MG	2A	3829	1/1	0.96	0.15	43,43,43,43	0
56	MG	1a	1649	1/1	0.96	0.13	49,49,49,49	0
56	MG	1A	3598	1/1	0.96	0.25	33,33,33,33	0
56	MG	2A	3147	1/1	0.96	0.18	40,40,40,40	0
56	MG	1A	3159	1/1	0.96	0.18	28,28,28,28	0
56	MG	2A	3844	1/1	0.96	0.17	47,47,47,47	0
56	MG	1a	1653	1/1	0.96	0.12	45,45,45,45	0
56	MG	1a	1654	1/1	0.96	0.13	47,47,47,47	0
56	MG	2A	3571	1/1	0.96	0.14	40,40,40,40	0
56	MG	1A	3330	1/1	0.96	0.14	28,28,28,28	0
56	MG	2a	3175	1/1	0.96	0.09	53,53,53,53	0
56	MG	2A	3574	1/1	0.96	0.12	51,51,51,51	0
56	MG	2A	3152	1/1	0.96	0.17	46,46,46,46	0
56	MG	2A	3339	1/1	0.96	0.18	43,43,43,43	0
56	MG	1A	3771	1/1	0.96	0.13	47,47,47,47	0
56	MG	2a	3180	1/1	0.96	0.07	54,54,54,54	0
56	MG	2a	3181	1/1	0.96	0.21	52,52,52,52	0
56	MG	2a	3182	1/1	0.96	0.22	47,47,47,47	0
56	MG	1A	4016	1/1	0.96	0.08	52,52,52,52	0
56	MG	2A	3582	1/1	0.96	0.16	30,30,30,30	0
56	MG	1a	1659	1/1	0.96	0.30	58,58,58,58	0
56	MG	1A	3884	1/1	0.96	0.18	47,47,47,47	0
56	MG	1A	3056	1/1	0.96	0.19	32,32,32,32	0
56	MG	2A	3864	1/1	0.96	0.17	32,32,32,32	0
56	MG	1A	3887	1/1	0.96	0.14	26,26,26,26	0
56	MG	2A	3866	1/1	0.96	0.20	44,44,44,44	0
56	MG	1A	3889	1/1	0.96	0.20	44,44,44,44	0
56	MG	2A	3868	1/1	0.96	0.24	41,41,41,41	0
56	MG	2A	3869	1/1	0.96	0.09	50,50,50,50	0
56	MG	1A	3162	1/1	0.96	0.28	25,25,25,25	0
56	MG	1A	3676	1/1	0.96	0.21	19,19,19,19	0
56	MG	2A	3873	1/1	0.96	0.19	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4024	1/1	0.96	0.15	20,20,20,20	0
56	MG	1A	3775	1/1	0.96	0.19	26,26,26,26	0
56	MG	2A	3593	1/1	0.96	0.26	34,34,34,34	0
56	MG	1A	4028	1/1	0.96	0.20	66,66,66,66	0
56	MG	1A	3333	1/1	0.96	0.19	24,24,24,24	0
56	MG	2a	3205	1/1	0.96	0.22	51,51,51,51	0
56	MG	1A	3778	1/1	0.96	0.28	52,52,52,52	0
56	MG	1x	104	1/1	0.96	0.18	53,53,53,53	0
56	MG	1A	3779	1/1	0.96	0.11	47,47,47,47	0
56	MG	2B	204	1/1	0.96	0.10	71,71,71,71	0
56	MG	1A	3191	1/1	0.96	0.18	28,28,28,28	0
56	MG	1A	3606	1/1	0.96	0.21	32,32,32,32	0
56	MG	2B	207	1/1	0.96	0.14	55,55,55,55	0
56	MG	2A	3604	1/1	0.96	0.21	50,50,50,50	0
56	MG	2a	3215	1/1	0.96	0.14	61,61,61,61	0
56	MG	1a	1674	1/1	0.96	0.21	43,43,43,43	0
56	MG	2A	3606	1/1	0.96	0.21	52,52,52,52	0
56	MG	1O	202	1/1	0.96	0.29	49,49,49,49	0
56	MG	2A	3361	1/1	0.96	0.14	47,47,47,47	0
56	MG	1O	205	1/1	0.96	0.13	47,47,47,47	0
56	MG	2a	3223	1/1	0.96	0.18	58,58,58,58	0
56	MG	1A	4035	1/1	0.96	0.11	27,27,27,27	0
56	MG	1A	3119	1/1	0.96	0.17	27,27,27,27	0
56	MG	1A	4038	1/1	0.96	0.19	30,30,30,30	0
56	MG	1A	3337	1/1	0.96	0.18	35,35,35,35	0
56	MG	1A	3684	1/1	0.96	0.20	35,35,35,35	0
56	MG	2A	3618	1/1	0.96	0.18	58,58,58,58	0
56	MG	1A	3338	1/1	0.96	0.27	41,41,41,41	0
56	MG	1a	1684	1/1	0.96	0.11	47,47,47,47	0
56	MG	1Q	201	1/1	0.96	0.20	22,22,22,22	0
56	MG	1A	4043	1/1	0.96	0.16	55,55,55,55	0
56	MG	1A	3139	1/1	0.96	0.27	25,25,25,25	0
56	MG	2D	305	1/1	0.96	0.53	40,40,40,40	0
56	MG	1A	4046	1/1	0.96	0.16	34,34,34,34	0
56	MG	1A	3441	1/1	0.96	0.14	39,39,39,39	0
56	MG	1A	3790	1/1	0.96	0.22	39,39,39,39	0
56	MG	2A	3627	1/1	0.96	0.11	59,59,59,59	0
56	MG	1A	4049	1/1	0.96	0.16	33,33,33,33	0
56	MG	2E	306	1/1	0.96	0.17	40,40,40,40	0
56	MG	1S	201	1/1	0.96	0.20	43,43,43,43	0
56	MG	1A	3911	1/1	0.96	0.12	31,31,31,31	0
56	MG	1a	1694	1/1	0.96	0.11	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	2A	3198	1/1	0.96	0.18	48,48,48,48	0
56	MG	2A	3634	1/1	0.96	0.13	26,26,26,26	0
