Full wwPDB X-ray Structure Validation Report (i)

Nov 4, 2024 – 06:23 PM EST

PDB ID	:	9D7T
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with Api137 antimicrobial peptide, mRNA, A-site release factor 1, and deacylated P-site and E-site tRNAphe at 2.70A resolution
Authors	:	Aleksandrova, E.V.; Huang, W.; Baliga, C.; Atkinson, G.C.; Vazquez-Laslop, N.; Mankin, A.S.; Polikanov, Y.S.
Deposited on	:	2024-08-17
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 (i) symbol.

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

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

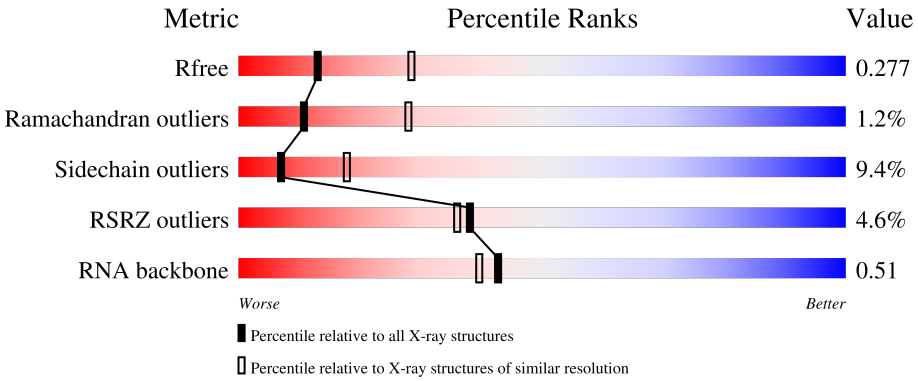
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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}	164625	3333 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)
RNA backbone	3690	1028 (2.94-2.46)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	3% 81% 17%
1	2A	2915	3% 78% 17%
2	1B	121	90% 9%
2	2B	121	5% 84% 15%

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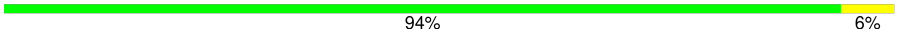
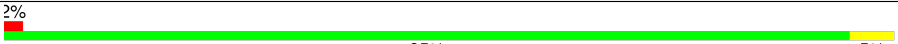
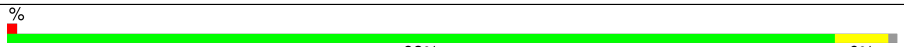
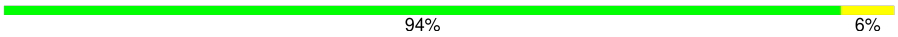
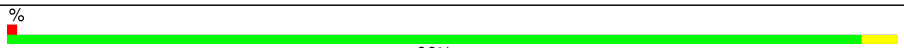
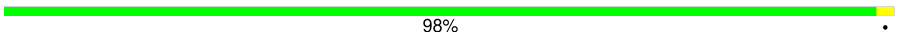
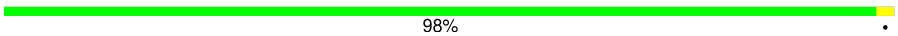
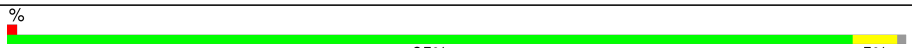
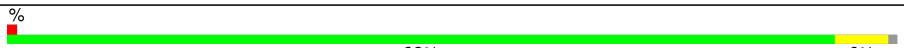
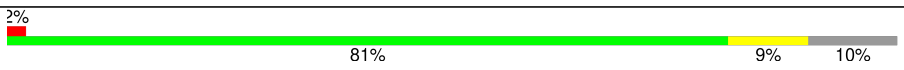
Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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Mol	Chain	Length	Quality of chain
15	2T	146	2% 87% 10%
16	1U	118	% 95%
16	2U	118	95%
17	1V	101	95%
17	2V	101	94% 5%
18	1W	113	94% 5%
18	2W	113	97%
19	1X	96	% 94% 5%
19	2X	96	4% 95%
20	1Y	110	89% 8%
20	2Y	110	2% 86% 11%
21	1Z	206	82% 7% 11%
21	2Z	206	% 81% 10% 10%
22	10	85	81% 8% 11%
22	20	85	11% 85% 6% 9%
23	11	98	% 95%
23	21	98	3% 92% 7%
24	12	72	3% 92% 6%
24	22	72	% 89% 8%
25	13	60	93% 5%
25	23	60	93% 5%
26	14	71	13% 80% 14%
26	24	71	18% 77% 15%
27	15	60	93% 5%
27	25	60	3% 93% 5%

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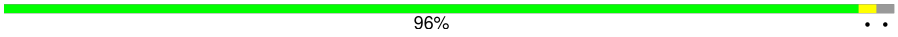
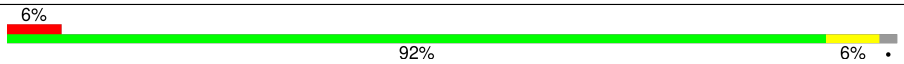
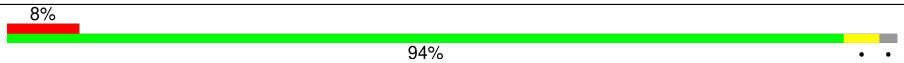
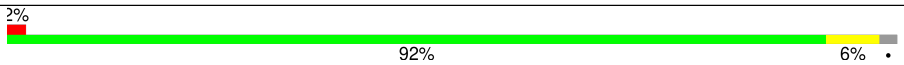
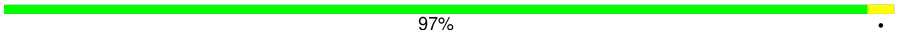
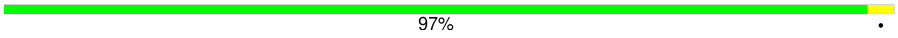
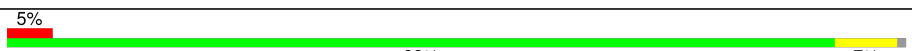
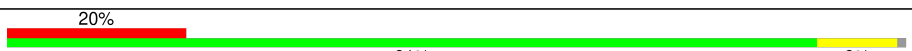
Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
40	2i	128	42% 85% 10%
41	1j	105	18% 85% 8% 7%
41	2j	105	35% 81% 10% 9%
42	1k	129	4% 81% 7% 12%
42	2k	129	7% 83% 5% 12%
43	1l	132	3% 84% 8% 8%
43	2l	132	2% 87% 5% 8%
44	1m	126	6% 84% 10% 6%
44	2m	126	17% 86% 6% 9%
45	1n	61	18% 89% 10%
45	2n	61	39% 85% 13%
46	1o	89	7% 94%
46	2o	89	2% 92% 7%
47	1p	88	17% 86% 7% 7%
47	2p	88	% 85% 8% 7%
48	1q	105	2% 87% 8% 6%
48	2q	105	2% 85% 10% 6%
49	1r	88	69% 8% 23%
49	2r	88	66% 11% 23%
50	1s	93	13% 83% 6% 11%
50	2s	93	13% 77% 12% 11%
51	1t	106	5% 78% 11% 9%
51	2t	106	7% 80% 8% 9%
52	1u	27	15% 85% 15%
52	2u	27	37% 81% 15%

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Mol	Chain	Length	Quality of chain
53	1v	24	12% 42% 12% 46%
53	2v	24	21% 46% 8% 46%
54	1w	354	% 62% 8% 30%
54	2w	354	3% 61% 11% 29%
55	1x	76	71% 28%
55	1y	76	9% 55% 39%
55	2x	76	72% 26%
55	2y	76	11% 55% 39%
56	1z	18	17% 67% 11% 22%
56	2z	18	28% 61% 17% 22%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1A	3634	-	-	-	X
57	MG	2A	3116	-	-	-	X

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 299179 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			746	485	134	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	183	Total	C	N	O	S	0	0	0
			1437	919	256	260	2			
21	2Z	186	Total	C	N	O	S	0	0	0
			1451	928	256	265	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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
			548	347	99	97	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	68	Total	C	N	O	S	0	0	0
			517	330	92	90	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
			511	328	99	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
			1554	977	302	274	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
			1659	1040	326	286	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
			1130	714	214	199	3			

- 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	513	143	151	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	123	Total	C	N	O	0	0	0
			940	593	185	162			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	98	Total	C	N	O	0	0	0
			721	449	140	132			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	118	Total	C	N	O	S	0	0	0
			923	569	191	161	2			
44	2m	115	Total	C	N	O	S	0	0	0
			889	546	183	158	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			486	309	101	72	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
49	2r	68	Total	C	N	O	0	0	0
			551	353	108	90			

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

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

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

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

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

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

- Molecule 53 is a RNA chain called PHE-Stop mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			274	124	48	89	13			
53	2v	13	Total	C	N	O	P	0	0	0
			274	124	48	89	13			

- Molecule 54 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	249	Total	C	N	O	S	0	0	0
			1939	1199	360	371	9			
54	2w	253	Total	C	N	O	S	0	0	0
			1954	1208	361	377	8			

- Molecule 55 is a RNA chain called P-site and E-site Deacylated tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	75	Total	C	N	O	P	S	0	0	0
			1612	722	288	525	75	2			
55	1y	74	Total	C	N	O	P	S	0	0	0
			1590	712	285	517	74	2			
55	2x	75	Total	C	N	O	P	S	0	0	0
			1612	722	288	525	75	2			
55	2y	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			

- Molecule 56 is a protein called Api137 Antimicrobial Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	1z	14	Total	C	N	O	0	0	0
			121	80	25	16			
56	2z	14	Total	C	N	O	0	0	0
			121	80	25	16			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	807	Total	Mg	0	0
			807	807		
57	1B	20	Total	Mg	0	0
			20	20		
57	1D	6	Total	Mg	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1E	7	Total Mg 7 7	0	0
57	1F	8	Total Mg 8 8	0	0
57	1G	3	Total Mg 3 3	0	0
57	1N	4	Total Mg 4 4	0	0
57	1O	2	Total Mg 2 2	0	0
57	1P	4	Total Mg 4 4	0	0
57	1Q	5	Total Mg 5 5	0	0
57	1R	2	Total Mg 2 2	0	0
57	1T	1	Total Mg 1 1	0	0
57	1U	6	Total Mg 6 6	0	0
57	1V	5	Total Mg 5 5	0	0
57	1W	4	Total Mg 4 4	0	0
57	1X	3	Total Mg 3 3	0	0
57	1Z	2	Total Mg 2 2	0	0
57	10	5	Total Mg 5 5	0	0
57	11	4	Total Mg 4 4	0	0
57	12	2	Total Mg 2 2	0	0
57	13	1	Total Mg 1 1	0	0
57	14	1	Total Mg 1 1	0	0
57	15	4	Total Mg 4 4	0	0
57	16	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	17	7	Total Mg 7 7	0	0
57	18	2	Total Mg 2 2	0	0
57	19	1	Total Mg 1 1	0	0
57	1a	187	Total Mg 187 187	0	0
57	1c	1	Total Mg 1 1	0	0
57	1d	1	Total Mg 1 1	0	0
57	1f	1	Total Mg 1 1	0	0
57	1k	1	Total Mg 1 1	0	0
57	1m	1	Total Mg 1 1	0	0
57	1n	1	Total Mg 1 1	0	0
57	1v	3	Total Mg 3 3	0	0
57	1w	4	Total Mg 4 4	0	0
57	1x	8	Total Mg 8 8	0	0
57	1y	2	Total Mg 2 2	0	0
57	2A	665	Total Mg 665 665	0	0
57	2B	11	Total Mg 11 11	0	0
57	2D	9	Total Mg 9 9	0	0
57	2E	5	Total Mg 5 5	0	0
57	2F	6	Total Mg 6 6	0	0
57	2N	1	Total Mg 1 1	0	0
57	2O	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2Q	3	Total Mg 3 3	0	0
57	2R	1	Total Mg 1 1	0	0
57	2U	1	Total Mg 1 1	0	0
57	2V	2	Total Mg 2 2	0	0
57	2W	1	Total Mg 1 1	0	0
57	2X	4	Total Mg 4 4	0	0
57	2Y	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	21	1	Total Mg 1 1	0	0
57	23	2	Total Mg 2 2	0	0
57	25	1	Total Mg 1 1	0	0
57	28	3	Total Mg 3 3	0	0
57	29	1	Total Mg 1 1	0	0
57	2a	172	Total Mg 172 172	0	0
57	2d	1	Total Mg 1 1	0	0
57	2e	2	Total Mg 2 2	0	0
57	2f	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0
57	2k	2	Total Mg 2 2	0	0
57	2t	1	Total Mg 1 1	0	0
57	2u	1	Total Mg 1 1	0	0

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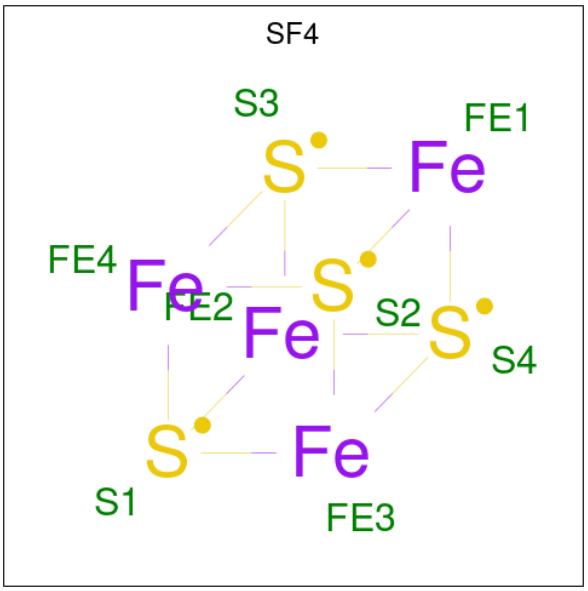
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2v	2	Total Mg 2 2	0	0
57	2w	2	Total Mg 2 2	0	0
57	2x	9	Total Mg 9 9	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1Y	1	Total Zn 1 1	0	0
58	14	1	Total Zn 1 1	0	0
58	15	1	Total Zn 1 1	0	0
58	16	1	Total Zn 1 1	0	0
58	19	1	Total Zn 1 1	0	0
58	1n	1	Total Zn 1 1	0	0
58	2Y	1	Total Zn 1 1	0	0
58	24	1	Total Zn 1 1	0	0
58	25	1	Total Zn 1 1	0	0
58	26	1	Total Zn 1 1	0	0
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: Fe_4S_4).



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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	1394	Total O 1394 1394	0	0
60	1B	31	Total O 31 31	0	0
60	1D	15	Total O 15 15	0	0
60	1E	12	Total O 12 12	0	0
60	1F	6	Total O 6 6	0	0
60	1G	1	Total O 1 1	0	0
60	1N	3	Total O 3 3	0	0
60	1O	3	Total O 3 3	0	0
60	1P	15	Total O 15 15	0	0
60	1Q	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1R	2	Total O 2 2	0	0
60	1T	1	Total O 1 1	0	0
60	1U	5	Total O 5 5	0	0
60	1V	1	Total O 1 1	0	0
60	1W	2	Total O 2 2	0	0
60	1X	4	Total O 4 4	0	0
60	10	1	Total O 1 1	0	0
60	11	3	Total O 3 3	0	0
60	13	2	Total O 2 2	0	0
60	15	5	Total O 5 5	0	0
60	16	1	Total O 1 1	0	0
60	17	2	Total O 2 2	0	0
60	18	7	Total O 7 7	0	0
60	1a	194	Total O 194 194	0	0
60	1d	1	Total O 1 1	0	0
60	1l	1	Total O 1 1	0	0
60	1p	1	Total O 1 1	0	0
60	1v	3	Total O 3 3	0	0
60	1w	5	Total O 5 5	0	0
60	1x	22	Total O 22 22	0	0
60	1y	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1z	4	Total O 4 4	0	0
60	2A	997	Total O 997 997	0	0
60	2B	7	Total O 7 7	0	0
60	2D	16	Total O 16 16	0	0
60	2E	11	Total O 11 11	0	0
60	2F	5	Total O 5 5	0	0
60	2N	1	Total O 1 1	0	0
60	2O	1	Total O 1 1	0	0
60	2P	12	Total O 12 12	0	0
60	2Q	1	Total O 1 1	0	0
60	2R	3	Total O 3 3	0	0
60	2T	1	Total O 1 1	0	0
60	2U	2	Total O 2 2	0	0
60	2W	1	Total O 1 1	0	0
60	2X	2	Total O 2 2	0	0
60	2Y	2	Total O 2 2	0	0
60	20	6	Total O 6 6	0	0
60	21	2	Total O 2 2	0	0
60	23	2	Total O 2 2	0	0
60	25	1	Total O 1 1	0	0
60	27	3	Total O 3 3	0	0

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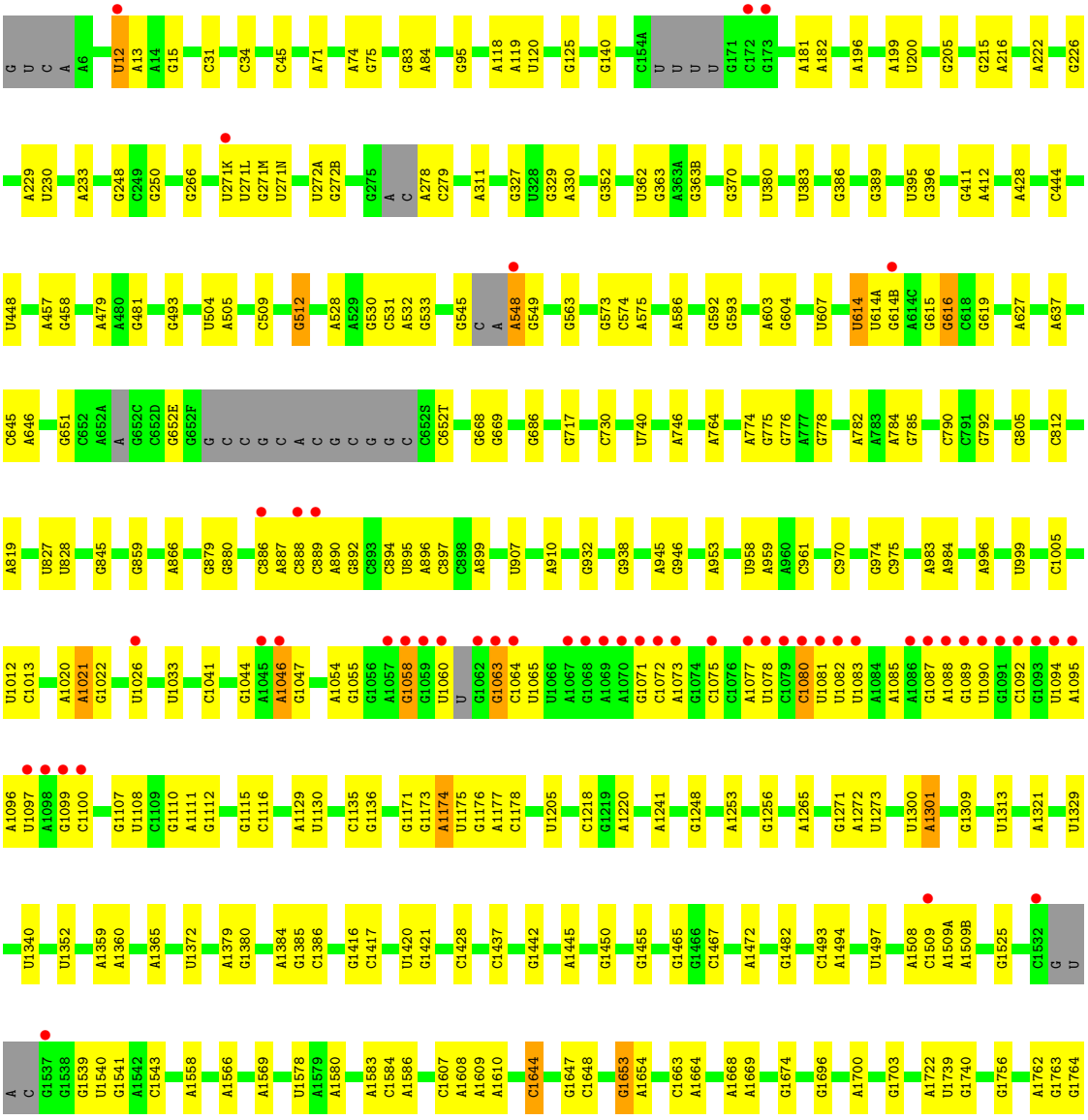
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	28	3	Total O 3 3	0	0
60	2a	154	Total O 154 154	0	0
60	2d	1	Total O 1 1	0	0
60	2j	1	Total O 1 1	0	0
60	2t	2	Total O 2 2	0	0
60	2v	2	Total O 2 2	0	0
60	2w	2	Total O 2 2	0	0
60	2x	13	Total O 13 13	0	0

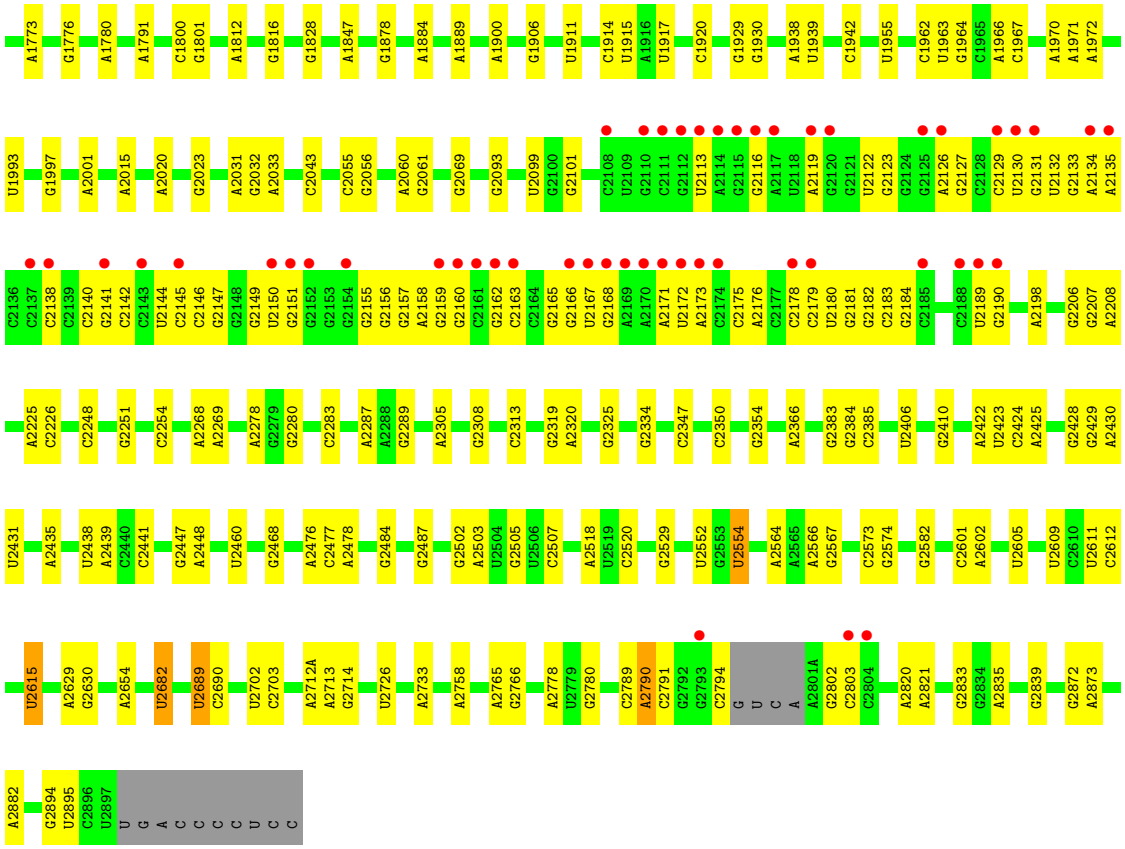
3 Residue-property plots (i)

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

- Molecule 1: 23S Ribosomal RNA

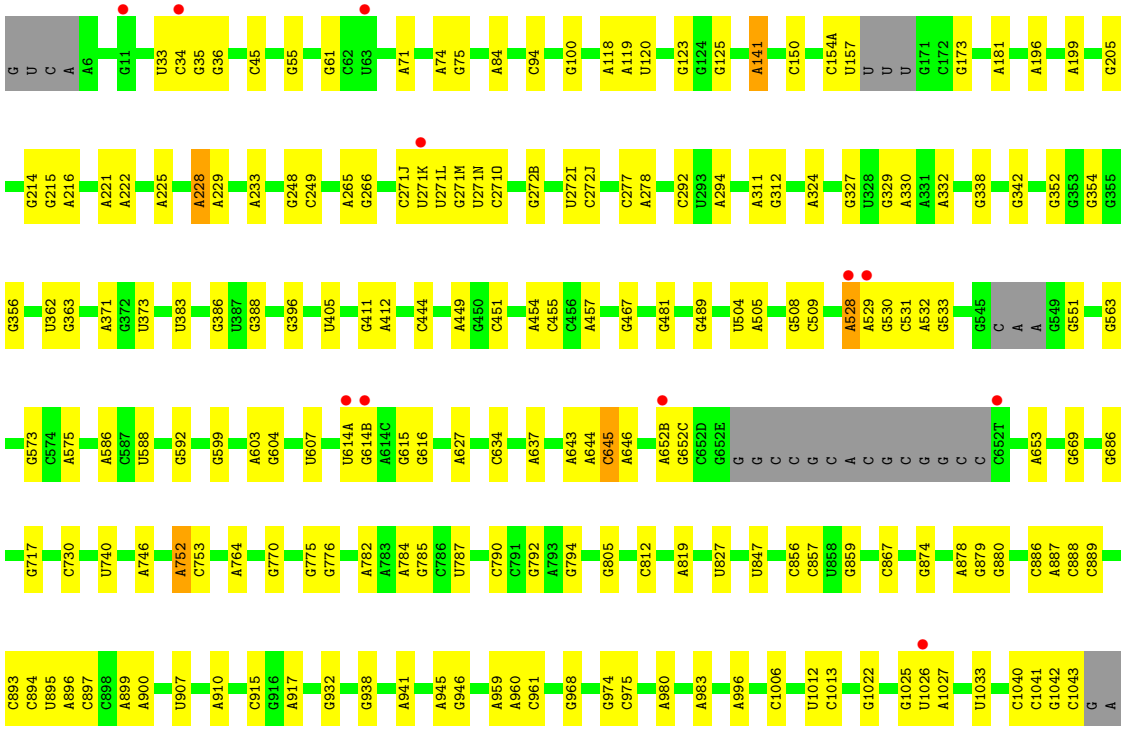
Chain 1A:

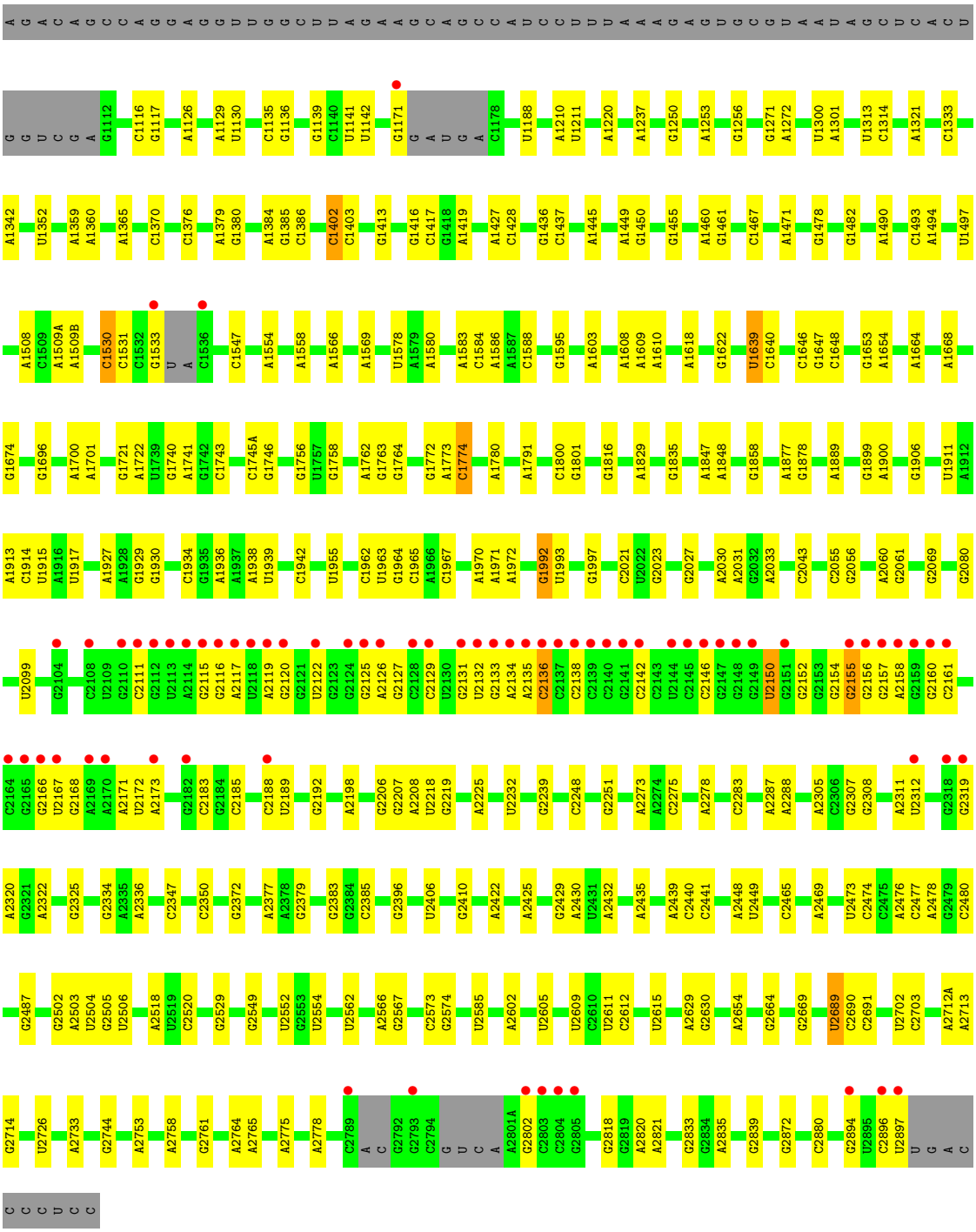




• Molecule 1: 23S Ribosomal RNA

Chain 2A:



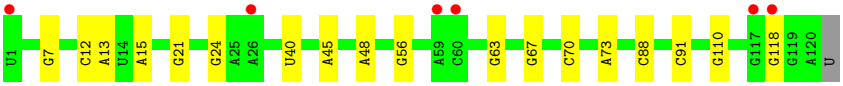


• Molecule 2: 5S Ribosomal RNA

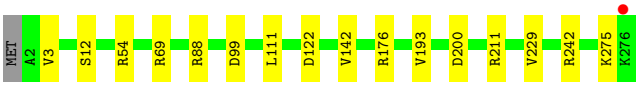
Chain 1B:

• Molecule 2: 5S Ribosomal RNA

Chain 2B:

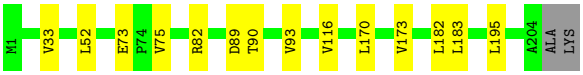


• Molecule 3: 50S ribosomal protein L2



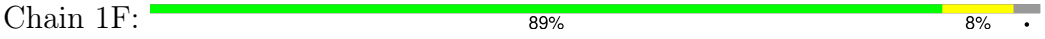
• Molecule 3: 50S ribosomal protein L2

• Molecule 4: 50S ribosomal protein L3

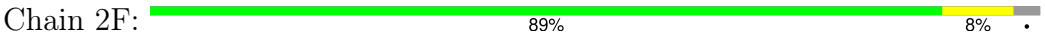


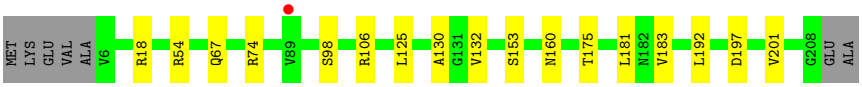
• Molecule 4: 50S ribosomal protein L3

• Molecule 5: 50S ribosomal protein L4



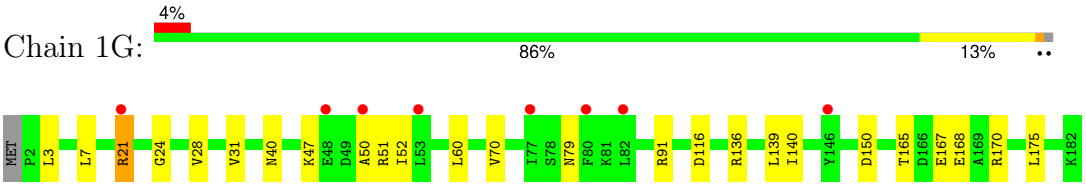
• Molecule 5: 50S ribosomal protein L4





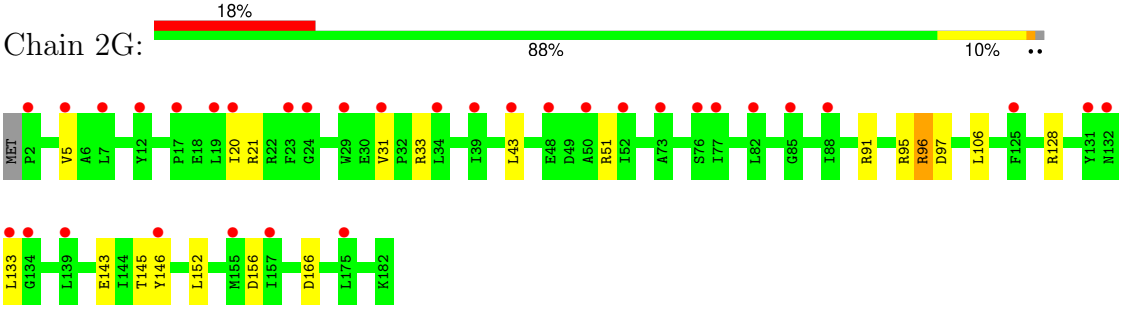
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



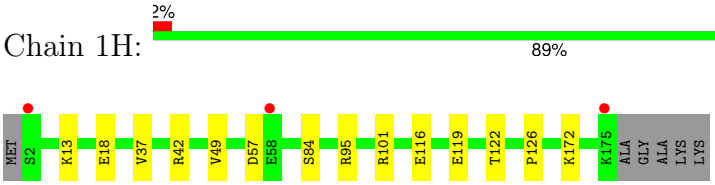
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



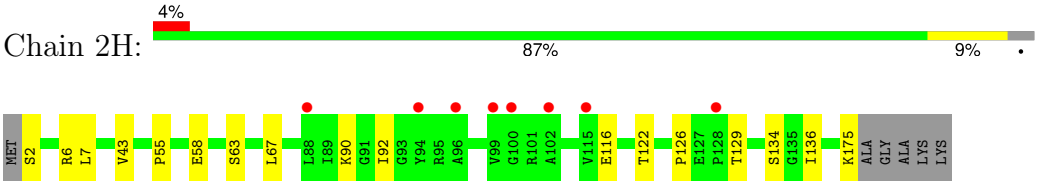
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



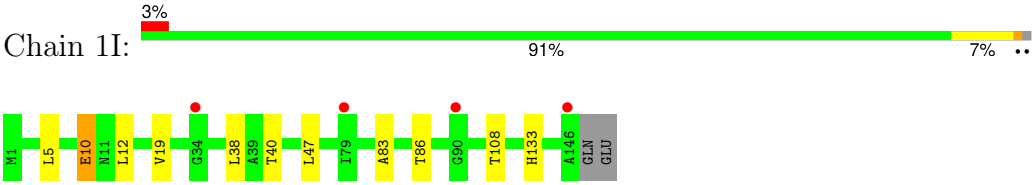
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



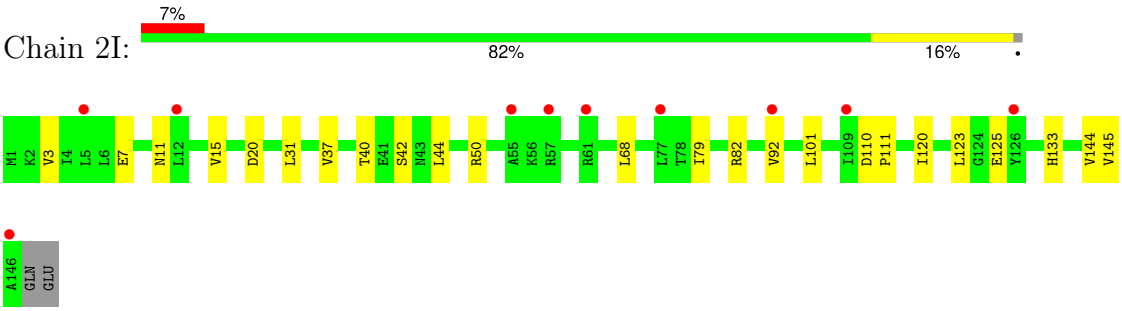
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



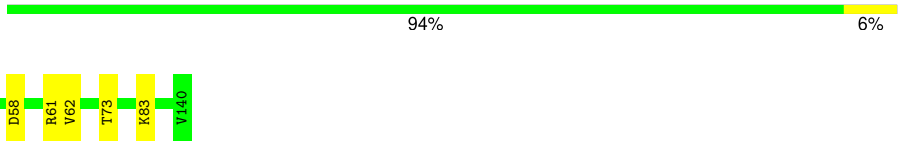
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



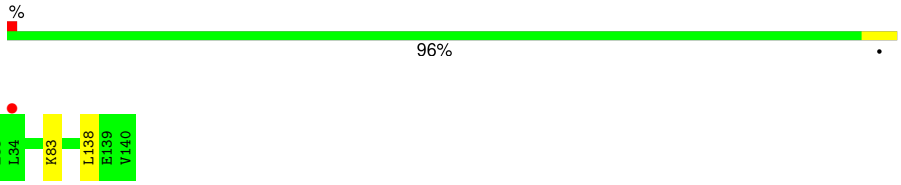
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



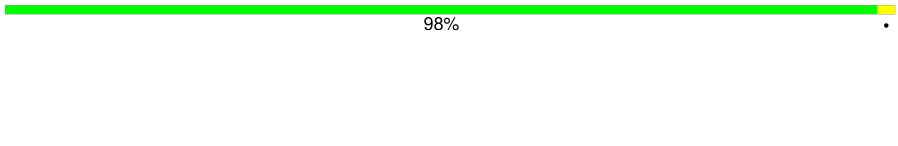
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



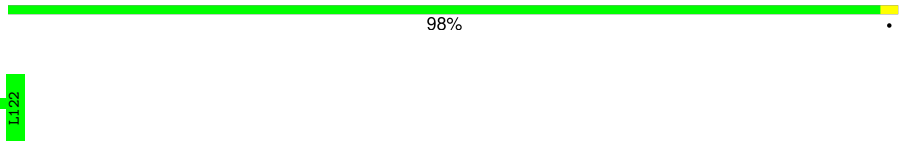
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



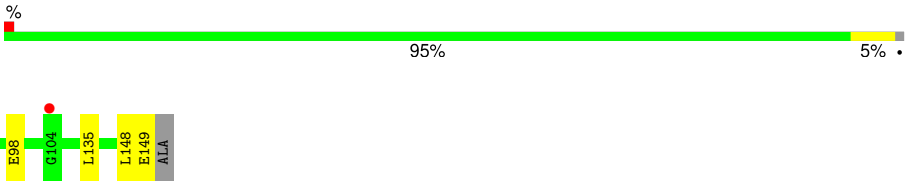
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



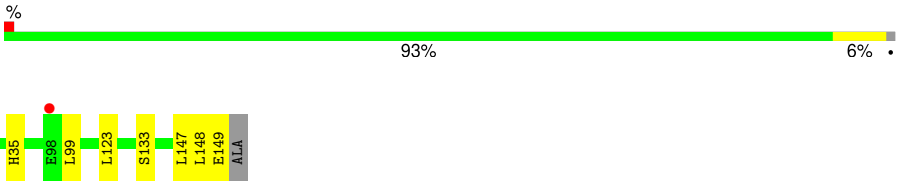
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



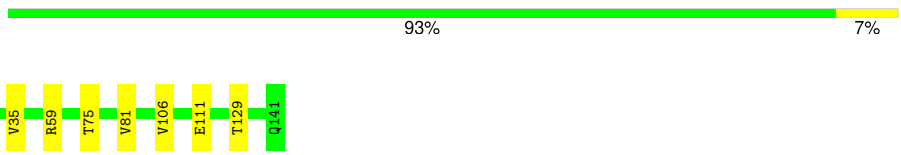
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



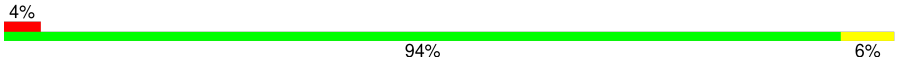
• Molecule 12: 50S ribosomal protein L16

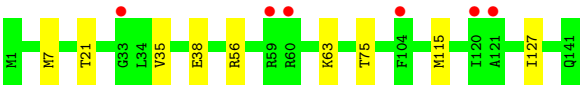
Chain 1Q:



• Molecule 12: 50S ribosomal protein L16

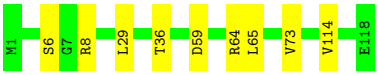
Chain 2Q:





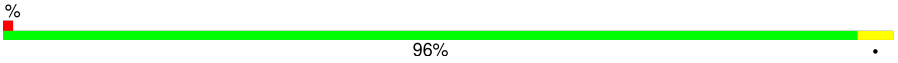
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



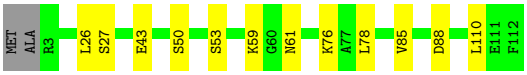
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



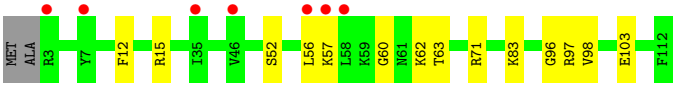
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



• Molecule 14: 50S ribosomal protein L18

Chain 2S:

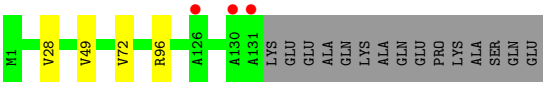


• Molecule 15: 50S ribosomal protein L19

Chain 1T:

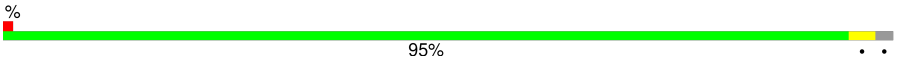
• Molecule 15: 50S ribosomal protein L19

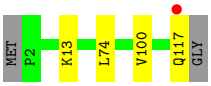
Chain 2T:



• Molecule 16: 50S ribosomal protein L20

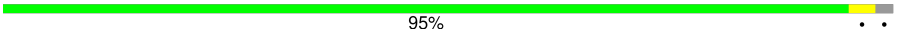
Chain 1U:





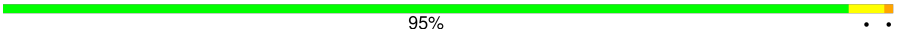
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



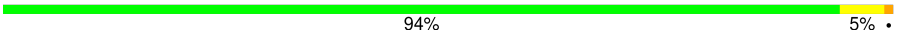
• Molecule 17: 50S ribosomal protein L21

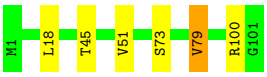
Chain 1V:



• Molecule 17: 50S ribosomal protein L21

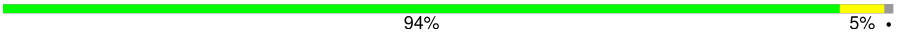
Chain 2V:





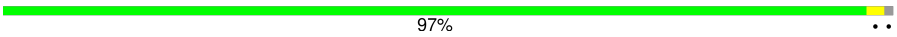
• Molecule 18: 50S ribosomal protein L22

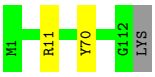
Chain 1W:



• Molecule 18: 50S ribosomal protein L22

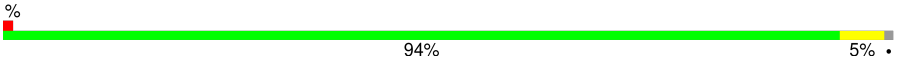
Chain 2W:

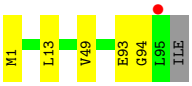




• Molecule 19: 50S ribosomal protein L23

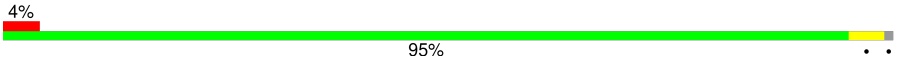
Chain 1X:

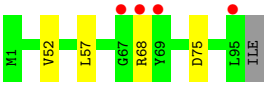




• Molecule 19: 50S ribosomal protein L23

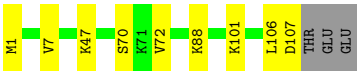
Chain 2X:





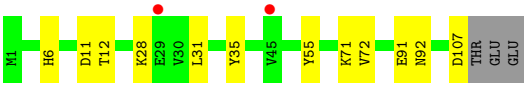
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



• Molecule 20: 50S ribosomal protein L24

Chain 2Y:

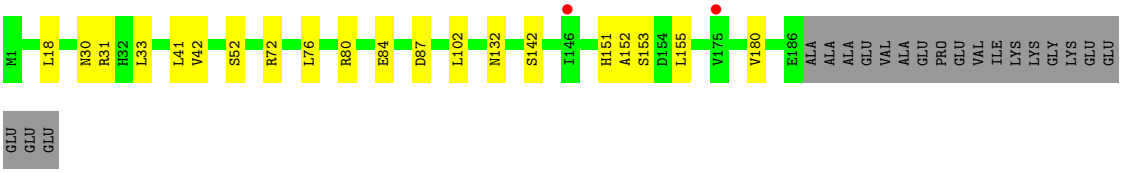


• Molecule 21: 50S ribosomal protein L25

Chain 1Z:

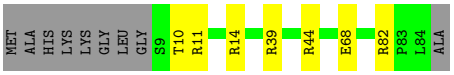
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



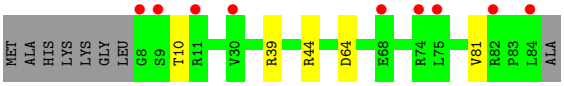
• Molecule 22: 50S ribosomal protein L27

Chain 10:



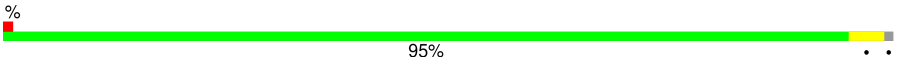
• Molecule 22: 50S ribosomal protein L27

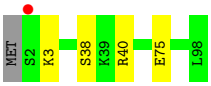
Chain 20:



• Molecule 23: 50S ribosomal protein L28

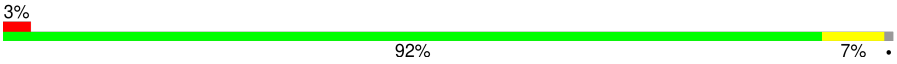
Chain 11:





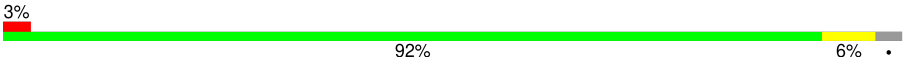
• Molecule 23: 50S ribosomal protein L28

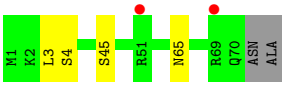
Chain 21:



• Molecule 24: 50S ribosomal protein L29

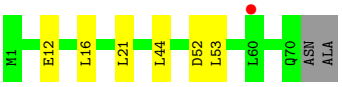
Chain 12:





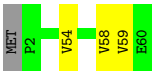
• Molecule 24: 50S ribosomal protein L29

Chain 22:



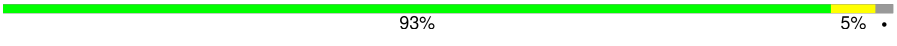
• Molecule 25: 50S ribosomal protein L30

Chain 13:



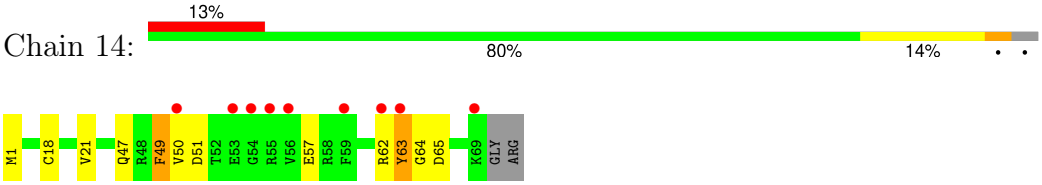
• Molecule 25: 50S ribosomal protein L30

Chain 23:



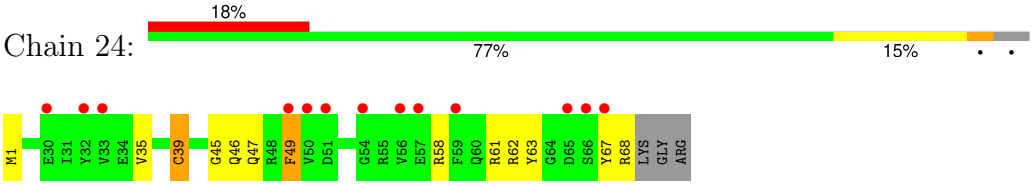
• Molecule 26: 50S ribosomal protein L31

Chain 14:



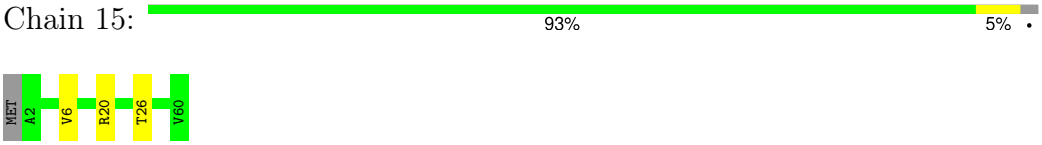
• Molecule 26: 50S ribosomal protein L31

Chain 24:



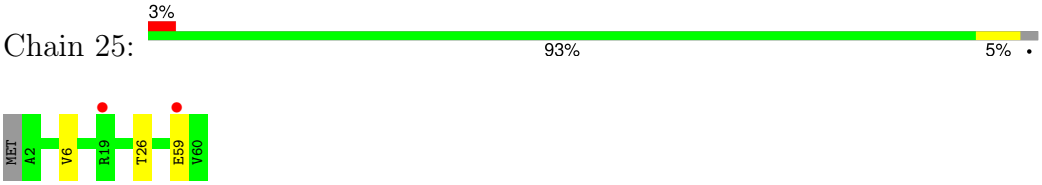
• Molecule 27: 50S ribosomal protein L32

Chain 15:



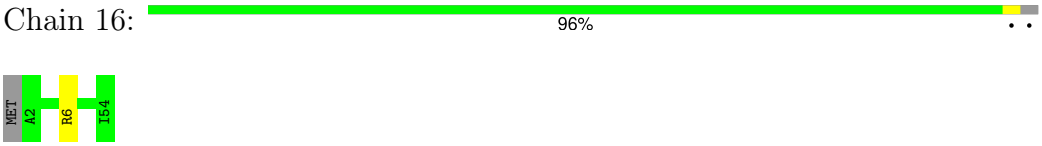
• Molecule 27: 50S ribosomal protein L32

Chain 25:



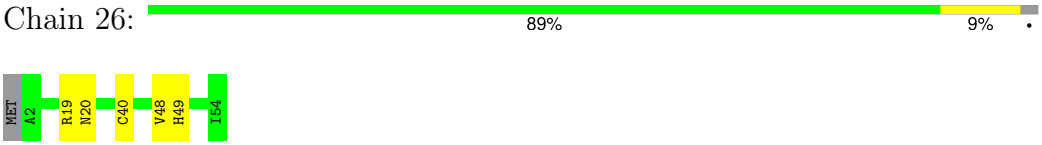
• Molecule 28: 50S ribosomal protein L33

Chain 16:



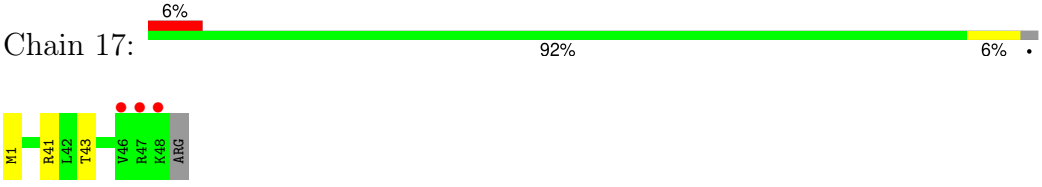
• Molecule 28: 50S ribosomal protein L33

Chain 26:



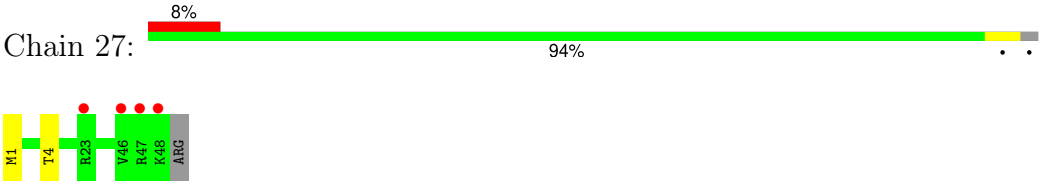
• Molecule 29: 50S ribosomal protein L34

Chain 17:



