



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 06:03 AM EST

PDB ID : 6CFL
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with lysyl-CAM and bound to protein Y (YfiA) at 2.6Å resolution
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Deposited on : 2018-02-15
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)

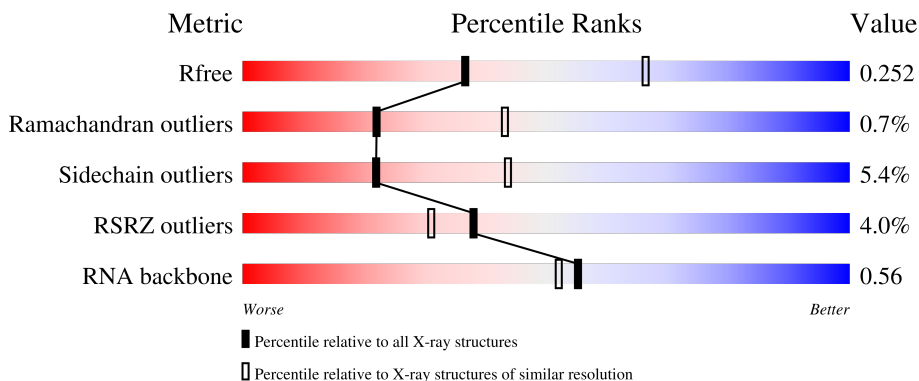
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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

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

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

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Mol	Chain	Length	Quality of chain
2	2B	121	86% 13%
3	1D	276	92% 7%
3	2D	276	2% 95%
4	1E	206	93% 6%
4	2E	206	% 92% 7%
5	1F	210	89% 8%
5	2F	210	90% 7%
6	1G	182	93% 6%
6	2G	182	6% 93% 6%
7	1H	180	93%
7	2H	180	7% 91% 6%
8	1I	148	94% 5%
8	2I	148	6% 95%
9	1N	140	91% 9%
9	2N	140	% 96%
10	1O	122	97%
10	2O	122	93% 7%
11	1P	150	% 97%
11	2P	150	3% 97%
12	1Q	141	95% 5%
12	2Q	141	4% 97%
13	1R	118	91% 9%
13	2R	118	93% 7%
14	1S	112	93%
14	2S	112	10% 94%

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Mol	Chain	Length	Quality of chain
15	1T	146	84% 5% 10%
15	2T	146	86% 5% 10%
16	1U	118	94% 5% . .
16	2U	118	93% 5% .
17	1V	101	92% 7% .
17	2V	101	95% . .
18	1W	113	90% 9% .
18	2W	113	93% 6% .
19	1X	96	95% . .
19	2X	96	95% . . .
20	1Y	110	92% 5% .
20	2Y	110	93% 5% .
21	1Z	206	92% 6% .
21	2Z	206	93% 5% .
22	10	85	87% . 9%
22	20	85	86% 5% 9%
23	11	98	96% . .
23	21	98	93% 6% .
24	12	72	96% . .
24	22	72	90% 7% .
25	13	60	93% 5% .
25	23	60	95% . .
26	14	71	92% . . .
26	24	71	90% 7% .
27	15	60	88% 10% .

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Mol	Chain	Length	Quality of chain
27	25	60	95%
28	16	54	87%
28	26	54	93%
29	17	49	8%
29	27	49	4%
30	18	65	2%
30	28	65	3%
31	19	37	100%
31	29	37	11%
32	1a	1521	2%
32	2a	1521	3%
33	1b	256	7%
33	2b	256	15%
34	1c	239	4%
34	2c	239	18%
35	1d	209	5%
35	2d	209	8%
36	1e	162	2%
36	2e	162	7%
37	1f	101	94%
37	2f	101	97%
38	1g	156	3%
38	2g	156	11%
39	1h	138	%
39	2h	138	7%

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Mol	Chain	Length	Quality of chain
40	1i	128	10% 95%
40	2i	128	48% 95%
41	1j	105	9% 87% 6% 8%
41	2j	105	33% 88% 9%
42	1k	129	% 88% 12%
42	2k	129	3% 82% 6% 12%
43	1l	132	2% 89% 8%
43	2l	132	8% 90% 8%
44	1m	126	2% 88% 8%
44	2m	126	13% 87% 10%
45	1n	61	11% 97%
45	2n	61	57% 95%
46	1o	89	2% 93% 6%
46	2o	89	2% 97%
47	1p	88	88% 6% 7%
47	2p	88	% 88% 6% 7%
48	1q	105	5% 90% 5% 6%
48	2q	105	4% 92% 6%
49	1r	88	% 75% 23%
49	2r	88	% 74% 23%
50	1s	93	84% 5% 11%
50	2s	93	32% 86% 11%
51	1t	106	10% 85% 6% 9%
51	2t	106	3% 87% 5% 8%
52	1u	27	7% 85% 15%

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Mol	Chain	Length	Quality of chain
52	2u	27	
53	1y	113	
53	2y	113	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	1A	3233	-	-	-	X
54	MG	1A	3855	-	-	-	X
54	MG	1A	3900	-	-	-	X
54	MG	1A	3939	-	-	-	X
54	MG	1A	3957	-	-	-	X
54	MG	1A	3970	-	-	-	X

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 295545 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	1G	181	Total 1426	C 916	N 253	O 253	S 4	0	0	0
6	2G	181	Total 1424	C 912	N 259	O 249	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	1H	174	Total 1330	C 845	N 248	O 236	S 1	0	0	0
7	2H	173	Total 1324	C 842	N 247	O 234	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	1I	147	Total 1094	C 699	N 191	O 203	S 1	0	0	0
8	2I	146	Total 1076	C 687	N 186	O 202	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	1N	140	Total 1121	C 722	N 208	O 187	S 4	0	0	0
9	2N	140	Total 1117	C 719	N 207	O 187	S 4	0	0	0

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

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

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

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

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	1V	101	Total 775	C 498	N 141	O 135	S 1	0	0	0
17	2V	101	Total 771	C 495	N 140	O 135	S 1	0	0	0

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

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

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

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

- Molecule 20 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	1Y	107	Total 810	C 520	N 153	O 131	S 6	0	0	0
20	2Y	107	Total 810	C 519	N 153	O 132	S 6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	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
			592	368	119	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
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- 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
			1842	1175	330	332	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
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	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
			1133	716	214	199	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	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
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	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
			1098	694	210	192	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
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	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
			834	520	156	155	3			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1m	116	914	564	189	159	2	0	0	0
44	2m	114	895	550	186	157	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	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
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	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 protein called Protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1071	Total	Mg	0	0
			1071	1071		
54	1B	32	Total	Mg	0	0
			32	32		
54	1D	13	Total	Mg	0	0
			13	13		
54	1E	5	Total	Mg	0	0
			5	5		
54	1F	10	Total	Mg	0	0
			10	10		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	3	Total	Mg	0	0
			3	3		
54	1N	3	Total	Mg	0	0
			3	3		
54	1O	1	Total	Mg	0	0
			1	1		
54	1P	2	Total	Mg	0	0
			2	2		
54	1Q	4	Total	Mg	0	0
			4	4		
54	1R	2	Total	Mg	0	0
			2	2		
54	1T	4	Total	Mg	0	0
			4	4		
54	1U	3	Total	Mg	0	0
			3	3		
54	1V	3	Total	Mg	0	0
			3	3		
54	1W	3	Total	Mg	0	0
			3	3		
54	1X	2	Total	Mg	0	0
			2	2		
54	1Z	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	10	5	Total 5	Mg 5	0	0
54	11	2	Total 2	Mg 2	0	0
54	13	3	Total 3	Mg 3	0	0
54	14	1	Total 1	Mg 1	0	0
54	15	3	Total 3	Mg 3	0	0
54	17	1	Total 1	Mg 1	0	0
54	18	1	Total 1	Mg 1	0	0
54	19	2	Total 2	Mg 2	0	0
54	1a	260	Total 260	Mg 260	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	4	Total 4	Mg 4	0	0
54	1e	3	Total 3	Mg 3	0	0
54	1f	2	Total 2	Mg 2	0	0
54	1g	3	Total 3	Mg 3	0	0
54	1h	2	Total 2	Mg 2	0	0
54	1i	1	Total 1	Mg 1	0	0
54	1k	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0
54	1n	2	Total 2	Mg 2	0	0
54	1o	1	Total 1	Mg 1	0	0
54	1p	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1q	2	Total Mg 2 2	0	0
54	1t	1	Total Mg 1 1	0	0
54	1y	4	Total Mg 4 4	0	0
54	2A	699	Total Mg 699 699	0	0
54	2B	21	Total Mg 21 21	0	0
54	2D	6	Total Mg 6 6	0	0
54	2E	6	Total Mg 6 6	0	0
54	2F	3	Total Mg 3 3	0	0
54	2G	3	Total Mg 3 3	0	0
54	2I	1	Total Mg 1 1	0	0
54	2N	1	Total Mg 1 1	0	0
54	2O	3	Total Mg 3 3	0	0
54	2P	1	Total Mg 1 1	0	0
54	2Q	3	Total Mg 3 3	0	0
54	2R	2	Total Mg 2 2	0	0
54	2T	4	Total Mg 4 4	0	0
54	2V	1	Total Mg 1 1	0	0
54	2W	2	Total Mg 2 2	0	0
54	2X	1	Total Mg 1 1	0	0
54	20	2	Total Mg 2 2	0	0
54	21	2	Total Mg 2 2	0	0

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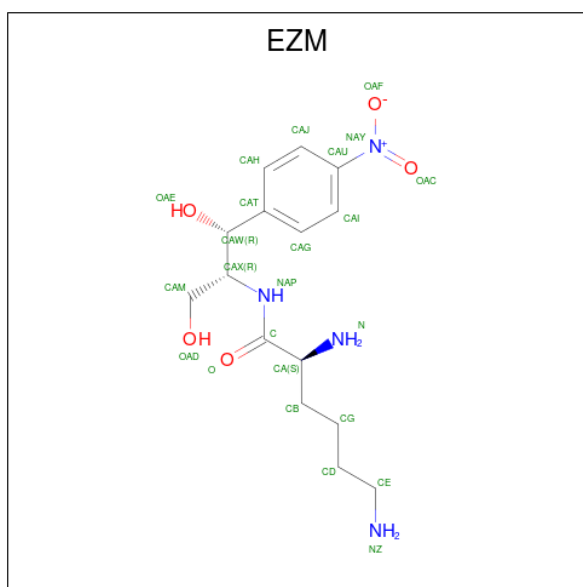
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	23	1	Total Mg 1 1	0	0
54	25	1	Total Mg 1 1	0	0
54	28	3	Total Mg 3 3	0	0
54	2a	184	Total Mg 184 184	0	0
54	2d	1	Total Mg 1 1	0	0
54	2e	1	Total Mg 1 1	0	0
54	2f	1	Total Mg 1 1	0	0
54	2j	1	Total Mg 1 1	0	0
54	2t	1	Total Mg 1 1	0	0

- Molecule 55 is POTASSIUM ION (three-letter code: K) (formula: K).

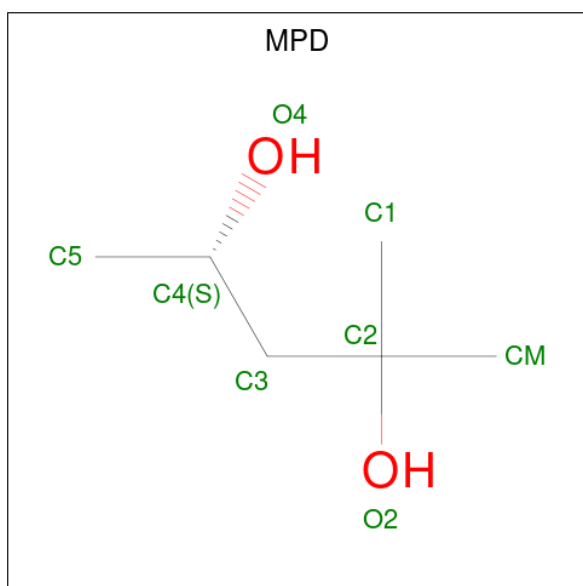
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1A	1	Total K 1 1	0	0
55	2A	1	Total K 1 1	0	0

- Molecule 56 is N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]-L-lysineamide (three-letter code: EZM) (formula: C₁₅H₂₄N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	1A	1	Total	C	N	O	0	0
			24	15	4	5		
56	2A	1	Total	C	N	O	0	0
			24	15	4	5		

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



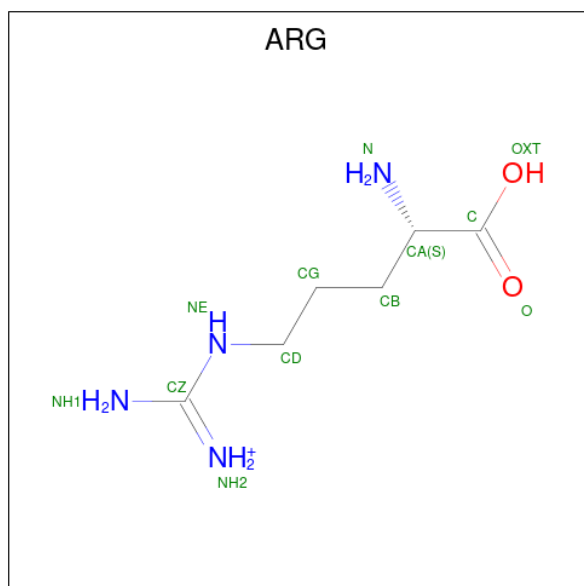
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	1A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	1T	1	Total	C	O	0	0
			8	6	2		
57	18	1	Total	C	O	0	0
			8	6	2		
57	1a	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 58 is ARGinine (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1B	1	Total	C	N	O	0	0
			12	6	4	2		
58	1F	1	Total	C	N	O	0	0
			12	6	4	2		

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

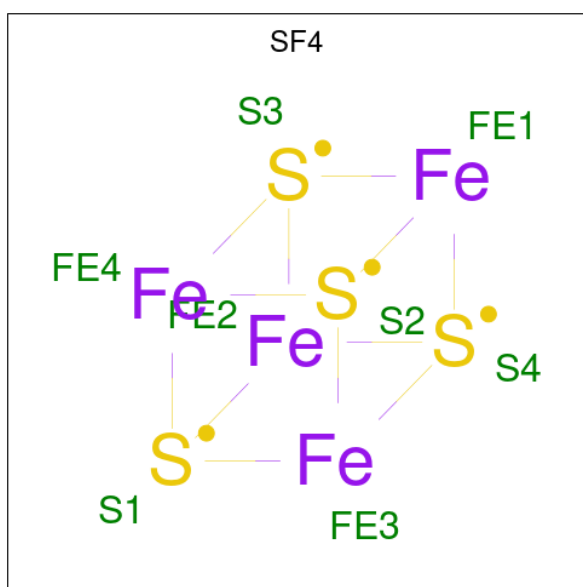
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	14	1	Total 1	Zn 1	0	0
59	15	1	Total 1	Zn 1	0	0
59	16	1	Total 1	Zn 1	0	0
59	19	1	Total 1	Zn 1	0	0
59	1n	1	Total 1	Zn 1	0	0
59	2Y	1	Total 1	Zn 1	0	0
59	24	1	Total 1	Zn 1	0	0
59	25	1	Total 1	Zn 1	0	0
59	26	1	Total 1	Zn 1	0	0
59	29	1	Total 1	Zn 1	0	0
59	2n	1	Total 1	Zn 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	3290	Total	O	0	0
			3290	3290		
61	1B	108	Total	O	0	0
			108	108		
61	1D	113	Total	O	0	0
			113	113		
61	1E	82	Total	O	0	0
			82	82		
61	1F	64	Total	O	0	0
			64	64		
61	1G	20	Total	O	0	0
			20	20		
61	1H	15	Total	O	0	0
			15	15		
61	1I	7	Total	O	0	0
			7	7		
61	1N	54	Total	O	0	0
			54	54		
61	1O	23	Total	O	0	0
			23	23		
61	1P	53	Total	O	0	0
			53	53		
61	1Q	46	Total	O	0	0
			46	46		
61	1R	32	Total	O	0	0
			32	32		
61	1S	13	Total	O	0	0
			13	13		
61	1T	35	Total	O	0	0
			35	35		
61	1U	42	Total	O	0	0
			42	42		
61	1V	36	Total	O	0	0
			36	36		
61	1W	26	Total	O	0	0
			26	26		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1X	23	Total 23	O 23	0	0
61	1Y	14	Total 14	O 14	0	0
61	1Z	13	Total 13	O 13	0	0
61	10	22	Total 22	O 22	0	0
61	11	25	Total 25	O 25	0	0
61	12	13	Total 13	O 13	0	0
61	13	25	Total 25	O 25	0	0
61	14	3	Total 3	O 3	0	0
61	15	24	Total 24	O 24	0	0
61	16	20	Total 20	O 20	0	0
61	17	9	Total 9	O 9	0	0
61	18	27	Total 27	O 27	0	0
61	19	6	Total 6	O 6	0	0
61	1a	343	Total 343	O 343	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	8	Total 8	O 8	0	0
61	1e	6	Total 6	O 6	0	0
61	1f	3	Total 3	O 3	0	0
61	1i	1	Total 1	O 1	0	0
61	1j	2	Total 2	O 2	0	0
61	1k	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1l	4	Total O 4 4	0	0
61	1o	4	Total O 4 4	0	0
61	1p	3	Total O 3 3	0	0
61	1t	1	Total O 1 1	0	0
61	1y	4	Total O 4 4	0	0
61	2A	1236	Total O 1236 1236	0	0
61	2B	73	Total O 73 73	0	0
61	2D	50	Total O 50 50	0	0
61	2E	25	Total O 25 25	0	0
61	2F	19	Total O 19 19	0	0
61	2G	8	Total O 8 8	0	0
61	2H	4	Total O 4 4	0	0
61	2I	4	Total O 4 4	0	0
61	2N	5	Total O 5 5	0	0
61	2O	21	Total O 21 21	0	0
61	2P	18	Total O 18 18	0	0
61	2Q	26	Total O 26 26	0	0
61	2R	15	Total O 15 15	0	0
61	2S	5	Total O 5 5	0	0
61	2T	10	Total O 10 10	0	0
61	2U	14	Total O 14 14	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2V	6	Total O 6 6	0	0
61	2W	18	Total O 18 18	0	0
61	2X	8	Total O 8 8	0	0
61	2Y	3	Total O 3 3	0	0
61	2Z	12	Total O 12 12	0	0
61	20	12	Total O 12 12	0	0
61	21	18	Total O 18 18	0	0
61	22	4	Total O 4 4	0	0
61	23	2	Total O 2 2	0	0
61	24	2	Total O 2 2	0	0
61	25	7	Total O 7 7	0	0
61	26	3	Total O 3 3	0	0
61	27	6	Total O 6 6	0	0
61	28	13	Total O 13 13	0	0
61	29	2	Total O 2 2	0	0
61	2a	259	Total O 259 259	0	0
61	2d	5	Total O 5 5	0	0
61	2e	2	Total O 2 2	0	0
61	2f	1	Total O 1 1	0	0
61	2j	2	Total O 2 2	0	0
61	2l	1	Total O 1 1	0	0

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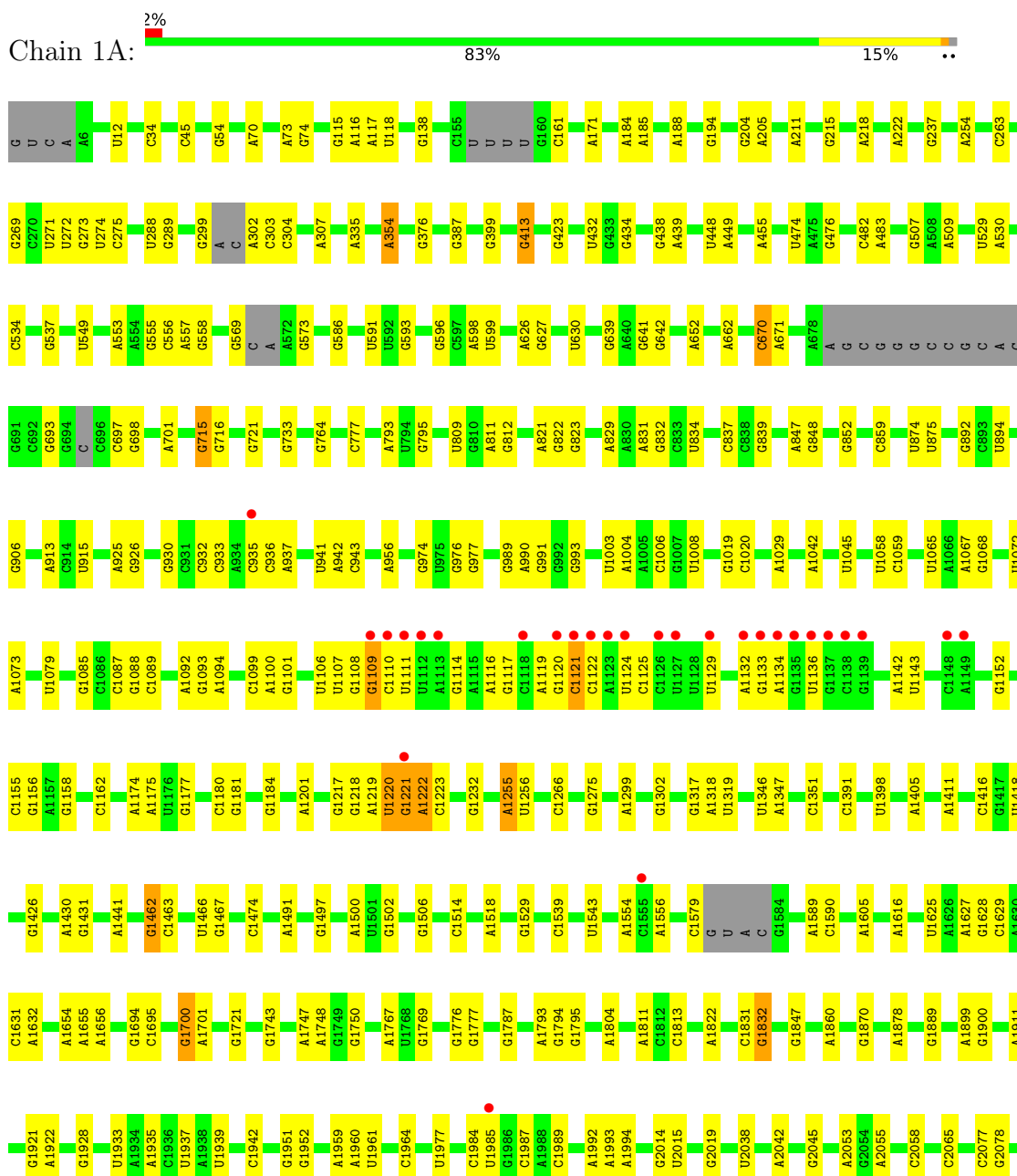
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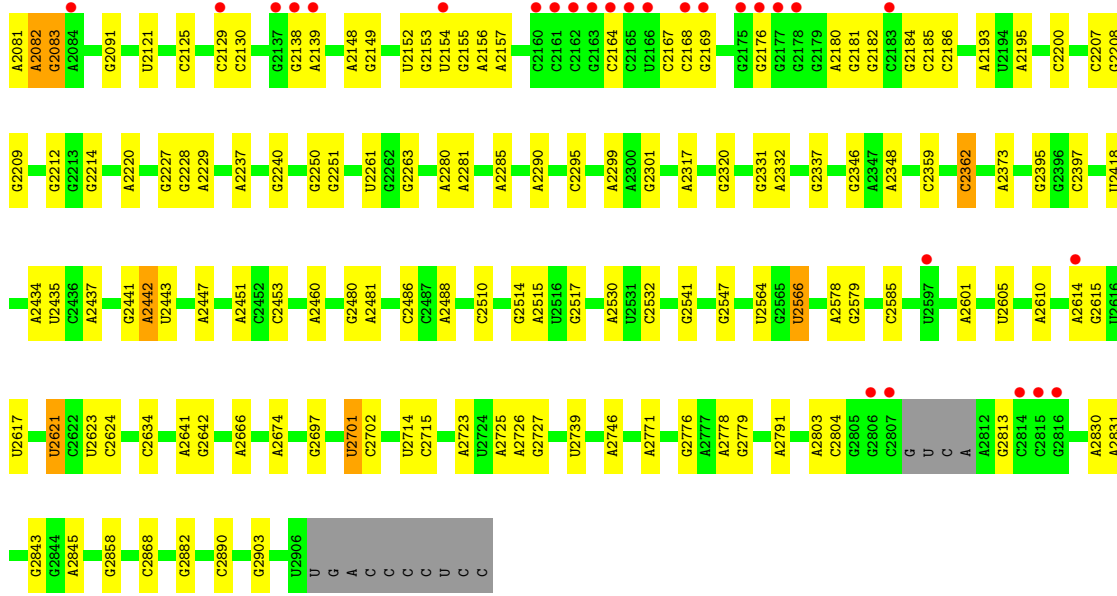
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2m	1	Total O 1 1	0	0
61	2o	2	Total O 2 2	0	0
61	2p	1	Total O 1 1	0	0
61	2q	1	Total O 1 1	0	0
61	2r	5	Total O 5 5	0	0
61	2s	1	Total O 1 1	0	0
61	2t	1	Total O 1 1	0	0
61	2u	1	Total O 1 1	0	0
61	2y	1	Total O 1 1	0	0

3 Residue-property plots

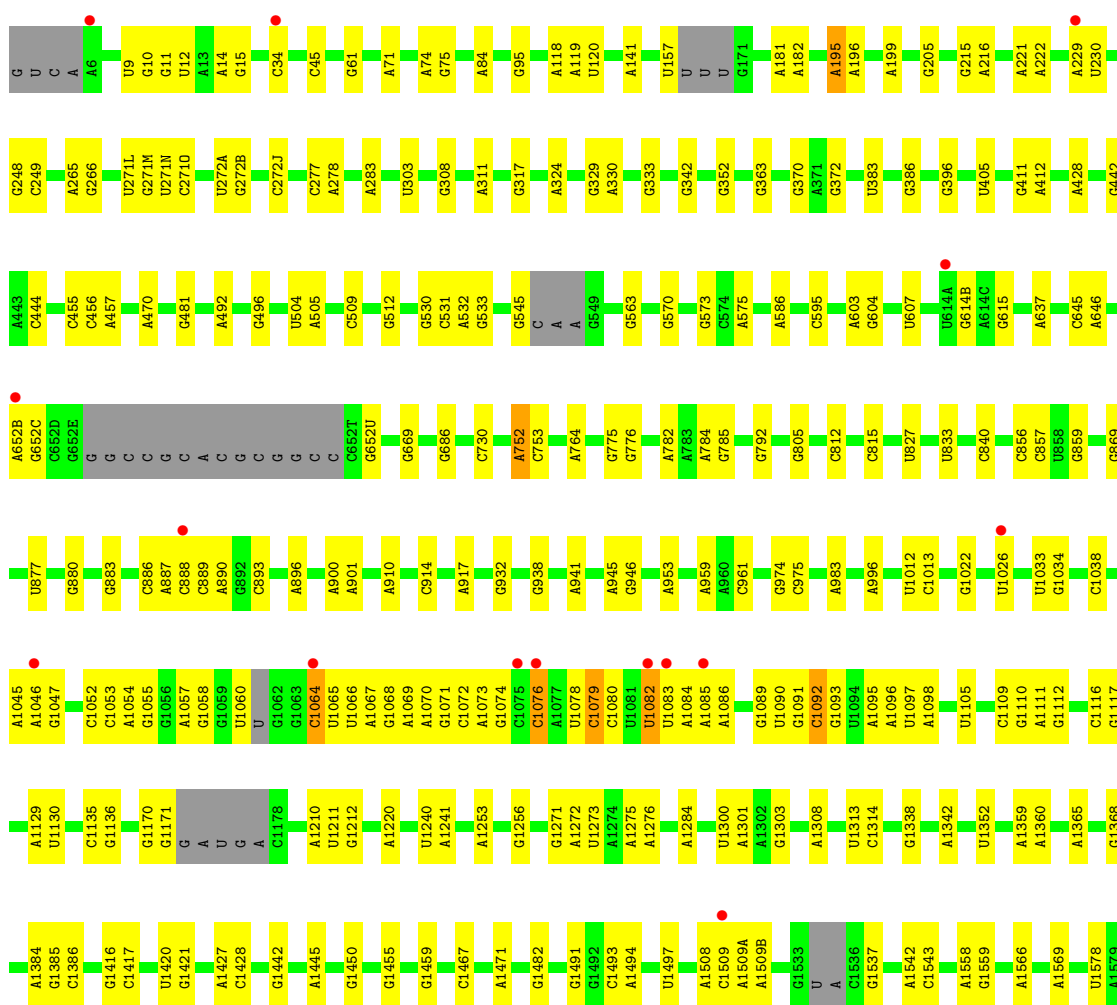
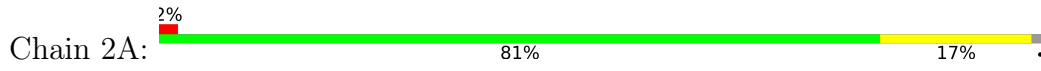
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S Ribosomal RNA

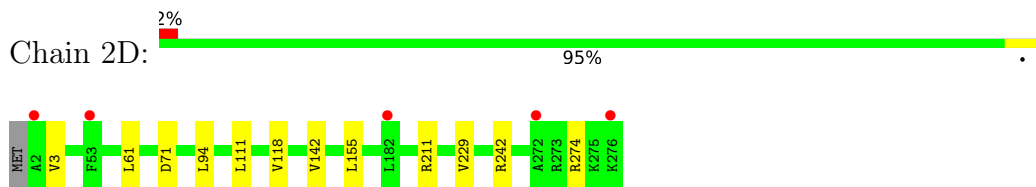




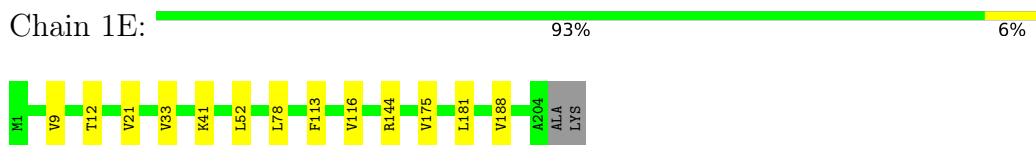
● Molecule 1: 23S Ribosomal RNA



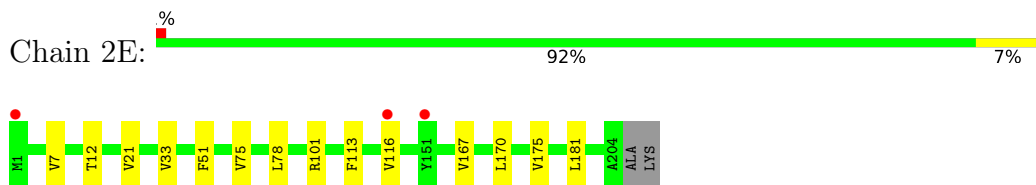
- Molecule 3: 50S ribosomal protein L2



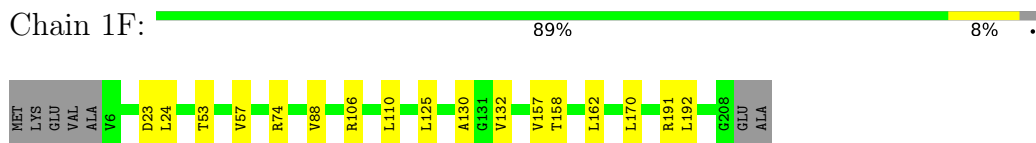
- Molecule 4: 50S Ribosomal Protein L3



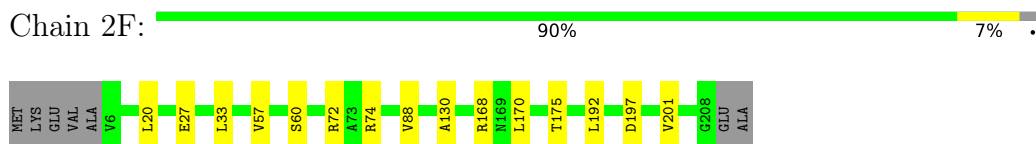
- Molecule 4: 50S Ribosomal Protein L3



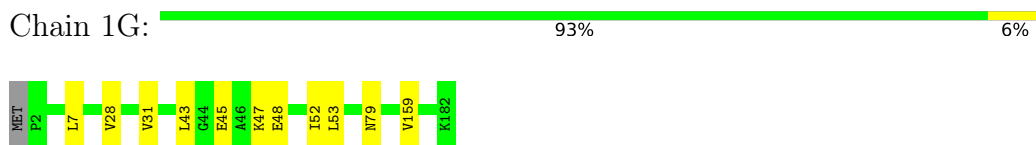
- Molecule 5: 50S ribosomal protein L4



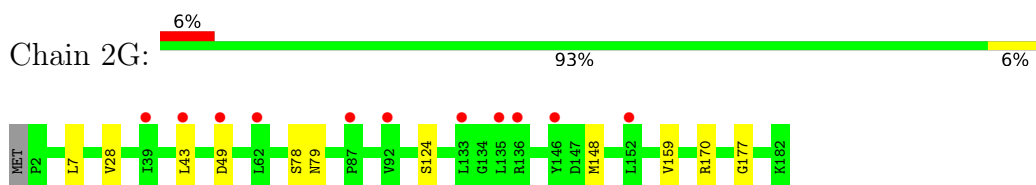
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5

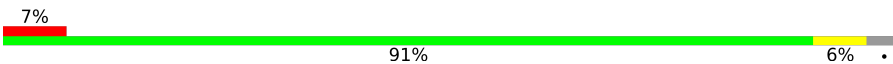


- Molecule 7: 50S ribosomal protein L6

Chain 1H:  93%



- Molecule 7: 50S ribosomal protein L6

Chain 2H:  91% 7% 6%



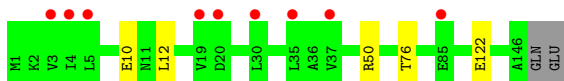
- Molecule 8: 50S ribosomal protein L9

Chain 1I:  94% 5%



- Molecule 8: 50S ribosomal protein L9

Chain 2I:  95% 6%



- Molecule 9: 50S ribosomal protein L13

Chain 1N:  91% 9%



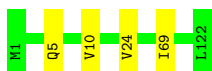
- Molecule 9: 50S ribosomal protein L13

Chain 2N:  96%



- Molecule 10: 50S ribosomal protein L14

Chain 1O:  97%



- Molecule 10: 50S ribosomal protein L14

Chain 2O:  93% 7%



- Molecule 11: 50S ribosomal protein L15

Chain 1P:  97% ..