56	MG	1A	3294	1/1	0.96	0.32	27,27,27,27	0
56	MG	1A	3792	1/1	0.96	0.15	38,38,38,38	0
56	MG	1A	3035	1/1	0.96	0.11	38,38,38,38	0
56	MG	2r	101	1/1	0.96	0.11	56,56,56,56	0
56	MG	1A	3693	1/1	0.96	0.18	18,18,18,18	0
56	MG	2A	3642	1/1	0.96	0.20	39,39,39,39	0
56	MG	2O	201	1/1	0.96	0.17	46,46,46,46	0
56	MG	1A	3694	1/1	0.96	0.23	17,17,17,17	0
56	MG	2A	3389	1/1	0.96	0.26	53,53,53,53	0
56	MG	2Q	201	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3444	1/1	0.96	0.15	36,36,36,36	0
56	MG	1A	3919	1/1	0.96	0.23	17,17,17,17	0
56	MG	1A	3141	1/1	0.96	0.15	30,30,30,30	0
56	MG	1A	4062	1/1	0.96	0.12	36,36,36,36	0
56	MG	2A	3208	1/1	0.96	0.18	32,32,32,32	0
56	MG	1A	3260	1/1	0.96	0.11	51,51,51,51	0
56	MG	2A	3654	1/1	0.96	0.17	60,60,60,60	0
56	MG	2A	3024	1/1	0.96	0.33	46,46,46,46	0
56	MG	2A	3025	1/1	0.96	0.43	44,44,44,44	0
56	MG	2A	3026	1/1	0.96	0.39	43,43,43,43	0
56	MG	1A	3923	1/1	0.96	0.14	22,22,22,22	0
56	MG	1A	3063	1/1	0.96	0.18	46,46,46,46	0
56	MG	2A	3215	1/1	0.96	0.13	41,41,41,41	0
56	MG	1V	205	1/1	0.96	0.09	30,30,30,30	0
56	MG	1A	3925	1/1	0.96	0.14	54,54,54,54	0
57	TYK	2A	3879	64/64	0.96	0.21	26,33,41,50	0
56	MG	1W	201	1/1	0.96	0.15	33,33,33,33	0
56	MG	2I	101	1/1	0.96	0.70	44,44,44,44	0
56	MG	1W	202	1/1	0.96	0.28	34,34,34,34	0
58	ZN	25	105	1/1	0.96	0.09	74,74,74,74	0
58	ZN	29	102	1/1	0.96	0.12	64,64,64,64	0
56	MG	2A	3220	1/1	0.96	0.19	49,49,49,49	0
56	MG	1A	3058	1/1	0.96	0.24	36,36,36,36	0
56	MG	1W	206	1/1	0.96	0.14	34,34,34,34	0
56	MG	1Q	202	1/1	0.97	0.26	34,34,34,34	0
56	MG	1Q	203	1/1	0.97	0.15	33,33,33,33	0
56	MG	1A	3716	1/1	0.97	0.15	20,20,20,20	0
56	MG	2A	3422	1/1	0.97	0.20	46,46,46,46	0
56	MG	1A	3095	1/1	0.97	0.30	44,44,44,44	0
56	MG	2A	3017	1/1	0.97	0.15	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	3425	1/1	0.97	0.17	43,43,43,43	0
56	MG	1R	201	1/1	0.97	0.23	31,31,31,31	0
56	MG	1A	3362	1/1	0.97	0.17	34,34,34,34	0
56	MG	1A	3001	1/1	0.97	0.19	34,34,34,34	0
56	MG	1A	4051	1/1	0.97	0.18	35,35,35,35	0
56	MG	1A	3212	1/1	0.97	0.23	29,29,29,29	0
56	MG	1A	3575	1/1	0.97	0.14	17,17,17,17	0
56	MG	1S	202	1/1	0.97	0.18	49,49,49,49	0
56	MG	1A	3815	1/1	0.97	0.23	23,23,23,23	0
56	MG	2A	3688	1/1	0.97	0.16	36,36,36,36	0
56	MG	1A	3725	1/1	0.97	0.22	19,19,19,19	0
56	MG	1A	3928	1/1	0.97	0.17	23,23,23,23	0
56	MG	2A	3691	1/1	0.97	0.09	46,46,46,46	0
56	MG	2A	3028	1/1	0.97	0.33	47,47,47,47	0
56	MG	2A	3693	1/1	0.97	0.16	57,57,57,57	0
56	MG	2A	3437	1/1	0.97	0.17	46,46,46,46	0
56	MG	1a	1698	1/1	0.97	0.06	53,53,53,53	0
56	MG	2A	3439	1/1	0.97	0.20	45,45,45,45	0
56	MG	1A	3817	1/1	0.97	0.19	39,39,39,39	0
56	MG	1a	1700	1/1	0.97	0.26	42,42,42,42	0
56	MG	1A	3182	1/1	0.97	0.26	17,17,17,17	0
56	MG	1A	3112	1/1	0.97	0.15	23,23,23,23	0
56	MG	2A	3034	1/1	0.97	0.10	38,38,38,38	0
56	MG	2A	3445	1/1	0.97	0.15	46,46,46,46	0
56	MG	1U	203	1/1	0.97	0.15	23,23,23,23	0
56	MG	2a	3023	1/1	0.97	0.18	65,65,65,65	0
56	MG	1U	204	1/1	0.97	0.22	26,26,26,26	0
56	MG	1A	3640	1/1	0.97	0.14	24,24,24,24	0
56	MG	1A	3641	1/1	0.97	0.16	50,50,50,50	0
56	MG	1A	3935	1/1	0.97	0.08	53,53,53,53	0
56	MG	1A	3184	1/1	0.97	0.20	29,29,29,29	0
56	MG	2a	3029	1/1	0.97	0.13	51,51,51,51	0
56	MG	1A	3937	1/1	0.97	0.18	27,27,27,27	0
56	MG	2A	3711	1/1	0.97	0.14	24,24,24,24	0
56	MG	1A	3643	1/1	0.97	0.18	37,37,37,37	0
56	MG	1V	201	1/1	0.97	0.44	25,25,25,25	0
56	MG	1A	3040	1/1	0.97	0.25	44,44,44,44	0