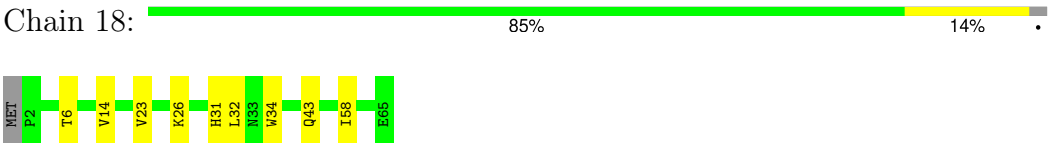
• Molecule 29: 50S ribosomal protein L34

Chain 27:



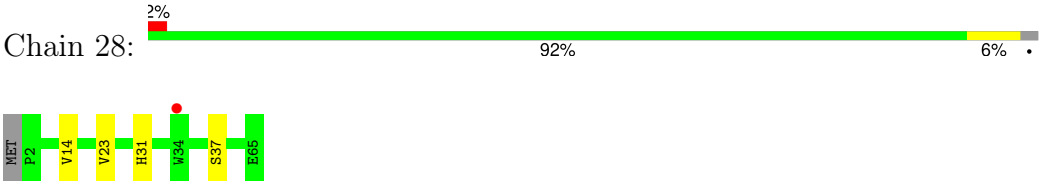
• Molecule 30: 50S ribosomal protein L35

Chain 18:



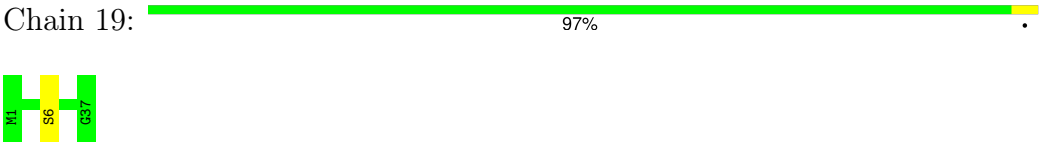
• Molecule 30: 50S ribosomal protein L35

Chain 28:



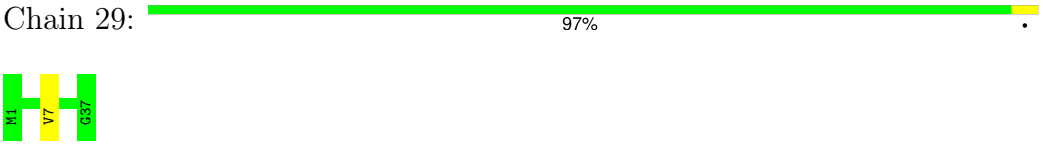
• Molecule 31: 50S ribosomal protein L36

Chain 19:



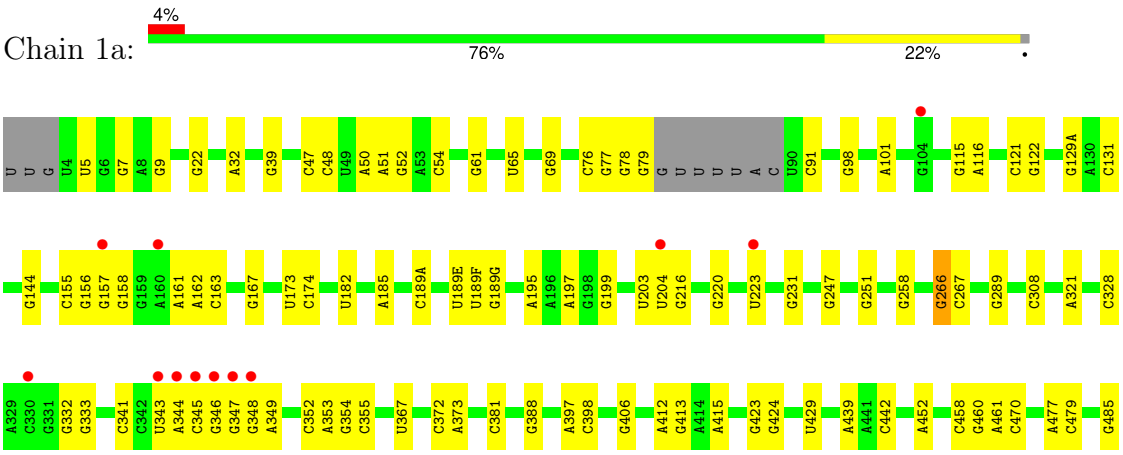
• Molecule 31: 50S ribosomal protein L36

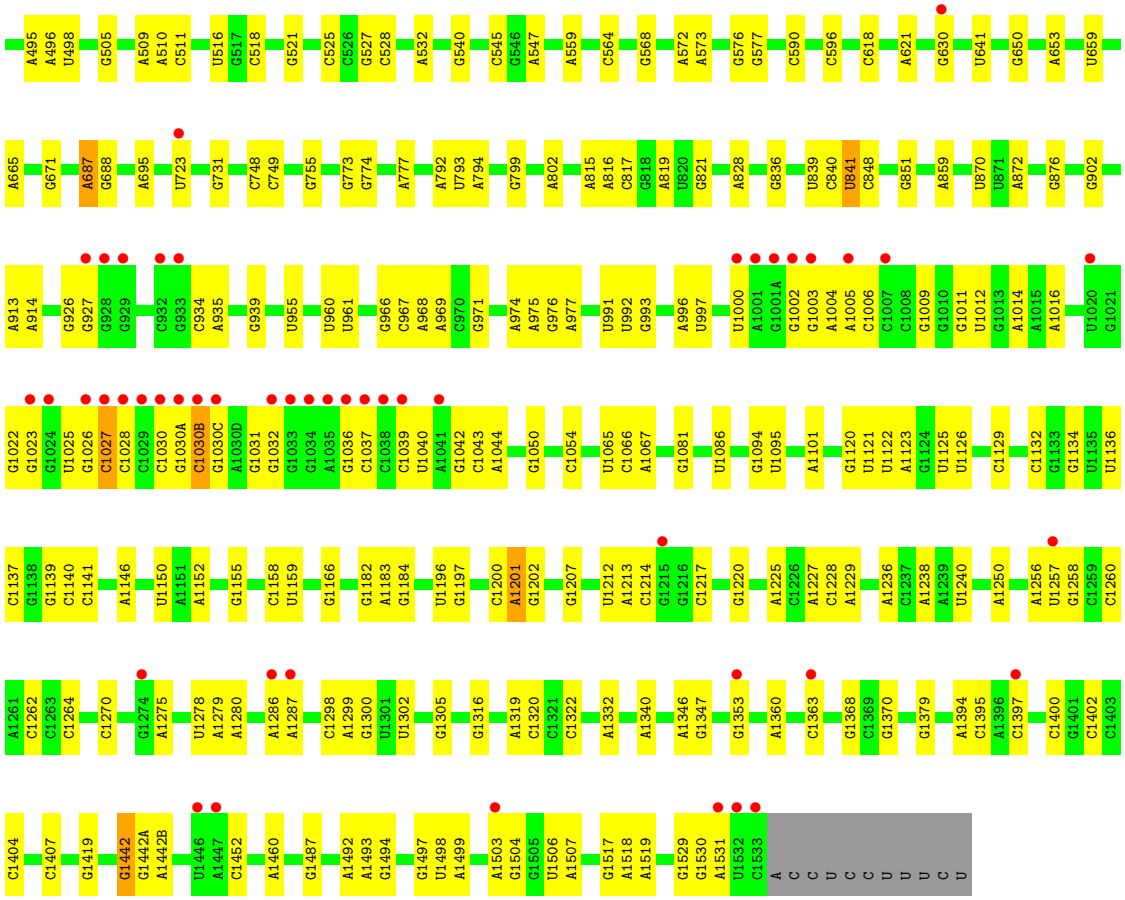
Chain 29:



• Molecule 32: 16S Ribosomal RNA

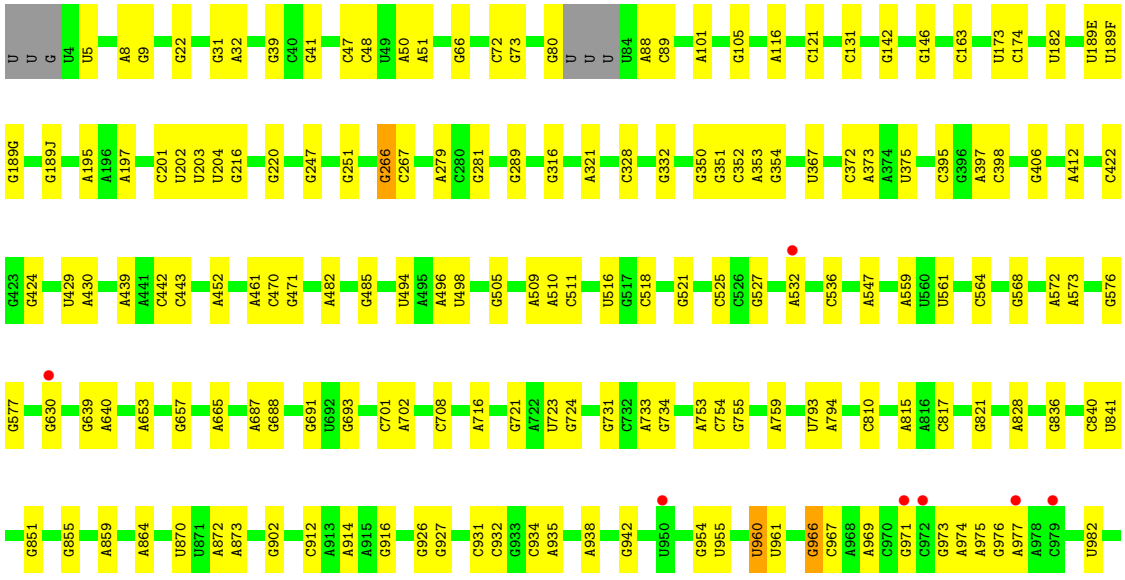
Chain 1a:

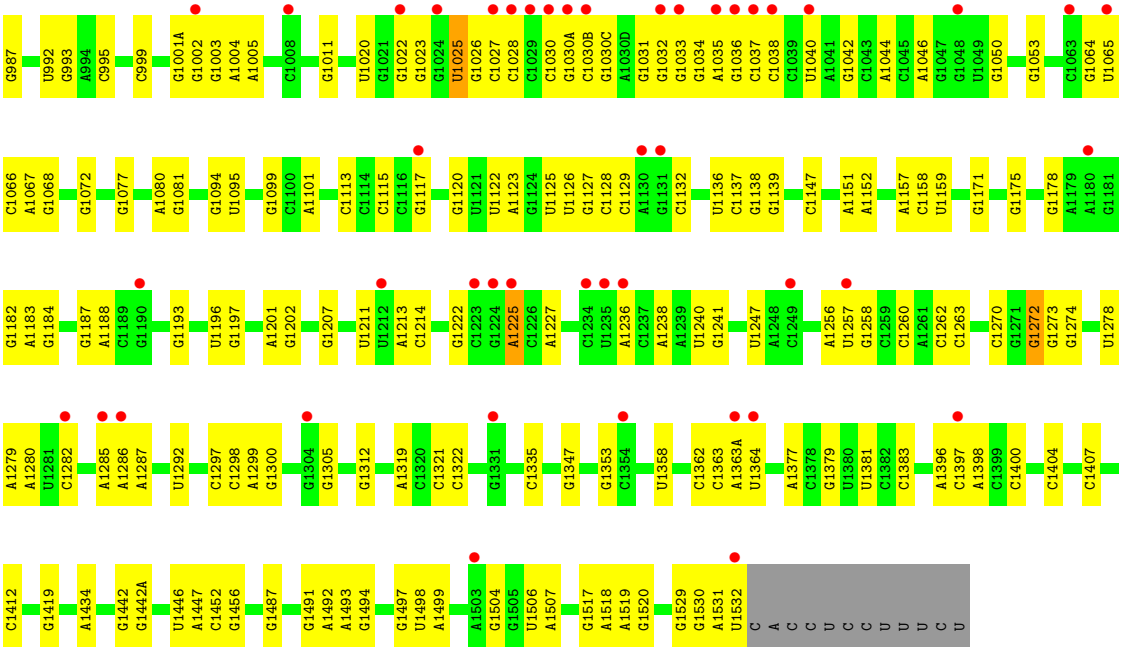




• Molecule 32: 16S Ribosomal RNA

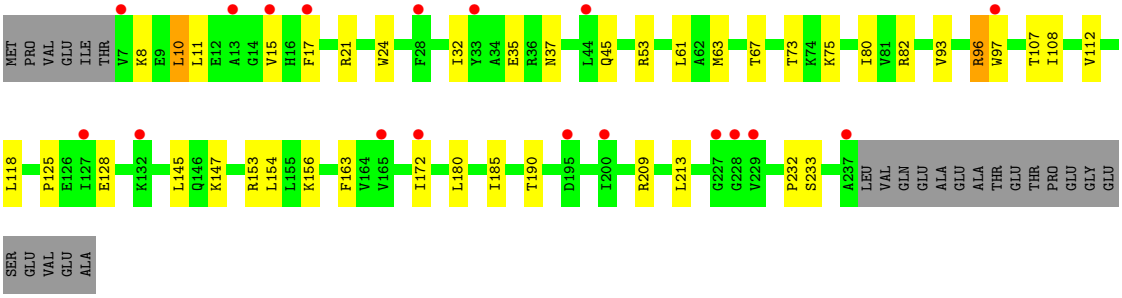
Chain 2a:





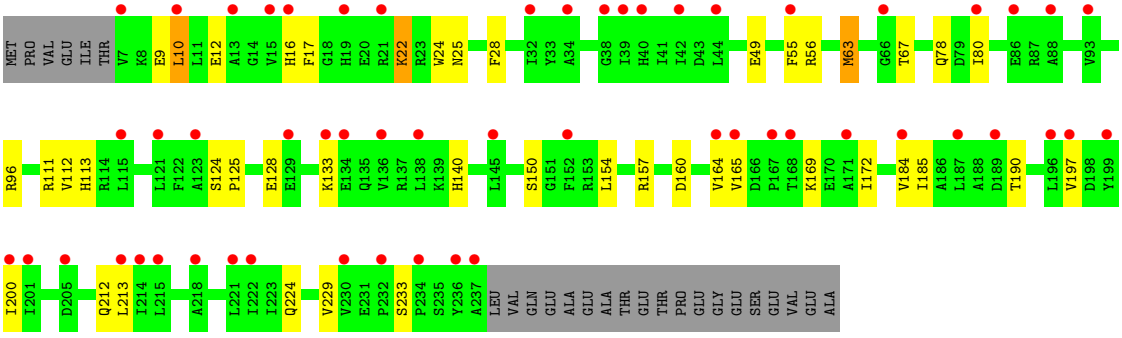
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



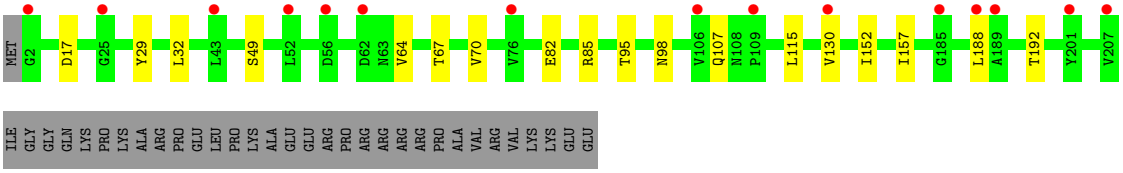
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



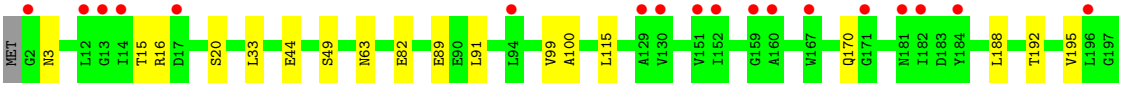
• Molecule 34: 30S ribosomal protein S3

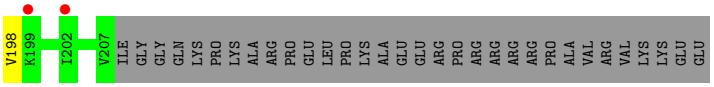
Chain 1c:



• Molecule 34: 30S ribosomal protein S3

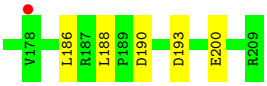
Chain 2c:





• Molecule 35: 30S ribosomal protein S4

Chain 1d:

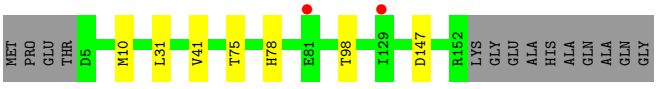


• Molecule 35: 30S ribosomal protein S4

Chain 2d:

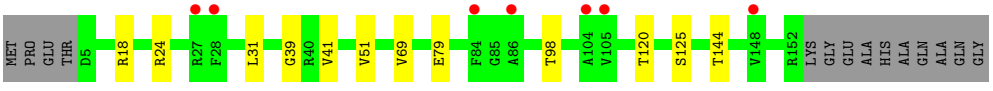
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



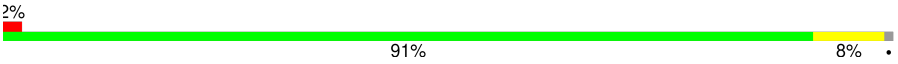
• Molecule 36: 30S ribosomal protein S5

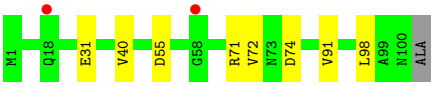
Chain 2e:



• Molecule 37: 30S ribosomal protein S6

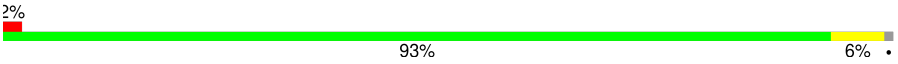
Chain 1f:





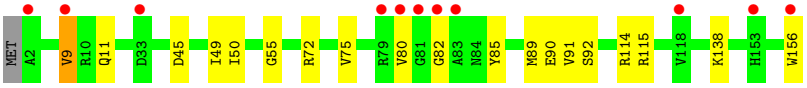
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



• Molecule 38: 30S ribosomal protein S7

Chain 1g:

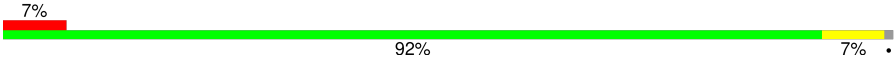


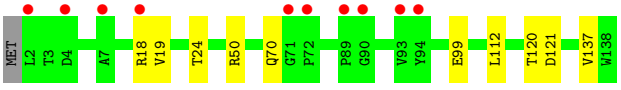
• Molecule 38: 30S ribosomal protein S7

Chain 2g:

• Molecule 39: 30S ribosomal protein S8

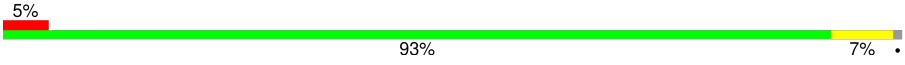
Chain 1h:

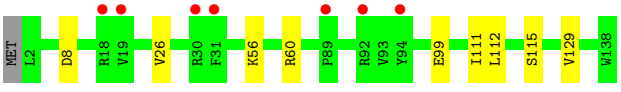




• Molecule 39: 30S ribosomal protein S8

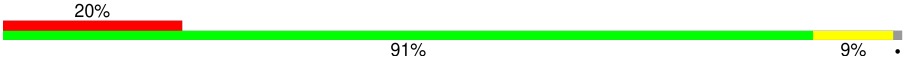
Chain 2h:

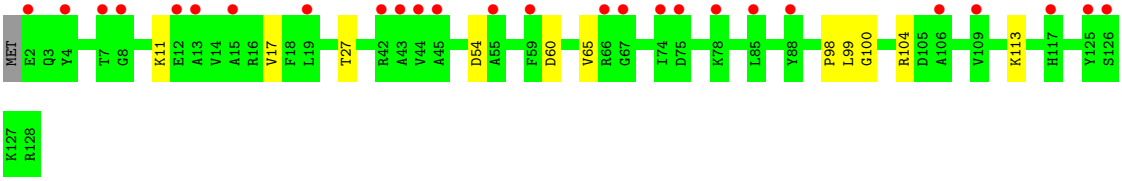




• Molecule 40: 30S ribosomal protein S9

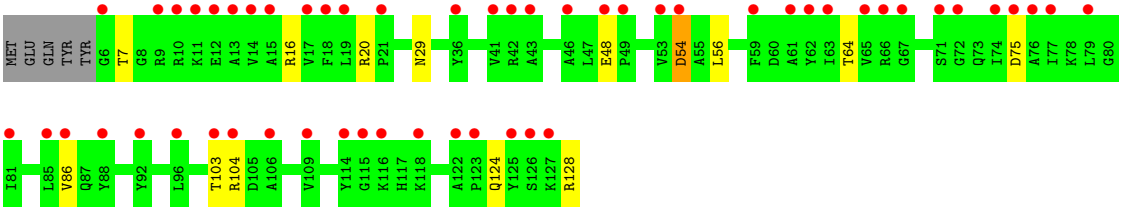
Chain 1i:





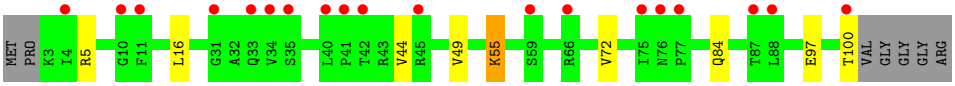
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



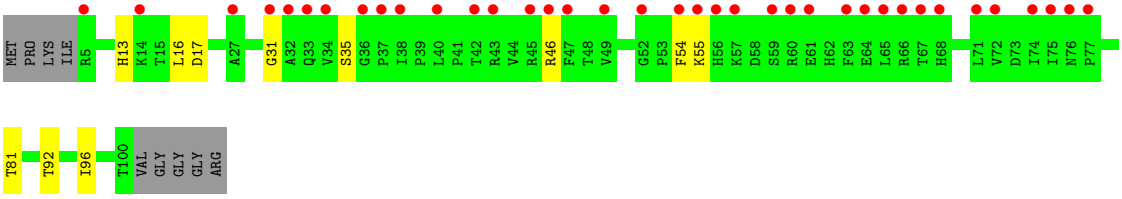
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



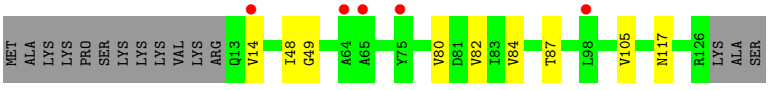
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



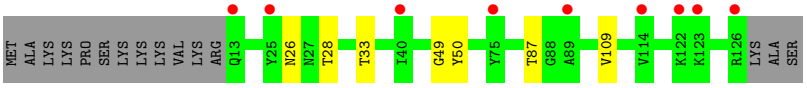
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



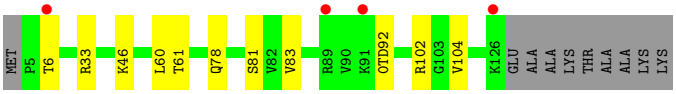
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



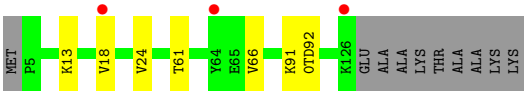
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



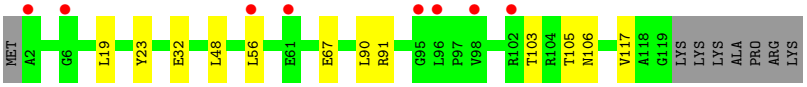
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



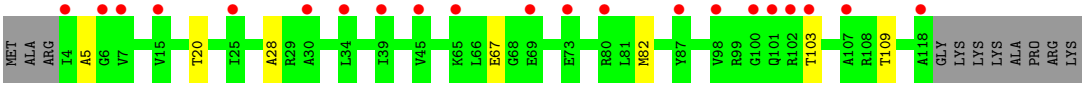
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



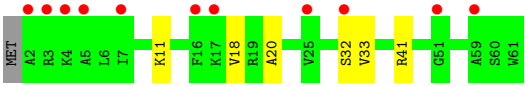
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



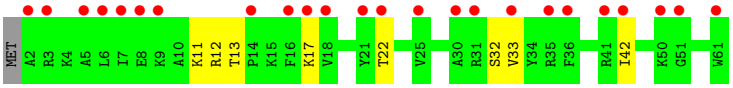
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



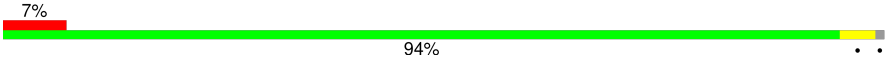
• Molecule 45: 30S ribosomal protein S14 type Z

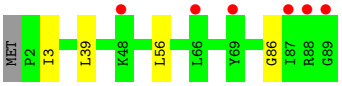
Chain 2n:



• Molecule 46: 30S ribosomal protein S15

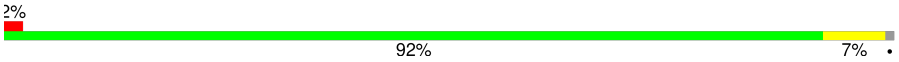
Chain 1o:

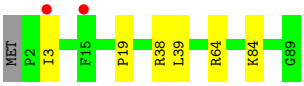




• Molecule 46: 30S ribosomal protein S15

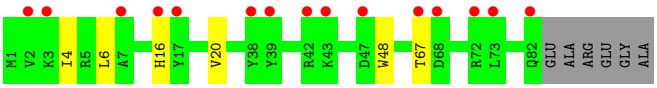
Chain 2o:





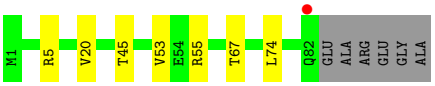
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



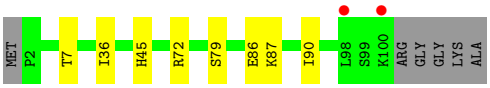
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



• Molecule 48: 30S ribosomal protein S17

Chain 1q:

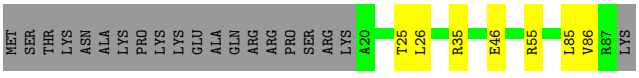


• Molecule 48: 30S ribosomal protein S17

Chain 2q:

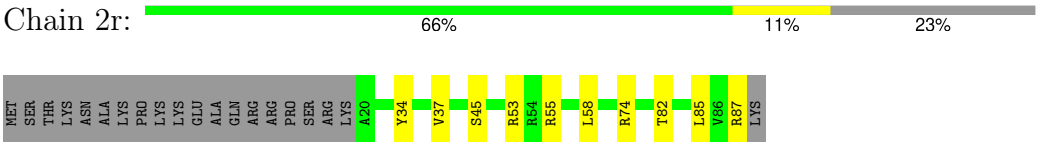
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



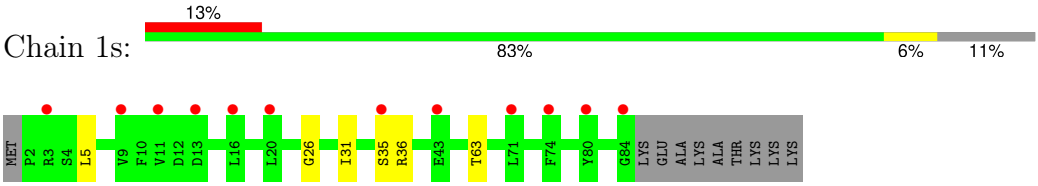
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



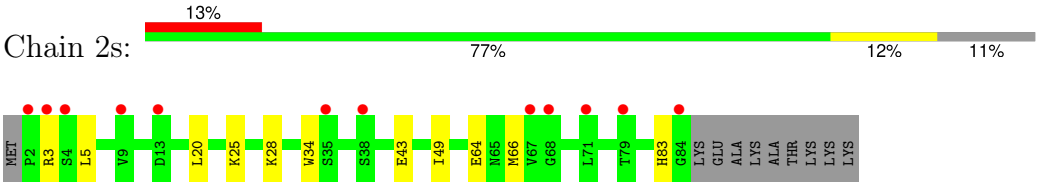
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



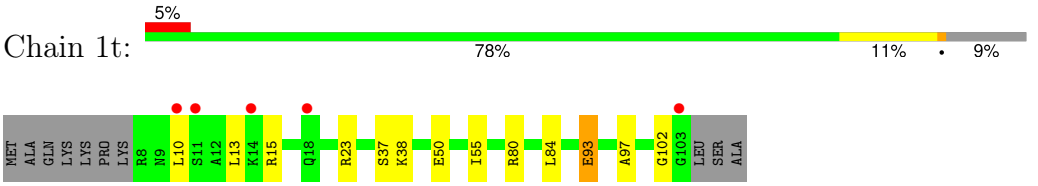
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



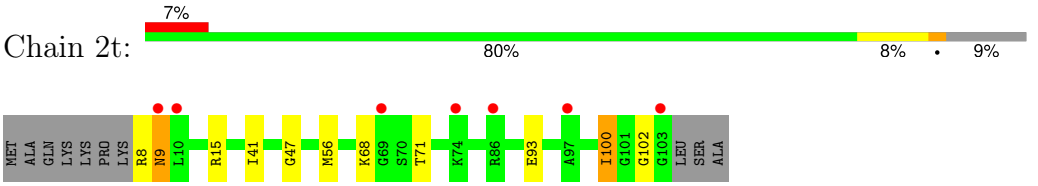
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



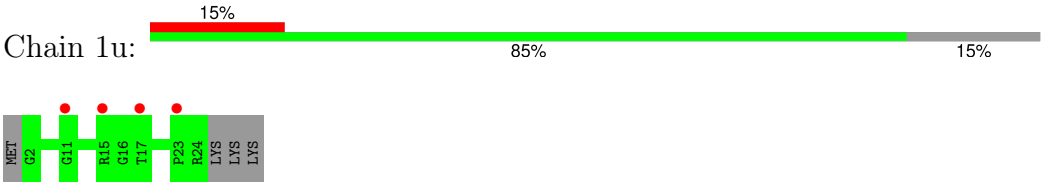
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



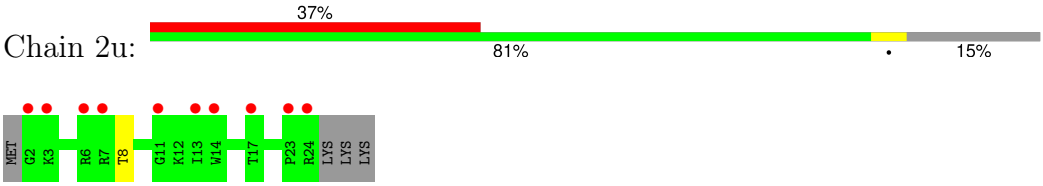
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



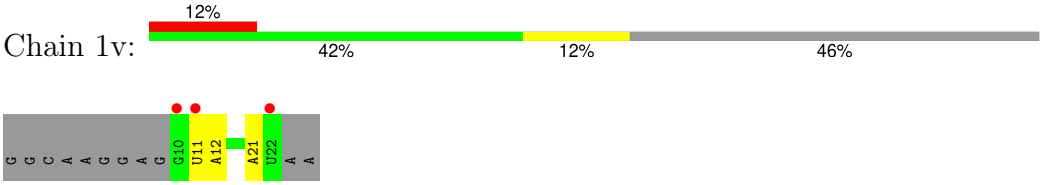
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



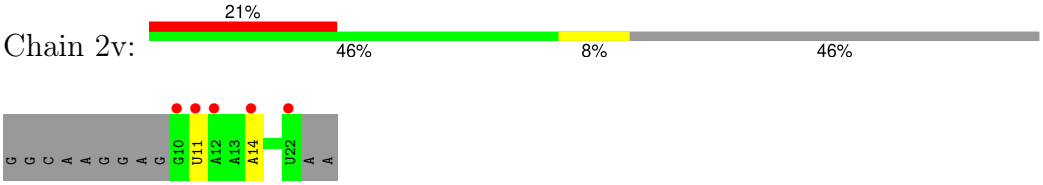
• Molecule 53: PHE-Stop mRNA

Chain 1v:



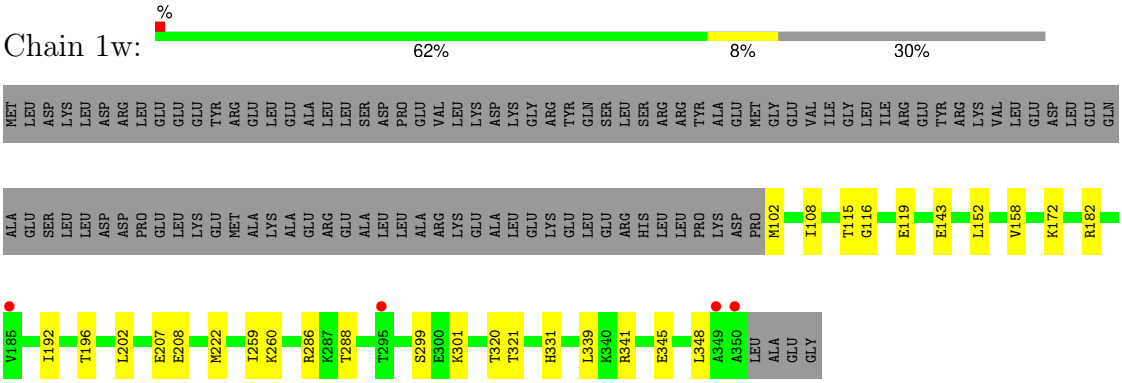
• Molecule 53: PHE-Stop mRNA

Chain 2v:



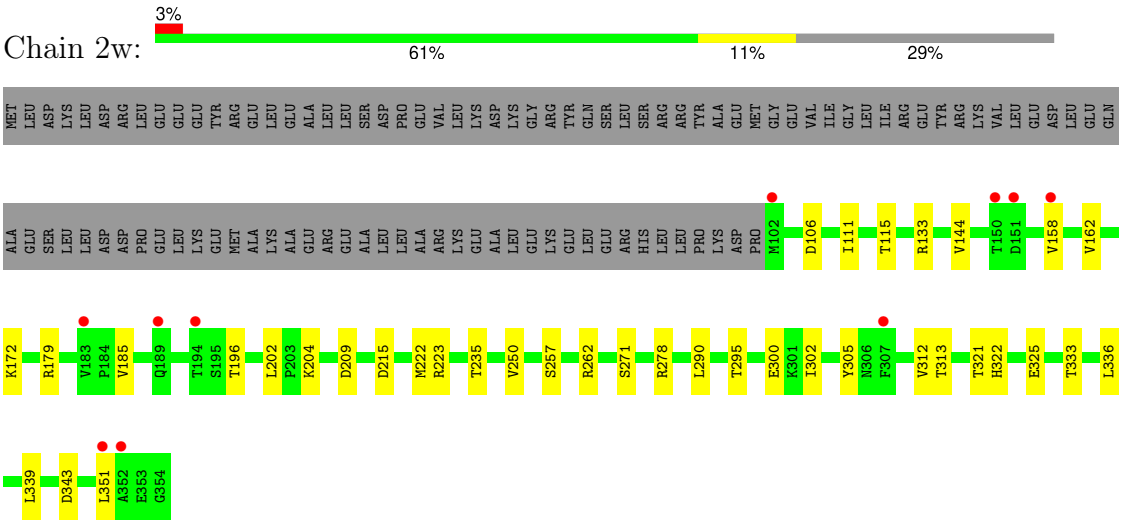
• Molecule 54: Peptide chain release factor 1

Chain 1w:



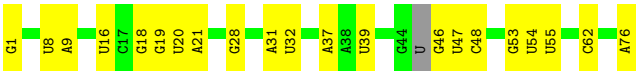
• Molecule 54: Peptide chain release factor 1

Chain 2w:

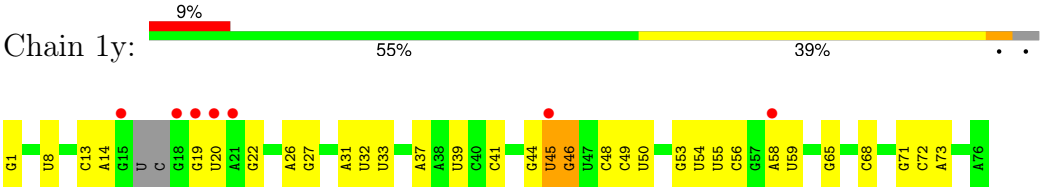


• Molecule 55: P-site and E-site Deacylated tRNAphe

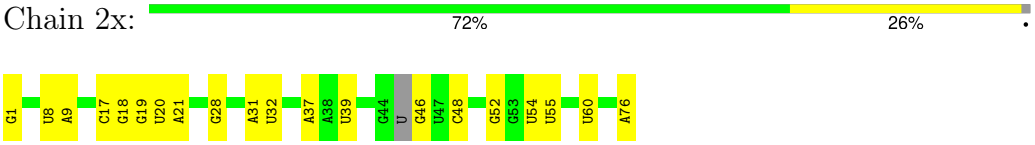
Chain 1x:



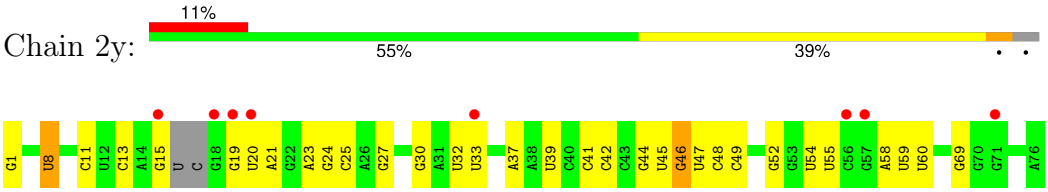
• Molecule 55: P-site and E-site Deacylated tRNAphe



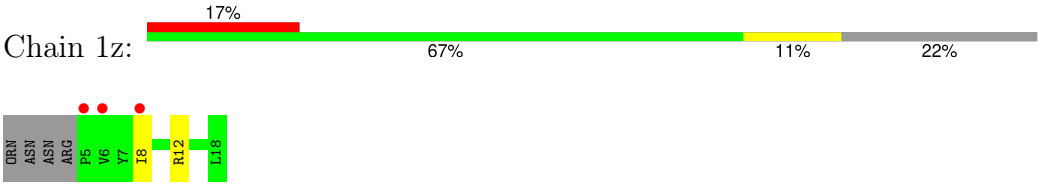
• Molecule 55: P-site and E-site Deacylated tRNAphe



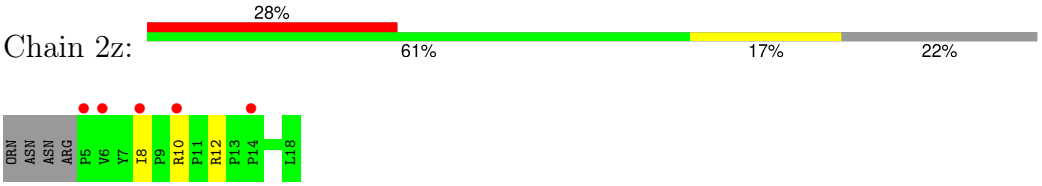
• Molecule 55: P-site and E-site Deacylated tRNAphe



• Molecule 56: Api137 Antimicrobial Peptide



• Molecule 56: Api137 Antimicrobial Peptide



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.60Å 450.81Å 624.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.87 – 2.70 152.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (152.87-2.70) 99.1 (152.87-2.70)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.227 , 0.278 0.229 , 0.277	Depositor DCC
R_{free} test set	80081 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	56.7	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	299179	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.53	1/69011 (0.0%)	0.98	52/107720 (0.0%)
1	2A	0.39	0/67295	0.87	26/105042 (0.0%)
2	1B	0.42	0/2881	0.87	0/4494
2	2B	0.33	0/2881	0.81	0/4494
3	1D	0.35	0/2186	0.57	0/2944
3	2D	0.30	0/2186	0.50	0/2944
4	1E	0.35	0/1592	0.57	0/2149
4	2E	0.29	0/1592	0.50	0/2149
5	1F	0.35	0/1619	0.52	0/2193
5	2F	0.32	0/1615	0.49	0/2188
6	1G	0.30	0/1450	0.49	0/1959
6	2G	0.31	0/1449	0.52	0/1958
7	1H	0.34	0/1356	0.52	0/1834
7	2H	0.29	0/1356	0.48	0/1834
8	1I	0.28	0/1100	0.49	0/1501
8	2I	0.28	0/1076	0.48	0/1471
9	1N	0.33	0/1144	0.52	0/1543
9	2N	0.28	0/1144	0.46	0/1543
10	1O	0.34	0/943	0.55	0/1269
10	2O	0.32	0/943	0.53	0/1269
11	1P	0.35	0/1152	0.59	0/1533
11	2P	0.31	0/1152	0.53	0/1533
12	1Q	0.37	0/1143	0.54	0/1527
12	2Q	0.31	0/1143	0.48	0/1527
13	1R	0.35	0/982	0.55	0/1312
13	2R	0.28	0/982	0.49	0/1312
14	1S	0.31	0/887	0.53	0/1180
14	2S	0.28	0/880	0.49	0/1172
15	1T	0.32	0/1105	0.52	0/1477
15	2T	0.30	0/1097	0.47	0/1468
16	1U	0.40	0/977	0.53	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.30	0/977	0.43	0/1301
17	1V	0.39	0/782	0.56	0/1049
17	2V	0.28	0/782	0.51	0/1049
18	1W	0.37	0/897	0.54	0/1205
18	2W	0.30	0/897	0.49	0/1205
19	1X	0.37	0/764	0.55	0/1025
19	2X	0.30	0/760	0.46	0/1021
20	1Y	0.37	0/819	0.52	0/1095
20	2Y	0.31	0/823	0.51	0/1100
21	1Z	0.30	0/1469	0.53	0/1998
21	2Z	0.30	0/1483	0.52	0/2018
22	10	0.36	0/612	0.54	0/816
22	20	0.30	0/616	0.52	0/821
23	11	0.35	0/762	0.53	0/1014
23	21	0.31	0/762	0.48	0/1014
24	12	0.33	0/590	0.48	0/781
24	22	0.27	0/590	0.44	0/781
25	13	0.33	0/474	0.51	0/635
25	23	0.29	0/469	0.47	0/630
26	14	0.33	0/561	0.52	0/756
26	24	0.37	0/530	0.57	0/719
27	15	0.36	0/469	0.55	0/635
27	25	0.31	0/469	0.47	0/635
28	16	0.34	0/460	0.55	0/613
28	26	0.30	0/456	0.49	0/608
29	17	0.38	0/426	0.53	0/561
29	27	0.29	0/426	0.48	0/561
30	18	0.36	0/519	0.54	0/684
30	28	0.28	0/525	0.50	0/691
31	19	0.36	0/310	0.54	0/407
31	29	0.32	0/310	0.54	0/407
32	1a	0.36	0/35795	0.86	25/55864 (0.0%)
32	2a	0.35	3/35886 (0.0%)	0.88	37/56005 (0.1%)
33	1b	0.30	0/1881	0.48	0/2542
33	2b	0.34	0/1860	0.53	0/2518
34	1c	0.30	0/1578	0.47	0/2133
34	2c	0.29	0/1566	0.47	0/2119
35	1d	0.29	0/1689	0.47	0/2267
35	2d	0.29	0/1704	0.47	0/2284
36	1e	0.30	0/1145	0.50	0/1543
36	2e	0.29	0/1146	0.50	0/1545
37	1f	0.29	0/823	0.48	0/1116
37	2f	0.29	0/829	0.46	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.30	0/1250	0.44	0/1679
38	2g	0.29	0/1254	0.44	0/1683
39	1h	0.29	0/1108	0.47	0/1494
39	2h	0.30	0/1108	0.49	0/1494
40	1i	0.31	0/1002	0.51	0/1346
40	2i	0.30	0/957	0.50	0/1288
41	1j	0.28	0/734	0.47	0/997
41	2j	0.29	0/727	0.49	0/988
42	1k	0.28	0/844	0.48	0/1145
42	2k	0.29	0/848	0.48	0/1149
43	1l	0.30	0/937	0.53	0/1260
43	2l	0.30	0/937	0.49	0/1260
44	1m	0.30	0/933	0.50	0/1254
44	2m	0.29	0/899	0.51	0/1212
45	1n	0.30	0/501	0.48	0/664
45	2n	0.29	0/495	0.48	0/657
46	1o	0.28	0/739	0.44	0/985
46	2o	0.27	0/739	0.42	0/985
47	1p	0.30	0/697	0.53	0/939
47	2p	0.28	0/693	0.52	0/935
48	1q	0.29	0/836	0.48	0/1117
48	2q	0.31	0/836	0.49	0/1117
49	1r	0.30	0/560	0.46	0/746
49	2r	0.28	0/556	0.48	0/741
50	1s	0.30	0/667	0.51	0/900
50	2s	0.28	0/661	0.47	0/893
51	1t	0.30	0/730	0.48	0/965
51	2t	0.27	0/729	0.44	0/965
52	1u	0.27	0/203	0.46	0/266
52	2u	0.25	0/203	0.46	0/266
53	1v	0.43	0/306	0.89	0/473
53	2v	0.40	0/306	0.90	0/473
54	1w	0.29	0/1956	0.47	0/2634
54	2w	0.30	0/1971	0.48	0/2654
55	1x	0.49	1/1629 (0.1%)	0.97	0/2535
55	1y	0.54	1/1602 (0.1%)	1.14	4/2488 (0.2%)
55	2x	0.45	1/1629 (0.1%)	0.89	0/2535
55	2y	0.54	1/1606 (0.1%)	0.97	0/2497
56	1z	0.34	0/128	0.53	0/175
56	2z	0.28	0/128	0.46	0/175
All	All	0.40	8/317654 (0.0%)	0.82	144/474763 (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	2P	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	1	G	OP3-P	-10.27	1.48	1.61
55	1y	1	G	OP3-P	-10.19	1.49	1.61
55	2y	1	G	OP3-P	-10.19	1.49	1.61
55	2x	1	G	OP3-P	-10.04	1.49	1.61
32	2a	1272	G	N1-C2	-7.84	1.31	1.37
32	2a	1272	G	C6-N1	-6.14	1.35	1.39
32	2a	1263	C	N3-C4	-5.26	1.30	1.33
1	1A	2790	A	N9-C4	5.05	1.40	1.37