- Molecule 11: 50S ribosomal protein L15

Chain 2P:  97% ..



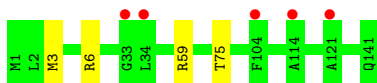
- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  95% 5%



- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  97% .



- Molecule 13: 50S ribosomal protein L17

Chain 1R:  91% 9%



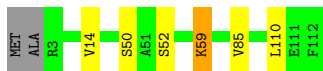
- Molecule 13: 50S ribosomal protein L17

Chain 2R:  93% 7%



- Molecule 14: 50S Ribosomal Protein L18

Chain 1S:  93%




- Molecule 14: 50S Ribosomal Protein L18

Chain 2S:  10% 94%




- Molecule 15: 50S ribosomal protein L19

Chain 1T:  84% 5% 10%



- Molecule 15: 50S ribosomal protein L19

Chain 2T:  % 86% 10%



- Molecule 16: 50S Ribosomal Protein L20

Chain 1U:  94%



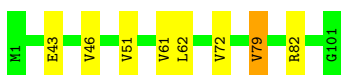
- Molecule 16: 50S Ribosomal Protein L20

Chain 2U:  93% 5%



- Molecule 17: 50S ribosomal protein L21

Chain 1V:  92% 7%



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  95% ..



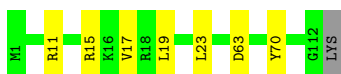
- Molecule 18: 50S ribosomal protein L22

Chain 1W:  90% 9% .



- Molecule 18: 50S ribosomal protein L22

Chain 2W:  93% 6% .



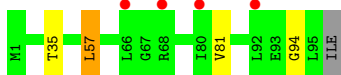
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  95% ..



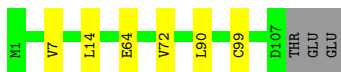
- Molecule 19: 50S ribosomal protein L23

Chain 2X:  4% 95% ...



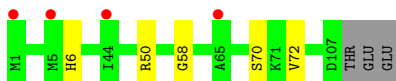
- Molecule 20: 50S Ribosomal Protein L24

Chain 1Y:  92% 5% .



- Molecule 20: 50S Ribosomal Protein L24

Chain 2Y:  4% 93% 5% .



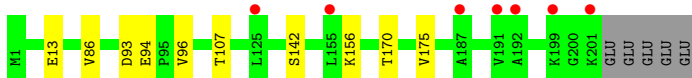
- Molecule 21: 50S ribosomal protein L25

Chain 1Z:  92% 6%




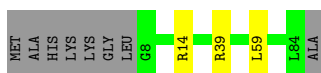
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:  93% 5% 3%




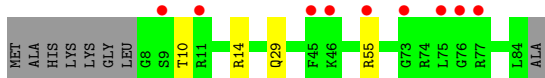
• Molecule 22: 50S ribosomal protein L27

Chain 10:  87% 9%



• Molecule 22: 50S ribosomal protein L27

Chain 20:  86% 5% 9% 11%

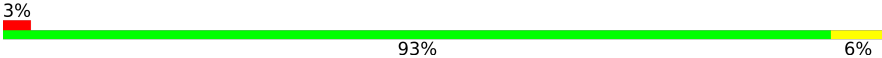


• Molecule 23: 50S ribosomal protein L28

Chain 11:  96% 3%



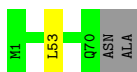
• Molecule 23: 50S ribosomal protein L28

Chain 21:  93% 6% 3%



• Molecule 24: 50S ribosomal protein L29

Chain 12:  96%



• Molecule 24: 50S ribosomal protein L29

Chain 22:  90% 7%



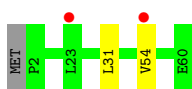
- Molecule 25: 50S ribosomal protein L30

Chain 13:  93% 5%

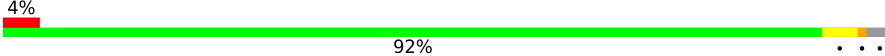


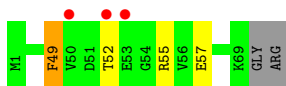
- Molecule 25: 50S ribosomal protein L30

Chain 23:  3% 95%




- Molecule 26: 50S Ribosomal Protein L31

Chain 14:  4% 92%




- Molecule 26: 50S Ribosomal Protein L31

Chain 24:  14% 90% 7%



- Molecule 27: 50S ribosomal protein L32

Chain 15:  88% 10%




- Molecule 27: 50S ribosomal protein L32

Chain 25:  95%



- Molecule 28: 50S ribosomal protein L33

Chain 16:  87% 11%




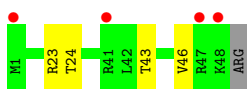
- Molecule 28: 50S ribosomal protein L33

Chain 26:  93% 6%



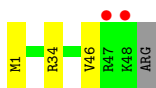
- Molecule 29: 50S ribosomal protein L34

Chain 17:  8% 90% 8%

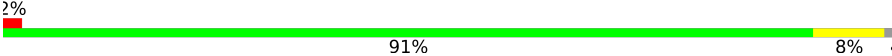


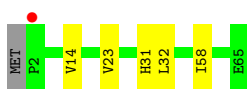
- Molecule 29: 50S ribosomal protein L34

Chain 27:  4% 92% 6%



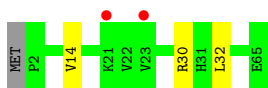
- Molecule 30: 50S ribosomal protein L35

Chain 18:  2% 91% 8%



- Molecule 30: 50S ribosomal protein L35

Chain 28:  3% 94% 5%

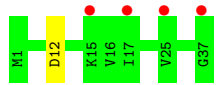


- Molecule 31: 50S ribosomal protein L36

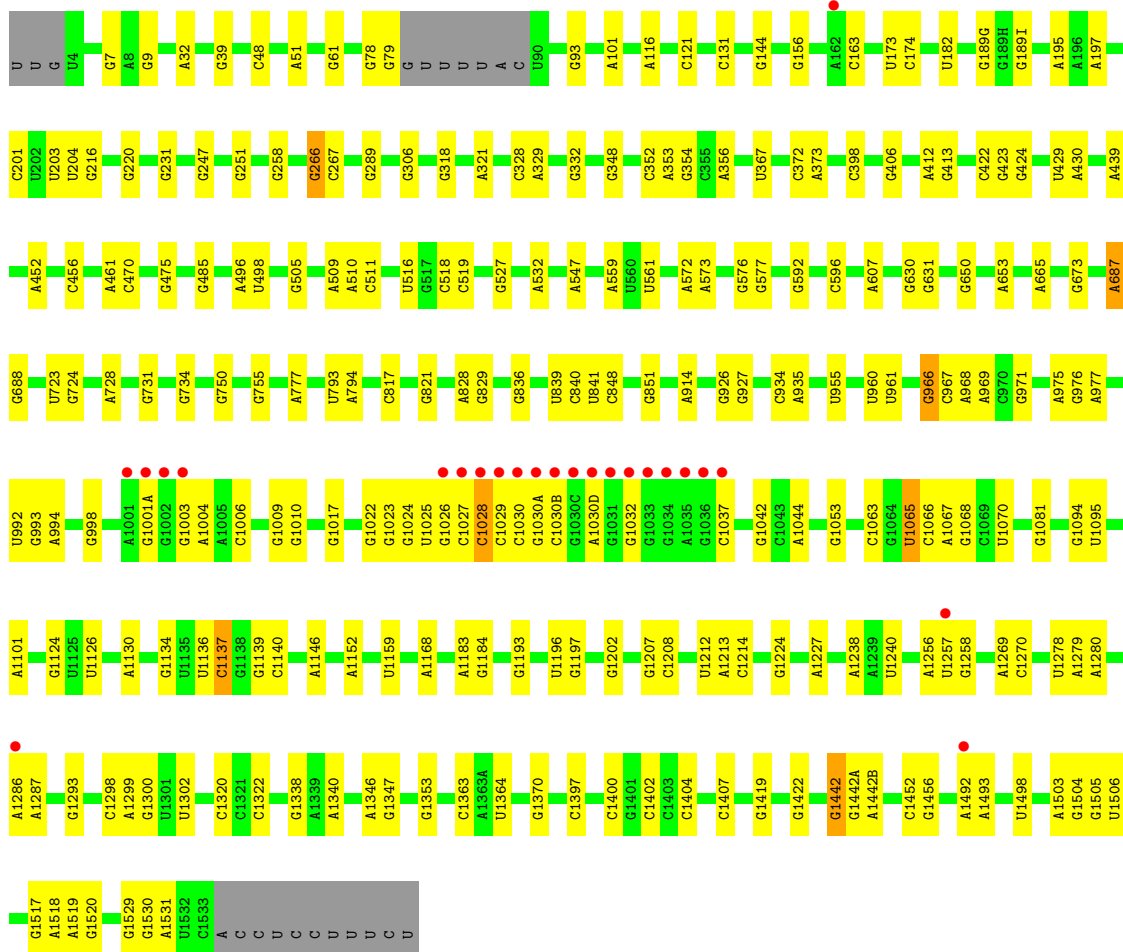
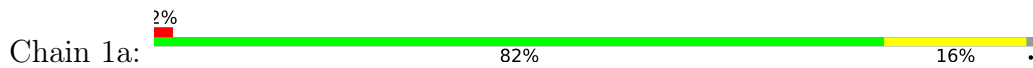
Chain 19:  100%

There are no outlier residues recorded for this chain.

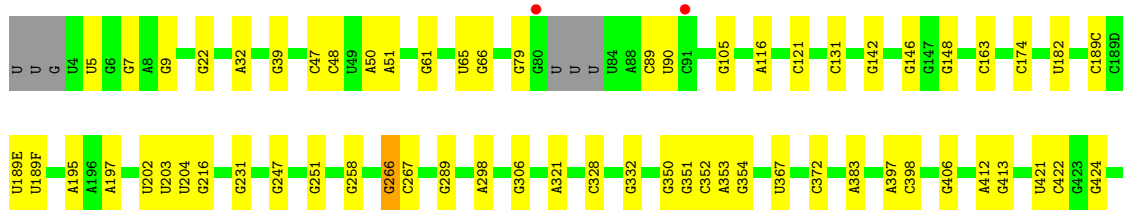
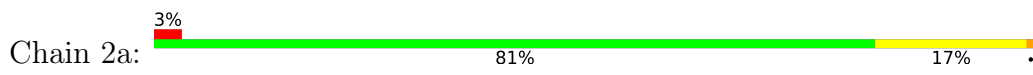
- Molecule 31: 50S ribosomal protein L36

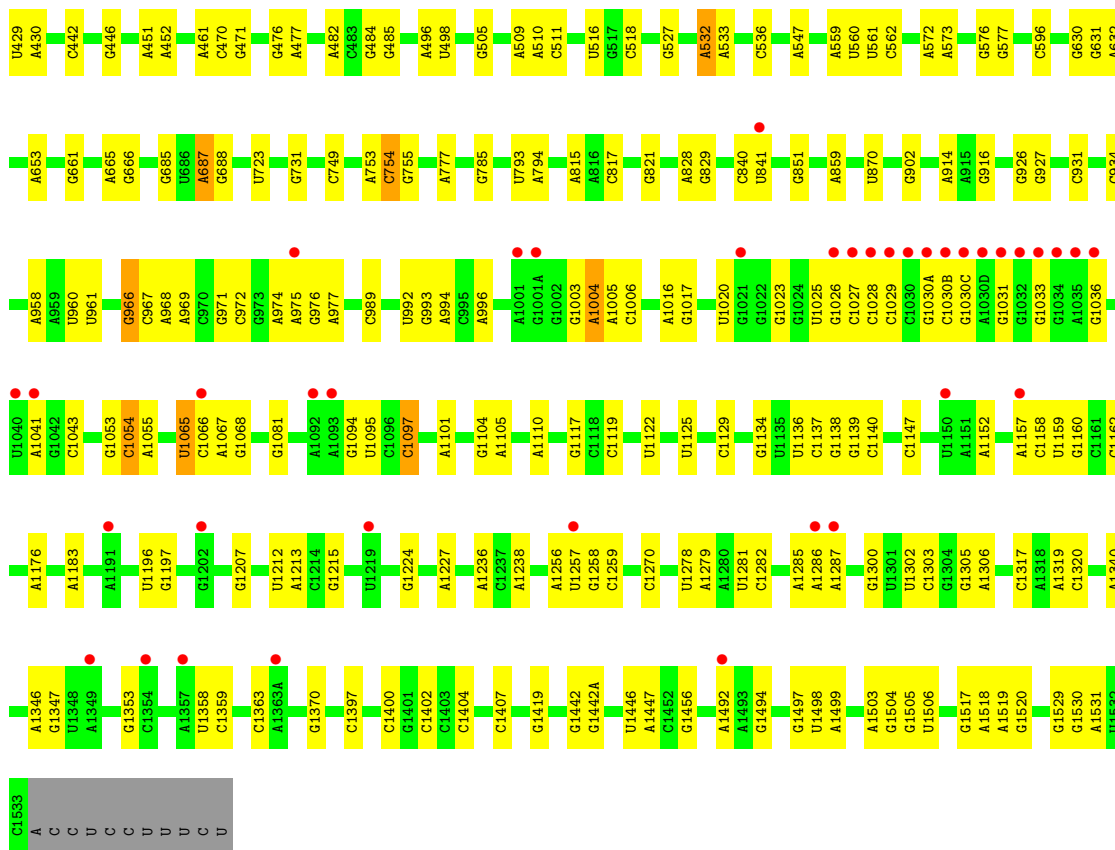


• Molecule 32: 16S Ribosomal RNA

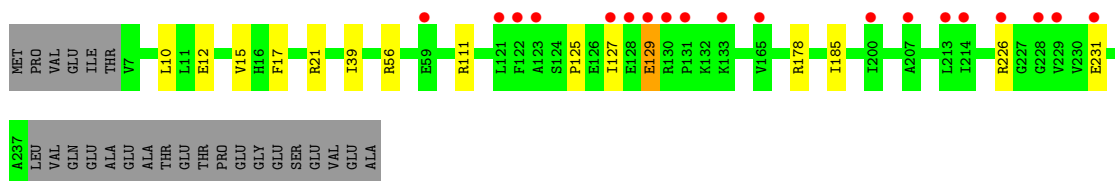
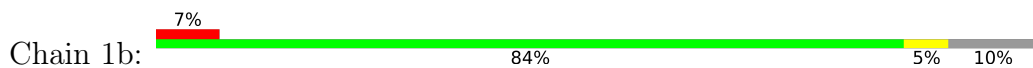


• Molecule 32: 16S Ribosomal RNA

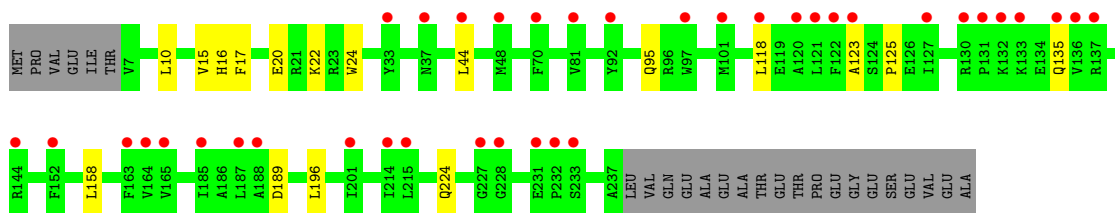
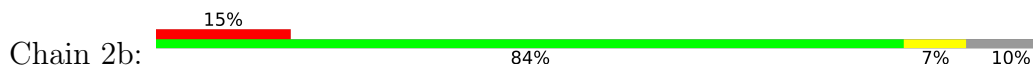




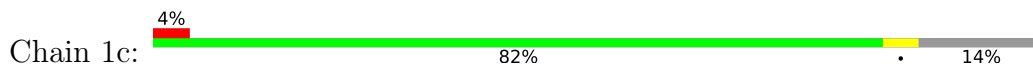
• Molecule 33: 30S ribosomal protein S2

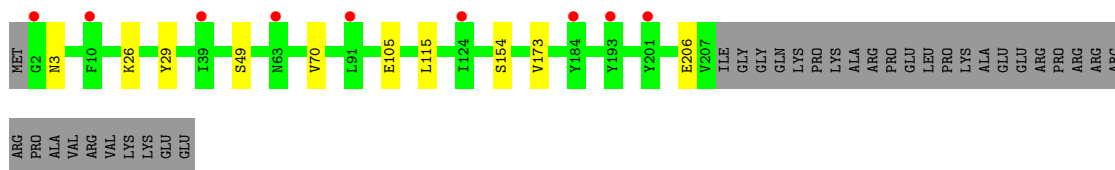


• Molecule 33: 30S ribosomal protein S2

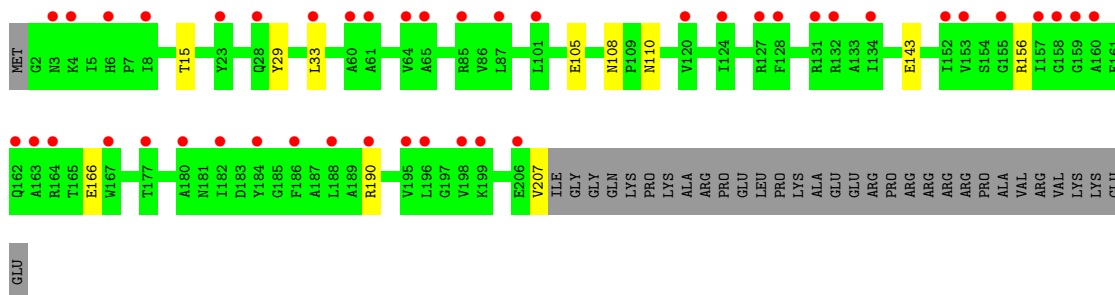
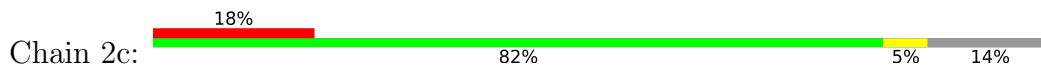


• Molecule 34: 30S ribosomal protein S3





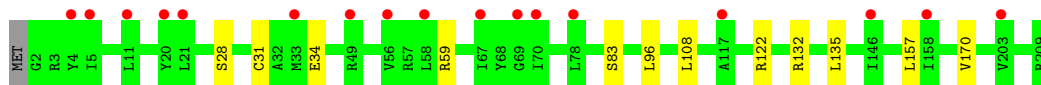
• Molecule 34: 30S ribosomal protein S3



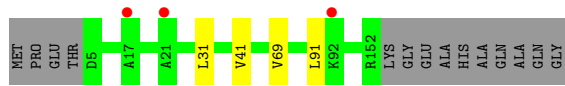
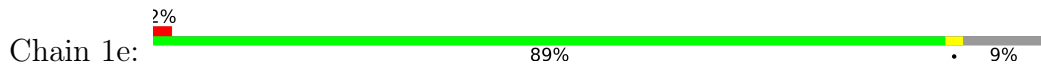
• Molecule 35: 30S ribosomal protein S4



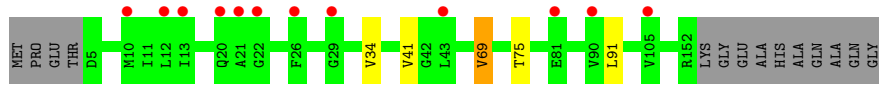
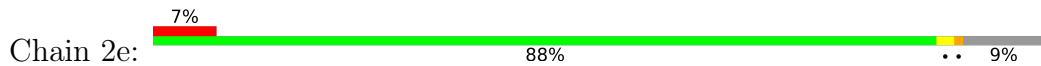
• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5



• Molecule 36: 30S ribosomal protein S5



• Molecule 37: 30S ribosomal protein S6

Chain 1f:  94% 5%



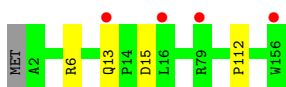
• Molecule 37: 30S ribosomal protein S6

Chain 2f:  97%



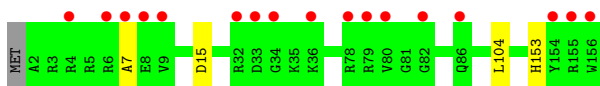
• Molecule 38: 30S ribosomal protein S7

Chain 1g:  3% 97%



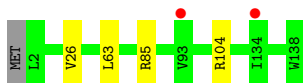
• Molecule 38: 30S ribosomal protein S7

Chain 2g:  11% 97%



• Molecule 39: 30S Ribosomal Protein S8

Chain 1h:  1% 96%



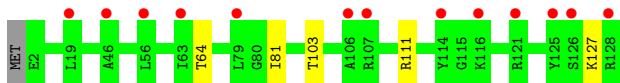
• Molecule 39: 30S Ribosomal Protein S8

Chain 2h:  7% 93% 7%

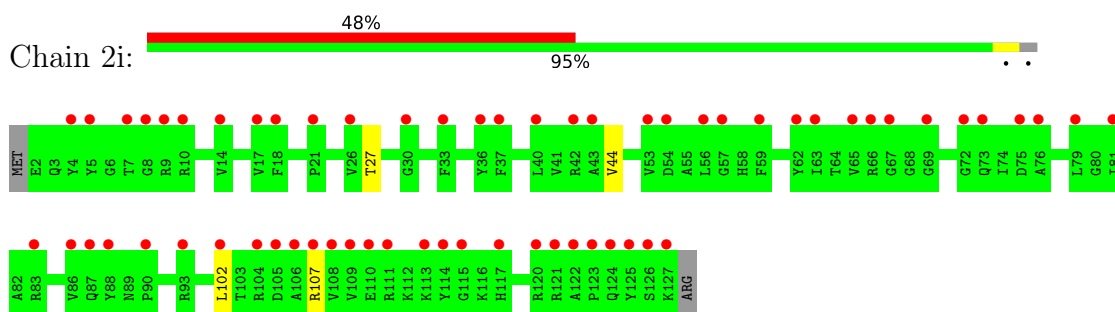


• Molecule 40: 30S ribosomal protein S9

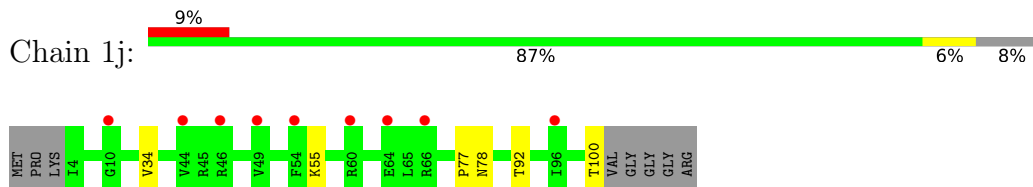
Chain 1i:  10% 95%



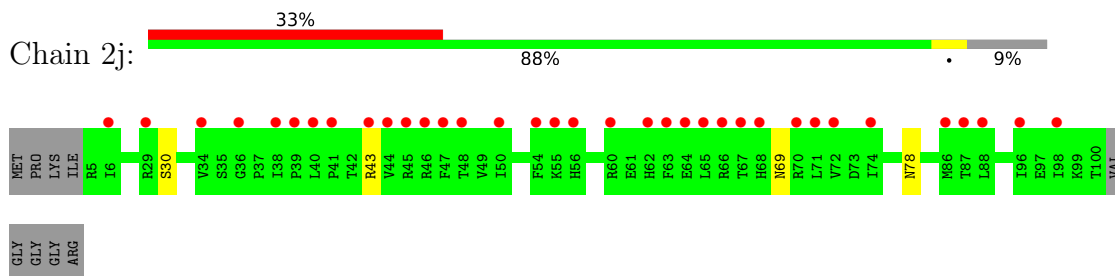
• Molecule 40: 30S ribosomal protein S9



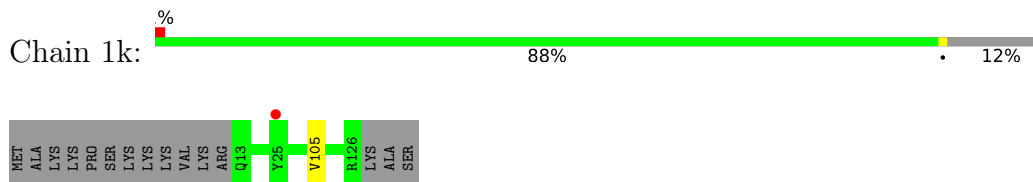
- Molecule 41: 30S ribosomal protein S10



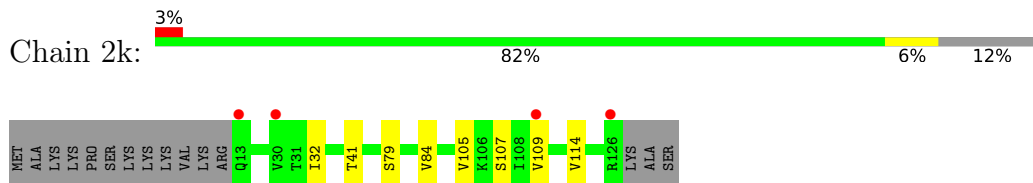
- Molecule 41: 30S ribosomal protein S10



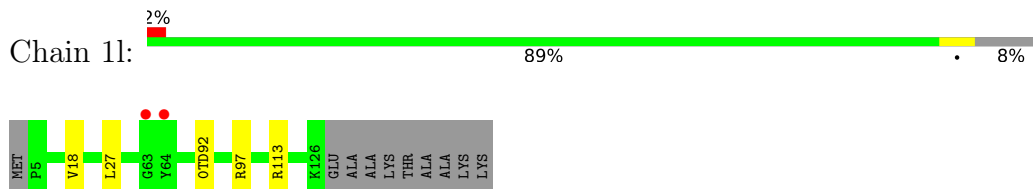
- Molecule 42: 30S ribosomal protein S11



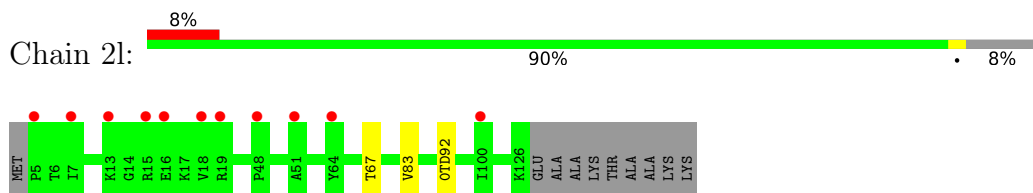
- Molecule 42: 30S ribosomal protein S11



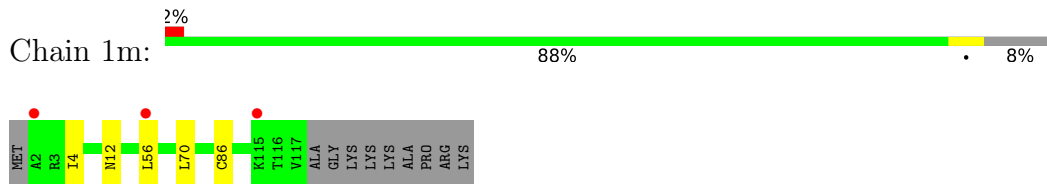
- Molecule 43: 30S ribosomal protein S12



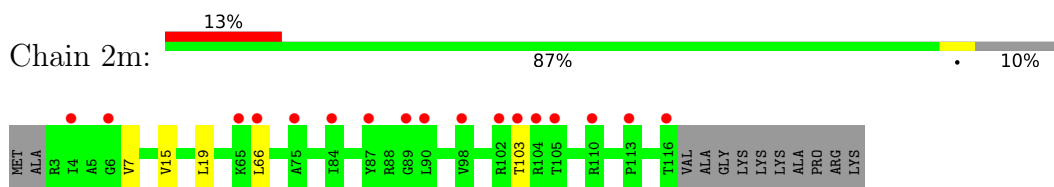
- Molecule 43: 30S ribosomal protein S12



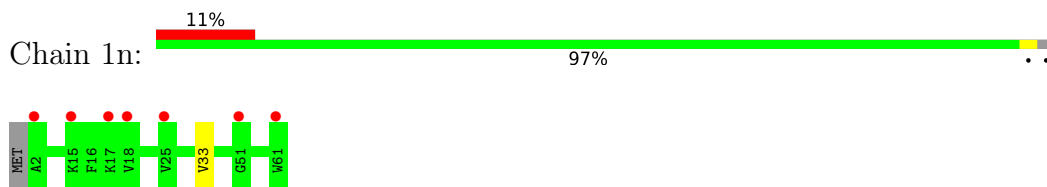
• Molecule 44: 30S ribosomal protein S13



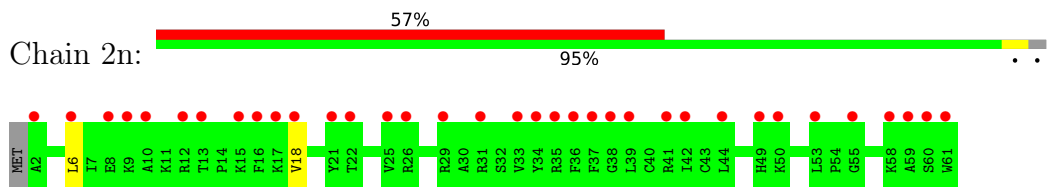
• Molecule 44: 30S ribosomal protein S13



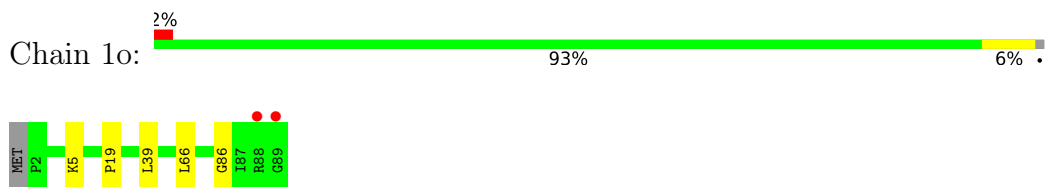
• Molecule 45: 30S ribosomal protein S14 type Z



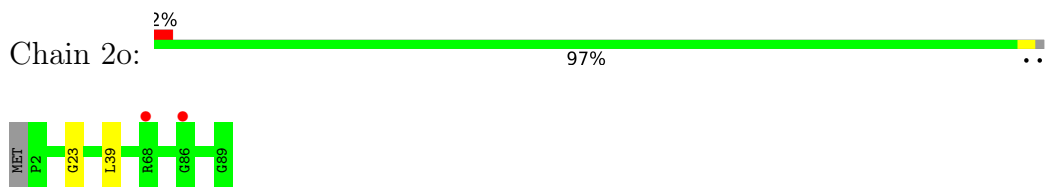
• Molecule 45: 30S ribosomal protein S14 type Z




• Molecule 46: 30S ribosomal protein S15



• Molecule 46: 30S ribosomal protein S15




- Molecule 47: 30S ribosomal protein S16

Chain 1p:  88% 6% 7%

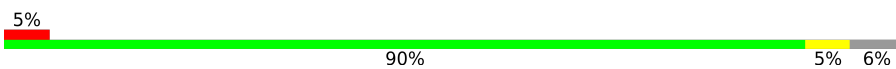


- Molecule 47: 30S ribosomal protein S16

Chain 2p:  88% 6% 7%

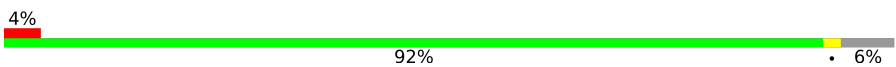


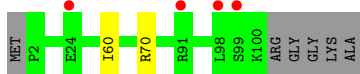
- Molecule 48: 30S ribosomal protein S17