56	MG	1A	3828	1/1	0.97	0.23	15,15,15,15	0
56	MG	2A	3716	1/1	0.97	0.19	37,37,37,37	0
56	MG	1A	4073	1/1	0.97	0.17	47,47,47,47	0
56	MG	2A	3718	1/1	0.97	0.16	43,43,43,43	0
56	MG	2A	3048	1/1	0.97	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3943	1/1	0.97	0.16	19,19,19,19	0
56	MG	1A	3733	1/1	0.97	0.12	22,22,22,22	0
56	MG	1A	3945	1/1	0.97	0.15	15,15,15,15	0
56	MG	1W	205	1/1	0.97	0.21	28,28,28,28	0
56	MG	2A	3724	1/1	0.97	0.12	32,32,32,32	0
56	MG	1A	4077	1/1	0.97	0.12	35,35,35,35	0
56	MG	1A	4078	1/1	0.97	0.24	42,42,42,42	0
56	MG	1A	3034	1/1	0.97	0.25	27,27,27,27	0
56	MG	1a	1722	1/1	0.97	0.20	54,54,54,54	0
56	MG	1a	1723	1/1	0.97	0.34	44,44,44,44	0
56	MG	1A	3101	1/1	0.97	0.09	58,58,58,58	0
56	MG	1A	4081	1/1	0.97	0.12	21,21,21,21	0
56	MG	1A	3948	1/1	0.97	0.26	40,40,40,40	0
56	MG	1A	3736	1/1	0.97	0.14	18,18,18,18	0
56	MG	1A	3051	1/1	0.97	0.29	25,25,25,25	0
56	MG	2A	3063	1/1	0.97	0.15	57,57,57,57	0
56	MG	1A	3017	1/1	0.97	0.14	48,48,48,48	0
56	MG	1A	3649	1/1	0.97	0.26	27,27,27,27	0
56	MG	1A	3223	1/1	0.97	0.17	36,36,36,36	0
56	MG	2A	3067	1/1	0.97	0.23	40,40,40,40	0
56	MG	1A	4090	1/1	0.97	0.16	31,31,31,31	0
56	MG	1A	4091	1/1	0.97	0.25	37,37,37,37	0
56	MG	2A	3483	1/1	0.97	0.08	40,40,40,40	0
56	MG	1A	3741	1/1	0.97	0.11	49,49,49,49	0
56	MG	2A	3486	1/1	0.97	0.24	41,41,41,41	0
56	MG	2a	3066	1/1	0.97	0.12	38,38,38,38	0
56	MG	2A	3487	1/1	0.97	0.14	45,45,45,45	0
56	MG	2A	3749	1/1	0.97	0.21	47,47,47,47	0
56	MG	2A	3488	1/1	0.97	0.08	40,40,40,40	0
56	MG	2a	3070	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	3652	1/1	0.97	0.19	20,20,20,20	0
56	MG	1a	1736	1/1	0.97	0.36	45,45,45,45	0
56	MG	2A	3073	1/1	0.97	0.16	59,59,59,59	0
56	MG	10	105	1/1	0.97	0.12	45,45,45,45	0
56	MG	2a	3075	1/1	0.97	0.12	46,46,46,46	0
56	MG	1A	3840	1/1	0.97	0.15	17,17,17,17	0
56	MG	1A	3586	1/1	0.97	0.26	26,26,26,26	0
56	MG	2A	3495	1/1	0.97	0.15	47,47,47,47	0
56	MG	1A	3161	1/1	0.97	0.18	28,28,28,28	0
56	MG	2a	3080	1/1	0.97	0.16	53,53,53,53	0
56	MG	1A	3424	1/1	0.97	0.21	34,34,34,34	0
56	MG	1A	3293	1/1	0.97	0.29	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1746	1/1	0.97	0.15	39,39,39,39	0
56	MG	1a	1747	1/1	0.97	0.14	58,58,58,58	0
56	MG	2A	3501	1/1	0.97	0.15	53,53,53,53	0
56	MG	1A	3118	1/1	0.97	0.28	22,22,22,22	0
56	MG	1A	3748	1/1	0.97	0.13	22,22,22,22	0
56	MG	2a	3088	1/1	0.97	0.15	53,53,53,53	0
56	MG	13	102	1/1	0.97	0.19	31,31,31,31	0
56	MG	13	103	1/1	0.97	0.17	30,30,30,30	0
56	MG	2a	3091	1/1	0.97	0.20	47,47,47,47	0
56	MG	1A	4103	1/1	0.97	0.31	47,47,47,47	0
56	MG	2a	3093	1/1	0.97	0.26	72,72,72,72	0
56	MG	13	105	1/1	0.97	0.24	19,19,19,19	0
56	MG	13	106	1/1	0.97	0.15	35,35,35,35	0
56	MG	1a	1756	1/1	0.97	0.20	28,28,28,28	0
56	MG	1A	3592	1/1	0.97	0.14	21,21,21,21	0
56	MG	2A	3512	1/1	0.97	0.14	44,44,44,44	0
56	MG	1A	3256	1/1	0.97	0.25	40,40,40,40	0
56	MG	15	104	1/1	0.97	0.20	27,27,27,27	0
56	MG	1A	3335	1/1	0.97	0.20	45,45,45,45	0
56	MG	16	101	1/1	0.97	0.16	37,37,37,37	0
56	MG	1A	3296	1/1	0.97	0.12	33,33,33,33	0
56	MG	1a	1764	1/1	0.97	0.15	33,33,33,33	0
56	MG	1a	1765	1/1	0.97	0.19	52,52,52,52	0
56	MG	1A	3163	1/1	0.97	0.29	32,32,32,32	0
56	MG	2a	3107	1/1	0.97	0.26	61,61,61,61	0
56	MG	1A	3969	1/1	0.97	0.17	28,28,28,28	0
56	MG	1B	204	1/1	0.97	0.24	39,39,39,39	0
56	MG	17	103	1/1	0.97	0.15	35,35,35,35	0
56	MG	2a	3111	1/1	0.97	0.21	52,52,52,52	0