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1263	C	N1-C2-O2	21.71	131.93	118.90
32	2a	1272	G	N3-C2-N2	18.63	132.94	119.90
32	2a	1272	G	C5-C6-O6	17.58	139.15	128.60
32	2a	1272	G	N1-C2-N2	-14.63	103.03	116.20
32	2a	1272	G	C6-N1-C2	13.88	133.43	125.10
32	2a	1263	C	C2-N3-C4	11.88	125.84	119.90
32	2a	1263	C	N3-C2-O2	-11.50	113.85	121.90
32	2a	1272	G	C5-C6-N1	-11.45	105.78	111.50
32	2a	1263	C	C5-C6-N1	9.22	125.61	121.00
1	1A	1075	C	N1-C2-O2	8.51	124.00	118.90
32	1a	1027	C	N3-C2-O2	-8.43	116.00	121.90
32	1a	1027	C	C6-N1-C2	-8.36	116.95	120.30
1	2A	787	U	O5'-P-OP1	-8.21	98.31	105.70
1	1A	1075	C	C2-N3-C4	8.19	124.00	119.90
32	2a	1272	G	N1-C6-O6	-8.14	115.02	119.90
1	2A	1774	C	O5'-P-OP1	-8.11	98.40	105.70
32	2a	1158	C	N1-C2-O2	8.09	123.75	118.90
1	2A	2136	C	N1-C2-O2	8.00	123.70	118.90
32	1a	841	U	C2-N1-C1'	7.95	127.24	117.70
1	1A	1372	U	N3-C4-O4	7.94	124.96	119.40
32	2a	1263	C	C2-N1-C1'	7.93	127.52	118.80
32	2a	1263	C	C4-C5-C6	-7.82	113.49	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1372	U	C5-C4-O4	-7.72	121.27	125.90
1	1A	1090	U	C2-N1-C1'	7.57	126.78	117.70
1	1A	999	U	O5'-P-OP2	-7.53	98.92	105.70
32	2a	1263	C	N3-C4-N4	-7.37	112.84	118.00
1	1A	1090	U	N1-C2-O2	7.17	127.82	122.80
1	2A	2155	G	C6-N1-C2	7.16	129.40	125.10
32	2a	1263	C	N1-C2-N3	-7.15	114.20	119.20
32	2a	1272	G	C2-N3-C4	-7.10	108.35	111.90
1	2A	2155	G	N3-C2-N2	7.08	124.86	119.90
1	1A	2248	C	O5'-P-OP2	-7.08	99.33	105.70
32	2a	1158	C	C2-N1-C1'	7.07	126.57	118.80
32	2a	1158	C	N3-C2-O2	-7.01	116.99	121.90
1	1A	1063	G	C5-C6-O6	6.90	132.74	128.60
32	2a	754	C	C2-N1-C1'	6.73	126.20	118.80
32	1a	1030(B)	C	C2-N1-C1'	6.73	126.20	118.80
32	1a	1027	C	N3-C4-C5	-6.71	119.22	121.90
1	1A	1021	A	C8-N9-C4	-6.67	103.13	105.80
1	1A	1265	A	O5'-P-OP2	-6.60	99.76	105.70
1	2A	2136	C	N3-C2-O2	-6.58	117.29	121.90
1	1A	31	C	O5'-P-OP1	-6.55	99.81	105.70
32	2a	1263	C	C5-C4-N4	6.51	124.76	120.20
32	1a	266	G	P-O3'-C3'	6.45	127.44	119.70
1	2A	1992	G	P-O3'-C3'	6.45	127.43	119.70
1	1A	1080	C	N1-C2-O2	6.44	122.76	118.90
1	1A	512	G	O4'-C1'-N9	6.44	113.35	108.20
32	1a	1027	C	C5-C4-N4	6.28	124.59	120.20
32	1a	841	U	N3-C2-O2	-6.16	117.89	122.20
32	2a	955	U	C2-N3-C4	6.10	130.66	127.00
1	1A	1090	U	N3-C2-O2	-6.02	117.98	122.20
1	2A	2440	C	N1-C2-O2	-6.00	115.30	118.90
1	2A	1899	G	N3-C4-N9	5.99	129.59	126.00
32	2a	1225	A	C6-N1-C2	5.99	122.19	118.60
1	1A	1021	A	N7-C8-N9	5.97	116.78	113.80
1	1A	389	G	C8-N9-C4	5.97	108.79	106.40
1	1A	984	A	O5'-P-OP1	-5.93	100.36	105.70
32	1a	1158	C	C2-N1-C1'	5.93	125.32	118.80
1	1A	2615	U	N3-C2-O2	-5.91	118.06	122.20
55	1y	50	U	C5-C4-O4	5.89	129.43	125.90
32	1a	841	U	N1-C2-O2	5.87	126.91	122.80
1	1A	2689	U	P-O3'-C3'	5.86	126.73	119.70
32	2a	1158	C	C6-N1-C2	-5.86	117.96	120.30
1	1A	1776	G	O5'-P-OP2	-5.81	100.47	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2319	G	N3-C4-C5	5.77	131.49	128.60
1	1A	2254	C	N1-C2-O2	-5.77	115.44	118.90
1	1A	12	U	C2-N1-C1'	5.73	124.58	117.70
1	1A	2615	U	N1-C2-O2	5.69	126.78	122.80
32	1a	955	U	C5-C4-O4	5.65	129.29	125.90
32	2a	1225	A	C5-C6-N6	5.65	128.22	123.70
1	1A	2789	C	C2-N1-C1'	-5.65	112.58	118.80
1	1A	1063	G	C6-N1-C2	5.65	128.49	125.10
32	1a	1030(B)	C	N1-C2-O2	5.63	122.28	118.90
1	1A	226	G	O4'-C1'-N9	5.63	112.70	108.20
55	1y	56	C	N1-C2-O2	5.62	122.27	118.90
32	1a	841	U	C6-N1-C2	-5.61	117.63	121.00
1	2A	847	U	C2-N1-C1'	5.61	124.43	117.70
32	2a	266	G	P-O3'-C3'	5.61	126.43	119.70
32	2a	1263	C	C6-N1-C1'	-5.60	114.08	120.80
1	2A	752	A	P-O3'-C3'	5.60	126.42	119.70
32	1a	841	U	C5-C6-N1	5.59	125.50	122.70
1	1A	1174	A	P-O3'-C3'	5.58	126.40	119.70
1	1A	1090	U	C6-N1-C1'	-5.56	113.41	121.20
32	1a	1395	C	C2-N3-C4	5.53	122.67	119.90
1	1A	1046	A	O4'-C1'-N9	5.53	112.62	108.20
1	1A	1313	U	C2-N1-C1'	5.51	124.31	117.70
32	2a	955	U	C5-C4-O4	5.50	129.20	125.90
32	1a	1442	G	N3-C4-C5	-5.50	125.85	128.60
32	2a	1025	U	N1-C2-O2	5.49	126.64	122.80
1	1A	1653	G	P-O3'-C3'	5.48	126.28	119.70
1	1A	2682	U	O5'-P-OP2	-5.48	100.77	105.70
1	1A	614	U	C2-N1-C1'	5.46	124.25	117.70
32	1a	687	A	P-O3'-C3'	5.46	126.25	119.70
1	2A	2150	U	N1-C2-O2	5.46	126.62	122.80
1	1A	2873	A	O4'-C1'-N9	5.46	112.57	108.20
1	2A	1530	C	P-O3'-C3'	5.46	126.25	119.70
1	1A	2689	U	N3-C2-O2	-5.45	118.38	122.20
32	2a	1262	C	N1-C2-O2	5.45	122.17	118.90
1	2A	1639	U	O5'-P-OP2	-5.45	100.80	105.70
1	2A	1772	G	C2-N3-C4	-5.44	109.18	111.90
1	1A	2790	A	C2-N3-C4	5.42	113.31	110.60
55	1y	33	U	C2-N1-C1'	5.41	124.19	117.70
1	2A	2155	G	N9-C4-C5	-5.41	103.24	105.40
1	1A	616	G	O5'-P-OP2	-5.40	100.84	105.70
32	1a	1225	A	C5-C6-N6	5.39	128.01	123.70
1	2A	645	C	C2-N1-C1'	5.38	124.72	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1313	U	C2-N1-C1'	5.37	124.14	117.70
1	2A	228	A	P-O3'-C3'	5.36	126.14	119.70
32	2a	754	C	N1-C2-O2	5.36	122.11	118.90
32	1a	346	G	C2-N3-C4	5.35	114.57	111.90
1	2A	383	U	O4'-C1'-N1	5.30	112.44	108.20
32	2a	960	U	C2-N1-C1'	5.30	124.06	117.70
32	2a	1025	U	C2-N1-C1'	5.29	124.05	117.70
1	1A	1301	A	C8-N9-C4	-5.27	103.69	105.80
1	2A	141	A	N7-C8-N9	5.26	116.43	113.80
32	2a	1272	G	C4-N9-C1'	5.26	133.34	126.50
32	2a	1272	G	C8-N9-C1'	-5.24	120.19	127.00
32	2a	1292	U	C5-C4-O4	5.24	129.04	125.90
32	1a	748	C	P-O3'-C3'	5.22	125.97	119.70
32	1a	115	G	P-O3'-C3'	5.20	125.94	119.70
55	1y	45	U	N1-C2-O2	5.19	126.43	122.80
1	2A	528	A	P-O3'-C3'	5.17	125.91	119.70
32	1a	1027	C	N1-C2-O2	5.17	122.00	118.90
32	2a	1067	A	P-O3'-C3'	5.17	125.90	119.70
1	1A	458	G	O4'-C1'-N9	5.17	112.33	108.20
1	1A	1129	A	O4'-C1'-N9	5.16	112.33	108.20
1	2A	2689	U	P-O3'-C3'	5.15	125.88	119.70
32	2a	1263	C	C6-N1-C2	-5.15	118.24	120.30
1	1A	2447	G	C4-N9-C1'	-5.14	119.82	126.50
1	1A	2554	U	O5'-P-OP1	-5.13	101.08	105.70
1	1A	383	U	O4'-C1'-N1	5.12	112.30	108.20
1	1A	548	A	P-O3'-C3'	5.12	125.85	119.70
1	2A	1402	C	N1-C2-O2	5.10	121.96	118.90
1	1A	845	G	O4'-C1'-N9	5.09	112.27	108.20
32	1a	1030(B)	C	C6-N1-C2	-5.08	118.27	120.30
1	2A	2155	G	N1-C2-N3	-5.08	120.85	123.90
32	1a	1201	A	P-O3'-C3'	5.08	125.79	119.70
1	1A	1313	U	N3-C2-O2	-5.08	118.65	122.20
1	2A	646	A	O4'-C1'-N9	5.07	112.25	108.20
1	1A	1340	U	C5-C6-N1	-5.07	120.17	122.70
1	1A	1058	G	N9-C4-C5	-5.04	103.38	105.40
1	1A	2015	A	OP2-P-O3'	5.02	116.24	105.20
1	1A	1644	C	N1-C2-O2	5.02	121.91	118.90
32	1a	913	A	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	2P	35	HIS	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	257 (94%)	16 (6%)	0	100 100
3	2D	273/276 (99%)	254 (93%)	19 (7%)	0	100 100
4	1E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	25 49
4	2E	202/206 (98%)	184 (91%)	17 (8%)	1 (0%)	25 49
5	1F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	13 33
5	2F	201/210 (96%)	187 (93%)	11 (6%)	3 (2%)	8 22
6	1G	179/182 (98%)	155 (87%)	19 (11%)	5 (3%)	4 10
6	2G	179/182 (98%)	155 (87%)	22 (12%)	2 (1%)	12 30
7	1H	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	22 45
7	2H	172/180 (96%)	149 (87%)	20 (12%)	3 (2%)	7 20
8	1I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	9 24
8	2I	144/148 (97%)	122 (85%)	20 (14%)	2 (1%)	9 24
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100 100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100 100
10	1O	120/122 (98%)	109 (91%)	11 (9%)	0	100 100
10	2O	120/122 (98%)	110 (92%)	10 (8%)	0	100 100
11	1P	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	9 24
11	2P	147/150 (98%)	127 (86%)	19 (13%)	1 (1%)	19 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	1Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	19 42
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100 100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100 100
13	2R	116/118 (98%)	107 (92%)	9 (8%)	0	100 100
14	1S	108/112 (96%)	98 (91%)	10 (9%)	0	100 100
14	2S	108/112 (96%)	91 (84%)	11 (10%)	6 (6%)	1 2
15	1T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16 38
15	2T	129/146 (88%)	117 (91%)	12 (9%)	0	100 100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100 100
17	1V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	13 33
17	2V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6 16
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
19	1X	93/96 (97%)	90 (97%)	1 (1%)	2 (2%)	5 15
19	2X	93/96 (97%)	87 (94%)	6 (6%)	0	100 100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	13 33
20	2Y	105/110 (96%)	88 (84%)	17 (16%)	0	100 100
21	1Z	181/206 (88%)	159 (88%)	19 (10%)	3 (2%)	7 20
21	2Z	184/206 (89%)	159 (86%)	21 (11%)	4 (2%)	5 15
22	10	74/85 (87%)	70 (95%)	3 (4%)	1 (1%)	9 24
22	20	75/85 (88%)	67 (89%)	8 (11%)	0	100 100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	12 30
23	21	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	12 30
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100 100
25	13	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	7 18
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
26	14	67/71 (94%)	48 (72%)	11 (16%)	8 (12%)	0 0
26	24	66/71 (93%)	43 (65%)	18 (27%)	5 (8%)	1 1
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	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%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	193 (84%)	29 (13%)	7 (3%)	3	8
33	2b	229/256 (90%)	193 (84%)	24 (10%)	12 (5%)	1	3
34	1c	204/239 (85%)	175 (86%)	27 (13%)	2 (1%)	13	33
34	2c	204/239 (85%)	166 (81%)	36 (18%)	2 (1%)	13	33
35	1d	206/209 (99%)	180 (87%)	24 (12%)	2 (1%)	13	33
35	2d	206/209 (99%)	177 (86%)	27 (13%)	2 (1%)	13	33
36	1e	146/162 (90%)	129 (88%)	17 (12%)	0	100	100
36	2e	146/162 (90%)	124 (85%)	19 (13%)	3 (2%)	5	15
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	85 (87%)	12 (12%)	1 (1%)	13	33
38	1g	153/156 (98%)	134 (88%)	15 (10%)	4 (3%)	4	11
38	2g	153/156 (98%)	135 (88%)	13 (8%)	5 (3%)	3	7
39	1h	135/138 (98%)	125 (93%)	9 (7%)	1 (1%)	19	42
39	2h	135/138 (98%)	123 (91%)	11 (8%)	1 (1%)	19	42
40	1i	125/128 (98%)	103 (82%)	18 (14%)	4 (3%)	3	8
40	2i	121/128 (94%)	99 (82%)	20 (16%)	2 (2%)	7	20
41	1j	96/105 (91%)	88 (92%)	7 (7%)	1 (1%)	13	33
41	2j	94/105 (90%)	80 (85%)	12 (13%)	2 (2%)	5	15
42	1k	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	7	18
42	2k	112/129 (87%)	96 (86%)	15 (13%)	1 (1%)	14	35
43	1l	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
43	2l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
44	1m	116/126 (92%)	102 (88%)	13 (11%)	1 (1%)	14 35
44	2m	113/126 (90%)	96 (85%)	14 (12%)	3 (3%)	4 10
45	1n	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	7 20
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100 100
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	11 28
46	2o	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	11 28
47	1p	80/88 (91%)	66 (82%)	13 (16%)	1 (1%)	10 26
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100 100
48	1q	97/105 (92%)	91 (94%)	6 (6%)	0	100 100
48	2q	97/105 (92%)	85 (88%)	12 (12%)	0	100 100
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100 100
49	2r	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	8 22
50	1s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	11 28
50	2s	81/93 (87%)	67 (83%)	12 (15%)	2 (2%)	4 12
51	1t	94/106 (89%)	80 (85%)	10 (11%)	4 (4%)	2 4
51	2t	94/106 (89%)	85 (90%)	5 (5%)	4 (4%)	2 4
52	1u	21/27 (78%)	21 (100%)	0	0	100 100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
54	1w	246/354 (70%)	228 (93%)	13 (5%)	5 (2%)	6 16
54	2w	250/354 (71%)	235 (94%)	14 (6%)	1 (0%)	30 55
56	1z	12/18 (67%)	11 (92%)	1 (8%)	0	100 100
56	2z	12/18 (67%)	10 (83%)	2 (17%)	0	100 100
All	All	11922/12872 (93%)	10772 (90%)	1007 (8%)	143 (1%)	11 28

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	50	ALA
8	1I	10	GLU
17	1V	79	VAL
23	11	3	LYS
26	14	18	CYS
33	1b	17	PHE

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Mol	Chain	Res	Type
33	1b	125	PRO
34	1c	107	GLN
35	1d	44	GLY
40	1i	100	GLY
44	1m	67	GLU
5	2F	130	ALA
6	2G	96	ARG
7	2H	126	PRO
21	2Z	31	ARG
33	2b	10	LEU
33	2b	22	LYS
34	2c	100	ALA
38	2g	80	VAL
41	2j	55	LYS
54	2w	209	ASP
6	1G	24	GLY
15	1T	37	GLY
20	1Y	101	LYS
21	1Z	52	SER
22	10	10	THR
26	14	49	PHE
26	14	62	ARG
38	1g	55	GLY
40	1i	99	LEU
54	1w	299	SER
54	1w	331	HIS
8	2I	42	SER
14	2S	62	LYS
17	2V	79	VAL
17	2V	100	ARG
21	2Z	52	SER
26	24	39	CYS
26	24	45	GLY
26	24	49	PHE
33	2b	17	PHE
33	2b	78	GLN
36	2e	98	THR
38	2g	55	GLY
38	2g	79	ARG
41	2j	31	GLY
42	2k	49	GLY
44	2m	5	ALA

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Mol	Chain	Res	Type
44	2m	28	ALA
46	2o	19	PRO
50	2s	25	LYS
51	2t	47	GLY
6	1G	47	LYS
6	1G	51	ARG
11	1P	29	LYS
12	1Q	59	ARG
26	14	47	GLN
33	1b	96	ARG
34	1c	157	ILE
38	1g	80	VAL
40	1i	54	ASP
41	1j	55	LYS
47	1p	48	TRP
54	1w	207	GLU
5	2F	54	ARG
7	2H	55	PRO
7	2H	92	ILE
14	2S	57	LYS
21	2Z	152	ALA
33	2b	16	HIS
33	2b	128	GLU
33	2b	150	SER
34	2c	99	VAL
38	2g	82	GLY
40	2i	29	ASN
44	2m	67	GLU
5	1F	145	GLU
8	1I	83	ALA
19	1X	94	GLY
21	1Z	137	ILE
26	14	64	GLY
26	14	65	ASP
33	1b	10	LEU
35	1d	137	SER
38	1g	82	GLY
45	1n	20	ALA
51	1t	38	LYS
51	1t	93	GLU
54	1w	116	GLY
54	1w	208	GLU

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Mol	Chain	Res	Type
4	2E	52	LEU
5	2F	18	ARG
6	2G	143	GLU
11	2P	6	LEU
14	2S	63	THR
14	2S	97	ARG
21	2Z	153	SER
23	21	3	LYS
26	24	62	ARG
33	2b	63	MET
33	2b	96	ARG
35	2d	147	ALA
35	2d	166	LYS
39	2h	115	SER
50	2s	3	ARG
4	1E	52	LEU
19	1X	93	GLU
26	14	63	TYR
33	1b	21	ARG
33	1b	232	PRO
39	1h	70	GLN
26	24	47	GLN
33	2b	124	SER
37	2f	80	ARG
38	2g	81	GLY
40	2i	54	ASP
49	2r	53	ARG
51	2t	9	ASN
7	1H	126	PRO
21	1Z	53	ILE
26	14	51	ASP
33	1b	15	VAL
40	1i	98	PRO
51	1t	97	ALA
51	1t	102	GLY
36	2e	69	VAL
11	1P	44	GLY
42	1k	49	GLY
46	1o	86	GLY
14	2S	96	GLY
33	2b	165	VAL
36	2e	39	GLY

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Mol	Chain	Res	Type
25	13	59	VAL
42	1k	105	VAL
14	2S	60	GLY
51	2t	100	ILE
38	1g	9	VAL
50	1s	26	GLY
8	2I	111	PRO
33	2b	125	PRO
51	2t	102	GLY
6	1G	52	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%)	199 (93%)	16 (7%)	11 28
3	2D	215/218 (99%)	201 (94%)	14 (6%)	14 34
4	1E	164/166 (99%)	151 (92%)	13 (8%)	10 25
4	2E	164/166 (99%)	153 (93%)	11 (7%)	13 33
5	1F	160/166 (96%)	146 (91%)	14 (9%)	8 20
5	2F	159/166 (96%)	145 (91%)	14 (9%)	8 20
6	1G	143/156 (92%)	123 (86%)	20 (14%)	3 7
6	2G	142/156 (91%)	123 (87%)	19 (13%)	3 8
7	1H	144/148 (97%)	131 (91%)	13 (9%)	8 19
7	2H	144/148 (97%)	130 (90%)	14 (10%)	6 17
8	1I	110/124 (89%)	100 (91%)	10 (9%)	7 19
8	2I	104/124 (84%)	82 (79%)	22 (21%)	1 2
9	1N	118/119 (99%)	110 (93%)	8 (7%)	13 32
9	2N	118/119 (99%)	113 (96%)	5 (4%)	25 53
10	1O	100/100 (100%)	98 (98%)	2 (2%)	50 78
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	1P	115/116 (99%)	110 (96%)	5 (4%)	25 52
11	2P	115/116 (99%)	108 (94%)	7 (6%)	15 36
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	9 23
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	9 23
13	1R	101/101 (100%)	92 (91%)	9 (9%)	8 20
13	2R	101/101 (100%)	96 (95%)	5 (5%)	20 46
14	1S	87/88 (99%)	75 (86%)	12 (14%)	3 7
14	2S	85/88 (97%)	77 (91%)	8 (9%)	7 18
15	1T	115/127 (91%)	103 (90%)	12 (10%)	5 14
15	2T	113/127 (89%)	109 (96%)	4 (4%)	31 60
16	1U	93/94 (99%)	89 (96%)	4 (4%)	25 52
16	2U	93/94 (99%)	89 (96%)	4 (4%)	25 52
17	1V	80/82 (98%)	75 (94%)	5 (6%)	15 35
17	2V	80/82 (98%)	75 (94%)	5 (6%)	15 35
18	1W	90/92 (98%)	84 (93%)	6 (7%)	13 33
18	2W	90/92 (98%)	88 (98%)	2 (2%)	47 76
19	1X	77/78 (99%)	74 (96%)	3 (4%)	27 56
19	2X	76/78 (97%)	72 (95%)	4 (5%)	19 43
20	1Y	85/91 (93%)	77 (91%)	8 (9%)	7 18
20	2Y	86/91 (94%)	74 (86%)	12 (14%)	3 7
21	1Z	155/179 (87%)	144 (93%)	11 (7%)	12 30
21	2Z	155/179 (87%)	139 (90%)	16 (10%)	6 14
22	10	61/67 (91%)	55 (90%)	6 (10%)	6 16
22	20	61/67 (91%)	56 (92%)	5 (8%)	9 23
23	11	80/83 (96%)	77 (96%)	3 (4%)	28 56
23	21	80/83 (96%)	74 (92%)	6 (8%)	11 28
24	12	65/67 (97%)	61 (94%)	4 (6%)	15 36
24	22	65/67 (97%)	59 (91%)	6 (9%)	7 18
25	13	51/52 (98%)	49 (96%)	2 (4%)	27 56
25	23	50/52 (96%)	47 (94%)	3 (6%)	16 38
26	14	58/63 (92%)	52 (90%)	6 (10%)	6 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	24	51/63 (81%)	41 (80%)	10 (20%)	1 3
27	15	50/52 (96%)	47 (94%)	3 (6%)	16 38
27	25	50/52 (96%)	47 (94%)	3 (6%)	16 38
28	16	51/52 (98%)	50 (98%)	1 (2%)	50 78
28	26	50/52 (96%)	45 (90%)	5 (10%)	6 16
29	17	41/42 (98%)	38 (93%)	3 (7%)	11 29
29	27	41/42 (98%)	39 (95%)	2 (5%)	21 47
30	18	53/55 (96%)	44 (83%)	9 (17%)	1 4
30	28	54/55 (98%)	50 (93%)	4 (7%)	11 28
31	19	34/34 (100%)	33 (97%)	1 (3%)	37 67
31	29	34/34 (100%)	33 (97%)	1 (3%)	37 67
33	1b	192/220 (87%)	155 (81%)	37 (19%)	1 3
33	2b	187/220 (85%)	153 (82%)	34 (18%)	1 4
34	1c	144/188 (77%)	128 (89%)	16 (11%)	5 12
34	2c	140/188 (74%)	123 (88%)	17 (12%)	4 10
35	1d	170/181 (94%)	139 (82%)	31 (18%)	1 4
35	2d	173/181 (96%)	153 (88%)	20 (12%)	4 11
36	1e	113/123 (92%)	106 (94%)	7 (6%)	15 36
36	2e	113/123 (92%)	104 (92%)	9 (8%)	10 24
37	1f	84/90 (93%)	76 (90%)	8 (10%)	7 17
37	2f	85/90 (94%)	80 (94%)	5 (6%)	16 38
38	1g	119/127 (94%)	103 (87%)	16 (13%)	3 8
38	2g	120/127 (94%)	111 (92%)	9 (8%)	11 28
39	1h	114/119 (96%)	105 (92%)	9 (8%)	10 25
39	2h	114/119 (96%)	106 (93%)	8 (7%)	12 31
40	1i	90/99 (91%)	83 (92%)	7 (8%)	10 26
40	2i	86/99 (87%)	73 (85%)	13 (15%)	2 6
41	1j	68/92 (74%)	59 (87%)	9 (13%)	3 8
41	2j	69/92 (75%)	60 (87%)	9 (13%)	3 8
42	1k	82/99 (83%)	75 (92%)	7 (8%)	8 21
42	2k	83/99 (84%)	77 (93%)	6 (7%)	12 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
43	1l	96/108 (89%)	86 (90%)	10 (10%)	5 14
43	2l	96/108 (89%)	90 (94%)	6 (6%)	15 35
44	1m	90/101 (89%)	79 (88%)	11 (12%)	4 9
44	2m	85/101 (84%)	81 (95%)	4 (5%)	22 49
45	1n	49/50 (98%)	44 (90%)	5 (10%)	6 15
45	2n	48/50 (96%)	40 (83%)	8 (17%)	2 5
46	1o	78/80 (98%)	75 (96%)	3 (4%)	28 56
46	2o	78/80 (98%)	73 (94%)	5 (6%)	14 34
47	1p	69/74 (93%)	64 (93%)	5 (7%)	12 30
47	2p	68/74 (92%)	61 (90%)	7 (10%)	6 14
48	1q	94/97 (97%)	86 (92%)	8 (8%)	8 21
48	2q	94/97 (97%)	84 (89%)	10 (11%)	5 13
49	1r	59/77 (77%)	52 (88%)	7 (12%)	4 10
49	2r	58/77 (75%)	49 (84%)	9 (16%)	2 6
50	1s	69/80 (86%)	64 (93%)	5 (7%)	12 30
50	2s	67/80 (84%)	58 (87%)	9 (13%)	3 8
51	1t	70/82 (85%)	60 (86%)	10 (14%)	2 7
51	2t	70/82 (85%)	61 (87%)	9 (13%)	3 8
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	17 41
54	1w	203/298 (68%)	179 (88%)	24 (12%)	4 10
54	2w	202/298 (68%)	165 (82%)	37 (18%)	1 3
56	1z	14/17 (82%)	12 (86%)	2 (14%)	2 7
56	2z	14/17 (82%)	11 (79%)	3 (21%)	1 2
All	All	9747/10694 (91%)	8831 (91%)	916 (9%)	7 18

All (916) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	12	SER
3	1D	54	ARG
3	1D	69	ARG
3	1D	88	ARG

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Mol	Chain	Res	Type
3	1D	99	ASP
3	1D	111	LEU
3	1D	122	ASP
3	1D	142	VAL
3	1D	176	ARG
3	1D	193	VAL
3	1D	200	ASP
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	275	LYS
4	1E	33	VAL
4	1E	73	GLU
4	1E	75	VAL
4	1E	82	ARG
4	1E	89	ASP
4	1E	90	THR
4	1E	93	VAL
4	1E	116	VAL
4	1E	170	LEU
4	1E	173	VAL
4	1E	182	LEU
4	1E	183	LEU
4	1E	195	LEU
5	1F	24	LEU
5	1F	40	GLN
5	1F	53	THR
5	1F	57	VAL
5	1F	106	ARG
5	1F	119	ARG
5	1F	120	GLU
5	1F	137	LYS
5	1F	162	LEU
5	1F	170	LEU
5	1F	176	LEU
5	1F	191	ARG
5	1F	192	LEU
5	1F	204	ASN
6	1G	3	LEU
6	1G	7	LEU
6	1G	21	ARG
6	1G	28	VAL

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Mol	Chain	Res	Type
6	1G	31	VAL
6	1G	40	ASN
6	1G	60	LEU
6	1G	70	VAL
6	1G	79	ASN
6	1G	91	ARG
6	1G	116	ASP
6	1G	136	ARG
6	1G	139	LEU
6	1G	140	ILE
6	1G	150	ASP
6	1G	165	THR
6	1G	167	GLU
6	1G	168	GLU
6	1G	170	ARG
6	1G	175	LEU
7	1H	13	LYS
7	1H	18	GLU
7	1H	37	VAL
7	1H	42	ARG
7	1H	49	VAL
7	1H	57	ASP
7	1H	84	SER
7	1H	95	ARG
7	1H	101	ARG
7	1H	116	GLU
7	1H	119	GLU
7	1H	122	THR
7	1H	172	LYS
8	1I	5	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	19	VAL
8	1I	38	LEU
8	1I	40	THR
8	1I	47	LEU
8	1I	86	THR
8	1I	108	THR
8	1I	133	HIS
9	1N	12	ARG
9	1N	33	LEU
9	1N	48	MET

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Mol	Chain	Res	Type
9	1N	58	ASP
9	1N	61	ARG
9	1N	62	VAL
9	1N	73	THR
9	1N	83	LYS
10	1O	47	ILE
10	1O	66	LYS
11	1P	1	MET
11	1P	98	GLU
11	1P	135	LEU
11	1P	148	LEU
11	1P	149	GLU
12	1Q	3	MET
12	1Q	7	MET
12	1Q	17	LEU
12	1Q	35	VAL
12	1Q	75	THR
12	1Q	81	VAL
12	1Q	106	VAL
12	1Q	111	GLU
12	1Q	129	THR
13	1R	6	SER
13	1R	8	ARG
13	1R	29	LEU
13	1R	36	THR
13	1R	59	ASP
13	1R	64	ARG
13	1R	65	LEU
13	1R	73	VAL
13	1R	114	VAL
14	1S	26	LEU
14	1S	27	SER
14	1S	43	GLU
14	1S	50	SER
14	1S	53	SER
14	1S	59	LYS
14	1S	61	ASN
14	1S	76	LYS
14	1S	78	LEU
14	1S	85	VAL
14	1S	88	ASP
14	1S	110	LEU

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Mol	Chain	Res	Type
15	1T	17	THR
15	1T	21	GLU
15	1T	28	VAL
15	1T	36	GLU
15	1T	49	VAL
15	1T	64	ARG
15	1T	66	VAL
15	1T	84	GLN
15	1T	96	ARG
15	1T	112	ARG
15	1T	118	ARG
15	1T	124	ASP
16	1U	13	LYS
16	1U	74	LEU
16	1U	100	VAL
16	1U	117	GLN
17	1V	13	ARG
17	1V	32	THR
17	1V	73	SER
17	1V	79	VAL
17	1V	85	LYS
18	1W	11	ARG
18	1W	17	VAL
18	1W	68	ARG
18	1W	90	ARG
18	1W	101	SER
18	1W	111	HIS
19	1X	1	MET
19	1X	13	LEU
19	1X	49	VAL
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	47	LYS
20	1Y	70	SER
20	1Y	72	VAL
20	1Y	88	LYS
20	1Y	106	LEU
20	1Y	107	ASP
21	1Z	31	ARG
21	1Z	86	VAL
21	1Z	87	ASP
21	1Z	121	HIS

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Mol	Chain	Res	Type
21	1Z	136	PHE
21	1Z	142	SER
21	1Z	155	LEU
21	1Z	156	LYS
21	1Z	165	VAL
21	1Z	170	THR
21	1Z	175	VAL
22	10	11	ARG
22	10	14	ARG
22	10	39	ARG
22	10	44	ARG
22	10	68	GLU
22	10	82	ARG
23	11	38	SER
23	11	40	ARG
23	11	75	GLU
24	12	3	LEU
24	12	4	SER
24	12	45	SER
24	12	65	ASN
25	13	54	VAL
25	13	58	VAL
26	14	1	MET
26	14	21	VAL
26	14	49	PHE
26	14	50	VAL
26	14	57	GLU
26	14	63	TYR
27	15	6	VAL
27	15	20	ARG
27	15	26	THR
28	16	6	ARG
29	17	1	MET
29	17	41	ARG
29	17	43	THR
30	18	6	THR
30	18	14	VAL
30	18	23	VAL
30	18	26	LYS
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP

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Mol	Chain	Res	Type
30	18	43	GLN
30	18	58	ILE
31	19	6	SER
33	1b	8	LYS
33	1b	10	LEU
33	1b	11	LEU
33	1b	24	TRP
33	1b	32	ILE
33	1b	35	GLU
33	1b	37	ASN
33	1b	45	GLN
33	1b	53	ARG
33	1b	61	LEU
33	1b	63	MET
33	1b	67	THR
33	1b	73	THR
33	1b	75	LYS
33	1b	80	ILE
33	1b	82	ARG
33	1b	93	VAL
33	1b	96	ARG
33	1b	97	TRP
33	1b	107	THR
33	1b	108	ILE
33	1b	112	VAL
33	1b	118	LEU
33	1b	128	GLU
33	1b	145	LEU
33	1b	147	LYS
33	1b	153	ARG
33	1b	154	LEU
33	1b	156	LYS
33	1b	163	PHE
33	1b	172	ILE
33	1b	180	LEU
33	1b	185	ILE
33	1b	190	THR
33	1b	209	ARG
33	1b	213	LEU
33	1b	233	SER
34	1c	17	ASP
34	1c	29	TYR

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Mol	Chain	Res	Type
34	1c	32	LEU
34	1c	49	SER
34	1c	64	VAL
34	1c	67	THR
34	1c	70	VAL
34	1c	82	GLU
34	1c	85	ARG
34	1c	95	THR
34	1c	98	ASN
34	1c	115	LEU
34	1c	130	VAL
34	1c	152	ILE
34	1c	188	LEU
34	1c	192	THR
35	1d	17	VAL
35	1d	18	LYS
35	1d	30	LYS
35	1d	31	CYS
35	1d	33	MET
35	1d	35	ARG
35	1d	42	GLN
35	1d	47	ARG
35	1d	56	VAL
35	1d	85	LYS
35	1d	88	VAL
35	1d	93	PHE
35	1d	94	LEU
35	1d	106	TYR
35	1d	110	PHE
35	1d	122	ARG
35	1d	127	THR
35	1d	129	ASN
35	1d	132	ARG
35	1d	135	LEU
35	1d	141	ARG
35	1d	150	GLU
35	1d	155	LEU
35	1d	163	GLU
35	1d	166	LYS
35	1d	174	LEU
35	1d	186	LEU
35	1d	188	LEU

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Mol	Chain	Res	Type
35	1d	190	ASP
35	1d	193	ASP
35	1d	200	GLU
36	1e	10	MET
36	1e	31	LEU
36	1e	41	VAL
36	1e	75	THR
36	1e	78	HIS
36	1e	98	THR
36	1e	147	ASP
37	1f	31	GLU
37	1f	40	VAL
37	1f	55	ASP
37	1f	71	ARG
37	1f	72	VAL
37	1f	74	ASP
37	1f	91	VAL
37	1f	98	LEU
38	1g	9	VAL
38	1g	11	GLN
38	1g	45	ASP
38	1g	49	ILE
38	1g	50	ILE
38	1g	72	ARG
38	1g	75	VAL
38	1g	85	TYR
38	1g	89	MET
38	1g	90	GLU
38	1g	91	VAL
38	1g	92	SER
38	1g	114	ARG
38	1g	115	ARG
38	1g	138	LYS
38	1g	156	TRP
39	1h	18	ARG
39	1h	19	VAL
39	1h	24	THR
39	1h	50	ARG
39	1h	99	GLU
39	1h	112	LEU
39	1h	120	THR
39	1h	121	ASP

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Mol	Chain	Res	Type
39	1h	137	VAL
40	1i	11	LYS
40	1i	17	VAL
40	1i	27	THR
40	1i	60	ASP
40	1i	65	VAL
40	1i	104	ARG
40	1i	113	LYS
41	1j	5	ARG
41	1j	16	LEU
41	1j	44	VAL
41	1j	49	VAL
41	1j	55	LYS
41	1j	72	VAL
41	1j	84	GLN
41	1j	97	GLU
41	1j	100	THR
42	1k	14	VAL
42	1k	48	ILE
42	1k	80	VAL
42	1k	82	VAL
42	1k	84	VAL
42	1k	87	THR
42	1k	117	ASN
43	1l	6	THR
43	1l	33	ARG
43	1l	46	LYS
43	1l	60	LEU
43	1l	61	THR
43	1l	78	GLN
43	1l	81	SER
43	1l	83	VAL
43	1l	102	ARG
43	1l	104	VAL
44	1m	19	LEU
44	1m	23	TYR
44	1m	32	GLU
44	1m	48	LEU
44	1m	56	LEU
44	1m	90	LEU
44	1m	91	ARG
44	1m	103	THR

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Mol	Chain	Res	Type
44	1m	105	THR
44	1m	106	ASN
44	1m	117	VAL
45	1n	11	LYS
45	1n	18	VAL
45	1n	32	SER
45	1n	33	VAL
45	1n	41	ARG
46	1o	3	ILE
46	1o	39	LEU
46	1o	56	LEU
47	1p	4	ILE
47	1p	6	LEU
47	1p	16	HIS
47	1p	20	VAL
47	1p	67	THR
48	1q	7	THR
48	1q	36	ILE
48	1q	45	HIS
48	1q	72	ARG
48	1q	79	SER
48	1q	86	GLU
48	1q	87	LYS
48	1q	90	ILE
49	1r	25	THR
49	1r	26	LEU
49	1r	35	ARG
49	1r	46	GLU
49	1r	55	ARG
49	1r	85	LEU
49	1r	86	VAL
50	1s	5	LEU
50	1s	31	ILE
50	1s	35	SER
50	1s	36	ARG
50	1s	63	THR
51	1t	10	LEU
51	1t	13	LEU
51	1t	15	ARG
51	1t	23	ARG
51	1t	37	SER
51	1t	50	GLU

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Mol	Chain	Res	Type
51	1t	55	ILE
51	1t	80	ARG
51	1t	84	LEU
51	1t	93	GLU
54	1w	102	MET
54	1w	108	ILE
54	1w	115	THR
54	1w	119	GLU
54	1w	143	GLU
54	1w	152	LEU
54	1w	158	VAL
54	1w	172	LYS
54	1w	182	ARG
54	1w	192	ILE
54	1w	196	THR
54	1w	202	LEU
54	1w	222	MET
54	1w	259	ILE
54	1w	260	LYS
54	1w	286	ARG
54	1w	288	THR
54	1w	301	LYS
54	1w	320	THR
54	1w	321	THR
54	1w	339	LEU
54	1w	341	ARG
54	1w	345	GLU
54	1w	348	LEU
56	1z	8	ILE
56	1z	12	ARG
3	2D	4	LYS
3	2D	27	THR
3	2D	28	GLU
3	2D	88	ARG
3	2D	134	ARG
3	2D	142	VAL
3	2D	193	VAL
3	2D	204	ILE
3	2D	211	ARG
3	2D	218	ARG
3	2D	229	VAL
3	2D	237	GLU

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Mol	Chain	Res	Type
3	2D	242	ARG
3	2D	275	LYS
4	2E	69	LYS
4	2E	72	VAL
4	2E	75	VAL
4	2E	82	ARG
4	2E	90	THR
4	2E	93	VAL
4	2E	113	PHE
4	2E	116	VAL
4	2E	128	SER
4	2E	170	LEU
4	2E	184	VAL
5	2F	67	GLN
5	2F	74	ARG
5	2F	98	SER
5	2F	106	ARG
5	2F	125	LEU
5	2F	132	VAL
5	2F	153	SER
5	2F	160	ASN
5	2F	175	THR
5	2F	181	LEU
5	2F	183	VAL
5	2F	192	LEU
5	2F	197	ASP
5	2F	201	VAL
6	2G	5	VAL
6	2G	20	ILE
6	2G	21	ARG
6	2G	31	VAL
6	2G	33	ARG
6	2G	43	LEU
6	2G	51	ARG
6	2G	91	ARG
6	2G	95	ARG
6	2G	96	ARG
6	2G	97	ASP
6	2G	106	LEU
6	2G	128	ARG
6	2G	133	LEU
6	2G	145	THR

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Mol	Chain	Res	Type
6	2G	146	TYR
6	2G	152	LEU
6	2G	156	ASP
6	2G	166	ASP
7	2H	2	SER
7	2H	6	ARG
7	2H	7	LEU
7	2H	43	VAL
7	2H	58	GLU
7	2H	63	SER
7	2H	67	LEU
7	2H	90	LYS
7	2H	116	GLU
7	2H	122	THR
7	2H	129	THR
7	2H	134	SER
7	2H	136	ILE
7	2H	175	LYS
8	2I	3	VAL
8	2I	7	GLU
8	2I	11	ASN
8	2I	15	VAL
8	2I	20	ASP
8	2I	31	LEU
8	2I	37	VAL
8	2I	40	THR
8	2I	44	LEU
8	2I	50	ARG
8	2I	68	LEU
8	2I	79	ILE
8	2I	82	ARG
8	2I	92	VAL
8	2I	101	LEU
8	2I	110	ASP
8	2I	120	ILE
8	2I	123	LEU
8	2I	125	GLU
8	2I	133	HIS
8	2I	144	VAL
8	2I	145	VAL
9	2N	9	VAL
9	2N	12	ARG

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Mol	Chain	Res	Type
9	2N	32	THR
9	2N	83	LYS
9	2N	138	LEU
10	2O	21	CYS
10	2O	42	SER
10	2O	78	ARG
11	2P	30	THR
11	2P	99	LEU
11	2P	123	LEU
11	2P	133	SER
11	2P	147	LEU
11	2P	148	LEU
11	2P	149	GLU
12	2Q	7	MET
12	2Q	21	THR
12	2Q	35	VAL
12	2Q	38	GLU
12	2Q	56	ARG
12	2Q	63	LYS
12	2Q	75	THR
12	2Q	115	MET
12	2Q	127	ILE
13	2R	29	LEU
13	2R	36	THR
13	2R	65	LEU
13	2R	86	ARG
13	2R	114	VAL
14	2S	12	PHE
14	2S	15	ARG
14	2S	52	SER
14	2S	56	LEU
14	2S	71	ARG
14	2S	83	LYS
14	2S	98	VAL
14	2S	103	GLU
15	2T	28	VAL
15	2T	49	VAL
15	2T	72	VAL
15	2T	96	ARG
16	2U	5	LYS
16	2U	13	LYS
16	2U	31	SER

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Mol	Chain	Res	Type
16	2U	74	LEU
17	2V	18	LEU
17	2V	45	THR
17	2V	51	VAL
17	2V	73	SER
17	2V	79	VAL
18	2W	11	ARG
18	2W	70	TYR
19	2X	52	VAL
19	2X	57	LEU
19	2X	68	ARG
19	2X	75	ASP
20	2Y	6	HIS
20	2Y	11	ASP
20	2Y	12	THR
20	2Y	28	LYS
20	2Y	31	LEU
20	2Y	35	TYR
20	2Y	55	TYR
20	2Y	71	LYS
20	2Y	72	VAL
20	2Y	91	GLU
20	2Y	92	ASN
20	2Y	107	ASP
21	2Z	18	LEU
21	2Z	30	ASN
21	2Z	33	LEU
21	2Z	41	LEU
21	2Z	42	VAL
21	2Z	72	ARG
21	2Z	76	LEU
21	2Z	80	ARG
21	2Z	84	GLU
21	2Z	87	ASP
21	2Z	102	LEU
21	2Z	132	ASN
21	2Z	142	SER
21	2Z	151	HIS
21	2Z	155	LEU
21	2Z	180	VAL
22	20	10	THR
22	20	39	ARG

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Mol	Chain	Res	Type
22	20	44	ARG
22	20	64	ASP
22	20	81	VAL
23	21	21	ARG
23	21	30	VAL
23	21	35	THR
23	21	40	ARG
23	21	46	LEU
23	21	80	LEU
24	22	12	GLU
24	22	16	LEU
24	22	21	LEU
24	22	44	LEU
24	22	52	ASP
24	22	53	LEU
25	23	31	LEU
25	23	40	THR
25	23	54	VAL
26	24	1	MET
26	24	35	VAL
26	24	39	CYS
26	24	46	GLN
26	24	49	PHE
26	24	58	ARG
26	24	61	ARG
26	24	63	TYR
26	24	67	TYR
26	24	68	ARG
27	25	6	VAL
27	25	26	THR
27	25	59	GLU
28	26	19	ARG
28	26	20	ASN
28	26	40	CYS
28	26	48	VAL
28	26	49	HIS
29	27	1	MET
29	27	4	THR
30	28	14	VAL
30	28	23	VAL
30	28	31	HIS
30	28	37	SER

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Mol	Chain	Res	Type
31	29	7	VAL
33	2b	9	GLU
33	2b	10	LEU
33	2b	12	GLU
33	2b	22	LYS
33	2b	24	TRP
33	2b	25	ASN
33	2b	28	PHE
33	2b	49	GLU
33	2b	55	PHE
33	2b	56	ARG
33	2b	63	MET
33	2b	67	THR
33	2b	80	ILE
33	2b	111	ARG
33	2b	112	VAL
33	2b	113	HIS
33	2b	133	LYS
33	2b	140	HIS
33	2b	154	LEU
33	2b	157	ARG
33	2b	160	ASP
33	2b	164	VAL
33	2b	169	LYS
33	2b	172	ILE
33	2b	184	VAL
33	2b	185	ILE
33	2b	190	THR
33	2b	197	VAL
33	2b	200	ILE
33	2b	212	GLN
33	2b	213	LEU
33	2b	224	GLN
33	2b	229	VAL
33	2b	233	SER
34	2c	3	ASN
34	2c	15	THR
34	2c	16	ARG
34	2c	20	SER
34	2c	33	LEU
34	2c	44	GLU
34	2c	49	SER

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Mol	Chain	Res	Type
34	2c	63	ASN
34	2c	82	GLU
34	2c	89	GLU
34	2c	91	LEU
34	2c	115	LEU
34	2c	170	GLN
34	2c	188	LEU
34	2c	192	THR
34	2c	195	VAL
34	2c	198	VAL
35	2d	3	ARG
35	2d	12	CYS
35	2d	17	VAL
35	2d	18	LYS
35	2d	19	LEU
35	2d	21	LEU
35	2d	108	LEU
35	2d	115	ARG
35	2d	127	THR
35	2d	132	ARG
35	2d	135	LEU
35	2d	137	SER
35	2d	141	ARG
35	2d	144	ASP
35	2d	150	GLU
35	2d	155	LEU
35	2d	162	LEU
35	2d	175	SER
35	2d	200	GLU
35	2d	202	LEU
36	2e	18	ARG
36	2e	24	ARG
36	2e	31	LEU
36	2e	41	VAL
36	2e	51	VAL
36	2e	79	GLU
36	2e	120	THR
36	2e	125	SER
36	2e	144	THR
37	2f	30	LEU
37	2f	65	VAL
37	2f	69	GLU

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Mol	Chain	Res	Type
37	2f	72	VAL
37	2f	73	ASN
38	2g	8	GLU
38	2g	9	VAL
38	2g	35	LYS
38	2g	50	ILE
38	2g	75	VAL
38	2g	76	ARG
38	2g	91	VAL
38	2g	115	ARG
38	2g	155	ARG
39	2h	8	ASP
39	2h	26	VAL
39	2h	56	LYS
39	2h	60	ARG
39	2h	99	GLU
39	2h	111	ILE
39	2h	112	LEU
39	2h	129	VAL
40	2i	7	THR
40	2i	16	ARG
40	2i	20	ARG
40	2i	48	GLU
40	2i	54	ASP
40	2i	56	LEU
40	2i	64	THR
40	2i	75	ASP
40	2i	86	VAL
40	2i	103	THR
40	2i	104	ARG
40	2i	124	GLN
40	2i	128	ARG
41	2j	13	HIS
41	2j	16	LEU
41	2j	17	ASP
41	2j	35	SER
41	2j	46	ARG
41	2j	54	PHE
41	2j	81	THR
41	2j	92	THR
41	2j	96	ILE
42	2k	26	ASN

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Mol	Chain	Res	Type
42	2k	28	THR
42	2k	33	THR
42	2k	50	TYR
42	2k	87	THR
42	2k	109	VAL
43	2l	13	LYS
43	2l	18	VAL
43	2l	24	VAL
43	2l	61	THR
43	2l	66	VAL
43	2l	91	LYS
44	2m	20	THR
44	2m	82	MET
44	2m	103	THR
44	2m	109	THR
45	2n	11	LYS
45	2n	12	ARG
45	2n	13	THR
45	2n	17	LYS
45	2n	22	THR
45	2n	32	SER
45	2n	33	VAL
45	2n	42	ILE
46	2o	3	ILE
46	2o	38	ARG
46	2o	39	LEU
46	2o	64	ARG
46	2o	84	LYS
47	2p	5	ARG
47	2p	20	VAL
47	2p	45	THR
47	2p	53	VAL
47	2p	55	ARG
47	2p	67	THR
47	2p	74	LEU
48	2q	3	LYS
48	2q	7	THR
48	2q	31	LEU
48	2q	36	ILE
48	2q	63	ARG
48	2q	76	LEU
48	2q	83	ASP

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Mol	Chain	Res	Type
48	2q	86	GLU
48	2q	89	LEU
48	2q	96	GLU
49	2r	34	TYR
49	2r	37	VAL
49	2r	45	SER
49	2r	55	ARG
49	2r	58	LEU
49	2r	74	ARG
49	2r	82	THR
49	2r	85	LEU
49	2r	87	ARG
50	2s	5	LEU
50	2s	20	LEU
50	2s	28	LYS
50	2s	34	TRP
50	2s	43	GLU
50	2s	49	ILE
50	2s	64	GLU
50	2s	66	MET
50	2s	83	HIS
51	2t	8	ARG
51	2t	9	ASN
51	2t	15	ARG
51	2t	41	ILE
51	2t	56	MET
51	2t	68	LYS
51	2t	71	THR
51	2t	93	GLU
51	2t	100	ILE
52	2u	8	THR
54	2w	106	ASP
54	2w	111	ILE
54	2w	115	THR
54	2w	133	ARG
54	2w	144	VAL
54	2w	158	VAL
54	2w	162	VAL
54	2w	172	LYS
54	2w	179	ARG
54	2w	185	VAL
54	2w	196	THR

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Mol	Chain	Res	Type
54	2w	202	LEU
54	2w	204	LYS
54	2w	215	ASP
54	2w	222	MET
54	2w	223	ARG
54	2w	235	THR
54	2w	250	VAL
54	2w	257	SER
54	2w	262	ARG
54	2w	271	SER
54	2w	278	ARG
54	2w	290	LEU
54	2w	295	THR
54	2w	300	GLU
54	2w	302	ILE
54	2w	305	TYR
54	2w	312	VAL
54	2w	313	THR
54	2w	321	THR
54	2w	322	HIS
54	2w	325	GLU
54	2w	333	THR
54	2w	336	LEU
54	2w	339	LEU
54	2w	343	ASP
54	2w	351	LEU
56	2z	8	ILE
56	2z	10	ARG
56	2z	12	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
4	1E	48	GLN
4	1E	143	ASN
5	1F	40	GLN
5	1F	204	ASN
6	1G	66	GLN
6	1G	138	GLN
8	1I	104	GLN
9	1N	131	GLN

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Mol	Chain	Res	Type
10	1O	3	GLN
12	1Q	57	HIS
13	1R	71	GLN
14	1S	38	GLN
15	1T	58	ASN
18	1W	111	HIS
19	1X	31	HIS
21	1Z	34	ASN
21	1Z	50	GLN
21	1Z	65	GLN
21	1Z	73	GLN
22	10	29	GLN
24	12	38	GLN
31	19	34	GLN
33	1b	37	ASN
33	1b	40	HIS
33	1b	78	GLN
33	1b	212	GLN
35	1d	125	HIS
35	1d	129	ASN
36	1e	78	HIS
37	1f	94	GLN
38	1g	13	GLN
38	1g	64	GLN
39	1h	15	ASN
39	1h	82	HIS
40	1i	3	GLN
40	1i	73	GLN
40	1i	124	GLN
41	1j	13	HIS
41	1j	56	HIS
42	1k	38	ASN
42	1k	93	GLN
43	1l	80	HIS
44	1m	92	HIS
45	1n	49	HIS
46	1o	28	GLN
46	1o	62	GLN
47	1p	13	HIS
47	1p	76	GLN
48	1q	26	GLN
54	1w	331	HIS

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Mol	Chain	Res	Type
3	2D	87	ASN
4	2E	48	GLN
4	2E	121	ASN
5	2F	69	HIS
5	2F	75	HIS
5	2F	160	ASN
6	2G	66	GLN
7	2H	74	ASN
7	2H	143	GLN
7	2H	147	ASN
8	2I	11	ASN
8	2I	139	GLN
10	2O	5	GLN
11	2P	68	GLN
12	2Q	123	HIS
13	2R	13	HIS
13	2R	24	GLN
14	2S	38	GLN
15	2T	43	GLN
18	2W	60	ASN
18	2W	111	HIS
20	2Y	6	HIS
21	2Z	73	GLN
21	2Z	121	HIS
21	2Z	151	HIS
22	20	29	GLN
24	22	38	GLN
31	29	34	GLN
33	2b	135	GLN
33	2b	212	GLN
34	2c	69	HIS
34	2c	110	ASN
34	2c	123	GLN
34	2c	136	GLN
34	2c	181	ASN
35	2d	42	GLN
35	2d	45	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
36	2e	73	ASN
37	2f	7	ASN

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Mol	Chain	Res	Type
37	2f	13	ASN
37	2f	57	GLN
37	2f	73	ASN
38	2g	13	GLN
38	2g	28	ASN
38	2g	86	GLN
38	2g	97	GLN
40	2i	29	ASN
40	2i	87	GLN
44	2m	77	ASN
44	2m	101	GLN
46	2o	28	GLN
47	2p	76	GLN
49	2r	63	GLN
50	2s	56	GLN
50	2s	57	HIS
50	2s	69	HIS
51	2t	16	HIS
54	2w	253	GLN
54	2w	315	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	465 (16%)	28 (0%)
1	2A	2790/2915 (95%)	490 (17%)	25 (0%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	119/121 (98%)	18 (15%)	0
32	1a	1494/1521 (98%)	318 (21%)	0
32	2a	1498/1521 (98%)	321 (21%)	0
53	1v	11/24 (45%)	3 (27%)	0
53	2v	11/24 (45%)	2 (18%)	0
55	1x	72/76 (94%)	13 (18%)	0
55	1y	70/76 (92%)	22 (31%)	0
55	2x	72/76 (94%)	12 (16%)	0
55	2y	71/76 (93%)	26 (36%)	0
All	All	9190/9466 (97%)	1701 (18%)	53 (0%)

All (1701) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	83	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	140	G
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	199	A
1	1A	200	U
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	229	A
1	1A	230	U
1	1A	233	A
1	1A	248	G
1	1A	250	G
1	1A	266	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	279	C
1	1A	311	A
1	1A	327	G
1	1A	329	G
1	1A	330	A
1	1A	352	G

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Mol	Chain	Res	Type
1	1A	362	U
1	1A	363	G
1	1A	363(B)	G
1	1A	370	G
1	1A	380	U
1	1A	386	G
1	1A	395	U
1	1A	396	G
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	457	A
1	1A	479	A
1	1A	481	G
1	1A	493	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	512	G
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	586	A
1	1A	592	G
1	1A	593	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614	U
1	1A	614(A)	U
1	1A	614(B)	G
1	1A	615	G

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Mol	Chain	Res	Type
1	1A	616	G
1	1A	619	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	651	G
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	740	U
1	1A	775	G
1	1A	776	G
1	1A	778	G
1	1A	782	A
1	1A	784	A
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	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	892	G
1	1A	894	C
1	1A	896	A
1	1A	897	C
1	1A	899	A

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Mol	Chain	Res	Type
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	958	U
1	1A	959	A
1	1A	961	C
1	1A	970	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1005	C
1	1A	1012	U
1	1A	1013	C
1	1A	1020	A
1	1A	1021	A
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1041	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	1060	U
1	1A	1063	G
1	1A	1064	C
1	1A	1071	G
1	1A	1072	C
1	1A	1073	A
1	1A	1077	A
1	1A	1078	U
1	1A	1080	C
1	1A	1081	U
1	1A	1082	U
1	1A	1083	U

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Mol	Chain	Res	Type
1	1A	1085	A
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1092	C
1	1A	1094	U
1	1A	1095	A
1	1A	1096	A
1	1A	1097	U
1	1A	1099	G
1	1A	1100	C
1	1A	1108	U
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1205	U
1	1A	1218	C
1	1A	1220	A
1	1A	1241	A
1	1A	1248	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1309	G
1	1A	1321	A
1	1A	1329	U

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Mol	Chain	Res	Type
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
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	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1465	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1497	U
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1509(B)	A
1	1A	1525	G
1	1A	1539	G
1	1A	1540	U
1	1A	1541	G
1	1A	1543	C
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1583	A
1	1A	1584	C
1	1A	1586	A
1	1A	1607	C
1	1A	1608	A

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Mol	Chain	Res	Type
1	1A	1609	A
1	1A	1610	A
1	1A	1644	C
1	1A	1647	G
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1668	A
1	1A	1669	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1740	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A
1	1A	1816	G
1	1A	1828	G
1	1A	1847	A
1	1A	1878	G
1	1A	1884	A
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1914	C
1	1A	1929	G
1	1A	1930	G
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1964	G
1	1A	1966	A

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Mol	Chain	Res	Type
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2001	A
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
1	1A	2061	G
1	1A	2069	G
1	1A	2093	G
1	1A	2099	U
1	1A	2101	G
1	1A	2113	U
1	1A	2116	G
1	1A	2119	A
1	1A	2122	U
1	1A	2123	G
1	1A	2126	A
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	2138	C
1	1A	2140	C
1	1A	2141	G
1	1A	2142	C
1	1A	2144	U
1	1A	2145	C
1	1A	2146	C

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Mol	Chain	Res	Type
1	1A	2147	G
1	1A	2149	G
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	2160	G
1	1A	2162	G
1	1A	2163	C
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2175	C
1	1A	2176	A
1	1A	2178	C
1	1A	2179	C
1	1A	2180	U
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2190	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2225	A
1	1A	2226	C
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

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Mol	Chain	Res	Type
1	1A	2305	A
1	1A	2308	G
1	1A	2313	C
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2366	A
1	1A	2383	G
1	1A	2384	G
1	1A	2385	C
1	1A	2406	U
1	1A	2410	G
1	1A	2422	A
1	1A	2423	U
1	1A	2424	C
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2438	U
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2460	U
1	1A	2468	G
1	1A	2476	A
1	1A	2477	C
1	1A	2478	A
1	1A	2484	G
1	1A	2487	G
1	1A	2502	G
1	1A	2505	G
1	1A	2507	C
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2554	U

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Mol	Chain	Res	Type
1	1A	2564	A
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2582	G
1	1A	2601	C
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2615	U
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2682	U
1	1A	2689	U
1	1A	2690	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
1	1A	2733	A
1	1A	2758	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2780	G
1	1A	2790	A
1	1A	2791	C
1	1A	2794	C
1	1A	2802	G
1	1A	2803	C
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2839	G
1	1A	2872	G
1	1A	2882	A

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Mol	Chain	Res	Type
1	1A	2894	G
1	1A	2895	U
2	1B	7	G
2	1B	13	A
2	1B	42	C
2	1B	45	A
2	1B	52	A
2	1B	56	G
2	1B	66	A
2	1B	73	A
2	1B	85	G
2	1B	106	G
2	1B	110	G
32	1a	5	U
32	1a	7	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	52	G
32	1a	54	C
32	1a	61	G
32	1a	65	U
32	1a	69	G
32	1a	76	C
32	1a	77	G
32	1a	78	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	122	G
32	1a	129(A)	G
32	1a	131	C
32	1a	144	G
32	1a	155	C