Chain 1q:  90% 5% 6%




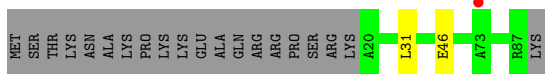
- Molecule 48: 30S ribosomal protein S17

Chain 2q:  92% 6%




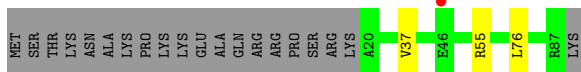
- Molecule 49: 30S ribosomal protein S18

Chain 1r:  75% 23%




- Molecule 49: 30S ribosomal protein S18

Chain 2r:  74% 23%

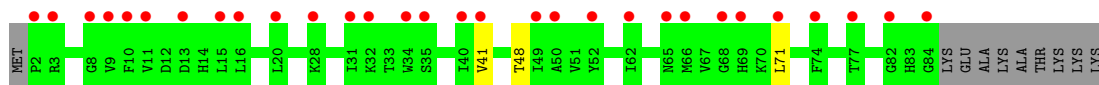
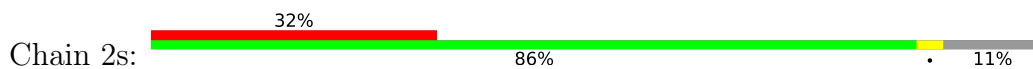


- Molecule 50: 30S ribosomal protein S19

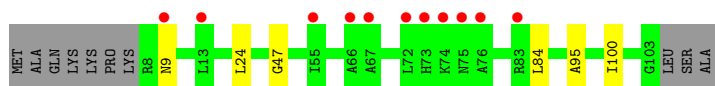
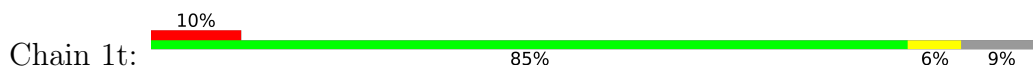
Chain 1s:  84% 5% 11%



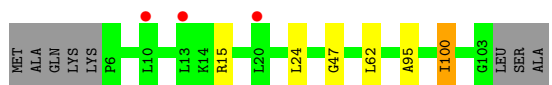
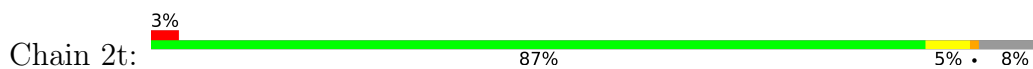
• Molecule 50: 30S ribosomal protein S19



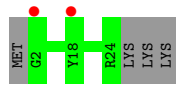
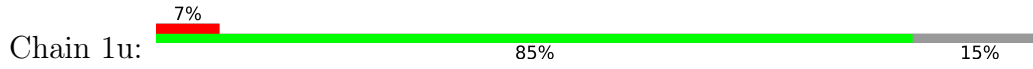
• Molecule 51: 30S ribosomal protein S20



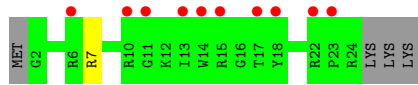
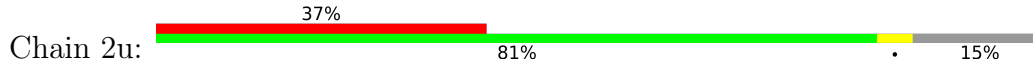
• Molecule 51: 30S ribosomal protein S20



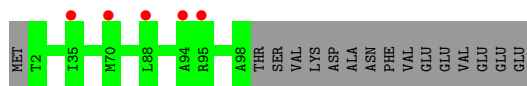
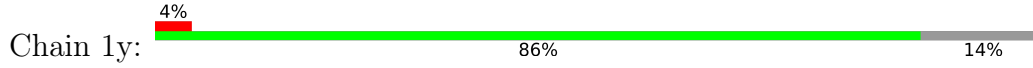
• Molecule 52: 30S Ribosomal Protein THX



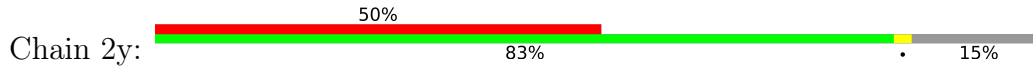
• Molecule 52: 30S Ribosomal Protein THX

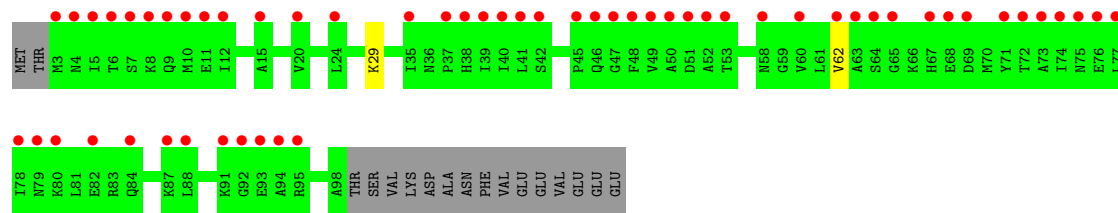


• Molecule 53: Protein Y



• Molecule 53: Protein Y





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.15Å 449.33Å 623.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.66 – 2.60 311.73 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (224.66-2.60) 99.8 (311.73-2.60)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.62Å)	Xtrriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.209 , 0.252 0.209 , 0.252	Depositor DCC
R_{free} test set	89415 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtrriage
Anisotropy	0.112	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	295545	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.54	1/69029 (0.0%)	1.01	84/107746 (0.1%)
1	2A	0.42	0/68901	0.90	29/107544 (0.0%)
2	1B	0.45	0/2876	0.93	2/4486 (0.0%)
2	2B	0.38	0/2878	0.86	0/4490
3	1D	0.38	0/2181	0.60	1/2940 (0.0%)
3	2D	0.33	0/2186	0.54	0/2944
4	1E	0.36	0/1592	0.57	0/2149
4	2E	0.33	0/1592	0.54	0/2149
5	1F	0.37	1/1619 (0.1%)	0.58	0/2193
5	2F	0.32	0/1615	0.52	0/2188
6	1G	0.30	0/1451	0.50	0/1961
6	2G	0.32	0/1449	0.47	0/1957
7	1H	0.35	0/1356	0.51	0/1834
7	2H	0.30	0/1350	0.48	0/1826
8	1I	0.31	0/1109	0.50	0/1512
8	2I	0.28	0/1091	0.50	0/1490
9	1N	0.35	0/1148	0.54	0/1547
9	2N	0.31	0/1144	0.48	0/1543
10	1O	0.39	0/943	0.58	0/1269
10	2O	0.33	0/943	0.52	0/1269
11	1P	0.34	0/1152	0.56	0/1533
11	2P	0.33	0/1152	0.54	0/1533
12	1Q	0.35	0/1143	0.52	0/1527
12	2Q	0.31	0/1143	0.49	0/1527
13	1R	0.33	0/982	0.59	0/1312
13	2R	0.29	0/982	0.54	0/1312
14	1S	0.31	0/887	0.52	0/1180
14	2S	0.31	0/880	0.49	0/1172
15	1T	0.33	0/1105	0.55	0/1477
15	2T	0.31	0/1097	0.51	0/1468
16	1U	0.38	0/977	0.54	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.31	0/977	0.44	0/1301
17	1V	0.38	0/786	0.57	0/1053
17	2V	0.33	0/782	0.52	0/1049
18	1W	0.35	0/897	0.54	0/1205
18	2W	0.31	0/897	0.50	0/1205
19	1X	0.37	0/764	0.56	0/1025
19	2X	0.31	0/764	0.55	1/1025 (0.1%)
20	1Y	0.37	0/823	0.54	0/1099
20	2Y	0.31	0/823	0.51	0/1100
21	1Z	0.32	0/1620	0.51	0/2200
21	2Z	0.34	1/1590 (0.1%)	0.50	0/2162
22	10	0.36	0/616	0.55	0/821
22	20	0.32	0/616	0.51	0/821
23	11	0.35	0/761	0.55	0/1013
23	21	0.33	0/766	0.51	0/1018
24	12	0.31	0/590	0.51	0/781
24	22	0.31	0/594	0.42	0/785
25	13	0.33	0/474	0.55	0/635
25	23	0.30	0/469	0.49	0/630
26	14	0.34	0/559	0.54	0/754
26	24	0.37	0/549	0.56	0/741
27	15	0.39	0/473	0.68	2/639 (0.3%)
27	25	0.31	0/469	0.52	0/635
28	16	0.32	0/460	0.55	0/613
28	26	0.31	0/456	0.49	0/608
29	17	0.36	0/426	0.60	0/561
29	27	0.32	0/426	0.51	0/561
30	18	0.35	0/525	0.59	0/691
30	28	0.30	0/525	0.51	0/691
31	19	0.36	0/310	0.54	0/407
31	29	0.30	0/310	0.51	0/407
32	1a	0.39	0/35795	0.88	13/55864 (0.0%)
32	2a	0.37	0/35890	0.87	21/56012 (0.0%)
33	1b	0.30	0/1876	0.49	1/2533 (0.0%)
33	2b	0.33	0/1860	0.49	0/2518
34	1c	0.36	1/1582 (0.1%)	0.47	0/2137
34	2c	0.30	0/1566	0.49	0/2119
35	1d	0.30	0/1695	0.48	0/2274
35	2d	0.29	0/1698	0.46	0/2277
36	1e	0.32	0/1149	0.52	0/1548
36	2e	0.35	1/1149 (0.1%)	0.49	0/1548
37	1f	0.31	0/827	0.51	0/1120
37	2f	0.29	0/829	0.51	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.29	0/1254	0.42	0/1683
38	2g	0.29	0/1248	0.42	0/1676
39	1h	0.29	0/1118	0.48	0/1506
39	2h	0.28	0/1108	0.47	0/1494
40	1i	0.29	0/1005	0.51	0/1351
40	2i	0.31	0/985	0.47	0/1329
41	1j	0.30	0/732	0.50	0/993
41	2j	0.30	0/723	0.49	0/984
42	1k	0.29	0/849	0.48	0/1150
42	2k	0.30	0/848	0.52	0/1149
43	1l	0.30	0/937	0.50	0/1260
43	2l	0.28	0/937	0.52	0/1260
44	1m	0.29	0/924	0.48	0/1242
44	2m	0.30	0/905	0.47	0/1217
45	1n	0.31	0/501	0.46	0/664
45	2n	0.32	0/501	0.47	0/664
46	1o	0.30	0/739	0.46	0/985
46	2o	0.28	0/739	0.44	0/985
47	1p	0.31	0/697	0.53	0/939
47	2p	0.30	0/693	0.51	0/935
48	1q	0.30	0/836	0.49	0/1117
48	2q	0.31	0/836	0.50	0/1117
49	1r	0.29	0/560	0.49	0/746
49	2r	0.29	0/560	0.45	0/746
50	1s	0.28	0/663	0.50	0/895
50	2s	0.30	0/660	0.47	0/893
51	1t	0.28	0/734	0.45	0/969
51	2t	0.28	0/736	0.42	0/976
52	1u	0.26	0/203	0.48	0/266
52	2u	0.31	0/203	0.56	0/266
53	1y	0.29	0/776	0.49	0/1048
53	2y	0.28	0/761	0.47	0/1030
All	All	0.42	5/309937 (0.0%)	0.83	154/463223 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1c	173	VAL	C-N	8.18	1.49	1.34
1	1A	354	A	N9-C4	-6.29	1.34	1.37
36	2e	69	VAL	C-N	6.14	1.46	1.34
21	2Z	13	GLU	C-N	5.16	1.46	1.34
5	1F	23	ASP	C-N	-5.07	1.22	1.34

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1045	U	O5'-P-OP2	-11.85	95.03	105.70
1	1A	848	G	O5'-P-OP2	-9.23	97.39	105.70
1	1A	537	G	O4'-C1'-N9	8.97	115.38	108.20
1	1A	354	A	C2-N3-C4	-8.79	106.20	110.60
32	1a	1028	C	C5-C6-N1	8.53	125.26	121.00
1	1A	974	G	N1-C6-O6	-8.15	115.01	119.90
1	1A	1418	U	C5-C4-O4	-8.05	121.07	125.90
1	1A	2566	U	O5'-P-OP1	-7.80	98.68	105.70
1	1A	354	A	N1-C2-N3	7.75	133.18	129.30
32	2a	1003	G	N3-C4-C5	-7.75	124.72	128.60
1	1A	591	U	C5-C4-O4	-7.67	121.30	125.90
1	1A	1222	A	O5'-P-OP1	-7.54	98.91	105.70
1	2A	1092	C	N1-C2-O2	7.51	123.41	118.90
1	1A	1120	G	N3-C2-N2	7.37	125.06	119.90
32	2a	1004	A	O4'-C1'-N9	7.30	114.04	108.20
1	1A	2083	G	O5'-P-OP2	-7.23	99.19	105.70
1	1A	1418	U	N3-C4-O4	7.16	124.42	119.40
1	1A	1184	G	O5'-P-OP2	-7.16	99.26	105.70
1	1A	2601	A	O5'-P-OP1	-7.15	99.27	105.70
1	1A	1110	C	C2-N3-C4	7.07	123.44	119.90
1	1A	2058	C	O5'-P-OP1	-7.07	99.34	105.70
1	1A	1700	G	C8-N9-C4	-7.02	103.59	106.40
1	1A	2723	A	O5'-P-OP2	-6.95	99.44	105.70
1	1A	1121	C	N1-C2-O2	6.81	122.98	118.90
1	1A	2442	A	O5'-P-OP2	-6.80	99.58	105.70
1	1A	215	G	O4'-C1'-N9	6.79	113.63	108.20
1	1A	834	U	O5'-P-OP1	-6.71	99.67	105.70
32	2a	266	G	P-O3'-C3'	6.59	127.61	119.70
1	1A	1221	G	OP1-P-O3'	6.50	119.51	105.20
32	1a	1028	C	C2-N3-C4	6.46	123.13	119.90
1	1A	1232	G	N1-C6-O6	-6.44	116.03	119.90
1	1A	12	U	N3-C2-O2	-6.44	117.69	122.20
32	2a	1003	G	C8-N9-C4	-6.43	103.83	106.40
1	1A	892	G	O4'-C1'-N9	6.40	113.32	108.20
1	1A	1132	A	N1-C6-N6	-6.34	114.80	118.60
1	1A	1255	A	P-O3'-C3'	6.29	127.25	119.70
1	1A	2261	U	N3-C4-O4	-6.29	114.99	119.40
1	2A	512	G	O4'-C1'-N9	6.27	113.21	108.20
32	1a	1137	C	C5-C6-N1	6.26	124.13	121.00
1	1A	591	U	N3-C4-C5	6.24	118.34	114.60
1	1A	2697	G	N1-C6-O6	-6.23	116.16	119.90
1	1A	2858	G	O4'-C1'-N9	6.19	113.15	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1832	G	C5-C6-O6	-6.19	124.89	128.60
19	2X	57	LEU	CA-CB-CG	6.16	129.47	115.30
1	2A	2108	C	C2-N3-C4	6.11	122.95	119.90
1	2A	2689	U	N3-C2-O2	-6.11	117.92	122.20
1	2A	1082	U	C2-N1-C1'	6.10	125.02	117.70
2	1B	57	A	N9-C4-C5	-6.09	103.37	105.80
1	1A	593	G	C5-C6-O6	-6.08	124.95	128.60
32	2a	1097	C	C2-N1-C1'	6.05	125.46	118.80
1	1A	974	G	C5-C6-O6	6.04	132.23	128.60
1	1A	795	G	C4-N9-C1'	-6.01	118.69	126.50
32	1a	1137	C	C6-N1-C2	-6.00	117.90	120.30
32	1a	1028	C	C6-N1-C2	-6.00	117.90	120.30
1	1A	1101	G	C6-N1-C2	5.99	128.69	125.10
1	1A	354	A	N3-C4-N9	-5.97	122.62	127.40
1	1A	2082	A	C8-N9-C4	5.95	108.18	105.80
1	1A	847	A	O5'-P-OP1	-5.94	100.35	105.70
1	1A	1110	C	N1-C2-O2	5.94	122.46	118.90
2	1B	1	U	C2-N1-C1'	5.93	124.82	117.70
1	2A	1082	U	N3-C2-O2	-5.91	118.06	122.20
1	1A	2442	A	C2-N3-C4	5.88	113.54	110.60
1	1A	2634	C	N1-C2-O2	-5.88	115.37	118.90
1	2A	2103	C	C2-N3-C4	5.87	122.83	119.90
32	2a	754	C	C2-N1-C1'	5.84	125.23	118.80
27	15	58	LEU	CA-CB-CG	5.79	128.62	115.30
1	2A	1936	A	O4'-C1'-N9	5.77	112.81	108.20
32	2a	79	G	C5-C6-O6	5.76	132.06	128.60
1	2A	2689	U	P-O3'-C3'	5.76	126.61	119.70
1	1A	184	A	P-O3'-C3'	5.75	126.60	119.70
32	2a	1158	C	C6-N1-C2	-5.74	118.00	120.30
1	1A	1120	G	N9-C4-C5	-5.73	103.11	105.40
1	2A	1992	G	P-O3'-C3'	5.71	126.55	119.70
1	1A	1266	C	C6-N1-C2	-5.66	118.03	120.30
1	2A	383	U	O4'-C1'-N1	5.65	112.72	108.20
32	1a	1442	G	N3-C4-C5	-5.64	125.78	128.60
32	2a	1065	U	P-O3'-C3'	5.62	126.45	119.70
32	1a	1067	A	P-O3'-C3'	5.62	126.45	119.70
32	1a	1442	G	P-O3'-C3'	5.62	126.45	119.70
1	2A	1313	U	C2-N1-C1'	5.61	124.43	117.70
32	1a	1442	G	C2-N3-C4	5.61	114.70	111.90
1	2A	1082	U	N1-C2-O2	5.58	126.71	122.80
1	2A	1064	C	C6-N1-C2	-5.58	118.07	120.30
1	1A	2331	G	O4'-C1'-N9	5.56	112.65	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	591	U	C2-N3-C4	-5.55	123.67	127.00
1	1A	721	G	C5-C6-O6	-5.55	125.27	128.60
1	2A	2104	G	C4-N9-C1'	5.53	133.69	126.50
1	1A	593	G	N9-C4-C5	-5.51	103.20	105.40
1	1A	1232	G	N3-C2-N2	5.50	123.75	119.90
1	1A	993	G	O5'-P-OP1	-5.49	100.76	105.70
1	1A	809	U	C5-C4-O4	-5.49	122.61	125.90
1	1A	1109	G	C5-C6-O6	5.47	131.88	128.60
1	1A	1121	C	C2-N3-C4	5.46	122.63	119.90
32	2a	560	U	C2-N1-C1'	5.46	124.25	117.70
1	2A	1092	C	C5-C6-N1	5.42	123.71	121.00
1	1A	715	G	OP2-P-O3'	5.42	117.12	105.20
1	1A	1255	A	C8-N9-C4	-5.42	103.63	105.80
1	1A	476	G	C5-C6-N1	5.41	114.20	111.50
32	2a	1054	C	N1-C2-O2	5.40	122.14	118.90
33	1b	129	GLU	C-N-CA	5.37	135.12	121.70
1	1A	2240	G	N1-C6-O6	-5.36	116.68	119.90
1	1A	593	G	N3-C4-N9	5.35	129.21	126.00
32	2a	687	A	P-O3'-C3'	5.35	126.12	119.70
32	2a	266	G	OP2-P-O3'	5.33	116.94	105.20
32	1a	266	G	P-O3'-C3'	5.33	126.10	119.70
1	1A	1177	G	O4'-C1'-N9	5.33	112.46	108.20
1	1A	1921	G	N3-C4-N9	5.32	129.19	126.00
1	1A	894	U	C2-N1-C1'	5.30	124.07	117.70
1	2A	2870	C	C6-N1-C2	-5.30	118.18	120.30
1	2A	752	A	P-O3'-C3'	5.29	126.05	119.70
1	1A	1700	G	P-O3'-C3'	5.29	126.04	119.70
32	2a	65	U	P-O3'-C3'	5.28	126.03	119.70
1	2A	1092	C	C2-N1-C1'	5.27	124.60	118.80
1	1A	413	G	O4'-C1'-N9	5.27	112.42	108.20
3	1D	242	ARG	NE-CZ-NH1	5.26	122.93	120.30
32	2a	1033	G	C8-N9-C4	-5.25	104.30	106.40
32	2a	1003	G	C2-N3-C4	5.25	114.52	111.90
32	2a	1003	G	C4-N9-C1'	5.25	133.32	126.50
1	1A	2610	A	O5'-P-OP1	-5.24	100.98	105.70
1	1A	2701	U	P-O3'-C3'	5.24	125.99	119.70
1	2A	195	A	P-O3'-C3'	5.23	125.98	119.70
1	1A	1462	G	O4'-C1'-N9	5.22	112.38	108.20
1	2A	2108	C	N1-C2-O2	5.21	122.03	118.90
32	1a	955	U	C5-C4-O4	5.20	129.02	125.90
32	2a	532	A	OP1-P-O3'	5.20	116.63	105.20
1	1A	2362	C	C6-N1-C2	-5.19	118.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1092	C	N3-C2-O2	-5.17	118.28	121.90
1	1A	599	U	O5'-P-OP1	-5.16	101.05	105.70
1	2A	2107	C	C2-N3-C4	5.16	122.48	119.90
1	2A	2161	C	C5-C4-N4	5.15	123.81	120.20
1	1A	2081	A	O4'-C1'-N9	5.15	112.32	108.20
1	1A	1220	U	P-O3'-C3'	5.13	125.86	119.70
1	2A	570	G	C4-C5-N7	5.13	112.85	110.80
1	1A	399	G	O4'-C1'-N9	5.10	112.28	108.20
27	15	25	LEU	C-N-CA	-5.09	108.97	121.70
1	2A	1079	C	C2-N1-C1'	5.09	124.40	118.80
1	2A	1064	C	C5-C6-N1	5.07	123.54	121.00
1	1A	670	C	N1-C2-O2	5.06	121.94	118.90
1	2A	1076	C	O4'-C1'-N1	5.06	112.25	108.20
1	1A	2038	U	O5'-P-OP2	-5.05	101.15	105.70
1	2A	570	G	C5-C6-O6	-5.05	125.57	128.60
1	1A	721	G	N1-C6-O6	5.05	122.93	119.90
1	1A	989	G	C4-N9-C1'	5.05	133.06	126.50
1	1A	670	C	C2-N1-C1'	5.04	124.35	118.80
32	1a	687	A	P-O3'-C3'	5.04	125.75	119.70
1	1A	2605	U	N3-C4-O4	-5.03	115.88	119.40
1	1A	2621	U	O4'-C1'-N1	5.03	112.22	108.20
1	1A	2176	G	N3-C4-N9	-5.02	122.98	126.00
32	2a	1067	A	P-O3'-C3'	5.02	125.72	119.70
32	2a	1036	G	N7-C8-N9	5.01	115.61	113.10
1	1A	2776	G	OP2-P-O3'	5.01	116.22	105.20
32	1a	1065	U	P-O3'-C3'	5.01	125.71	119.70
32	2a	90	U	N1-C2-O2	-5.00	119.30	122.80
1	1A	549	U	N3-C4-O4	-5.00	115.90	119.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles

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%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	29	52
4	2E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	29	52
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	29	52
5	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	29	52
6	1G	179/182 (98%)	163 (91%)	14 (8%)	2 (1%)	14	30
6	2G	179/182 (98%)	160 (89%)	14 (8%)	5 (3%)	5	7
7	1H	172/180 (96%)	164 (95%)	6 (4%)	2 (1%)	13	27
7	2H	171/180 (95%)	152 (89%)	17 (10%)	2 (1%)	13	27
8	1I	145/148 (98%)	128 (88%)	16 (11%)	1 (1%)	22	43
8	2I	144/148 (97%)	134 (93%)	8 (6%)	2 (1%)	11	22
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	134 (97%)	3 (2%)	1 (1%)	22	43
10	1O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	19	39
10	2O	120/122 (98%)	111 (92%)	7 (6%)	2 (2%)	9	18
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
11	2P	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	22	43
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	43
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	17	35
14	2S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
15	1T	129/146 (88%)	124 (96%)	3 (2%)	2 (2%)	9	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	122 (95%)	7 (5%)	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%)	94 (95%)	3 (3%)	2 (2%)	7	14
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	32
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	14	30
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	30
20	1Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
20	2Y	105/110 (96%)	101 (96%)	3 (3%)	1 (1%)	15	32
21	1Z	201/206 (98%)	191 (95%)	10 (5%)	0	100	100
21	2Z	199/206 (97%)	187 (94%)	12 (6%)	0	100	100
22	10	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	20	75/85 (88%)	70 (93%)	5 (7%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	30
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	30
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	2	3
26	24	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	1
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	196 (86%)	27 (12%)	6 (3%)	5	9
33	2b	229/256 (90%)	200 (87%)	21 (9%)	8 (4%)	3	5
34	1c	204/239 (85%)	186 (91%)	18 (9%)	0	100	100
34	2c	204/239 (85%)	174 (85%)	26 (13%)	4 (2%)	7	14
35	1d	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	52
35	2d	206/209 (99%)	195 (95%)	11 (5%)	0	100	100
36	1e	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
36	2e	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
38	1g	153/156 (98%)	147 (96%)	5 (3%)	1 (1%)	22	43
38	2g	153/156 (98%)	143 (94%)	9 (6%)	1 (1%)	22	43
39	1h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
39	2h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
40	1i	125/128 (98%)	108 (86%)	17 (14%)	0	100	100
40	2i	124/128 (97%)	110 (89%)	12 (10%)	2 (2%)	9	19
41	1j	95/105 (90%)	80 (84%)	12 (13%)	3 (3%)	4	6
41	2j	94/105 (90%)	80 (85%)	13 (14%)	1 (1%)	14	30
42	1k	112/129 (87%)	103 (92%)	8 (7%)	1 (1%)	17	35
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	17	35
43	1l	119/132 (90%)	116 (98%)	3 (2%)	0	100	100
43	2l	119/132 (90%)	104 (87%)	15 (13%)	0	100	100
44	1m	114/126 (90%)	101 (89%)	12 (10%)	1 (1%)	17	35
44	2m	112/126 (89%)	100 (89%)	11 (10%)	1 (1%)	17	35
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	6	11
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	27
47	1p	80/88 (91%)	70 (88%)	10 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
48	1q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
48	2q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
49	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	74 (91%)	5 (6%)	2 (2%)	5	9
50	2s	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
51	1t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	4	6
51	2t	96/106 (91%)	91 (95%)	2 (2%)	3 (3%)	4	6
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	2
53	1y	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
53	2y	94/113 (83%)	91 (97%)	3 (3%)	0	100	100
All	All	11629/12354 (94%)	10866 (93%)	678 (6%)	85 (1%)	22	43

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	47	LYS
41	1j	77	PRO
46	1o	19	PRO
4	2E	51	PHE
5	2F	130	ALA
6	2G	43	LEU
6	2G	78	SER
6	2G	148	MET
8	2I	10	GLU
26	24	55	ARG
26	24	62	ARG
33	2b	10	LEU
33	2b	16	HIS
33	2b	17	PHE
34	2c	29	TYR
40	2i	44	VAL
7	1H	92	ILE
14	1S	59	LYS

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Mol	Chain	Res	Type
17	1V	79	VAL
19	1X	94	GLY
26	14	49	PHE
33	1b	17	PHE
35	1d	5	ILE
51	1t	47	GLY
7	2H	65	HIS
10	2O	5	GLN
23	21	3	LYS
26	24	45	GLY
33	2b	22	LYS
33	2b	95	GLN
51	2t	47	GLY
51	2t	95	ALA
4	1E	52	LEU
17	1V	43	GLU
26	14	55	ARG
26	14	57	GLU
33	1b	21	ARG
33	1b	231	GLU
41	1j	55	LYS
51	1t	95	ALA
9	2N	129	PRO
19	2X	94	GLY
41	2j	78	ASN
46	2o	23	GLY
6	1G	48	GLU
8	1I	85	GLU
10	1O	5	GLN
23	11	3	LYS
41	1j	78	ASN
42	1k	105	VAL
50	1s	12	ASP
50	1s	13	ASP
6	2G	124	SER
6	2G	177	GLY
11	2P	122	PRO
12	2Q	59	ARG
17	2V	79	VAL
33	2b	123	ALA
33	2b	125	PRO
34	2c	110	ASN

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Mol	Chain	Res	Type
51	2t	100	ILE
52	2u	7	ARG
7	1H	159	GLU
15	1T	127	ALA
33	1b	129	GLU
44	1m	12	ASN
8	2I	12	LEU
10	2O	29	ASN
26	24	49	PHE
33	2b	20	GLU
34	2c	156	ARG
15	1T	55	ASN
33	1b	127	ILE
46	1o	86	GLY
51	1t	100	ILE
38	2g	7	ALA
40	2i	107	ARG
7	2H	126	PRO
44	2m	7	VAL
38	1g	112	PRO
20	2Y	58	GLY
34	2c	108	ASN
42	2k	105	VAL
33	1b	125	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	214/218 (98%)	194 (91%)	20 (9%)	9 17
3	2D	215/218 (99%)	203 (94%)	12 (6%)	21 42
4	1E	164/166 (99%)	152 (93%)	12 (7%)	14 28
4	2E	164/166 (99%)	151 (92%)	13 (8%)	12 24
5	1F	160/166 (96%)	145 (91%)	15 (9%)	8 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/166 (96%)	145 (91%)	14 (9%)	10	19
6	1G	144/156 (92%)	135 (94%)	9 (6%)	18	36
6	2G	142/156 (91%)	136 (96%)	6 (4%)	30	55
7	1H	144/148 (97%)	140 (97%)	4 (3%)	43	69
7	2H	143/148 (97%)	135 (94%)	8 (6%)	21	42
8	1I	111/124 (90%)	104 (94%)	7 (6%)	18	36
8	2I	108/124 (87%)	105 (97%)	3 (3%)	43	69
9	1N	119/119 (100%)	107 (90%)	12 (10%)	7	14
9	2N	118/119 (99%)	114 (97%)	4 (3%)	37	63
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	67
10	2O	100/100 (100%)	94 (94%)	6 (6%)	19	39
11	1P	115/116 (99%)	111 (96%)	4 (4%)	36	62
11	2P	115/116 (99%)	112 (97%)	3 (3%)	46	72
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18	36
12	2Q	111/111 (100%)	108 (97%)	3 (3%)	44	71
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6	11
13	2R	101/101 (100%)	93 (92%)	8 (8%)	12	24
14	1S	87/88 (99%)	81 (93%)	6 (7%)	15	31
14	2S	85/88 (97%)	80 (94%)	5 (6%)	19	39
15	1T	115/127 (91%)	109 (95%)	6 (5%)	23	46
15	2T	113/127 (89%)	108 (96%)	5 (4%)	28	53
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22	44
16	2U	93/94 (99%)	87 (94%)	6 (6%)	17	34
17	1V	81/82 (99%)	74 (91%)	7 (9%)	10	20
17	2V	80/82 (98%)	75 (94%)	5 (6%)	18	36
18	1W	90/92 (98%)	80 (89%)	10 (11%)	6	11
18	2W	90/92 (98%)	83 (92%)	7 (8%)	12	25
19	1X	77/78 (99%)	74 (96%)	3 (4%)	32	58
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	58
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	15	30
20	2Y	86/91 (94%)	82 (95%)	4 (5%)	26	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	169/179 (94%)	156 (92%)	13 (8%)	13	25
21	2Z	165/179 (92%)	156 (94%)	9 (6%)	21	43
22	10	61/67 (91%)	58 (95%)	3 (5%)	25	48
22	20	61/67 (91%)	57 (93%)	4 (7%)	16	33
23	11	79/83 (95%)	77 (98%)	2 (2%)	47	73
23	21	81/83 (98%)	76 (94%)	5 (6%)	18	37
24	12	65/67 (97%)	64 (98%)	1 (2%)	65	83
24	22	66/67 (98%)	61 (92%)	5 (8%)	13	26
25	13	51/52 (98%)	48 (94%)	3 (6%)	19	39
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	57
26	14	58/63 (92%)	56 (97%)	2 (3%)	37	63
26	24	54/63 (86%)	53 (98%)	1 (2%)	57	79
27	15	51/52 (98%)	47 (92%)	4 (8%)	12	25
27	25	50/52 (96%)	48 (96%)	2 (4%)	31	57
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	9
28	26	50/52 (96%)	47 (94%)	3 (6%)	19	39
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	15
29	27	41/42 (98%)	38 (93%)	3 (7%)	14	28
30	18	54/55 (98%)	49 (91%)	5 (9%)	9	17
30	28	54/55 (98%)	51 (94%)	3 (6%)	21	42
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	68
33	1b	191/220 (87%)	182 (95%)	9 (5%)	26	50
33	2b	187/220 (85%)	178 (95%)	9 (5%)	25	49
34	1c	144/188 (77%)	135 (94%)	9 (6%)	18	36
34	2c	140/188 (74%)	133 (95%)	7 (5%)	24	47
35	1d	171/181 (94%)	159 (93%)	12 (7%)	15	30
35	2d	172/181 (95%)	160 (93%)	12 (7%)	15	30
36	1e	114/123 (93%)	110 (96%)	4 (4%)	36	62
36	2e	114/123 (93%)	109 (96%)	5 (4%)	28	53
37	1f	85/90 (94%)	80 (94%)	5 (6%)	19	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	83 (98%)	2 (2%)	49	74
38	1g	120/127 (94%)	117 (98%)	3 (2%)	47	73
38	2g	119/127 (94%)	116 (98%)	3 (2%)	47	73
39	1h	116/119 (98%)	112 (97%)	4 (3%)	37	63
39	2h	114/119 (96%)	105 (92%)	9 (8%)	12	24
40	1i	91/99 (92%)	86 (94%)	5 (6%)	21	43
40	2i	88/99 (89%)	86 (98%)	2 (2%)	50	75
41	1j	68/92 (74%)	65 (96%)	3 (4%)	28	53
41	2j	68/92 (74%)	65 (96%)	3 (4%)	28	53
42	1k	83/99 (84%)	83 (100%)	0	100	100
42	2k	83/99 (84%)	76 (92%)	7 (8%)	11	21
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	55
43	2l	96/108 (89%)	94 (98%)	2 (2%)	53	77
44	1m	90/101 (89%)	86 (96%)	4 (4%)	28	53
44	2m	87/101 (86%)	83 (95%)	4 (5%)	27	51
45	1n	49/50 (98%)	48 (98%)	1 (2%)	55	78
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30	56
46	1o	78/80 (98%)	75 (96%)	3 (4%)	33	59
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69	86
47	1p	69/74 (93%)	64 (93%)	5 (7%)	14	29
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13	28
48	1q	94/97 (97%)	89 (95%)	5 (5%)	22	45
48	2q	94/97 (97%)	92 (98%)	2 (2%)	53	77
49	1r	59/77 (77%)	57 (97%)	2 (3%)	37	63
49	2r	59/77 (77%)	56 (95%)	3 (5%)	24	46
50	1s	68/80 (85%)	65 (96%)	3 (4%)	28	53
50	2s	67/80 (84%)	64 (96%)	3 (4%)	27	52
51	1t	71/82 (87%)	68 (96%)	3 (4%)	30	55
51	2t	70/82 (85%)	66 (94%)	4 (6%)	20	41
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	1y	82/98 (84%)	82 (100%)	0	100	100
53	2y	79/98 (81%)	77 (98%)	2 (2%)	47	73
All	All	9524/10260 (93%)	9010 (95%)	514 (5%)	22	44