56	MG	2A	3527	1/1	0.97	0.14	47,47,47,47	0
56	MG	1a	1770	1/1	0.97	0.26	46,46,46,46	0
56	MG	1A	3971	1/1	0.97	0.11	31,31,31,31	0
56	MG	1B	206	1/1	0.97	0.22	36,36,36,36	0
56	MG	2A	3531	1/1	0.97	0.10	54,54,54,54	0
56	MG	1A	3382	1/1	0.97	0.33	38,38,38,38	0
56	MG	2A	3309	1/1	0.97	0.13	49,49,49,49	0
56	MG	2A	3310	1/1	0.97	0.17	45,45,45,45	0
56	MG	2A	3795	1/1	0.97	0.18	42,42,42,42	0
56	MG	1a	1775	1/1	0.97	0.15	41,41,41,41	0
56	MG	18	105	1/1	0.97	0.26	51,51,51,51	0
56	MG	1A	3854	1/1	0.97	0.17	35,35,35,35	0
56	MG	2a	3125	1/1	0.97	0.08	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3112	1/1	0.97	0.23	57,57,57,57	0
56	MG	1a	1778	1/1	0.97	0.20	54,54,54,54	0
56	MG	1A	3259	1/1	0.97	0.12	40,40,40,40	0
56	MG	1A	3975	1/1	0.97	0.11	45,45,45,45	0
56	MG	1A	3856	1/1	0.97	0.21	31,31,31,31	0
56	MG	1A	3977	1/1	0.97	0.15	30,30,30,30	0
56	MG	2A	3546	1/1	0.97	0.13	42,42,42,42	0
56	MG	1A	3858	1/1	0.97	0.15	27,27,27,27	0
56	MG	1A	3339	1/1	0.97	0.26	31,31,31,31	0
56	MG	1A	3434	1/1	0.97	0.19	30,30,30,30	0
56	MG	2A	3550	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3862	1/1	0.97	0.23	57,57,57,57	0
56	MG	2A	3552	1/1	0.97	0.18	38,38,38,38	0
56	MG	2A	3812	1/1	0.97	0.23	63,63,63,63	0
56	MG	2A	3813	1/1	0.97	0.06	67,67,67,67	0
56	MG	2a	3143	1/1	0.97	0.10	62,62,62,62	0
56	MG	1A	3863	1/1	0.97	0.23	35,35,35,35	0
56	MG	1a	1610	1/1	0.97	0.20	17,17,17,17	0
56	MG	2A	3556	1/1	0.97	0.20	28,28,28,28	0
56	MG	1B	219	1/1	0.97	0.24	31,31,31,31	0
56	MG	1A	3760	1/1	0.97	0.18	31,31,31,31	0
56	MG	2a	3150	1/1	0.97	0.17	38,38,38,38	0
56	MG	1a	1794	1/1	0.97	0.16	48,48,48,48	0
56	MG	2A	3561	1/1	0.97	0.13	32,32,32,32	0
56	MG	1A	3985	1/1	0.97	0.10	40,40,40,40	0
56	MG	1A	3761	1/1	0.97	0.12	30,30,30,30	0
56	MG	2A	3825	1/1	0.97	0.16	43,43,43,43	0
56	MG	1A	3866	1/1	0.97	0.14	32,32,32,32	0
56	MG	1A	3762	1/1	0.97	0.20	17,17,17,17	0
56	MG	1A	3299	1/1	0.97	0.27	41,41,41,41	0
56	MG	1A	3043	1/1	0.97	0.21	27,27,27,27	0
56	MG	2a	3161	1/1	0.97	0.15	60,60,60,60	0
56	MG	2A	3568	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3673	1/1	0.97	0.14	55,55,55,55	0
56	MG	2A	3834	1/1	0.97	0.10	38,38,38,38	0
56	MG	2A	3570	1/1	0.97	0.18	51,51,51,51	0
56	MG	2A	3842	1/1	0.97	0.19	60,60,60,60	0
56	MG	1a	1621	1/1	0.97	0.17	50,50,50,50	0
56	MG	2A	3572	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	3993	1/1	0.97	0.14	19,19,19,19	0
56	MG	1A	3071	1/1	0.97	0.18	18,18,18,18	0
56	MG	2a	3172	1/1	0.97	0.11	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3121	1/1	0.97	0.17	30,30,30,30	0
56	MG	2A	3340	1/1	0.97	0.09	56,56,56,56	0
56	MG	2A	3578	1/1	0.97	0.10	33,33,33,33	0
56	MG	1B	232	1/1	0.97	0.13	69,69,69,69	0
56	MG	2A	3140	1/1	0.97	0.14	39,39,39,39	0
56	MG	2A	3581	1/1	0.97	0.13	41,41,41,41	0
56	MG	1A	3996	1/1	0.97	0.14	40,40,40,40	0
56	MG	1A	3142	1/1	0.97	0.23	33,33,33,33	0
56	MG	2A	3858	1/1	0.97	0.04	55,55,55,55	0
56	MG	2A	3859	1/1	0.97	0.10	51,51,51,51	0
56	MG	2A	3860	1/1	0.97	0.14	28,28,28,28	0
56	MG	1a	1811	1/1	0.97	0.12	56,56,56,56	0
56	MG	1a	1812	1/1	0.97	0.20	46,46,46,46	0
56	MG	1A	3106	1/1	0.97	0.17	28,28,28,28	0
56	MG	1a	1814	1/1	0.97	0.21	51,51,51,51	0
56	MG	1A	3391	1/1	0.97	0.23	47,47,47,47	0
56	MG	2A	3589	1/1	0.97	0.15	54,54,54,54	0
56	MG	1D	305	1/1	0.97	0.32	33,33,33,33	0
56	MG	2a	3192	1/1	0.97	0.24	55,55,55,55	0
56	MG	2a	3193	1/1	0.97	0.06	53,53,53,53	0