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Mol	Chain	Res	Type
32	1a	156	G
32	1a	157	G
32	1a	158	G
32	1a	161	A
32	1a	162	A
32	1a	163	C
32	1a	167	G
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	185	A
32	1a	189(A)	C
32	1a	189(E)	U
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	223	U
32	1a	231	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	308	C
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	333	G
32	1a	341	C
32	1a	343	U
32	1a	344	A
32	1a	345	C
32	1a	347	G
32	1a	348	G
32	1a	349	A

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Mol	Chain	Res	Type
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	355	C
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	381	C
32	1a	388	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	415	A
32	1a	423	G
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	460	G
32	1a	461	A
32	1a	470	C
32	1a	477	A
32	1a	479	C
32	1a	485	G
32	1a	495	A
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	525	C
32	1a	528	C
32	1a	532	A
32	1a	540	G
32	1a	545	C

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Mol	Chain	Res	Type
32	1a	547	A
32	1a	559	A
32	1a	564	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	590	C
32	1a	596	C
32	1a	618	C
32	1a	621	A
32	1a	630	G
32	1a	641	U
32	1a	650	G
32	1a	653	A
32	1a	659	U
32	1a	665	A
32	1a	671	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	773	G
32	1a	774	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	799	G
32	1a	802	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	819	A
32	1a	821	G
32	1a	828	A
32	1a	836	G
32	1a	839	U

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Mol	Chain	Res	Type
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	859	A
32	1a	870	U
32	1a	872	A
32	1a	876	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	939	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	991	U
32	1a	992	U
32	1a	993	G
32	1a	996	A
32	1a	997	U
32	1a	1000	U
32	1a	1002	G
32	1a	1003	G
32	1a	1004	A
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1011	G
32	1a	1012	U
32	1a	1014	A
32	1a	1016	A
32	1a	1022	G
32	1a	1023	G

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Mol	Chain	Res	Type
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1032	G
32	1a	1036	G
32	1a	1037	C
32	1a	1039	C
32	1a	1040	U
32	1a	1042	G
32	1a	1043	C
32	1a	1044	A
32	1a	1050	G
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1067	A
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1120	G
32	1a	1121	U
32	1a	1122	U
32	1a	1123	A
32	1a	1125	U
32	1a	1126	U
32	1a	1129	C
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1141	C
32	1a	1146	A

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Mol	Chain	Res	Type
32	1a	1150	U
32	1a	1152	A
32	1a	1155	G
32	1a	1159	U
32	1a	1166	G
32	1a	1182	G
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1200	C
32	1a	1201	A
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1217	C
32	1a	1220	G
32	1a	1227	A
32	1a	1228	C
32	1a	1229	A
32	1a	1236	A
32	1a	1238	A
32	1a	1240	U
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1262	C
32	1a	1264	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1298	C
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U

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Mol	Chain	Res	Type
32	1a	1305	G
32	1a	1316	G
32	1a	1319	A
32	1a	1320	C
32	1a	1322	C
32	1a	1332	A
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1360	A
32	1a	1363	C
32	1a	1368	G
32	1a	1370	G
32	1a	1379	G
32	1a	1394	A
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1452	C
32	1a	1460	A
32	1a	1487	G
32	1a	1492	A
32	1a	1493	A
32	1a	1494	G
32	1a	1497	G
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
53	1v	11	U
53	1v	12	A
53	1v	21	A
55	1x	9	A
55	1x	16	U

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Mol	Chain	Res	Type
55	1x	18	G
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	28	G
55	1x	31	A
55	1x	47	U
55	1x	48	C
55	1x	53	G
55	1x	62	C
55	1x	76	A
55	1y	13	C
55	1y	14	A
55	1y	19	G
55	1y	20	U
55	1y	22	G
55	1y	26	A
55	1y	27	G
55	1y	31	A
55	1y	41	C
55	1y	44	G
55	1y	45	U
55	1y	46	G7M
55	1y	48	C
55	1y	49	C
55	1y	53	G
55	1y	58	A
55	1y	59	U
55	1y	65	G
55	1y	68	C
55	1y	71	G
55	1y	72	C
55	1y	73	A
1	2A	33	U
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	55	G
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G

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Mol	Chain	Res	Type
1	2A	84	A
1	2A	94	C
1	2A	100	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	123	G
1	2A	125	G
1	2A	141	A
1	2A	150	C
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
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	225	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	265	A
1	2A	266	G
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	272(I)	U
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	292	C

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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	338	G
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	371	A
1	2A	373	U
1	2A	386	G
1	2A	388	G
1	2A	396	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	444	C
1	2A	449	A
1	2A	451	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	467	G
1	2A	481	G
1	2A	489	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	551	G

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Mol	Chain	Res	Type
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	592	G
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	643	A
1	2A	644	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	740	U
1	2A	753	C
1	2A	770	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	794	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U

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Mol	Chain	Res	Type
1	2A	857	C
1	2A	859	G
1	2A	867	C
1	2A	874	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	886	C
1	2A	887	A
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	897	C
1	2A	899	A
1	2A	900	A
1	2A	907	U
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	959	A
1	2A	961	C
1	2A	968	G
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G
1	2A	1025	G
1	2A	1027	A
1	2A	1033	U
1	2A	1040	C

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Mol	Chain	Res	Type
1	2A	1041	C
1	2A	1042	G
1	2A	1043	C
1	2A	1116	C
1	2A	1117	G
1	2A	1126	A
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1141	U
1	2A	1142	U
1	2A	1171	G
1	2A	1188	U
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1237	A
1	2A	1250	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1321	A
1	2A	1333	C
1	2A	1342	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1370	C
1	2A	1376	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1402	C
1	2A	1403	C

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Mol	Chain	Res	Type
1	2A	1413	G
1	2A	1416	G
1	2A	1417	C
1	2A	1419	A
1	2A	1427	A
1	2A	1428	C
1	2A	1436	G
1	2A	1437	C
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	1467	C
1	2A	1471	A
1	2A	1478	G
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509(A)	A
1	2A	1509(B)	A
1	2A	1531	C
1	2A	1533	G
1	2A	1547	C
1	2A	1554	A
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1588	C
1	2A	1595	G
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A

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Mol	Chain	Res	Type
1	2A	1610	A
1	2A	1618	A
1	2A	1622	G
1	2A	1639	U
1	2A	1640	C
1	2A	1646	C
1	2A	1647	G
1	2A	1648	C
1	2A	1653	G
1	2A	1654	A
1	2A	1664	A
1	2A	1668	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1741	A
1	2A	1743	C
1	2A	1745(A)	C
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1774	C
1	2A	1780	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1877	A
1	2A	1878	G

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Mol	Chain	Res	Type
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1934	C
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1964	G
1	2A	1965	C
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2021	C
1	2A	2023	G
1	2A	2027	G
1	2A	2030	A
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2080	G
1	2A	2099	U
1	2A	2111	C
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G

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Mol	Chain	Res	Type
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2138	C
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2152	G
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2160	G
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2171	A
1	2A	2172	U
1	2A	2173	A
1	2A	2183	C
1	2A	2185	C
1	2A	2188	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2219	G
1	2A	2225	A
1	2A	2232	U

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Mol	Chain	Res	Type
1	2A	2239	G
1	2A	2248	C
1	2A	2273	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2305	A
1	2A	2307	G
1	2A	2308	G
1	2A	2311	A
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2372	G
1	2A	2377	A
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2406	U
1	2A	2410	G
1	2A	2422	A
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2432	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2449	U
1	2A	2465	C
1	2A	2469	A
1	2A	2473	U

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Mol	Chain	Res	Type
1	2A	2474	C
1	2A	2476	A
1	2A	2477	C
1	2A	2478	A
1	2A	2480	C
1	2A	2487	G
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2549	G
1	2A	2554	U
1	2A	2562	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2574	G
1	2A	2585	U
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2664	G
1	2A	2669	G
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G

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Mol	Chain	Res	Type
1	2A	2753	A
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2775	A
1	2A	2778	A
1	2A	2802	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2880	C
1	2A	2894	G
1	2A	2896	C
1	2A	2897	U
2	2B	7	G
2	2B	12	C
2	2B	13	A
2	2B	15	A
2	2B	21	G
2	2B	24	G
2	2B	40	U
2	2B	45	A
2	2B	48	A
2	2B	56	G
2	2B	63	G
2	2B	67	G
2	2B	70	C
2	2B	73	A
2	2B	88	C
2	2B	91	C
2	2B	110	G
2	2B	118	G
32	2a	5	U
32	2a	8	A
32	2a	9	G
32	2a	22	G
32	2a	31	G

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Mol	Chain	Res	Type
32	2a	32	A
32	2a	39	G
32	2a	41	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	66	G
32	2a	72	C
32	2a	73	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	105	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	142	G
32	2a	146	G
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	189(G)	G
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	220	G
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	279	A
32	2a	281	G

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Mol	Chain	Res	Type
32	2a	289	G
32	2a	316	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	375	U
32	2a	395	C
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	422	C
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	443	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	482	A
32	2a	485	G
32	2a	494	U
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	525	C

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Mol	Chain	Res	Type
32	2a	532	A
32	2a	536	C
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	630	G
32	2a	639	G
32	2a	640	A
32	2a	653	A
32	2a	657	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	691	G
32	2a	693	G
32	2a	701	C
32	2a	702	A
32	2a	708	C
32	2a	716	A
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	733	A
32	2a	734	G
32	2a	753	A
32	2a	755	G
32	2a	759	A
32	2a	793	U
32	2a	794	A
32	2a	810	C
32	2a	815	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	836	G

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Mol	Chain	Res	Type
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	855	G
32	2a	859	A
32	2a	864	A
32	2a	870	U
32	2a	872	A
32	2a	873	A
32	2a	902	G
32	2a	912	C
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	932	C
32	2a	934	C
32	2a	935	A
32	2a	938	A
32	2a	942	G
32	2a	954	G
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	969	A
32	2a	971	G
32	2a	973	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	987	G
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	999	C
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A

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Mol	Chain	Res	Type
32	2a	1005	A
32	2a	1011	G
32	2a	1020	U
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1030(C)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1033	G
32	2a	1034	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C
32	2a	1038	C
32	2a	1040	U
32	2a	1042	G
32	2a	1044	A
32	2a	1046	A
32	2a	1050	G
32	2a	1053	G
32	2a	1064	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1072	G
32	2a	1077	G
32	2a	1080	A
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1099	G
32	2a	1101	A
32	2a	1113	C
32	2a	1115	C
32	2a	1117	G

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Mol	Chain	Res	Type
32	2a	1120	G
32	2a	1122	U
32	2a	1123	A
32	2a	1125	U
32	2a	1126	U
32	2a	1127	G
32	2a	1128	C
32	2a	1129	C
32	2a	1132	C
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1147	C
32	2a	1151	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1171	G
32	2a	1175	G
32	2a	1178	G
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1187	G
32	2a	1188	A
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1202	G
32	2a	1211	U
32	2a	1213	A
32	2a	1214	C
32	2a	1222	G
32	2a	1225	A
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1247	U

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Mol	Chain	Res	Type
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1274	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1282	C
32	2a	1285	A
32	2a	1286	A
32	2a	1287	A
32	2a	1297	C
32	2a	1298	C
32	2a	1299	A
32	2a	1300	G
32	2a	1305	G
32	2a	1312	G
32	2a	1319	A
32	2a	1321	C
32	2a	1322	C
32	2a	1335	C
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U
32	2a	1362	C
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1364	U
32	2a	1377	A
32	2a	1379	G
32	2a	1381	U
32	2a	1383	C
32	2a	1396	A
32	2a	1397	C
32	2a	1398	A
32	2a	1412	C
32	2a	1419	G
32	2a	1434	A

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Mol	Chain	Res	Type
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1487	G
32	2a	1491	G
32	2a	1492	A
32	2a	1493	A
32	2a	1494	G
32	2a	1497	G
32	2a	1499	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	11	U
53	2v	14	A
55	2x	9	A
55	2x	17	C
55	2x	18	G
55	2x	19	G
55	2x	20	U
55	2x	21	A
55	2x	28	G
55	2x	31	A
55	2x	48	C
55	2x	52	G
55	2x	60	U
55	2x	76	A
55	2y	8	4SU
55	2y	11	C
55	2y	13	C
55	2y	15	G
55	2y	19	G
55	2y	20	U

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Mol	Chain	Res	Type
55	2y	21	A
55	2y	23	A
55	2y	24	G
55	2y	25	C
55	2y	27	G
55	2y	30	G
55	2y	33	U
55	2y	41	C
55	2y	42	C
55	2y	44	G
55	2y	45	U
55	2y	46	G7M
55	2y	47	U
55	2y	48	C
55	2y	49	C
55	2y	52	G
55	2y	58	A
55	2y	59	U
55	2y	60	U
55	2y	69	G

All (53) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	278	A
1	1A	548	A
1	1A	573	G
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	887	A
1	1A	895	U
1	1A	974	G
1	1A	1065	U
1	1A	1107	G
1	1A	1174	A
1	1A	1176	G
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A

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Mol	Chain	Res	Type
1	1A	1653	G
1	1A	1663	C
1	1A	2131	G
1	1A	2134	A
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2439	A
1	1A	2601	C
1	1A	2689	U
1	2A	34	C
1	2A	196	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	764	A
1	2A	827	U
1	2A	856	C
1	2A	888	C
1	2A	960	A
1	2A	1026	U
1	2A	1210	A
1	2A	1379	A
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2406	U
1	2A	2689	U

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

78 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	5MC	2a	1404	32	19,22,23	1.60	2 (10%)	26,32,35	1.16	3 (11%)
1	PSU	1A	1917	1	18,21,22	1.42	2 (11%)	21,30,33	2.12	5 (23%)
55	PSU	1y	32	55	18,21,22	1.40	3 (16%)	21,30,33	1.94	3 (14%)
32	5MC	1a	1400	32	19,22,23	1.75	3 (15%)	26,32,35	1.15	2 (7%)
54	MEQ	2w	230	54	8,9,10	0.91	0	5,10,12	0.50	0
55	PSU	1y	39	55	18,21,22	1.38	2 (11%)	21,30,33	1.94	3 (14%)
32	5MC	2a	967	32	19,22,23	1.61	3 (15%)	26,32,35	1.11	2 (7%)
1	5MU	2A	1915	1,57	19,22,23	1.44	5 (26%)	27,32,35	2.14	6 (22%)
1	5MU	1A	1939	1,57	19,22,23	1.46	6 (31%)	27,32,35	2.30	6 (22%)
55	G7M	2y	46	55	20,26,27	1.34	2 (10%)	16,39,42	0.48	0
32	2MG	1a	1207	32	18,26,27	0.88	1 (5%)	16,38,41	1.46	4 (25%)
55	5MU	1y	54	55	19,22,23	1.43	4 (21%)	27,32,35	1.68	6 (22%)
32	2MG	2a	1207	32	18,26,27	0.88	0	16,38,41	1.61	4 (25%)
1	5MU	2A	1939	1,57	19,22,23	1.48	6 (31%)	27,32,35	2.15	6 (22%)
32	5MC	2a	1400	32	19,22,23	1.65	3 (15%)	26,32,35	1.24	4 (15%)
32	UR3	1a	1498	32	19,22,23	1.08	2 (10%)	26,32,35	1.66	4 (15%)
55	4SU	1x	8	55	18,21,22	1.78	5 (27%)	25,30,33	2.16	5 (20%)
55	PSU	2x	32	55	18,21,22	1.37	2 (11%)	21,30,33	2.03	3 (14%)
1	PSU	1A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.12	5 (23%)
32	MA6	2a	1518	32	19,26,27	1.01	2 (10%)	18,38,41	1.97	3 (16%)
32	PSU	2a	516	57,32	18,21,22	1.37	2 (11%)	21,30,33	2.02	5 (23%)
32	5MC	1a	967	32	19,22,23	1.65	3 (15%)	26,32,35	1.14	2 (7%)
55	MIA	1x	37	55	24,31,32	2.23	4 (16%)	22,44,47	2.44	7 (31%)
32	M2G	2a	966	32	20,27,28	1.32	3 (15%)	19,40,43	1.03	2 (10%)
32	4OC	2a	1402	57,32	20,23,24	0.79	0	25,32,35	0.92	0
32	5MC	2a	1407	32	19,22,23	1.59	3 (15%)	26,32,35	1.14	3 (11%)
1	OMG	1A	2251	1,55,57	19,26,27	0.94	1 (5%)	21,38,41	1.14	3 (14%)
32	MA6	1a	1519	32	19,26,27	1.03	2 (10%)	18,38,41	2.04	3 (16%)
1	OMC	2A	1920	1,57	19,22,23	0.82	0	25,31,34	0.89	0
1	PSU	1A	2605	1,57	18,21,22	1.49	4 (22%)	21,30,33	1.99	4 (19%)
55	MIA	1y	37	55	24,31,32	2.22	4 (16%)	22,44,47	2.22	6 (27%)
55	5MU	2x	54	55	19,22,23	1.40	5 (26%)	27,32,35	1.80	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	4OC	1a	1402	57,32	20,23,24	0.80	1 (5%)	25,32,35	0.96	1 (4%)
1	5MC	2A	1962	1,57	19,22,23	1.57	3 (15%)	26,32,35	1.14	2 (7%)
55	PSU	1x	55	55	18,21,22	1.36	2 (11%)	21,30,33	1.98	4 (19%)
1	OMG	2A	2251	1,55,57	19,26,27	0.97	1 (5%)	21,38,41	0.94	1 (4%)
55	G7M	2x	46	55	20,26,27	1.22	2 (10%)	16,39,42	0.64	0
32	G7M	2a	527	32	20,26,27	1.21	2 (10%)	16,39,42	0.66	0
43	0TD	2l	92	43	8,9,10	4.44	2 (25%)	6,11,13	5.67	1 (16%)
55	PSU	2y	39	55	18,21,22	1.42	2 (11%)	21,30,33	1.66	3 (14%)
55	G7M	1y	46	55	20,26,27	1.29	2 (10%)	16,39,42	0.58	0
43	0TD	1l	92	43	8,9,10	4.34	1 (12%)	6,11,13	7.76	1 (16%)
32	UR3	2a	1498	57,32	19,22,23	0.96	0	26,32,35	1.70	2 (7%)
1	5MU	1A	1915	1,57	19,22,23	1.48	5 (26%)	27,32,35	2.11	6 (22%)
55	PSU	1x	32	55	18,21,22	1.38	3 (16%)	21,30,33	2.09	5 (23%)
55	PSU	2y	55	55	18,21,22	1.37	3 (16%)	21,30,33	1.98	3 (14%)
32	5MC	1a	1407	32	19,22,23	1.43	2 (10%)	26,32,35	1.06	2 (7%)
55	5MU	1x	54	55	19,22,23	1.40	4 (21%)	27,32,35	1.78	7 (25%)
1	PSU	2A	1911	1	18,21,22	1.40	3 (16%)	21,30,33	2.10	5 (23%)
55	MIA	2x	37	55	24,31,32	2.31	4 (16%)	22,44,47	2.41	7 (31%)
1	2MA	2A	2503	1,57	17,25,26	1.02	1 (5%)	16,37,40	1.53	3 (18%)
55	PSU	1x	39	55	18,21,22	1.42	2 (11%)	21,30,33	1.86	3 (14%)
32	5MC	1a	1404	32	19,22,23	1.62	3 (15%)	26,32,35	1.10	2 (7%)
55	5MU	2y	54	55	19,22,23	1.44	5 (26%)	27,32,35	2.15	8 (29%)
55	PSU	2x	55	55	18,21,22	1.39	2 (11%)	21,30,33	2.02	3 (14%)
1	OMU	2A	2552	1,57	19,22,23	1.25	3 (15%)	25,31,34	1.90	5 (20%)
55	PSU	2x	39	55	18,21,22	1.40	2 (11%)	21,30,33	1.86	3 (14%)
1	2MA	1A	2503	1,57	17,25,26	1.00	1 (5%)	16,37,40	1.29	2 (12%)
55	4SU	2x	8	55	18,21,22	1.87	5 (27%)	25,30,33	2.04	5 (20%)
1	PSU	2A	2605	1	18,21,22	1.30	2 (11%)	21,30,33	2.08	3 (14%)
32	G7M	1a	527	57,32	20,26,27	1.26	2 (10%)	16,39,42	0.52	0
55	PSU	1y	55	55	18,21,22	1.41	2 (11%)	21,30,33	1.91	3 (14%)
1	5MC	2A	1942	1	19,22,23	1.74	3 (15%)	26,32,35	1.21	2 (7%)
54	MEQ	1w	230	54	8,9,10	1.00	0	5,10,12	0.78	0
1	OMU	1A	2552	1,57	19,22,23	1.27	3 (15%)	25,31,34	1.93	5 (20%)
32	MA6	2a	1519	32	19,26,27	1.01	1 (5%)	18,38,41	2.02	3 (16%)
55	4SU	1y	8	55	18,21,22	1.74	4 (22%)	25,30,33	2.46	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
55	PSU	2y	32	55	18,21,22	1.40	2 (11%)	21,30,33	1.90	3 (14%)
1	5MC	1A	1942	1	19,22,23	1.50	3 (15%)	26,32,35	1.14	3 (11%)
1	OMC	1A	1920	1	19,22,23	0.80	0	25,31,34	1.03	2 (8%)
55	MIA	2y	37	55	24,31,32	2.33	4 (16%)	22,44,47	2.72	6 (27%)
55	4SU	2y	8	55	18,21,22	1.83	6 (33%)	25,30,33	1.67	5 (20%)
55	G7M	1x	46	55	20,26,27	1.26	2 (10%)	16,39,42	0.70	0
32	M2G	1a	966	32	20,27,28	1.37	3 (15%)	19,40,43	1.04	1 (5%)
1	PSU	2A	1917	1	18,21,22	1.36	3 (16%)	21,30,33	2.09	4 (19%)
1	5MC	1A	1962	1,57	19,22,23	1.55	3 (15%)	26,32,35	1.11	2 (7%)
32	MA6	1a	1518	32	19,26,27	1.02	2 (10%)	18,38,41	1.94	3 (16%)
32	PSU	1a	516	57,32	18,21,22	1.40	2 (11%)	21,30,33	2.00	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	PSU	1y	32	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
54	MEQ	2w	230	54	-	2/8/9/11	-
55	PSU	1y	39	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1,57	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
55	G7M	2y	46	55	-	0/3/25/26	0/3/3/3
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
55	5MU	1y	54	55	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	1/5/27/28	0/3/3/3
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
55	PSU	2x	32	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	PSU	2a	516	57,32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	MIA	1x	37	55	-	5/11/33/34	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	4OC	2a	1402	57,32	-	2/9/29/30	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,55,57	-	0/5/27/28	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
1	OMC	2A	1920	1,57	-	0/9/27/28	0/2/2/2
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
55	MIA	1y	37	55	-	4/11/33/34	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	57,32	-	2/9/29/30	0/2/2/2
1	5MC	2A	1962	1,57	-	2/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55,57	-	0/5/27/28	0/3/3/3
55	G7M	2x	46	55	-	3/3/25/26	0/3/3/3
32	G7M	2a	527	32	-	0/3/25/26	0/3/3/3
43	0TD	2l	92	43	-	5/7/12/14	-
55	PSU	2y	39	55	-	0/7/25/26	0/2/2/2
55	G7M	1y	46	55	-	3/3/25/26	0/3/3/3
43	0TD	1l	92	43	-	3/7/12/14	-
32	UR3	2a	1498	57,32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1,57	-	0/7/25/26	0/2/2/2
55	PSU	1x	32	55	-	0/7/25/26	0/2/2/2
55	PSU	2y	55	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	MIA	2x	37	55	-	3/11/33/34	0/3/3/3
1	2MA	2A	2503	1,57	-	2/3/25/26	0/3/3/3
55	PSU	1x	39	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
55	5MU	2y	54	55	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
55	PSU	2x	39	55	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,57	-	2/3/25/26	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	57,32	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	1y	55	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	MEQ	1w	230	54	-	3/8/9/11	-
1	OMU	1A	2552	1,57	-	0/9/27/28	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
55	4SU	1y	8	55	-	0/7/25/26	0/2/2/2
55	PSU	2y	32	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	3/9/27/28	0/2/2/2
55	MIA	2y	37	55	-	2/11/33/34	0/3/3/3
55	4SU	2y	8	55	-	0/7/25/26	0/2/2/2
55	G7M	1x	46	55	-	3/3/25/26	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,57	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	PSU	1a	516	57,32	-	0/7/25/26	0/2/2/2

All (199) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.01	1.70	1.82
43	1l	92	0TD	CB-SB	-11.84	1.70	1.82
55	2y	37	MIA	C2-S10	-7.45	1.69	1.75
55	1x	37	MIA	C2-S10	-7.12	1.69	1.75
55	2x	37	MIA	C13-C14	7.06	1.53	1.32
55	2x	37	MIA	C2-S10	-6.97	1.70	1.75
55	2y	37	MIA	C13-C14	6.91	1.53	1.32
55	1y	37	MIA	C13-C14	6.87	1.53	1.32
55	1x	37	MIA	C13-C14	6.86	1.53	1.32
55	1y	37	MIA	C2-S10	-6.68	1.70	1.75
1	2A	1942	5MC	C5-C4	6.40	1.49	1.44
32	1a	1400	5MC	C5-C4	6.38	1.48	1.44
32	2a	1400	5MC	C5-C4	6.07	1.48	1.44
32	1a	967	5MC	C5-C4	6.03	1.48	1.44
32	1a	1404	5MC	C5-C4	5.88	1.48	1.44
32	2a	967	5MC	C5-C4	5.73	1.48	1.44
32	2a	1407	5MC	C5-C4	5.66	1.48	1.44
1	2A	1962	5MC	C5-C4	5.59	1.48	1.44
32	2a	1404	5MC	C5-C4	5.50	1.48	1.44
1	1A	1962	5MC	C5-C4	5.40	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1942	5MC	C5-C4	5.09	1.48	1.44
55	2x	8	4SU	C4-S4	-4.97	1.59	1.68
55	1y	8	4SU	C4-S4	-4.88	1.60	1.68
55	1x	8	4SU	C4-S4	-4.84	1.60	1.68
32	1a	1407	5MC	C5-C4	4.70	1.47	1.44
55	2y	8	4SU	C4-S4	-4.64	1.60	1.68
55	2x	55	PSU	C6-C5	4.22	1.40	1.35
55	2y	46	G7M	C5-C4	4.09	1.47	1.39
55	1y	32	PSU	C6-C5	4.08	1.39	1.35
32	1a	966	M2G	C2-N3	4.03	1.36	1.30
55	1y	55	PSU	C6-C5	3.98	1.39	1.35
55	2y	32	PSU	C6-C5	3.96	1.39	1.35
1	1A	1911	PSU	C6-C5	3.91	1.39	1.35
55	1y	46	G7M	C5-C4	3.88	1.46	1.39
55	1x	39	PSU	C6-C5	3.88	1.39	1.35
1	1A	1917	PSU	C6-C5	3.88	1.39	1.35
32	1a	516	PSU	C6-C5	3.85	1.39	1.35
32	2a	966	M2G	C2-N3	3.84	1.36	1.30
55	2y	39	PSU	C6-C5	3.79	1.39	1.35
55	1x	46	G7M	C5-C4	3.77	1.46	1.39
32	1a	527	G7M	C5-C4	3.71	1.46	1.39
55	2y	55	PSU	C6-C5	3.69	1.39	1.35
55	2x	46	G7M	C5-C4	3.68	1.46	1.39
55	2x	39	PSU	C6-C5	3.67	1.39	1.35
55	2x	32	PSU	C6-C5	3.65	1.39	1.35
55	1y	39	PSU	C6-C5	3.65	1.39	1.35
32	2a	516	PSU	C6-C5	3.57	1.39	1.35
32	2a	527	G7M	C5-C4	3.53	1.46	1.39
55	2x	37	MIA	C6-C5	3.52	1.50	1.44
1	2A	1911	PSU	C6-C5	3.51	1.39	1.35
55	1x	55	PSU	C6-C5	3.44	1.39	1.35
1	2A	2605	PSU	C6-C5	3.41	1.39	1.35
1	2A	1917	PSU	C6-C5	3.37	1.39	1.35
55	2y	8	4SU	C4-N3	-3.34	1.34	1.37
1	1A	1915	5MU	C6-C5	3.26	1.39	1.34
32	2a	1404	5MC	C6-C5	3.17	1.39	1.34
55	1x	32	PSU	C6-C5	3.16	1.38	1.35
1	1A	2605	PSU	C6-C5	3.15	1.38	1.35
55	2x	8	4SU	C5-C4	-3.14	1.38	1.42
1	1A	2605	PSU	C4-N3	-3.13	1.33	1.38
55	1x	8	4SU	C4-N3	-3.06	1.34	1.37
55	1y	37	MIA	C6-C5	3.05	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	8	4SU	C4-N3	-3.04	1.34	1.37
1	2A	1939	5MU	C6-C5	3.00	1.39	1.34
32	1a	1407	5MC	C6-C5	2.98	1.39	1.34
55	2y	37	MIA	C6-C5	2.96	1.49	1.44
55	1x	54	5MU	C6-C5	2.95	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.93	1.33	1.38
55	1y	54	5MU	C6-C5	2.92	1.39	1.34
1	2A	1915	5MU	C2-N1	2.91	1.43	1.38
32	2a	967	5MC	C6-C5	2.90	1.39	1.34
32	1a	966	M2G	C2-N2	2.89	1.40	1.35
1	1A	1915	5MU	C4-N3	-2.89	1.33	1.38
55	2y	54	5MU	C6-C5	2.88	1.39	1.34
55	2y	54	5MU	C4-C5	2.87	1.49	1.44
1	2A	1942	5MC	C6-C5	2.86	1.39	1.34
1	1A	1939	5MU	C6-C5	2.85	1.39	1.34
1	2A	2552	OMU	C4-N3	-2.83	1.33	1.38
1	2A	1915	5MU	C6-C5	2.82	1.39	1.34
55	2x	54	5MU	C4-N3	-2.82	1.33	1.38
32	2a	966	M2G	C2-N2	2.81	1.40	1.35
1	2A	1911	PSU	C4-N3	-2.80	1.33	1.38
32	1a	1400	5MC	C6-C5	2.79	1.39	1.34
55	2y	39	PSU	C4-N3	-2.78	1.33	1.38
1	1A	1942	5MC	C6-C5	2.77	1.39	1.34
55	1x	32	PSU	C4-N3	-2.77	1.33	1.38
32	2a	1407	5MC	C6-C5	2.74	1.39	1.34
1	2A	2251	OMG	C6-N1	-2.70	1.33	1.37
55	1y	8	4SU	C4-N3	-2.70	1.34	1.37
55	2y	54	5MU	C2-N1	2.68	1.42	1.38
55	1x	54	5MU	C4-N3	-2.68	1.33	1.38
55	2x	54	5MU	C6-C5	2.67	1.39	1.34
55	1x	8	4SU	C5-C4	-2.67	1.39	1.42
1	2A	1917	PSU	C4-N3	-2.66	1.33	1.38
1	2A	2605	PSU	C4-N3	-2.65	1.33	1.38
1	1A	1962	5MC	C6-N1	-2.64	1.33	1.38
1	2A	1962	5MC	C6-C5	2.64	1.38	1.34
55	1x	39	PSU	C4-N3	-2.63	1.33	1.38
55	2y	8	4SU	C5-C4	-2.63	1.39	1.42
55	2y	55	PSU	C4-N3	-2.62	1.33	1.38
55	1x	55	PSU	C4-N3	-2.62	1.33	1.38
32	2a	516	PSU	C4-N3	-2.61	1.34	1.38
55	1y	8	4SU	C5-C4	-2.60	1.39	1.42
1	1A	2552	OMU	C4-N3	-2.57	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1404	5MC	C6-C5	2.57	1.38	1.34
55	1x	37	MIA	C6-C5	2.56	1.48	1.44
1	1A	1917	PSU	C4-N3	-2.56	1.34	1.38
55	1y	39	PSU	C4-N3	-2.54	1.34	1.38
1	1A	2251	OMG	C6-N1	-2.54	1.33	1.37
32	1a	967	5MC	C6-C5	2.53	1.38	1.34
1	1A	1939	5MU	C4-N3	-2.51	1.34	1.38
55	1y	54	5MU	C4-C5	2.51	1.48	1.44
32	1a	527	G7M	C6-N1	-2.50	1.34	1.37
1	1A	1939	5MU	C6-N1	-2.49	1.33	1.38
32	1a	516	PSU	C4-N3	-2.49	1.34	1.38
32	2a	1400	5MC	C6-C5	2.49	1.38	1.34
32	1a	1518	MA6	C6-C5	-2.48	1.41	1.44
32	1a	1498	UR3	C2-N1	2.48	1.41	1.38
55	2x	32	PSU	C4-N3	-2.46	1.34	1.38
55	1y	54	5MU	C2-N1	2.45	1.42	1.38
1	2A	1939	5MU	C6-N1	-2.44	1.33	1.38
32	1a	1404	5MC	C6-N1	-2.44	1.33	1.38
55	1y	54	5MU	C4-N3	-2.41	1.34	1.38
1	2A	1915	5MU	C4-C5	2.41	1.48	1.44
55	2x	39	PSU	C4-N3	-2.41	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.40	1.34	1.38
55	2y	8	4SU	C2-N1	2.40	1.42	1.38
32	2a	1518	MA6	C6-C5	-2.39	1.41	1.44
55	2x	8	4SU	C2-N1	2.38	1.42	1.38
32	2a	1519	MA6	C6-C5	-2.37	1.41	1.44
1	2A	2552	OMU	C2-N3	-2.36	1.33	1.38
55	2y	32	PSU	C4-N3	-2.36	1.34	1.38
1	1A	1939	5MU	C2-N1	2.35	1.42	1.38
1	2A	1939	5MU	C2-N3	-2.34	1.33	1.38
32	1a	1519	MA6	C6-C5	-2.34	1.41	1.44
55	2x	54	5MU	C2-N3	-2.33	1.33	1.38
1	1A	2552	OMU	C5-C4	-2.32	1.38	1.43
55	1y	8	4SU	C2-N1	2.31	1.42	1.38
1	1A	1939	5MU	C2-N3	-2.31	1.33	1.38
32	2a	966	M2G	C6-N1	-2.31	1.34	1.37
32	2a	1400	5MC	C6-N1	-2.30	1.34	1.38
55	2x	54	5MU	C4-C5	2.30	1.48	1.44
32	2a	527	G7M	C6-N1	-2.29	1.34	1.37
1	2A	1939	5MU	C4-C5	2.29	1.48	1.44
1	1A	2605	PSU	C2-N3	-2.27	1.33	1.37
1	1A	1915	5MU	C4-C5	2.27	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	967	5MC	C6-N1	-2.27	1.34	1.38
1	1A	1962	5MC	C6-C5	2.26	1.38	1.34
43	2l	92	0TD	CB-CA	2.26	1.55	1.54
1	1A	2552	OMU	C2-N3	-2.26	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.25	1.34	1.38
1	1A	1911	PSU	C4-N3	-2.25	1.34	1.38
55	2y	54	5MU	C4-N3	-2.25	1.34	1.38
55	1y	46	G7M	C6-N1	-2.25	1.34	1.37
55	1x	54	5MU	C4-C5	2.24	1.48	1.44
55	2y	37	MIA	C6-N1	2.24	1.36	1.33
1	1A	1915	5MU	C2-N1	2.23	1.41	1.38
1	1A	1942	5MC	C6-N1	-2.22	1.34	1.38
55	1y	32	PSU	C4-N3	-2.22	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.22	1.34	1.38
55	2x	55	PSU	C4-N3	-2.21	1.34	1.38
55	1y	55	PSU	C4-N3	-2.21	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.20	1.34	1.37
55	1x	54	5MU	C2-N1	2.20	1.41	1.38
55	2y	8	4SU	C2-N3	-2.19	1.34	1.38
55	2y	46	G7M	C6-N1	-2.19	1.34	1.37
55	1x	8	4SU	C2-N1	2.18	1.41	1.38
32	1a	1498	UR3	C6-C5	2.16	1.40	1.35
1	1A	1915	5MU	C2-N3	-2.15	1.34	1.38
55	2x	46	G7M	C6-N1	-2.12	1.34	1.37
55	2x	54	5MU	C6-N1	-2.11	1.34	1.38
32	2a	1518	MA6	C6-N1	2.11	1.35	1.32
1	2A	2552	OMU	C5-C4	-2.11	1.39	1.43
1	2A	1942	5MC	C6-N1	-2.10	1.34	1.38
1	2A	1939	5MU	C2-N1	2.10	1.41	1.38
55	2y	54	5MU	C6-N1	-2.09	1.34	1.38
1	1A	1939	5MU	C4-C5	2.09	1.48	1.44
55	1x	8	4SU	C2-N3	-2.09	1.34	1.38
55	1x	46	G7M	C6-N1	-2.08	1.34	1.37
1	2A	2503	2MA	C6-N1	-2.07	1.33	1.37
32	2a	967	5MC	C6-N1	-2.07	1.34	1.38
1	1A	2605	PSU	C2-N1	-2.07	1.34	1.36
55	2x	8	4SU	C2-N3	-2.07	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.07	1.34	1.38
55	1x	32	PSU	C2-N3	-2.05	1.34	1.37
55	2x	37	MIA	C6-N1	2.05	1.35	1.33
32	1a	1518	MA6	C6-N1	2.04	1.35	1.32
1	1A	2503	2MA	C6-N6	2.04	1.35	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2y	8	4SU	O2-C2	2.04	1.26	1.23
1	2A	1911	PSU	C2-N3	-2.04	1.34	1.37
1	2A	1917	PSU	C2-N3	-2.03	1.34	1.37
32	1a	966	M2G	C6-N1	-2.03	1.34	1.37
55	2y	55	PSU	C4-C5	2.03	1.50	1.44
55	1y	37	MIA	C6-N1	2.02	1.35	1.33
55	1y	32	PSU	C4-C5	2.01	1.49	1.44
32	1a	1402	4OC	C6-N1	-2.01	1.33	1.38
32	1a	1519	MA6	C6-N1	2.01	1.35	1.32
32	2a	1407	5MC	C6-N1	-2.01	1.34	1.38
55	1x	37	MIA	C6-N1	2.01	1.35	1.33

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	18.90	136.33	102.36
43	2l	92	0TD	CSB-SB-CB	13.78	127.14	102.36
55	2y	37	MIA	C12-C13-C14	-8.81	111.21	127.01
55	1x	37	MIA	C12-C13-C14	-8.09	112.49	127.01
55	2x	37	MIA	C12-C13-C14	-7.78	113.04	127.01
55	1y	8	4SU	C4-N3-C2	-7.51	120.12	127.31
32	2a	1498	UR3	C4-N3-C2	-6.92	119.01	124.58
55	1y	37	MIA	C12-C13-C14	-6.81	114.79	127.01
1	1A	1917	PSU	N1-C2-N3	6.76	122.30	115.17
1	2A	1911	PSU	N1-C2-N3	6.68	122.21	115.17
1	2A	1917	PSU	N1-C2-N3	6.55	122.07	115.17
32	1a	1498	UR3	C4-N3-C2	-6.35	119.47	124.58
55	1x	32	PSU	N1-C2-N3	6.34	121.86	115.17
55	2x	32	PSU	N1-C2-N3	6.31	121.82	115.17
55	1x	8	4SU	C4-N3-C2	-6.31	121.27	127.31
1	1A	1911	PSU	N1-C2-N3	6.29	121.80	115.17
55	1y	8	4SU	C5-C4-N3	6.20	120.52	114.75
55	2y	55	PSU	N1-C2-N3	6.18	121.69	115.17
32	1a	516	PSU	N1-C2-N3	6.17	121.68	115.17
1	2A	2605	PSU	N1-C2-N3	6.16	121.67	115.17
55	1y	55	PSU	N1-C2-N3	6.15	121.66	115.17
32	2a	516	PSU	N1-C2-N3	6.12	121.63	115.17
55	1y	32	PSU	N1-C2-N3	6.10	121.60	115.17
55	1x	55	PSU	N1-C2-N3	6.09	121.60	115.17
55	2x	55	PSU	N1-C2-N3	6.09	121.59	115.17
55	2y	32	PSU	N1-C2-N3	6.08	121.58	115.17
1	1A	2605	PSU	N1-C2-N3	6.06	121.56	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1y	39	PSU	N1-C2-N3	5.97	121.47	115.17
55	1x	39	PSU	N1-C2-N3	5.89	121.38	115.17
32	2a	1518	MA6	N3-C2-N1	-5.77	120.84	128.67
55	1x	8	4SU	C5-C4-N3	5.68	120.03	114.75
55	2y	37	MIA	C11-S10-C2	-5.63	98.03	102.25
32	2a	1519	MA6	N3-C2-N1	-5.61	121.06	128.67
55	2x	39	PSU	N1-C2-N3	5.60	121.08	115.17
32	1a	1518	MA6	N3-C2-N1	-5.59	121.08	128.67
1	2A	1939	5MU	N3-C2-N1	5.57	122.14	114.89
1	1A	1939	5MU	O4-C4-C5	-5.50	118.62	124.92
1	1A	1939	5MU	C5-C4-N3	5.49	120.10	115.32
1	1A	1915	5MU	N3-C2-N1	5.45	121.98	114.89
1	1A	1939	5MU	C4-N3-C2	-5.42	120.23	127.34
55	2x	8	4SU	C5-C4-N3	5.42	119.79	114.75
55	2y	39	PSU	N1-C2-N3	5.31	120.77	115.17
32	1a	1519	MA6	N3-C2-N1	-5.28	121.51	128.67
55	2y	54	5MU	C4-N3-C2	-5.26	120.44	127.34
1	2A	1939	5MU	C4-N3-C2	-5.26	120.44	127.34
1	2A	2552	OMU	C4-N3-C2	-5.24	120.10	126.61
1	1A	1915	5MU	C4-N3-C2	-5.18	120.55	127.34
55	2y	54	5MU	N3-C2-N1	5.14	121.58	114.89
1	2A	1915	5MU	C4-N3-C2	-5.12	120.63	127.34
1	1A	2552	OMU	C4-N3-C2	-5.00	120.40	126.61
1	2A	1915	5MU	N3-C2-N1	4.94	121.32	114.89
32	1a	1519	MA6	C2-N1-C6	4.93	121.67	116.84
55	2y	8	4SU	C5-C4-N3	4.85	119.26	114.75
32	1a	1518	MA6	C2-N1-C6	4.83	121.58	116.84
55	1y	8	4SU	C5-C4-S4	-4.80	118.82	124.31
55	2x	8	4SU	C4-N3-C2	-4.76	122.76	127.31
32	2a	1518	MA6	C2-N1-C6	4.70	121.45	116.84
55	2x	8	4SU	C5-C4-S4	-4.67	118.97	124.31
55	1x	54	5MU	N3-C2-N1	4.66	120.95	114.89
32	2a	1519	MA6	C2-N1-C6	4.61	121.36	116.84
1	2A	1915	5MU	C5-C4-N3	4.49	119.23	115.32
55	2x	54	5MU	N3-C2-N1	4.49	120.74	114.89
1	1A	1915	5MU	C5-C4-N3	4.47	119.21	115.32
1	2A	1915	5MU	O4-C4-C5	-4.42	119.86	124.92
1	2A	2605	PSU	C4-N3-C2	-4.42	120.29	126.37
1	2A	1917	PSU	C4-N3-C2	-4.39	120.33	126.37
1	2A	1911	PSU	C4-N3-C2	-4.38	120.33	126.37
1	1A	1939	5MU	N3-C2-N1	4.37	120.58	114.89
1	1A	1939	5MU	C5-C6-N1	-4.34	118.60	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1917	PSU	C4-N3-C2	-4.30	120.44	126.37
55	1x	32	PSU	C4-N3-C2	-4.30	120.45	126.37
1	2A	2552	OMU	N3-C2-N1	4.29	120.48	114.89
55	2y	54	5MU	C5-C4-N3	4.29	119.05	115.32
1	1A	1911	PSU	C4-N3-C2	-4.29	120.46	126.37
1	1A	1911	PSU	O2-C2-N1	-4.21	118.44	122.79
32	2a	516	PSU	C4-N3-C2	-4.19	120.60	126.37
1	1A	2552	OMU	N3-C2-N1	4.18	120.33	114.89
55	1y	37	MIA	C15-C14-C13	-4.17	110.14	122.66
1	1A	2552	OMU	C5-C4-N3	4.17	120.64	114.80
32	1a	516	PSU	C4-N3-C2	-4.16	120.64	126.37
55	1y	8	4SU	N3-C2-N1	4.15	120.30	114.89
1	2A	2552	OMU	C5-C4-N3	4.13	120.59	114.80
1	2A	1939	5MU	C5-C4-N3	4.11	118.90	115.32
55	2x	54	5MU	C4-N3-C2	-4.10	121.97	127.34
55	1x	37	MIA	C16-C14-C13	-4.08	110.40	122.66
55	1y	54	5MU	N3-C2-N1	4.06	120.18	114.89
55	2x	32	PSU	C4-N3-C2	-3.99	120.88	126.37
1	2A	2503	2MA	C4-N3-C2	-3.95	120.27	123.30
55	2x	55	PSU	C4-N3-C2	-3.95	120.93	126.37
55	2y	55	PSU	C4-N3-C2	-3.93	120.96	126.37
1	2A	1939	5MU	C5-C6-N1	-3.92	119.06	123.31
55	1y	39	PSU	C4-N3-C2	-3.92	120.97	126.37
1	1A	2605	PSU	C4-N3-C2	-3.91	120.99	126.37
55	1x	8	4SU	C5-C4-S4	-3.89	119.87	124.31
55	2y	8	4SU	C4-N3-C2	-3.88	123.59	127.31
55	1x	55	PSU	C4-N3-C2	-3.86	121.05	126.37
55	2x	32	PSU	O2-C2-N1	-3.86	118.81	122.79
55	2y	37	MIA	C15-C14-C13	-3.86	111.08	122.66
1	1A	1915	5MU	C5-C6-N1	-3.86	119.12	123.31
1	2A	1939	5MU	O4-C4-C5	-3.85	120.52	124.92
55	2y	54	5MU	O4-C4-C5	-3.85	120.52	124.92
55	1y	55	PSU	O2-C2-N1	-3.83	118.83	122.79
55	1x	8	4SU	N3-C2-N1	3.81	119.86	114.89
32	1a	1404	5MC	C5-C6-N1	-3.80	119.19	123.31
55	1y	32	PSU	C4-N3-C2	-3.78	121.16	126.37
32	2a	1207	2MG	N1-C2-N2	3.77	120.41	116.56
55	1x	54	5MU	C4-N3-C2	-3.73	122.45	127.34
55	2y	37	MIA	C16-C14-C13	-3.72	111.50	122.66
1	1A	2552	OMU	O4-C4-C5	-3.71	118.77	125.16
1	1A	1915	5MU	O4-C4-C5	-3.68	120.70	124.92
1	2A	1942	5MC	C5-C6-N1	-3.67	119.33	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	37	MIA	C4-C5-N7	-3.64	105.49	109.34
55	2x	37	MIA	C16-C14-C13	-3.63	111.77	122.66
32	1a	1519	MA6	C4-C5-N7	-3.62	105.52	109.34
55	1x	39	PSU	C4-N3-C2	-3.61	121.40	126.37
55	1x	32	PSU	O2-C2-N1	-3.58	119.09	122.79
55	2x	54	5MU	C5-C4-N3	3.54	118.40	115.32
55	1x	55	PSU	O2-C2-N1	-3.53	119.15	122.79
55	2y	32	PSU	C4-N3-C2	-3.52	121.53	126.37
55	1x	37	MIA	C15-C14-C13	-3.50	112.14	122.66
55	2x	37	MIA	C15-C14-C13	-3.50	112.17	122.66
55	2x	39	PSU	C4-N3-C2	-3.46	121.61	126.37
55	2x	39	PSU	O2-C2-N1	-3.43	119.25	122.79
32	2a	1400	5MC	C5-C6-N1	-3.40	119.62	123.31
55	1y	37	MIA	C16-C14-C13	-3.39	112.48	122.66
55	2y	32	PSU	O2-C2-N1	-3.39	119.29	122.79
1	2A	1962	5MC	C5-C6-N1	-3.38	119.64	123.31
1	1A	2605	PSU	O2-C2-N1	-3.38	119.30	122.79
55	2x	55	PSU	O2-C2-N1	-3.38	119.30	122.79
32	1a	967	5MC	C5-C6-N1	-3.38	119.65	123.31
32	2a	967	5MC	C5-C6-N1	-3.36	119.66	123.31
55	1y	54	5MU	C4-N3-C2	-3.33	122.98	127.34
55	1y	55	PSU	C4-N3-C2	-3.32	121.80	126.37
32	2a	1498	UR3	C5-C4-N3	3.28	119.36	115.04
1	1A	1917	PSU	O2-C2-N1	-3.26	119.42	122.79
55	1y	32	PSU	O2-C2-N1	-3.26	119.42	122.79
1	2A	1915	5MU	C5-C6-N1	-3.24	119.79	123.31
55	2x	54	5MU	O4-C4-C5	-3.21	121.24	124.92
32	2a	1519	MA6	C4-C5-N7	-3.19	105.96	109.34
1	1A	2503	2MA	C4-N3-C2	-3.18	120.86	123.30
55	2y	55	PSU	O2-C2-N1	-3.18	119.51	122.79
1	2A	1917	PSU	O2-C2-N1	-3.17	119.52	122.79
55	1x	54	5MU	O4-C4-C5	-3.17	121.29	124.92
55	1y	54	5MU	O4-C4-C5	-3.16	121.30	124.92
32	1a	966	M2G	C8-N7-C5	3.15	107.92	102.55
32	1a	1400	5MC	C5-C6-N1	-3.14	119.90	123.31
55	2x	54	5MU	C5-C6-N1	-3.14	119.90	123.31
32	2a	1404	5MC	C5-C6-N1	-3.11	119.93	123.31
32	2a	1404	5MC	C5-C4-N3	-3.11	118.57	121.75
55	2y	54	5MU	C5-C6-N1	-3.10	119.94	123.31
32	2a	1407	5MC	C5-C4-N3	-3.10	118.57	121.75
1	1A	1942	5MC	C5-C6-N1	-3.09	119.96	123.31
55	1y	54	5MU	C5-C4-N3	3.09	118.01	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1942	5MC	C5-C4-N3	-3.09	118.59	121.75
55	1y	39	PSU	O2-C2-N1	-3.08	119.61	122.79
32	1a	1207	2MG	C8-N7-C5	3.05	107.74	102.55
55	2x	8	4SU	C1'-N1-C2	3.05	123.06	117.59
32	1a	1498	UR3	C5-C4-N3	2.99	118.97	115.04
55	1x	37	MIA	C4-C5-N7	-2.96	106.21	109.34
1	2A	2503	2MA	C8-N7-C5	2.96	107.59	102.55
55	1x	54	5MU	C5-C4-N3	2.95	117.89	115.32
55	2y	39	PSU	C4-N3-C2	-2.95	122.30	126.37
55	1y	37	MIA	C2-N1-C6	2.95	122.66	117.42
32	1a	1407	5MC	C5-C4-N3	-2.94	118.74	121.75
1	2A	1911	PSU	O2-C2-N1	-2.93	119.76	122.79
1	2A	2552	OMU	O4-C4-C5	-2.92	120.12	125.16
1	2A	2605	PSU	O2-C2-N1	-2.92	119.78	122.79
32	2a	1207	2MG	N2-C2-N3	-2.90	116.81	120.51
55	1y	37	MIA	C4-C5-N7	-2.88	106.30	109.34
32	2a	1207	2MG	C8-N7-C5	2.87	107.44	102.55
1	1A	1942	5MC	C5-C4-N3	-2.87	118.81	121.75
55	2y	37	MIA	C2-N1-C6	2.87	122.52	117.42
32	1a	1400	5MC	C5-C4-N3	-2.86	118.82	121.75
1	1A	1962	5MC	C5-C6-N1	-2.86	120.20	123.31
55	2y	8	4SU	C5-C4-S4	-2.84	121.06	124.31
1	1A	2251	OMG	C8-N7-C5	2.83	107.37	102.55
32	2a	516	PSU	O2-C2-N1	-2.83	119.87	122.79
32	2a	1518	MA6	C4-C5-N7	-2.83	106.35	109.34
32	2a	966	M2G	C8-N7-C5	2.82	107.34	102.55
32	1a	516	PSU	O2-C2-N1	-2.81	119.89	122.79
55	1x	39	PSU	O2-C2-N1	-2.80	119.90	122.79
55	2x	37	MIA	C11-S10-C2	-2.78	100.16	102.25
1	2A	2552	OMU	O2-C2-N1	-2.77	119.20	122.80
1	1A	2503	2MA	C8-N7-C5	2.76	107.25	102.55
55	1x	37	MIA	C2-N1-C6	2.76	122.32	117.42
55	1y	54	5MU	C5M-C5-C4	2.74	121.71	118.78
32	2a	1407	5MC	C5-C6-N1	-2.71	120.37	123.31
55	2y	54	5MU	O2-C2-N1	-2.69	119.30	122.80
55	2x	8	4SU	N3-C2-N1	2.67	118.37	114.89
32	1a	1207	2MG	N1-C2-N2	2.65	119.27	116.56
1	1A	1915	5MU	O2-C2-N1	-2.65	119.35	122.80
32	1a	967	5MC	C5-C4-N3	-2.64	119.04	121.75
55	2y	8	4SU	N3-C2-N1	2.64	118.33	114.89
1	1A	2605	PSU	C5-C6-N1	-2.63	118.50	122.14
1	2A	1939	5MU	O2-C2-N1	-2.61	119.39	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	37	MIA	C2-N1-C6	2.56	121.97	117.42
32	1a	1207	2MG	N2-C2-N3	-2.55	117.26	120.51
55	1x	37	MIA	C11-S10-C2	-2.55	100.34	102.25
32	1a	1498	UR3	C6-N1-C2	-2.55	119.72	121.80
32	2a	967	5MC	C5-C4-N3	-2.54	119.15	121.75
1	2A	1962	5MC	C5-C4-N3	-2.53	119.16	121.75
55	2y	37	MIA	C4-C5-N7	-2.52	106.67	109.34
1	1A	2251	OMG	C5-C6-N1	2.52	118.87	114.07
1	1A	1920	OMC	C1'-N1-C2	2.51	123.98	118.44
55	1x	54	5MU	O2-C2-N1	-2.45	119.60	122.80
1	2A	2251	OMG	C8-N7-C5	2.45	106.73	102.55
55	1y	37	MIA	N3-C2-N1	-2.41	122.63	127.03
32	1a	1402	4OC	C6-C5-C4	2.39	119.88	117.00
55	2y	54	5MU	C5M-C5-C4	2.38	121.32	118.78
32	2a	516	PSU	O4'-C1'-C2'	2.36	108.42	105.15
55	1x	37	MIA	N3-C2-N1	-2.36	122.72	127.03
55	1x	32	PSU	C5-C6-N1	-2.35	118.88	122.14
32	2a	1400	5MC	C1'-N1-C6	-2.34	117.30	121.15
1	1A	1920	OMC	O2-C2-N3	-2.34	118.64	122.33
55	2y	39	PSU	O2-C2-N1	-2.34	120.38	122.79
1	2A	1911	PSU	C5-C6-N1	-2.33	118.90	122.14
55	2y	8	4SU	C1'-N1-C2	2.33	121.77	117.59
1	1A	2552	OMU	O2-C2-N1	-2.32	119.78	122.80
32	1a	1407	5MC	O2-C2-N3	-2.32	118.68	122.33
32	1a	1518	MA6	C4-C5-N7	-2.31	106.89	109.34
32	2a	1400	5MC	C5-C4-N3	-2.31	119.39	121.75
55	2x	37	MIA	N3-C2-N1	-2.30	122.83	127.03
32	1a	1404	5MC	C5-C4-N3	-2.29	119.41	121.75
32	1a	516	PSU	C5-C6-N1	-2.28	118.98	122.14
1	1A	1917	PSU	C5-C6-N1	-2.27	118.98	122.14
55	1y	8	4SU	O2-C2-N1	-2.27	119.85	122.80
1	1A	1911	PSU	C5-C6-N1	-2.25	119.02	122.14
1	2A	2503	2MA	O4'-C1'-N9	-2.24	105.77	108.75
1	2A	1917	PSU	C5-C6-N1	-2.23	119.05	122.14
1	1A	2251	OMG	O6-C6-C5	-2.20	119.96	124.32
32	2a	1407	5MC	O2-C2-N3	-2.20	118.87	122.33
55	1x	32	PSU	O4'-C1'-C2'	2.19	108.19	105.15
55	1x	54	5MU	C5-C6-N1	-2.16	120.97	123.31
1	2A	1911	PSU	O2-C2-N3	-2.16	118.03	121.86
32	2a	516	PSU	C5-C6-N1	-2.16	119.15	122.14
32	2a	1400	5MC	O2-C2-N3	-2.15	118.95	122.33
55	1x	54	5MU	C5M-C5-C4	2.14	121.07	118.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1498	UR3	C3U-N3-C2	2.13	121.05	117.33
1	1A	1962	5MC	CM5-C5-C6	-2.11	120.00	122.85
32	2a	1207	2MG	CM2-N2-C2	-2.10	119.13	123.65
55	1y	54	5MU	C1'-N1-C2	2.09	121.35	117.59
55	1y	8	4SU	C1'-N1-C2	2.09	121.34	117.59
55	1x	8	4SU	C1'-N1-C2	2.08	121.32	117.59
1	1A	1939	5MU	O2-C2-N1	-2.07	120.10	122.80
1	2A	1915	5MU	C1'-N1-C2	2.07	121.30	117.59
32	1a	1207	2MG	CM2-N2-C2	-2.07	119.21	123.65
32	1a	516	PSU	O4'-C1'-C2'	2.06	108.00	105.15
32	2a	966	M2G	C5-C6-N1	2.06	117.99	114.07
32	2a	1404	5MC	O2-C2-N3	-2.06	119.09	122.33
1	1A	1911	PSU	O4'-C1'-C2'	2.04	107.97	105.15
55	2y	54	5MU	C5M-C5-C6	-2.03	120.10	122.85
1	1A	1917	PSU	O2-C2-N3	-2.02	118.28	121.86
1	1A	1942	5MC	N4-C4-N3	2.01	122.15	118.51
55	2x	54	5MU	O2-C2-N1	-2.01	120.18	122.80
55	1x	55	PSU	C5-C6-N1	-2.00	119.36	122.14