All (514) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	13	ARG
3	1D	34	VAL
3	1D	39	LYS
3	1D	61	LEU
3	1D	63	ARG
3	1D	99	ASP
3	1D	103	ARG
3	1D	111	LEU
3	1D	116	GLN
3	1D	140	THR
3	1D	142	VAL
3	1D	155	LEU
3	1D	183	ARG
3	1D	193	VAL
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	9	VAL
4	1E	12	THR
4	1E	21	VAL
4	1E	33	VAL
4	1E	41	LYS
4	1E	78	LEU
4	1E	113	PHE
4	1E	116	VAL
4	1E	144	ARG
4	1E	175	VAL
4	1E	181	LEU
4	1E	188	VAL
5	1F	24	LEU
5	1F	53	THR

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Mol	Chain	Res	Type
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	110	LEU
5	1F	125	LEU
5	1F	132	VAL
5	1F	157	VAL
5	1F	158	THR
5	1F	162	LEU
5	1F	170	LEU
5	1F	191	ARG
5	1F	192	LEU
6	1G	7	LEU
6	1G	28	VAL
6	1G	31	VAL
6	1G	43	LEU
6	1G	45	GLU
6	1G	52	ILE
6	1G	53	LEU
6	1G	79	ASN
6	1G	159	VAL
7	1H	6	ARG
7	1H	24	VAL
7	1H	71	LEU
7	1H	122	THR
8	1I	3	VAL
8	1I	5	LEU
8	1I	12	LEU
8	1I	92	VAL
8	1I	109	ILE
8	1I	127	VAL
8	1I	140	LEU
9	1N	9	VAL
9	1N	14	VAL
9	1N	33	LEU
9	1N	34	LEU
9	1N	48	MET
9	1N	60	ILE
9	1N	62	VAL
9	1N	67	LEU
9	1N	73	THR

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Mol	Chain	Res	Type
9	1N	83	LYS
9	1N	99	LEU
9	1N	121	LYS
10	1O	10	VAL
10	1O	24	VAL
10	1O	69	ILE
11	1P	59	LEU
11	1P	95	VAL
11	1P	112	LEU
11	1P	147	LEU
12	1Q	2	LEU
12	1Q	6	ARG
12	1Q	55	VAL
12	1Q	60	ARG
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	133	ARG
13	1R	6	SER
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	75	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	50	SER
14	1S	52	SER
14	1S	59	LYS
14	1S	85	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	39	ARG
15	1T	59	THR
15	1T	67	SER
15	1T	89	VAL
15	1T	118	ARG
16	1U	8	VAL
16	1U	31	SER

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Mol	Chain	Res	Type
16	1U	77	SER
16	1U	83	LEU
16	1U	95	LEU
17	1V	46	VAL
17	1V	51	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
17	1V	82	ARG
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	49	LYS
18	1W	90	ARG
18	1W	96	ILE
18	1W	100	THR
18	1W	107	LEU
19	1X	35	THR
19	1X	38	GLU
19	1X	66	LEU
20	1Y	7	VAL
20	1Y	14	LEU
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	90	LEU
20	1Y	99	CYS
21	1Z	18	LEU
21	1Z	20	ARG
21	1Z	41	LEU
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	94	GLU
21	1Z	107	THR
21	1Z	142	SER
21	1Z	150	LEU
21	1Z	155	LEU
21	1Z	161	VAL
21	1Z	170	THR

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Mol	Chain	Res	Type
22	10	14	ARG
22	10	39	ARG
22	10	59	LEU
23	11	30	VAL
23	11	95	LEU
24	12	53	LEU
25	13	6	VAL
25	13	23	LEU
25	13	54	VAL
26	14	49	PHE
26	14	52	THR
27	15	26	THR
27	15	29	THR
27	15	40	LYS
27	15	60	VAL
28	16	6	ARG
28	16	14	THR
28	16	19	ARG
28	16	47	THR
28	16	48	VAL
28	16	52	VAL
29	17	23	ARG
29	17	24	THR
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	23	VAL
30	18	31	HIS
30	18	32	LEU
30	18	58	ILE
33	1b	10	LEU
33	1b	12	GLU
33	1b	15	VAL
33	1b	39	ILE
33	1b	56	ARG
33	1b	111	ARG
33	1b	178	ARG
33	1b	185	ILE
33	1b	226	ARG
34	1c	3	ASN
34	1c	26	LYS
34	1c	29	TYR

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Mol	Chain	Res	Type
34	1c	49	SER
34	1c	70	VAL
34	1c	105	GLU
34	1c	115	LEU
34	1c	154	SER
34	1c	206	GLU
35	1d	8	VAL
35	1d	19	LEU
35	1d	31	CYS
35	1d	58	LEU
35	1d	115	ARG
35	1d	127	THR
35	1d	135	LEU
35	1d	140	VAL
35	1d	168	ARG
35	1d	188	LEU
35	1d	193	ASP
35	1d	194	LEU
36	1e	31	LEU
36	1e	41	VAL
36	1e	69	VAL
36	1e	91	LEU
37	1f	17	SER
37	1f	40	VAL
37	1f	45	LEU
37	1f	69	GLU
37	1f	73	ASN
38	1g	6	ARG
38	1g	13	GLN
38	1g	15	ASP
39	1h	26	VAL
39	1h	63	LEU
39	1h	85	ARG
39	1h	104	ARG
40	1i	64	THR
40	1i	81	ILE
40	1i	103	THR
40	1i	111	ARG
40	1i	127	LYS
41	1j	34	VAL
41	1j	92	THR
41	1j	100	THR

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Mol	Chain	Res	Type
43	1l	18	VAL
43	1l	27	LEU
43	1l	97	ARG
43	1l	113	ARG
44	1m	4	ILE
44	1m	56	LEU
44	1m	70	LEU
44	1m	86	CYS
45	1n	33	VAL
46	1o	5	LYS
46	1o	39	LEU
46	1o	66	LEU
47	1p	2	VAL
47	1p	42	ARG
47	1p	61	SER
47	1p	62	VAL
47	1p	67	THR
48	1q	45	HIS
48	1q	61	GLU
48	1q	63	ARG
48	1q	85	VAL
48	1q	97	SER
49	1r	31	LEU
49	1r	46	GLU
50	1s	5	LEU
50	1s	41	VAL
50	1s	79	THR
51	1t	9	ASN
51	1t	24	LEU
51	1t	84	LEU
3	2D	3	VAL
3	2D	61	LEU
3	2D	71	ASP
3	2D	94	LEU
3	2D	111	LEU
3	2D	118	VAL
3	2D	142	VAL
3	2D	155	LEU
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
3	2D	274	ARG

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Mol	Chain	Res	Type
4	2E	7	VAL
4	2E	12	THR
4	2E	21	VAL
4	2E	33	VAL
4	2E	75	VAL
4	2E	78	LEU
4	2E	101	ARG
4	2E	113	PHE
4	2E	116	VAL
4	2E	167	VAL
4	2E	170	LEU
4	2E	175	VAL
4	2E	181	LEU
5	2F	20	LEU
5	2F	27	GLU
5	2F	33	LEU
5	2F	57	VAL
5	2F	60	SER
5	2F	72	ARG
5	2F	74	ARG
5	2F	88	VAL
5	2F	168	ARG
5	2F	170	LEU
5	2F	175	THR
5	2F	192	LEU
5	2F	197	ASP
5	2F	201	VAL
6	2G	7	LEU
6	2G	28	VAL
6	2G	49	ASP
6	2G	79	ASN
6	2G	159	VAL
6	2G	170	ARG
7	2H	13	LYS
7	2H	18	GLU
7	2H	45	VAL
7	2H	68	THR
7	2H	71	LEU
7	2H	98	LEU
7	2H	127	GLU
7	2H	139	GLN
8	2I	50	ARG

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Mol	Chain	Res	Type
8	2I	76	THR
8	2I	122	GLU
9	2N	12	ARG
9	2N	28	THR
9	2N	62	VAL
9	2N	99	LEU
10	2O	10	VAL
10	2O	24	VAL
10	2O	35	VAL
10	2O	78	ARG
10	2O	98	VAL
10	2O	108	GLU
11	2P	86	LYS
11	2P	112	LEU
11	2P	148	LEU
12	2Q	3	MET
12	2Q	6	ARG
12	2Q	75	THR
13	2R	36	THR
13	2R	44	LEU
13	2R	65	LEU
13	2R	67	LEU
13	2R	86	ARG
13	2R	96	ARG
13	2R	111	LEU
13	2R	114	VAL
14	2S	19	LYS
14	2S	25	ARG
14	2S	36	TYR
14	2S	50	SER
14	2S	52	SER
15	2T	17	THR
15	2T	42	ILE
15	2T	53	ARG
15	2T	89	VAL
15	2T	96	ARG
16	2U	31	SER
16	2U	52	ARG
16	2U	55	ARG
16	2U	74	LEU
16	2U	83	LEU
16	2U	95	LEU

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Mol	Chain	Res	Type
17	2V	46	VAL
17	2V	51	VAL
17	2V	56	SER
17	2V	72	VAL
17	2V	79	VAL
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	23	LEU
18	2W	63	ASP
18	2W	70	TYR
19	2X	35	THR
19	2X	57	LEU
19	2X	81	VAL
20	2Y	6	HIS
20	2Y	50	ARG
20	2Y	70	SER
20	2Y	72	VAL
21	2Z	86	VAL
21	2Z	93	ASP
21	2Z	94	GLU
21	2Z	96	VAL
21	2Z	107	THR
21	2Z	142	SER
21	2Z	156	LYS
21	2Z	170	THR
21	2Z	175	VAL
22	20	10	THR
22	20	14	ARG
22	20	29	GLN
22	20	55	ARG
23	21	35	THR
23	21	40	ARG
23	21	51	VAL
23	21	85	LEU
23	21	95	LEU
24	22	25	VAL
24	22	40	SER
24	22	53	LEU
24	22	62	THR
24	22	64	LEU

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Mol	Chain	Res	Type
25	23	31	LEU
25	23	54	VAL
26	24	52	THR
27	25	6	VAL
27	25	29	THR
28	26	6	ARG
28	26	8	LYS
28	26	48	VAL
29	27	1	MET
29	27	34	ARG
29	27	46	VAL
30	28	14	VAL
30	28	30	ARG
30	28	32	LEU
31	29	12	ASP
33	2b	15	VAL
33	2b	24	TRP
33	2b	44	LEU
33	2b	118	LEU
33	2b	135	GLN
33	2b	158	LEU
33	2b	189	ASP
33	2b	196	LEU
33	2b	224	GLN
34	2c	15	THR
34	2c	33	LEU
34	2c	105	GLU
34	2c	143	GLU
34	2c	166	GLU
34	2c	190	ARG
34	2c	207	VAL
35	2d	28	SER
35	2d	31	CYS
35	2d	34	GLU
35	2d	59	ARG
35	2d	83	SER
35	2d	96	LEU
35	2d	108	LEU
35	2d	122	ARG
35	2d	132	ARG
35	2d	135	LEU
35	2d	157	LEU

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Mol	Chain	Res	Type
35	2d	170	VAL
36	2e	34	VAL
36	2e	41	VAL
36	2e	69	VAL
36	2e	75	THR
36	2e	91	LEU
37	2f	63	TYR
37	2f	81	ILE
38	2g	15	ASP
38	2g	104	LEU
38	2g	153	HIS
39	2h	23	SER
39	2h	25	ASP
39	2h	45	ILE
39	2h	85	ARG
39	2h	91	ARG
39	2h	104	ARG
39	2h	105	ARG
39	2h	114	THR
39	2h	115	SER
40	2i	27	THR
40	2i	102	LEU
41	2j	30	SER
41	2j	43	ARG
41	2j	69	ASN
42	2k	32	ILE
42	2k	41	THR
42	2k	79	SER
42	2k	84	VAL
42	2k	107	SER
42	2k	109	VAL
42	2k	114	VAL
43	2l	67	THR
43	2l	83	VAL
44	2m	15	VAL
44	2m	19	LEU
44	2m	66	LEU
44	2m	103	THR
45	2n	6	LEU
45	2n	18	VAL
46	2o	39	LEU
47	2p	1	MET

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Mol	Chain	Res	Type
47	2p	2	VAL
47	2p	45	THR
47	2p	62	VAL
47	2p	69	THR
48	2q	60	ILE
48	2q	70	ARG
49	2r	37	VAL
49	2r	55	ARG
49	2r	76	LEU
50	2s	41	VAL
50	2s	48	THR
50	2s	71	LEU
51	2t	15	ARG
51	2t	24	LEU
51	2t	62	LEU
51	2t	100	ILE
53	2y	29	LYS
53	2y	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
4	1E	48	GLN
5	1F	8	GLN
6	1G	26	GLN
6	1G	108	ASN
7	1H	158	HIS
8	1I	104	GLN
8	1I	105	HIS
12	1Q	89	ASN
13	1R	13	HIS
15	1T	58	ASN
15	1T	123	GLN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	92	ASN
21	1Z	34	ASN
21	1Z	73	GLN
21	1Z	151	HIS
22	10	35	ASN
23	11	56	GLN

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Mol	Chain	Res	Type
25	13	32	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	69	HIS
34	1c	102	ASN
34	1c	104	GLN
34	1c	162	GLN
35	1d	45	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
35	1d	129	ASN
37	1f	64	GLN
37	1f	73	ASN
38	1g	28	ASN
38	1g	64	GLN
38	1g	86	GLN
38	1g	148	ASN
40	1i	73	GLN
40	1i	87	GLN
40	1i	124	GLN
41	1j	56	HIS
41	1j	84	GLN
43	1l	80	HIS
43	1l	99	HIS
46	1o	28	GLN
47	1p	16	HIS
48	1q	16	GLN
50	1s	69	HIS
50	1s	83	HIS
51	1t	18	GLN
53	1y	38	HIS
3	2D	126	GLN
4	2E	48	GLN
5	2F	69	HIS
5	2F	75	HIS
5	2F	203	GLN
6	2G	41	GLN
7	2H	74	ASN
8	2I	43	ASN
9	2N	133	GLN
10	2O	3	GLN

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Mol	Chain	Res	Type
12	2Q	89	ASN
13	2R	24	GLN
13	2R	31	HIS
16	2U	94	ASN
16	2U	117	GLN
17	2V	64	HIS
18	2W	60	ASN
19	2X	31	HIS
21	2Z	73	GLN
24	22	65	ASN
25	23	32	GLN
30	28	35	GLN
33	2b	19	HIS
33	2b	40	HIS
34	2c	37	GLN
34	2c	176	HIS
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	160	GLN
36	2e	78	HIS
37	2f	73	ASN
38	2g	28	ASN
38	2g	64	GLN
38	2g	68	ASN
39	2h	78	GLN
40	2i	3	GLN
40	2i	34	ASN
40	2i	73	GLN
40	2i	87	GLN
41	2j	56	HIS
41	2j	62	HIS
41	2j	68	HIS
41	2j	69	ASN
43	2l	99	HIS
46	2o	28	GLN
50	2s	57	HIS
50	2s	69	HIS
50	2s	83	HIS
53	2y	38	HIS

5.3.3 RNA 

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	396 (13%)	30 (1%)
1	2A	2855/2915 (97%)	475 (16%)	38 (1%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	119/121 (98%)	16 (13%)	0
32	1a	1494/1521 (98%)	234 (15%)	0
32	2a	1498/1521 (98%)	255 (17%)	0
All	All	8947/9114 (98%)	1388 (15%)	68 (0%)

All (1388) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	34	C
1	1A	45	C
1	1A	54	G
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	138	G
1	1A	161	C
1	1A	171	A
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	254	A
1	1A	263	C
1	1A	269	G
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	274	U
1	1A	275	C
1	1A	288	U

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Mol	Chain	Res	Type
1	1A	289	G
1	1A	299	G
1	1A	303	C
1	1A	304	C
1	1A	307	A
1	1A	335	A
1	1A	354	A
1	1A	376	G
1	1A	387	G
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	434	G
1	1A	438	G
1	1A	439	A
1	1A	448	U
1	1A	449	A
1	1A	455	A
1	1A	474	U
1	1A	482	C
1	1A	483	A
1	1A	507	G
1	1A	529	U
1	1A	530	A
1	1A	534	C
1	1A	553	A
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	639	G
1	1A	641	G
1	1A	642	G
1	1A	652	A

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Mol	Chain	Res	Type
1	1A	662	A
1	1A	670	C
1	1A	671	A
1	1A	693	G
1	1A	697	C
1	1A	698	G
1	1A	701	A
1	1A	715	G
1	1A	716	G
1	1A	733	G
1	1A	764	G
1	1A	777	C
1	1A	812	G
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	831	A
1	1A	832	G
1	1A	837	C
1	1A	839	G
1	1A	852	G
1	1A	859	C
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	913	A
1	1A	915	U
1	1A	925	A
1	1A	926	G
1	1A	930	G
1	1A	932	C
1	1A	933	C
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	942	A
1	1A	943	C
1	1A	956	A
1	1A	976	G
1	1A	977	G
1	1A	990	A
1	1A	991	G

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Mol	Chain	Res	Type
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1008	U
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1072	U
1	1A	1073	A
1	1A	1079	U
1	1A	1085	G
1	1A	1087	C
1	1A	1088	G
1	1A	1089	C
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1099	C
1	1A	1100	A
1	1A	1106	U
1	1A	1107	U
1	1A	1108	G
1	1A	1109	G
1	1A	1111	U
1	1A	1114	G
1	1A	1116	A
1	1A	1117	G
1	1A	1119	A
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1125	C
1	1A	1129	U
1	1A	1133	G
1	1A	1134	A
1	1A	1136	U
1	1A	1142	A
1	1A	1143	U

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Mol	Chain	Res	Type
1	1A	1152	G
1	1A	1155	C
1	1A	1156	G
1	1A	1158	G
1	1A	1162	C
1	1A	1174	A
1	1A	1175	A
1	1A	1180	C
1	1A	1181	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1223	C
1	1A	1255	A
1	1A	1256	U
1	1A	1275	G
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1346	U
1	1A	1347	A
1	1A	1351	C
1	1A	1391	C
1	1A	1398	U
1	1A	1405	A
1	1A	1411	A
1	1A	1416	C
1	1A	1426	G
1	1A	1430	A
1	1A	1431	G
1	1A	1441	A
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A

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Mol	Chain	Res	Type
1	1A	1497	G
1	1A	1500	A
1	1A	1502	G
1	1A	1506	G
1	1A	1514	C
1	1A	1518	A
1	1A	1529	G
1	1A	1539	C
1	1A	1543	U
1	1A	1554	A
1	1A	1556	A
1	1A	1579	C
1	1A	1589	A
1	1A	1590	C
1	1A	1605	A
1	1A	1616	A
1	1A	1625	U
1	1A	1627	A
1	1A	1628	G
1	1A	1629	C
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1656	A
1	1A	1694	G
1	1A	1695	C
1	1A	1701	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1748	A
1	1A	1750	G
1	1A	1767	A
1	1A	1769	G
1	1A	1776	G
1	1A	1777	G
1	1A	1787	G
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A

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Mol	Chain	Res	Type
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1870	G
1	1A	1878	A
1	1A	1889	G
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1922	A
1	1A	1928	G
1	1A	1935	A
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1987	C
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2055	A
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2091	G
1	1A	2121	U
1	1A	2125	C

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Mol	Chain	Res	Type
1	1A	2129	C
1	1A	2130	C
1	1A	2138	G
1	1A	2139	A
1	1A	2148	A
1	1A	2149	G
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2164	C
1	1A	2167	C
1	1A	2168	C
1	1A	2169	G
1	1A	2180	A
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2185	C
1	1A	2186	C
1	1A	2193	A
1	1A	2195	A
1	1A	2200	C
1	1A	2207	C
1	1A	2208	G
1	1A	2209	G
1	1A	2212	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2285	A
1	1A	2290	A
1	1A	2295	C

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Mol	Chain	Res	Type
1	1A	2299	A
1	1A	2301	G
1	1A	2317	A
1	1A	2320	G
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2373	A
1	1A	2395	G
1	1A	2397	C
1	1A	2418	U
1	1A	2434	A
1	1A	2435	U
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A
1	1A	2443	U
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2480	G
1	1A	2481	A
1	1A	2486	C
1	1A	2488	A
1	1A	2510	C
1	1A	2514	G
1	1A	2517	G
1	1A	2530	A
1	1A	2532	C
1	1A	2541	G
1	1A	2547	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2614	A
1	1A	2615	G
1	1A	2621	U

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Mol	Chain	Res	Type
1	1A	2623	U
1	1A	2624	C
1	1A	2641	A
1	1A	2642	G
1	1A	2666	A
1	1A	2674	A
1	1A	2701	U
1	1A	2702	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2771	A
1	1A	2778	A
1	1A	2779	G
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C
1	1A	2813	G
1	1A	2830	A
1	1A	2831	A
1	1A	2843	G
1	1A	2845	A
1	1A	2868	C
1	1A	2882	G
1	1A	2890	C
1	1A	2903	G
2	1B	2	C
2	1B	7	G
2	1B	13	A
2	1B	15	A
2	1B	30	C
2	1B	45	A
2	1B	53	A
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	106	G
2	1B	110	G

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Mol	Chain	Res	Type
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	93	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	156	G
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(G)	G
32	1a	189(I)	G
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G
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	306	G
32	1a	318	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G

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Mol	Chain	Res	Type
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	452	A
32	1a	456	C
32	1a	461	A
32	1a	470	C
32	1a	475	G
32	1a	485	G
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	519	C
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	596	C

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Mol	Chain	Res	Type
32	1a	607	A
32	1a	630	G
32	1a	631	G
32	1a	650	G
32	1a	653	A
32	1a	665	A
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	724	G
32	1a	728	A
32	1a	731	G
32	1a	734	G
32	1a	750	G
32	1a	755	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G
32	1a	836	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	966	M2G
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	975	A
32	1a	976	G

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Mol	Chain	Res	Type
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	998	G
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1004	A
32	1a	1006	C
32	1a	1009	G
32	1a	1010	G
32	1a	1017	G
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(D)	A
32	1a	1032	G
32	1a	1037	C
32	1a	1042	G
32	1a	1044	A
32	1a	1053	G
32	1a	1063	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1124	G
32	1a	1126	U
32	1a	1130	A
32	1a	1134	G

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Mol	Chain	Res	Type
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1208	C
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1224	G
32	1a	1227	A
32	1a	1238	A
32	1a	1240	U
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1269	A
32	1a	1270	C
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1293	G
32	1a	1298	C
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A

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Mol	Chain	Res	Type
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1422	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1452	C
32	1a	1456	G
32	1a	1492	A
32	1a	1493	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	9	U
1	2A	10	G
1	2A	11	G
1	2A	12	U
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	95	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	141	A

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Mol	Chain	Res	Type
1	2A	157	U
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	229	A
1	2A	230	U
1	2A	248	G
1	2A	265	A
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	303	U
1	2A	308	G
1	2A	311	A
1	2A	317	G
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	342	G
1	2A	352	G
1	2A	363	G
1	2A	370	G
1	2A	372	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	411	G
1	2A	412	A

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Mol	Chain	Res	Type
1	2A	428	A
1	2A	442	G
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	492	A
1	2A	496	G
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	595	C
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	669	G
1	2A	686	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A

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Mol	Chain	Res	Type
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	815	C
1	2A	827	U
1	2A	833	U
1	2A	857	C
1	2A	859	G
1	2A	869	G
1	2A	877	U
1	2A	880	G
1	2A	883	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	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	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G
1	2A	1026	U

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Mol	Chain	Res	Type
1	2A	1033	U
1	2A	1034	G
1	2A	1038	C
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1052	C
1	2A	1054	A
1	2A	1055	G
1	2A	1058	G
1	2A	1060	U
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1069	A
1	2A	1070	A
1	2A	1071	G
1	2A	1072	C
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1078	U
1	2A	1079	C
1	2A	1080	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1089	G
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1095	A
1	2A	1096	A
1	2A	1097	U
1	2A	1098	A
1	2A	1105	U
1	2A	1109	C

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Mol	Chain	Res	Type
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1117	G
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1170	G
1	2A	1171	G
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1241	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1276	A
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1308	A
1	2A	1314	C
1	2A	1338	G
1	2A	1342	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A

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Mol	Chain	Res	Type
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1494	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1509(B)	A
1	2A	1537	G
1	2A	1542	A
1	2A	1543	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1595	G
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1647	G
1	2A	1648	C
1	2A	1674	G
1	2A	1675	C
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A

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Mol	Chain	Res	Type
1	2A	1756	G
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A
1	2A	1831	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1860	G
1	2A	1877	A
1	2A	1878	G
1	2A	1896	G
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C

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Mol	Chain	Res	Type
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2096	U
1	2A	2099	U
1	2A	2103	C
1	2A	2104	G
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2112	G
1	2A	2113	U
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2120	G
1	2A	2121	G
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2138	C
1	2A	2141	G
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2149	G
1	2A	2150	U
1	2A	2151	G
1	2A	2158	A

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Mol	Chain	Res	Type
1	2A	2159	G
1	2A	2161	C
1	2A	2162	G
1	2A	2163	C
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G
1	2A	2172	U
1	2A	2173	A
1	2A	2176	A
1	2A	2178	C
1	2A	2181	G
1	2A	2184	G
1	2A	2186	G
1	2A	2187	G
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	2239	G
1	2A	2269	A
1	2A	2273	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2312	U
1	2A	2318	G
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A

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Mol	Chain	Res	Type
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2396	G
1	2A	2406	U
1	2A	2410	G
1	2A	2414	G
1	2A	2422	A
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2468	G
1	2A	2470	G
1	2A	2474	C
1	2A	2478	A
1	2A	2494	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	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2602	A
1	2A	2603	G
1	2A	2611	U

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Mol	Chain	Res	Type
1	2A	2612	C
1	2A	2630	G
1	2A	2663	G
1	2A	2669	G
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2703	C
1	2A	2707	G
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2752	C
1	2A	2757	A
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2769	C
1	2A	2778	A
1	2A	2789	C
1	2A	2802	G
1	2A	2803	C
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2872	G
1	2A	2880	C
1	2A	2891	G
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	7	G
2	2B	9	G
2	2B	13	A
2	2B	30	C

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Mol	Chain	Res	Type
2	2B	32	C
2	2B	42	C
2	2B	45	A
2	2B	46	A
2	2B	51	G
2	2B	56	G
2	2B	64	C
2	2B	73	A
2	2B	84	C
2	2B	85	G
2	2B	110	G
32	2a	5	U
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	61	G
32	2a	66	G
32	2a	89	C
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	148	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(C)	C
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U

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Mol	Chain	Res	Type
32	2a	216	G
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	298	A
32	2a	306	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	383	A
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	422	C
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	442	C
32	2a	446	G
32	2a	451	A
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	476	G
32	2a	477	A
32	2a	482	A
32	2a	484	G

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Mol	Chain	Res	Type
32	2a	485	G
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	532	A
32	2a	533	A
32	2a	536	C
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	562	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	631	G
32	2a	632	A
32	2a	653	A
32	2a	661	G
32	2a	665	A
32	2a	666	G
32	2a	685	G
32	2a	687	A
32	2a	688	G
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	753	A
32	2a	754	C
32	2a	755	G
32	2a	777	A
32	2a	785	G
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	817	C

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Mol	Chain	Res	Type
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	870	U
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	996	A
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1016	A
32	2a	1017	G
32	2a	1020	U
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C

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Mol	Chain	Res	Type
32	2a	1028	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1030(C)	G
32	2a	1031	G
32	2a	1041	A
32	2a	1043	C
32	2a	1053	G
32	2a	1054	C
32	2a	1055	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1097	C
32	2a	1101	A
32	2a	1104	G
32	2a	1105	A
32	2a	1110	A
32	2a	1117	G
32	2a	1119	C
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1162	C
32	2a	1176	A
32	2a	1183	A
32	2a	1196	U

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Mol	Chain	Res	Type
32	2a	1197	G
32	2a	1212	U
32	2a	1213	A
32	2a	1215	G
32	2a	1224	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1259	C
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1281	U
32	2a	1282	C
32	2a	1285	A
32	2a	1286	A
32	2a	1287	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1317	C
32	2a	1319	A
32	2a	1320	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U
32	2a	1359	C
32	2a	1363	C
32	2a	1370	G
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A

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Mol	Chain	Res	Type
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1505	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A

All (68) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	185	A
1	1A	271	U
1	1A	302	A
1	1A	509	A
1	1A	793	A
1	1A	811	A
1	1A	821	A
1	1A	874	U
1	1A	913	A
1	1A	935	C
1	1A	941	U
1	1A	1003	U
1	1A	1019	G
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1201	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1654	A
1	1A	1700	G
1	1A	2148	A

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Mol	Chain	Res	Type
1	1A	2418	U
1	1A	2434	A
1	1A	2442	A
1	1A	2614	A
1	1A	2623	U
1	1A	2701	U
1	2A	9	U
1	2A	195	A
1	2A	196	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	532	A
1	2A	645	C
1	2A	752	A
1	2A	764	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	900	A
1	2A	974	G
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1210	A
1	2A	1240	U
1	2A	1275	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2317	C
1	2A	2321	G
1	2A	2406	U
1	2A	2601	C
1	2A	2602	A

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Mol	Chain	Res	Type
1	2A	2689	U
1	2A	2756	U