56	MG	1A	3680	1/1	0.97	0.17	37,37,37,37	0
56	MG	1A	4001	1/1	0.97	0.15	30,30,30,30	0
56	MG	1A	3305	1/1	0.97	0.16	32,32,32,32	0
56	MG	1A	3547	1/1	0.97	0.17	28,28,28,28	0
56	MG	1A	3548	1/1	0.97	0.28	30,30,30,30	0
56	MG	1a	1636	1/1	0.97	0.32	45,45,45,45	0
56	MG	1A	3685	1/1	0.97	0.08	48,48,48,48	0
56	MG	2A	3156	1/1	0.97	0.09	33,33,33,33	0
56	MG	1A	3107	1/1	0.97	0.18	20,20,20,20	0
56	MG	1A	3171	1/1	0.97	0.13	19,19,19,19	0
56	MG	2a	3204	1/1	0.97	0.09	65,65,65,65	0
56	MG	2A	3602	1/1	0.97	0.12	41,41,41,41	0
56	MG	2A	3603	1/1	0.97	0.17	47,47,47,47	0
56	MG	1A	3445	1/1	0.97	0.17	40,40,40,40	0
56	MG	1A	3689	1/1	0.97	0.16	39,39,39,39	0
56	MG	1E	306	1/1	0.97	0.16	20,20,20,20	0
56	MG	1A	3885	1/1	0.97	0.29	47,47,47,47	0
56	MG	1h	201	1/1	0.97	0.11	62,62,62,62	0
56	MG	1A	3036	1/1	0.97	0.22	29,29,29,29	0
56	MG	1E	309	1/1	0.97	0.21	19,19,19,19	0
56	MG	2A	3611	1/1	0.97	0.18	53,53,53,53	0
56	MG	1A	3147	1/1	0.97	0.25	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1a	1647	1/1	0.97	0.11	40,40,40,40	0
56	MG	1A	3888	1/1	0.97	0.21	23,23,23,23	0
56	MG	1A	3784	1/1	0.97	0.10	35,35,35,35	0
56	MG	2A	3172	1/1	0.97	0.08	44,44,44,44	0
56	MG	1A	3890	1/1	0.97	0.14	26,26,26,26	0
56	MG	2B	217	1/1	0.97	0.15	49,49,49,49	0
56	MG	1A	3148	1/1	0.97	0.29	19,19,19,19	0
56	MG	1a	1652	1/1	0.97	0.08	45,45,45,45	0
56	MG	1A	3352	1/1	0.97	0.34	32,32,32,32	0
56	MG	2A	3177	1/1	0.97	0.19	36,36,36,36	0
56	MG	1A	3270	1/1	0.97	0.23	48,48,48,48	0
56	MG	2A	3380	1/1	0.97	0.10	45,45,45,45	0
56	MG	1A	3451	1/1	0.97	0.16	26,26,26,26	0
56	MG	1A	3697	1/1	0.97	0.14	29,29,29,29	0
56	MG	2A	3628	1/1	0.97	0.10	54,54,54,54	0
56	MG	1A	3127	1/1	0.97	0.26	35,35,35,35	0
56	MG	1w	107	1/1	0.97	0.19	45,45,45,45	0
56	MG	1a	1658	1/1	0.97	0.12	51,51,51,51	0
56	MG	1A	3238	1/1	0.97	0.10	36,36,36,36	0
56	MG	1A	3403	1/1	0.97	0.54	44,44,44,44	0
56	MG	2E	305	1/1	0.97	0.16	27,27,27,27	0
56	MG	1A	4025	1/1	0.97	0.17	29,29,29,29	0
56	MG	2E	307	1/1	0.97	0.14	26,26,26,26	0
56	MG	1x	106	1/1	0.97	0.21	52,52,52,52	0
56	MG	2A	3636	1/1	0.97	0.17	28,28,28,28	0
56	MG	2E	310	1/1	0.97	0.16	47,47,47,47	0
56	MG	2A	3637	1/1	0.97	0.13	53,53,53,53	0
56	MG	1A	3793	1/1	0.97	0.16	28,28,28,28	0
56	MG	1G	202	1/1	0.97	0.16	46,46,46,46	0
56	MG	1A	3703	1/1	0.97	0.13	18,18,18,18	0
56	MG	2A	3641	1/1	0.97	0.13	33,33,33,33	0
56	MG	2F	306	1/1	0.97	0.22	47,47,47,47	0
56	MG	2A	3394	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3404	1/1	0.97	0.39	24,24,24,24	0
56	MG	2A	3644	1/1	0.97	0.13	52,52,52,52	0
56	MG	2A	3396	1/1	0.97	0.10	38,38,38,38	0
56	MG	2P	201	1/1	0.97	0.22	46,46,46,46	0
56	MG	1A	3705	1/1	0.97	0.15	15,15,15,15	0
56	MG	1N	201	1/1	0.97	0.40	43,43,43,43	0
56	MG	1A	3508	1/1	0.97	0.09	42,42,42,42	0
56	MG	1A	3904	1/1	0.97	0.16	25,25,25,25	0
56	MG	1x	115	1/1	0.97	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	3798	1/1	0.97	0.12	25,25,25,25	0
56	MG	2A	3653	1/1	0.97	0.15	38,38,38,38	0
56	MG	1A	4034	1/1	0.97	0.18	19,19,19,19	0
56	MG	1A	3356	1/1	0.97	0.25	27,27,27,27	0
56	MG	1A	4036	1/1	0.97	0.10	28,28,28,28	0
56	MG	1O	203	1/1	0.97	0.22	43,43,43,43	0
56	MG	1A	3909	1/1	0.97	0.14	42,42,42,42	0
56	MG	1A	3627	1/1	0.97	0.27	29,29,29,29	0
56	MG	2A	3660	1/1	0.97	0.22	55,55,55,55	0
56	MG	1A	3239	1/1	0.97	0.16	39,39,39,39	0
56	MG	1A	3567	1/1	0.97	0.15	32,32,32,32	0
57	TYK	1A	4107	64/64	0.97	0.22	13,21,29,34	0