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
54	1w	230	MEQ	C-CA-CB-CG
55	1x	37	MIA	C12-C13-C14-C15
55	1x	37	MIA	C12-C13-C14-C16
55	1x	46	G7M	C4'-C5'-O5'-P
55	1y	37	MIA	C12-C13-C14-C15
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	O-C-CA-CB
43	2l	92	0TD	CG-CB-SB-CSB
55	2x	37	MIA	C12-C13-C14-C15
55	2x	37	MIA	C12-C13-C14-C16
55	2y	37	MIA	C12-C13-C14-C15
55	2y	37	MIA	C12-C13-C14-C16
32	1a	1402	4OC	O4'-C4'-C5'-O5'
55	1x	46	G7M	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
55	2x	46	G7M	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
55	1x	46	G7M	O4'-C4'-C5'-O5'
55	1y	46	G7M	O4'-C4'-C5'-O5'
55	2x	46	G7M	O4'-C4'-C5'-O5'
55	1y	46	G7M	C4'-C5'-O5'-P
54	1w	230	MEQ	NE2-CD-CG-CB
54	1w	230	MEQ	OE1-CD-CG-CB
55	1y	37	MIA	N1-C6-N6-C12
55	1x	37	MIA	N1-C6-N6-C12
55	1y	46	G7M	C3'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	1l	92	0TD	SB-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD1
1	1A	2503	2MA	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
55	1x	37	MIA	N6-C12-C13-C14
55	1y	37	MIA	C13-C12-N6-C6
1	1A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
55	2x	46	G7M	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'
55	2x	37	MIA	C3'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD2
43	2l	92	0TD	SB-CB-CG-OD2
1	1A	1920	OMC	C1'-C2'-O2'-CM2
1	1A	1920	OMC	C3'-C2'-O2'-CM2
43	2l	92	0TD	CA-CB-CG-OD2
1	1A	1920	OMC	C2'-C1'-N1-C2
1	2A	2503	2MA	C4'-C5'-O5'-P
54	2w	230	MEQ	OE1-CD-CG-CB
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	2a	1207	2MG	O4'-C4'-C5'-O5'
1	2A	1962	5MC	C2'-C1'-N1-C6
54	2w	230	MEQ	NE2-CD-CG-CB
55	1x	37	MIA	C5-C6-N6-C12
55	1y	37	MIA	C5-C6-N6-C12
1	2A	1962	5MC	O4'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2056 ligands modelled in this entry, 2054 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	SF4	2d	302	35	0,12,12	-	-	-		
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	302	35	-	-	0/6/5/5
59	SF4	1d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1A	2860/2915 (98%)	-0.52	101 (3%) 47 45	16, 33, 90, 104	0
1	2A	2789/2915 (95%)	-0.02	80 (2%) 54 52	29, 56, 89, 104	0
2	1B	120/121 (99%)	-0.44	0 100 100	25, 48, 61, 77	0
2	2B	120/121 (99%)	0.68	6 (5%) 35 33	59, 79, 88, 98	0
3	1D	275/276 (99%)	-0.32	1 (0%) 89 88	17, 35, 51, 75	0
3	2D	275/276 (99%)	0.29	5 (1%) 67 67	31, 50, 64, 77	0
4	1E	204/206 (99%)	-0.28	0 100 100	17, 36, 55, 67	0
4	2E	204/206 (99%)	0.25	2 (0%) 79 79	35, 56, 69, 77	0
5	1F	203/210 (96%)	-0.28	1 (0%) 87 86	18, 38, 65, 82	0
5	2F	203/210 (96%)	0.35	1 (0%) 87 86	36, 63, 76, 89	0
6	1G	181/182 (99%)	0.47	8 (4%) 39 38	43, 56, 71, 84	0
6	2G	181/182 (99%)	1.23	33 (18%) 4 4	63, 79, 85, 89	0
7	1H	174/180 (96%)	0.05	3 (1%) 69 68	34, 51, 65, 69	0
7	2H	174/180 (96%)	0.79	8 (4%) 38 36	64, 77, 84, 91	0
8	1I	146/148 (98%)	0.39	4 (2%) 56 54	42, 67, 76, 80	0
8	2I	146/148 (98%)	0.89	10 (6%) 25 23	55, 72, 79, 83	0
9	1N	140/140 (100%)	-0.44	0 100 100	21, 32, 54, 61	0
9	2N	140/140 (100%)	0.31	1 (0%) 84 83	45, 61, 72, 80	0
10	1O	122/122 (100%)	-0.26	0 100 100	27, 38, 54, 60	0
10	2O	122/122 (100%)	-0.04	0 100 100	38, 53, 63, 73	0
11	1P	149/150 (99%)	-0.10	2 (1%) 74 74	15, 39, 59, 67	0
11	2P	149/150 (99%)	0.48	2 (1%) 74 74	37, 65, 77, 88	0
12	1Q	141/141 (100%)	-0.24	0 100 100	23, 37, 52, 71	0
12	2Q	141/141 (100%)	0.47	6 (4%) 40 39	48, 60, 70, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.35	0 100 100	21, 31, 44, 57	0
13	2R	118/118 (100%)	0.20	1 (0%) 82 82	38, 53, 64, 71	0
14	1S	110/112 (98%)	-0.02	0 100 100	37, 47, 60, 64	0
14	2S	110/112 (98%)	0.93	7 (6%) 27 24	62, 71, 76, 81	0
15	1T	131/146 (89%)	-0.13	3 (2%) 61 60	29, 41, 66, 81	0
15	2T	131/146 (89%)	0.35	3 (2%) 61 60	46, 56, 72, 83	0
16	1U	116/118 (98%)	-0.41	1 (0%) 81 80	18, 26, 39, 58	0
16	2U	116/118 (98%)	0.19	0 100 100	41, 57, 70, 76	0
17	1V	101/101 (100%)	-0.40	0 100 100	18, 35, 52, 58	0
17	2V	101/101 (100%)	0.33	0 100 100	40, 65, 75, 81	0
18	1W	112/113 (99%)	-0.50	0 100 100	21, 27, 42, 81	0
18	2W	112/113 (99%)	0.02	0 100 100	40, 50, 66, 84	0
19	1X	95/96 (98%)	-0.22	1 (1%) 77 77	24, 35, 54, 68	0
19	2X	95/96 (98%)	0.61	4 (4%) 41 39	49, 61, 69, 80	0
20	1Y	107/110 (97%)	0.02	0 100 100	27, 44, 63, 74	0
20	2Y	107/110 (97%)	0.66	2 (1%) 66 65	56, 69, 77, 82	0
21	1Z	183/206 (88%)	0.17	1 (0%) 87 86	35, 54, 69, 74	0
21	2Z	186/206 (90%)	0.57	2 (1%) 77 77	59, 73, 80, 89	0
22	10	76/85 (89%)	-0.21	0 100 100	25, 35, 48, 61	0
22	20	77/85 (90%)	0.90	9 (11%) 10 10	50, 62, 70, 77	0
23	11	97/98 (98%)	-0.04	1 (1%) 79 79	26, 40, 66, 70	0
23	21	97/98 (98%)	0.51	3 (3%) 51 49	41, 58, 74, 79	0
24	12	70/72 (97%)	-0.01	2 (2%) 54 52	34, 46, 58, 74	0
24	22	70/72 (97%)	0.28	1 (1%) 73 73	57, 67, 73, 78	0
25	13	59/60 (98%)	-0.40	0 100 100	20, 31, 55, 72	0
25	23	59/60 (98%)	0.28	0 100 100	50, 58, 71, 78	0
26	14	69/71 (97%)	0.80	9 (13%) 9 8	53, 73, 86, 88	0
26	24	68/71 (95%)	1.17	13 (19%) 4 4	76, 84, 89, 94	0
27	15	59/60 (98%)	-0.59	0 100 100	16, 28, 45, 55	0
27	25	59/60 (98%)	0.24	2 (3%) 48 46	34, 50, 66, 82	0
28	16	53/54 (98%)	-0.27	0 100 100	30, 40, 54, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.44	0 100 100	54, 61, 68, 73	0
29	17	48/49 (97%)	-0.23	3 (6%) 27 25	21, 26, 64, 66	0
29	27	48/49 (97%)	0.19	4 (8%) 19 17	36, 44, 65, 79	0
30	18	64/65 (98%)	-0.09	0 100 100	24, 30, 37, 46	0
30	28	64/65 (98%)	0.39	1 (1%) 70 70	43, 51, 60, 62	0
31	19	37/37 (100%)	-0.13	0 100 100	27, 39, 52, 57	0
31	29	37/37 (100%)	0.59	0 100 100	56, 64, 73, 76	0
32	1a	1488/1521 (97%)	0.47	60 (4%) 43 41	35, 71, 92, 103	0
32	2a	1491/1521 (98%)	0.52	52 (3%) 47 45	44, 74, 92, 104	0
33	1b	231/256 (90%)	0.89	18 (7%) 20 19	63, 75, 85, 90	0
33	2b	231/256 (90%)	1.31	55 (23%) 2 3	63, 79, 87, 96	0
34	1c	206/239 (86%)	0.94	15 (7%) 22 20	63, 77, 84, 91	0
34	2c	206/239 (86%)	0.95	20 (9%) 15 14	67, 78, 84, 87	0
35	1d	208/209 (99%)	0.87	7 (3%) 48 46	53, 72, 79, 89	0
35	2d	208/209 (99%)	0.74	8 (3%) 44 42	53, 68, 76, 86	0
36	1e	148/162 (91%)	0.51	2 (1%) 73 73	53, 64, 73, 81	0
36	2e	148/162 (91%)	0.77	7 (4%) 37 35	58, 70, 76, 88	0
37	1f	100/101 (99%)	0.50	2 (2%) 64 64	55, 68, 75, 80	0
37	2f	100/101 (99%)	0.62	2 (2%) 64 64	57, 70, 76, 79	0
38	1g	155/156 (99%)	0.73	11 (7%) 23 21	60, 73, 82, 90	0
38	2g	155/156 (99%)	0.91	15 (9%) 15 14	66, 79, 85, 91	0
39	1h	137/138 (99%)	0.47	10 (7%) 22 20	56, 65, 73, 76	0
39	2h	137/138 (99%)	0.75	7 (5%) 34 32	59, 70, 77, 83	0
40	1i	127/128 (99%)	1.29	26 (20%) 3 3	60, 77, 83, 89	0
40	2i	123/128 (96%)	2.00	54 (43%) 1 1	70, 82, 87, 91	0
41	1j	98/105 (93%)	1.34	19 (19%) 4 4	63, 79, 85, 89	0
41	2j	96/105 (91%)	1.83	37 (38%) 1 1	72, 82, 88, 91	0
42	1k	114/129 (88%)	0.44	5 (4%) 39 38	45, 65, 75, 78	0
42	2k	114/129 (88%)	0.80	9 (7%) 20 18	62, 73, 80, 85	0
43	1l	121/132 (91%)	0.39	4 (3%) 49 47	47, 59, 70, 73	0
43	2l	121/132 (91%)	0.45	3 (2%) 58 57	49, 61, 69, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	118/126 (93%)	1.04	8 (6%) 25 23	60, 73, 78, 84	0
44	2m	115/126 (91%)	1.37	21 (18%) 4 4	69, 81, 87, 88	0
45	1n	60/61 (98%)	1.31	11 (18%) 4 4	67, 74, 80, 81	0
45	2n	60/61 (98%)	2.14	24 (40%) 1 1	72, 80, 86, 92	0
46	1o	88/89 (98%)	0.59	6 (6%) 25 23	49, 63, 73, 79	0
46	2o	88/89 (98%)	0.73	2 (2%) 61 60	60, 69, 77, 81	0
47	1p	82/88 (93%)	1.24	15 (18%) 4 4	58, 71, 80, 82	0
47	2p	82/88 (93%)	0.73	1 (1%) 76 76	56, 67, 74, 78	0
48	1q	99/105 (94%)	0.58	2 (2%) 64 64	50, 63, 71, 75	0
48	2q	99/105 (94%)	0.55	2 (2%) 64 64	57, 67, 74, 78	0
49	1r	68/88 (77%)	0.31	0 100 100	53, 64, 74, 80	0
49	2r	68/88 (77%)	0.68	0 100 100	61, 71, 76, 80	0
50	1s	83/93 (89%)	1.31	12 (14%) 7 6	66, 76, 81, 83	0
50	2s	83/93 (89%)	1.34	12 (14%) 7 6	74, 82, 88, 90	0
51	1t	96/106 (90%)	0.76	5 (5%) 34 31	54, 67, 78, 83	0
51	2t	96/106 (90%)	0.69	7 (7%) 22 20	56, 68, 78, 83	0
52	1u	23/27 (85%)	1.43	4 (17%) 5 5	65, 71, 74, 79	0
52	2u	23/27 (85%)	1.70	10 (43%) 1 1	72, 82, 85, 86	0
53	1v	13/24 (54%)	0.74	3 (23%) 2 3	52, 64, 92, 92	0
53	2v	13/24 (54%)	1.48	5 (38%) 1 1	68, 75, 98, 100	0
54	1w	248/354 (70%)	0.16	4 (1%) 70 70	29, 65, 79, 87	0
54	2w	252/354 (71%)	0.56	10 (3%) 43 41	48, 73, 83, 88	0
55	1x	68/76 (89%)	-0.20	0 100 100	27, 59, 73, 82	0
55	1y	67/76 (88%)	0.84	7 (10%) 13 12	41, 91, 97, 99	0
55	2x	68/76 (89%)	0.23	0 100 100	48, 74, 82, 94	0
55	2y	67/76 (88%)	1.31	8 (11%) 10 9	61, 97, 101, 103	0
56	1z	14/18 (77%)	1.07	3 (21%) 3 3	31, 49, 71, 80	0
56	2z	14/18 (77%)	1.66	5 (35%) 1 1	52, 65, 77, 82	0
All	All	21290/22338 (95%)	0.28	982 (4%) 38 36	15, 62, 86, 104	0

All (982) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	2	ALA	7.5
23	11	2	SER	6.3
44	1m	2	ALA	5.8
40	2i	14	VAL	5.7
1	1A	1088	A	5.7
32	1a	1531	A	5.4
1	2A	2134	A	5.2
1	2A	2158	A	5.1
32	1a	1532	U	5.1
32	2a	1030(B)	C	5.1
32	1a	1002	G	5.1
1	2A	2113	U	5.1
40	2i	15	ALA	5.0
1	2A	2146	C	5.0
23	21	2	SER	4.9
1	2A	1536	C	4.8
43	1l	126	LYS	4.8
44	2m	4	ILE	4.8
1	2A	2157	G	4.8
40	2i	106	ALA	4.8
45	2n	3	ARG	4.7
33	2b	7	VAL	4.7
12	2Q	121	ALA	4.7
40	2i	126	SER	4.6
32	1a	344	A	4.6
1	1A	2113	U	4.6
19	2X	69	TYR	4.6
1	2A	2138	C	4.5
1	1A	2115	G	4.5
1	2A	2115	G	4.5
1	2A	2156	G	4.5
1	2A	2147	G	4.5
1	2A	2114	A	4.5
45	1n	2	ALA	4.5
32	2a	1236	A	4.4
45	2n	33	VAL	4.4
1	1A	1058	G	4.4
1	2A	2136	C	4.4
11	2P	15	ARG	4.4
1	2A	2159	G	4.3
14	2S	3	ARG	4.3
1	1A	1068	G	4.3
40	1i	2	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
40	2i	46	ALA	4.3
56	2z	10	ARG	4.3
50	2s	9	VAL	4.2
1	2A	2116	G	4.2
50	1s	16	LEU	4.2
40	2i	6	GLY	4.2
1	1A	1059	G	4.2
5	2F	89	VAL	4.2
3	2D	236	GLY	4.2
32	1a	1028	C	4.2
50	1s	9	VAL	4.1
43	1l	91	LYS	4.1
51	1t	14	LYS	4.1
53	2v	10	G	4.1
45	2n	30	ALA	4.1
38	1g	79	ARG	4.1
32	1a	1029	C	4.1
26	24	56	VAL	4.1
38	1g	156	TRP	4.1
42	1k	64	ALA	4.0
40	2i	10	ARG	4.0
45	2n	17	LYS	4.0
40	1i	8	GLY	4.0
38	2g	16	LEU	4.0
1	1A	1087	G	4.0
1	1A	1057	A	3.9
1	2A	2119	A	3.9
32	1a	1447	A	3.9
33	2b	123	ALA	3.9
40	2i	43	ALA	3.9
41	2j	47	PHE	3.9
3	2D	38	LYS	3.9
6	2G	48	GLU	3.9
33	2b	19	HIS	3.9
32	2a	977	A	3.9
38	1g	80	VAL	3.9
51	2t	9	ASN	3.9
35	1d	155	LEU	3.9
7	2H	96	ALA	3.8
40	1i	126	SER	3.8
56	2z	6	VAL	3.8
32	1a	1030(B)	C	3.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2169	A	3.8
1	2A	2133	G	3.8
51	1t	10	LEU	3.8
32	1a	1397	C	3.8
38	2g	156	TRP	3.8
1	1A	1092	C	3.8
1	2A	2111	C	3.8
1	2A	2137	C	3.8
41	2j	71	LEU	3.8
40	2i	123	PRO	3.8
33	2b	236	TYR	3.8
1	1A	1063	G	3.7
3	2D	55	GLY	3.7
40	2i	109	VAL	3.7
1	2A	2112	G	3.7
32	1a	1026	G	3.7
32	2a	1331	G	3.7
1	1A	2114	A	3.7
14	2S	7	TYR	3.7
41	2j	65	LEU	3.7
50	1s	20	LEU	3.7
41	1j	66	ARG	3.7
32	1a	346	G	3.7
32	2a	1002	G	3.7
32	2a	1224	G	3.7
38	1g	2	ALA	3.6
32	1a	1001(A)	G	3.6
44	2m	7	VAL	3.6
44	2m	102	ARG	3.6
22	20	9	SER	3.6
33	2b	88	ALA	3.6
7	2H	115	VAL	3.6
1	1A	1060	U	3.6
40	2i	11	LYS	3.6
40	2i	19	LEU	3.6
15	1T	131	ALA	3.6
15	2T	131	ALA	3.6
38	2g	83	ALA	3.6
56	1z	6	VAL	3.6
1	2A	2160	G	3.6
1	1A	2170	A	3.6
1	2A	2135	A	3.6

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Mol	Chain	Res	Type	RSRZ
1	2A	2145	C	3.6
41	2j	75	ILE	3.5
3	2D	276	LYS	3.5
45	2n	21	TYR	3.5
44	2m	6	GLY	3.5
46	1o	66	LEU	3.5
54	2w	183	VAL	3.5
41	2j	55	LYS	3.5
41	2j	61	GLU	3.5
40	1i	15	ALA	3.5
56	1z	5	PRO	3.5
1	2A	2144	U	3.5
41	2j	76	ASN	3.5
1	1A	2112	G	3.5
41	2j	54	PHE	3.5
1	1A	1082	U	3.5
40	2i	62	TYR	3.5
40	2i	122	ALA	3.4
26	14	56	VAL	3.4
1	2A	2131	G	3.4
32	1a	630	G	3.4
55	1y	18	G	3.4
1	2A	2118	U	3.4
41	2j	56	HIS	3.4
44	2m	100	GLY	3.4
46	2o	15	PHE	3.4
44	2m	65	LYS	3.4
1	2A	2155	G	3.4
1	2A	2170	A	3.4
47	1p	47	ASP	3.4
45	1n	3	ARG	3.4
43	2l	64	TYR	3.3
41	1j	34	VAL	3.3
1	1A	271(K)	U	3.3
1	1A	2189	U	3.3
32	1a	1003	G	3.3
40	2i	13	ALA	3.3
33	2b	44	LEU	3.3
34	2c	2	GLY	3.3
1	1A	2172	U	3.3
32	1a	345	C	3.3
33	2b	200	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	1A	2166	G	3.3
6	2G	43	LEU	3.3
32	1a	1533	C	3.3
40	2i	66	ARG	3.3
1	1A	1093	G	3.3
32	1a	928	G	3.3
14	2S	56	LEU	3.2
33	2b	10	LEU	3.2
40	1i	19	LEU	3.2
32	1a	1030	C	3.2
40	2i	9	ARG	3.2
15	1T	130	ALA	3.2
40	2i	36	TYR	3.2
45	2n	18	VAL	3.2
44	1m	102	ARG	3.2
51	2t	103	GLY	3.2
1	1A	2150	U	3.2
44	1m	98	VAL	3.2
1	2A	2166	G	3.2
11	1P	15	ARG	3.2
12	2Q	104	PHE	3.2
45	2n	41	ARG	3.2
55	1y	19	G	3.2
40	2i	115	GLY	3.2
54	2w	151	ASP	3.2
33	2b	80	ILE	3.2
15	2T	130	ALA	3.2
38	2g	2	ALA	3.2
41	2j	40	LEU	3.2
47	1p	82	GLN	3.2
23	21	28	GLY	3.2
38	2g	81	GLY	3.2
41	2j	52	GLY	3.2
1	2A	2110	G	3.1
1	2A	2148	G	3.1
47	1p	16	HIS	3.1
41	2j	46	ARG	3.1
1	1A	2129	C	3.1
50	1s	71	LEU	3.1
1	2A	2125	G	3.1
50	2s	35	SER	3.1
35	1d	2	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
3	1D	276	LYS	3.1
50	2s	13	ASP	3.1
1	1A	1064	C	3.1
33	2b	15	VAL	3.1
45	2n	31	ARG	3.1
22	20	8	GLY	3.1
1	1A	2119	A	3.1
50	2s	2	PRO	3.1
33	2b	221	LEU	3.1
1	1A	1100	C	3.1
1	2A	2139	C	3.1
32	1a	1037	C	3.1
12	2Q	60	ARG	3.1
41	2j	72	VAL	3.1
45	1n	5	ALA	3.1
52	2u	24	ARG	3.1
34	2c	13	GLY	3.1
33	2b	234	PRO	3.1
32	1a	1257	U	3.0
32	2a	1235	U	3.0
1	2A	2117	A	3.0
32	2a	1363(A)	A	3.0
41	2j	42	THR	3.0
45	2n	7	ILE	3.0
1	1A	2125	G	3.0
32	1a	1036	G	3.0
6	1G	50	ALA	3.0
35	2d	88	VAL	3.0
1	1A	2145	C	3.0
1	1A	2178	C	3.0
1	1A	2188	C	3.0
32	2a	1234	C	3.0
52	2u	23	PRO	3.0
22	20	68	GLU	3.0
1	1A	1090	U	3.0
6	2G	133	LEU	3.0
33	2b	39	ILE	3.0
45	2n	22	THR	3.0
34	1c	189	ALA	3.0
32	1a	1024	G	3.0
45	2n	9	LYS	3.0
40	2i	48	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
45	2n	42	ILE	3.0
41	2j	60	ARG	3.0
1	1A	1026	U	3.0
33	2b	165	VAL	3.0
38	2g	40	ALA	3.0
44	2m	118	ALA	3.0
1	1A	548	A	3.0
7	1H	2	SER	3.0
33	2b	167	PRO	3.0
1	1A	2190	G	3.0
41	1j	100	THR	3.0
39	1h	4	ASP	3.0
47	1p	68	ASP	3.0
26	14	50	VAL	3.0
40	2i	41	VAL	3.0
42	2k	114	VAL	3.0
32	2a	1532	U	3.0
55	2y	20	U	3.0
40	1i	13	ALA	2.9
40	2i	17	VAL	2.9
55	2y	15	G	2.9
55	2y	19	G	2.9
1	1A	2111	C	2.9
26	24	54	GLY	2.9
46	2o	3	ILE	2.9
52	2u	13	ILE	2.9
1	1A	2117	A	2.9
26	14	69	LYS	2.9
7	2H	102	ALA	2.9
8	1I	146	ALA	2.9
33	2b	136	VAL	2.9
32	1a	1030(A)	G	2.9
56	2z	8	ILE	2.9
1	2A	2897	U	2.9
34	1c	207	VAL	2.9
50	1s	13	ASP	2.9
26	14	59	PHE	2.9
40	2i	18	PHE	2.9
36	1e	81	GLU	2.9
44	2m	80	ARG	2.9
1	1A	173	G	2.9
1	1A	2116	G	2.9

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Mol	Chain	Res	Type	RSRZ
4	2E	151	TYR	2.9
26	14	63	TYR	2.9
32	1a	932	C	2.9
6	1G	80	PHE	2.9
41	2j	63	PHE	2.9
40	2i	21	PRO	2.9
45	2n	6	LEU	2.9
36	2e	27	ARG	2.8
40	1i	78	LYS	2.8
41	2j	57	LYS	2.8
45	1n	32	SER	2.8
44	2m	30	ALA	2.8
1	1A	2168	G	2.8
32	1a	204	U	2.8
32	2a	971	G	2.8
26	14	54	GLY	2.8
6	2G	34	LEU	2.8
22	20	84	LEU	2.8
35	1d	154	ASN	2.8
40	2i	79	LEU	2.8
41	1j	76	ASN	2.8
54	2w	351	LEU	2.8
33	1b	200	ILE	2.8
32	1a	1035	A	2.8
36	2e	105	VAL	2.8
47	1p	7	ALA	2.8
6	2G	12	TYR	2.8
40	2i	49	PRO	2.8
34	2c	17	ASP	2.8
33	2b	215	LEU	2.8
42	1k	98	LEU	2.8
44	1m	56	LEU	2.8
1	1A	1094	U	2.8
38	2g	84	ASN	2.8
53	2v	11	U	2.8
6	1G	21	ARG	2.8
40	2i	81	ILE	2.8
1	1A	1071	G	2.8
1	2A	2805	G	2.8
2	2B	118	G	2.8
26	14	53	GLU	2.8
32	1a	1007	C	2.8

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Mol	Chain	Res	Type	RSRZ
41	2j	59	SER	2.8
50	1s	35	SER	2.8
41	2j	49	VAL	2.8
40	1i	43	ALA	2.8
40	2i	76	ALA	2.8
54	1w	350	ALA	2.8
38	1g	82	GLY	2.8
1	1A	1072	C	2.8
1	2A	1533	G	2.8
1	2A	2149	G	2.8
21	2Z	175	VAL	2.8
8	2I	5	LEU	2.8
41	1j	40	LEU	2.8
15	1T	37	GLY	2.8
1	1A	2126	A	2.8
1	1A	2169	A	2.8
1	1A	2171	A	2.8
32	1a	160	A	2.8
40	2i	74	ILE	2.7
44	2m	25	ILE	2.7
26	24	57	GLU	2.7
1	1A	1081	U	2.7
1	2A	1026	U	2.7
32	2a	950	U	2.7
33	1b	229	VAL	2.7
40	2i	65	VAL	2.7
45	1n	59	ALA	2.7
45	2n	61	TRP	2.7
6	2G	2	PRO	2.7
7	2H	128	PRO	2.7
50	1s	74	PHE	2.7
1	1A	2174	C	2.7
1	2A	2142	C	2.7
1	2A	2803	C	2.7
32	1a	1039	C	2.7
32	2a	979	C	2.7
32	2a	1397	C	2.7
33	2b	199	TYR	2.7
34	1c	185	GLY	2.7
40	2i	67	GLY	2.7
42	2k	75	TYR	2.7
1	2A	2319	G	2.7

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Mol	Chain	Res	Type	RSRZ
19	2X	68	ARG	2.7
32	2a	1304	G	2.7
38	1g	153	HIS	2.7
40	2i	42	ARG	2.7
7	1H	58	GLU	2.7
41	2j	34	VAL	2.7
38	1g	83	ALA	2.7
40	1i	55	ALA	2.7
34	1c	109	PRO	2.7
40	2i	71	SER	2.7
44	2m	107	ALA	2.7
7	2H	88	LEU	2.7
39	2h	18	ARG	2.7
40	1i	66	ARG	2.7
50	1s	84	GLY	2.7
51	1t	103	GLY	2.7
39	1h	94	TYR	2.7
1	1A	1079	C	2.7
32	2a	1249	C	2.7
1	1A	614(B)	G	2.7
32	1a	157	G	2.7
1	1A	2135	A	2.7
32	1a	1287	A	2.7
32	2a	1225	A	2.7
45	2n	50	LYS	2.7
33	2b	13	ALA	2.7
39	1h	89	PRO	2.7
54	1w	349	ALA	2.7
33	1b	28	PHE	2.7
56	2z	5	PRO	2.7
45	1n	51	GLY	2.7
34	2c	182	ILE	2.7
50	1s	80	TYR	2.7
32	1a	1027	C	2.7
8	2I	146	ALA	2.7
43	1l	6	THR	2.7
44	2m	103	THR	2.7
1	1A	2151	G	2.7
1	2A	2141	G	2.7
32	1a	1023	G	2.7
32	2a	1036	G	2.7
22	20	82	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
29	27	47	ARG	2.7
32	2a	1286	A	2.7
41	1j	59	SER	2.7
51	1t	11	SER	2.7
52	1u	11	GLY	2.7
33	1b	127	ILE	2.7
41	2j	38	ILE	2.7
26	24	32	TYR	2.6
33	2b	134	GLU	2.6
40	2i	118	LYS	2.6
40	2i	86	VAL	2.6
6	2G	50	ALA	2.6
8	2I	77	LEU	2.6
1	1A	2803	C	2.6
1	2A	2188	C	2.6
6	2G	24	GLY	2.6
35	2d	87	GLY	2.6
40	2i	72	GLY	2.6
52	2u	11	GLY	2.6
32	1a	927	G	2.6
32	1a	929	G	2.6
40	2i	12	GLU	2.6
55	1y	15	G	2.6
26	24	51	ASP	2.6
29	27	48	LYS	2.6
1	1A	2130	U	2.6
6	2G	175	LEU	2.6
45	2n	25	VAL	2.6
47	2p	82	GLN	2.6
42	2k	126	ARG	2.6
7	2H	94	TYR	2.6
8	2I	126	TYR	2.6
42	2k	25	TYR	2.6
34	1c	56	ASP	2.6
1	1A	1077	A	2.6
1	1A	2159	G	2.6
1	2A	2318	G	2.6
33	2b	196	LEU	2.6
33	2b	232	PRO	2.6
26	24	49	PHE	2.6
32	2a	1212	U	2.6
41	2j	5	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
45	2n	16	PHE	2.6
54	2w	194	THR	2.6
40	1i	74	ILE	2.6
34	2c	184	TYR	2.6
33	1b	165	VAL	2.6
34	1c	76	VAL	2.6
34	1c	130	VAL	2.6
38	1g	9	VAL	2.6
38	2g	80	VAL	2.6
32	2a	1008	C	2.6
33	1b	228	GLY	2.6
33	2b	222	ILE	2.6
1	1A	1091	G	2.6
1	1A	1537	G	2.6
1	1A	2120	G	2.6
1	2A	614(B)	G	2.6
32	1a	1032	G	2.6
32	2a	1033	G	2.6
40	2i	114	TYR	2.5
41	1j	88	LEU	2.5
47	1p	2	VAL	2.5
29	17	47	ARG	2.5
41	2j	66	ARG	2.5
46	1o	88	ARG	2.5
42	1k	65	ALA	2.5
41	2j	74	ILE	2.5
1	2A	2804	C	2.5
1	1A	1073	A	2.5
1	1A	1078	U	2.5
1	2A	2132	U	2.5
27	25	59	GLU	2.5
52	2u	14	TRP	2.5
1	1A	1062	G	2.5
1	1A	2152	G	2.5
1	1A	2162	G	2.5
32	1a	1030(C)	G	2.5
32	2a	630	G	2.5
6	1G	53	LEU	2.5
34	2c	12	LEU	2.5
40	2i	88	TYR	2.5
41	1j	33	GLN	2.5
43	1l	89	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
45	1n	16	PHE	2.5
33	1b	237	ALA	2.5
42	2k	89	ALA	2.5
6	2G	85	GLY	2.5
34	2c	171	GLY	2.5
1	1A	2161	C	2.5
32	2a	1282	C	2.5
55	2y	56	C	2.5
32	1a	723	U	2.5
33	2b	187	LEU	2.5
26	14	55	ARG	2.5
41	1j	77	PRO	2.5
38	2g	85	TYR	2.5
39	2h	94	TYR	2.5
41	2j	45	ARG	2.5
44	2m	98	VAL	2.5
45	1n	25	VAL	2.5
47	1p	38	TYR	2.5
36	2e	104	ALA	2.5
40	1i	45	ALA	2.5
1	1A	1099	G	2.5
1	1A	2141	G	2.5
32	1a	1034	G	2.5
32	2a	1030(A)	G	2.5
55	2y	18	G	2.5
6	2G	88	ILE	2.5
45	1n	7	ILE	2.5
33	2b	66	GLY	2.5
40	2i	103	THR	2.5
6	2G	139	LEU	2.5
8	2I	12	LEU	2.5
44	1m	96	LEU	2.5
39	1h	72	PRO	2.5
45	2n	35	ARG	2.5
7	2H	99	VAL	2.5
33	2b	93	VAL	2.5
33	2b	164	VAL	2.5
1	1A	1083	U	2.5
1	2A	614(A)	U	2.5
1	2A	2126	A	2.5
1	2A	2164	C	2.5
32	1a	1000	U	2.5

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Mol	Chain	Res	Type	RSRZ
32	1a	1503	A	2.5
40	2i	125	TYR	2.5
14	2S	57	LYS	2.5
34	2c	160	ALA	2.5
41	2j	27	ALA	2.5
51	2t	74	LYS	2.5
33	2b	42	ILE	2.5
38	1g	81	GLY	2.5
51	2t	69	GLY	2.5
6	1G	48	GLU	2.4
33	2b	121	LEU	2.4
33	2b	213	LEU	2.4
41	1j	35	SER	2.4
48	2q	91	ARG	2.4
29	17	46	VAL	2.4
33	1b	15	VAL	2.4
54	2w	158	VAL	2.4
42	2k	13	GLN	2.4
44	2m	101	GLN	2.4
33	2b	171	ALA	2.4
38	2g	154	TYR	2.4
6	1G	77	ILE	2.4
41	1j	4	ILE	2.4
1	2A	271(K)	U	2.4
1	2A	2312	U	2.4
32	1a	1446	U	2.4
32	2a	1364	U	2.4
53	1v	22	U	2.4
1	1A	1067	A	2.4
1	2A	2129	C	2.4
39	1h	71	GLY	2.4
22	20	75	LEU	2.4
26	24	66	SER	2.4
1	2A	2120	G	2.4
32	1a	933	G	2.4
32	1a	1353	G	2.4
32	2a	1190	G	2.4
33	2b	133	LYS	2.4
41	2j	14	LYS	2.4
6	1G	146	TYR	2.4
6	2G	157	ILE	2.4
40	2i	63	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
41	1j	75	ILE	2.4
44	2m	39	ILE	2.4
40	1i	75	ASP	2.4
52	2u	17	THR	2.4
32	1a	1020	U	2.4
6	2G	7	LEU	2.4
32	1a	1001	A	2.4
32	1a	1286	A	2.4
1	1A	2108	C	2.4
32	2a	972	C	2.4
34	2c	167	TRP	2.4
45	1n	4	LYS	2.4
6	2G	76	SER	2.4
26	24	33	VAL	2.4
33	2b	40	HIS	2.4
34	2c	151	VAL	2.4
50	2s	4	SER	2.4
50	2s	38	SER	2.4
33	2b	218	ALA	2.4
40	1i	106	ALA	2.4
33	1b	33	TYR	2.4
44	2m	87	TYR	2.4
6	2G	134	GLY	2.4
1	2A	2894	G	2.4
3	2D	28	GLU	2.4
33	2b	129	GLU	2.4
35	1d	139	ARG	2.4
50	2s	3	ARG	2.4
53	2v	22	U	2.4
52	2u	3	LYS	2.4
1	1A	1509	C	2.4
33	1b	17	PHE	2.4
8	1I	79	ILE	2.4
35	2d	164	ALA	2.4
35	2d	195	ALA	2.4
33	1b	227	GLY	2.4
33	2b	168	THR	2.3
14	2S	58	LEU	2.3
20	2Y	29	GLU	2.3
35	2d	132	ARG	2.3
39	2h	30	ARG	2.3
51	2t	86	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
29	17	48	LYS	2.3
34	2c	199	LYS	2.3
6	2G	29	TRP	2.3
33	1b	7	VAL	2.3
54	2w	189	GLN	2.3
15	2T	126	ALA	2.3
23	21	77	ALA	2.3
36	2e	86	ALA	2.3
1	1A	1086	A	2.3
2	2B	26	A	2.3
32	2a	532	A	2.3
32	2a	1035	A	2.3
32	2a	1130	A	2.3
45	2n	51	GLY	2.3
1	2A	652(T)	C	2.3
1	2A	2128	C	2.3
2	2B	60	C	2.3
34	1c	52	LEU	2.3
35	2d	155	LEU	2.3
41	2j	67	THR	2.3
6	2G	155	MET	2.3
41	1j	45	ARG	2.3
41	1j	41	PRO	2.3
39	2h	19	VAL	2.3
26	24	59	PHE	2.3
33	2b	55	PHE	2.3
6	2G	20	ILE	2.3
34	2c	152	ILE	2.3
46	1o	87	ILE	2.3
1	1A	2131	G	2.3
1	2A	1171	G	2.3
32	2a	1032	G	2.3
33	2b	237	ALA	2.3
55	1y	20	U	2.3
12	2Q	33	GLY	2.3
50	2s	84	GLY	2.3
26	24	67	TYR	2.3
39	1h	2	LEU	2.3
44	2m	34	LEU	2.3
34	1c	62	ASP	2.3
55	1y	58	A	2.3
24	12	51	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
47	1p	72	ARG	2.3
1	1A	2163	C	2.3
1	1A	2185	C	2.3
1	2A	2896	C	2.3
39	1h	93	VAL	2.3
42	1k	14	VAL	2.3
44	2m	15	VAL	2.3
8	2I	55	ALA	2.3
34	2c	129	ALA	2.3
38	2g	7	ALA	2.3
13	2R	14	SER	2.3
5	1F	208	GLY	2.3
1	1A	12	U	2.3
1	2A	2167	U	2.3
24	22	60	LEU	2.3
54	2w	102	MET	2.3
1	1A	2154	G	2.3
1	2A	2104	G	2.3
35	1d	153	ARG	2.3
44	2m	69	GLU	2.3
50	1s	3	ARG	2.3
53	1v	10	G	2.3
6	2G	17	PRO	2.3
1	1A	2134	A	2.3
32	2a	1285	A	2.3
53	2v	14	A	2.3
32	2a	1027	C	2.3
32	2a	1063	C	2.3
36	2e	84	PHE	2.3
33	2b	201	ILE	2.3
6	2G	73	ALA	2.3
33	2b	34	ALA	2.3
45	2n	5	ALA	2.3
7	2H	100	GLY	2.3
33	2b	138	LEU	2.3
40	2i	116	LYS	2.2
48	1q	98	LEU	2.3
29	27	23	ARG	2.2
11	2P	98	GLU	2.2
40	1i	7	THR	2.2
1	1A	2167	U	2.2
32	2a	1065	U	2.2

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Mol	Chain	Res	Type	RSRZ
41	2j	37	PRO	2.2
1	2A	2151	G	2.2
1	2A	2793	G	2.2
22	20	30	VAL	2.2
32	1a	348	G	2.2
37	1f	18	GLN	2.2
40	2i	53	VAL	2.2
6	2G	39	ILE	2.2
14	2S	35	ILE	2.2
1	1A	1045	A	2.2
1	1A	1070	A	2.2
55	1y	21	A	2.2
39	1h	7	ALA	2.2
8	1I	90	GLY	2.2
33	1b	44	LEU	2.2
33	2b	38	GLY	2.2
35	2d	157	LEU	2.2
37	1f	58	GLY	2.2
40	2i	96	LEU	2.2
47	1p	73	LEU	2.2
1	1A	1532	C	2.2
38	2g	155	ARG	2.2
26	24	30	GLU	2.2
40	1i	12	GLU	2.2
44	2m	73	GLU	2.2
41	1j	87	THR	2.2
6	2G	132	ASN	2.2
34	1c	201	TYR	2.2
33	2b	205	ASP	2.2
40	1i	117	HIS	2.2
1	2A	63	U	2.2
8	2I	92	VAL	2.2
32	1a	223	U	2.2
35	1d	178	VAL	2.2
51	2t	97	ALA	2.2
33	1b	97	TRP	2.2
34	2c	159	GLY	2.2
50	2s	68	GLY	2.2
2	2B	117	G	2.2
4	2E	149	ARG	2.2
32	2a	1048	G	2.2
54	2w	150	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	1A	1075	C	2.2
1	2A	34	C	2.2
1	2A	2140	C	2.2
6	2G	131	TYR	2.2
33	2b	16	HIS	2.2
47	1p	17	TYR	2.2
33	2b	184	VAL	2.2
34	2c	130	VAL	2.2
37	2f	6	VAL	2.2
33	1b	172	ILE	2.2
33	1b	132	LYS	2.2
43	2l	126	LYS	2.2
33	1b	13	ALA	2.2
55	1y	45	U	2.2
8	2I	57	ARG	2.2
34	1c	2	GLY	2.2
41	1j	31	GLY	2.2
52	2u	6	ARG	2.2
41	2j	77	PRO	2.2
52	1u	17	THR	2.2
1	2A	652(B)	A	2.2
1	2A	2173	A	2.2
32	1a	1041	A	2.2
53	2v	12	A	2.2
1	1A	2793	G	2.2
1	2A	2165	G	2.2
1	2A	2182	G	2.2
32	1a	1274	G	2.2
32	2a	1022	G	2.2
32	2a	1024	G	2.2
32	2a	1117	G	2.2
12	2Q	120	ILE	2.2
33	2b	152	PHE	2.2
33	2b	214	ILE	2.2
40	1i	59	PHE	2.2
41	2j	33	GLN	2.2
54	1w	185	VAL	2.2
1	1A	889	C	2.2
1	1A	2137	C	2.2
1	2A	2789	C	2.2
32	1a	330	C	2.2
47	1p	3	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
6	1G	82	LEU	2.2
19	2X	95	LEU	2.2
33	2b	145	LEU	2.2
34	1c	188	LEU	2.2
39	1h	90	GLY	2.2
39	2h	92	ARG	2.2
52	2u	2	GLY	2.2
32	1a	343	U	2.1
55	2y	33	U	2.1
38	2g	112	PRO	2.1
41	2j	64	GLU	2.1
41	1j	42	THR	2.1
38	1g	33	ASP	2.1
20	2Y	45	VAL	2.1
26	24	50	VAL	2.1
33	2b	230	VAL	2.1
38	1g	118	VAL	2.1
40	2i	127	LYS	2.1
41	1j	11	PHE	2.1
48	1q	100	LYS	2.1
1	1A	1095	A	2.1
1	2A	529	A	2.1
1	2A	2124	G	2.1
32	1a	347	G	2.1
40	2i	85	LEU	2.1
55	2y	57	G	2.1
22	20	11	ARG	2.1
24	12	69	ARG	2.1
27	25	19	ARG	2.1
40	1i	42	ARG	2.1
41	1j	10	GLY	2.1
41	2j	36	GLY	2.1
46	1o	89	GLY	2.1
1	1A	888	C	2.1
1	1A	2138	C	2.1
1	2A	2161	C	2.1
32	1a	1038	C	2.1
32	1a	1363	C	2.1
32	2a	1223	C	2.1
32	2a	1354	C	2.1
44	1m	61	GLU	2.1
32	2a	1257	U	2.1