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

48 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$
1	OMG	2A	2251	54,1	18,26,27	0.97	1 (5%)	19,38,41	1.01	2 (10%)
1	PSU	1A	1939	1	18,21,22	1.30	2 (11%)	22,30,33	1.84	3 (13%)
1	OMG	1A	2263	54,1	18,26,27	1.14	1 (5%)	19,38,41	1.06	2 (10%)
1	4OC	1A	1942	1	19,22,24	0.82	0	26,31,35	0.87	1 (3%)
32	7MG	1a	527	32	22,26,27	1.41	4 (18%)	29,39,42	2.45	7 (24%)
43	0TD	1l	92	43	7,9,10	4.88	1 (14%)	6,11,13	4.70	3 (50%)
1	2MA	2A	2503	54,1	17,25,26	1.02	1 (5%)	17,37,40	1.03	2 (11%)
1	5MC	1A	1964	1	18,22,23	0.95	2 (11%)	26,32,35	1.13	2 (7%)
32	M2G	2a	966	54,32	20,27,28	1.46	3 (15%)	22,40,43	0.93	2 (9%)
32	MA6	2a	1519	32	19,26,27	1.02	1 (5%)	18,38,41	1.88	5 (27%)
1	5MU	2A	1915	1	19,22,23	1.40	4 (21%)	28,32,35	2.18	8 (28%)
43	0TD	2l	92	43	7,9,10	4.60	1 (14%)	6,11,13	2.77	3 (50%)
32	5MC	1a	1404	32	18,22,23	0.93	2 (11%)	26,32,35	1.09	3 (11%)
1	PSU	1A	2617	1	18,21,22	1.35	3 (16%)	22,30,33	1.78	4 (18%)
32	5MC	2a	1404	32	18,22,23	0.98	2 (11%)	26,32,35	1.14	2 (7%)
1	5MC	2A	1962	54,1	18,22,23	0.97	2 (11%)	26,32,35	1.17	2 (7%)
1	2MU	1A	2564	54,1	19,22,24	1.29	3 (15%)	26,31,36	1.68	4 (15%)
32	5MC	1a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.11	2 (7%)
32	5MC	1a	1400	32	18,22,23	1.03	2 (11%)	26,32,35	1.19	2 (7%)
32	5MC	1a	1407	32	18,22,23	0.96	1 (5%)	26,32,35	1.16	4 (15%)
1	PSU	1A	1933	1	18,21,22	1.38	2 (11%)	22,30,33	1.89	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	4OC	1a	1402	32	20,23,24	0.76	1 (5%)	26,32,35	1.01	3 (11%)
1	5MC	1A	1984	54,1	18,22,23	1.00	2 (11%)	26,32,35	1.22	3 (11%)
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	4 (18%)
1	5MC	2A	1942	1	18,22,23	0.94	2 (11%)	26,32,35	1.30	3 (11%)
32	5MC	2a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.20	3 (11%)
32	5MC	2a	1400	32	18,22,23	0.97	2 (11%)	26,32,35	1.29	3 (11%)
32	5MC	2a	1407	32	18,22,23	0.96	2 (11%)	26,32,35	1.16	3 (11%)
1	5MU	1A	1961	54,1	19,22,23	1.32	3 (15%)	28,32,35	2.23	6 (21%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	22,30,33	1.94	3 (13%)
32	MA6	1a	1519	32	19,26,27	1.06	1 (5%)	18,38,41	1.62	4 (22%)
1	PSU	2A	2605	1	18,21,22	1.29	3 (16%)	22,30,33	1.86	4 (18%)
1	5MU	2A	1939	1	19,22,23	1.49	5 (26%)	28,32,35	2.25	6 (21%)
32	7MG	2a	527	32	22,26,27	1.35	4 (18%)	29,39,42	2.42	6 (20%)
32	UR3	1a	1498	32	19,22,23	0.98	1 (5%)	26,32,35	1.48	3 (11%)
32	M2G	1a	966	32	20,27,28	1.38	3 (15%)	22,40,43	0.94	2 (9%)
1	4OC	2A	1920	1	19,22,24	0.82	0	26,31,35	0.96	1 (3%)
32	UR3	2a	1498	54,32	19,22,23	1.00	1 (5%)	26,32,35	1.41	1 (3%)
32	PSU	1a	516	54,32	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)
1	5MU	1A	1937	1	19,22,23	1.47	4 (21%)	28,32,35	2.17	10 (35%)
32	MA6	1a	1518	32	19,26,27	1.01	1 (5%)	18,38,41	1.64	5 (27%)
32	MA6	2a	1518	32	19,26,27	1.04	1 (5%)	18,38,41	1.70	6 (33%)
1	2MA	1A	2515	54,1	17,25,26	1.03	2 (11%)	17,37,40	1.10	2 (11%)
32	2MG	1a	1207	32	18,26,27	1.00	1 (5%)	16,38,41	1.48	4 (25%)
32	2MG	2a	1207	32	18,26,27	0.89	1 (5%)	16,38,41	1.04	1 (6%)
32	PSU	2a	516	54,32	18,21,22	1.30	3 (16%)	22,30,33	1.90	5 (22%)
1	2MU	2A	2552	54,1	19,22,24	1.26	3 (15%)	26,31,36	1.90	6 (23%)
32	4OC	2a	1402	32	20,23,24	0.78	0	26,32,35	1.05	2 (7%)

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
1	OMG	2A	2251	54,1	-	0/5/27/28	0/3/3/3
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1A	2263	54,1	-	0/5/27/28	0/3/3/3
1	4OC	1A	1942	1	-	2/9/27/30	0/2/2/2
32	7MG	1a	527	32	-	1/7/37/38	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
1	2MA	2A	2503	54,1	-	1/3/25/26	0/3/3/3
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	54,32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	54,1	-	3/7/25/26	0/2/2/2
1	2MU	1A	2564	54,1	-	0/9/27/28	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	5MC	1A	1984	54,1	-	2/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	2/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	54,1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	1/7/37/38	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	4OC	2A	1920	1	-	2/9/27/30	0/2/2/2
32	UR3	2a	1498	54,32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	54,32	-	2/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	2/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1518	32	-	1/7/29/30	0/3/3/3
1	2MA	1A	2515	54,1	-	2/3/25/26	0/3/3/3
32	2MG	1a	1207	32	-	4/5/27/28	0/3/3/3
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	PSU	2a	516	54,32	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	54,1	-	0/9/27/28	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.53	1.69	1.82
43	2l	92	0TD	CB-SB	-11.85	1.70	1.82
32	2a	966	M2G	C2-N3	4.57	1.36	1.30
32	1a	966	M2G	C2-N3	4.01	1.35	1.30
1	1A	1933	PSU	C6-C5	3.60	1.39	1.35
1	2A	1911	PSU	C6-C5	3.56	1.39	1.35
1	1A	2263	OMG	C6-N1	-3.53	1.32	1.37
32	1a	527	7MG	C4-N9	-3.50	1.33	1.37
32	1a	516	PSU	C6-C5	3.38	1.39	1.35
1	1A	1939	PSU	C6-C5	3.22	1.39	1.35
32	2a	527	7MG	C4-N9	-3.20	1.34	1.37
1	2A	1917	PSU	C6-C5	3.07	1.38	1.35
32	2a	516	PSU	C6-C5	3.06	1.38	1.35
32	1a	527	7MG	C5-C4	3.02	1.47	1.38
32	2a	527	7MG	C5-C4	2.97	1.47	1.38
1	1A	2617	PSU	C4-N3	-2.95	1.33	1.38
1	2A	1939	5MU	C6-C5	2.94	1.39	1.34
1	1A	1937	5MU	C2-N1	2.93	1.43	1.38
1	2A	1915	5MU	C2-N1	2.93	1.43	1.38
32	2a	966	M2G	C2-N2	2.91	1.40	1.35
32	1a	966	M2G	C6-N1	-2.90	1.33	1.37
1	2A	1939	5MU	C4-N3	-2.88	1.33	1.38
32	1a	1407	5MC	C6-C5	2.87	1.39	1.34
1	2A	1962	5MC	C6-C5	2.87	1.39	1.34
32	2a	1518	MA6	C5-C4	2.86	1.48	1.40
1	2A	1939	5MU	C4-C5	2.85	1.49	1.44
32	2a	1407	5MC	C6-C5	2.84	1.39	1.34
1	1A	1961	5MU	C6-C5	2.81	1.39	1.34
32	1a	1400	5MC	C6-C5	2.78	1.39	1.34
1	2A	1915	5MU	C6-C5	2.76	1.39	1.34
1	1A	1937	5MU	C6-C5	2.75	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1984	5MC	C6-N1	-2.75	1.33	1.38
1	2A	2605	PSU	C4-N3	-2.72	1.33	1.38
1	1A	1937	5MU	C4-N3	-2.71	1.33	1.38
32	2a	967	5MC	C6-C5	2.70	1.39	1.34
32	2a	1404	5MC	C6-C5	2.70	1.39	1.34
1	2A	2552	2MU	C4-N3	-2.68	1.33	1.38
32	1a	966	M2G	C2-N2	2.68	1.40	1.35
32	1a	1404	5MC	C6-C5	2.67	1.39	1.34
32	2a	1400	5MC	C6-C5	2.67	1.39	1.34
1	2A	1911	PSU	C4-N3	-2.66	1.33	1.38
32	1a	967	5MC	C6-C5	2.66	1.39	1.34
32	1a	1519	MA6	C5-C4	2.62	1.47	1.40
1	1A	1964	5MC	C6-C5	2.59	1.38	1.34
32	1a	1400	5MC	C6-N1	-2.58	1.33	1.38
1	1A	2617	PSU	C6-C5	2.57	1.38	1.35
1	1A	1984	5MC	C6-C5	2.57	1.38	1.34
1	2A	1917	PSU	C4-N3	-2.56	1.34	1.38
32	2a	1519	MA6	C5-C4	2.55	1.47	1.40
1	1A	1937	5MU	C4-C5	2.53	1.49	1.44
32	1a	1518	MA6	C5-C4	2.51	1.47	1.40
1	1A	1933	PSU	C4-N3	-2.50	1.34	1.38
1	1A	1964	5MC	C6-N1	-2.49	1.33	1.38
1	1A	2564	2MU	C4-N3	-2.48	1.34	1.38
1	2A	1942	5MC	C6-C5	2.48	1.38	1.34
32	1a	1207	2MG	C6-N1	-2.48	1.34	1.37
1	1A	1961	5MU	C6-N1	-2.47	1.33	1.38
1	1A	1961	5MU	C4-N3	-2.45	1.34	1.38
1	2A	2605	PSU	C6-C5	2.45	1.38	1.35
1	2A	2251	OMG	C6-N1	-2.44	1.34	1.37
1	2A	1915	5MU	C4-C5	2.43	1.48	1.44
1	2A	1942	5MC	C6-N1	-2.41	1.33	1.38
32	2a	1400	5MC	C6-N1	-2.40	1.34	1.38
32	2a	527	7MG	C6-N1	-2.39	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.39	1.34	1.38
32	2a	516	PSU	C4-N3	-2.38	1.34	1.38
32	2a	966	M2G	C6-N1	-2.37	1.34	1.37
1	1A	1939	PSU	C4-N3	-2.35	1.34	1.38
1	1A	2515	2MA	C2-N3	2.33	1.36	1.31
32	1a	516	PSU	C4-N3	-2.30	1.34	1.38
1	1A	2564	2MU	C5-C4	2.30	1.48	1.43
1	1A	2617	PSU	C2-N3	-2.30	1.33	1.37
1	2A	2605	PSU	C2-N3	-2.29	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	527	7MG	C6-N1	-2.28	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.28	1.33	1.38
1	2A	1962	5MC	C6-N1	-2.26	1.34	1.38
32	2a	967	5MC	C6-N1	-2.25	1.34	1.38
32	1a	967	5MC	C6-N1	-2.22	1.34	1.38
32	1a	527	7MG	C5-N7	-2.22	1.33	1.35
1	2A	1939	5MU	C6-N1	-2.17	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.17	1.34	1.38
1	2A	2552	2MU	C5-C4	2.15	1.48	1.43
32	2a	1498	UR3	C6-C5	2.14	1.40	1.35
32	2a	1207	2MG	C6-N1	-2.13	1.34	1.37
1	1A	2515	2MA	C6-N1	-2.12	1.33	1.38
1	1A	2564	2MU	C2-N3	-2.11	1.34	1.38
1	2A	2503	2MA	C2-N3	2.09	1.35	1.31
1	2A	2552	2MU	C2-N3	-2.08	1.34	1.38
32	1a	1498	UR3	C6-C5	2.07	1.39	1.35
1	2A	1915	5MU	C4-N3	-2.04	1.35	1.38
32	2a	527	7MG	C8-N9	2.03	1.47	1.46
32	2a	1407	5MC	C6-N1	-2.02	1.34	1.38
32	2a	516	PSU	O4'-C1'	-2.01	1.41	1.43
32	1a	1402	4OC	C6-C5	2.01	1.39	1.35

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-10.49	83.46	102.44
32	1a	527	7MG	N9-C4-N3	8.68	138.46	125.47
32	2a	527	7MG	N9-C4-N3	8.16	137.67	125.47
1	2A	1911	PSU	N1-C2-N3	6.20	122.15	115.13
1	1A	1933	PSU	N1-C2-N3	5.97	121.89	115.13
32	1a	1498	UR3	C4-N3-C2	-5.90	119.01	124.56
1	2A	1939	5MU	C4-N3-C2	-5.82	119.81	127.35
1	2A	1917	PSU	N1-C2-N3	5.82	121.72	115.13
1	2A	1939	5MU	N3-C2-N1	5.73	122.50	114.89
32	1a	516	PSU	N1-C2-N3	5.72	121.61	115.13
32	2a	1498	UR3	C4-N3-C2	-5.70	119.19	124.56
32	2a	516	PSU	N1-C2-N3	5.70	121.59	115.13
43	2l	92	0TD	CSB-SB-CB	-5.67	92.17	102.44
1	1A	1939	PSU	N1-C2-N3	5.55	121.42	115.13
1	1A	1961	5MU	O4-C4-C5	-5.53	118.49	124.90
1	2A	2605	PSU	N1-C2-N3	5.49	121.35	115.13
1	1A	2617	PSU	N1-C2-N3	5.48	121.34	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	N9-C8-N7	-5.46	95.57	103.38
1	2A	2552	2MU	N3-C2-N1	5.34	121.98	114.89
1	1A	1937	5MU	N3-C2-N1	5.33	121.97	114.89
32	1a	527	7MG	C5-C4-N3	-5.29	118.05	128.13
1	1A	1961	5MU	C4-N3-C2	-5.21	120.61	127.35
32	2a	527	7MG	C5-C4-N3	-5.07	118.47	128.13
32	1a	527	7MG	N9-C8-N7	-4.83	96.47	103.38
1	1A	2564	2MU	N3-C2-N1	4.82	121.29	114.89
1	1A	1937	5MU	C4-N3-C2	-4.76	121.19	127.35
1	2A	1939	5MU	C5-C4-N3	4.73	119.35	115.31
1	2A	2552	2MU	C4-N3-C2	-4.73	120.34	126.58
1	1A	1961	5MU	C5-C4-N3	4.56	119.21	115.31
1	2A	1939	5MU	C5-C6-N1	-4.56	118.65	123.34
1	2A	1915	5MU	C4-N3-C2	-4.52	121.50	127.35
1	1A	1961	5MU	N3-C2-N1	4.51	120.88	114.89
32	2a	1400	5MC	C5-C6-N1	-4.40	118.81	123.34
1	2A	1915	5MU	N3-C2-N1	4.40	120.73	114.89
1	2A	1915	5MU	O4-C4-C5	-4.34	119.88	124.90
1	2A	1942	5MC	C5-C6-N1	-4.28	118.94	123.34
1	2A	1915	5MU	C1 [?] -N1-C2	4.26	125.28	117.57
32	2a	967	5MC	C5-C6-N1	-4.24	118.98	123.34
32	2a	527	7MG	C2-N3-C4	4.22	119.82	112.30
1	2A	2605	PSU	C4-N3-C2	-4.22	120.26	126.34
32	1a	1400	5MC	C5-C6-N1	-4.05	119.17	123.34
32	2a	516	PSU	C4-N3-C2	-4.05	120.51	126.34
32	1a	527	7MG	C2-N3-C4	4.04	119.50	112.30
1	1A	1961	5MU	O2-C2-N1	-4.04	117.42	122.79
32	2a	1519	MA6	C4-C5-N7	-4.01	105.22	109.40
1	2A	1911	PSU	C4-N3-C2	-3.99	120.59	126.34
32	1a	516	PSU	C4-N3-C2	-3.98	120.61	126.34
1	1A	1937	5MU	C5-C4-N3	3.97	118.70	115.31
1	2A	1915	5MU	C5-C4-N3	3.97	118.70	115.31
1	1A	1937	5MU	C1 [?] -N1-C2	3.95	124.72	117.57
1	1A	2617	PSU	C4-N3-C2	-3.93	120.68	126.34
1	1A	1939	PSU	C4-N3-C2	-3.89	120.73	126.34
32	1a	967	5MC	C5-C6-N1	-3.87	119.36	123.34
1	1A	1961	5MU	C5-C6-N1	-3.86	119.36	123.34
1	1A	1964	5MC	C5-C6-N1	-3.86	119.37	123.34
1	1A	1933	PSU	C4-N3-C2	-3.84	120.80	126.34
1	2A	1917	PSU	O2-C2-N1	-3.81	118.59	122.79
1	2A	1915	5MU	C1 [?] -N1-C6	-3.72	114.92	121.12
43	1l	92	0TD	OD2-CG-CB	3.69	121.11	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1962	5MC	C5-C6-N1	-3.68	119.55	123.34
32	1a	1518	MA6	C4-C5-N7	-3.68	105.56	109.40
1	2A	1917	PSU	C4-N3-C2	-3.66	121.07	126.34
32	1a	1519	MA6	N1-C6-N6	3.65	120.90	117.06
32	2a	1404	5MC	C5-C6-N1	-3.63	119.60	123.34
1	1A	2564	2MU	C4-N3-C2	-3.60	121.83	126.58
32	2a	1519	MA6	C10-N6-C6	-3.58	108.66	119.51
1	1A	1984	5MC	C5-C6-N1	-3.55	119.69	123.34
32	1a	516	PSU	O2-C2-N1	-3.51	118.92	122.79
1	1A	1939	PSU	O2-C2-N1	-3.44	119.01	122.79
1	2A	2552	2MU	O2-C2-N1	-3.40	118.27	122.79
1	1A	1933	PSU	O2-C2-N1	-3.38	119.07	122.79
1	1A	2564	2MU	C2'-C1'-N1	-3.34	107.75	114.22
32	2a	1518	MA6	C4-C5-N7	-3.28	105.98	109.40
32	2a	516	PSU	O2-C2-N1	-3.26	119.20	122.79
32	1a	1519	MA6	C9-N6-C6	-3.26	109.64	119.51
32	2a	1519	MA6	N3-C2-N1	-3.25	123.60	128.68
32	2a	1519	MA6	C10-N6-C9	-3.20	105.82	116.12
1	2A	1911	PSU	O2-C2-N1	-3.19	119.28	122.79
32	2a	1407	5MC	C5-C6-N1	-3.18	120.07	123.34
1	2A	1939	5MU	O2-C2-N1	-3.16	118.59	122.79
32	2a	1518	MA6	N3-C2-N1	-3.12	123.80	128.68
1	1A	1937	5MU	O4-C4-C5	-3.09	121.32	124.90
32	1a	1407	5MC	C5-C6-N1	-3.09	120.16	123.34
32	2a	1518	MA6	C9-N6-C6	-3.08	110.18	119.51
32	1a	1404	5MC	C5-C6-N1	-3.03	120.22	123.34
32	1a	1518	MA6	C9-N6-C6	-3.01	110.41	119.51
1	2A	1939	5MU	O4-C4-C5	-2.99	121.43	124.90
1	1A	2515	2MA	C5-C6-N1	2.95	119.10	114.02
32	1a	1519	MA6	N3-C2-N1	-2.94	124.09	128.68
32	2a	1407	5MC	C5-C4-N3	-2.89	118.55	121.67
32	1a	1518	MA6	N3-C2-N1	-2.83	124.26	128.68
32	1a	1519	MA6	C4-C5-N7	-2.79	106.50	109.40
1	1A	1937	5MU	C1'-N1-C6	-2.78	116.49	121.12
43	2l	92	0TD	OD2-CG-CB	2.77	119.13	113.15
32	2a	1404	5MC	C5-C4-N3	-2.76	118.69	121.67
32	1a	1402	4OC	CM4-N4-C4	-2.74	117.09	122.45
1	2A	2552	2MU	C5-C4-N3	2.73	118.92	114.84
32	2a	1518	MA6	C10-N6-C9	-2.70	107.43	116.12
1	1A	1937	5MU	O2-C2-N3	-2.64	116.58	121.50
32	2a	527	7MG	C5-C6-N1	2.62	115.61	110.99
1	2A	2503	2MA	C8-N7-C5	2.62	107.99	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2552	2MU	C2'-C1'-N1	-2.61	109.16	114.22
1	2A	1920	4OC	O2-C2-N3	-2.56	118.17	122.33
32	1a	1498	UR3	C6-N1-C2	-2.55	119.50	121.79
1	2A	2552	2MU	O4-C4-C5	-2.55	120.68	125.16
32	1a	1407	5MC	C5-C4-N3	-2.53	118.94	121.67
32	1a	1207	2MG	CM2-N2-C2	-2.51	118.31	123.86
32	2a	1519	MA6	C9-N6-C6	-2.50	111.93	119.51
32	2a	1518	MA6	N1-C6-N6	2.49	119.68	117.06
32	1a	527	7MG	C5-C6-N1	2.48	115.36	110.99
1	1A	1937	5MU	C6-N1-C2	-2.47	118.79	121.30
43	1l	92	0TD	OD1-CG-CB	-2.46	117.28	122.44
32	1a	1207	2MG	C8-N7-C5	2.46	107.68	102.99
32	1a	1404	5MC	C5-C4-N3	-2.46	119.02	121.67
1	1A	2263	OMG	C8-N7-C5	2.46	107.67	102.99
1	2A	2605	PSU	O2-C2-N1	-2.44	120.11	122.79
1	1A	2263	OMG	C5-C6-N1	2.43	118.24	113.95
1	1A	2564	2MU	O2-C2-N1	-2.42	119.57	122.79
32	2a	1400	5MC	C5-C4-N3	-2.40	119.08	121.67
1	2A	2503	2MA	C5-C6-N1	2.40	118.16	114.02
1	2A	1917	PSU	C6-C5-C4	-2.39	116.53	118.20
1	2A	1942	5MC	C5-C4-N3	-2.38	119.10	121.67
32	1a	1400	5MC	C5-C4-N3	-2.38	119.10	121.67
32	1a	966	M2G	C5-C6-N1	2.37	118.13	113.95
32	2a	1518	MA6	C10-N6-C6	-2.35	112.39	119.51
32	1a	1518	MA6	C10-N6-C9	-2.35	108.55	116.12
1	2A	2605	PSU	C5-C6-N1	-2.35	118.59	122.11
32	1a	1207	2MG	O3'-C3'-C2'	2.33	119.36	111.82
1	1A	2515	2MA	C8-N7-C5	2.33	107.43	102.99
1	2A	2251	OMG	C8-N7-C5	2.33	107.43	102.99
32	2a	516	PSU	O4'-C1'-C2'	2.32	108.42	105.14
1	1A	2617	PSU	C5-C6-N1	-2.32	118.63	122.11
32	1a	1498	UR3	C3U-N3-C2	2.32	121.37	117.31
1	1A	1984	5MC	CM5-C5-C6	-2.31	119.76	122.85
32	1a	1407	5MC	O2-C2-N3	-2.31	118.58	122.33
32	2a	967	5MC	CM5-C5-C6	-2.31	119.77	122.85
32	1a	527	7MG	O6-C6-C5	-2.30	121.89	127.54
32	2a	967	5MC	C5-C4-N3	-2.29	119.20	121.67
32	2a	1207	2MG	C8-N7-C5	2.29	107.36	102.99
1	2A	1962	5MC	C5-C4-N3	-2.29	119.21	121.67
32	1a	516	PSU	O4'-C1'-C2'	2.28	108.36	105.14
1	1A	1937	5MU	C5-C6-N1	-2.27	121.01	123.34
1	2A	1942	5MC	CM5-C5-C6	-2.25	119.85	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	966	M2G	C5-C6-N1	2.25	117.92	113.95
32	1a	1404	5MC	CM5-C5-C6	-2.21	119.89	122.85
32	1a	966	M2G	C8-N7-C5	2.21	107.20	102.99
32	1a	527	7MG	C5-C4-N9	-2.20	103.49	106.35
1	2A	1915	5MU	C5-C6-N1	-2.20	121.08	123.34
1	1A	1937	5MU	C5M-C5-C4	2.19	121.17	118.77
32	1a	1207	2MG	C5-C6-N1	2.18	117.81	113.95
1	1A	1984	5MC	C5-C4-N3	-2.18	119.33	121.67
32	2a	966	M2G	C8-N7-C5	2.16	107.11	102.99
32	2a	1402	4OC	C6-C5-C4	2.16	119.61	116.96
32	1a	1407	5MC	CM5-C5-C6	-2.16	119.97	122.85
1	1A	1964	5MC	C5-C4-N3	-2.13	119.38	121.67
1	1A	2617	PSU	O2-C2-N1	-2.11	120.47	122.79
1	2A	1915	5MU	C5M-C5-C4	2.10	121.08	118.77
32	2a	516	PSU	C5-C6-N1	-2.10	118.96	122.11
32	1a	1518	MA6	C10-N6-C6	-2.09	113.18	119.51
32	1a	1402	4OC	C6-C5-C4	2.09	119.52	116.96
1	1A	1933	PSU	O4'-C1'-C2'	2.08	108.08	105.14
43	2l	92	0TD	OD1-CG-CB	-2.07	118.10	122.44
32	2a	1400	5MC	O2-C2-N3	-2.06	118.99	122.33
1	2A	2251	OMG	C5-C6-N1	2.04	117.56	113.95
32	1a	1402	4OC	O2-C2-N3	-2.04	119.02	122.33
32	2a	1402	4OC	C5-C4-N4	-2.03	118.48	122.61
1	1A	1942	4OC	O2-C2-N3	-2.02	119.04	122.33
32	1a	967	5MC	C5-C4-N3	-2.02	119.50	121.67
32	2a	1407	5MC	O2-C2-N3	-2.01	119.06	122.33
32	2a	527	7MG	CM7-N7-C5	2.00	131.57	126.40

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1937	5MU	O4'-C1'-N1-C2
1	1A	1937	5MU	O4'-C1'-N1-C6
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
32	1a	1518	MA6	C5-C6-N6-C10
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
1	2A	1917	PSU	C2'-C1'-C5-C4
1	2A	1917	PSU	C2'-C1'-C5-C6
32	2a	1402	4OC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	C5-C6-N6-C9
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C5-C6-N6-C10
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	1207	2MG	C3'-C4'-C5'-O5'
1	1A	1942	4OC	C3'-C2'-O2'-CM2
1	2A	1962	5MC	C2'-C1'-N1-C6
1	1A	2515	2MA	C4'-C5'-O5'-P
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	516	PSU	O4'-C1'-C5-C4
1	2A	1920	4OC	C3'-C2'-O2'-CM2
1	2A	1962	5MC	O4'-C1'-N1-C6
1	1A	1984	5MC	C2'-C1'-N1-C6
1	2A	2503	2MA	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD2
1	1A	1984	5MC	O4'-C1'-N1-C6
32	1a	1207	2MG	O4'-C4'-C5'-O5'
32	1a	516	PSU	O4'-C1'-C5-C6
32	1a	527	7MG	C4'-C5'-O5'-P
43	2l	92	0TD	SB-CB-CG-OD1
1	2A	1962	5MC	O4'-C1'-N1-C2
1	1A	1942	4OC	C2'-C1'-N1-C2
1	2A	1920	4OC	C2'-C1'-N1-C2
1	1A	2515	2MA	O4'-C4'-C5'-O5'
32	2a	527	7MG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates i

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2456 ligands modelled in this entry, 2443 are monoatomic - leaving 13 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
57	MPD	1A	4036	-	7,7,7	0.31	0	9,10,10	0.20	0
57	MPD	1T	205	-	7,7,7	0.30	0	9,10,10	0.14	0
60	SF4	1d	501	35	0,12,12	-	-	-	-	-
58	ARG	1B	232	54	10,11,11	0.78	1 (10%)	11,13,13	1.11	1 (9%)
56	EZM	2A	3691	-	23,24,24	3.10	3 (13%)	28,31,31	0.74	1 (3%)
60	SF4	2d	302	35	0,12,12	-	-	-	-	-
57	MPD	18	102	-	7,7,7	0.30	0	9,10,10	0.47	0
57	MPD	2A	3692	-	7,7,7	0.34	0	9,10,10	0.33	0
57	MPD	2B	222	-	7,7,7	0.32	0	9,10,10	0.19	0
57	MPD	1a	1860	-	7,7,7	0.40	0	9,10,10	0.46	0
57	MPD	2A	3693	-	7,7,7	0.32	0	9,10,10	0.34	0
56	EZM	1A	4035	-	23,24,24	1.95	3 (13%)	28,31,31	1.16	2 (7%)
58	ARG	1F	311	-	10,11,11	0.75	1 (10%)	11,13,13	1.20	2 (18%)

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
57	MPD	1A	4036	-	-	1/5/5/5	-
57	MPD	1T	205	-	-	0/5/5/5	-
60	SF4	1d	501	35	-	-	0/6/5/5
58	ARG	1B	232	54	-	3/11/11/11	-
56	EZM	2A	3691	-	-	4/25/27/27	0/1/1/1
60	SF4	2d	302	35	-	-	0/6/5/5
57	MPD	18	102	-	-	0/5/5/5	-
57	MPD	2A	3692	-	-	0/5/5/5	-
57	MPD	2B	222	-	-	2/5/5/5	-
57	MPD	1a	1860	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	2A	3693	-	-	1/5/5/5	-
56	EZM	1A	4035	-	-	4/25/27/27	0/1/1/1
58	ARG	1F	311	-	-	2/11/11/11	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2A	3691	EZM	OAC-NAY	11.74	1.42	1.22
56	2A	3691	EZM	CAT-CAW	-7.83	1.40	1.51
56	1A	4035	EZM	CAT-CAW	-7.35	1.41	1.51
56	1A	4035	EZM	CAU-NAY	-4.52	1.34	1.45
56	2A	3691	EZM	CAU-NAY	-4.38	1.34	1.45
56	1A	4035	EZM	OAC-NAY	2.33	1.26	1.22
58	1B	232	ARG	OXT-C	-2.11	1.23	1.30
58	1F	311	ARG	OXT-C	-2.10	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	4035	EZM	CAT-CAW-CAX	4.27	119.17	111.64
58	1F	311	ARG	OXT-C-O	-3.16	116.91	124.09
58	1B	232	ARG	OXT-C-O	-2.75	117.85	124.09
58	1F	311	ARG	OXT-C-CA	2.31	121.24	113.38
56	1A	4035	EZM	CAI-CAU-NAY	2.10	120.96	119.38
56	2A	3691	EZM	CAX-NAP-C	-2.06	119.43	123.07

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	1a	1860	MPD	C2-C3-C4-O4
56	1A	4035	EZM	CE-CD-CG-CB
56	1A	4035	EZM	CA-CB-CG-CD
56	2A	3691	EZM	CA-CB-CG-CD
58	1B	232	ARG	O-C-CA-N
56	2A	3691	EZM	OAD-CAM-CAX-CAW
56	1A	4035	EZM	CG-CD-CE-NZ
58	1B	232	ARG	OXT-C-CA-N
57	2B	222	MPD	C2-C3-C4-C5
56	2A	3691	EZM	CE-CD-CG-CB
58	1B	232	ARG	CA-CB-CG-CD