56	MG	2Y	201	1/1	0.97	0.17	48,48,48,48	0
56	MG	2Z	301	1/1	0.97	0.18	68,68,68,68	0
56	MG	2A	3007	1/1	0.97	0.20	43,43,43,43	0
58	ZN	2Y	202	1/1	0.97	0.08	83,83,83,83	0
56	MG	1A	3458	1/1	0.97	0.19	33,33,33,33	0
56	MG	1A	3177	1/1	0.97	0.18	34,34,34,34	0
56	MG	1A	3807	1/1	0.97	0.12	22,22,22,22	0
56	MG	1A	3038	1/1	0.97	0.14	28,28,28,28	0
56	MG	2A	3417	1/1	0.97	0.12	39,39,39,39	0
56	MG	1a	1683	1/1	0.97	0.12	64,64,64,64	0
56	MG	1a	1809	1/1	0.98	0.22	38,38,38,38	0
56	MG	1A	3011	1/1	0.98	0.16	31,31,31,31	0
56	MG	2A	3161	1/1	0.98	0.28	32,32,32,32	0
56	MG	1a	1612	1/1	0.98	0.08	57,57,57,57	0
56	MG	1A	3482	1/1	0.98	0.14	24,24,24,24	0
56	MG	1A	3258	1/1	0.98	0.12	49,49,49,49	0
56	MG	1A	3970	1/1	0.98	0.14	44,44,44,44	0
56	MG	1A	3682	1/1	0.98	0.21	20,20,20,20	0
56	MG	2U	201	1/1	0.98	0.28	49,49,49,49	0
56	MG	1A	4041	1/1	0.98	0.19	40,40,40,40	0
56	MG	1R	206	1/1	0.98	0.25	29,29,29,29	0
56	MG	2A	3652	1/1	0.98	0.09	49,49,49,49	0
56	MG	2A	3523	1/1	0.98	0.14	31,31,31,31	0
56	MG	1A	3845	1/1	0.98	0.09	48,48,48,48	0
56	MG	1a	1820	1/1	0.98	0.28	27,27,27,27	0
56	MG	2A	3792	1/1	0.98	0.07	46,46,46,46	0
56	MG	1B	216	1/1	0.98	0.19	42,42,42,42	0
56	MG	1A	3557	1/1	0.98	0.25	17,17,17,17	0
56	MG	2a	3137	1/1	0.98	0.15	48,48,48,48	0
56	MG	1A	4044	1/1	0.98	0.27	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	3907	1/1	0.98	0.18	25,25,25,25	0
56	MG	1A	3028	1/1	0.98	0.24	25,25,25,25	0
56	MG	1A	3016	1/1	0.98	0.26	38,38,38,38	0
56	MG	1A	3910	1/1	0.98	0.15	23,23,23,23	0
56	MG	1A	3211	1/1	0.98	0.14	40,40,40,40	0
56	MG	2a	3145	1/1	0.98	0.06	45,45,45,45	0
56	MG	2A	3534	1/1	0.98	0.17	29,29,29,29	0
56	MG	23	104	1/1	0.98	0.13	53,53,53,53	0
56	MG	1A	3318	1/1	0.98	0.27	38,38,38,38	0
56	MG	1A	3044	1/1	0.98	0.20	29,29,29,29	0
56	MG	2A	3411	1/1	0.98	0.08	41,41,41,41	0
56	MG	1A	3602	1/1	0.98	0.12	30,30,30,30	0
56	MG	1A	3289	1/1	0.98	0.19	19,19,19,19	0
56	MG	1k	201	1/1	0.98	0.17	36,36,36,36	0
56	MG	2A	3184	1/1	0.98	0.09	37,37,37,37	0
56	MG	1U	208	1/1	0.98	0.14	34,34,34,34	0
56	MG	2A	3673	1/1	0.98	0.15	48,48,48,48	0
56	MG	2A	3674	1/1	0.98	0.18	34,34,34,34	0
56	MG	2A	3543	1/1	0.98	0.13	39,39,39,39	0
56	MG	1A	4055	1/1	0.98	0.16	16,16,16,16	0
56	MG	2a	3160	1/1	0.98	0.12	58,58,58,58	0
56	MG	2A	3814	1/1	0.98	0.13	56,56,56,56	0
56	MG	2A	3677	1/1	0.98	0.24	44,44,44,44	0
56	MG	2A	3075	1/1	0.98	0.26	33,33,33,33	0
56	MG	1A	3419	1/1	0.98	0.17	36,36,36,36	0
56	MG	2a	3006	1/1	0.98	0.11	42,42,42,42	0
56	MG	1A	3984	1/1	0.98	0.15	38,38,38,38	0
56	MG	1A	3290	1/1	0.98	0.23	25,25,25,25	0
56	MG	2a	3009	1/1	0.98	0.38	68,68,68,68	0
56	MG	1V	202	1/1	0.98	0.17	25,25,25,25	0
56	MG	2a	3170	1/1	0.98	0.10	65,65,65,65	0
56	MG	1A	3918	1/1	0.98	0.08	39,39,39,39	0
56	MG	1B	235	1/1	0.98	0.15	39,39,39,39	0
56	MG	2a	3173	1/1	0.98	0.19	45,45,45,45	0
56	MG	2A	3308	1/1	0.98	0.20	60,60,60,60	0
56	MG	1A	3045	1/1	0.98	0.18	22,22,22,22	0
56	MG	2A	3195	1/1	0.98	0.16	41,41,41,41	0
56	MG	2A	3555	1/1	0.98	0.11	41,41,41,41	0
56	MG	1D	302	1/1	0.98	0.20	23,23,23,23	0
56	MG	1A	3857	1/1	0.98	0.15	33,33,33,33	0
56	MG	1A	3292	1/1	0.98	0.19	26,26,26,26	0
56	MG	1W	204	1/1	0.98	0.13	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3832	1/1	0.98	0.26	30,30,30,30	0
56	MG	2A	3833	1/1	0.98	0.16	54,54,54,54	0
56	MG	1A	3151	1/1	0.98	0.19	20,20,20,20	0
56	MG	2A	3835	1/1	0.98	0.20	33,33,33,33	0
56	MG	2A	3836	1/1	0.98	0.15	27,27,27,27	0