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Mol	Chain	Res	Type	RSRZ
41	2j	68	HIS	2.1
53	1v	11	U	2.1
34	2c	14	ILE	2.1
36	1e	129	ILE	2.1
39	2h	31	PHE	2.1
40	1i	125	TYR	2.1
40	2i	92	TYR	2.1
42	1k	75	TYR	2.1
43	2l	18	VAL	2.1
6	2G	19	LEU	2.1
8	2I	61	ARG	2.1
47	1p	42	ARG	2.1
48	2q	68	ARG	2.1
1	1A	1046	A	2.1
1	1A	1098	A	2.1
1	2A	528	A	2.1
19	2X	67	GLY	2.1
34	1c	25	GLY	2.1
1	1A	2160	G	2.1
1	2A	2802	G	2.1
39	2h	89	PRO	2.1
52	1u	23	PRO	2.1
55	2y	71	G	2.1
1	2A	2108	C	2.1
32	2a	1028	C	2.1
42	2k	122	LYS	2.1
1	1A	1097	U	2.1
6	2G	31	VAL	2.1
6	2G	77	ILE	2.1
16	1U	117	GLN	2.1
21	2Z	146	ILE	2.1
29	27	46	VAL	2.1
33	2b	197	VAL	2.1
36	2e	28	PHE	2.1
38	2g	21	VAL	2.1
38	2g	105	VAL	2.1
44	2m	45	VAL	2.1
50	2s	67	VAL	2.1
51	1t	18	GLN	2.1
56	1z	8	ILE	2.1
54	2w	307	PHE	2.1
47	1p	39	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
19	1X	95	LEU	2.1
21	1Z	70	LEU	2.1
34	2c	94	LEU	2.1
26	14	62	ARG	2.1
39	1h	18	ARG	2.1
41	2j	32	ALA	2.1
52	1u	15	ARG	2.1
52	2u	7	ARG	2.1
40	1i	67	GLY	2.1
41	2j	31	GLY	2.1
44	1m	6	GLY	2.1
45	2n	8	GLU	2.1
45	2n	14	PRO	2.1
2	2B	59	A	2.1
32	2a	1180	A	2.1
42	2k	123	LYS	2.1
46	1o	48	LYS	2.1
42	2k	40	ILE	2.1
1	1A	1089	G	2.1
1	1A	2110	G	2.1
6	2G	5	VAL	2.1
32	1a	1033	G	2.1
32	1a	1215	G	2.1
36	2e	148	VAL	2.1
40	2i	59	PHE	2.1
50	1s	11	VAL	2.1
1	1A	2143	C	2.1
1	1A	2179	C	2.1
1	1A	2804	C	2.1
6	2G	82	LEU	2.1
32	2a	1029	C	2.1
32	2a	1030	C	2.1
32	2a	1037	C	2.1
32	2a	1038	C	2.1
34	1c	43	LEU	2.1
50	2s	71	LEU	2.1
51	2t	10	LEU	2.1
2	2B	1	U	2.1
32	2a	1040	U	2.1
33	1b	195	ASP	2.1
40	1i	88	TYR	2.1
40	2i	75	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
46	1o	69	TYR	2.1
40	2i	104	ARG	2.1
41	2j	43	ARG	2.1
40	2i	61	ALA	2.1
54	2w	352	ALA	2.1
33	2b	86	GLU	2.0
47	1p	43	LYS	2.0
30	28	34	TRP	2.0
8	2I	109	ILE	2.0
40	2i	77	ILE	2.0
1	1A	2173	A	2.0
6	2G	125	PHE	2.0
32	2a	1503	A	2.0
33	2b	115	LEU	2.0
34	2c	196	LEU	2.0
40	1i	85	LEU	2.0
26	24	65	ASP	2.0
33	2b	189	ASP	2.0
40	2i	54	ASP	2.0
1	2A	11	G	2.0
1	2A	2122	U	2.0
8	1I	34	GLY	2.0
11	1P	104	GLY	2.0
32	1a	104	G	2.0
32	2a	1131	G	2.0
35	2d	2	GLY	2.0
44	1m	95	GLY	2.0
1	1A	172	C	2.0
1	1A	886	C	2.0
1	1A	1080	C	2.0
56	2z	14	PRO	2.0
7	1H	175	LYS	2.0
35	1d	156	GLU	2.0
45	1n	17	LYS	2.0
50	1s	43	GLU	2.0
6	2G	52	ILE	2.0
33	2b	32	ILE	2.0
34	2c	202	ILE	2.0
47	1p	67	THR	2.0
50	2s	79	THR	2.0
54	1w	295	THR	2.0
6	2G	23	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
9	2N	34	LEU	2.0
14	2S	46	VAL	2.0
34	1c	106	VAL	2.0
40	1i	44	VAL	2.0
40	1i	109	VAL	2.0
45	2n	36	PHE	2.0
12	2Q	59	ARG	2.0
22	20	74	ARG	2.0
33	2b	21	ARG	2.0
34	2c	181	ASN	2.0
1	1A	1069	A	2.0
6	2G	146	TYR	2.0
32	1a	1005	A	2.0
37	2f	59	TYR	2.0
40	1i	4	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MIA	2y	37	29/30	0.56	0.18	82,91,98,107	0
55	PSU	2y	32	20/21	0.61	0.15	86,94,101,104	0
55	G7M	2y	46	24/25	0.61	0.13	85,97,109,126	0
55	4SU	2y	8	20/21	0.62	0.13	94,98,108,118	0
55	5MU	1y	54	21/22	0.63	0.12	82,90,99,103	0
55	PSU	2y	55	20/21	0.63	0.16	88,99,107,107	0
55	5MU	2y	54	21/22	0.65	0.14	89,97,103,117	0
55	PSU	1y	55	20/21	0.66	0.13	82,96,103,107	0
55	PSU	2y	39	20/21	0.68	0.13	87,96,107,118	0
55	G7M	1y	46	24/25	0.69	0.14	79,92,98,111	0
55	MIA	1y	37	29/30	0.71	0.16	73,88,99,113	0
55	4SU	1y	8	20/21	0.75	0.12	80,92,98,103	0
55	PSU	1y	32	20/21	0.81	0.12	72,83,91,96	0
55	PSU	1y	39	20/21	0.81	0.09	76,87,94,98	0
32	2MG	2a	1207	24/25	0.83	0.13	72,83,87,87	0
55	G7M	2x	46	24/25	0.85	0.12	65,73,81,100	0
43	0TD	1l	92	10/11	0.86	0.15	60,63,67,79	0
55	PSU	2x	32	20/21	0.86	0.13	72,79,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	MIA	2x	37	29/30	0.88	0.15	65,76,83,102	0
55	G7M	1x	46	24/25	0.88	0.10	50,60,73,97	0
32	2MG	1a	1207	24/25	0.88	0.11	73,78,83,84	0
55	PSU	2x	55	20/21	0.89	0.09	70,76,82,90	0
32	PSU	2a	516	20/21	0.90	0.10	69,77,84,86	0
32	5MC	2a	967	21/22	0.90	0.15	63,69,76,76	0
32	5MC	2a	1400	21/22	0.91	0.14	57,73,74,79	0
55	5MU	1x	54	21/22	0.92	0.09	58,64,70,73	0
55	4SU	2x	8	20/21	0.92	0.09	60,70,77,78	0
32	G7M	2a	527	24/25	0.92	0.11	60,68,71,73	0
32	M2G	2a	966	25/26	0.92	0.13	61,67,78,83	0
55	MIA	1x	37	29/30	0.92	0.11	43,58,65,90	0
55	5MU	2x	54	21/22	0.92	0.09	62,70,78,80	0
1	5MU	2A	1915	21/22	0.92	0.09	62,68,75,79	0
32	M2G	1a	966	25/26	0.93	0.12	49,61,69,75	0
55	PSU	1x	32	20/21	0.93	0.10	52,61,71,71	0
32	PSU	1a	516	20/21	0.93	0.10	51,67,75,75	0
55	PSU	2x	39	20/21	0.93	0.09	56,72,78,78	0
55	PSU	1x	39	20/21	0.93	0.09	54,59,63,69	0
32	MA6	2a	1518	24/25	0.93	0.13	51,57,62,63	0
43	0TD	2l	92	10/11	0.93	0.11	52,64,68,81	0
1	5MU	1A	1915	21/22	0.94	0.10	46,51,58,62	0
1	PSU	2A	1917	20/21	0.94	0.09	59,63,67,68	0
32	5MC	1a	1400	21/22	0.94	0.11	47,60,68,73	0
32	4OC	2a	1402	22/23	0.94	0.12	54,61,65,66	0
32	5MC	1a	967	21/22	0.94	0.10	55,62,67,69	0
1	PSU	2A	1911	20/21	0.94	0.09	52,61,66,68	0
54	MEQ	2w	230	10/11	0.94	0.12	52,54,56,57	0
32	G7M	1a	527	24/25	0.95	0.10	51,62,71,74	0
32	5MC	2a	1404	21/22	0.95	0.10	49,58,65,67	0
32	5MC	2a	1407	21/22	0.95	0.10	47,56,61,64	0
55	PSU	1x	55	20/21	0.95	0.08	55,60,64,71	0
1	PSU	1A	1917	20/21	0.96	0.07	42,48,53,54	0
1	5MC	1A	1962	21/22	0.96	0.09	22,29,36,37	0
32	4OC	1a	1402	22/23	0.96	0.09	41,47,53,54	0
32	5MC	1a	1404	21/22	0.96	0.09	40,46,52,59	0
32	5MC	1a	1407	21/22	0.96	0.09	36,42,48,50	0
32	MA6	1a	1518	24/25	0.96	0.10	36,43,48,60	0
1	PSU	1A	1911	20/21	0.96	0.09	36,47,55,55	0
55	4SU	1x	8	20/21	0.96	0.07	39,48,55,59	0
1	OMC	2A	1920	21/22	0.96	0.09	53,57,62,63	0
32	UR3	2a	1498	21/22	0.96	0.10	48,53,62,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MC	2A	1962	21/22	0.96	0.09	37,43,47,57	0
32	MA6	2a	1519	24/25	0.96	0.11	51,57,62,63	0
1	OMG	2A	2251	24/25	0.96	0.09	24,39,45,50	0
1	2MA	2A	2503	23/24	0.96	0.07	31,35,41,42	0
1	OMU	2A	2552	21/22	0.97	0.08	30,36,41,48	0
1	PSU	2A	2605	20/21	0.97	0.07	33,39,46,49	0
32	MA6	1a	1519	24/25	0.97	0.09	38,42,48,50	0
1	OMU	1A	2552	21/22	0.97	0.08	19,26,30,35	0
54	MEQ	1w	230	10/11	0.97	0.07	25,30,33,33	0
1	5MU	2A	1939	21/22	0.97	0.08	36,41,46,48	0
1	5MC	2A	1942	21/22	0.97	0.07	44,52,56,63	0
1	PSU	1A	2605	20/21	0.97	0.07	20,25,35,36	0
1	5MC	1A	1942	21/22	0.97	0.07	30,33,39,45	0
1	OMC	1A	1920	21/22	0.97	0.08	34,43,46,50	0
1	OMG	1A	2251	24/25	0.98	0.06	19,23,26,29	0
1	5MU	1A	1939	21/22	0.98	0.07	18,26,30,31	0
32	UR3	1a	1498	21/22	0.98	0.07	38,45,50,53	0
1	2MA	1A	2503	23/24	0.99	0.05	14,19,22,22	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3490	1/1	0.57	0.20	75,75,75,75	0
57	MG	1A	3658	1/1	0.60	0.22	68,68,68,68	0
57	MG	1A	3726	1/1	0.62	0.14	46,46,46,46	0
57	MG	1A	3634	1/1	0.64	0.59	60,60,60,60	0
57	MG	2A	3116	1/1	0.66	0.45	81,81,81,81	0
57	MG	2A	3148	1/1	0.69	0.27	69,69,69,69	0
57	MG	2a	1694	1/1	0.69	0.26	78,78,78,78	0
57	MG	2A	3182	1/1	0.70	0.28	65,65,65,65	0
57	MG	1a	1638	1/1	0.70	0.32	79,79,79,79	0
57	MG	1A	3641	1/1	0.71	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3110	1/1	0.71	0.13	75,75,75,75	0
57	MG	2A	3410	1/1	0.72	0.20	69,69,69,69	0
57	MG	1A	3219	1/1	0.73	0.19	69,69,69,69	0
57	MG	2A	3379	1/1	0.73	0.16	67,67,67,67	0
57	MG	1A	3624	1/1	0.73	0.29	72,72,72,72	0
57	MG	2A	3431	1/1	0.73	0.21	50,50,50,50	0
57	MG	2A	3639	1/1	0.73	0.16	78,78,78,78	0
57	MG	2a	1602	1/1	0.73	0.14	68,68,68,68	0
57	MG	1A	3650	1/1	0.73	0.21	54,54,54,54	0
57	MG	2a	1759	1/1	0.74	0.16	78,78,78,78	0
57	MG	1A	3644	1/1	0.75	0.19	32,32,32,32	0
57	MG	1w	404	1/1	0.75	0.18	69,69,69,69	0
57	MG	1A	3021	1/1	0.75	0.17	56,56,56,56	0
57	MG	2A	3481	1/1	0.75	0.21	60,60,60,60	0
57	MG	2a	1769	1/1	0.75	0.36	77,77,77,77	0
57	MG	2A	3598	1/1	0.76	0.19	82,82,82,82	0
57	MG	2a	1720	1/1	0.76	0.21	76,76,76,76	0
57	MG	2a	1752	1/1	0.76	0.28	69,69,69,69	0
57	MG	1a	1738	1/1	0.76	0.22	64,64,64,64	0
57	MG	2A	3535	1/1	0.76	0.24	67,67,67,67	0
57	MG	2A	3511	1/1	0.77	0.19	77,77,77,77	0
57	MG	1a	1612	1/1	0.77	0.23	54,54,54,54	0
57	MG	1A	3336	1/1	0.77	0.13	34,34,34,34	0
57	MG	2A	3638	1/1	0.77	0.18	65,65,65,65	0
57	MG	2a	1758	1/1	0.77	0.24	69,69,69,69	0
57	MG	2A	3486	1/1	0.77	0.16	65,65,65,65	0
57	MG	2A	3648	1/1	0.77	0.15	77,77,77,77	0
57	MG	2A	3144	1/1	0.78	0.16	71,71,71,71	0
57	MG	2A	3578	1/1	0.78	0.14	54,54,54,54	0
57	MG	2A	3055	1/1	0.78	0.23	64,64,64,64	0
57	MG	1A	3371	1/1	0.78	0.13	66,66,66,66	0
57	MG	2A	3262	1/1	0.78	0.28	68,68,68,68	0
57	MG	1a	1707	1/1	0.78	0.23	71,71,71,71	0
57	MG	2A	3662	1/1	0.78	0.29	73,73,73,73	0
57	MG	1O	202	1/1	0.79	0.16	67,67,67,67	0
57	MG	2A	3665	1/1	0.79	0.12	63,63,63,63	0
57	MG	2X	104	1/1	0.79	0.16	83,83,83,83	0
57	MG	2A	3434	1/1	0.79	0.17	57,57,57,57	0
57	MG	2A	3284	1/1	0.79	0.23	49,49,49,49	0
57	MG	2A	3603	1/1	0.79	0.14	69,69,69,69	0
57	MG	1A	3314	1/1	0.79	0.14	39,39,39,39	0
57	MG	2A	3244	1/1	0.79	0.33	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3647	1/1	0.79	0.17	67,67,67,67	0
57	MG	2A	3532	1/1	0.79	0.20	68,68,68,68	0
57	MG	2e	201	1/1	0.79	0.12	70,70,70,70	0
57	MG	1A	3664	1/1	0.80	0.11	45,45,45,45	0
57	MG	2A	3572	1/1	0.80	0.19	75,75,75,75	0
57	MG	2A	3422	1/1	0.80	0.23	47,47,47,47	0
57	MG	2a	1643	1/1	0.80	0.23	60,60,60,60	0
57	MG	2a	1657	1/1	0.80	0.17	72,72,72,72	0
57	MG	1a	1783	1/1	0.80	0.27	60,60,60,60	0
57	MG	2A	3137	1/1	0.80	0.15	69,69,69,69	0
57	MG	2a	1735	1/1	0.80	0.19	65,65,65,65	0
57	MG	1A	3771	1/1	0.80	0.17	66,66,66,66	0
57	MG	2A	3348	1/1	0.80	0.14	56,56,56,56	0
57	MG	2A	3505	1/1	0.80	0.17	70,70,70,70	0
57	MG	2A	3354	1/1	0.80	0.19	72,72,72,72	0
57	MG	1a	1733	1/1	0.80	0.27	62,62,62,62	0
57	MG	2a	1665	1/1	0.81	0.42	68,68,68,68	0
57	MG	1A	3455	1/1	0.81	0.14	16,16,16,16	0
57	MG	2A	3305	1/1	0.81	0.24	67,67,67,67	0
57	MG	1c	301	1/1	0.81	0.28	71,71,71,71	0
57	MG	2A	3195	1/1	0.81	0.23	60,60,60,60	0
57	MG	2A	3359	1/1	0.81	0.23	60,60,60,60	0
57	MG	1A	3516	1/1	0.81	0.23	54,54,54,54	0
57	MG	1a	1669	1/1	0.81	0.30	59,59,59,59	0
57	MG	2A	3513	1/1	0.81	0.15	60,60,60,60	0
57	MG	2A	3025	1/1	0.82	0.26	67,67,67,67	0
57	MG	1A	3328	1/1	0.82	0.22	51,51,51,51	0
57	MG	2a	1674	1/1	0.82	0.27	65,65,65,65	0
57	MG	2a	1684	1/1	0.82	0.20	61,61,61,61	0
57	MG	1a	1771	1/1	0.82	0.14	60,60,60,60	0
57	MG	2a	1708	1/1	0.82	0.22	66,66,66,66	0
57	MG	2A	3473	1/1	0.82	0.22	71,71,71,71	0
57	MG	2A	3654	1/1	0.82	0.28	56,56,56,56	0
57	MG	1a	1683	1/1	0.82	0.19	63,63,63,63	0
57	MG	1A	3746	1/1	0.82	0.15	25,25,25,25	0
57	MG	2A	3501	1/1	0.82	0.28	70,70,70,70	0
57	MG	1a	1652	1/1	0.82	0.25	76,76,76,76	0
57	MG	2a	1771	1/1	0.82	0.14	78,78,78,78	0
57	MG	2A	3618	1/1	0.82	0.14	58,58,58,58	0
57	MG	2x	108	1/1	0.82	0.29	77,77,77,77	0
57	MG	2A	3256	1/1	0.83	0.17	53,53,53,53	0
57	MG	1A	3610	1/1	0.83	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3610	1/1	0.83	0.16	41,41,41,41	0
57	MG	1A	3102	1/1	0.83	0.24	52,52,52,52	0
57	MG	2A	3288	1/1	0.83	0.14	61,61,61,61	0
57	MG	1a	1750	1/1	0.83	0.25	66,66,66,66	0
57	MG	1a	1759	1/1	0.83	0.11	63,63,63,63	0
57	MG	1A	3404	1/1	0.83	0.18	37,37,37,37	0
57	MG	2A	3652	1/1	0.83	0.16	49,49,49,49	0
57	MG	1A	3775	1/1	0.83	0.20	59,59,59,59	0
57	MG	2A	3655	1/1	0.83	0.21	70,70,70,70	0
57	MG	2A	3374	1/1	0.83	0.17	63,63,63,63	0
57	MG	1B	211	1/1	0.83	0.23	57,57,57,57	0
57	MG	1E	307	1/1	0.83	0.20	31,31,31,31	0
57	MG	1A	3153	1/1	0.83	0.09	76,76,76,76	0
57	MG	2A	3048	1/1	0.83	0.31	61,61,61,61	0
57	MG	11	103	1/1	0.83	0.26	52,52,52,52	0
57	MG	1A	3049	1/1	0.83	0.31	63,63,63,63	0
57	MG	1A	3492	1/1	0.83	0.14	52,52,52,52	0
57	MG	1A	3370	1/1	0.83	0.21	66,66,66,66	0
57	MG	2A	3140	1/1	0.83	0.13	64,64,64,64	0
57	MG	1A	3596	1/1	0.83	0.17	62,62,62,62	0
57	MG	1A	3674	1/1	0.83	0.14	54,54,54,54	0
57	MG	1a	1688	1/1	0.83	0.19	57,57,57,57	0
57	MG	1A	3690	1/1	0.83	0.19	58,58,58,58	0
57	MG	2A	3201	1/1	0.83	0.13	57,57,57,57	0
57	MG	2A	3211	1/1	0.83	0.10	81,81,81,81	0
57	MG	1a	1718	1/1	0.83	0.21	69,69,69,69	0
57	MG	2A	3583	1/1	0.83	0.27	73,73,73,73	0
57	MG	2A	3584	1/1	0.83	0.14	81,81,81,81	0
57	MG	2A	3589	1/1	0.83	0.26	70,70,70,70	0
57	MG	1A	3807	1/1	0.84	0.20	49,49,49,49	0
57	MG	1a	1701	1/1	0.84	0.10	62,62,62,62	0
57	MG	2A	3314	1/1	0.84	0.12	64,64,64,64	0
57	MG	2A	3503	1/1	0.84	0.10	54,54,54,54	0
57	MG	1a	1702	1/1	0.84	0.22	57,57,57,57	0
57	MG	1a	1623	1/1	0.84	0.16	58,58,58,58	0
57	MG	1a	1633	1/1	0.84	0.20	57,57,57,57	0
57	MG	2A	3523	1/1	0.84	0.14	62,62,62,62	0
57	MG	2B	206	1/1	0.84	0.36	69,69,69,69	0
57	MG	2A	3369	1/1	0.84	0.14	66,66,66,66	0
57	MG	1a	1725	1/1	0.84	0.26	53,53,53,53	0
57	MG	2a	1626	1/1	0.84	0.28	60,60,60,60	0
57	MG	2A	3555	1/1	0.84	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1652	1/1	0.84	0.18	67,67,67,67	0
57	MG	2A	3556	1/1	0.84	0.27	61,61,61,61	0
57	MG	2A	3564	1/1	0.84	0.20	65,65,65,65	0
57	MG	1A	3496	1/1	0.84	0.12	32,32,32,32	0
57	MG	2A	3405	1/1	0.84	0.14	63,63,63,63	0
57	MG	2A	3580	1/1	0.84	0.20	61,61,61,61	0
57	MG	2a	1701	1/1	0.84	0.19	82,82,82,82	0
57	MG	2A	3105	1/1	0.84	0.33	67,67,67,67	0
57	MG	2A	3416	1/1	0.84	0.31	59,59,59,59	0
57	MG	2a	1727	1/1	0.84	0.22	76,76,76,76	0
57	MG	2A	3248	1/1	0.84	0.13	38,38,38,38	0
57	MG	1A	3552	1/1	0.84	0.10	16,16,16,16	0
57	MG	1A	3589	1/1	0.84	0.10	21,21,21,21	0
57	MG	2A	3443	1/1	0.84	0.14	65,65,65,65	0
57	MG	2A	3617	1/1	0.84	0.28	57,57,57,57	0
57	MG	2A	3472	1/1	0.84	0.18	65,65,65,65	0
57	MG	2A	3622	1/1	0.84	0.16	81,81,81,81	0
57	MG	1A	3798	1/1	0.84	0.20	64,64,64,64	0
57	MG	2A	3661	1/1	0.85	0.14	58,58,58,58	0
57	MG	1a	1756	1/1	0.85	0.17	63,63,63,63	0
57	MG	1a	1656	1/1	0.85	0.25	53,53,53,53	0
57	MG	2B	205	1/1	0.85	0.18	61,61,61,61	0
57	MG	2A	3423	1/1	0.85	0.23	61,61,61,61	0
57	MG	2X	102	1/1	0.85	0.14	74,74,74,74	0
57	MG	1a	1767	1/1	0.85	0.26	52,52,52,52	0
57	MG	20	101	1/1	0.85	0.10	77,77,77,77	0
57	MG	2A	3115	1/1	0.85	0.34	61,61,61,61	0
57	MG	1a	1769	1/1	0.85	0.15	56,56,56,56	0
57	MG	2A	3461	1/1	0.85	0.23	46,46,46,46	0
57	MG	1a	1661	1/1	0.85	0.25	56,56,56,56	0
57	MG	2A	3138	1/1	0.85	0.15	71,71,71,71	0
57	MG	1A	3661	1/1	0.85	0.13	52,52,52,52	0
57	MG	2a	1668	1/1	0.85	0.34	70,70,70,70	0
57	MG	2A	3482	1/1	0.85	0.11	41,41,41,41	0
57	MG	1A	3524	1/1	0.85	0.11	49,49,49,49	0
57	MG	2A	3613	1/1	0.85	0.11	43,43,43,43	0
57	MG	1a	1686	1/1	0.85	0.10	75,75,75,75	0
57	MG	1a	1611	1/1	0.85	0.23	68,68,68,68	0
57	MG	2A	3037	1/1	0.85	0.26	59,59,59,59	0
57	MG	2A	3626	1/1	0.85	0.18	58,58,58,58	0
57	MG	2A	3197	1/1	0.85	0.20	64,64,64,64	0
57	MG	2A	3046	1/1	0.85	0.16	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3401	1/1	0.85	0.11	39,39,39,39	0
57	MG	2A	3210	1/1	0.85	0.11	57,57,57,57	0
57	MG	1A	3753	1/1	0.85	0.10	50,50,50,50	0
57	MG	2A	3537	1/1	0.85	0.17	75,75,75,75	0
57	MG	2A	3542	1/1	0.85	0.15	58,58,58,58	0
57	MG	2x	101	1/1	0.85	0.20	72,72,72,72	0
57	MG	2A	3656	1/1	0.85	0.13	45,45,45,45	0
57	MG	2A	3161	1/1	0.86	0.28	59,59,59,59	0
57	MG	2A	3173	1/1	0.86	0.18	65,65,65,65	0
57	MG	1A	3111	1/1	0.86	0.17	42,42,42,42	0
57	MG	1A	3761	1/1	0.86	0.15	45,45,45,45	0
57	MG	1A	3020	1/1	0.86	0.26	65,65,65,65	0
57	MG	1a	1667	1/1	0.86	0.39	64,64,64,64	0
57	MG	1A	3423	1/1	0.86	0.09	18,18,18,18	0
57	MG	1a	1673	1/1	0.86	0.30	66,66,66,66	0
57	MG	2A	3227	1/1	0.86	0.25	54,54,54,54	0
57	MG	2A	3500	1/1	0.86	0.11	54,54,54,54	0
57	MG	2A	3240	1/1	0.86	0.14	47,47,47,47	0
57	MG	1A	3646	1/1	0.86	0.17	46,46,46,46	0
57	MG	1A	3647	1/1	0.86	0.19	54,54,54,54	0
57	MG	1A	3543	1/1	0.86	0.12	17,17,17,17	0
57	MG	1A	3105	1/1	0.86	0.18	50,50,50,50	0
57	MG	1A	3466	1/1	0.86	0.11	25,25,25,25	0
57	MG	1a	1703	1/1	0.86	0.17	64,64,64,64	0
57	MG	2a	1605	1/1	0.86	0.18	66,66,66,66	0
57	MG	2A	3295	1/1	0.86	0.13	74,74,74,74	0
57	MG	2a	1632	1/1	0.86	0.20	69,69,69,69	0
57	MG	2A	3059	1/1	0.86	0.12	58,58,58,58	0
57	MG	2a	1648	1/1	0.86	0.17	51,51,51,51	0
57	MG	2A	3071	1/1	0.86	0.11	44,44,44,44	0
57	MG	2A	3543	1/1	0.86	0.13	71,71,71,71	0
57	MG	2A	3334	1/1	0.86	0.12	35,35,35,35	0
57	MG	2a	1667	1/1	0.86	0.16	69,69,69,69	0
57	MG	2A	3074	1/1	0.86	0.25	62,62,62,62	0
57	MG	1A	3362	1/1	0.86	0.09	39,39,39,39	0
57	MG	1A	3604	1/1	0.86	0.09	23,23,23,23	0
57	MG	1a	1721	1/1	0.86	0.16	62,62,62,62	0
57	MG	1A	3491	1/1	0.86	0.18	49,49,49,49	0
57	MG	2A	3129	1/1	0.86	0.32	64,64,64,64	0
57	MG	2A	3393	1/1	0.86	0.13	58,58,58,58	0
57	MG	2A	3397	1/1	0.86	0.15	49,49,49,49	0
57	MG	2A	3591	1/1	0.86	0.29	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1744	1/1	0.86	0.23	67,67,67,67	0
57	MG	2A	3399	1/1	0.86	0.30	68,68,68,68	0
57	MG	2a	1756	1/1	0.86	0.17	47,47,47,47	0
57	MG	1a	1731	1/1	0.86	0.11	54,54,54,54	0
57	MG	1A	3615	1/1	0.86	0.22	47,47,47,47	0
57	MG	2A	3406	1/1	0.86	0.13	51,51,51,51	0
57	MG	1a	1624	1/1	0.86	0.12	59,59,59,59	0
57	MG	1A	3274	1/1	0.86	0.23	43,43,43,43	0
57	MG	2A	3147	1/1	0.86	0.16	58,58,58,58	0
57	MG	1A	3749	1/1	0.86	0.13	30,30,30,30	0
57	MG	2A	3039	1/1	0.87	0.12	51,51,51,51	0
57	MG	2A	3468	1/1	0.87	0.13	54,54,54,54	0
57	MG	1A	3770	1/1	0.87	0.40	43,43,43,43	0
57	MG	1a	1711	1/1	0.87	0.20	76,76,76,76	0
57	MG	1a	1626	1/1	0.87	0.35	70,70,70,70	0
57	MG	1A	3470	1/1	0.87	0.20	60,60,60,60	0
57	MG	1A	3016	1/1	0.87	0.19	40,40,40,40	0
57	MG	2A	3274	1/1	0.87	0.11	44,44,44,44	0
57	MG	1A	3670	1/1	0.87	0.24	53,53,53,53	0
57	MG	1A	3544	1/1	0.87	0.15	37,37,37,37	0
57	MG	1a	1659	1/1	0.87	0.20	56,56,56,56	0
57	MG	2F	303	1/1	0.87	0.12	64,64,64,64	0
57	MG	2R	201	1/1	0.87	0.15	66,66,66,66	0
57	MG	1a	1740	1/1	0.87	0.21	73,73,73,73	0
57	MG	1a	1744	1/1	0.87	0.28	74,74,74,74	0
57	MG	2A	3319	1/1	0.87	0.12	55,55,55,55	0
57	MG	21	101	1/1	0.87	0.14	57,57,57,57	0
57	MG	2A	3126	1/1	0.87	0.25	55,55,55,55	0
57	MG	2A	3335	1/1	0.87	0.18	59,59,59,59	0
57	MG	2A	3536	1/1	0.87	0.19	72,72,72,72	0
57	MG	2A	3339	1/1	0.87	0.12	46,46,46,46	0
57	MG	2A	3346	1/1	0.87	0.12	58,58,58,58	0
57	MG	2A	3347	1/1	0.87	0.14	40,40,40,40	0
57	MG	2A	3544	1/1	0.87	0.15	67,67,67,67	0
57	MG	1A	3250	1/1	0.87	0.10	33,33,33,33	0
57	MG	2a	1658	1/1	0.87	0.22	59,59,59,59	0
57	MG	1B	212	1/1	0.87	0.29	67,67,67,67	0
57	MG	1a	1758	1/1	0.87	0.23	73,73,73,73	0
57	MG	1A	3188	1/1	0.87	0.25	51,51,51,51	0
57	MG	2A	3141	1/1	0.87	0.12	41,41,41,41	0
57	MG	1A	3594	1/1	0.87	0.10	33,33,33,33	0
57	MG	1A	3281	1/1	0.87	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	14	502	1/1	0.87	0.30	69,69,69,69	0
57	MG	2A	3159	1/1	0.87	0.14	53,53,53,53	0
57	MG	2a	1713	1/1	0.87	0.12	63,63,63,63	0
57	MG	2a	1717	1/1	0.87	0.21	73,73,73,73	0
57	MG	1a	1773	1/1	0.87	0.15	70,70,70,70	0
57	MG	2A	3171	1/1	0.87	0.26	53,53,53,53	0
57	MG	2A	3601	1/1	0.87	0.12	52,52,52,52	0
57	MG	1a	1778	1/1	0.87	0.17	58,58,58,58	0
57	MG	18	101	1/1	0.87	0.29	64,64,64,64	0
57	MG	2a	1754	1/1	0.87	0.22	67,67,67,67	0
57	MG	2A	3611	1/1	0.87	0.13	66,66,66,66	0
57	MG	2A	3186	1/1	0.87	0.15	54,54,54,54	0
57	MG	1a	1693	1/1	0.87	0.20	66,66,66,66	0
57	MG	2a	1764	1/1	0.87	0.11	51,51,51,51	0
57	MG	1w	402	1/1	0.87	0.22	44,44,44,44	0
57	MG	1A	3286	1/1	0.87	0.13	60,60,60,60	0
57	MG	1A	3758	1/1	0.87	0.13	51,51,51,51	0
57	MG	2f	201	1/1	0.87	0.19	59,59,59,59	0
57	MG	2j	201	1/1	0.87	0.16	74,74,74,74	0
57	MG	1A	3518	1/1	0.87	0.13	39,39,39,39	0
57	MG	2x	102	1/1	0.87	0.25	68,68,68,68	0
57	MG	2A	3455	1/1	0.87	0.12	56,56,56,56	0
57	MG	1A	3247	1/1	0.88	0.17	54,54,54,54	0
57	MG	1A	3503	1/1	0.88	0.12	52,52,52,52	0
57	MG	1A	3085	1/1	0.88	0.28	51,51,51,51	0
57	MG	2A	3341	1/1	0.88	0.16	60,60,60,60	0
57	MG	1A	3175	1/1	0.88	0.29	43,43,43,43	0
57	MG	2B	209	1/1	0.88	0.31	63,63,63,63	0
57	MG	2D	306	1/1	0.88	0.14	54,54,54,54	0
57	MG	1y	101	1/1	0.88	0.21	77,77,77,77	0
57	MG	2A	3526	1/1	0.88	0.28	67,67,67,67	0
57	MG	2A	3531	1/1	0.88	0.18	64,64,64,64	0
57	MG	2A	3168	1/1	0.88	0.32	64,64,64,64	0
57	MG	1a	1634	1/1	0.88	0.34	62,62,62,62	0
57	MG	1A	3613	1/1	0.88	0.47	30,30,30,30	0
57	MG	2A	3368	1/1	0.88	0.12	55,55,55,55	0
57	MG	1a	1639	1/1	0.88	0.23	62,62,62,62	0
57	MG	2a	1610	1/1	0.88	0.17	64,64,64,64	0
57	MG	2a	1612	1/1	0.88	0.12	50,50,50,50	0
57	MG	1a	1729	1/1	0.88	0.21	58,58,58,58	0
57	MG	2a	1630	1/1	0.88	0.19	60,60,60,60	0
57	MG	1a	1648	1/1	0.88	0.24	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1636	1/1	0.88	0.18	65,65,65,65	0
57	MG	2a	1639	1/1	0.88	0.15	44,44,44,44	0
57	MG	2A	3383	1/1	0.88	0.21	57,57,57,57	0
57	MG	2a	1645	1/1	0.88	0.17	59,59,59,59	0
57	MG	1a	1649	1/1	0.88	0.13	58,58,58,58	0
57	MG	1A	3346	1/1	0.88	0.13	49,49,49,49	0
57	MG	1B	201	1/1	0.88	0.08	56,56,56,56	0
57	MG	1A	3350	1/1	0.88	0.14	56,56,56,56	0
57	MG	2A	3579	1/1	0.88	0.20	53,53,53,53	0
57	MG	2A	3220	1/1	0.88	0.14	56,56,56,56	0
57	MG	2A	3083	1/1	0.88	0.23	53,53,53,53	0
57	MG	2A	3239	1/1	0.88	0.23	63,63,63,63	0
57	MG	2a	1680	1/1	0.88	0.21	50,50,50,50	0
57	MG	2A	3588	1/1	0.88	0.22	64,64,64,64	0
57	MG	2a	1691	1/1	0.88	0.16	39,39,39,39	0
57	MG	2A	3084	1/1	0.88	0.15	54,54,54,54	0
57	MG	2A	3418	1/1	0.88	0.19	60,60,60,60	0
57	MG	1A	3045	1/1	0.88	0.13	30,30,30,30	0
57	MG	2a	1711	1/1	0.88	0.15	52,52,52,52	0
57	MG	1A	3716	1/1	0.88	0.12	50,50,50,50	0
57	MG	2A	3428	1/1	0.88	0.09	42,42,42,42	0
57	MG	1A	3636	1/1	0.88	0.30	41,41,41,41	0
57	MG	1A	3736	1/1	0.88	0.24	30,30,30,30	0
57	MG	2a	1730	1/1	0.88	0.19	71,71,71,71	0
57	MG	1A	3122	1/1	0.88	0.21	56,56,56,56	0
57	MG	2A	3448	1/1	0.88	0.10	40,40,40,40	0
57	MG	2A	3281	1/1	0.88	0.14	65,65,65,65	0
57	MG	2A	3620	1/1	0.88	0.13	46,46,46,46	0
57	MG	2A	3621	1/1	0.88	0.13	48,48,48,48	0
57	MG	1A	3571	1/1	0.88	0.12	37,37,37,37	0
57	MG	2A	3467	1/1	0.88	0.20	54,54,54,54	0
57	MG	2a	1761	1/1	0.88	0.11	59,59,59,59	0
57	MG	2A	3634	1/1	0.88	0.07	57,57,57,57	0
57	MG	2A	3134	1/1	0.88	0.19	46,46,46,46	0
57	MG	2A	3292	1/1	0.88	0.14	66,66,66,66	0
57	MG	1A	3645	1/1	0.88	0.17	53,53,53,53	0
57	MG	2A	3478	1/1	0.88	0.18	70,70,70,70	0
57	MG	2A	3298	1/1	0.88	0.20	50,50,50,50	0
57	MG	1A	3287	1/1	0.88	0.25	49,49,49,49	0
57	MG	1a	1617	1/1	0.88	0.17	59,59,59,59	0
57	MG	2x	105	1/1	0.88	0.13	40,40,40,40	0
57	MG	1a	1782	1/1	0.88	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3002	1/1	0.89	0.19	57,57,57,57	0
57	MG	2A	3212	1/1	0.89	0.09	58,58,58,58	0
57	MG	1A	3064	1/1	0.89	0.18	40,40,40,40	0
57	MG	1A	3288	1/1	0.89	0.40	40,40,40,40	0
57	MG	2A	3233	1/1	0.89	0.13	62,62,62,62	0
57	MG	2A	3476	1/1	0.89	0.24	52,52,52,52	0
57	MG	1A	3538	1/1	0.89	0.20	41,41,41,41	0
57	MG	1a	1618	1/1	0.89	0.26	53,53,53,53	0
57	MG	1A	3765	1/1	0.89	0.16	49,49,49,49	0
57	MG	2Q	203	1/1	0.89	0.29	56,56,56,56	0
57	MG	1A	3767	1/1	0.89	0.23	29,29,29,29	0
57	MG	1A	3488	1/1	0.89	0.22	62,62,62,62	0
57	MG	1A	3629	1/1	0.89	0.11	34,34,34,34	0
57	MG	2A	3072	1/1	0.89	0.18	57,57,57,57	0
57	MG	1A	3302	1/1	0.89	0.36	34,34,34,34	0
57	MG	2A	3081	1/1	0.89	0.16	59,59,59,59	0
57	MG	1A	3776	1/1	0.89	0.10	29,29,29,29	0
57	MG	1A	3796	1/1	0.89	0.26	69,69,69,69	0
57	MG	1a	1732	1/1	0.89	0.25	56,56,56,56	0
57	MG	2a	1620	1/1	0.89	0.21	59,59,59,59	0
57	MG	2a	1624	1/1	0.89	0.23	61,61,61,61	0
57	MG	1a	1646	1/1	0.89	0.19	66,66,66,66	0
57	MG	2A	3112	1/1	0.89	0.26	60,60,60,60	0
57	MG	1a	1734	1/1	0.89	0.26	71,71,71,71	0
57	MG	1a	1647	1/1	0.89	0.21	60,60,60,60	0
57	MG	2A	3322	1/1	0.89	0.17	46,46,46,46	0
57	MG	2A	3121	1/1	0.89	0.23	55,55,55,55	0
57	MG	1A	3103	1/1	0.89	0.27	53,53,53,53	0
57	MG	1a	1743	1/1	0.89	0.15	51,51,51,51	0
57	MG	2a	1650	1/1	0.89	0.33	57,57,57,57	0
57	MG	2A	3546	1/1	0.89	0.16	56,56,56,56	0
57	MG	2a	1653	1/1	0.89	0.15	61,61,61,61	0
57	MG	2A	3340	1/1	0.89	0.14	47,47,47,47	0
57	MG	1A	3695	1/1	0.89	0.10	30,30,30,30	0
57	MG	2A	3557	1/1	0.89	0.10	46,46,46,46	0
57	MG	2A	3135	1/1	0.89	0.29	53,53,53,53	0
57	MG	1A	3375	1/1	0.89	0.09	31,31,31,31	0
57	MG	2a	1671	1/1	0.89	0.30	53,53,53,53	0
57	MG	1A	3077	1/1	0.89	0.17	51,51,51,51	0
57	MG	2a	1677	1/1	0.89	0.26	65,65,65,65	0
57	MG	1a	1657	1/1	0.89	0.21	57,57,57,57	0
57	MG	1A	3108	1/1	0.89	0.18	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3362	1/1	0.89	0.13	48,48,48,48	0
57	MG	2A	3142	1/1	0.89	0.25	48,48,48,48	0
57	MG	2A	3587	1/1	0.89	0.11	73,73,73,73	0
57	MG	1a	1660	1/1	0.89	0.13	48,48,48,48	0
57	MG	1E	303	1/1	0.89	0.12	42,42,42,42	0
57	MG	1A	3741	1/1	0.89	0.28	68,68,68,68	0
57	MG	2A	3151	1/1	0.89	0.21	53,53,53,53	0
57	MG	2A	3153	1/1	0.89	0.15	60,60,60,60	0
57	MG	2a	1722	1/1	0.89	0.24	51,51,51,51	0
57	MG	2A	3602	1/1	0.89	0.18	44,44,44,44	0
57	MG	2a	1728	1/1	0.89	0.25	49,49,49,49	0
57	MG	2A	3395	1/1	0.89	0.20	68,68,68,68	0
57	MG	1a	1668	1/1	0.89	0.30	60,60,60,60	0
57	MG	1A	3744	1/1	0.89	0.12	40,40,40,40	0
57	MG	2a	1747	1/1	0.89	0.17	64,64,64,64	0
57	MG	2A	3162	1/1	0.89	0.23	45,45,45,45	0
57	MG	2A	3163	1/1	0.89	0.23	62,62,62,62	0
57	MG	2A	3164	1/1	0.89	0.15	56,56,56,56	0
57	MG	1P	201	1/1	0.89	0.25	28,28,28,28	0
57	MG	2A	3413	1/1	0.89	0.15	50,50,50,50	0
57	MG	2a	1760	1/1	0.89	0.15	65,65,65,65	0
57	MG	1a	1679	1/1	0.89	0.17	42,42,42,42	0
57	MG	1A	3514	1/1	0.89	0.09	31,31,31,31	0
57	MG	2a	1768	1/1	0.89	0.20	73,73,73,73	0
57	MG	2A	3629	1/1	0.89	0.21	70,70,70,70	0
57	MG	1v	101	1/1	0.89	0.13	71,71,71,71	0
57	MG	1w	401	1/1	0.89	0.41	46,46,46,46	0
57	MG	2A	3194	1/1	0.89	0.36	65,65,65,65	0
57	MG	1a	1685	1/1	0.89	0.11	53,53,53,53	0
57	MG	2t	201	1/1	0.89	0.21	54,54,54,54	0
57	MG	1A	3030	1/1	0.89	0.12	43,43,43,43	0
57	MG	2A	3198	1/1	0.89	0.16	45,45,45,45	0
57	MG	1x	107	1/1	0.89	0.07	43,43,43,43	0
57	MG	1A	3751	1/1	0.89	0.12	56,56,56,56	0
57	MG	1N	203	1/1	0.90	0.08	36,36,36,36	0
57	MG	2B	202	1/1	0.90	0.19	70,70,70,70	0
57	MG	1A	3211	1/1	0.90	0.08	33,33,33,33	0
57	MG	1A	3275	1/1	0.90	0.19	65,65,65,65	0
57	MG	2A	3490	1/1	0.90	0.19	75,75,75,75	0
57	MG	1Z	301	1/1	0.90	0.17	53,53,53,53	0
57	MG	2A	3131	1/1	0.90	0.13	50,50,50,50	0
57	MG	2Q	201	1/1	0.90	0.27	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3452	1/1	0.90	0.12	35,35,35,35	0
57	MG	2A	3504	1/1	0.90	0.16	64,64,64,64	0
57	MG	2V	202	1/1	0.90	0.21	49,49,49,49	0
57	MG	1A	3173	1/1	0.90	0.10	43,43,43,43	0
57	MG	1a	1671	1/1	0.90	0.33	71,71,71,71	0
57	MG	1a	1775	1/1	0.90	0.14	71,71,71,71	0
57	MG	2A	3514	1/1	0.90	0.09	59,59,59,59	0
57	MG	28	101	1/1	0.90	0.20	63,63,63,63	0
57	MG	1A	3542	1/1	0.90	0.13	30,30,30,30	0
57	MG	1a	1779	1/1	0.90	0.18	56,56,56,56	0
57	MG	1a	1605	1/1	0.90	0.36	54,54,54,54	0
57	MG	2a	1611	1/1	0.90	0.14	54,54,54,54	0
57	MG	1a	1609	1/1	0.90	0.21	65,65,65,65	0
57	MG	2a	1613	1/1	0.90	0.24	56,56,56,56	0
57	MG	2A	3533	1/1	0.90	0.14	65,65,65,65	0
57	MG	1A	3459	1/1	0.90	0.23	58,58,58,58	0
57	MG	1A	3028	1/1	0.90	0.17	52,52,52,52	0
57	MG	1a	1614	1/1	0.90	0.13	74,74,74,74	0
57	MG	1A	3355	1/1	0.90	0.12	45,45,45,45	0
57	MG	2a	1634	1/1	0.90	0.22	50,50,50,50	0
57	MG	1A	3477	1/1	0.90	0.09	31,31,31,31	0
57	MG	1a	1620	1/1	0.90	0.10	49,49,49,49	0
57	MG	2a	1642	1/1	0.90	0.23	60,60,60,60	0
57	MG	2A	3356	1/1	0.90	0.14	65,65,65,65	0
57	MG	1a	1622	1/1	0.90	0.27	55,55,55,55	0
57	MG	2a	1646	1/1	0.90	0.17	60,60,60,60	0
57	MG	1A	3360	1/1	0.90	0.10	59,59,59,59	0
57	MG	2A	3006	1/1	0.90	0.22	54,54,54,54	0
57	MG	1A	3591	1/1	0.90	0.12	28,28,28,28	0
57	MG	2A	3566	1/1	0.90	0.14	55,55,55,55	0
57	MG	2A	3570	1/1	0.90	0.16	50,50,50,50	0
57	MG	2A	3026	1/1	0.90	0.25	57,57,57,57	0
57	MG	2a	1659	1/1	0.90	0.15	48,48,48,48	0
57	MG	2a	1660	1/1	0.90	0.20	63,63,63,63	0
57	MG	2a	1663	1/1	0.90	0.31	54,54,54,54	0
57	MG	2A	3027	1/1	0.90	0.36	51,51,51,51	0
57	MG	2A	3177	1/1	0.90	0.22	52,52,52,52	0
57	MG	2A	3033	1/1	0.90	0.20	69,69,69,69	0
57	MG	1a	1717	1/1	0.90	0.15	51,51,51,51	0
57	MG	2A	3191	1/1	0.90	0.13	45,45,45,45	0
57	MG	2a	1675	1/1	0.90	0.11	59,59,59,59	0
57	MG	2A	3585	1/1	0.90	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3361	1/1	0.90	0.09	40,40,40,40	0
57	MG	1A	3059	1/1	0.90	0.18	35,35,35,35	0
57	MG	2a	1685	1/1	0.90	0.28	65,65,65,65	0
57	MG	2a	1688	1/1	0.90	0.28	64,64,64,64	0
57	MG	1a	1724	1/1	0.90	0.21	51,51,51,51	0
57	MG	2A	3590	1/1	0.90	0.20	48,48,48,48	0
57	MG	1A	3671	1/1	0.90	0.17	49,49,49,49	0
57	MG	2A	3407	1/1	0.90	0.16	43,43,43,43	0
57	MG	2A	3409	1/1	0.90	0.14	76,76,76,76	0
57	MG	2A	3058	1/1	0.90	0.16	61,61,61,61	0
57	MG	2A	3207	1/1	0.90	0.16	39,39,39,39	0
57	MG	2A	3608	1/1	0.90	0.09	67,67,67,67	0
57	MG	1A	3368	1/1	0.90	0.10	10,10,10,10	0
57	MG	1A	3261	1/1	0.90	0.11	52,52,52,52	0
57	MG	2A	3612	1/1	0.90	0.17	54,54,54,54	0
57	MG	2a	1729	1/1	0.90	0.22	62,62,62,62	0
57	MG	2A	3419	1/1	0.90	0.21	65,65,65,65	0
57	MG	1A	3263	1/1	0.90	0.17	39,39,39,39	0
57	MG	2A	3214	1/1	0.90	0.20	57,57,57,57	0
57	MG	1A	3709	1/1	0.90	0.13	55,55,55,55	0
57	MG	2a	1748	1/1	0.90	0.22	62,62,62,62	0
57	MG	2A	3221	1/1	0.90	0.33	66,66,66,66	0
57	MG	2A	3433	1/1	0.90	0.14	40,40,40,40	0
57	MG	2A	3075	1/1	0.90	0.17	59,59,59,59	0
57	MG	1B	210	1/1	0.90	0.29	59,59,59,59	0
57	MG	2A	3632	1/1	0.90	0.25	53,53,53,53	0
57	MG	2A	3633	1/1	0.90	0.08	67,67,67,67	0
57	MG	1A	3508	1/1	0.90	0.11	42,42,42,42	0
57	MG	2a	1763	1/1	0.90	0.15	64,64,64,64	0
57	MG	1a	1651	1/1	0.90	0.25	36,36,36,36	0
57	MG	2A	3086	1/1	0.90	0.14	53,53,53,53	0
57	MG	2A	3640	1/1	0.90	0.13	57,57,57,57	0
57	MG	2A	3645	1/1	0.90	0.41	69,69,69,69	0
57	MG	2A	3463	1/1	0.90	0.33	48,48,48,48	0
57	MG	2e	202	1/1	0.90	0.13	60,60,60,60	0
57	MG	1a	1741	1/1	0.90	0.16	71,71,71,71	0
57	MG	2A	3250	1/1	0.90	0.26	67,67,67,67	0
57	MG	2k	201	1/1	0.90	0.27	68,68,68,68	0
57	MG	2A	3470	1/1	0.90	0.11	43,43,43,43	0
57	MG	1A	3267	1/1	0.90	0.23	48,48,48,48	0
57	MG	2A	3261	1/1	0.90	0.12	57,57,57,57	0
57	MG	1A	3626	1/1	0.90	0.13	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3739	1/1	0.90	0.10	38,38,38,38	0
57	MG	1A	3619	1/1	0.91	0.11	47,47,47,47	0
57	MG	1A	3738	1/1	0.91	0.17	63,63,63,63	0
57	MG	1A	3622	1/1	0.91	0.14	32,32,32,32	0
57	MG	1A	3107	1/1	0.91	0.23	55,55,55,55	0
57	MG	2A	3157	1/1	0.91	0.24	66,66,66,66	0
57	MG	2A	3420	1/1	0.91	0.21	48,48,48,48	0
57	MG	2A	3657	1/1	0.91	0.16	48,48,48,48	0
57	MG	1A	3191	1/1	0.91	0.11	35,35,35,35	0
57	MG	1a	1753	1/1	0.91	0.20	58,58,58,58	0
57	MG	1a	1754	1/1	0.91	0.15	41,41,41,41	0
57	MG	1A	3194	1/1	0.91	0.24	37,37,37,37	0
57	MG	2B	203	1/1	0.91	0.23	65,65,65,65	0
57	MG	2B	204	1/1	0.91	0.23	56,56,56,56	0
57	MG	1A	3539	1/1	0.91	0.10	31,31,31,31	0
57	MG	1A	3750	1/1	0.91	0.14	32,32,32,32	0
57	MG	2A	3440	1/1	0.91	0.11	59,59,59,59	0
57	MG	2D	301	1/1	0.91	0.25	52,52,52,52	0
57	MG	1a	1762	1/1	0.91	0.16	50,50,50,50	0
57	MG	1a	1763	1/1	0.91	0.16	69,69,69,69	0
57	MG	1A	3635	1/1	0.91	0.20	63,63,63,63	0
57	MG	2A	3458	1/1	0.91	0.21	57,57,57,57	0
57	MG	1a	1627	1/1	0.91	0.35	65,65,65,65	0
57	MG	2U	201	1/1	0.91	0.10	48,48,48,48	0
57	MG	1A	3279	1/1	0.91	0.27	56,56,56,56	0
57	MG	1A	3467	1/1	0.91	0.12	25,25,25,25	0
57	MG	1A	3019	1/1	0.91	0.12	31,31,31,31	0
57	MG	1A	3086	1/1	0.91	0.10	27,27,27,27	0
57	MG	1a	1642	1/1	0.91	0.11	50,50,50,50	0
57	MG	1A	3553	1/1	0.91	0.11	19,19,19,19	0
57	MG	2A	3200	1/1	0.91	0.18	57,57,57,57	0
57	MG	2a	1604	1/1	0.91	0.20	56,56,56,56	0
57	MG	1A	3224	1/1	0.91	0.11	35,35,35,35	0
57	MG	1a	1787	1/1	0.91	0.17	49,49,49,49	0
57	MG	1A	3648	1/1	0.91	0.16	47,47,47,47	0
57	MG	1A	3773	1/1	0.91	0.14	55,55,55,55	0
57	MG	1A	3580	1/1	0.91	0.07	32,32,32,32	0
57	MG	2A	3493	1/1	0.91	0.18	57,57,57,57	0
57	MG	2A	3497	1/1	0.91	0.08	63,63,63,63	0
57	MG	1A	3651	1/1	0.91	0.15	40,40,40,40	0
57	MG	2a	1629	1/1	0.91	0.13	67,67,67,67	0
57	MG	2A	3216	1/1	0.91	0.23	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3781	1/1	0.91	0.11	43,43,43,43	0
57	MG	1A	3785	1/1	0.91	0.14	45,45,45,45	0
57	MG	2A	3225	1/1	0.91	0.18	46,46,46,46	0
57	MG	1A	3789	1/1	0.91	0.23	57,57,57,57	0
57	MG	2a	1640	1/1	0.91	0.21	49,49,49,49	0
57	MG	2A	3512	1/1	0.91	0.10	61,61,61,61	0
57	MG	1A	3101	1/1	0.91	0.19	45,45,45,45	0
57	MG	1A	3066	1/1	0.91	0.31	46,46,46,46	0
57	MG	2A	3013	1/1	0.91	0.16	57,57,57,57	0
57	MG	2A	3019	1/1	0.91	0.27	40,40,40,40	0
57	MG	2A	3528	1/1	0.91	0.13	68,68,68,68	0
57	MG	2A	3245	1/1	0.91	0.12	62,62,62,62	0
57	MG	1a	1665	1/1	0.91	0.17	66,66,66,66	0
57	MG	1A	3802	1/1	0.91	0.07	20,20,20,20	0
57	MG	1A	3592	1/1	0.91	0.09	18,18,18,18	0
57	MG	2A	3029	1/1	0.91	0.22	50,50,50,50	0
57	MG	2A	3032	1/1	0.91	0.16	48,48,48,48	0
57	MG	2A	3266	1/1	0.91	0.08	49,49,49,49	0
57	MG	2A	3267	1/1	0.91	0.15	54,54,54,54	0
57	MG	1A	3668	1/1	0.91	0.08	46,46,46,46	0
57	MG	2A	3279	1/1	0.91	0.14	61,61,61,61	0
57	MG	2A	3553	1/1	0.91	0.23	65,65,65,65	0
57	MG	1B	209	1/1	0.91	0.24	58,58,58,58	0
57	MG	1A	3253	1/1	0.91	0.10	73,73,73,73	0
57	MG	1a	1675	1/1	0.91	0.18	59,59,59,59	0
57	MG	2a	1679	1/1	0.91	0.14	73,73,73,73	0
57	MG	2A	3559	1/1	0.91	0.11	48,48,48,48	0
57	MG	1A	3401	1/1	0.91	0.16	46,46,46,46	0
57	MG	2A	3051	1/1	0.91	0.21	67,67,67,67	0
57	MG	2A	3568	1/1	0.91	0.10	70,70,70,70	0
57	MG	2a	1689	1/1	0.91	0.14	61,61,61,61	0
57	MG	1a	1681	1/1	0.91	0.20	66,66,66,66	0
57	MG	1A	3599	1/1	0.91	0.11	31,31,31,31	0
57	MG	2a	1698	1/1	0.91	0.22	73,73,73,73	0
57	MG	2A	3307	1/1	0.91	0.11	47,47,47,47	0
57	MG	1B	219	1/1	0.91	0.20	57,57,57,57	0
57	MG	1E	302	1/1	0.91	0.09	17,17,17,17	0
57	MG	2A	3320	1/1	0.91	0.09	38,38,38,38	0
57	MG	1A	3683	1/1	0.91	0.18	46,46,46,46	0
57	MG	1a	1691	1/1	0.91	0.19	52,52,52,52	0
57	MG	1a	1692	1/1	0.91	0.12	32,32,32,32	0