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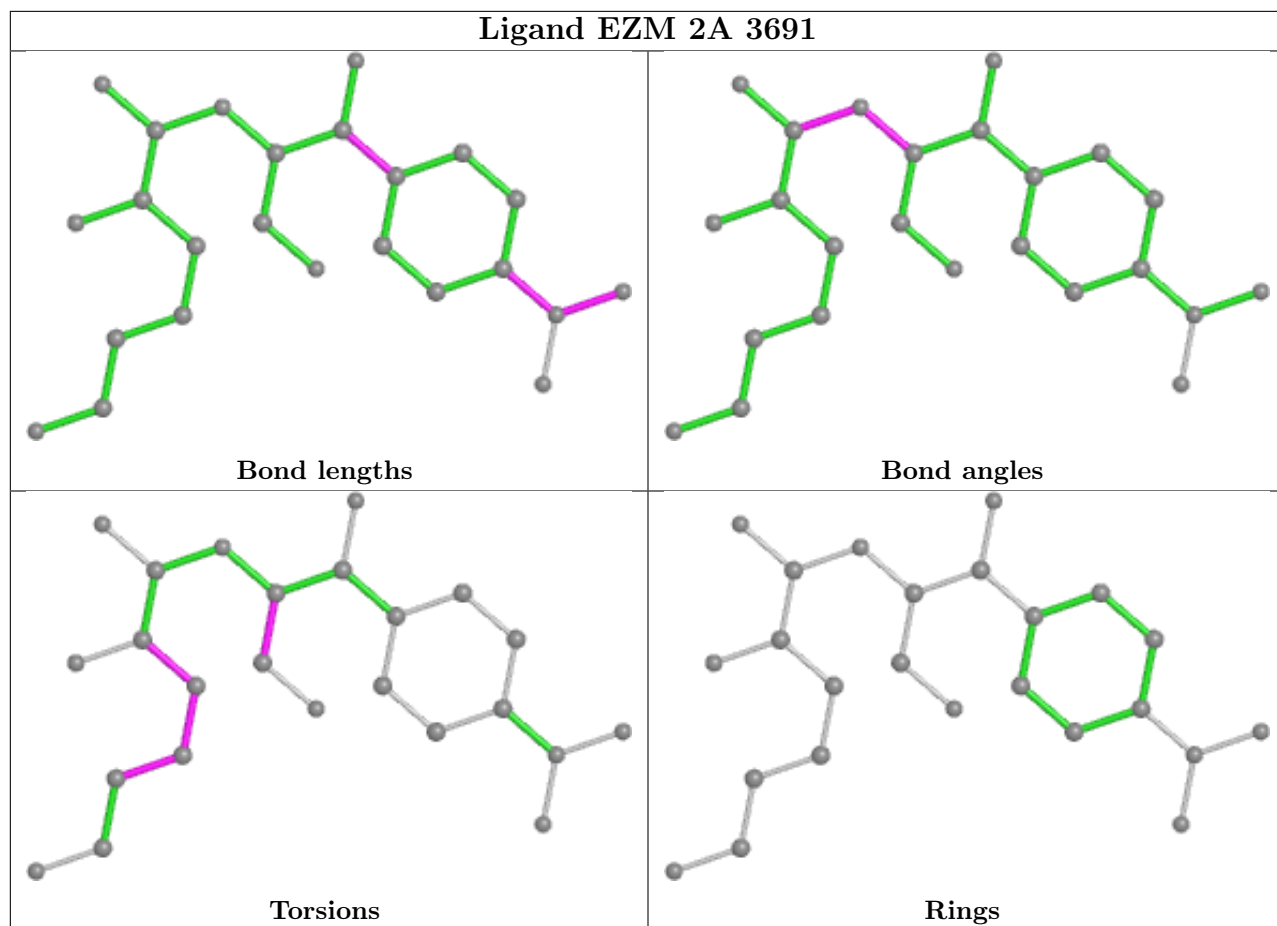
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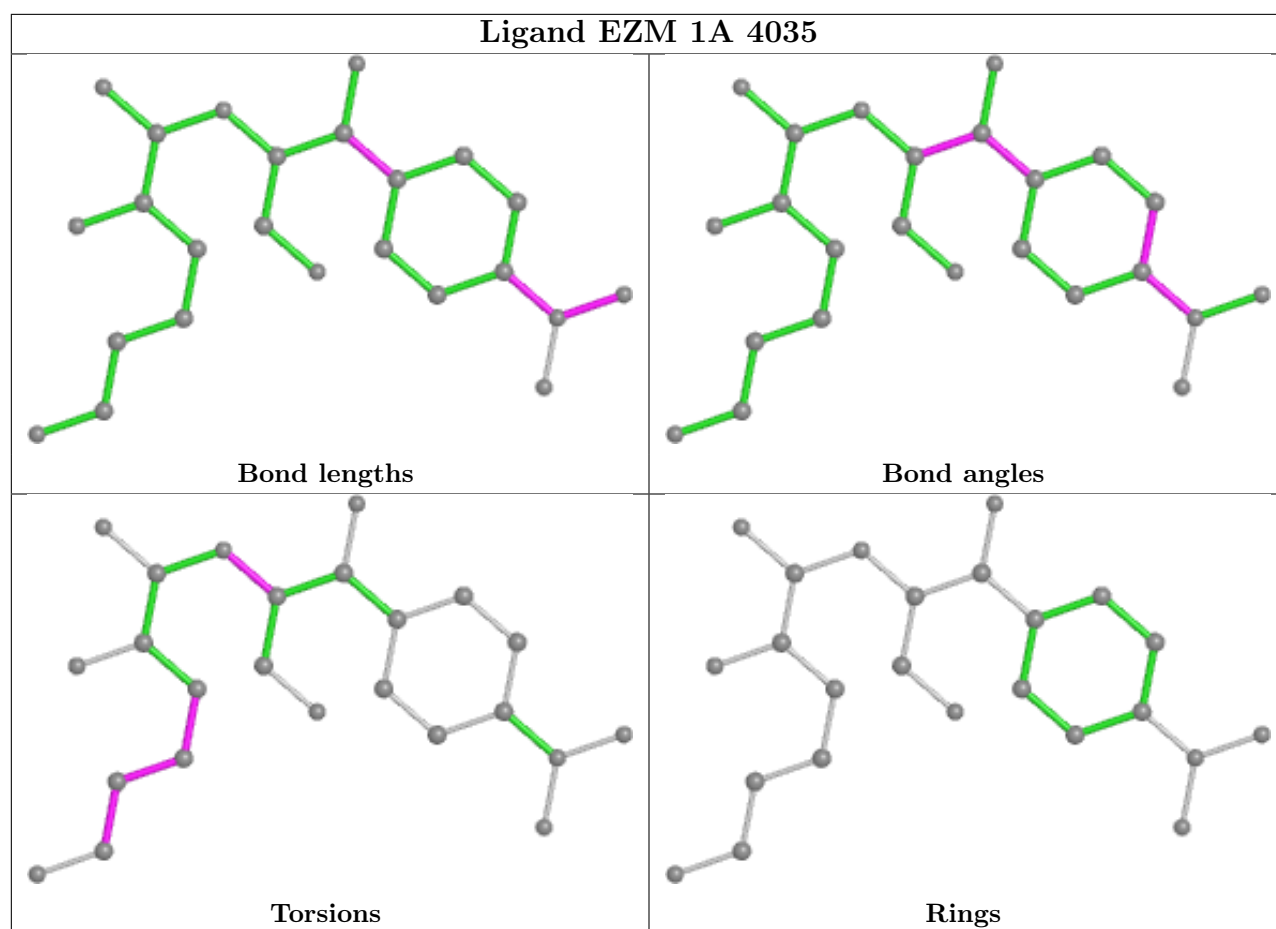
Mol	Chain	Res	Type	Atoms
57	1a	1860	MPD	C1-C2-C3-C4
58	1F	311	ARG	O-C-CA-CB
58	1F	311	ARG	OXT-C-CA-CB
56	1A	4035	EZM	CAM-CAX-NAP-C
56	2A	3691	EZM	C-CA-CB-CG
57	1A	4036	MPD	C2-C3-C4-C5
57	2A	3693	MPD	C2-C3-C4-C5
57	2B	222	MPD	C2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2861/2915 (98%)	0.31	55 (1%) 66 62	16, 32, 88, 100	0
1	2A	2856/2915 (97%)	0.11	68 (2%) 59 53	28, 52, 90, 101	0
2	1B	120/121 (99%)	-0.05	0 100 100	27, 46, 60, 76	0
2	2B	120/121 (99%)	-0.21	0 100 100	56, 74, 82, 87	0
3	1D	275/276 (99%)	0.45	1 (0%) 92 91	19, 34, 48, 67	0
3	2D	275/276 (99%)	0.51	5 (1%) 68 64	29, 47, 60, 75	0
4	1E	204/206 (99%)	0.36	0 100 100	16, 35, 56, 69	0
4	2E	204/206 (99%)	0.34	3 (1%) 73 70	31, 51, 68, 74	0
5	1F	203/210 (96%)	0.29	0 100 100	17, 38, 66, 81	0
5	2F	203/210 (96%)	0.13	0 100 100	30, 60, 74, 83	0
6	1G	181/182 (99%)	-0.00	0 100 100	44, 57, 72, 81	0
6	2G	181/182 (99%)	0.52	11 (6%) 21 16	69, 77, 83, 89	0
7	1H	174/180 (96%)	0.10	0 100 100	34, 49, 62, 67	0
7	2H	173/180 (96%)	0.70	13 (7%) 14 10	63, 75, 81, 86	0
8	1I	147/148 (99%)	-0.01	0 100 100	37, 67, 77, 84	0
8	2I	146/148 (98%)	0.21	9 (6%) 20 15	53, 70, 79, 82	0
9	1N	140/140 (100%)	0.28	0 100 100	22, 34, 55, 71	0
9	2N	140/140 (100%)	0.31	2 (1%) 75 71	41, 59, 71, 79	0
10	1O	122/122 (100%)	0.38	0 100 100	25, 36, 55, 61	0
10	2O	122/122 (100%)	0.19	0 100 100	40, 51, 65, 70	0
11	1P	149/150 (99%)	0.18	1 (0%) 87 86	17, 40, 60, 74	0
11	2P	149/150 (99%)	0.38	4 (2%) 54 48	33, 62, 76, 80	0
12	1Q	141/141 (100%)	0.25	0 100 100	24, 36, 48, 66	0
12	2Q	141/141 (100%)	0.42	5 (3%) 44 36	38, 58, 69, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.37	0 100 100	23, 32, 45, 53	0
13	2R	118/118 (100%)	0.29	0 100 100	34, 48, 59, 67	0
14	1S	110/112 (98%)	0.09	0 100 100	35, 47, 59, 66	0
14	2S	110/112 (98%)	0.45	11 (10%) 7 4	59, 70, 76, 80	0
15	1T	131/146 (89%)	0.23	0 100 100	30, 41, 64, 74	0
15	2T	131/146 (89%)	0.30	2 (1%) 73 70	45, 55, 71, 77	0
16	1U	116/118 (98%)	0.38	0 100 100	19, 26, 40, 57	0
16	2U	116/118 (98%)	0.33	0 100 100	35, 53, 68, 78	0
17	1V	101/101 (100%)	0.22	0 100 100	20, 36, 53, 61	0
17	2V	101/101 (100%)	0.18	0 100 100	35, 64, 73, 76	0
18	1W	112/113 (99%)	0.33	0 100 100	21, 27, 47, 77	0
18	2W	112/113 (99%)	0.39	0 100 100	35, 45, 63, 79	0
19	1X	95/96 (98%)	0.33	0 100 100	24, 35, 60, 69	0
19	2X	95/96 (98%)	0.55	4 (4%) 36 29	44, 56, 70, 77	0
20	1Y	107/110 (97%)	0.16	0 100 100	33, 44, 62, 70	0
20	2Y	107/110 (97%)	0.49	4 (3%) 41 34	54, 64, 74, 80	0
21	1Z	203/206 (98%)	0.06	1 (0%) 91 89	33, 53, 68, 78	0
21	2Z	201/206 (97%)	0.26	7 (3%) 44 36	60, 71, 78, 83	0
22	10	77/85 (90%)	0.31	0 100 100	24, 33, 49, 58	0
22	20	77/85 (90%)	0.80	9 (11%) 4 3	45, 57, 67, 72	0
23	11	97/98 (98%)	0.55	3 (3%) 49 42	25, 40, 62, 70	0
23	21	97/98 (98%)	0.69	3 (3%) 49 42	37, 52, 70, 73	0
24	12	70/72 (97%)	0.14	0 100 100	34, 46, 57, 79	0
24	22	70/72 (97%)	0.26	0 100 100	52, 65, 71, 74	0
25	13	59/60 (98%)	0.36	0 100 100	22, 32, 57, 67	0
25	23	59/60 (98%)	0.51	2 (3%) 45 38	47, 56, 70, 78	0
26	14	69/71 (97%)	-0.01	3 (4%) 35 28	52, 70, 83, 89	0
26	24	69/71 (97%)	0.69	10 (14%) 2 1	75, 82, 87, 92	0
27	15	59/60 (98%)	0.40	0 100 100	18, 28, 44, 57	0
27	25	59/60 (98%)	0.26	0 100 100	29, 46, 59, 68	0
28	16	53/54 (98%)	0.11	0 100 100	27, 38, 52, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.23	0 100 100	50, 56, 65, 68	0
29	17	48/49 (97%)	0.59	4 (8%) 11 8	15, 24, 53, 61	0
29	27	48/49 (97%)	0.69	2 (4%) 36 29	28, 38, 58, 67	0
30	18	64/65 (98%)	0.42	1 (1%) 72 68	24, 31, 38, 53	0
30	28	64/65 (98%)	0.76	2 (3%) 49 42	42, 51, 59, 66	0
31	19	37/37 (100%)	0.35	0 100 100	25, 36, 52, 55	0
31	29	37/37 (100%)	0.94	4 (10%) 5 3	53, 60, 70, 72	0
32	1a	1488/1521 (97%)	-0.04	24 (1%) 72 68	34, 63, 87, 100	0
32	2a	1492/1521 (98%)	0.13	40 (2%) 54 48	42, 72, 89, 98	0
33	1b	231/256 (90%)	0.55	19 (8%) 11 8	58, 73, 82, 86	0
33	2b	231/256 (90%)	0.88	38 (16%) 1 1	68, 79, 84, 89	0
34	1c	206/239 (86%)	0.53	9 (4%) 34 27	56, 68, 77, 82	0
34	2c	206/239 (86%)	1.07	44 (21%) 0 0	68, 77, 82, 84	0
35	1d	208/209 (99%)	0.38	10 (4%) 30 24	51, 66, 75, 82	0
35	2d	208/209 (99%)	0.73	17 (8%) 11 8	57, 67, 76, 81	0
36	1e	148/162 (91%)	0.37	3 (2%) 65 60	45, 60, 69, 76	0
36	2e	148/162 (91%)	0.62	12 (8%) 12 8	55, 68, 75, 86	0
37	1f	100/101 (99%)	0.15	0 100 100	47, 62, 70, 74	0
37	2f	100/101 (99%)	-0.04	0 100 100	52, 64, 72, 77	0
38	1g	155/156 (99%)	0.24	4 (2%) 56 50	57, 66, 74, 81	0
38	2g	155/156 (99%)	0.62	17 (10%) 5 3	67, 74, 80, 84	0
39	1h	137/138 (99%)	0.41	2 (1%) 73 70	51, 63, 70, 75	0
39	2h	137/138 (99%)	0.61	9 (6%) 18 13	60, 69, 74, 79	0
40	1i	127/128 (99%)	0.74	13 (10%) 6 4	58, 72, 80, 82	0
40	2i	126/128 (98%)	2.01	62 (49%) 0 0	70, 79, 83, 85	0
41	1j	97/105 (92%)	0.73	9 (9%) 8 6	54, 73, 82, 84	0
41	2j	96/105 (91%)	1.57	35 (36%) 0 0	71, 80, 85, 87	0
42	1k	114/129 (88%)	0.30	1 (0%) 84 82	41, 60, 69, 74	0
42	2k	114/129 (88%)	0.55	4 (3%) 44 36	52, 66, 76, 82	0
43	1l	121/132 (91%)	0.26	2 (1%) 70 66	44, 55, 67, 72	0
43	2l	121/132 (91%)	0.53	11 (9%) 9 6	53, 62, 70, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.06	3 (2%) 56 50	53, 68, 74, 77	0
44	2m	114/126 (90%)	0.81	17 (14%) 2 1	71, 79, 83, 84	0
45	1n	60/61 (98%)	1.09	7 (11%) 4 3	55, 65, 74, 81	0
45	2n	60/61 (98%)	2.33	35 (58%) 0 0	71, 77, 82, 86	0
46	1o	88/89 (98%)	0.32	2 (2%) 60 54	43, 61, 71, 77	0
46	2o	88/89 (98%)	0.57	2 (2%) 60 54	55, 67, 76, 81	0
47	1p	82/88 (93%)	0.57	0 100 100	58, 66, 76, 82	0
47	2p	82/88 (93%)	0.38	1 (1%) 79 76	56, 65, 74, 78	0
48	1q	99/105 (94%)	0.56	5 (5%) 28 22	53, 63, 70, 73	0
48	2q	99/105 (94%)	0.54	4 (4%) 38 31	55, 64, 73, 77	0
49	1r	68/88 (77%)	0.21	1 (1%) 73 70	53, 59, 72, 79	0
49	2r	68/88 (77%)	0.23	1 (1%) 73 70	57, 67, 75, 79	0
50	1s	83/93 (89%)	-0.04	0 100 100	61, 70, 78, 80	0
50	2s	83/93 (89%)	1.64	30 (36%) 0 0	73, 81, 85, 87	0
51	1t	96/106 (90%)	0.74	11 (11%) 4 3	56, 67, 75, 80	0
51	2t	98/106 (92%)	0.43	3 (3%) 49 42	54, 65, 76, 79	0
52	1u	23/27 (85%)	0.94	2 (8%) 10 7	59, 66, 70, 74	0
52	2u	23/27 (85%)	1.91	10 (43%) 0 0	71, 75, 79, 80	0
53	1y	97/113 (85%)	0.68	5 (5%) 27 21	46, 56, 69, 74	0
53	2y	96/113 (84%)	2.31	57 (59%) 0 0	61, 72, 79, 82	0
All	All	20766/21468 (96%)	0.33	830 (3%) 38 31	15, 59, 82, 101	0

All (830) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	2a	1030(B)	C	8.3
44	2m	102	ARG	7.6
1	1A	1122	C	7.4
1	1A	1137	G	7.2
32	2a	1030(A)	G	7.1
1	1A	1110	C	6.8
1	2A	2146	C	6.8
1	1A	2614	A	6.5
26	24	49	PHE	6.5
53	1y	95	ARG	6.2

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Mol	Chain	Res	Type	RSRZ
1	2A	2169	A	6.1
42	2k	13	GLN	6.1
1	1A	1136	U	6.1
45	2n	2	ALA	6.0
1	2A	2147	G	6.0
1	1A	1133	G	5.9
53	2y	9	GLN	5.9
53	2y	8	LYS	5.9
23	21	2	SER	5.8
34	2c	8	ILE	5.7
53	2y	40	ILE	5.7
23	11	2	SER	5.6
50	2s	49	ILE	5.6
40	2i	7	THR	5.6
20	2Y	1	MET	5.6
40	2i	109	VAL	5.5
1	2A	2145	C	5.5
52	2u	14	TRP	5.5
1	2A	2602	A	5.5
26	24	45	GLY	5.5
33	2b	123	ALA	5.4
32	1a	1030(B)	C	5.3
32	1a	1036	G	5.2
6	2G	152	LEU	5.2
32	1a	1257	U	5.1
45	2n	12	ARG	5.1
40	2i	126	SER	5.1
44	2m	116	THR	5.1
53	2y	88	LEU	5.0
1	2A	2140	C	4.9
1	2A	2153	G	4.9
40	2i	75	ASP	4.9
34	2c	124	ILE	4.9
53	2y	38	HIS	4.9
34	2c	196	LEU	4.8
40	2i	36	TYR	4.7
40	1i	125	TYR	4.7
32	1a	1030	C	4.7
33	1b	129	GLU	4.7
31	29	37	GLY	4.7
1	2A	2141	G	4.7
45	2n	25	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
39	2h	2	LEU	4.6
29	27	48	LYS	4.6
40	2i	66	ARG	4.6
26	24	54	GLY	4.6
40	2i	63	ILE	4.6
1	2A	2139	C	4.6
1	2A	2142	C	4.6
40	2i	76	ALA	4.6
50	2s	16	LEU	4.6
41	2j	67	THR	4.5
32	2a	1030	C	4.5
1	2A	2138	C	4.5
32	2a	1036	G	4.5
40	2i	127	LYS	4.5
1	2A	2144	U	4.4
45	2n	34	TYR	4.4
40	2i	114	TYR	4.4
1	1A	1113	A	4.4
41	2j	6	ILE	4.4
1	2A	2793	G	4.4
41	2j	46	ARG	4.3
1	1A	1135	G	4.3
8	2I	3	VAL	4.3
48	2q	98	LEU	4.3
41	2j	72	VAL	4.3
45	2n	44	LEU	4.3
50	2s	71	LEU	4.3
45	2n	61	TRP	4.3
40	2i	18	PHE	4.3
40	2i	113	LYS	4.2
32	1a	1001	A	4.2
33	1b	228	GLY	4.2
53	2y	41	LEU	4.2
1	2A	1046	A	4.2
1	2A	2168	G	4.2
32	1a	1034	G	4.1
34	1c	193	TYR	4.1
53	2y	71	TYR	4.1
1	1A	1121	C	4.1
41	2j	62	HIS	4.1
1	2A	1509	C	4.1
50	2s	15	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	1A	1221	G	4.1
33	2b	214	ILE	4.0
21	2Z	192	ALA	4.0
32	2a	1001(A)	G	4.0
7	2H	115	VAL	4.0
33	2b	118	LEU	4.0
7	2H	166	GLY	4.0
41	2j	45	ARG	4.0
41	2j	48	THR	4.0
19	2X	92	LEU	4.0
34	2c	159	GLY	4.0
35	1d	2	GLY	4.0
33	2b	131	PRO	4.0
53	2y	11	GLU	4.0
41	2j	44	VAL	4.0
52	2u	6	ARG	3.9
1	2A	2132	U	3.9
36	2e	13	ILE	3.9
1	1A	2154	U	3.9
33	2b	37	ASN	3.9
43	2l	18	VAL	3.9
32	2a	1030(C)	G	3.9
41	2j	40	LEU	3.9
45	2n	10	ALA	3.9
38	2g	6	ARG	3.9
32	2a	1257	U	3.9
40	2i	110	GLU	3.8
40	2i	115	GLY	3.8
6	2G	146	TYR	3.8
34	2c	157	ILE	3.8
6	2G	39	ILE	3.8
53	2y	64	SER	3.8
1	2A	2805	G	3.8
45	2n	35	ARG	3.8
50	2s	11	VAL	3.8
32	1a	1030(C)	G	3.8
32	2a	1492	A	3.8
33	1b	214	ILE	3.8
41	2j	65	LEU	3.8
53	2y	73	ALA	3.8
45	2n	31	ARG	3.8
1	1A	2163	G	3.8

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Mol	Chain	Res	Type	RSRZ
41	2j	63	PHE	3.8
1	2A	2179	C	3.8
21	1Z	192	ALA	3.8
53	2y	49	VAL	3.8
40	2i	108	VAL	3.7
1	2A	2118	U	3.7
41	2j	54	PHE	3.7
35	2d	146	ILE	3.7
51	1t	74	LYS	3.7
53	2y	5	ILE	3.7
1	1A	1120	G	3.7
12	2Q	104	PHE	3.7
41	2j	47	PHE	3.7
1	1A	1124	U	3.7
1	2A	1076	C	3.7
45	2n	6	LEU	3.7
33	1b	128	GLU	3.7
38	2g	154	TYR	3.7
48	1q	98	LEU	3.7
53	2y	77	LEU	3.7
51	1t	9	ASN	3.7
1	1A	2169	G	3.7
1	1A	1134	A	3.6
32	1a	1029	C	3.6
38	2g	32	ARG	3.6
3	2D	2	ALA	3.6
45	2n	13	THR	3.6
34	2c	33	LEU	3.6
1	2A	2143	C	3.6
34	2c	65	ALA	3.6
41	2j	60	ARG	3.6
40	2i	125	TYR	3.6
53	2y	4	ASN	3.6
52	2u	11	GLY	3.6
35	2d	33	MET	3.6
32	2a	1034	G	3.6
41	1j	66	ARG	3.6
1	1A	2177	G	3.6
32	1a	1031	G	3.6
1	2A	1085	A	3.6
40	2i	104	ARG	3.5
53	2y	10	MET	3.5

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Mol	Chain	Res	Type	RSRZ
26	24	66	SER	3.5
53	2y	39	ILE	3.5
53	2y	79	ASN	3.5
1	1A	2807	C	3.5
44	2m	6	GLY	3.5
53	2y	48	PHE	3.5
52	2u	15	ARG	3.5
40	2i	90	PRO	3.5
45	2n	38	GLY	3.5
45	2n	42	ILE	3.5
32	1a	1001(A)	G	3.5
43	1l	64	TYR	3.5
51	1t	66	ALA	3.5
40	2i	88	TYR	3.5
50	2s	52	TYR	3.5
53	2y	80	LYS	3.5
53	2y	58	ASN	3.5
32	1a	1035	A	3.4
50	2s	9	VAL	3.4
53	2y	12	ILE	3.4
50	2s	82	GLY	3.4
1	2A	2154	G	3.4
32	1a	1030(A)	G	3.4
52	2u	17	THR	3.4
40	2i	69	GLY	3.4
53	2y	52	ALA	3.4
33	2b	201	ILE	3.4
1	2A	2109	U	3.4
34	2c	163	ALA	3.4
1	2A	652(B)	A	3.4
21	2Z	191	VAL	3.4
53	2y	78	ILE	3.4
33	2b	120	ALA	3.4
40	2i	42	ARG	3.3
1	1A	1126	C	3.3
1	1A	2084	A	3.3
51	1t	72	LEU	3.3
40	1i	126	SER	3.3
32	1a	1028	C	3.3
40	2i	121	ARG	3.3
38	2g	34	GLY	3.3
1	1A	1111	U	3.3

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Mol	Chain	Res	Type	RSRZ
1	2A	229	A	3.3
35	2d	11	LEU	3.3
1	2A	2116	G	3.3
1	2A	2802	G	3.3
41	2j	74	ILE	3.3
33	1b	131	PRO	3.3
35	2d	49	ARG	3.3
45	2n	36	PHE	3.3
38	2g	156	TRP	3.3
26	24	68	ARG	3.2
40	1i	128	ARG	3.2
1	2A	2162	G	3.2
1	1A	1138	C	3.2
1	1A	1148	C	3.2
7	2H	95	ARG	3.2
34	2c	87	LEU	3.2
43	1l	63	GLY	3.2
32	2a	1030(D)	A	3.2
40	1i	46	ALA	3.2
44	1m	115	LYS	3.2
36	2e	12	LEU	3.2
1	2A	2174	C	3.2
38	2g	82	GLY	3.2
40	2i	111	ARG	3.2
40	2i	65	VAL	3.2
1	1A	1132	A	3.2
35	1d	167	GLY	3.2
1	1A	1112	U	3.2
45	2n	37	PHE	3.2
32	2a	1202	G	3.2
38	1g	16	LEU	3.2
43	2l	13	LYS	3.2
53	2y	45	PRO	3.2
53	2y	87	LYS	3.1
40	2i	123	PRO	3.1
43	2l	5	PRO	3.1
45	1n	61	TRP	3.1
33	1b	165	VAL	3.1
34	2c	177	THR	3.1
51	2t	10	LEU	3.1
53	2y	67	HIS	3.1
1	1A	1123	A	3.1

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Mol	Chain	Res	Type	RSRZ
40	2i	73	GLN	3.1
40	2i	86	VAL	3.1
1	2A	2106	G	3.1
1	2A	2120	G	3.1
1	1A	1129	U	3.1
33	2b	70	PHE	3.1
34	2c	164	ARG	3.1
45	2n	18	VAL	3.1
6	2G	135	LEU	3.1
40	1i	106	ALA	3.1
53	2y	42	SER	3.1
42	1k	25	TYR	3.1
19	2X	68	ARG	3.1
12	2Q	33	GLY	3.1
34	2c	155	GLY	3.1
26	24	56	VAL	3.1
36	2e	21	ALA	3.1
34	2c	152	ILE	3.1
41	2j	38	ILE	3.1
52	2u	22	ARG	3.1
32	1a	1492	A	3.1
33	2b	97	TRP	3.0
1	2A	2155	G	3.0
32	2a	80	G	3.0
26	24	51	ASP	3.0
53	2y	94	ALA	3.0
1	1A	1127	U	3.0
8	2I	35	LEU	3.0
34	2c	160	ALA	3.0
6	2G	136	ARG	3.0
33	1b	229	VAL	3.0
34	2c	162	GLN	3.0
41	2j	34	VAL	3.0
1	1A	2806	G	3.0
40	2i	5	TYR	3.0
1	1A	1118	C	3.0
1	1A	2183	C	3.0
44	2m	110	ARG	3.0
45	2n	41	ARG	3.0
33	2b	187	LEU	3.0
40	2i	102	LEU	3.0
50	2s	69	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
33	2b	122	PHE	3.0
1	2A	2152	G	3.0
45	2n	29	ARG	3.0
38	2g	9	VAL	3.0
41	2j	64	GLU	3.0
53	2y	93	GLU	3.0
1	2A	1083	U	3.0
53	2y	74	ILE	3.0
40	1i	19	LEU	3.0
29	27	47	ARG	3.0
53	2y	63	ALA	3.0
32	1a	1026	G	2.9
32	1a	1033	G	2.9
40	2i	54	ASP	2.9
1	2A	2119	A	2.9
33	1b	121	LEU	2.9
34	1c	2	GLY	2.9
52	1u	2	GLY	2.9
33	2b	130	ARG	2.9
34	2c	167	TRP	2.9
33	2b	233	SER	2.9
34	2c	184	TYR	2.9
32	2a	1001	A	2.9
1	2A	2124	G	2.9
32	2a	1286	A	2.9
53	2y	68	GLU	2.9
35	2d	70	ILE	2.9
51	1t	73	HIS	2.9
50	2s	35	SER	2.9
1	1A	1555	C	2.9
1	1A	2160	C	2.9
35	2d	20	TYR	2.9
14	2S	20	ARG	2.9
22	20	11	ARG	2.9
34	2c	199	LYS	2.9
32	1a	1027	C	2.9
40	2i	67	GLY	2.9
1	2A	2165	G	2.9
51	2t	13	LEU	2.9
26	24	50	VAL	2.9
41	1j	44	VAL	2.9
53	2y	20	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
40	2i	93	ARG	2.9
1	1A	2164	C	2.9
36	2e	26	PHE	2.9
33	2b	121	LEU	2.9
40	2i	122	ALA	2.9
48	2q	91	ARG	2.9
1	1A	2166	U	2.8
41	1j	10	GLY	2.8
8	2I	4	ILE	2.8
45	2n	60	SER	2.8
33	1b	130	ARG	2.8
39	2h	4	ASP	2.8
40	2i	9	ARG	2.8
40	2i	105	ASP	2.8
14	2S	12	PHE	2.8
35	1d	157	LEU	2.8
41	2j	66	ARG	2.8
43	2l	64	TYR	2.8
48	1q	99	SER	2.8
39	1h	134	ILE	2.8
21	2Z	125	LEU	2.8
45	2n	53	LEU	2.8
53	2y	24	LEU	2.8
38	2g	8	GLU	2.8
53	2y	3	MET	2.8
40	2i	56	LEU	2.8
1	2A	2125	G	2.8
1	2A	2804	C	2.8
22	20	76	GLY	2.8
33	2b	92	TYR	2.8
40	2i	62	TYR	2.8
38	2g	4	ARG	2.8
35	1d	179	GLU	2.8
32	2a	1035	A	2.8
44	2m	90	LEU	2.8
1	1A	2165	C	2.8
40	2i	57	GLY	2.8
40	2i	10	ARG	2.8
7	2H	159	GLU	2.7
33	1b	123	ALA	2.7
36	2e	20	GLN	2.7
40	2i	53	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
45	1n	25	VAL	2.7
38	2g	33	ASP	2.7
40	1i	114	TYR	2.7
44	2m	87	TYR	2.7
33	1b	213	LEU	2.7
41	2j	96	ILE	2.7
50	2s	62	ILE	2.7
34	2c	64	VAL	2.7
33	2b	48	MET	2.7
45	2n	49	HIS	2.7
33	2b	152	PHE	2.7
32	1a	1037	C	2.7
33	1b	133	LYS	2.7
33	2b	133	LYS	2.7
33	2b	136	VAL	2.7
1	1A	935	C	2.7
1	2A	2110	G	2.7
1	2A	2148	G	2.7
26	24	63	TYR	2.7
32	2a	1219	U	2.7
7	2H	35	VAL	2.7
43	2l	51	ALA	2.7
53	2y	51	ASP	2.7
34	2c	190	ARG	2.7
1	1A	1149	A	2.7
32	1a	1030(D)	A	2.7
8	2I	5	LEU	2.7
50	2s	65	ASN	2.7
48	2q	99	SER	2.7
51	1t	67	ALA	2.7
40	2i	117	HIS	2.7
7	2H	103	LEU	2.7
19	2X	80	ILE	2.7
41	1j	96	ILE	2.7
32	2a	1031	G	2.7
34	2c	132	ARG	2.7
45	2n	26	ARG	2.7
38	2g	80	VAL	2.7
40	2i	30	GLY	2.7
45	1n	15	LYS	2.7
41	1j	54	PHE	2.7
50	2s	74	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	34	C	2.7
33	2b	231	GLU	2.7
53	2y	72	THR	2.7
1	2A	2126	A	2.7
34	2c	4	LYS	2.7
45	1n	2	ALA	2.7
45	1n	18	VAL	2.7
34	2c	3	ASN	2.7
7	2H	89	ILE	2.7
47	2p	19	ILE	2.7
50	2s	34	TRP	2.7
33	2b	232	PRO	2.6
40	2i	8	GLY	2.6
1	2A	2801(A)	A	2.6
36	2e	10	MET	2.6
12	2Q	34	LEU	2.6
32	2a	1032	G	2.6
34	1c	10	PHE	2.6
3	1D	275	LYS	2.6
15	2T	111	ARG	2.6
44	2m	104	ARG	2.6
41	2j	98	ILE	2.6
53	2y	50	ALA	2.6
33	2b	165	VAL	2.6
1	2A	2896	C	2.6
34	2c	186	PHE	2.6
38	2g	155	ARG	2.6
1	1A	2175	G	2.6
7	2H	165	ALA	2.6
9	2N	68	GLU	2.6
33	2b	215	LEU	2.6
40	2i	79	LEU	2.6
41	2j	68	HIS	2.6
43	2l	15	ARG	2.6
50	2s	66	MET	2.6
40	2i	59	PHE	2.6
45	2n	55	GLY	2.6
8	2I	19	VAL	2.6
34	2c	153	VAL	2.6
45	2n	8	GLU	2.6
1	2A	1075	C	2.6
1	1A	2138	G	2.6