56	MG	2A	3837	1/1	0.98	0.09	50,50,50,50	0
56	MG	2A	3838	1/1	0.98	0.18	32,32,32,32	0
56	MG	2A	3839	1/1	0.98	0.23	51,51,51,51	0
56	MG	2A	3840	1/1	0.98	0.09	37,37,37,37	0
56	MG	1A	4064	1/1	0.98	0.23	28,28,28,28	0
56	MG	1A	4065	1/1	0.98	0.23	22,22,22,22	0
56	MG	1a	1743	1/1	0.98	0.17	38,38,38,38	0
56	MG	2A	3092	1/1	0.98	0.15	48,48,48,48	0
56	MG	2A	3698	1/1	0.98	0.10	37,37,37,37	0
56	MG	1A	3070	1/1	0.98	0.22	12,12,12,12	0
56	MG	1a	1745	1/1	0.98	0.17	35,35,35,35	0
56	MG	2A	3848	1/1	0.98	0.14	27,27,27,27	0
56	MG	1A	3992	1/1	0.98	0.16	37,37,37,37	0
56	MG	1X	103	1/1	0.98	0.20	42,42,42,42	0
56	MG	1A	3650	1/1	0.98	0.12	54,54,54,54	0
56	MG	1A	3803	1/1	0.98	0.14	18,18,18,18	0
56	MG	1E	301	1/1	0.98	0.25	30,30,30,30	0
56	MG	2A	3854	1/1	0.98	0.06	64,64,64,64	0
56	MG	1A	3804	1/1	0.98	0.17	47,47,47,47	0
56	MG	1A	3700	1/1	0.98	0.20	12,12,12,12	0
56	MG	2A	3857	1/1	0.98	0.10	28,28,28,28	0
56	MG	1Y	203	1/1	0.98	0.39	39,39,39,39	0
56	MG	2A	3576	1/1	0.98	0.15	43,43,43,43	0
56	MG	2a	3210	1/1	0.98	0.15	54,54,54,54	0
56	MG	1Z	3700	1/1	0.98	0.25	57,57,57,57	0
56	MG	1A	4072	1/1	0.98	0.14	18,18,18,18	0
56	MG	1A	3357	1/1	0.98	0.33	28,28,28,28	0
56	MG	1A	3753	1/1	0.98	0.20	13,13,13,13	0
56	MG	1A	3013	1/1	0.98	0.25	23,23,23,23	0
56	MG	1A	3392	1/1	0.98	0.15	35,35,35,35	0
56	MG	1A	3072	1/1	0.98	0.42	27,27,27,27	0
56	MG	2a	3218	1/1	0.98	0.13	42,42,42,42	0
56	MG	1A	3174	1/1	0.98	0.17	29,29,29,29	0
56	MG	2A	3003	1/1	0.98	0.19	47,47,47,47	0
56	MG	1A	3195	1/1	0.98	0.21	27,27,27,27	0
56	MG	2a	3222	1/1	0.98	0.11	68,68,68,68	0
56	MG	1A	3155	1/1	0.98	0.12	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	11	101	1/1	0.98	0.31	29,29,29,29	0
56	MG	2A	3872	1/1	0.98	0.13	30,30,30,30	0
56	MG	1A	3222	1/1	0.98	0.22	28,28,28,28	0
56	MG	2a	3063	1/1	0.98	0.14	48,48,48,48	0
56	MG	1F	301	1/1	0.98	0.16	30,30,30,30	0
56	MG	1A	3364	1/1	0.98	0.28	28,28,28,28	0
56	MG	1A	3579	1/1	0.98	0.21	33,33,33,33	0
56	MG	2A	3726	1/1	0.98	0.06	50,50,50,50	0
56	MG	1a	1771	1/1	0.98	0.19	48,48,48,48	0
56	MG	2A	3728	1/1	0.98	0.16	39,39,39,39	0
56	MG	1A	3941	1/1	0.98	0.17	29,29,29,29	0
56	MG	2A	3465	1/1	0.98	0.24	56,56,56,56	0
56	MG	1A	3942	1/1	0.98	0.20	26,26,26,26	0
56	MG	1A	3122	1/1	0.98	0.26	38,38,38,38	0
56	MG	1A	4087	1/1	0.98	0.22	28,28,28,28	0
56	MG	1A	3199	1/1	0.98	0.33	29,29,29,29	0
56	MG	1A	4089	1/1	0.98	0.17	20,20,20,20	0
56	MG	2A	3601	1/1	0.98	0.10	29,29,29,29	0
56	MG	1A	3664	1/1	0.98	0.12	54,54,54,54	0
56	MG	1A	3820	1/1	0.98	0.09	24,24,24,24	0
56	MG	2A	3474	1/1	0.98	0.17	20,20,20,20	0
56	MG	1A	3073	1/1	0.98	0.18	12,12,12,12	0
56	MG	1A	4093	1/1	0.98	0.26	42,42,42,42	0
56	MG	1A	3666	1/1	0.98	0.18	13,13,13,13	0
56	MG	2A	3131	1/1	0.98	0.09	46,46,46,46	0
56	MG	2A	3244	1/1	0.98	0.18	43,43,43,43	0
56	MG	1A	3718	1/1	0.98	0.14	18,18,18,18	0
56	MG	1A	4017	1/1	0.98	0.09	49,49,49,49	0
56	MG	1A	3719	1/1	0.98	0.15	17,17,17,17	0
56	MG	1A	4098	1/1	0.98	0.17	29,29,29,29	0
56	MG	17	102	1/1	0.98	0.17	23,23,23,23	0
56	MG	2A	3615	1/1	0.98	0.15	41,41,41,41	0
56	MG	1A	3097	1/1	0.98	0.26	25,25,25,25	0
56	MG	1a	1789	1/1	0.98	0.13	53,53,53,53	0
56	MG	18	101	1/1	0.98	0.21	33,33,33,33	0
56	MG	1a	1791	1/1	0.98	0.08	61,61,61,61	0
56	MG	1A	3827	1/1	0.98	0.16	17,17,17,17	0
56	MG	1a	1793	1/1	0.98	0.17	50,50,50,50	0
56	MG	1A	3014	1/1	0.98	0.13	19,19,19,19	0
56	MG	1A	3126	1/1	0.98	0.29	28,28,28,28	0