57	MG	1A	3689	1/1	0.91	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3082	1/1	0.91	0.16	48,48,48,48	0
57	MG	1N	201	1/1	0.91	0.24	41,41,41,41	0
57	MG	1A	3603	1/1	0.91	0.10	44,44,44,44	0
57	MG	1A	3076	1/1	0.91	0.10	28,28,28,28	0
57	MG	2a	1742	1/1	0.91	0.17	50,50,50,50	0
57	MG	2A	3096	1/1	0.91	0.14	48,48,48,48	0
57	MG	2A	3352	1/1	0.91	0.19	54,54,54,54	0
57	MG	1a	1706	1/1	0.91	0.15	70,70,70,70	0
57	MG	1A	3703	1/1	0.91	0.12	47,47,47,47	0
57	MG	1P	204	1/1	0.91	0.15	42,42,42,42	0
57	MG	1a	1712	1/1	0.91	0.26	64,64,64,64	0
57	MG	2A	3366	1/1	0.91	0.10	56,56,56,56	0
57	MG	1A	3706	1/1	0.91	0.15	49,49,49,49	0
57	MG	2A	3120	1/1	0.91	0.25	55,55,55,55	0
57	MG	1A	3707	1/1	0.91	0.08	42,42,42,42	0
57	MG	1a	1720	1/1	0.91	0.24	64,64,64,64	0
57	MG	12	101	1/1	0.91	0.13	36,36,36,36	0
57	MG	2A	3390	1/1	0.91	0.22	64,64,64,64	0
57	MG	2A	3624	1/1	0.91	0.27	66,66,66,66	0
57	MG	1A	3061	1/1	0.91	0.25	57,57,57,57	0
57	MG	15	101	1/1	0.91	0.20	38,38,38,38	0
57	MG	1A	3424	1/1	0.91	0.10	17,17,17,17	0
57	MG	1a	1730	1/1	0.91	0.15	46,46,46,46	0
57	MG	1a	1604	1/1	0.91	0.11	69,69,69,69	0
57	MG	2A	3635	1/1	0.91	0.09	49,49,49,49	0
57	MG	2A	3636	1/1	0.91	0.11	49,49,49,49	0
57	MG	1A	3431	1/1	0.91	0.07	16,16,16,16	0
57	MG	1a	1607	1/1	0.91	0.09	67,67,67,67	0
57	MG	1A	3730	1/1	0.91	0.17	29,29,29,29	0
57	MG	1A	3731	1/1	0.91	0.26	32,32,32,32	0
57	MG	1a	1757	1/1	0.92	0.10	70,70,70,70	0
57	MG	1a	1628	1/1	0.92	0.16	56,56,56,56	0
57	MG	1A	3380	1/1	0.92	0.16	31,31,31,31	0
57	MG	1a	1761	1/1	0.92	0.15	66,66,66,66	0
57	MG	1A	3393	1/1	0.92	0.16	42,42,42,42	0
57	MG	1a	1637	1/1	0.92	0.17	58,58,58,58	0
57	MG	2A	3641	1/1	0.92	0.07	44,44,44,44	0
57	MG	1A	3537	1/1	0.92	0.10	22,22,22,22	0
57	MG	2A	3160	1/1	0.92	0.20	65,65,65,65	0
57	MG	1A	3395	1/1	0.92	0.09	34,34,34,34	0
57	MG	1A	3138	1/1	0.92	0.20	30,30,30,30	0
57	MG	1a	1772	1/1	0.92	0.20	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1645	1/1	0.92	0.31	55,55,55,55	0
57	MG	1A	3778	1/1	0.92	0.09	40,40,40,40	0
57	MG	1A	3780	1/1	0.92	0.15	48,48,48,48	0
57	MG	2A	3658	1/1	0.92	0.17	52,52,52,52	0
57	MG	2A	3659	1/1	0.92	0.27	63,63,63,63	0
57	MG	1A	3402	1/1	0.92	0.08	26,26,26,26	0
57	MG	2A	3174	1/1	0.92	0.19	71,71,71,71	0
57	MG	2A	3176	1/1	0.92	0.10	40,40,40,40	0
57	MG	1a	1781	1/1	0.92	0.16	73,73,73,73	0
57	MG	1A	3783	1/1	0.92	0.11	43,43,43,43	0
57	MG	1A	3151	1/1	0.92	0.06	32,32,32,32	0
57	MG	2A	3438	1/1	0.92	0.09	32,32,32,32	0
57	MG	1A	3230	1/1	0.92	0.14	47,47,47,47	0
57	MG	2A	3192	1/1	0.92	0.14	41,41,41,41	0
57	MG	2B	210	1/1	0.92	0.14	66,66,66,66	0
57	MG	1A	3791	1/1	0.92	0.12	20,20,20,20	0
57	MG	2A	3450	1/1	0.92	0.11	58,58,58,58	0
57	MG	1A	3546	1/1	0.92	0.08	36,36,36,36	0
57	MG	1A	3017	1/1	0.92	0.11	41,41,41,41	0
57	MG	1A	3303	1/1	0.92	0.12	59,59,59,59	0
57	MG	2A	3199	1/1	0.92	0.20	57,57,57,57	0
57	MG	2A	3466	1/1	0.92	0.16	46,46,46,46	0
57	MG	2V	201	1/1	0.92	0.18	58,58,58,58	0
57	MG	1A	3555	1/1	0.92	0.08	39,39,39,39	0
57	MG	1A	3433	1/1	0.92	0.18	38,38,38,38	0
57	MG	1B	202	1/1	0.92	0.20	44,44,44,44	0
57	MG	2A	3471	1/1	0.92	0.17	58,58,58,58	0
57	MG	1y	102	1/1	0.92	0.12	73,73,73,73	0
57	MG	23	101	1/1	0.92	0.15	51,51,51,51	0
57	MG	1A	3677	1/1	0.92	0.10	71,71,71,71	0
57	MG	29	101	1/1	0.92	0.21	64,64,64,64	0
57	MG	2A	3474	1/1	0.92	0.16	52,52,52,52	0
57	MG	1A	3678	1/1	0.92	0.08	43,43,43,43	0
57	MG	1a	1670	1/1	0.92	0.12	41,41,41,41	0
57	MG	1A	3679	1/1	0.92	0.09	34,34,34,34	0
57	MG	1A	3442	1/1	0.92	0.08	43,43,43,43	0
57	MG	1A	3583	1/1	0.92	0.11	19,19,19,19	0
57	MG	1A	3585	1/1	0.92	0.11	45,45,45,45	0
57	MG	2a	1614	1/1	0.92	0.13	52,52,52,52	0
57	MG	2a	1615	1/1	0.92	0.17	59,59,59,59	0
57	MG	1A	3156	1/1	0.92	0.10	54,54,54,54	0
57	MG	2a	1623	1/1	0.92	0.19	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3700	1/1	0.92	0.25	57,57,57,57	0
57	MG	2a	1625	1/1	0.92	0.09	51,51,51,51	0
57	MG	2A	3236	1/1	0.92	0.18	60,60,60,60	0
57	MG	2A	3237	1/1	0.92	0.19	44,44,44,44	0
57	MG	1F	308	1/1	0.92	0.12	53,53,53,53	0
57	MG	2A	3036	1/1	0.92	0.09	53,53,53,53	0
57	MG	2A	3241	1/1	0.92	0.09	64,64,64,64	0
57	MG	2A	3508	1/1	0.92	0.23	55,55,55,55	0
57	MG	2A	3509	1/1	0.92	0.15	56,56,56,56	0
57	MG	1A	3315	1/1	0.92	0.11	35,35,35,35	0
57	MG	1a	1687	1/1	0.92	0.19	60,60,60,60	0
57	MG	1N	202	1/1	0.92	0.06	40,40,40,40	0
57	MG	1A	3007	1/1	0.92	0.07	33,33,33,33	0
57	MG	2A	3518	1/1	0.92	0.17	49,49,49,49	0
57	MG	2A	3519	1/1	0.92	0.12	56,56,56,56	0
57	MG	1A	3461	1/1	0.92	0.07	24,24,24,24	0
57	MG	2A	3257	1/1	0.92	0.14	42,42,42,42	0
57	MG	2A	3258	1/1	0.92	0.13	51,51,51,51	0
57	MG	1A	3259	1/1	0.92	0.10	57,57,57,57	0
57	MG	2A	3057	1/1	0.92	0.17	36,36,36,36	0
57	MG	1A	3710	1/1	0.92	0.09	23,23,23,23	0
57	MG	1Q	205	1/1	0.92	0.11	42,42,42,42	0
57	MG	2A	3060	1/1	0.92	0.18	66,66,66,66	0
57	MG	2a	1664	1/1	0.92	0.26	52,52,52,52	0
57	MG	2A	3276	1/1	0.92	0.10	33,33,33,33	0
57	MG	2a	1666	1/1	0.92	0.11	62,62,62,62	0
57	MG	2A	3540	1/1	0.92	0.09	51,51,51,51	0
57	MG	2A	3278	1/1	0.92	0.15	49,49,49,49	0
57	MG	2A	3067	1/1	0.92	0.15	42,42,42,42	0
57	MG	2a	1673	1/1	0.92	0.14	80,80,80,80	0
57	MG	1U	201	1/1	0.92	0.16	33,33,33,33	0
57	MG	1U	203	1/1	0.92	0.07	27,27,27,27	0
57	MG	2a	1676	1/1	0.92	0.40	57,57,57,57	0
57	MG	2A	3548	1/1	0.92	0.20	56,56,56,56	0
57	MG	2A	3286	1/1	0.92	0.17	63,63,63,63	0
57	MG	2A	3554	1/1	0.92	0.14	65,65,65,65	0
57	MG	2A	3287	1/1	0.92	0.11	44,44,44,44	0
57	MG	1A	3337	1/1	0.92	0.12	37,37,37,37	0
57	MG	10	102	1/1	0.92	0.20	40,40,40,40	0
57	MG	1A	3724	1/1	0.92	0.14	22,22,22,22	0
57	MG	2A	3296	1/1	0.92	0.13	40,40,40,40	0
57	MG	2A	3565	1/1	0.92	0.21	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3052	1/1	0.92	0.10	32,32,32,32	0
57	MG	2A	3303	1/1	0.92	0.07	55,55,55,55	0
57	MG	2a	1703	1/1	0.92	0.22	56,56,56,56	0
57	MG	1A	3474	1/1	0.92	0.08	59,59,59,59	0
57	MG	1A	3090	1/1	0.92	0.24	34,34,34,34	0
57	MG	15	103	1/1	0.92	0.13	43,43,43,43	0
57	MG	2a	1715	1/1	0.92	0.10	70,70,70,70	0
57	MG	1A	3485	1/1	0.92	0.10	41,41,41,41	0
57	MG	1a	1603	1/1	0.92	0.24	57,57,57,57	0
57	MG	2A	3108	1/1	0.92	0.35	48,48,48,48	0
57	MG	2a	1726	1/1	0.92	0.09	58,58,58,58	0
57	MG	2A	3327	1/1	0.92	0.15	50,50,50,50	0
57	MG	1A	3190	1/1	0.92	0.23	54,54,54,54	0
57	MG	1A	3616	1/1	0.92	0.07	55,55,55,55	0
57	MG	1A	3068	1/1	0.92	0.33	54,54,54,54	0
57	MG	1A	3031	1/1	0.92	0.36	38,38,38,38	0
57	MG	2a	1736	1/1	0.92	0.13	63,63,63,63	0
57	MG	2a	1741	1/1	0.92	0.13	58,58,58,58	0
57	MG	2A	3118	1/1	0.92	0.09	53,53,53,53	0
57	MG	2A	3343	1/1	0.92	0.08	61,61,61,61	0
57	MG	2A	3593	1/1	0.92	0.10	45,45,45,45	0
57	MG	2A	3595	1/1	0.92	0.30	63,63,63,63	0
57	MG	2A	3119	1/1	0.92	0.10	58,58,58,58	0
57	MG	1A	3278	1/1	0.92	0.34	56,56,56,56	0
57	MG	1A	3195	1/1	0.92	0.17	42,42,42,42	0
57	MG	1a	1735	1/1	0.92	0.09	54,54,54,54	0
57	MG	2A	3606	1/1	0.92	0.23	69,69,69,69	0
57	MG	2A	3127	1/1	0.92	0.18	54,54,54,54	0
57	MG	1A	3123	1/1	0.92	0.08	32,32,32,32	0
57	MG	2A	3358	1/1	0.92	0.20	56,56,56,56	0
57	MG	2A	3130	1/1	0.92	0.26	59,59,59,59	0
57	MG	1A	3504	1/1	0.92	0.10	47,47,47,47	0
57	MG	2A	3615	1/1	0.92	0.26	49,49,49,49	0
57	MG	2a	1770	1/1	0.92	0.24	67,67,67,67	0
57	MG	1A	3282	1/1	0.92	0.11	44,44,44,44	0
57	MG	1A	3754	1/1	0.92	0.09	47,47,47,47	0
57	MG	2A	3619	1/1	0.92	0.12	50,50,50,50	0
57	MG	1A	3283	1/1	0.92	0.25	51,51,51,51	0
57	MG	2A	3370	1/1	0.92	0.24	48,48,48,48	0
57	MG	1A	3515	1/1	0.92	0.10	29,29,29,29	0
57	MG	1A	3763	1/1	0.92	0.18	59,59,59,59	0
57	MG	2u	101	1/1	0.92	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2v	101	1/1	0.92	0.17	63,63,63,63	0
57	MG	2v	102	1/1	0.92	0.20	59,59,59,59	0
57	MG	2A	3380	1/1	0.92	0.18	58,58,58,58	0
57	MG	1A	3642	1/1	0.92	0.08	19,19,19,19	0
57	MG	2x	103	1/1	0.92	0.17	59,59,59,59	0
57	MG	1A	3378	1/1	0.92	0.06	23,23,23,23	0
57	MG	2A	3143	1/1	0.92	0.28	56,56,56,56	0
57	MG	1a	1616	1/1	0.93	0.20	55,55,55,55	0
57	MG	1A	3618	1/1	0.93	0.12	41,41,41,41	0
57	MG	2A	3386	1/1	0.93	0.16	60,60,60,60	0
57	MG	1A	3359	1/1	0.93	0.08	38,38,38,38	0
57	MG	1A	3189	1/1	0.93	0.28	45,45,45,45	0
57	MG	1A	3757	1/1	0.93	0.11	41,41,41,41	0
57	MG	2A	3396	1/1	0.93	0.12	49,49,49,49	0
57	MG	1A	3623	1/1	0.93	0.12	51,51,51,51	0
57	MG	2A	3643	1/1	0.93	0.08	43,43,43,43	0
57	MG	1A	3039	1/1	0.93	0.09	31,31,31,31	0
57	MG	1a	1760	1/1	0.93	0.19	71,71,71,71	0
57	MG	2A	3404	1/1	0.93	0.14	58,58,58,58	0
57	MG	1a	1625	1/1	0.93	0.13	57,57,57,57	0
57	MG	2A	3152	1/1	0.93	0.16	52,52,52,52	0
57	MG	1A	3133	1/1	0.93	0.07	30,30,30,30	0
57	MG	2A	3155	1/1	0.93	0.12	45,45,45,45	0
57	MG	1A	3364	1/1	0.93	0.11	29,29,29,29	0
57	MG	2A	3412	1/1	0.93	0.11	44,44,44,44	0
57	MG	1a	1764	1/1	0.93	0.20	69,69,69,69	0
57	MG	1A	3633	1/1	0.93	0.09	40,40,40,40	0
57	MG	1a	1632	1/1	0.93	0.26	55,55,55,55	0
57	MG	1A	3136	1/1	0.93	0.11	32,32,32,32	0
57	MG	2B	201	1/1	0.93	0.13	61,61,61,61	0
57	MG	1A	3003	1/1	0.93	0.08	21,21,21,21	0
57	MG	1A	3196	1/1	0.93	0.24	52,52,52,52	0
57	MG	1a	1774	1/1	0.93	0.08	62,62,62,62	0
57	MG	2A	3426	1/1	0.93	0.17	61,61,61,61	0
57	MG	1A	3637	1/1	0.93	0.25	49,49,49,49	0
57	MG	2A	3172	1/1	0.93	0.09	33,33,33,33	0
57	MG	1a	1776	1/1	0.93	0.19	56,56,56,56	0
57	MG	1A	3372	1/1	0.93	0.14	62,62,62,62	0
57	MG	1A	3139	1/1	0.93	0.15	23,23,23,23	0
57	MG	2D	307	1/1	0.93	0.10	60,60,60,60	0
57	MG	2E	305	1/1	0.93	0.10	46,46,46,46	0
57	MG	1A	3377	1/1	0.93	0.08	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2F	304	1/1	0.93	0.10	41,41,41,41	0
57	MG	2A	3178	1/1	0.93	0.13	56,56,56,56	0
57	MG	1A	3140	1/1	0.93	0.12	41,41,41,41	0
57	MG	2A	3183	1/1	0.93	0.10	37,37,37,37	0
57	MG	2A	3185	1/1	0.93	0.19	53,53,53,53	0
57	MG	1A	3379	1/1	0.93	0.07	32,32,32,32	0
57	MG	1A	3285	1/1	0.93	0.18	45,45,45,45	0
57	MG	2X	101	1/1	0.93	0.19	53,53,53,53	0
57	MG	1A	3386	1/1	0.93	0.09	34,34,34,34	0
57	MG	2A	3464	1/1	0.93	0.27	58,58,58,58	0
57	MG	2A	3465	1/1	0.93	0.16	67,67,67,67	0
57	MG	2A	3193	1/1	0.93	0.11	68,68,68,68	0
57	MG	1A	3520	1/1	0.93	0.09	32,32,32,32	0
57	MG	1A	3794	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3469	1/1	0.93	0.22	59,59,59,59	0
57	MG	2A	3196	1/1	0.93	0.12	39,39,39,39	0
57	MG	2a	1603	1/1	0.93	0.20	64,64,64,64	0
57	MG	1a	1653	1/1	0.93	0.12	50,50,50,50	0
57	MG	1A	3523	1/1	0.93	0.16	42,42,42,42	0
57	MG	2a	1606	1/1	0.93	0.17	52,52,52,52	0
57	MG	2a	1609	1/1	0.93	0.24	68,68,68,68	0
57	MG	1A	3388	1/1	0.93	0.11	44,44,44,44	0
57	MG	1a	1658	1/1	0.93	0.15	62,62,62,62	0
57	MG	1A	3221	1/1	0.93	0.07	30,30,30,30	0
57	MG	2A	3205	1/1	0.93	0.18	54,54,54,54	0
57	MG	2A	3001	1/1	0.93	0.18	59,59,59,59	0
57	MG	1A	3804	1/1	0.93	0.12	44,44,44,44	0
57	MG	2a	1616	1/1	0.93	0.22	61,61,61,61	0
57	MG	2A	3484	1/1	0.93	0.17	43,43,43,43	0
57	MG	2A	3005	1/1	0.93	0.11	58,58,58,58	0
57	MG	2A	3489	1/1	0.93	0.08	39,39,39,39	0
57	MG	1A	3806	1/1	0.93	0.08	34,34,34,34	0
57	MG	2A	3491	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	3070	1/1	0.93	0.09	33,33,33,33	0
57	MG	1A	3399	1/1	0.93	0.10	38,38,38,38	0
57	MG	2a	1631	1/1	0.93	0.23	63,63,63,63	0
57	MG	2A	3498	1/1	0.93	0.10	57,57,57,57	0
57	MG	2A	3219	1/1	0.93	0.16	46,46,46,46	0
57	MG	2a	1635	1/1	0.93	0.16	55,55,55,55	0
57	MG	2A	3021	1/1	0.93	0.14	56,56,56,56	0
57	MG	2a	1637	1/1	0.93	0.20	49,49,49,49	0
57	MG	2A	3024	1/1	0.93	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3669	1/1	0.93	0.28	43,43,43,43	0
57	MG	1B	203	1/1	0.93	0.15	50,50,50,50	0
57	MG	2A	3229	1/1	0.93	0.11	56,56,56,56	0
57	MG	2a	1644	1/1	0.93	0.10	48,48,48,48	0
57	MG	1B	205	1/1	0.93	0.14	49,49,49,49	0
57	MG	1A	3227	1/1	0.93	0.18	36,36,36,36	0
57	MG	1a	1672	1/1	0.93	0.14	56,56,56,56	0
57	MG	1A	3293	1/1	0.93	0.13	48,48,48,48	0
57	MG	2A	3034	1/1	0.93	0.21	44,44,44,44	0
57	MG	2A	3035	1/1	0.93	0.11	68,68,68,68	0
57	MG	1A	3229	1/1	0.93	0.09	34,34,34,34	0
57	MG	2A	3520	1/1	0.93	0.18	47,47,47,47	0
57	MG	1A	3545	1/1	0.93	0.10	19,19,19,19	0
57	MG	2A	3525	1/1	0.93	0.07	63,63,63,63	0
57	MG	1a	1680	1/1	0.93	0.13	51,51,51,51	0
57	MG	2A	3040	1/1	0.93	0.10	54,54,54,54	0
57	MG	2A	3529	1/1	0.93	0.09	40,40,40,40	0
57	MG	2A	3045	1/1	0.93	0.09	58,58,58,58	0
57	MG	1A	3406	1/1	0.93	0.07	22,22,22,22	0
57	MG	1D	305	1/1	0.93	0.12	38,38,38,38	0
57	MG	2a	1669	1/1	0.93	0.16	64,64,64,64	0
57	MG	2A	3049	1/1	0.93	0.16	62,62,62,62	0
57	MG	2A	3050	1/1	0.93	0.22	59,59,59,59	0
57	MG	2A	3264	1/1	0.93	0.07	47,47,47,47	0
57	MG	2A	3538	1/1	0.93	0.13	43,43,43,43	0
57	MG	1A	3407	1/1	0.93	0.07	21,21,21,21	0
57	MG	2A	3052	1/1	0.93	0.14	46,46,46,46	0
57	MG	1A	3411	1/1	0.93	0.09	39,39,39,39	0
57	MG	1E	306	1/1	0.93	0.12	24,24,24,24	0
57	MG	2a	1681	1/1	0.93	0.09	57,57,57,57	0
57	MG	2a	1683	1/1	0.93	0.16	55,55,55,55	0
57	MG	2A	3277	1/1	0.93	0.23	67,67,67,67	0
57	MG	1A	3100	1/1	0.93	0.08	38,38,38,38	0
57	MG	2a	1687	1/1	0.93	0.18	62,62,62,62	0
57	MG	2A	3552	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	3232	1/1	0.93	0.14	25,25,25,25	0
57	MG	1A	3011	1/1	0.93	0.17	43,43,43,43	0
57	MG	2a	1692	1/1	0.93	0.15	49,49,49,49	0
57	MG	2a	1693	1/1	0.93	0.20	47,47,47,47	0
57	MG	2A	3066	1/1	0.93	0.11	52,52,52,52	0
57	MG	2A	3285	1/1	0.93	0.12	33,33,33,33	0
57	MG	1A	3582	1/1	0.93	0.20	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1698	1/1	0.93	0.20	65,65,65,65	0
57	MG	2a	1706	1/1	0.93	0.26	69,69,69,69	0
57	MG	2a	1707	1/1	0.93	0.19	60,60,60,60	0
57	MG	1A	3701	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3432	1/1	0.93	0.09	36,36,36,36	0
57	MG	1A	3325	1/1	0.93	0.17	45,45,45,45	0
57	MG	2a	1714	1/1	0.93	0.16	52,52,52,52	0
57	MG	2A	3076	1/1	0.93	0.18	52,52,52,52	0
57	MG	2a	1716	1/1	0.93	0.13	65,65,65,65	0
57	MG	2A	3569	1/1	0.93	0.12	47,47,47,47	0
57	MG	2A	3078	1/1	0.93	0.07	51,51,51,51	0
57	MG	1A	3435	1/1	0.93	0.16	70,70,70,70	0
57	MG	2a	1723	1/1	0.93	0.14	67,67,67,67	0
57	MG	2A	3576	1/1	0.93	0.17	60,60,60,60	0
57	MG	1A	3590	1/1	0.93	0.10	50,50,50,50	0
57	MG	1A	3441	1/1	0.93	0.07	19,19,19,19	0
57	MG	1A	3159	1/1	0.93	0.12	34,34,34,34	0
57	MG	2A	3317	1/1	0.93	0.15	32,32,32,32	0
57	MG	2a	1731	1/1	0.93	0.09	45,45,45,45	0
57	MG	2a	1734	1/1	0.93	0.13	47,47,47,47	0
57	MG	1a	1714	1/1	0.93	0.14	62,62,62,62	0
57	MG	2A	3090	1/1	0.93	0.11	45,45,45,45	0
57	MG	2a	1738	1/1	0.93	0.19	49,49,49,49	0
57	MG	2a	1740	1/1	0.93	0.15	64,64,64,64	0
57	MG	2A	3321	1/1	0.93	0.13	37,37,37,37	0
57	MG	2A	3092	1/1	0.93	0.15	56,56,56,56	0
57	MG	2a	1743	1/1	0.93	0.22	59,59,59,59	0
57	MG	2A	3323	1/1	0.93	0.10	40,40,40,40	0
57	MG	2a	1746	1/1	0.93	0.14	62,62,62,62	0
57	MG	2A	3324	1/1	0.93	0.09	29,29,29,29	0
57	MG	2A	3326	1/1	0.93	0.16	46,46,46,46	0
57	MG	2a	1750	1/1	0.93	0.11	60,60,60,60	0
57	MG	2A	3095	1/1	0.93	0.24	62,62,62,62	0
57	MG	2A	3332	1/1	0.93	0.13	50,50,50,50	0
57	MG	2a	1755	1/1	0.93	0.21	57,57,57,57	0
57	MG	1A	3717	1/1	0.93	0.20	55,55,55,55	0
57	MG	2A	3104	1/1	0.93	0.19	55,55,55,55	0
57	MG	1A	3112	1/1	0.93	0.20	42,42,42,42	0
57	MG	2A	3106	1/1	0.93	0.10	46,46,46,46	0
57	MG	1A	3119	1/1	0.93	0.14	47,47,47,47	0
57	MG	2a	1762	1/1	0.93	0.18	65,65,65,65	0
57	MG	1A	3727	1/1	0.93	0.35	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3456	1/1	0.93	0.09	32,32,32,32	0
57	MG	2a	1765	1/1	0.93	0.15	72,72,72,72	0
57	MG	2a	1766	1/1	0.93	0.16	48,48,48,48	0
57	MG	1A	3602	1/1	0.93	0.13	62,62,62,62	0
57	MG	1A	3733	1/1	0.93	0.26	34,34,34,34	0
57	MG	1A	3457	1/1	0.93	0.08	42,42,42,42	0
57	MG	1A	3341	1/1	0.93	0.13	39,39,39,39	0
57	MG	1A	3606	1/1	0.93	0.07	44,44,44,44	0
57	MG	1A	3740	1/1	0.93	0.18	32,32,32,32	0
57	MG	1A	3344	1/1	0.93	0.21	43,43,43,43	0
57	MG	1a	1608	1/1	0.93	0.12	52,52,52,52	0
57	MG	1A	3181	1/1	0.93	0.08	36,36,36,36	0
57	MG	1A	3050	1/1	0.93	0.06	26,26,26,26	0
57	MG	2A	3623	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	3264	1/1	0.93	0.08	32,32,32,32	0
57	MG	1a	1613	1/1	0.93	0.09	47,47,47,47	0
57	MG	2A	3627	1/1	0.93	0.09	61,61,61,61	0
57	MG	2A	3628	1/1	0.93	0.08	54,54,54,54	0
57	MG	1A	3617	1/1	0.93	0.17	49,49,49,49	0
57	MG	2A	3631	1/1	0.93	0.10	56,56,56,56	0
57	MG	2x	106	1/1	0.93	0.18	65,65,65,65	0
57	MG	1a	1748	1/1	0.93	0.18	42,42,42,42	0
57	MG	1a	1722	1/1	0.94	0.16	66,66,66,66	0
57	MG	2A	3109	1/1	0.94	0.09	42,42,42,42	0
57	MG	1A	3687	1/1	0.94	0.23	42,42,42,42	0
57	MG	1P	202	1/1	0.94	0.26	24,24,24,24	0
57	MG	1a	1726	1/1	0.94	0.17	49,49,49,49	0
57	MG	2A	3364	1/1	0.94	0.12	53,53,53,53	0
57	MG	1A	3046	1/1	0.94	0.14	27,27,27,27	0
57	MG	1A	3271	1/1	0.94	0.08	37,37,37,37	0
57	MG	1A	3272	1/1	0.94	0.15	25,25,25,25	0
57	MG	1A	3697	1/1	0.94	0.24	35,35,35,35	0
57	MG	1W	202	1/1	0.94	0.09	35,35,35,35	0
57	MG	2A	3375	1/1	0.94	0.17	44,44,44,44	0
57	MG	1A	3699	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3048	1/1	0.94	0.13	35,35,35,35	0
57	MG	2A	3381	1/1	0.94	0.06	36,36,36,36	0
57	MG	2A	3128	1/1	0.94	0.30	53,53,53,53	0
57	MG	2A	3384	1/1	0.94	0.14	56,56,56,56	0
57	MG	1A	3394	1/1	0.94	0.12	48,48,48,48	0
57	MG	2A	3387	1/1	0.94	0.14	55,55,55,55	0
57	MG	1a	1739	1/1	0.94	0.16	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3177	1/1	0.94	0.31	43,43,43,43	0
57	MG	2A	3394	1/1	0.94	0.06	55,55,55,55	0
57	MG	12	102	1/1	0.94	0.07	49,49,49,49	0
57	MG	1A	3032	1/1	0.94	0.17	34,34,34,34	0
57	MG	1A	3182	1/1	0.94	0.33	29,29,29,29	0
57	MG	1a	1746	1/1	0.94	0.10	49,49,49,49	0
57	MG	1a	1747	1/1	0.94	0.20	41,41,41,41	0
57	MG	15	102	1/1	0.94	0.22	27,27,27,27	0
57	MG	1A	3187	1/1	0.94	0.32	32,32,32,32	0
57	MG	1a	1752	1/1	0.94	0.10	63,63,63,63	0
57	MG	1A	3403	1/1	0.94	0.07	14,14,14,14	0
57	MG	2B	208	1/1	0.94	0.23	47,47,47,47	0
57	MG	1a	1601	1/1	0.94	0.10	52,52,52,52	0
57	MG	1a	1602	1/1	0.94	0.23	56,56,56,56	0
57	MG	2B	211	1/1	0.94	0.13	47,47,47,47	0
57	MG	2A	3150	1/1	0.94	0.08	37,37,37,37	0
57	MG	1A	3560	1/1	0.94	0.07	38,38,38,38	0
57	MG	2A	3414	1/1	0.94	0.14	36,36,36,36	0
57	MG	2D	308	1/1	0.94	0.10	54,54,54,54	0
57	MG	2D	309	1/1	0.94	0.10	64,64,64,64	0
57	MG	1A	3036	1/1	0.94	0.33	30,30,30,30	0
57	MG	1A	3720	1/1	0.94	0.08	39,39,39,39	0
57	MG	1A	3721	1/1	0.94	0.07	25,25,25,25	0
57	MG	2O	3700	1/1	0.94	0.14	45,45,45,45	0
57	MG	1A	3117	1/1	0.94	0.07	36,36,36,36	0
57	MG	1A	3084	1/1	0.94	0.24	50,50,50,50	0
57	MG	1A	3408	1/1	0.94	0.08	34,34,34,34	0
57	MG	1A	3121	1/1	0.94	0.09	36,36,36,36	0
57	MG	1A	3587	1/1	0.94	0.06	16,16,16,16	0
57	MG	2A	3430	1/1	0.94	0.23	53,53,53,53	0
57	MG	2W	201	1/1	0.94	0.10	52,52,52,52	0
57	MG	1A	3192	1/1	0.94	0.23	30,30,30,30	0
57	MG	1A	3193	1/1	0.94	0.07	26,26,26,26	0
57	MG	2A	3165	1/1	0.94	0.20	42,42,42,42	0
57	MG	2Y	201	1/1	0.94	0.09	55,55,55,55	0
57	MG	1A	3038	1/1	0.94	0.16	36,36,36,36	0
57	MG	2A	3169	1/1	0.94	0.24	44,44,44,44	0
57	MG	2A	3441	1/1	0.94	0.10	51,51,51,51	0
57	MG	25	101	1/1	0.94	0.11	58,58,58,58	0
57	MG	2A	3442	1/1	0.94	0.07	34,34,34,34	0
57	MG	1A	3299	1/1	0.94	0.08	42,42,42,42	0
57	MG	1A	3593	1/1	0.94	0.07	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3001	1/1	0.94	0.10	26,26,26,26	0
57	MG	2A	3451	1/1	0.94	0.11	38,38,38,38	0
57	MG	2A	3452	1/1	0.94	0.11	42,42,42,42	0
57	MG	2A	3453	1/1	0.94	0.10	41,41,41,41	0
57	MG	2a	1608	1/1	0.94	0.14	63,63,63,63	0
57	MG	1A	3124	1/1	0.94	0.20	36,36,36,36	0
57	MG	2A	3457	1/1	0.94	0.15	54,54,54,54	0
57	MG	2A	3175	1/1	0.94	0.10	51,51,51,51	0
57	MG	1a	1777	1/1	0.94	0.16	57,57,57,57	0
57	MG	1A	3597	1/1	0.94	0.11	28,28,28,28	0
57	MG	1A	3439	1/1	0.94	0.18	52,52,52,52	0
57	MG	1a	1780	1/1	0.94	0.06	43,43,43,43	0
57	MG	1A	3310	1/1	0.94	0.07	31,31,31,31	0
57	MG	2A	3184	1/1	0.94	0.13	51,51,51,51	0
57	MG	2a	1622	1/1	0.94	0.19	58,58,58,58	0
57	MG	1A	3129	1/1	0.94	0.29	36,36,36,36	0
57	MG	1A	3447	1/1	0.94	0.09	17,17,17,17	0
57	MG	2A	3187	1/1	0.94	0.33	58,58,58,58	0
57	MG	2A	3189	1/1	0.94	0.28	61,61,61,61	0
57	MG	1a	1784	1/1	0.94	0.21	51,51,51,51	0
57	MG	1a	1786	1/1	0.94	0.17	44,44,44,44	0
57	MG	1A	3449	1/1	0.94	0.13	55,55,55,55	0
57	MG	1A	3756	1/1	0.94	0.09	29,29,29,29	0
57	MG	1A	3607	1/1	0.94	0.09	24,24,24,24	0
57	MG	2A	3479	1/1	0.94	0.15	60,60,60,60	0
57	MG	2A	3480	1/1	0.94	0.17	48,48,48,48	0
57	MG	1v	103	1/1	0.94	0.15	78,78,78,78	0
57	MG	1A	3212	1/1	0.94	0.16	45,45,45,45	0
57	MG	2A	3483	1/1	0.94	0.08	51,51,51,51	0
57	MG	2a	1641	1/1	0.94	0.10	58,58,58,58	0
57	MG	1A	3454	1/1	0.94	0.07	28,28,28,28	0
57	MG	2A	3485	1/1	0.94	0.14	62,62,62,62	0
57	MG	1A	3317	1/1	0.94	0.18	61,61,61,61	0
57	MG	1x	102	1/1	0.94	0.11	51,51,51,51	0
57	MG	1x	103	1/1	0.94	0.12	60,60,60,60	0
57	MG	2a	1647	1/1	0.94	0.13	63,63,63,63	0
57	MG	1a	1641	1/1	0.94	0.11	44,44,44,44	0
57	MG	2a	1649	1/1	0.94	0.17	59,59,59,59	0
57	MG	2A	3206	1/1	0.94	0.20	55,55,55,55	0
57	MG	2A	3495	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3764	1/1	0.94	0.08	50,50,50,50	0
57	MG	2a	1656	1/1	0.94	0.23	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3209	1/1	0.94	0.11	63,63,63,63	0
57	MG	2A	3499	1/1	0.94	0.10	58,58,58,58	0
57	MG	1A	3324	1/1	0.94	0.10	26,26,26,26	0
57	MG	1A	3132	1/1	0.94	0.24	28,28,28,28	0
57	MG	2a	1661	1/1	0.94	0.12	53,53,53,53	0
57	MG	2a	1662	1/1	0.94	0.09	62,62,62,62	0
57	MG	2A	3502	1/1	0.94	0.13	53,53,53,53	0
57	MG	1A	3458	1/1	0.94	0.09	24,24,24,24	0
57	MG	1A	3220	1/1	0.94	0.25	46,46,46,46	0
57	MG	1A	3772	1/1	0.94	0.13	52,52,52,52	0
57	MG	2A	3218	1/1	0.94	0.09	45,45,45,45	0
57	MG	2A	3007	1/1	0.94	0.08	39,39,39,39	0
57	MG	2A	3009	1/1	0.94	0.16	57,57,57,57	0
57	MG	2a	1670	1/1	0.94	0.20	61,61,61,61	0
57	MG	2A	3011	1/1	0.94	0.13	43,43,43,43	0
57	MG	1a	1650	1/1	0.94	0.13	54,54,54,54	0
57	MG	2A	3017	1/1	0.94	0.08	55,55,55,55	0
57	MG	2A	3517	1/1	0.94	0.21	55,55,55,55	0
57	MG	1A	3620	1/1	0.94	0.06	19,19,19,19	0
57	MG	2A	3230	1/1	0.94	0.53	47,47,47,47	0
57	MG	2a	1678	1/1	0.94	0.08	70,70,70,70	0
57	MG	2A	3232	1/1	0.94	0.33	43,43,43,43	0
57	MG	1A	3621	1/1	0.94	0.10	42,42,42,42	0
57	MG	2A	3524	1/1	0.94	0.09	40,40,40,40	0
57	MG	2A	3023	1/1	0.94	0.13	52,52,52,52	0
57	MG	1A	3329	1/1	0.94	0.07	21,21,21,21	0
57	MG	1A	3777	1/1	0.94	0.15	51,51,51,51	0
57	MG	1A	3463	1/1	0.94	0.10	19,19,19,19	0
57	MG	1A	3334	1/1	0.94	0.09	33,33,33,33	0
57	MG	2A	3028	1/1	0.94	0.17	38,38,38,38	0
57	MG	1A	3089	1/1	0.94	0.27	48,48,48,48	0
57	MG	1A	3468	1/1	0.94	0.09	39,39,39,39	0
57	MG	1A	3469	1/1	0.94	0.11	32,32,32,32	0
57	MG	2A	3253	1/1	0.94	0.07	46,46,46,46	0
57	MG	2a	1697	1/1	0.94	0.15	58,58,58,58	0
57	MG	1a	1662	1/1	0.94	0.15	61,61,61,61	0
57	MG	2a	1700	1/1	0.94	0.09	57,57,57,57	0
57	MG	1A	3788	1/1	0.94	0.08	37,37,37,37	0
57	MG	1a	1666	1/1	0.94	0.12	47,47,47,47	0
57	MG	2A	3259	1/1	0.94	0.08	46,46,46,46	0
57	MG	2A	3260	1/1	0.94	0.14	62,62,62,62	0
57	MG	1A	3222	1/1	0.94	0.10	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1709	1/1	0.94	0.07	53,53,53,53	0
57	MG	1A	3060	1/1	0.94	0.11	37,37,37,37	0
57	MG	2a	1712	1/1	0.94	0.12	57,57,57,57	0
57	MG	2A	3551	1/1	0.94	0.07	64,64,64,64	0
57	MG	2A	3263	1/1	0.94	0.12	66,66,66,66	0
57	MG	1A	3792	1/1	0.94	0.07	40,40,40,40	0
57	MG	1A	3475	1/1	0.94	0.17	42,42,42,42	0
57	MG	1A	3094	1/1	0.94	0.16	40,40,40,40	0
57	MG	2a	1718	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3270	1/1	0.94	0.11	53,53,53,53	0
57	MG	1A	3639	1/1	0.94	0.09	45,45,45,45	0
57	MG	1A	3480	1/1	0.94	0.10	45,45,45,45	0
57	MG	2a	1724	1/1	0.94	0.12	55,55,55,55	0
57	MG	1A	3095	1/1	0.94	0.12	35,35,35,35	0
57	MG	1a	1677	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3040	1/1	0.94	0.15	36,36,36,36	0
57	MG	2A	3280	1/1	0.94	0.14	52,52,52,52	0
57	MG	2A	3053	1/1	0.94	0.21	65,65,65,65	0
57	MG	2A	3054	1/1	0.94	0.21	57,57,57,57	0
57	MG	1A	3142	1/1	0.94	0.28	31,31,31,31	0
57	MG	2A	3573	1/1	0.94	0.09	53,53,53,53	0
57	MG	2A	3574	1/1	0.94	0.07	47,47,47,47	0
57	MG	1A	3358	1/1	0.94	0.19	40,40,40,40	0
57	MG	2a	1739	1/1	0.94	0.13	67,67,67,67	0
57	MG	1A	3236	1/1	0.94	0.30	35,35,35,35	0
57	MG	1A	3494	1/1	0.94	0.13	43,43,43,43	0
57	MG	1A	3238	1/1	0.94	0.36	35,35,35,35	0
57	MG	2A	3582	1/1	0.94	0.09	58,58,58,58	0
57	MG	2A	3062	1/1	0.94	0.11	53,53,53,53	0
57	MG	2A	3065	1/1	0.94	0.14	46,46,46,46	0
57	MG	1B	206	1/1	0.94	0.14	30,30,30,30	0
57	MG	1A	3244	1/1	0.94	0.08	38,38,38,38	0
57	MG	1a	1689	1/1	0.94	0.17	61,61,61,61	0
57	MG	2a	1751	1/1	0.94	0.18	53,53,53,53	0
57	MG	1A	3145	1/1	0.94	0.15	27,27,27,27	0
57	MG	2a	1753	1/1	0.94	0.20	56,56,56,56	0
57	MG	2A	3309	1/1	0.94	0.08	39,39,39,39	0
57	MG	2A	3310	1/1	0.94	0.07	48,48,48,48	0
57	MG	2A	3592	1/1	0.94	0.15	53,53,53,53	0
57	MG	2A	3073	1/1	0.94	0.07	46,46,46,46	0
57	MG	2A	3316	1/1	0.94	0.12	46,46,46,46	0
57	MG	1A	3248	1/1	0.94	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3599	1/1	0.94	0.09	49,49,49,49	0
57	MG	1A	3512	1/1	0.94	0.06	21,21,21,21	0
57	MG	1a	1694	1/1	0.94	0.10	59,59,59,59	0
57	MG	1B	214	1/1	0.94	0.06	42,42,42,42	0
57	MG	2A	3604	1/1	0.94	0.12	50,50,50,50	0
57	MG	2A	3079	1/1	0.94	0.06	30,30,30,30	0
57	MG	2a	1767	1/1	0.94	0.15	53,53,53,53	0
57	MG	2A	3607	1/1	0.94	0.12	61,61,61,61	0
57	MG	1A	3063	1/1	0.94	0.06	24,24,24,24	0
57	MG	1A	3152	1/1	0.94	0.13	30,30,30,30	0
57	MG	1A	3257	1/1	0.94	0.09	34,34,34,34	0
57	MG	1A	3258	1/1	0.94	0.20	37,37,37,37	0
57	MG	2A	3328	1/1	0.94	0.09	59,59,59,59	0
57	MG	2A	3614	1/1	0.94	0.09	41,41,41,41	0
57	MG	2A	3085	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	3044	1/1	0.94	0.11	41,41,41,41	0
57	MG	1A	3675	1/1	0.94	0.06	60,60,60,60	0
57	MG	2A	3337	1/1	0.94	0.11	34,34,34,34	0
57	MG	1A	3154	1/1	0.94	0.16	40,40,40,40	0
57	MG	2A	3093	1/1	0.94	0.08	58,58,58,58	0
57	MG	2w	402	1/1	0.94	0.16	62,62,62,62	0
57	MG	1A	3065	1/1	0.94	0.21	25,25,25,25	0
57	MG	1A	3533	1/1	0.94	0.07	19,19,19,19	0
57	MG	2A	3099	1/1	0.94	0.12	53,53,53,53	0
57	MG	1A	3682	1/1	0.94	0.14	26,26,26,26	0
57	MG	1N	204	1/1	0.94	0.09	38,38,38,38	0
57	MG	1A	3005	1/1	0.94	0.12	48,48,48,48	0
57	MG	1A	3387	1/1	0.95	0.07	63,63,63,63	0
57	MG	2A	3087	1/1	0.95	0.12	44,44,44,44	0
57	MG	2A	3630	1/1	0.95	0.08	51,51,51,51	0
57	MG	2A	3089	1/1	0.95	0.13	43,43,43,43	0
57	MG	1A	3511	1/1	0.95	0.10	38,38,38,38	0
57	MG	2A	3351	1/1	0.95	0.11	40,40,40,40	0
57	MG	1A	3205	1/1	0.95	0.09	32,32,32,32	0
57	MG	1A	3390	1/1	0.95	0.23	42,42,42,42	0
57	MG	1A	3206	1/1	0.95	0.14	27,27,27,27	0
57	MG	2A	3637	1/1	0.95	0.12	38,38,38,38	0
57	MG	1A	3150	1/1	0.95	0.19	46,46,46,46	0
57	MG	1a	1704	1/1	0.95	0.07	64,64,64,64	0
57	MG	2A	3360	1/1	0.95	0.12	50,50,50,50	0
57	MG	2A	3101	1/1	0.95	0.08	46,46,46,46	0
57	MG	2A	3103	1/1	0.95	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1705	1/1	0.95	0.11	51,51,51,51	0
57	MG	1A	3659	1/1	0.95	0.07	30,30,30,30	0
57	MG	1B	207	1/1	0.95	0.10	33,33,33,33	0
57	MG	2A	3650	1/1	0.95	0.08	64,64,64,64	0
57	MG	2A	3651	1/1	0.95	0.10	61,61,61,61	0
57	MG	1a	1709	1/1	0.95	0.22	46,46,46,46	0
57	MG	1A	3284	1/1	0.95	0.07	20,20,20,20	0
57	MG	1A	3663	1/1	0.95	0.04	29,29,29,29	0
57	MG	2A	3376	1/1	0.95	0.16	45,45,45,45	0
57	MG	1A	3082	1/1	0.95	0.19	28,28,28,28	0
57	MG	1a	1716	1/1	0.95	0.17	60,60,60,60	0
57	MG	1A	3665	1/1	0.95	0.07	54,54,54,54	0
57	MG	1A	3667	1/1	0.95	0.08	36,36,36,36	0
57	MG	1B	215	1/1	0.95	0.09	34,34,34,34	0
57	MG	1A	3522	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3214	1/1	0.95	0.21	52,52,52,52	0
57	MG	2A	3389	1/1	0.95	0.08	64,64,64,64	0
57	MG	2A	3125	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3391	1/1	0.95	0.10	41,41,41,41	0
57	MG	1a	1723	1/1	0.95	0.17	50,50,50,50	0
57	MG	1A	3216	1/1	0.95	0.11	36,36,36,36	0
57	MG	2B	207	1/1	0.95	0.14	54,54,54,54	0
57	MG	1A	3532	1/1	0.95	0.14	22,22,22,22	0
57	MG	1A	3120	1/1	0.95	0.17	41,41,41,41	0
57	MG	1a	1728	1/1	0.95	0.08	51,51,51,51	0
57	MG	2A	3398	1/1	0.95	0.06	27,27,27,27	0
57	MG	1A	3009	1/1	0.95	0.07	21,21,21,21	0
57	MG	2D	304	1/1	0.95	0.49	46,46,46,46	0
57	MG	2A	3400	1/1	0.95	0.10	57,57,57,57	0
57	MG	1F	304	1/1	0.95	0.18	27,27,27,27	0
57	MG	2A	3402	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3004	1/1	0.95	0.09	31,31,31,31	0
57	MG	2E	303	1/1	0.95	0.15	48,48,48,48	0
57	MG	2A	3136	1/1	0.95	0.12	57,57,57,57	0
57	MG	2F	302	1/1	0.95	0.09	40,40,40,40	0
57	MG	1G	201	1/1	0.95	0.12	54,54,54,54	0
57	MG	1G	203	1/1	0.95	0.14	41,41,41,41	0
57	MG	2A	3139	1/1	0.95	0.27	56,56,56,56	0
57	MG	1A	3155	1/1	0.95	0.12	23,23,23,23	0
57	MG	2A	3411	1/1	0.95	0.17	45,45,45,45	0
57	MG	1A	3223	1/1	0.95	0.17	30,30,30,30	0
57	MG	1A	3680	1/1	0.95	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3308	1/1	0.95	0.09	44,44,44,44	0
57	MG	1O	201	1/1	0.95	0.13	58,58,58,58	0
57	MG	2A	3145	1/1	0.95	0.07	44,44,44,44	0
57	MG	2A	3146	1/1	0.95	0.15	56,56,56,56	0
57	MG	1A	3413	1/1	0.95	0.08	23,23,23,23	0
57	MG	1A	3686	1/1	0.95	0.12	55,55,55,55	0
57	MG	2A	3149	1/1	0.95	0.14	48,48,48,48	0
57	MG	2A	3424	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	3417	1/1	0.95	0.06	26,26,26,26	0
57	MG	2A	3427	1/1	0.95	0.09	48,48,48,48	0
57	MG	1a	1745	1/1	0.95	0.16	54,54,54,54	0
57	MG	1A	3688	1/1	0.95	0.19	56,56,56,56	0
57	MG	28	103	1/1	0.95	0.10	48,48,48,48	0
57	MG	1Q	201	1/1	0.95	0.22	38,38,38,38	0
57	MG	2A	3154	1/1	0.95	0.09	36,36,36,36	0
57	MG	1Q	203	1/1	0.95	0.13	34,34,34,34	0
57	MG	2A	3436	1/1	0.95	0.15	51,51,51,51	0
57	MG	1a	1749	1/1	0.95	0.06	40,40,40,40	0
57	MG	1A	3418	1/1	0.95	0.07	24,24,24,24	0
57	MG	1a	1751	1/1	0.95	0.12	68,68,68,68	0
57	MG	1T	201	1/1	0.95	0.08	37,37,37,37	0
57	MG	1A	3550	1/1	0.95	0.09	23,23,23,23	0
57	MG	2A	3445	1/1	0.95	0.06	60,60,60,60	0
57	MG	2A	3447	1/1	0.95	0.12	41,41,41,41	0
57	MG	1A	3691	1/1	0.95	0.10	48,48,48,48	0
57	MG	1U	204	1/1	0.95	0.12	28,28,28,28	0
57	MG	1V	204	1/1	0.95	0.20	44,44,44,44	0
57	MG	1A	3692	1/1	0.95	0.11	18,18,18,18	0
57	MG	2a	1618	1/1	0.95	0.12	56,56,56,56	0
57	MG	1X	101	1/1	0.95	0.09	41,41,41,41	0
57	MG	2a	1621	1/1	0.95	0.25	50,50,50,50	0
57	MG	1A	3420	1/1	0.95	0.08	24,24,24,24	0
57	MG	2A	3456	1/1	0.95	0.09	61,61,61,61	0
57	MG	1Z	302	1/1	0.95	0.14	40,40,40,40	0
57	MG	10	101	1/1	0.95	0.16	27,27,27,27	0
57	MG	1A	3422	1/1	0.95	0.08	34,34,34,34	0
57	MG	2a	1628	1/1	0.95	0.19	39,39,39,39	0
57	MG	11	102	1/1	0.95	0.38	42,42,42,42	0
57	MG	1A	3022	1/1	0.95	0.05	26,26,26,26	0
57	MG	1a	1768	1/1	0.95	0.06	42,42,42,42	0
57	MG	1A	3557	1/1	0.95	0.07	17,17,17,17	0
57	MG	2A	3179	1/1	0.95	0.15	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1770	1/1	0.95	0.11	42,42,42,42	0
57	MG	1A	3226	1/1	0.95	0.10	34,34,34,34	0
57	MG	1A	3702	1/1	0.95	0.13	46,46,46,46	0
57	MG	1A	3561	1/1	0.95	0.06	62,62,62,62	0
57	MG	1A	3704	1/1	0.95	0.14	21,21,21,21	0
57	MG	1A	3562	1/1	0.95	0.06	25,25,25,25	0
57	MG	15	104	1/1	0.95	0.16	29,29,29,29	0
57	MG	16	101	1/1	0.95	0.10	46,46,46,46	0
57	MG	17	103	1/1	0.95	0.18	32,32,32,32	0
57	MG	17	105	1/1	0.95	0.11	30,30,30,30	0
57	MG	1A	3568	1/1	0.95	0.06	22,22,22,22	0
57	MG	18	102	1/1	0.95	0.12	34,34,34,34	0
57	MG	1A	3088	1/1	0.95	0.08	62,62,62,62	0
57	MG	1A	3316	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3713	1/1	0.95	0.05	36,36,36,36	0
57	MG	1A	3715	1/1	0.95	0.18	60,60,60,60	0
57	MG	1A	3581	1/1	0.95	0.09	22,22,22,22	0
57	MG	2a	1654	1/1	0.95	0.31	57,57,57,57	0
57	MG	2A	3487	1/1	0.95	0.20	48,48,48,48	0
57	MG	2A	3488	1/1	0.95	0.15	47,47,47,47	0
57	MG	1A	3161	1/1	0.95	0.12	32,32,32,32	0
57	MG	2A	3202	1/1	0.95	0.25	56,56,56,56	0
57	MG	2A	3203	1/1	0.95	0.25	53,53,53,53	0
57	MG	2A	3492	1/1	0.95	0.09	42,42,42,42	0
57	MG	1d	301	1/1	0.95	0.23	37,37,37,37	0
57	MG	2A	3494	1/1	0.95	0.06	44,44,44,44	0
57	MG	1k	201	1/1	0.95	0.12	53,53,53,53	0
57	MG	2A	3496	1/1	0.95	0.19	29,29,29,29	0
57	MG	1n	101	1/1	0.95	0.20	62,62,62,62	0
57	MG	2A	3208	1/1	0.95	0.11	48,48,48,48	0
57	MG	1A	3718	1/1	0.95	0.07	42,42,42,42	0
57	MG	1v	102	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3322	1/1	0.95	0.09	41,41,41,41	0
57	MG	1A	3162	1/1	0.95	0.08	25,25,25,25	0
57	MG	2a	1672	1/1	0.95	0.14	47,47,47,47	0
57	MG	1A	3722	1/1	0.95	0.09	36,36,36,36	0
57	MG	1A	3723	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	3586	1/1	0.95	0.06	56,56,56,56	0
57	MG	1A	3171	1/1	0.95	0.13	37,37,37,37	0
57	MG	1A	3106	1/1	0.95	0.16	42,42,42,42	0
57	MG	1A	3444	1/1	0.95	0.06	23,23,23,23	0
57	MG	1A	3445	1/1	0.95	0.07	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3226	1/1	0.95	0.26	43,43,43,43	0
57	MG	1A	3130	1/1	0.95	0.33	22,22,22,22	0
57	MG	2A	3516	1/1	0.95	0.15	45,45,45,45	0
57	MG	1A	3072	1/1	0.95	0.30	47,47,47,47	0
57	MG	1A	3335	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3595	1/1	0.95	0.05	38,38,38,38	0
57	MG	1A	3246	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3179	1/1	0.95	0.14	43,43,43,43	0
57	MG	1A	3742	1/1	0.95	0.10	38,38,38,38	0
57	MG	1a	1630	1/1	0.95	0.18	51,51,51,51	0
57	MG	2A	3016	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3598	1/1	0.95	0.06	45,45,45,45	0
57	MG	2a	1695	1/1	0.95	0.09	48,48,48,48	0
57	MG	2A	3242	1/1	0.95	0.11	60,60,60,60	0
57	MG	2A	3530	1/1	0.95	0.08	55,55,55,55	0
57	MG	1A	3340	1/1	0.95	0.14	46,46,46,46	0
57	MG	1A	3601	1/1	0.95	0.07	41,41,41,41	0
57	MG	2a	1702	1/1	0.95	0.13	65,65,65,65	0
57	MG	2A	3247	1/1	0.95	0.17	48,48,48,48	0
57	MG	2a	1705	1/1	0.95	0.12	55,55,55,55	0
57	MG	1a	1636	1/1	0.95	0.18	49,49,49,49	0