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Mol	Chain	Res	Type	RSRZ
1	1A	2176	G	2.6
32	2a	1026	G	2.6
33	1b	226	ARG	2.6
1	1A	2129	C	2.6
32	2a	91	C	2.6
39	1h	93	VAL	2.6
33	2b	188	ALA	2.5
32	2a	1033	G	2.5
7	2H	24	VAL	2.5
50	2s	41	VAL	2.5
33	2b	101	MET	2.5
1	2A	2062	A	2.5
41	2j	41	PRO	2.5
35	1d	111	ALA	2.5
53	2y	53	THR	2.5
53	2y	60	VAL	2.5
22	20	9	SER	2.5
33	2b	127	ILE	2.5
34	1c	124	ILE	2.5
40	2i	81	ILE	2.5
11	2P	15	ARG	2.5
15	2T	66	VAL	2.5
41	2j	29	ARG	2.5
6	2G	49	ASP	2.5
36	2e	22	GLY	2.5
33	2b	164	VAL	2.5
51	1t	13	LEU	2.5
32	2a	1357	A	2.5
53	2y	7	SER	2.5
22	20	46	LYS	2.5
45	2n	22	THR	2.5
32	2a	1029	C	2.5
53	1y	94	ALA	2.5
14	2S	32	LEU	2.5
19	2X	66	LEU	2.5
35	2d	4	TYR	2.5
14	2S	57	LYS	2.5
40	2i	83	ARG	2.5
35	2d	158	ILE	2.5
39	2h	112	LEU	2.5
53	2y	62	VAL	2.5
11	2P	79	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
29	17	47	ARG	2.5
32	2a	841	U	2.5
53	2y	37	PRO	2.5
14	2S	35	ILE	2.5
14	2S	40	ILE	2.5
21	2Z	187	ALA	2.5
8	2I	30	LEU	2.5
32	2a	1349	A	2.5
44	2m	84	ILE	2.5
34	2c	195	VAL	2.5
45	2n	21	TYR	2.5
42	2k	126	ARG	2.5
1	2A	2151	G	2.5
26	14	53	GLU	2.4
35	1d	124	GLY	2.4
38	2g	86	GLN	2.4
40	2i	124	GLN	2.4
38	2g	36	LYS	2.4
45	2n	59	ALA	2.4
50	2s	40	ILE	2.4
52	2u	13	ILE	2.4
50	2s	10	PHE	2.4
1	1A	2162	C	2.4
1	2A	614(A)	U	2.4
6	2G	133	LEU	2.4
23	11	98	LEU	2.4
33	2b	185	ILE	2.4
40	1i	79	LEU	2.4
41	1j	46	ARG	2.4
33	2b	132	LYS	2.4
34	2c	28	GLN	2.4
44	2m	89	GLY	2.4
44	2m	105	THR	2.4
33	2b	137	ARG	2.4
50	2s	31	ILE	2.4
45	2n	33	VAL	2.4
38	2g	7	ALA	2.4
34	2c	206	GLU	2.4
44	1m	56	LEU	2.4
1	2A	2136	C	2.4
53	1y	35	ILE	2.4
45	2n	16	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
53	2y	47	GLY	2.4
53	2y	92	GLY	2.4
7	2H	128	PRO	2.4
39	2h	18	ARG	2.4
51	1t	76	ALA	2.4
1	1A	2139	A	2.4
34	1c	39	ILE	2.4
1	1A	2597	U	2.4
39	2h	93	VAL	2.4
14	2S	33	LYS	2.4
38	2g	78	ARG	2.4
53	2y	91	LYS	2.4
1	1A	1109	G	2.4
25	23	23	LEU	2.4
40	2i	106	ALA	2.4
33	1b	200	ILE	2.4
32	1a	162	A	2.4
51	1t	55	ILE	2.4
23	21	62	VAL	2.4
1	2A	1082	U	2.3
41	2j	86	MET	2.3
32	2a	1028	C	2.3
12	2Q	121	ALA	2.3
44	2m	65	LYS	2.3
45	2n	50	LYS	2.3
35	2d	5	ILE	2.3
53	2y	35	ILE	2.3
1	1A	2816	G	2.3
32	1a	1003	G	2.3
38	1g	156	TRP	2.3
53	1y	70	MET	2.3
29	17	48	LYS	2.3
34	1c	201	TYR	2.3
35	1d	166	LYS	2.3
45	2n	9	LYS	2.3
22	20	75	LEU	2.3
34	1c	91	LEU	2.3
1	1A	2161	C	2.3
1	2A	6	A	2.3
1	2A	1064	C	2.3
34	2c	60	ALA	2.3
8	2I	85	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
53	2y	65	GLY	2.3
14	2S	3	ARG	2.3
46	1o	88	ARG	2.3
53	2y	84	GLN	2.3
1	2A	2112	G	2.3
43	2l	19	ARG	2.3
53	2y	15	ALA	2.3
1	1A	2168	C	2.3
32	2a	1092	A	2.3
41	2j	50	ILE	2.3
34	2c	128	PHE	2.3
45	2n	58	LYS	2.3
34	2c	23	TYR	2.3
34	2c	188	LEU	2.3
41	2j	36	GLY	2.3
53	2y	75	ASN	2.3
1	2A	2127	G	2.3
33	2b	135	GLN	2.3
33	1b	122	PHE	2.3
40	2i	33	PHE	2.3
1	2A	888	C	2.3
32	1a	1286	A	2.3
33	1b	231	GLU	2.3
11	2P	109	GLY	2.3
39	2h	9	MET	2.3
40	2i	21	PRO	2.3
9	2N	140	VAL	2.3
33	2b	163	PHE	2.3
34	2c	120	VAL	2.3
36	2e	90	VAL	2.3
40	2i	17	VAL	2.3
1	1A	2178	G	2.3
40	2i	72	GLY	2.3
4	2E	1	MET	2.3
34	2c	101	LEU	2.3
45	2n	39	LEU	2.3
3	2D	272	ALA	2.3
33	2b	33	TYR	2.3
50	2s	77	THR	2.3
41	2j	55	LYS	2.3
50	2s	8	GLY	2.3
1	2A	2181	G	2.3

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Mol	Chain	Res	Type	RSRZ
6	2G	62	LEU	2.3
53	2y	82	GLU	2.3
43	2l	100	ILE	2.3
45	1n	17	LYS	2.3
45	2n	15	LYS	2.3
26	14	50	VAL	2.3
35	2d	21	LEU	2.2
41	2j	71	LEU	2.2
11	1P	15	ARG	2.2
32	1a	1032	G	2.2
40	2i	120	ARG	2.2
50	2s	3	ARG	2.2
34	1c	63	ASN	2.2
41	2j	56	HIS	2.2
49	2r	46	GLU	2.2
40	1i	116	LYS	2.2
40	1i	121	ARG	2.2
44	2m	103	THR	2.2
3	2D	53	PHE	2.2
1	1A	2137	G	2.2
33	2b	81	VAL	2.2
34	2c	182	ILE	2.2
36	2e	105	VAL	2.2
11	2P	149	GLU	2.2
43	2l	48	PRO	2.2
53	1y	88	LEU	2.2
1	1A	1985	U	2.2
1	2A	2172	U	2.2
41	2j	87	THR	2.2
43	2l	16	GLU	2.2
4	2E	116	VAL	2.2
50	2s	28	LYS	2.2
33	2b	44	LEU	2.2
34	2c	127	ARG	2.2
52	2u	23	PRO	2.2
53	2y	95	ARG	2.2
1	2A	1026	U	2.2
1	2A	2170	A	2.2
35	2d	56	VAL	2.2
35	2d	67	ILE	2.2
39	2h	19	VAL	2.2
40	1i	63	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
40	2i	26	VAL	2.2
34	2c	85	ARG	2.2
41	2j	88	LEU	2.2
20	2Y	65	ALA	2.2
34	2c	61	ALA	2.2
40	2i	87	GLN	2.2
1	1A	1139	G	2.2
33	2b	227	GLY	2.2
35	2d	69	GLY	2.2
50	2s	84	GLY	2.2
32	2a	975	A	2.2
40	2i	37	PHE	2.2
52	1u	18	TYR	2.2
35	1d	3	ARG	2.2
42	2k	30	VAL	2.2
51	1t	75	ASN	2.2
35	1d	120	LEU	2.2
39	2h	39	LEU	2.2
38	1g	13	GLN	2.2
53	2y	46	GLN	2.2
1	2A	2111	C	2.2
8	2I	20	ASP	2.2
29	17	1	MET	2.2
32	2a	1027	C	2.2
32	2a	1354	C	2.2
36	1e	21	ALA	2.2
40	2i	43	ALA	2.2
50	2s	13	ASP	2.2
40	2i	107	ARG	2.2
52	2u	18	TYR	2.2
6	2G	92	VAL	2.2
32	2a	1157	A	2.2
50	2s	32	LYS	2.2
46	2o	86	GLY	2.2
50	2s	50	ALA	2.2
21	2Z	199	LYS	2.1
34	2c	198	VAL	2.1
40	2i	40	LEU	2.1
45	1n	51	GLY	2.1
50	2s	68	GLY	2.1
7	2H	102	ALA	2.1
22	20	77	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
34	2c	180	ALA	2.1
1	2A	2108	C	2.1
33	1b	127	ILE	2.1
35	2d	58	LEU	2.1
33	2b	228	GLY	2.1
41	2j	39	PRO	2.1
35	1d	49	ARG	2.1
46	2o	68	ARG	2.1
51	1t	83	ARG	2.1
36	1e	17	ALA	2.1
32	1a	1002	G	2.1
41	1j	64	GLU	2.1
25	23	54	VAL	2.1
34	1c	184	TYR	2.1
35	2d	203	VAL	2.1
1	1A	2815	C	2.1
6	2G	43	LEU	2.1
32	2a	1066	C	2.1
32	2a	1150	U	2.1
33	2b	144	ARG	2.1
14	2S	5	THR	2.1
14	2S	4	LEU	2.1
36	2e	29	GLY	2.1
40	2i	4	TYR	2.1
40	2i	14	VAL	2.1
41	2j	70	ARG	2.1
1	1A	2814	C	2.1
53	2y	76	GLU	2.1
44	1m	2	ALA	2.1
38	1g	79	ARG	2.1
38	2g	79	ARG	2.1
40	1i	107	ARG	2.1
4	2E	151	TYR	2.1
20	2Y	44	ILE	2.1
31	29	25	VAL	2.1
40	1i	56	LEU	2.1
48	1q	36	ILE	2.1
51	2t	20	LEU	2.1
32	2a	1093	A	2.1
32	2a	1363(A)	A	2.1
33	1b	59	GLU	2.1
1	2A	2897	U	2.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2107	C	2.1
26	24	44	THR	2.1
31	29	15	LYS	2.1
14	2S	17	ARG	2.1
41	1j	60	ARG	2.1
22	20	73	GLY	2.1
30	18	2	PRO	2.1
48	1q	28	PRO	2.1
1	2A	1913	A	2.1
1	2A	2135	A	2.1
53	2y	6	THR	2.1
6	2G	87	PRO	2.1
23	21	7	ILE	2.1
36	1e	92	LYS	2.1
48	1q	37	LYS	2.1
12	2Q	114	ALA	2.1
44	2m	75	ALA	2.1
29	17	41	ARG	2.1
52	2u	10	ARG	2.1
26	14	52	THR	2.1
32	2a	1021	G	2.0
32	2a	1041	A	2.1
32	2a	1191	A	2.1
46	1o	89	GLY	2.1
7	2H	50	VAL	2.0
8	2I	37	VAL	2.0
41	1j	49	VAL	2.0
31	29	17	ILE	2.0
43	2l	7	ILE	2.0
44	2m	4	ILE	2.0
44	2m	113	PRO	2.0
22	20	55	ARG	2.0
35	2d	117	ALA	2.0
48	2q	24	GLU	2.0
49	1r	73	ALA	2.0
20	2Y	5	MET	2.0
53	2y	69	ASP	2.0
3	2D	276	LYS	2.0
22	20	45	PHE	2.0
45	2n	17	LYS	2.0
32	2a	1040	U	2.0
32	2a	1287	A	2.0