56	MG	2A	3373	1/1	0.98	0.08	41,41,41,41	0
56	MG	2A	3761	1/1	0.98	0.13	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3036	1/1	0.98	0.13	43,43,43,43	0
56	MG	1A	3278	1/1	0.98	0.16	28,28,28,28	0
56	MG	1A	3181	1/1	0.98	0.14	30,30,30,30	0
56	MG	1A	3776	1/1	0.98	0.15	42,42,42,42	0
56	MG	1A	3672	1/1	0.98	0.17	10,10,10,10	0
56	MG	1A	3143	1/1	0.98	0.21	17,17,17,17	0
56	MG	1A	3589	1/1	0.98	0.21	27,27,27,27	0
56	MG	1A	3961	1/1	0.98	0.06	28,28,28,28	0
56	MG	2A	3382	1/1	0.98	0.25	42,42,42,42	0
56	MG	1A	3099	1/1	0.98	0.18	19,19,19,19	0
56	MG	1A	3837	1/1	0.98	0.17	24,24,24,24	0
56	MG	1A	3781	1/1	0.98	0.09	30,30,30,30	0
56	MG	2a	3114	1/1	0.98	0.09	65,65,65,65	0
56	MG	2A	3507	1/1	0.98	0.11	47,47,47,47	0
56	MG	1A	3311	1/1	0.98	0.32	33,33,33,33	0
56	MG	1A	3032	1/1	0.98	0.21	20,20,20,20	0
56	MG	2A	3158	1/1	0.98	0.18	30,30,30,30	0
56	MG	1A	3657	1/1	0.99	0.18	23,23,23,23	0
56	MG	2A	3559	1/1	0.99	0.18	26,26,26,26	0
56	MG	1a	1808	1/1	0.99	0.10	40,40,40,40	0
56	MG	2a	3142	1/1	0.99	0.14	50,50,50,50	0
56	MG	1A	3707	1/1	0.99	0.19	20,20,20,20	0
56	MG	1A	4054	1/1	0.99	0.07	23,23,23,23	0
56	MG	2A	3520	1/1	0.99	0.17	21,21,21,21	0
56	MG	1A	3037	1/1	0.99	0.16	18,18,18,18	0
56	MG	2A	3522	1/1	0.99	0.18	40,40,40,40	0
56	MG	2A	3741	1/1	0.99	0.07	50,50,50,50	0
56	MG	1a	1741	1/1	0.99	0.23	39,39,39,39	0
56	MG	1A	3921	1/1	0.99	0.17	17,17,17,17	0
56	MG	1A	3170	1/1	0.99	0.11	24,24,24,24	0
56	MG	2A	3484	1/1	0.99	0.20	42,42,42,42	0
56	MG	1B	224	1/1	0.99	0.17	46,46,46,46	0
56	MG	15	102	1/1	0.99	0.24	32,32,32,32	0
56	MG	1A	3758	1/1	0.99	0.14	46,46,46,46	0
56	MG	2A	3616	1/1	0.99	0.12	35,35,35,35	0
56	MG	1a	1818	1/1	0.99	0.08	46,46,46,46	0
56	MG	1A	3003	1/1	0.99	0.13	22,22,22,22	0
56	MG	1A	3217	1/1	0.99	0.24	26,26,26,26	0
56	MG	2T	203	1/1	0.99	0.22	39,39,39,39	0
56	MG	1A	3905	1/1	0.99	0.20	24,24,24,24	0
56	MG	1a	1750	1/1	0.99	0.21	25,25,25,25	0
56	MG	1A	3698	1/1	0.99	0.19	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1X	107	1/1	0.99	0.24	32,32,32,32	0
56	MG	1A	3012	1/1	0.99	0.17	21,21,21,21	0
56	MG	1O	204	1/1	0.99	0.16	48,48,48,48	0
56	MG	1A	3714	1/1	0.99	0.20	17,17,17,17	0
56	MG	1A	3136	1/1	0.99	0.19	29,29,29,29	0
56	MG	1A	3675	1/1	0.99	0.25	19,19,19,19	0
56	MG	1B	234	1/1	0.99	0.12	33,33,33,33	0
56	MG	1A	3033	1/1	0.99	0.27	18,18,18,18	0
56	MG	1a	1760	1/1	0.99	0.12	39,39,39,39	0
56	MG	1U	209	1/1	0.99	0.17	23,23,23,23	0
56	MG	2A	3307	1/1	0.99	0.17	31,31,31,31	0
56	MG	1A	3077	1/1	0.99	0.21	37,37,37,37	0
56	MG	2A	3080	1/1	0.99	0.24	41,41,41,41	0
56	MG	1A	3934	1/1	0.99	0.21	22,22,22,22	0
56	MG	1A	3555	1/1	0.99	0.25	32,32,32,32	0
56	MG	1A	3197	1/1	0.99	0.26	29,29,29,29	0
58	ZN	15	106	1/1	0.99	0.13	52,52,52,52	0
58	ZN	19	102	1/1	0.99	0.17	39,39,39,39	0
58	ZN	1n	103	1/1	0.99	0.15	58,58,58,58	0
56	MG	1A	3721	1/1	0.99	0.19	29,29,29,29	0
56	MG	1V	203	1/1	0.99	0.19	27,27,27,27	0
56	MG	1A	3822	1/1	0.99	0.18	20,20,20,20	0
56	MG	1Q	205	1/1	0.99	0.16	38,38,38,38	0
56	MG	1A	4027	1/1	0.99	0.10	21,21,21,21	0
59	SF4	1d	302	8/8	0.99	0.11	51,55,66,66	0
59	SF4	2d	303	8/8	0.99	0.12	53,64,70,73	0
56	MG	2A	3822	1/1	0.99	0.11	26,26,26,26	0
56	MG	1A	3859	1/1	0.99	0.19	38,38,38,38	0
58	ZN	16	104	1/1	1.00	0.15	28,28,28,28	0
56	MG	1A	3691	1/1	1.00	0.20	19,19,19,19	0
58	ZN	26	102	1/1	1.00	0.14	57,57,57,57	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.