57	MG	1A	3073	1/1	0.95	0.29	46,46,46,46	0
57	MG	1A	3342	1/1	0.95	0.09	39,39,39,39	0
57	MG	2A	3254	1/1	0.95	0.11	28,28,28,28	0
57	MG	1A	3752	1/1	0.95	0.12	58,58,58,58	0
57	MG	1A	3134	1/1	0.95	0.14	27,27,27,27	0
57	MG	1A	3184	1/1	0.95	0.06	50,50,50,50	0
57	MG	1a	1644	1/1	0.95	0.18	49,49,49,49	0
57	MG	2A	3031	1/1	0.95	0.06	47,47,47,47	0
57	MG	1A	3135	1/1	0.95	0.08	29,29,29,29	0
57	MG	1A	3609	1/1	0.95	0.08	33,33,33,33	0
57	MG	1A	3109	1/1	0.95	0.17	49,49,49,49	0
57	MG	1A	3760	1/1	0.95	0.07	18,18,18,18	0
57	MG	1A	3023	1/1	0.95	0.18	45,45,45,45	0
57	MG	1A	3260	1/1	0.95	0.27	49,49,49,49	0
57	MG	2A	3038	1/1	0.95	0.14	46,46,46,46	0
57	MG	2a	1725	1/1	0.95	0.14	46,46,46,46	0
57	MG	2A	3271	1/1	0.95	0.09	48,48,48,48	0
57	MG	2A	3272	1/1	0.95	0.08	40,40,40,40	0
57	MG	2A	3562	1/1	0.95	0.15	31,31,31,31	0
57	MG	2A	3273	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3014	1/1	0.95	0.07	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3275	1/1	0.95	0.11	48,48,48,48	0
57	MG	2a	1732	1/1	0.95	0.13	54,54,54,54	0
57	MG	2a	1733	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3113	1/1	0.95	0.13	35,35,35,35	0
57	MG	2A	3042	1/1	0.95	0.16	48,48,48,48	0
57	MG	1A	3766	1/1	0.95	0.18	43,43,43,43	0
57	MG	1a	1655	1/1	0.95	0.32	60,60,60,60	0
57	MG	2A	3047	1/1	0.95	0.21	57,57,57,57	0
57	MG	1A	3471	1/1	0.95	0.11	50,50,50,50	0
57	MG	1A	3769	1/1	0.95	0.26	46,46,46,46	0
57	MG	1A	3472	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3141	1/1	0.95	0.10	32,32,32,32	0
57	MG	1A	3266	1/1	0.95	0.18	31,31,31,31	0
57	MG	2a	1745	1/1	0.95	0.15	63,63,63,63	0
57	MG	1A	3365	1/1	0.95	0.15	39,39,39,39	0
57	MG	1A	3774	1/1	0.95	0.24	28,28,28,28	0
57	MG	2A	3293	1/1	0.95	0.15	54,54,54,54	0
57	MG	1A	3479	1/1	0.95	0.17	30,30,30,30	0
57	MG	2A	3056	1/1	0.95	0.13	64,64,64,64	0
57	MG	2A	3297	1/1	0.95	0.14	41,41,41,41	0
57	MG	1A	3098	1/1	0.95	0.19	35,35,35,35	0
57	MG	2A	3299	1/1	0.95	0.06	57,57,57,57	0
57	MG	2A	3300	1/1	0.95	0.09	27,27,27,27	0
57	MG	1A	3118	1/1	0.95	0.19	45,45,45,45	0
57	MG	2A	3304	1/1	0.95	0.09	34,34,34,34	0
57	MG	1A	3146	1/1	0.95	0.24	40,40,40,40	0
57	MG	2A	3306	1/1	0.95	0.15	62,62,62,62	0
57	MG	1A	3630	1/1	0.95	0.09	45,45,45,45	0
57	MG	2A	3600	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3489	1/1	0.95	0.09	39,39,39,39	0
57	MG	2A	3063	1/1	0.95	0.15	42,42,42,42	0
57	MG	2A	3064	1/1	0.95	0.14	54,54,54,54	0
57	MG	1A	3782	1/1	0.95	0.15	55,55,55,55	0
57	MG	2A	3605	1/1	0.95	0.17	61,61,61,61	0
57	MG	1A	3273	1/1	0.95	0.13	28,28,28,28	0
57	MG	1A	3149	1/1	0.95	0.24	35,35,35,35	0
57	MG	2A	3070	1/1	0.95	0.06	47,47,47,47	0
57	MG	1A	3787	1/1	0.95	0.06	20,20,20,20	0
57	MG	1A	3198	1/1	0.95	0.08	48,48,48,48	0
57	MG	1A	3277	1/1	0.95	0.13	28,28,28,28	0
57	MG	1A	3638	1/1	0.95	0.36	26,26,26,26	0
57	MG	2A	3325	1/1	0.95	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3200	1/1	0.95	0.07	33,33,33,33	0
57	MG	2k	202	1/1	0.95	0.07	72,72,72,72	0
57	MG	2A	3616	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3640	1/1	0.95	0.13	34,34,34,34	0
57	MG	1A	3498	1/1	0.95	0.11	42,42,42,42	0
57	MG	1A	3797	1/1	0.95	0.08	40,40,40,40	0
57	MG	2w	401	1/1	0.95	0.07	38,38,38,38	0
57	MG	2A	3080	1/1	0.95	0.12	52,52,52,52	0
57	MG	1A	3202	1/1	0.95	0.40	31,31,31,31	0
57	MG	1A	3799	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3280	1/1	0.95	0.12	33,33,33,33	0
57	MG	1A	3803	1/1	0.95	0.08	35,35,35,35	0
57	MG	1A	3507	1/1	0.95	0.05	39,39,39,39	0
57	MG	2A	3342	1/1	0.95	0.07	40,40,40,40	0
57	MG	1F	302	1/1	0.96	0.26	34,34,34,34	0
57	MG	2D	303	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3313	1/1	0.96	0.06	18,18,18,18	0
57	MG	1A	3473	1/1	0.96	0.10	52,52,52,52	0
57	MG	2A	3235	1/1	0.96	0.16	48,48,48,48	0
57	MG	2A	3460	1/1	0.96	0.17	65,65,65,65	0
57	MG	1A	3055	1/1	0.96	0.16	14,14,14,14	0
57	MG	2E	301	1/1	0.96	0.12	46,46,46,46	0
57	MG	2E	302	1/1	0.96	0.15	44,44,44,44	0
57	MG	1G	202	1/1	0.96	0.11	35,35,35,35	0
57	MG	2A	3238	1/1	0.96	0.06	44,44,44,44	0
57	MG	2F	301	1/1	0.96	0.09	39,39,39,39	0
57	MG	1a	1695	1/1	0.96	0.12	34,34,34,34	0
57	MG	1A	3174	1/1	0.96	0.16	29,29,29,29	0
57	MG	1A	3207	1/1	0.96	0.09	17,17,17,17	0
57	MG	2F	306	1/1	0.96	0.12	44,44,44,44	0
57	MG	2N	201	1/1	0.96	0.05	41,41,41,41	0
57	MG	1A	3478	1/1	0.96	0.09	65,65,65,65	0
57	MG	1A	3208	1/1	0.96	0.05	29,29,29,29	0
57	MG	2Q	202	1/1	0.96	0.06	51,51,51,51	0
57	MG	1A	3398	1/1	0.96	0.10	49,49,49,49	0
57	MG	2A	3246	1/1	0.96	0.12	50,50,50,50	0
57	MG	1A	3712	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3483	1/1	0.96	0.12	42,42,42,42	0
57	MG	2A	3061	1/1	0.96	0.11	47,47,47,47	0
57	MG	2A	3475	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3714	1/1	0.96	0.07	30,30,30,30	0
57	MG	2A	3477	1/1	0.96	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3600	1/1	0.96	0.06	32,32,32,32	0
57	MG	1P	203	1/1	0.96	0.26	37,37,37,37	0
57	MG	1A	3319	1/1	0.96	0.07	48,48,48,48	0
57	MG	20	102	1/1	0.96	0.09	53,53,53,53	0
57	MG	1a	1713	1/1	0.96	0.13	58,58,58,58	0
57	MG	1A	3486	1/1	0.96	0.13	41,41,41,41	0
57	MG	23	102	1/1	0.96	0.11	50,50,50,50	0
57	MG	1A	3400	1/1	0.96	0.05	18,18,18,18	0
57	MG	1Q	204	1/1	0.96	0.12	41,41,41,41	0
57	MG	28	102	1/1	0.96	0.07	67,67,67,67	0
57	MG	1A	3024	1/1	0.96	0.06	23,23,23,23	0
57	MG	1A	3143	1/1	0.96	0.09	29,29,29,29	0
57	MG	2a	1601	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3213	1/1	0.96	0.12	29,29,29,29	0
57	MG	1A	3608	1/1	0.96	0.14	57,57,57,57	0
57	MG	1A	3178	1/1	0.96	0.18	36,36,36,36	0
57	MG	2A	3269	1/1	0.96	0.04	30,30,30,30	0
57	MG	2A	3077	1/1	0.96	0.13	47,47,47,47	0
57	MG	1V	202	1/1	0.96	0.14	26,26,26,26	0
57	MG	1A	3725	1/1	0.96	0.08	32,32,32,32	0
57	MG	1A	3405	1/1	0.96	0.11	35,35,35,35	0
57	MG	1W	204	1/1	0.96	0.07	40,40,40,40	0
57	MG	1A	3033	1/1	0.96	0.09	24,24,24,24	0
57	MG	1A	3497	1/1	0.96	0.12	43,43,43,43	0
57	MG	1A	3330	1/1	0.96	0.12	54,54,54,54	0
57	MG	1A	3218	1/1	0.96	0.19	40,40,40,40	0
57	MG	1A	3409	1/1	0.96	0.10	39,39,39,39	0
57	MG	10	103	1/1	0.96	0.12	48,48,48,48	0
57	MG	2a	1619	1/1	0.96	0.06	55,55,55,55	0
57	MG	10	105	1/1	0.96	0.13	46,46,46,46	0
57	MG	2A	3282	1/1	0.96	0.10	45,45,45,45	0
57	MG	2A	3283	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3737	1/1	0.96	0.10	33,33,33,33	0
57	MG	1A	3180	1/1	0.96	0.10	47,47,47,47	0
57	MG	1A	3412	1/1	0.96	0.06	26,26,26,26	0
57	MG	1A	3027	1/1	0.96	0.18	28,28,28,28	0
57	MG	2a	1627	1/1	0.96	0.28	55,55,55,55	0
57	MG	1A	3416	1/1	0.96	0.07	15,15,15,15	0
57	MG	2A	3289	1/1	0.96	0.10	38,38,38,38	0
57	MG	1A	3513	1/1	0.96	0.11	28,28,28,28	0
57	MG	1A	3743	1/1	0.96	0.12	22,22,22,22	0
57	MG	2A	3102	1/1	0.96	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3080	1/1	0.96	0.12	11,11,11,11	0
57	MG	1A	3625	1/1	0.96	0.15	30,30,30,30	0
57	MG	1A	3062	1/1	0.96	0.08	31,31,31,31	0
57	MG	2A	3522	1/1	0.96	0.08	63,63,63,63	0
57	MG	2a	1638	1/1	0.96	0.15	73,73,73,73	0
57	MG	1A	3627	1/1	0.96	0.05	37,37,37,37	0
57	MG	1A	3037	1/1	0.96	0.17	28,28,28,28	0
57	MG	2A	3301	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	3006	1/1	0.96	0.08	42,42,42,42	0
57	MG	2A	3527	1/1	0.96	0.07	62,62,62,62	0
57	MG	1A	3631	1/1	0.96	0.10	34,34,34,34	0
57	MG	2A	3111	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3519	1/1	0.96	0.19	35,35,35,35	0
57	MG	1A	3343	1/1	0.96	0.08	39,39,39,39	0
57	MG	2A	3308	1/1	0.96	0.06	47,47,47,47	0
57	MG	1a	1755	1/1	0.96	0.16	54,54,54,54	0
57	MG	1A	3225	1/1	0.96	0.07	32,32,32,32	0
57	MG	1A	3015	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3759	1/1	0.96	0.08	26,26,26,26	0
57	MG	1a	1606	1/1	0.96	0.10	34,34,34,34	0
57	MG	2a	1655	1/1	0.96	0.28	52,52,52,52	0
57	MG	2A	3124	1/1	0.96	0.20	39,39,39,39	0
57	MG	1A	3087	1/1	0.96	0.05	20,20,20,20	0
57	MG	1A	3525	1/1	0.96	0.05	36,36,36,36	0
57	MG	1A	3051	1/1	0.96	0.12	23,23,23,23	0
57	MG	2A	3545	1/1	0.96	0.09	90,90,90,90	0
57	MG	1A	3434	1/1	0.96	0.06	26,26,26,26	0
57	MG	2A	3547	1/1	0.96	0.06	51,51,51,51	0
57	MG	1A	3534	1/1	0.96	0.10	32,32,32,32	0
57	MG	2A	3550	1/1	0.96	0.12	51,51,51,51	0
57	MG	1a	1766	1/1	0.96	0.06	49,49,49,49	0
57	MG	1A	3357	1/1	0.96	0.08	20,20,20,20	0
57	MG	2A	3132	1/1	0.96	0.13	28,28,28,28	0
57	MG	1A	3438	1/1	0.96	0.10	37,37,37,37	0
57	MG	1A	3768	1/1	0.96	0.15	15,15,15,15	0
57	MG	1A	3002	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3069	1/1	0.96	0.08	24,24,24,24	0
57	MG	2A	3336	1/1	0.96	0.09	54,54,54,54	0
57	MG	2A	3560	1/1	0.96	0.09	52,52,52,52	0
57	MG	2A	3561	1/1	0.96	0.17	29,29,29,29	0
57	MG	1A	3234	1/1	0.96	0.23	32,32,32,32	0
57	MG	2A	3563	1/1	0.96	0.07	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3338	1/1	0.96	0.07	45,45,45,45	0
57	MG	1a	1621	1/1	0.96	0.07	52,52,52,52	0
57	MG	1A	3443	1/1	0.96	0.08	23,23,23,23	0
57	MG	2A	3567	1/1	0.96	0.06	58,58,58,58	0
57	MG	1A	3235	1/1	0.96	0.08	38,38,38,38	0
57	MG	2a	1682	1/1	0.96	0.13	66,66,66,66	0
57	MG	1A	3115	1/1	0.96	0.16	21,21,21,21	0
57	MG	1A	3652	1/1	0.96	0.12	46,46,46,46	0
57	MG	1A	3655	1/1	0.96	0.16	49,49,49,49	0
57	MG	1A	3657	1/1	0.96	0.04	30,30,30,30	0
57	MG	1A	3547	1/1	0.96	0.07	22,22,22,22	0
57	MG	2A	3350	1/1	0.96	0.08	33,33,33,33	0
57	MG	2A	3577	1/1	0.96	0.08	48,48,48,48	0
57	MG	1a	1629	1/1	0.96	0.18	41,41,41,41	0
57	MG	1A	3779	1/1	0.96	0.08	41,41,41,41	0
57	MG	1a	1631	1/1	0.96	0.13	53,53,53,53	0
57	MG	1A	3549	1/1	0.96	0.12	15,15,15,15	0
57	MG	2a	1696	1/1	0.96	0.17	54,54,54,54	0
57	MG	1a	1785	1/1	0.96	0.12	49,49,49,49	0
57	MG	1A	3660	1/1	0.96	0.05	24,24,24,24	0
57	MG	2a	1699	1/1	0.96	0.13	44,44,44,44	0
57	MG	1A	3054	1/1	0.96	0.17	40,40,40,40	0
57	MG	2A	3586	1/1	0.96	0.15	48,48,48,48	0
57	MG	2A	3361	1/1	0.96	0.08	41,41,41,41	0
57	MG	1A	3662	1/1	0.96	0.06	36,36,36,36	0
57	MG	2a	1704	1/1	0.96	0.15	57,57,57,57	0
57	MG	1A	3448	1/1	0.96	0.09	17,17,17,17	0
57	MG	2A	3365	1/1	0.96	0.12	45,45,45,45	0
57	MG	1f	201	1/1	0.96	0.12	42,42,42,42	0
57	MG	1A	3163	1/1	0.96	0.17	31,31,31,31	0
57	MG	1m	3001	1/1	0.96	0.09	64,64,64,64	0
57	MG	2A	3594	1/1	0.96	0.06	74,74,74,74	0
57	MG	1A	3292	1/1	0.96	0.11	25,25,25,25	0
57	MG	2A	3596	1/1	0.96	0.06	65,65,65,65	0
57	MG	1a	1640	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	3666	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3369	1/1	0.96	0.06	12,12,12,12	0
57	MG	2A	3378	1/1	0.96	0.05	51,51,51,51	0
57	MG	1a	1643	1/1	0.96	0.24	52,52,52,52	0
57	MG	2a	1719	1/1	0.96	0.09	70,70,70,70	0
57	MG	2A	3166	1/1	0.96	0.09	35,35,35,35	0
57	MG	2a	1721	1/1	0.96	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3558	1/1	0.96	0.09	33,33,33,33	0
57	MG	1A	3245	1/1	0.96	0.04	20,20,20,20	0
57	MG	2A	3170	1/1	0.96	0.15	49,49,49,49	0
57	MG	1A	3296	1/1	0.96	0.20	40,40,40,40	0
57	MG	1A	3170	1/1	0.96	0.15	42,42,42,42	0
57	MG	1x	104	1/1	0.96	0.05	55,55,55,55	0
57	MG	1x	106	1/1	0.96	0.04	40,40,40,40	0
57	MG	1A	3673	1/1	0.96	0.08	27,27,27,27	0
57	MG	1A	3564	1/1	0.96	0.06	22,22,22,22	0
57	MG	1A	3565	1/1	0.96	0.06	30,30,30,30	0
57	MG	1A	3676	1/1	0.96	0.12	43,43,43,43	0
57	MG	1A	3373	1/1	0.96	0.12	22,22,22,22	0
57	MG	2A	3180	1/1	0.96	0.17	56,56,56,56	0
57	MG	1A	3805	1/1	0.96	0.10	24,24,24,24	0
57	MG	1A	3569	1/1	0.96	0.05	68,68,68,68	0
57	MG	1A	3300	1/1	0.96	0.07	43,43,43,43	0
57	MG	2A	3008	1/1	0.96	0.07	41,41,41,41	0
57	MG	1A	3572	1/1	0.96	0.10	53,53,53,53	0
57	MG	2A	3010	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3681	1/1	0.96	0.08	42,42,42,42	0
57	MG	2A	3012	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3573	1/1	0.96	0.10	42,42,42,42	0
57	MG	2A	3408	1/1	0.96	0.05	48,48,48,48	0
57	MG	2A	3014	1/1	0.96	0.08	43,43,43,43	0
57	MG	2A	3015	1/1	0.96	0.10	45,45,45,45	0
57	MG	1B	204	1/1	0.96	0.08	26,26,26,26	0
57	MG	2a	1749	1/1	0.96	0.14	63,63,63,63	0
57	MG	1A	3575	1/1	0.96	0.07	48,48,48,48	0
57	MG	1A	3685	1/1	0.96	0.06	37,37,37,37	0
57	MG	2A	3020	1/1	0.96	0.06	25,25,25,25	0
57	MG	2A	3415	1/1	0.96	0.09	29,29,29,29	0
57	MG	1a	1663	1/1	0.96	0.09	50,50,50,50	0
57	MG	2A	3417	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3579	1/1	0.96	0.11	41,41,41,41	0
57	MG	2a	1757	1/1	0.96	0.04	52,52,52,52	0
57	MG	1B	208	1/1	0.96	0.07	40,40,40,40	0
57	MG	1A	3199	1/1	0.96	0.15	40,40,40,40	0
57	MG	1A	3071	1/1	0.96	0.20	48,48,48,48	0
57	MG	2A	3204	1/1	0.96	0.12	69,69,69,69	0
57	MG	2A	3644	1/1	0.96	0.07	60,60,60,60	0
57	MG	1A	3464	1/1	0.96	0.11	46,46,46,46	0
57	MG	1A	3306	1/1	0.96	0.07	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3584	1/1	0.96	0.08	48,48,48,48	0
57	MG	1A	3172	1/1	0.96	0.17	37,37,37,37	0
57	MG	1B	218	1/1	0.96	0.05	52,52,52,52	0
57	MG	1A	3693	1/1	0.96	0.08	42,42,42,42	0
57	MG	2A	3432	1/1	0.96	0.09	44,44,44,44	0
57	MG	1a	1676	1/1	0.96	0.07	41,41,41,41	0
57	MG	1B	220	1/1	0.96	0.06	33,33,33,33	0
57	MG	2a	1772	1/1	0.96	0.10	59,59,59,59	0
57	MG	2d	301	1/1	0.96	0.19	45,45,45,45	0
57	MG	1D	302	1/1	0.96	0.05	19,19,19,19	0
57	MG	2A	3437	1/1	0.96	0.15	50,50,50,50	0
57	MG	2A	3215	1/1	0.96	0.21	41,41,41,41	0
57	MG	1A	3382	1/1	0.96	0.15	39,39,39,39	0
57	MG	2A	3217	1/1	0.96	0.16	36,36,36,36	0
57	MG	2A	3663	1/1	0.96	0.17	45,45,45,45	0
57	MG	1D	306	1/1	0.96	0.18	35,35,35,35	0
57	MG	1A	3696	1/1	0.96	0.12	40,40,40,40	0
57	MG	2A	3444	1/1	0.96	0.13	50,50,50,50	0
57	MG	1a	1684	1/1	0.96	0.19	42,42,42,42	0
57	MG	2A	3446	1/1	0.96	0.09	34,34,34,34	0
57	MG	1A	3385	1/1	0.96	0.09	34,34,34,34	0
57	MG	2A	3044	1/1	0.96	0.17	41,41,41,41	0
57	MG	2A	3449	1/1	0.96	0.18	49,49,49,49	0
57	MG	1A	3309	1/1	0.96	0.08	32,32,32,32	0
57	MG	2x	104	1/1	0.96	0.13	61,61,61,61	0
57	MG	1A	3251	1/1	0.96	0.08	36,36,36,36	0
57	MG	2A	3228	1/1	0.96	0.35	54,54,54,54	0
57	MG	1F	301	1/1	0.96	0.17	24,24,24,24	0
57	MG	2x	109	1/1	0.96	0.08	55,55,55,55	0
57	MG	1Q	202	1/1	0.97	0.10	31,31,31,31	0
57	MG	1A	3304	1/1	0.97	0.33	32,32,32,32	0
57	MG	2A	3068	1/1	0.97	0.11	40,40,40,40	0
57	MG	2A	3069	1/1	0.97	0.12	53,53,53,53	0
57	MG	1A	3305	1/1	0.97	0.04	23,23,23,23	0
57	MG	1A	3166	1/1	0.97	0.05	15,15,15,15	0
57	MG	1R	201	1/1	0.97	0.12	31,31,31,31	0
57	MG	1R	202	1/1	0.97	0.30	40,40,40,40	0
57	MG	2A	3265	1/1	0.97	0.08	45,45,45,45	0
57	MG	1A	3392	1/1	0.97	0.11	36,36,36,36	0
57	MG	1a	1719	1/1	0.97	0.11	37,37,37,37	0
57	MG	2X	103	1/1	0.97	0.07	51,51,51,51	0
57	MG	2A	3268	1/1	0.97	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3307	1/1	0.97	0.12	40,40,40,40	0
57	MG	1A	3614	1/1	0.97	0.18	53,53,53,53	0
57	MG	1A	3732	1/1	0.97	0.34	29,29,29,29	0
57	MG	1U	206	1/1	0.97	0.13	28,28,28,28	0
57	MG	1A	3203	1/1	0.97	0.17	26,26,26,26	0
57	MG	1A	3734	1/1	0.97	0.16	26,26,26,26	0
57	MG	1W	201	1/1	0.97	0.23	41,41,41,41	0
57	MG	1a	1727	1/1	0.97	0.16	35,35,35,35	0
57	MG	1A	3735	1/1	0.97	0.13	42,42,42,42	0
57	MG	1W	203	1/1	0.97	0.17	27,27,27,27	0
57	MG	1A	3249	1/1	0.97	0.13	25,25,25,25	0
57	MG	1A	3495	1/1	0.97	0.05	44,44,44,44	0
57	MG	2A	3088	1/1	0.97	0.10	59,59,59,59	0
57	MG	1A	3396	1/1	0.97	0.18	37,37,37,37	0
57	MG	1A	3204	1/1	0.97	0.12	22,22,22,22	0
57	MG	2A	3091	1/1	0.97	0.11	26,26,26,26	0
57	MG	1A	3312	1/1	0.97	0.07	39,39,39,39	0
57	MG	2a	1607	1/1	0.97	0.25	46,46,46,46	0
57	MG	2A	3507	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3499	1/1	0.97	0.06	25,25,25,25	0
57	MG	2A	3094	1/1	0.97	0.12	49,49,49,49	0
57	MG	1a	1736	1/1	0.97	0.05	55,55,55,55	0
57	MG	1a	1737	1/1	0.97	0.10	48,48,48,48	0
57	MG	2A	3291	1/1	0.97	0.07	47,47,47,47	0
57	MG	2A	3097	1/1	0.97	0.12	54,54,54,54	0
57	MG	2A	3515	1/1	0.97	0.15	59,59,59,59	0
57	MG	1A	3137	1/1	0.97	0.09	27,27,27,27	0
57	MG	2A	3100	1/1	0.97	0.10	36,36,36,36	0
57	MG	10	104	1/1	0.97	0.06	53,53,53,53	0
57	MG	1A	3252	1/1	0.97	0.14	22,22,22,22	0
57	MG	1A	3075	1/1	0.97	0.07	40,40,40,40	0
57	MG	2A	3521	1/1	0.97	0.10	34,34,34,34	0
57	MG	1A	3254	1/1	0.97	0.08	36,36,36,36	0
57	MG	11	104	1/1	0.97	0.07	35,35,35,35	0
57	MG	1A	3747	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3509	1/1	0.97	0.12	56,56,56,56	0
57	MG	1A	3255	1/1	0.97	0.07	25,25,25,25	0
57	MG	1A	3318	1/1	0.97	0.07	27,27,27,27	0
57	MG	1A	3256	1/1	0.97	0.09	38,38,38,38	0
57	MG	1A	3320	1/1	0.97	0.10	35,35,35,35	0
57	MG	2A	3113	1/1	0.97	0.14	41,41,41,41	0
57	MG	2A	3114	1/1	0.97	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1633	1/1	0.97	0.23	61,61,61,61	0
57	MG	1A	3321	1/1	0.97	0.05	15,15,15,15	0
57	MG	2A	3312	1/1	0.97	0.09	40,40,40,40	0
57	MG	1A	3755	1/1	0.97	0.08	21,21,21,21	0
57	MG	2A	3117	1/1	0.97	0.20	35,35,35,35	0
57	MG	17	101	1/1	0.97	0.09	32,32,32,32	0
57	MG	17	102	1/1	0.97	0.15	34,34,34,34	0
57	MG	1A	3042	1/1	0.97	0.17	33,33,33,33	0
57	MG	1A	3323	1/1	0.97	0.05	39,39,39,39	0
57	MG	2A	3122	1/1	0.97	0.13	51,51,51,51	0
57	MG	2A	3123	1/1	0.97	0.07	41,41,41,41	0
57	MG	17	106	1/1	0.97	0.18	45,45,45,45	0
57	MG	1A	3043	1/1	0.97	0.28	26,26,26,26	0
57	MG	1A	3209	1/1	0.97	0.12	25,25,25,25	0
57	MG	19	101	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3414	1/1	0.97	0.07	18,18,18,18	0
57	MG	2A	3329	1/1	0.97	0.09	26,26,26,26	0
57	MG	2A	3330	1/1	0.97	0.08	49,49,49,49	0
57	MG	2a	1651	1/1	0.97	0.18	45,45,45,45	0
57	MG	2A	3331	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	3326	1/1	0.97	0.07	35,35,35,35	0
57	MG	1A	3762	1/1	0.97	0.07	16,16,16,16	0
57	MG	1A	3327	1/1	0.97	0.08	47,47,47,47	0
57	MG	1A	3104	1/1	0.97	0.08	21,21,21,21	0
57	MG	1A	3526	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3643	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3530	1/1	0.97	0.15	46,46,46,46	0
57	MG	1A	3079	1/1	0.97	0.13	33,33,33,33	0
57	MG	1a	1610	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	3176	1/1	0.97	0.30	27,27,27,27	0
57	MG	1A	3331	1/1	0.97	0.05	28,28,28,28	0
57	MG	2A	3344	1/1	0.97	0.07	38,38,38,38	0
57	MG	2A	3345	1/1	0.97	0.08	50,50,50,50	0
57	MG	1A	3536	1/1	0.97	0.20	47,47,47,47	0
57	MG	1A	3649	1/1	0.97	0.07	40,40,40,40	0
57	MG	1A	3332	1/1	0.97	0.14	10,10,10,10	0
57	MG	1A	3428	1/1	0.97	0.10	24,24,24,24	0
57	MG	1A	3429	1/1	0.97	0.05	20,20,20,20	0
57	MG	1a	1619	1/1	0.97	0.06	65,65,65,65	0
57	MG	2A	3353	1/1	0.97	0.07	55,55,55,55	0
57	MG	1A	3653	1/1	0.97	0.13	36,36,36,36	0
57	MG	2A	3355	1/1	0.97	0.06	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3540	1/1	0.97	0.05	19,19,19,19	0
57	MG	2A	3357	1/1	0.97	0.16	50,50,50,50	0
57	MG	2A	3581	1/1	0.97	0.08	41,41,41,41	0
57	MG	1A	3018	1/1	0.97	0.04	20,20,20,20	0
57	MG	1A	3265	1/1	0.97	0.13	19,19,19,19	0
57	MG	1A	3144	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3217	1/1	0.97	0.12	38,38,38,38	0
57	MG	1A	3338	1/1	0.97	0.06	19,19,19,19	0
57	MG	1A	3436	1/1	0.97	0.07	44,44,44,44	0
57	MG	1A	3784	1/1	0.97	0.06	52,52,52,52	0
57	MG	2A	3156	1/1	0.97	0.12	43,43,43,43	0
57	MG	2a	1686	1/1	0.97	0.19	48,48,48,48	0
57	MG	1A	3548	1/1	0.97	0.08	28,28,28,28	0
57	MG	2A	3158	1/1	0.97	0.13	33,33,33,33	0
57	MG	1A	3268	1/1	0.97	0.09	29,29,29,29	0
57	MG	2a	1690	1/1	0.97	0.14	36,36,36,36	0
57	MG	1A	3269	1/1	0.97	0.24	40,40,40,40	0
57	MG	1A	3551	1/1	0.97	0.15	29,29,29,29	0
57	MG	1A	3790	1/1	0.97	0.06	14,14,14,14	0
57	MG	2A	3377	1/1	0.97	0.10	46,46,46,46	0
57	MG	2A	3597	1/1	0.97	0.10	48,48,48,48	0
57	MG	1A	3091	1/1	0.97	0.14	27,27,27,27	0
57	MG	1A	3081	1/1	0.97	0.31	34,34,34,34	0
57	MG	1A	3793	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3554	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3167	1/1	0.97	0.17	41,41,41,41	0
57	MG	1A	3147	1/1	0.97	0.26	36,36,36,36	0
57	MG	2A	3385	1/1	0.97	0.11	41,41,41,41	0
57	MG	1w	403	1/1	0.97	0.13	31,31,31,31	0
57	MG	1A	3556	1/1	0.97	0.08	16,16,16,16	0
57	MG	1x	101	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3672	1/1	0.97	0.09	35,35,35,35	0
57	MG	2A	3609	1/1	0.97	0.10	40,40,40,40	0
57	MG	1A	3125	1/1	0.97	0.04	19,19,19,19	0
57	MG	1A	3348	1/1	0.97	0.05	22,22,22,22	0
57	MG	2a	1710	1/1	0.97	0.12	42,42,42,42	0
57	MG	1x	105	1/1	0.97	0.07	60,60,60,60	0
57	MG	1A	3349	1/1	0.97	0.06	23,23,23,23	0
57	MG	1A	3183	1/1	0.97	0.17	38,38,38,38	0
57	MG	1A	3352	1/1	0.97	0.06	13,13,13,13	0
57	MG	1A	3563	1/1	0.97	0.06	16,16,16,16	0
57	MG	1A	3450	1/1	0.97	0.06	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3181	1/1	0.97	0.26	50,50,50,50	0
57	MG	1A	3353	1/1	0.97	0.06	21,21,21,21	0
57	MG	2A	3004	1/1	0.97	0.15	34,34,34,34	0
57	MG	1A	3566	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3567	1/1	0.97	0.12	52,52,52,52	0
57	MG	1A	3453	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3684	1/1	0.97	0.06	14,14,14,14	0
57	MG	2A	3625	1/1	0.97	0.13	65,65,65,65	0
57	MG	2A	3188	1/1	0.97	0.07	45,45,45,45	0
57	MG	1a	1654	1/1	0.97	0.06	34,34,34,34	0
57	MG	1A	3126	1/1	0.97	0.06	27,27,27,27	0
57	MG	1A	3127	1/1	0.97	0.03	24,24,24,24	0
57	MG	1A	3128	1/1	0.97	0.16	28,28,28,28	0
57	MG	1A	3010	1/1	0.97	0.05	24,24,24,24	0
57	MG	1A	3096	1/1	0.97	0.16	29,29,29,29	0
57	MG	1A	3578	1/1	0.97	0.06	37,37,37,37	0
57	MG	1A	3228	1/1	0.97	0.17	36,36,36,36	0
57	MG	1B	213	1/1	0.97	0.09	40,40,40,40	0
57	MG	2A	3018	1/1	0.97	0.18	38,38,38,38	0
57	MG	1A	3460	1/1	0.97	0.08	26,26,26,26	0
57	MG	2a	1737	1/1	0.97	0.25	59,59,59,59	0
57	MG	1A	3131	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3462	1/1	0.97	0.06	8,8,8,8	0
57	MG	2A	3022	1/1	0.97	0.04	24,24,24,24	0
57	MG	1A	3097	1/1	0.97	0.09	32,32,32,32	0
57	MG	2A	3642	1/1	0.97	0.08	46,46,46,46	0
57	MG	1A	3157	1/1	0.97	0.04	37,37,37,37	0
57	MG	1D	301	1/1	0.97	0.28	43,43,43,43	0
57	MG	1A	3465	1/1	0.97	0.10	47,47,47,47	0
57	MG	1D	303	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	3366	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3008	1/1	0.97	0.13	22,22,22,22	0
57	MG	2A	3030	1/1	0.97	0.18	41,41,41,41	0
57	MG	1a	1674	1/1	0.97	0.16	40,40,40,40	0
57	MG	1E	301	1/1	0.97	0.25	28,28,28,28	0
57	MG	1A	3114	1/1	0.97	0.22	45,45,45,45	0
57	MG	1A	3067	1/1	0.97	0.14	40,40,40,40	0
57	MG	2A	3439	1/1	0.97	0.05	58,58,58,58	0
57	MG	1a	1678	1/1	0.97	0.06	47,47,47,47	0
57	MG	1E	305	1/1	0.97	0.07	46,46,46,46	0
57	MG	1A	3290	1/1	0.97	0.10	20,20,20,20	0
57	MG	1A	3705	1/1	0.97	0.05	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3197	1/1	0.97	0.07	33,33,33,33	0
57	MG	2A	3664	1/1	0.97	0.07	37,37,37,37	0
57	MG	2A	3224	1/1	0.97	0.10	48,48,48,48	0
57	MG	1A	3239	1/1	0.97	0.06	34,34,34,34	0
57	MG	2A	3041	1/1	0.97	0.21	32,32,32,32	0
57	MG	1F	303	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3708	1/1	0.97	0.12	31,31,31,31	0
57	MG	1F	305	1/1	0.97	0.18	34,34,34,34	0
57	MG	1F	306	1/1	0.97	0.06	42,42,42,42	0
57	MG	2A	3231	1/1	0.97	0.12	54,54,54,54	0
57	MG	1A	3295	1/1	0.97	0.06	31,31,31,31	0
57	MG	1A	3240	1/1	0.97	0.11	16,16,16,16	0
57	MG	1A	3711	1/1	0.97	0.11	48,48,48,48	0
57	MG	1A	3297	1/1	0.97	0.13	30,30,30,30	0
57	MG	1A	3243	1/1	0.97	0.12	31,31,31,31	0
57	MG	2D	302	1/1	0.97	0.14	32,32,32,32	0
57	MG	1A	3116	1/1	0.97	0.08	30,30,30,30	0
57	MG	1a	1696	1/1	0.97	0.16	54,54,54,54	0
57	MG	2D	305	1/1	0.97	0.06	43,43,43,43	0
57	MG	1a	1697	1/1	0.97	0.12	44,44,44,44	0
57	MG	1A	3301	1/1	0.97	0.13	28,28,28,28	0
57	MG	1a	1700	1/1	0.97	0.07	49,49,49,49	0
57	MG	1A	3383	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3481	1/1	0.97	0.06	34,34,34,34	0
57	MG	1A	3482	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3719	1/1	0.97	0.14	43,43,43,43	0
57	MG	2E	304	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	3164	1/1	0.97	0.12	37,37,37,37	0
57	MG	2A	3249	1/1	0.97	0.19	39,39,39,39	0
57	MG	1A	3484	1/1	0.97	0.07	17,17,17,17	0
57	MG	1A	3605	1/1	0.97	0.04	25,25,25,25	0
57	MG	1A	3165	1/1	0.97	0.07	29,29,29,29	0
57	MG	2F	305	1/1	0.97	0.19	47,47,47,47	0
57	MG	2A	3255	1/1	0.97	0.06	61,61,61,61	0
57	MG	1a	1710	1/1	0.97	0.07	29,29,29,29	0
58	ZN	2n	501	1/1	0.97	0.06	86,86,86,86	0
57	MG	2A	3646	1/1	0.98	0.07	34,34,34,34	0
57	MG	1B	217	1/1	0.98	0.05	47,47,47,47	0
57	MG	2A	3388	1/1	0.98	0.06	66,66,66,66	0
57	MG	2A	3649	1/1	0.98	0.03	35,35,35,35	0
57	MG	1A	3201	1/1	0.98	0.07	31,31,31,31	0
57	MG	17	107	1/1	0.98	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3057	1/1	0.98	0.11	26,26,26,26	0
57	MG	2A	3653	1/1	0.98	0.06	33,33,33,33	0
57	MG	2A	3392	1/1	0.98	0.04	58,58,58,58	0
57	MG	1A	3160	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3367	1/1	0.98	0.04	35,35,35,35	0
57	MG	1a	1690	1/1	0.98	0.09	40,40,40,40	0
57	MG	1A	3058	1/1	0.98	0.04	17,17,17,17	0
57	MG	1A	3026	1/1	0.98	0.04	15,15,15,15	0
57	MG	2A	3660	1/1	0.98	0.08	39,39,39,39	0
57	MG	1D	304	1/1	0.98	0.08	33,33,33,33	0
57	MG	1A	3291	1/1	0.98	0.06	23,23,23,23	0
57	MG	1A	3611	1/1	0.98	0.05	32,32,32,32	0
57	MG	1A	3476	1/1	0.98	0.06	15,15,15,15	0
57	MG	1A	3421	1/1	0.98	0.11	18,18,18,18	0
57	MG	2A	3403	1/1	0.98	0.10	49,49,49,49	0
57	MG	1A	3029	1/1	0.98	0.18	37,37,37,37	0
57	MG	1A	3231	1/1	0.98	0.19	23,23,23,23	0
57	MG	1A	3294	1/1	0.98	0.15	41,41,41,41	0
57	MG	2A	3534	1/1	0.98	0.17	43,43,43,43	0
57	MG	1A	3427	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3092	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3376	1/1	0.98	0.05	28,28,28,28	0
57	MG	1A	3430	1/1	0.98	0.03	27,27,27,27	0
57	MG	1a	1615	1/1	0.98	0.04	45,45,45,45	0
57	MG	2A	3541	1/1	0.98	0.07	57,57,57,57	0
57	MG	1A	3262	1/1	0.98	0.19	37,37,37,37	0
57	MG	2A	3290	1/1	0.98	0.08	45,45,45,45	0
57	MG	1A	3186	1/1	0.98	0.07	26,26,26,26	0
57	MG	1A	3298	1/1	0.98	0.09	33,33,33,33	0
57	MG	1F	307	1/1	0.98	0.10	32,32,32,32	0
57	MG	2A	3294	1/1	0.98	0.09	45,45,45,45	0
57	MG	1A	3148	1/1	0.98	0.18	31,31,31,31	0
57	MG	2A	3549	1/1	0.98	0.08	33,33,33,33	0
57	MG	1A	3694	1/1	0.98	0.11	22,22,22,22	0
57	MG	2A	3190	1/1	0.98	0.09	56,56,56,56	0
57	MG	1A	3381	1/1	0.98	0.07	39,39,39,39	0
57	MG	1a	1715	1/1	0.98	0.17	58,58,58,58	0
57	MG	1A	3210	1/1	0.98	0.06	27,27,27,27	0
57	MG	2A	3425	1/1	0.98	0.06	37,37,37,37	0
57	MG	1A	3628	1/1	0.98	0.11	34,34,34,34	0
57	MG	2A	3302	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3698	1/1	0.98	0.09	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3429	1/1	0.98	0.07	33,33,33,33	0
57	MG	2A	3098	1/1	0.98	0.10	39,39,39,39	0
57	MG	2A	3003	1/1	0.98	0.05	23,23,23,23	0
57	MG	1A	3559	1/1	0.98	0.06	14,14,14,14	0
57	MG	1A	3437	1/1	0.98	0.03	14,14,14,14	0
57	MG	1A	3493	1/1	0.98	0.07	35,35,35,35	0
57	MG	2A	3435	1/1	0.98	0.12	39,39,39,39	0
57	MG	1A	3632	1/1	0.98	0.04	51,51,51,51	0
57	MG	1A	3237	1/1	0.98	0.08	27,27,27,27	0
57	MG	2A	3311	1/1	0.98	0.09	30,30,30,30	0
57	MG	1A	3093	1/1	0.98	0.16	28,28,28,28	0
57	MG	2A	3571	1/1	0.98	0.12	46,46,46,46	0
57	MG	2A	3313	1/1	0.98	0.12	37,37,37,37	0
57	MG	1A	3339	1/1	0.98	0.05	23,23,23,23	0
57	MG	2A	3315	1/1	0.98	0.04	31,31,31,31	0
57	MG	2A	3575	1/1	0.98	0.05	59,59,59,59	0
57	MG	2A	3107	1/1	0.98	0.08	44,44,44,44	0
57	MG	1A	3167	1/1	0.98	0.08	39,39,39,39	0
57	MG	2A	3318	1/1	0.98	0.11	22,22,22,22	0
57	MG	1A	3168	1/1	0.98	0.09	48,48,48,48	0
57	MG	1a	1635	1/1	0.98	0.11	24,24,24,24	0
57	MG	1A	3389	1/1	0.98	0.08	21,21,21,21	0
57	MG	1A	3500	1/1	0.98	0.05	18,18,18,18	0
57	MG	1A	3502	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3270	1/1	0.98	0.08	26,26,26,26	0
57	MG	2A	3213	1/1	0.98	0.16	52,52,52,52	0
57	MG	1A	3786	1/1	0.98	0.05	22,22,22,22	0
57	MG	2A	3454	1/1	0.98	0.10	37,37,37,37	0
57	MG	1A	3391	1/1	0.98	0.14	46,46,46,46	0
57	MG	1A	3505	1/1	0.98	0.05	39,39,39,39	0
57	MG	1A	3506	1/1	0.98	0.10	40,40,40,40	0
57	MG	1U	202	1/1	0.98	0.14	34,34,34,34	0
57	MG	1A	3576	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3241	1/1	0.98	0.06	32,32,32,32	0
57	MG	2A	3462	1/1	0.98	0.07	36,36,36,36	0
57	MG	1U	205	1/1	0.98	0.21	30,30,30,30	0
57	MG	2A	3222	1/1	0.98	0.04	37,37,37,37	0
57	MG	2A	3223	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3242	1/1	0.98	0.04	21,21,21,21	0
57	MG	1a	1742	1/1	0.98	0.13	69,69,69,69	0
57	MG	1V	201	1/1	0.98	0.25	21,21,21,21	0
57	MG	1A	3345	1/1	0.98	0.04	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1V	203	1/1	0.98	0.36	26,26,26,26	0
57	MG	1A	3451	1/1	0.98	0.04	51,51,51,51	0
57	MG	2a	1617	1/1	0.98	0.18	40,40,40,40	0
57	MG	1V	205	1/1	0.98	0.18	25,25,25,25	0
57	MG	1A	3169	1/1	0.98	0.09	34,34,34,34	0
57	MG	1A	3215	1/1	0.98	0.16	28,28,28,28	0
57	MG	1A	3397	1/1	0.98	0.05	36,36,36,36	0
57	MG	2A	3234	1/1	0.98	0.10	55,55,55,55	0
57	MG	2A	3133	1/1	0.98	0.09	48,48,48,48	0
57	MG	2A	3349	1/1	0.98	0.14	32,32,32,32	0
57	MG	1A	3025	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3800	1/1	0.98	0.07	23,23,23,23	0
57	MG	1X	103	1/1	0.98	0.07	24,24,24,24	0
57	MG	1A	3654	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3311	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	3656	1/1	0.98	0.07	46,46,46,46	0
57	MG	1A	3517	1/1	0.98	0.07	41,41,41,41	0
57	MG	2A	3243	1/1	0.98	0.09	48,48,48,48	0
57	MG	1a	1664	1/1	0.98	0.04	61,61,61,61	0
57	MG	1A	3729	1/1	0.98	0.09	35,35,35,35	0
57	MG	1A	3351	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3276	1/1	0.98	0.16	29,29,29,29	0
57	MG	1A	3034	1/1	0.98	0.12	22,22,22,22	0
57	MG	1A	3053	1/1	0.98	0.11	26,26,26,26	0
57	MG	1A	3110	1/1	0.98	0.14	30,30,30,30	0
57	MG	2A	3251	1/1	0.98	0.06	40,40,40,40	0
57	MG	2A	3252	1/1	0.98	0.06	36,36,36,36	0
57	MG	1a	1765	1/1	0.98	0.05	58,58,58,58	0
57	MG	1A	3035	1/1	0.98	0.15	32,32,32,32	0
57	MG	2A	3373	1/1	0.98	0.07	44,44,44,44	0
57	MG	1A	3074	1/1	0.98	0.15	21,21,21,21	0
57	MG	13	101	1/1	0.98	0.13	28,28,28,28	0
57	MG	1A	3099	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3528	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	3529	1/1	0.98	0.06	37,37,37,37	0
57	MG	1A	3041	1/1	0.98	0.10	19,19,19,19	0
57	MG	1A	3158	1/1	0.98	0.15	29,29,29,29	0
57	MG	2A	3506	1/1	0.98	0.07	48,48,48,48	0
57	MG	1A	3410	1/1	0.98	0.07	40,40,40,40	0
57	MG	2A	3382	1/1	0.98	0.11	67,67,67,67	0
57	MG	1A	3363	1/1	0.98	0.06	12,12,12,12	0
57	MG	2A	3510	1/1	0.98	0.09	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2x	107	1/1	0.98	0.05	76,76,76,76	0
57	MG	1A	3535	1/1	0.98	0.06	36,36,36,36	0
57	MG	1a	1682	1/1	0.98	0.04	39,39,39,39	0
58	ZN	1n	102	1/1	0.98	0.04	97,97,97,97	0
58	ZN	2Y	202	1/1	0.98	0.04	89,89,89,89	0
58	ZN	24	501	1/1	0.98	0.09	125,125,125,125	0
57	MG	1A	3745	1/1	0.98	0.07	30,30,30,30	0
59	SF4	2d	302	8/8	0.98	0.04	55,65,83,89	0
57	MG	1A	3446	1/1	0.99	0.08	19,19,19,19	0
57	MG	1a	1708	1/1	0.99	0.04	29,29,29,29	0
57	MG	1A	3612	1/1	0.99	0.02	18,18,18,18	0
57	MG	2A	3371	1/1	0.99	0.04	34,34,34,34	0
57	MG	2A	3372	1/1	0.99	0.04	38,38,38,38	0
57	MG	1A	3078	1/1	0.99	0.07	32,32,32,32	0
57	MG	2A	3421	1/1	0.99	0.11	48,48,48,48	0
57	MG	1A	3531	1/1	0.99	0.04	38,38,38,38	0
57	MG	1A	3801	1/1	0.99	0.09	27,27,27,27	0
57	MG	17	104	1/1	0.99	0.10	24,24,24,24	0
57	MG	1E	304	1/1	0.99	0.07	16,16,16,16	0
57	MG	1A	3013	1/1	0.99	0.08	19,19,19,19	0
57	MG	1A	3487	1/1	0.99	0.03	17,17,17,17	0
57	MG	1A	3012	1/1	0.99	0.03	22,22,22,22	0
57	MG	2A	3333	1/1	0.99	0.06	38,38,38,38	0
57	MG	1A	3588	1/1	0.99	0.04	15,15,15,15	0
57	MG	1A	3354	1/1	0.99	0.07	13,13,13,13	0
57	MG	1A	3333	1/1	0.99	0.03	23,23,23,23	0
57	MG	1A	3356	1/1	0.99	0.07	20,20,20,20	0
57	MG	1A	3384	1/1	0.99	0.03	16,16,16,16	0
57	MG	1A	3415	1/1	0.99	0.08	14,14,14,14	0
57	MG	1A	3056	1/1	0.99	0.09	19,19,19,19	0
57	MG	1A	3541	1/1	0.99	0.09	23,23,23,23	0
57	MG	1x	108	1/1	0.99	0.03	42,42,42,42	0
57	MG	1A	3289	1/1	0.99	0.07	14,14,14,14	0
57	MG	1X	102	1/1	0.99	0.04	31,31,31,31	0
57	MG	2A	3539	1/1	0.99	0.06	44,44,44,44	0
57	MG	2A	3043	1/1	0.99	0.05	39,39,39,39	0
57	MG	1A	3748	1/1	0.99	0.05	19,19,19,19	0
57	MG	1A	3233	1/1	0.99	0.37	30,30,30,30	0
57	MG	1A	3347	1/1	0.99	0.05	37,37,37,37	0
57	MG	1A	3570	1/1	0.99	0.05	37,37,37,37	0
57	MG	1A	3374	1/1	0.99	0.04	27,27,27,27	0
57	MG	1A	3521	1/1	0.99	0.08	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3047	1/1	0.99	0.11	27,27,27,27	0
57	MG	1A	3574	1/1	0.99	0.09	34,34,34,34	0
57	MG	11	101	1/1	0.99	0.19	39,39,39,39	0
57	MG	1A	3185	1/1	0.99	0.04	20,20,20,20	0
57	MG	1B	216	1/1	0.99	0.04	34,34,34,34	0
57	MG	1A	3501	1/1	0.99	0.04	10,10,10,10	0
57	MG	1a	1699	1/1	0.99	0.03	38,38,38,38	0
57	MG	1A	3577	1/1	0.99	0.05	44,44,44,44	0
57	MG	1A	3083	1/1	0.99	0.03	12,12,12,12	0
57	MG	1A	3728	1/1	0.99	0.04	50,50,50,50	0
57	MG	1A	3425	1/1	0.99	0.02	26,26,26,26	0
57	MG	2A	3558	1/1	0.99	0.04	29,29,29,29	0
58	ZN	1Y	501	1/1	0.99	0.03	56,56,56,56	0
58	ZN	14	501	1/1	0.99	0.08	107,107,107,107	0
58	ZN	15	105	1/1	0.99	0.02	38,38,38,38	0
58	ZN	16	102	1/1	0.99	0.03	42,42,42,42	0
57	MG	2A	3459	1/1	0.99	0.03	34,34,34,34	0
57	MG	1A	3527	1/1	0.99	0.03	32,32,32,32	0
57	MG	1A	3795	1/1	0.99	0.04	37,37,37,37	0
58	ZN	25	102	1/1	0.99	0.05	52,52,52,52	0
58	ZN	26	501	1/1	0.99	0.02	55,55,55,55	0
58	ZN	29	102	1/1	0.99	0.04	69,69,69,69	0
57	MG	1A	3426	1/1	0.99	0.04	21,21,21,21	0
59	SF4	1d	302	8/8	0.99	0.04	61,72,77,81	0
57	MG	2A	3367	1/1	0.99	0.04	53,53,53,53	0
58	ZN	19	102	1/1	1.00	0.02	39,39,39,39	0
57	MG	1A	3419	1/1	1.00	0.01	21,21,21,21	0
57	MG	1A	3510	1/1	1.00	0.04	52,52,52,52	0
57	MG	1A	3440	1/1	1.00	0.07	17,17,17,17	0
57	MG	2A	3363	1/1	1.00	0.10	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.