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Mol	Chain	Res	Type	RSRZ
7	2H	29	PRO	2.0
39	2h	95	VAL	2.0
44	2m	98	VAL	2.0
34	2c	134	ILE	2.0
41	2j	43	ARG	2.0
36	2e	81	GLU	2.0
33	1b	207	ALA	2.0
3	2D	182	LEU	2.0
21	2Z	155	LEU	2.0
50	2s	20	LEU	2.0
30	28	23	VAL	2.0
34	2c	131	ARG	2.0
42	2k	109	VAL	2.0
50	2s	2	PRO	2.0
21	2Z	201	LYS	2.0
30	28	21	LYS	2.0
34	2c	158	GLY	2.0
23	11	46	LEU	2.0
35	2d	78	LEU	2.0
36	2e	43	LEU	2.0
44	2m	66	LEU	2.0
34	2c	6	HIS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	2MG	2a	1207	24/25	0.88	0.24	77,83,87,100	0
43	0TD	1l	92	10/11	0.89	0.27	50,56,62,88	0
43	0TD	2l	92	10/11	0.89	0.23	60,63,68,89	0
32	5MC	2a	967	21/22	0.90	0.19	62,69,79,81	0
1	PSU	1A	1939	20/21	0.90	0.15	56,69,73,74	0
1	5MU	1A	1937	21/22	0.90	0.16	71,76,82,90	0
1	PSU	2A	1911	20/21	0.91	0.13	64,69,79,81	0
1	5MU	2A	1915	21/22	0.91	0.17	75,81,84,94	0
1	PSU	2A	1917	20/21	0.91	0.15	70,76,84,90	0
32	M2G	2a	966	25/26	0.93	0.17	56,67,80,85	0
1	PSU	1A	1933	20/21	0.93	0.15	50,63,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	2MG	1a	1207	24/25	0.94	0.16	65,69,74,76	0
32	PSU	2a	516	20/21	0.94	0.13	67,74,77,80	0
1	4OC	2A	1920	21/23	0.95	0.17	60,65,71,73	0
32	5MC	2a	1404	21/22	0.95	0.22	55,61,64,66	0
32	MA6	2a	1518	24/25	0.95	0.18	55,61,65,67	0
32	7MG	2a	527	24/25	0.95	0.17	57,65,68,69	0
32	4OC	2a	1402	22/23	0.96	0.21	52,64,68,71	0
32	5MC	1a	967	21/22	0.96	0.19	50,57,65,68	0
32	5MC	2a	1407	21/22	0.96	0.15	55,62,65,71	0
32	PSU	1a	516	20/21	0.96	0.19	51,59,63,64	0
32	MA6	2a	1519	24/25	0.96	0.26	53,59,64,65	0
32	5MC	2a	1400	21/22	0.96	0.24	62,68,71,75	0
32	7MG	1a	527	24/25	0.97	0.18	44,50,54,62	0
32	5MC	1a	1407	21/22	0.97	0.20	41,50,54,58	0
32	UR3	1a	1498	21/22	0.97	0.20	41,47,51,62	0
1	5MC	2A	1962	21/22	0.97	0.16	39,43,54,60	0
32	MA6	1a	1518	24/25	0.97	0.26	38,43,50,53	0
32	UR3	2a	1498	21/22	0.97	0.21	56,60,64,69	0
32	MA6	1a	1519	24/25	0.97	0.23	39,43,47,48	0
32	M2G	1a	966	25/26	0.97	0.21	49,53,58,62	0
1	4OC	1A	1942	21/23	0.97	0.21	42,56,60,62	0
32	5MC	1a	1400	21/22	0.98	0.20	41,49,53,54	0
32	4OC	1a	1402	22/23	0.98	0.17	46,49,51,56	0
1	5MU	2A	1939	21/22	0.98	0.20	31,36,39,43	0
1	5MC	2A	1942	21/22	0.98	0.18	41,50,55,58	0
32	5MC	1a	1404	21/22	0.98	0.17	35,42,46,47	0
1	OMG	2A	2251	24/25	0.98	0.22	31,36,38,41	0
1	2MA	2A	2503	23/24	0.98	0.21	30,33,38,39	0
1	2MU	2A	2552	21/23	0.98	0.20	33,37,42,43	0
1	PSU	2A	2605	20/21	0.98	0.22	31,37,45,51	0
1	PSU	1A	2617	20/21	0.98	0.20	20,24,29,31	0
1	5MC	1A	1984	21/22	0.98	0.20	27,32,39,45	0
1	2MA	1A	2515	23/24	0.99	0.22	14,20,22,24	0
1	2MU	1A	2564	21/23	0.99	0.23	23,27,31,31	0
1	5MC	1A	1964	21/22	0.99	0.18	30,36,40,42	0
1	5MU	1A	1961	21/22	0.99	0.19	19,25,28,30	0
1	OMG	1A	2263	24/25	0.99	0.20	18,21,23,26	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
54	MG	1A	3986	1/1	0.33	0.16	99,99,99,99	0
54	MG	2B	202	1/1	0.34	0.32	93,93,93,93	0
54	MG	1A	3970	1/1	0.35	0.65	73,73,73,73	0
54	MG	2a	1777	1/1	0.38	0.22	85,85,85,85	0
54	MG	1a	1837	1/1	0.39	0.12	58,58,58,58	0
54	MG	2A	3633	1/1	0.39	0.23	66,66,66,66	0
54	MG	2B	220	1/1	0.42	0.22	81,81,81,81	0
54	MG	1a	1807	1/1	0.42	0.28	76,76,76,76	0
54	MG	2A	3627	1/1	0.43	0.19	76,76,76,76	0
54	MG	2A	3661	1/1	0.44	0.19	89,89,89,89	0
54	MG	2G	3001	1/1	0.47	0.14	80,80,80,80	0
54	MG	1a	1825	1/1	0.48	0.20	64,64,64,64	0
54	MG	1A	3807	1/1	0.49	0.20	58,58,58,58	0
54	MG	2a	1618	1/1	0.50	0.22	65,65,65,65	0
54	MG	1a	1755	1/1	0.52	0.22	73,73,73,73	0
54	MG	1a	1743	1/1	0.53	0.22	81,81,81,81	0
54	MG	1B	207	1/1	0.54	0.25	65,65,65,65	0
54	MG	1A	3953	1/1	0.54	0.23	84,84,84,84	0
54	MG	2a	1758	1/1	0.55	0.13	89,89,89,89	0
54	MG	1A	3949	1/1	0.55	0.17	72,72,72,72	0
54	MG	1A	3995	1/1	0.56	0.14	51,51,51,51	0
54	MG	2a	1752	1/1	0.56	0.12	72,72,72,72	0
54	MG	1A	3900	1/1	0.57	0.53	51,51,51,51	0
54	MG	2A	3436	1/1	0.57	0.24	76,76,76,76	0
54	MG	1A	3987	1/1	0.58	0.24	78,78,78,78	0
54	MG	2Q	3003	1/1	0.58	0.13	63,63,63,63	0
54	MG	2a	1765	1/1	0.58	0.15	78,78,78,78	0
54	MG	1A	3513	1/1	0.58	0.10	61,61,61,61	0
54	MG	1E	303	1/1	0.59	0.17	65,65,65,65	0
54	MG	2A	3387	1/1	0.59	0.21	56,56,56,56	0
54	MG	2A	3677	1/1	0.59	0.30	74,74,74,74	0
54	MG	2a	1603	1/1	0.60	0.25	69,69,69,69	0
54	MG	1A	3930	1/1	0.60	0.11	74,74,74,74	0
54	MG	2A	3261	1/1	0.60	0.32	71,71,71,71	0
54	MG	2A	3646	1/1	0.62	0.11	72,72,72,72	0
54	MG	2A	3648	1/1	0.63	0.18	62,62,62,62	0
54	MG	2a	1653	1/1	0.63	0.17	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	1A	3667	1/1	0.63	0.13	49,49,49,49	0
54	MG	2a	1763	1/1	0.64	0.15	63,63,63,63	0
54	MG	2A	3353	1/1	0.64	0.18	43,43,43,43	0
54	MG	1A	3809	1/1	0.64	0.20	66,66,66,66	0
54	MG	2a	1674	1/1	0.65	0.16	57,57,57,57	0
54	MG	1A	3920	1/1	0.65	0.19	69,69,69,69	0
54	MG	1a	1785	1/1	0.65	0.12	81,81,81,81	0
54	MG	2A	3670	1/1	0.66	0.09	78,78,78,78	0
54	MG	1A	4002	1/1	0.67	0.14	54,54,54,54	0
54	MG	1d	502	1/1	0.67	0.14	79,79,79,79	0
54	MG	1A	3957	1/1	0.67	0.41	66,66,66,66	0
54	MG	2A	3316	1/1	0.67	0.10	64,64,64,64	0
54	MG	1a	1828	1/1	0.67	0.24	70,70,70,70	0
54	MG	2a	1772	1/1	0.67	0.12	70,70,70,70	0
54	MG	2B	203	1/1	0.67	0.20	76,76,76,76	0
54	MG	2B	210	1/1	0.68	0.13	75,75,75,75	0
54	MG	1A	3336	1/1	0.68	0.17	56,56,56,56	0
54	MG	1A	3722	1/1	0.68	0.16	63,63,63,63	0
54	MG	2a	1661	1/1	0.68	0.13	66,66,66,66	0
54	MG	2A	3675	1/1	0.68	0.17	75,75,75,75	0
54	MG	2a	1713	1/1	0.68	0.34	67,67,67,67	0
54	MG	1A	3782	1/1	0.69	0.15	48,48,48,48	0
54	MG	2a	1664	1/1	0.69	0.19	73,73,73,73	0
54	MG	2A	3658	1/1	0.70	0.23	79,79,79,79	0
54	MG	1a	1848	1/1	0.70	0.17	61,61,61,61	0
54	MG	1A	3991	1/1	0.70	0.16	66,66,66,66	0
54	MG	1g	3002	1/1	0.70	0.18	75,75,75,75	0
54	MG	2A	3072	1/1	0.70	0.25	69,69,69,69	0
54	MG	2A	3219	1/1	0.70	0.25	67,67,67,67	0
54	MG	1a	1653	1/1	0.70	0.13	64,64,64,64	0
54	MG	1A	3516	1/1	0.70	0.14	58,58,58,58	0
54	MG	2A	3164	1/1	0.71	0.30	65,65,65,65	0
54	MG	2A	3173	1/1	0.71	0.14	53,53,53,53	0
54	MG	1T	201	1/1	0.71	0.18	65,65,65,65	0
54	MG	1I	102	1/1	0.71	0.15	56,56,56,56	0
54	MG	1A	3640	1/1	0.72	0.14	61,61,61,61	0
54	MG	1A	3653	1/1	0.72	0.06	73,73,73,73	0
54	MG	2a	1751	1/1	0.72	0.14	57,57,57,57	0
54	MG	1a	1752	1/1	0.72	0.21	70,70,70,70	0
54	MG	2A	3174	1/1	0.72	0.33	56,56,56,56	0
54	MG	1G	3002	1/1	0.72	0.19	57,57,57,57	0
54	MG	2A	3635	1/1	0.72	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3988	1/1	0.72	0.29	68,68,68,68	0
54	MG	1A	4018	1/1	0.72	0.11	29,29,29,29	0
54	MG	2B	217	1/1	0.73	0.10	73,73,73,73	0
54	MG	1a	1728	1/1	0.73	0.11	52,52,52,52	0
54	MG	1A	3142	1/1	0.73	0.20	45,45,45,45	0
54	MG	2A	3172	1/1	0.73	0.11	62,62,62,62	0
54	MG	1A	3990	1/1	0.73	0.10	43,43,43,43	0
54	MG	1a	1845	1/1	0.73	0.09	86,86,86,86	0
54	MG	1A	3721	1/1	0.73	0.12	59,59,59,59	0
54	MG	2a	1771	1/1	0.73	0.30	96,96,96,96	0
54	MG	1a	1608	1/1	0.73	0.13	52,52,52,52	0
54	MG	1A	3599	1/1	0.73	0.22	28,28,28,28	0
54	MG	2a	1779	1/1	0.73	0.20	76,76,76,76	0
54	MG	2A	3584	1/1	0.74	0.27	57,57,57,57	0
54	MG	1a	1853	1/1	0.74	0.15	60,60,60,60	0
54	MG	2A	3630	1/1	0.74	0.08	74,74,74,74	0
54	MG	1A	3709	1/1	0.74	0.15	54,54,54,54	0
54	MG	1A	3679	1/1	0.74	0.19	23,23,23,23	0
54	MG	2A	3641	1/1	0.74	0.15	83,83,83,83	0
54	MG	2A	3002	1/1	0.74	0.15	59,59,59,59	0
54	MG	1P	202	1/1	0.74	0.11	77,77,77,77	0
54	MG	2A	3563	1/1	0.74	0.14	78,78,78,78	0
54	MG	1A	3974	1/1	0.75	0.18	65,65,65,65	0
54	MG	1B	219	1/1	0.75	0.16	74,74,74,74	0
54	MG	2A	3407	1/1	0.75	0.13	62,62,62,62	0
54	MG	10	104	1/1	0.75	0.14	63,63,63,63	0
54	MG	2A	3481	1/1	0.75	0.15	58,58,58,58	0
54	MG	2A	3042	1/1	0.75	0.14	51,51,51,51	0
54	MG	2A	3319	1/1	0.75	0.13	71,71,71,71	0
54	MG	1A	3945	1/1	0.76	0.10	43,43,43,43	0
54	MG	2A	3154	1/1	0.76	0.21	59,59,59,59	0
54	MG	1a	1602	1/1	0.76	0.16	73,73,73,73	0
54	MG	2a	1635	1/1	0.76	0.16	67,67,67,67	0
54	MG	1q	201	1/1	0.76	0.15	62,62,62,62	0
54	MG	1A	3882	1/1	0.76	0.15	57,57,57,57	0
54	MG	2A	3660	1/1	0.76	0.11	78,78,78,78	0
54	MG	1A	3977	1/1	0.76	0.13	45,45,45,45	0
54	MG	2A	3195	1/1	0.76	0.17	62,62,62,62	0
54	MG	25	502	1/1	0.77	0.14	55,55,55,55	0
54	MG	2A	3080	1/1	0.77	0.19	51,51,51,51	0
54	MG	2a	1604	1/1	0.77	0.26	63,63,63,63	0
54	MG	1A	3222	1/1	0.77	0.23	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	2a	1632	1/1	0.77	0.12	82,82,82,82	0
54	MG	1A	3233	1/1	0.77	0.48	53,53,53,53	0
54	MG	1A	3582	1/1	0.77	0.11	64,64,64,64	0
54	MG	1A	3992	1/1	0.77	0.13	86,86,86,86	0
54	MG	1A	3994	1/1	0.77	0.17	53,53,53,53	0
54	MG	1A	3011	1/1	0.77	0.25	53,53,53,53	0
54	MG	2A	3587	1/1	0.77	0.13	57,57,57,57	0
54	MG	2a	1722	1/1	0.77	0.27	65,65,65,65	0
54	MG	2A	3687	1/1	0.77	0.06	70,70,70,70	0
54	MG	2A	3615	1/1	0.77	0.19	71,71,71,71	0
54	MG	1a	1786	1/1	0.77	0.14	59,59,59,59	0
54	MG	1A	3941	1/1	0.77	0.14	37,37,37,37	0
54	MG	2A	3632	1/1	0.77	0.12	48,48,48,48	0
54	MG	1A	3628	1/1	0.77	0.10	51,51,51,51	0
54	MG	1A	3844	1/1	0.77	0.11	57,57,57,57	0
54	MG	2A	3329	1/1	0.77	0.15	38,38,38,38	0
54	MG	2T	3003	1/1	0.77	0.11	62,62,62,62	0
54	MG	2a	1622	1/1	0.78	0.14	59,59,59,59	0
54	MG	1A	3939	1/1	0.78	0.62	51,51,51,51	0
54	MG	1A	3855	1/1	0.78	0.41	57,57,57,57	0
54	MG	2a	1639	1/1	0.78	0.25	67,67,67,67	0
54	MG	1y	3003	1/1	0.78	0.19	69,69,69,69	0
54	MG	1a	1694	1/1	0.78	0.17	55,55,55,55	0
54	MG	1a	1707	1/1	0.78	0.16	69,69,69,69	0
54	MG	1a	1829	1/1	0.78	0.24	63,63,63,63	0
54	MG	1A	3711	1/1	0.78	0.10	29,29,29,29	0
54	MG	2A	3122	1/1	0.78	0.10	58,58,58,58	0
54	MG	1A	3894	1/1	0.78	0.17	51,51,51,51	0
54	MG	1A	3756	1/1	0.78	0.17	45,45,45,45	0
54	MG	2A	3652	1/1	0.78	0.14	71,71,71,71	0
54	MG	1A	3828	1/1	0.78	0.15	25,25,25,25	0
54	MG	1A	3240	1/1	0.78	0.10	77,77,77,77	0
54	MG	28	102	1/1	0.78	0.18	65,65,65,65	0
54	MG	1g	3001	1/1	0.78	0.19	67,67,67,67	0
54	MG	2a	1776	1/1	0.78	0.13	71,71,71,71	0
54	MG	2A	3663	1/1	0.78	0.14	69,69,69,69	0
54	MG	2A	3668	1/1	0.78	0.14	63,63,63,63	0
54	MG	1a	1720	1/1	0.79	0.16	62,62,62,62	0
54	MG	2a	1724	1/1	0.79	0.18	61,61,61,61	0
54	MG	1A	3545	1/1	0.79	0.14	60,60,60,60	0
54	MG	1A	3378	1/1	0.79	0.16	33,33,33,33	0
54	MG	2A	3530	1/1	0.79	0.12	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2F	3001	1/1	0.79	0.16	41,41,41,41	0
54	MG	2A	3669	1/1	0.79	0.23	72,72,72,72	0
54	MG	1A	3810	1/1	0.79	0.16	55,55,55,55	0
54	MG	2A	3052	1/1	0.79	0.15	41,41,41,41	0
54	MG	1A	3596	1/1	0.79	0.14	32,32,32,32	0
54	MG	2A	3370	1/1	0.79	0.09	39,39,39,39	0
54	MG	1A	3996	1/1	0.79	0.31	70,70,70,70	0
54	MG	2A	3216	1/1	0.80	0.16	53,53,53,53	0
54	MG	1A	3910	1/1	0.80	0.25	77,77,77,77	0
54	MG	2A	3253	1/1	0.80	0.16	61,61,61,61	0
54	MG	2A	3624	1/1	0.80	0.13	78,78,78,78	0
54	MG	1A	3472	1/1	0.80	0.12	54,54,54,54	0
54	MG	1a	1849	1/1	0.80	0.17	68,68,68,68	0
54	MG	2a	1668	1/1	0.80	0.08	58,58,58,58	0
54	MG	2A	3076	1/1	0.80	0.25	56,56,56,56	0
54	MG	1a	1790	1/1	0.80	0.20	65,65,65,65	0
54	MG	1a	1601	1/1	0.80	0.10	63,63,63,63	0
54	MG	2A	3354	1/1	0.80	0.18	58,58,58,58	0
54	MG	1d	504	1/1	0.80	0.13	72,72,72,72	0
54	MG	1A	3921	1/1	0.80	0.10	62,62,62,62	0
54	MG	2A	3399	1/1	0.80	0.17	59,59,59,59	0
54	MG	1A	3192	1/1	0.80	0.16	50,50,50,50	0
54	MG	1A	3271	1/1	0.80	0.27	37,37,37,37	0
54	MG	1a	1656	1/1	0.80	0.15	59,59,59,59	0
54	MG	2A	3521	1/1	0.80	0.18	81,81,81,81	0
54	MG	2a	1605	1/1	0.80	0.10	60,60,60,60	0
54	MG	1a	1838	1/1	0.80	0.08	75,75,75,75	0
54	MG	2A	3196	1/1	0.80	0.28	41,41,41,41	0
54	MG	2a	1782	1/1	0.80	0.14	78,78,78,78	0
54	MG	1A	3968	1/1	0.81	0.20	48,48,48,48	0
54	MG	1A	3891	1/1	0.81	0.16	42,42,42,42	0
54	MG	2a	1602	1/1	0.81	0.16	57,57,57,57	0
54	MG	1A	3790	1/1	0.81	0.19	56,56,56,56	0
54	MG	1A	3543	1/1	0.81	0.16	39,39,39,39	0
54	MG	1R	202	1/1	0.81	0.20	39,39,39,39	0
54	MG	1A	3808	1/1	0.81	0.15	58,58,58,58	0
54	MG	1a	1792	1/1	0.81	0.15	73,73,73,73	0
54	MG	1a	1795	1/1	0.81	0.21	56,56,56,56	0
54	MG	2A	3053	1/1	0.81	0.11	53,53,53,53	0
54	MG	2a	1637	1/1	0.81	0.12	76,76,76,76	0
54	MG	1A	3075	1/1	0.81	0.24	40,40,40,40	0
54	MG	1A	3486	1/1	0.81	0.20	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3404	1/1	0.81	0.15	66,66,66,66	0
54	MG	1A	3664	1/1	0.81	0.06	45,45,45,45	0
54	MG	2A	3410	1/1	0.81	0.15	69,69,69,69	0
54	MG	2A	3120	1/1	0.81	0.15	41,41,41,41	0
54	MG	2a	1679	1/1	0.81	0.15	64,64,64,64	0
54	MG	1A	3841	1/1	0.81	0.09	56,56,56,56	0
54	MG	2A	3140	1/1	0.81	0.16	53,53,53,53	0
54	MG	1A	3940	1/1	0.81	0.10	72,72,72,72	0
54	MG	1A	3164	1/1	0.81	0.15	51,51,51,51	0
54	MG	2B	206	1/1	0.81	0.17	69,69,69,69	0
54	MG	1A	3852	1/1	0.81	0.11	62,62,62,62	0
54	MG	1A	3947	1/1	0.81	0.19	74,74,74,74	0
54	MG	1A	3853	1/1	0.81	0.21	52,52,52,52	0
54	MG	2E	305	1/1	0.81	0.21	70,70,70,70	0
54	MG	2A	3617	1/1	0.81	0.10	63,63,63,63	0
54	MG	1A	3775	1/1	0.81	0.16	53,53,53,53	0
54	MG	2G	3003	1/1	0.81	0.16	68,68,68,68	0
54	MG	1a	1855	1/1	0.81	0.17	68,68,68,68	0
54	MG	2a	1781	1/1	0.81	0.13	70,70,70,70	0
54	MG	1A	3081	1/1	0.81	0.28	41,41,41,41	0
57	MPD	2A	3692	8/8	0.81	0.32	41,48,53,56	0
54	MG	2A	3217	1/1	0.82	0.22	61,61,61,61	0
54	MG	1A	3919	1/1	0.82	0.14	74,74,74,74	0
54	MG	2A	3226	1/1	0.82	0.14	72,72,72,72	0
54	MG	2A	3250	1/1	0.82	0.12	71,71,71,71	0
54	MG	1l	201	1/1	0.82	0.18	64,64,64,64	0
54	MG	2a	1620	1/1	0.82	0.17	71,71,71,71	0
54	MG	1F	310	1/1	0.82	0.25	64,64,64,64	0
54	MG	1A	3826	1/1	0.82	0.20	25,25,25,25	0
54	MG	1A	3984	1/1	0.82	0.10	81,81,81,81	0
54	MG	2A	3027	1/1	0.82	0.25	60,60,60,60	0
54	MG	1A	3173	1/1	0.82	0.15	50,50,50,50	0
54	MG	1A	3757	1/1	0.82	0.10	45,45,45,45	0
54	MG	1A	3294	1/1	0.82	0.09	62,62,62,62	0
54	MG	2A	3059	1/1	0.82	0.30	50,50,50,50	0
54	MG	2A	3397	1/1	0.82	0.20	31,31,31,31	0
54	MG	1A	3699	1/1	0.82	0.18	42,42,42,42	0
54	MG	1A	3789	1/1	0.82	0.11	38,38,38,38	0
54	MG	1A	3565	1/1	0.82	0.22	28,28,28,28	0
54	MG	1A	3878	1/1	0.82	0.12	53,53,53,53	0
54	MG	1a	1636	1/1	0.82	0.16	54,54,54,54	0
54	MG	2a	1743	1/1	0.82	0.06	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	1746	1/1	0.82	0.21	74,74,74,74	0
54	MG	1A	3797	1/1	0.82	0.13	46,46,46,46	0
54	MG	1A	3263	1/1	0.82	0.13	70,70,70,70	0
54	MG	1a	1669	1/1	0.82	0.31	54,54,54,54	0
54	MG	1A	3659	1/1	0.82	0.15	32,32,32,32	0
54	MG	2A	3583	1/1	0.82	0.18	54,54,54,54	0
54	MG	2a	1766	1/1	0.82	0.12	75,75,75,75	0
54	MG	1A	3270	1/1	0.82	0.21	55,55,55,55	0
54	MG	1A	3753	1/1	0.82	0.19	49,49,49,49	0
54	MG	2A	3599	1/1	0.82	0.14	58,58,58,58	0
54	MG	2A	3175	1/1	0.82	0.22	45,45,45,45	0
54	MG	1A	3973	1/1	0.82	0.12	67,67,67,67	0
54	MG	2A	3621	1/1	0.82	0.14	75,75,75,75	0
54	MG	1a	1732	1/1	0.82	0.12	57,57,57,57	0
54	MG	1B	221	1/1	0.82	0.14	45,45,45,45	0
58	ARG	1F	311	12/12	0.82	0.25	52,70,77,82	0
54	MG	1A	3277	1/1	0.83	0.24	60,60,60,60	0
54	MG	1A	3692	1/1	0.83	0.16	63,63,63,63	0
54	MG	2A	3241	1/1	0.83	0.10	68,68,68,68	0
54	MG	1A	3369	1/1	0.83	0.16	32,32,32,32	0
54	MG	1A	3182	1/1	0.83	0.22	53,53,53,53	0
54	MG	1a	1764	1/1	0.83	0.13	69,69,69,69	0
54	MG	2A	3637	1/1	0.83	0.06	86,86,86,86	0
54	MG	2A	3293	1/1	0.83	0.15	60,60,60,60	0
54	MG	1A	3538	1/1	0.83	0.22	51,51,51,51	0
54	MG	1A	4000	1/1	0.83	0.15	46,46,46,46	0
54	MG	2a	1643	1/1	0.83	0.14	75,75,75,75	0
54	MG	2A	3043	1/1	0.83	0.17	72,72,72,72	0
54	MG	2A	3342	1/1	0.83	0.09	32,32,32,32	0
54	MG	1A	3460	1/1	0.83	0.15	61,61,61,61	0
54	MG	1A	3979	1/1	0.83	0.30	85,85,85,85	0
54	MG	2A	3360	1/1	0.83	0.17	52,52,52,52	0
54	MG	2a	1677	1/1	0.83	0.12	75,75,75,75	0
54	MG	1a	1605	1/1	0.83	0.14	65,65,65,65	0
54	MG	1A	4029	1/1	0.83	0.07	58,58,58,58	0
54	MG	1a	1612	1/1	0.83	0.17	52,52,52,52	0
54	MG	2a	1723	1/1	0.83	0.12	63,63,63,63	0
54	MG	2A	3078	1/1	0.83	0.14	52,52,52,52	0
54	MG	1A	3656	1/1	0.83	0.15	49,49,49,49	0
54	MG	2a	1744	1/1	0.83	0.18	73,73,73,73	0
54	MG	1a	1643	1/1	0.83	0.08	69,69,69,69	0
54	MG	1a	1831	1/1	0.83	0.17	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1B	211	1/1	0.83	0.27	67,67,67,67	0
54	MG	2A	3453	1/1	0.83	0.13	55,55,55,55	0
54	MG	1A	3747	1/1	0.83	0.15	67,67,67,67	0
54	MG	1a	1842	1/1	0.83	0.08	79,79,79,79	0
54	MG	1A	3461	1/1	0.83	0.19	58,58,58,58	0
54	MG	2a	1769	1/1	0.83	0.14	84,84,84,84	0
54	MG	2A	3551	1/1	0.83	0.17	59,59,59,59	0
54	MG	1a	1675	1/1	0.83	0.13	49,49,49,49	0
54	MG	1B	225	1/1	0.83	0.10	52,52,52,52	0
54	MG	1B	227	1/1	0.83	0.15	64,64,64,64	0
54	MG	1a	1709	1/1	0.83	0.13	50,50,50,50	0
54	MG	1A	3470	1/1	0.83	0.10	51,51,51,51	0
54	MG	2A	3208	1/1	0.83	0.23	66,66,66,66	0
54	MG	2e	201	1/1	0.83	0.29	68,68,68,68	0
54	MG	1a	1724	1/1	0.83	0.19	58,58,58,58	0
54	MG	1A	3329	1/1	0.83	0.16	43,43,43,43	0
54	MG	2A	3115	1/1	0.84	0.10	49,49,49,49	0
54	MG	1a	1606	1/1	0.84	0.12	54,54,54,54	0
54	MG	1A	3848	1/1	0.84	0.12	55,55,55,55	0
54	MG	2A	3355	1/1	0.84	0.11	52,52,52,52	0
54	MG	1A	3249	1/1	0.84	0.19	52,52,52,52	0
54	MG	1a	1615	1/1	0.84	0.14	54,54,54,54	0
54	MG	1a	1620	1/1	0.84	0.11	61,61,61,61	0
54	MG	2A	3392	1/1	0.84	0.14	71,71,71,71	0
54	MG	2A	3167	1/1	0.84	0.17	67,67,67,67	0
54	MG	1a	1779	1/1	0.84	0.11	76,76,76,76	0
54	MG	1A	3604	1/1	0.84	0.18	53,53,53,53	0
54	MG	1A	3614	1/1	0.84	0.15	58,58,58,58	0
54	MG	1a	1787	1/1	0.84	0.30	60,60,60,60	0
54	MG	1A	3616	1/1	0.84	0.11	68,68,68,68	0
54	MG	1y	3001	1/1	0.84	0.33	66,66,66,66	0
54	MG	2a	1711	1/1	0.84	0.09	62,62,62,62	0
54	MG	1A	3433	1/1	0.84	0.16	33,33,33,33	0
54	MG	2a	1714	1/1	0.84	0.12	58,58,58,58	0
54	MG	2A	3688	1/1	0.84	0.13	61,61,61,61	0
54	MG	2A	3497	1/1	0.84	0.20	69,69,69,69	0
54	MG	1A	3091	1/1	0.84	0.19	44,44,44,44	0
54	MG	2a	1726	1/1	0.84	0.18	74,74,74,74	0
54	MG	2a	1731	1/1	0.84	0.34	65,65,65,65	0
54	MG	1A	3942	1/1	0.84	0.22	41,41,41,41	0
54	MG	2B	209	1/1	0.84	0.12	73,73,73,73	0
54	MG	1A	3641	1/1	0.84	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1702	1/1	0.84	0.11	61,61,61,61	0
54	MG	2A	3575	1/1	0.84	0.12	65,65,65,65	0
54	MG	2A	3228	1/1	0.84	0.19	63,63,63,63	0
54	MG	1A	3985	1/1	0.84	0.10	70,70,70,70	0
54	MG	2F	3002	1/1	0.84	0.18	54,54,54,54	0
54	MG	1A	4034	1/1	0.84	0.40	58,58,58,58	0
54	MG	1a	1716	1/1	0.84	0.17	54,54,54,54	0
54	MG	1A	3342	1/1	0.84	0.21	17,17,17,17	0
54	MG	2A	3262	1/1	0.84	0.17	57,57,57,57	0
54	MG	2T	3004	1/1	0.84	0.21	61,61,61,61	0
54	MG	20	102	1/1	0.84	0.12	62,62,62,62	0
54	MG	2A	3074	1/1	0.84	0.19	46,46,46,46	0
54	MG	2A	3310	1/1	0.84	0.14	65,65,65,65	0
54	MG	1a	1839	1/1	0.84	0.22	73,73,73,73	0
54	MG	1A	3230	1/1	0.84	0.10	44,44,44,44	0
54	MG	2j	8001	1/1	0.84	0.16	81,81,81,81	0
54	MG	2A	3328	1/1	0.84	0.14	38,38,38,38	0
54	MG	1A	3950	1/1	0.84	0.16	60,60,60,60	0
54	MG	1A	3121	1/1	0.85	0.15	48,48,48,48	0
54	MG	1A	3280	1/1	0.85	0.22	34,34,34,34	0
54	MG	1a	1750	1/1	0.85	0.12	64,64,64,64	0
54	MG	1a	1604	1/1	0.85	0.11	61,61,61,61	0
54	MG	2A	3212	1/1	0.85	0.19	60,60,60,60	0
54	MG	1a	1754	1/1	0.85	0.13	63,63,63,63	0
54	MG	2A	3609	1/1	0.85	0.13	75,75,75,75	0
54	MG	2a	1612	1/1	0.85	0.10	54,54,54,54	0
54	MG	2a	1616	1/1	0.85	0.12	67,67,67,67	0
54	MG	1A	3759	1/1	0.85	0.14	48,48,48,48	0
54	MG	1A	3549	1/1	0.85	0.24	42,42,42,42	0
54	MG	1a	1773	1/1	0.85	0.16	67,67,67,67	0
54	MG	2A	3227	1/1	0.85	0.25	59,59,59,59	0
54	MG	1A	3779	1/1	0.85	0.10	29,29,29,29	0
54	MG	1A	3228	1/1	0.85	0.24	30,30,30,30	0
54	MG	2A	3245	1/1	0.85	0.14	50,50,50,50	0
54	MG	2A	3034	1/1	0.85	0.13	66,66,66,66	0
54	MG	1A	3467	1/1	0.85	0.12	31,31,31,31	0
54	MG	1a	1616	1/1	0.85	0.13	53,53,53,53	0
54	MG	1A	3673	1/1	0.85	0.18	60,60,60,60	0
54	MG	2A	3642	1/1	0.85	0.11	63,63,63,63	0
54	MG	2A	3645	1/1	0.85	0.17	72,72,72,72	0
54	MG	1a	1632	1/1	0.85	0.13	62,62,62,62	0
54	MG	2A	3057	1/1	0.85	0.45	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	1703	1/1	0.85	0.17	69,69,69,69	0
54	MG	1B	213	1/1	0.85	0.15	71,71,71,71	0
54	MG	1A	3250	1/1	0.85	0.22	61,61,61,61	0
54	MG	1a	1819	1/1	0.85	0.14	64,64,64,64	0
54	MG	1a	1648	1/1	0.85	0.22	57,57,57,57	0
54	MG	1A	3254	1/1	0.85	0.14	67,67,67,67	0
54	MG	1A	3229	1/1	0.85	0.13	61,61,61,61	0
54	MG	2A	3087	1/1	0.85	0.15	44,44,44,44	0
54	MG	2A	3090	1/1	0.85	0.33	51,51,51,51	0
54	MG	2a	1732	1/1	0.85	0.15	80,80,80,80	0
54	MG	2A	3094	1/1	0.85	0.13	45,45,45,45	0
54	MG	2A	3363	1/1	0.85	0.12	63,63,63,63	0
54	MG	1A	3026	1/1	0.85	0.08	60,60,60,60	0
54	MG	2A	3382	1/1	0.85	0.15	63,63,63,63	0
54	MG	1D	313	1/1	0.85	0.17	48,48,48,48	0
54	MG	1A	3111	1/1	0.85	0.19	61,61,61,61	0
54	MG	2A	3132	1/1	0.85	0.15	63,63,63,63	0
54	MG	1A	3933	1/1	0.85	0.13	56,56,56,56	0
54	MG	2A	3142	1/1	0.85	0.12	66,66,66,66	0
54	MG	2B	213	1/1	0.85	0.09	70,70,70,70	0
54	MG	2A	3144	1/1	0.85	0.13	62,62,62,62	0
54	MG	2A	3150	1/1	0.85	0.28	59,59,59,59	0
54	MG	2E	303	1/1	0.85	0.35	61,61,61,61	0
54	MG	2A	3419	1/1	0.85	0.14	66,66,66,66	0
54	MG	1A	3820	1/1	0.85	0.06	56,56,56,56	0
54	MG	1A	3527	1/1	0.85	0.17	37,37,37,37	0
54	MG	2A	3166	1/1	0.85	0.16	62,62,62,62	0
54	MG	1A	3638	1/1	0.85	0.34	58,58,58,58	0
54	MG	1A	3416	1/1	0.85	0.17	48,48,48,48	0
54	MG	1A	3541	1/1	0.85	0.21	64,64,64,64	0
54	MG	1A	3754	1/1	0.85	0.17	57,57,57,57	0
54	MG	1A	3553	1/1	0.86	0.23	61,61,61,61	0
54	MG	20	101	1/1	0.86	0.15	74,74,74,74	0
54	MG	2A	3564	1/1	0.86	0.17	59,59,59,59	0
54	MG	2A	3225	1/1	0.86	0.25	67,67,67,67	0
54	MG	1A	3559	1/1	0.86	0.14	48,48,48,48	0
54	MG	1A	3767	1/1	0.86	0.10	61,61,61,61	0
54	MG	1A	3861	1/1	0.86	0.19	42,42,42,42	0
54	MG	1A	3960	1/1	0.86	0.14	48,48,48,48	0
54	MG	2A	3242	1/1	0.86	0.15	33,33,33,33	0
54	MG	1A	3864	1/1	0.86	0.32	82,82,82,82	0
54	MG	2a	1614	1/1	0.86	0.14	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3870	1/1	0.86	0.20	53,53,53,53	0
54	MG	1B	223	1/1	0.86	0.18	36,36,36,36	0
54	MG	1a	1668	1/1	0.86	0.15	56,56,56,56	0
54	MG	1A	3306	1/1	0.86	0.12	27,27,27,27	0
54	MG	2A	3273	1/1	0.86	0.16	66,66,66,66	0
54	MG	2a	1633	1/1	0.86	0.23	67,67,67,67	0
54	MG	1A	3409	1/1	0.86	0.17	48,48,48,48	0
54	MG	2A	3086	1/1	0.86	0.25	67,67,67,67	0
54	MG	1A	3505	1/1	0.86	0.17	53,53,53,53	0
54	MG	2a	1640	1/1	0.86	0.17	69,69,69,69	0
54	MG	2A	3636	1/1	0.86	0.20	63,63,63,63	0
54	MG	1a	1835	1/1	0.86	0.19	70,70,70,70	0
54	MG	2a	1654	1/1	0.86	0.14	50,50,50,50	0
54	MG	1A	3308	1/1	0.86	0.19	62,62,62,62	0
54	MG	1a	1703	1/1	0.86	0.14	63,63,63,63	0
54	MG	2A	3339	1/1	0.86	0.25	70,70,70,70	0
54	MG	1A	3078	1/1	0.86	0.19	56,56,56,56	0
54	MG	1A	3906	1/1	0.86	0.12	71,71,71,71	0
54	MG	1a	1843	1/1	0.86	0.15	68,68,68,68	0
54	MG	2A	3654	1/1	0.86	0.13	72,72,72,72	0
54	MG	2a	1710	1/1	0.86	0.18	68,68,68,68	0
54	MG	2A	3656	1/1	0.86	0.12	69,69,69,69	0
54	MG	1A	3795	1/1	0.86	0.13	41,41,41,41	0
54	MG	1A	3435	1/1	0.86	0.20	42,42,42,42	0
54	MG	1A	3456	1/1	0.86	0.12	34,34,34,34	0
54	MG	1A	3625	1/1	0.86	0.27	67,67,67,67	0
54	MG	1A	3627	1/1	0.86	0.25	43,43,43,43	0
54	MG	1a	1734	1/1	0.86	0.14	59,59,59,59	0
54	MG	1a	1736	1/1	0.86	0.14	55,55,55,55	0
54	MG	1A	3259	1/1	0.86	0.15	55,55,55,55	0
54	MG	2a	1733	1/1	0.86	0.08	69,69,69,69	0
54	MG	1A	3637	1/1	0.86	0.09	31,31,31,31	0
54	MG	2A	3678	1/1	0.86	0.13	39,39,39,39	0
54	MG	1A	3053	1/1	0.86	0.49	32,32,32,32	0
54	MG	1l	202	1/1	0.86	0.09	72,72,72,72	0
54	MG	1A	3751	1/1	0.86	0.10	47,47,47,47	0
54	MG	1q	202	1/1	0.86	0.08	65,65,65,65	0
54	MG	2A	3429	1/1	0.86	0.28	56,56,56,56	0
54	MG	1A	3368	1/1	0.86	0.14	64,64,64,64	0
54	MG	2A	3440	1/1	0.86	0.22	53,53,53,53	0
54	MG	2A	3446	1/1	0.86	0.16	57,57,57,57	0
54	MG	2A	3207	1/1	0.86	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3461	1/1	0.86	0.35	55,55,55,55	0
54	MG	1A	4001	1/1	0.86	0.08	56,56,56,56	0
54	MG	2A	3494	1/1	0.86	0.24	50,50,50,50	0
54	MG	1A	3163	1/1	0.86	0.15	65,65,65,65	0
54	MG	2A	3511	1/1	0.86	0.22	45,45,45,45	0
54	MG	2A	3213	1/1	0.86	0.14	64,64,64,64	0
54	MG	1a	1776	1/1	0.86	0.12	68,68,68,68	0
54	MG	2A	3537	1/1	0.86	0.18	70,70,70,70	0
54	MG	2R	201	1/1	0.86	0.26	51,51,51,51	0
54	MG	1A	3643	1/1	0.86	0.17	36,36,36,36	0
54	MG	1G	3001	1/1	0.87	0.12	65,65,65,65	0
54	MG	2A	3184	1/1	0.87	0.16	64,64,64,64	0
54	MG	2A	3004	1/1	0.87	0.16	61,61,61,61	0
54	MG	2A	3008	1/1	0.87	0.38	44,44,44,44	0
54	MG	1A	3788	1/1	0.87	0.09	38,38,38,38	0
54	MG	1a	1802	1/1	0.87	0.12	50,50,50,50	0
54	MG	2A	3405	1/1	0.87	0.21	62,62,62,62	0
54	MG	1a	1685	1/1	0.87	0.17	66,66,66,66	0
54	MG	2A	3409	1/1	0.87	0.13	42,42,42,42	0
54	MG	1a	1808	1/1	0.87	0.17	64,64,64,64	0
54	MG	1A	3010	1/1	0.87	0.12	44,44,44,44	0
54	MG	1A	3859	1/1	0.87	0.25	44,44,44,44	0
54	MG	1A	3609	1/1	0.87	0.11	55,55,55,55	0
54	MG	2a	1656	1/1	0.87	0.12	70,70,70,70	0
54	MG	2A	3224	1/1	0.87	0.15	54,54,54,54	0
54	MG	1A	3490	1/1	0.87	0.17	66,66,66,66	0
54	MG	2A	3065	1/1	0.87	0.31	57,57,57,57	0
54	MG	1A	3253	1/1	0.87	0.22	48,48,48,48	0
54	MG	2A	3465	1/1	0.87	0.14	69,69,69,69	0
54	MG	1A	3803	1/1	0.87	0.19	22,22,22,22	0
54	MG	2A	3229	1/1	0.87	0.15	56,56,56,56	0
54	MG	1A	3317	1/1	0.87	0.17	27,27,27,27	0
54	MG	2A	3503	1/1	0.87	0.14	38,38,38,38	0
54	MG	1A	3515	1/1	0.87	0.34	55,55,55,55	0
54	MG	2B	204	1/1	0.87	0.14	63,63,63,63	0
54	MG	1A	3096	1/1	0.87	0.17	29,29,29,29	0
54	MG	1a	1840	1/1	0.87	0.14	62,62,62,62	0
54	MG	1A	3573	1/1	0.87	0.16	31,31,31,31	0
54	MG	1A	3905	1/1	0.87	0.08	39,39,39,39	0
54	MG	2A	3552	1/1	0.87	0.09	48,48,48,48	0
54	MG	1A	3814	1/1	0.87	0.23	45,45,45,45	0
54	MG	2A	3267	1/1	0.87	0.19	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3909	1/1	0.87	0.19	86,86,86,86	0
54	MG	2A	3576	1/1	0.87	0.17	60,60,60,60	0
54	MG	2A	3277	1/1	0.87	0.26	48,48,48,48	0
54	MG	1A	3763	1/1	0.87	0.25	42,42,42,42	0
54	MG	1a	1851	1/1	0.87	0.10	83,83,83,83	0
54	MG	2a	1756	1/1	0.87	0.12	80,80,80,80	0
54	MG	2A	3590	1/1	0.87	0.33	64,64,64,64	0
54	MG	2A	3591	1/1	0.87	0.31	71,71,71,71	0
54	MG	1A	3133	1/1	0.87	0.21	44,44,44,44	0
54	MG	1A	3425	1/1	0.87	0.25	66,66,66,66	0
54	MG	1a	1634	1/1	0.87	0.14	71,71,71,71	0
54	MG	1A	3778	1/1	0.87	0.15	54,54,54,54	0
54	MG	1a	1771	1/1	0.87	0.17	59,59,59,59	0
54	MG	1A	3597	1/1	0.87	0.17	22,22,22,22	0
54	MG	1a	1644	1/1	0.87	0.29	62,62,62,62	0
54	MG	1B	230	1/1	0.87	0.14	60,60,60,60	0
54	MG	1A	3781	1/1	0.87	0.22	61,61,61,61	0
54	MG	1A	3937	1/1	0.87	0.09	80,80,80,80	0
54	MG	2a	1609	1/1	0.87	0.16	65,65,65,65	0
54	MG	2a	1611	1/1	0.87	0.19	63,63,63,63	0
57	MPD	1A	4036	8/8	0.87	0.23	42,53,63,65	0
54	MG	1a	1659	1/1	0.87	0.16	53,53,53,53	0
54	MG	1A	3097	1/1	0.87	0.17	37,37,37,37	0
54	MG	1a	1836	1/1	0.88	0.18	64,64,64,64	0
54	MG	1B	220	1/1	0.88	0.10	54,54,54,54	0
54	MG	1A	3969	1/1	0.88	0.09	61,61,61,61	0
54	MG	1a	1672	1/1	0.88	0.18	65,65,65,65	0
54	MG	2A	3413	1/1	0.88	0.19	66,66,66,66	0
54	MG	2A	3162	1/1	0.88	0.21	66,66,66,66	0
54	MG	1A	3422	1/1	0.88	0.17	42,42,42,42	0
54	MG	2A	3433	1/1	0.88	0.10	64,64,64,64	0
54	MG	2G	3002	1/1	0.88	0.17	72,72,72,72	0
54	MG	1A	3561	1/1	0.88	0.11	64,64,64,64	0
54	MG	2A	3438	1/1	0.88	0.19	67,67,67,67	0
54	MG	1a	1693	1/1	0.88	0.18	66,66,66,66	0
54	MG	1A	3120	1/1	0.88	0.12	53,53,53,53	0
54	MG	2A	3452	1/1	0.88	0.16	63,63,63,63	0
54	MG	1A	3508	1/1	0.88	0.12	54,54,54,54	0
54	MG	2A	3459	1/1	0.88	0.15	57,57,57,57	0
54	MG	1A	3916	1/1	0.88	0.13	56,56,56,56	0
54	MG	1A	3983	1/1	0.88	0.09	66,66,66,66	0
54	MG	2a	1601	1/1	0.88	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3180	1/1	0.88	0.32	56,56,56,56	0
54	MG	1A	3429	1/1	0.88	0.20	37,37,37,37	0
54	MG	2A	3186	1/1	0.88	0.22	42,42,42,42	0
54	MG	1a	1712	1/1	0.88	0.15	51,51,51,51	0
54	MG	2a	1607	1/1	0.88	0.09	65,65,65,65	0
54	MG	1A	3586	1/1	0.88	0.17	39,39,39,39	0
54	MG	2A	3199	1/1	0.88	0.20	49,49,49,49	0
54	MG	2A	3200	1/1	0.88	0.09	50,50,50,50	0
54	MG	1A	3589	1/1	0.88	0.21	58,58,58,58	0
54	MG	1e	3001	1/1	0.88	0.15	65,65,65,65	0
54	MG	1A	3225	1/1	0.88	0.36	51,51,51,51	0
54	MG	1A	3931	1/1	0.88	0.10	71,71,71,71	0
54	MG	1h	3002	1/1	0.88	0.17	74,74,74,74	0
54	MG	2a	1628	1/1	0.88	0.07	83,83,83,83	0
54	MG	1A	3079	1/1	0.88	0.38	36,36,36,36	0
54	MG	1U	201	1/1	0.88	0.17	34,34,34,34	0
54	MG	1p	8001	1/1	0.88	0.23	64,64,64,64	0
54	MG	1A	3935	1/1	0.88	0.15	67,67,67,67	0
54	MG	1A	3598	1/1	0.88	0.23	64,64,64,64	0
54	MG	1a	1746	1/1	0.88	0.13	70,70,70,70	0
54	MG	2a	1641	1/1	0.88	0.14	78,78,78,78	0
54	MG	1A	3351	1/1	0.88	0.20	22,22,22,22	0
54	MG	2a	1645	1/1	0.88	0.08	71,71,71,71	0
54	MG	2a	1648	1/1	0.88	0.17	65,65,65,65	0
54	MG	1A	3600	1/1	0.88	0.14	56,56,56,56	0
54	MG	2A	3608	1/1	0.88	0.22	70,70,70,70	0
54	MG	1A	3602	1/1	0.88	0.18	40,40,40,40	0
54	MG	1A	3998	1/1	0.88	0.18	58,58,58,58	0
54	MG	2A	3019	1/1	0.88	0.16	65,65,65,65	0
54	MG	2A	3248	1/1	0.88	0.11	48,48,48,48	0
54	MG	2A	3622	1/1	0.88	0.29	67,67,67,67	0
54	MG	2A	3022	1/1	0.88	0.34	52,52,52,52	0
54	MG	2A	3251	1/1	0.88	0.21	33,33,33,33	0
54	MG	2a	1685	1/1	0.88	0.12	70,70,70,70	0
54	MG	2a	1692	1/1	0.88	0.25	65,65,65,65	0
54	MG	1A	3130	1/1	0.88	0.12	55,55,55,55	0
54	MG	1a	1767	1/1	0.88	0.15	55,55,55,55	0
54	MG	1A	3786	1/1	0.88	0.14	53,53,53,53	0
54	MG	2A	3263	1/1	0.88	0.10	63,63,63,63	0
54	MG	1A	3298	1/1	0.88	0.15	31,31,31,31	0
54	MG	2a	1716	1/1	0.88	0.13	70,70,70,70	0
54	MG	2a	1717	1/1	0.88	0.27	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3271	1/1	0.88	0.21	56,56,56,56	0
54	MG	1A	3948	1/1	0.88	0.10	70,70,70,70	0
54	MG	1A	4025	1/1	0.88	0.15	38,38,38,38	0
54	MG	2A	3278	1/1	0.88	0.20	39,39,39,39	0
54	MG	2a	1727	1/1	0.88	0.22	65,65,65,65	0
54	MG	2A	3054	1/1	0.88	0.27	44,44,44,44	0
54	MG	1a	1780	1/1	0.88	0.10	53,53,53,53	0
54	MG	2A	3649	1/1	0.88	0.09	49,49,49,49	0
54	MG	2A	3651	1/1	0.88	0.16	84,84,84,84	0
54	MG	1A	3032	1/1	0.88	0.27	41,41,41,41	0
54	MG	1a	1622	1/1	0.88	0.13	59,59,59,59	0
54	MG	2A	3324	1/1	0.88	0.30	62,62,62,62	0
54	MG	1a	1629	1/1	0.88	0.12	38,38,38,38	0
54	MG	2a	1753	1/1	0.88	0.15	63,63,63,63	0
54	MG	2a	1754	1/1	0.88	0.10	85,85,85,85	0
54	MG	1a	1789	1/1	0.88	0.17	64,64,64,64	0
54	MG	1a	1631	1/1	0.88	0.21	62,62,62,62	0
54	MG	1A	3391	1/1	0.88	0.19	70,70,70,70	0
54	MG	1A	4040	1/1	0.88	0.17	22,22,22,22	0
54	MG	2A	3083	1/1	0.88	0.12	51,51,51,51	0
54	MG	2A	3084	1/1	0.88	0.11	52,52,52,52	0
54	MG	2A	3359	1/1	0.88	0.16	57,57,57,57	0
54	MG	1B	202	1/1	0.88	0.26	54,54,54,54	0
54	MG	1a	1638	1/1	0.88	0.18	68,68,68,68	0
54	MG	1B	206	1/1	0.88	0.26	42,42,42,42	0
54	MG	1A	3186	1/1	0.88	0.21	36,36,36,36	0
54	MG	2A	3700	1/1	0.88	0.13	49,49,49,49	0
54	MG	1A	3021	1/1	0.88	0.16	43,43,43,43	0
54	MG	1A	3728	1/1	0.88	0.11	62,62,62,62	0
54	MG	2A	3396	1/1	0.88	0.15	54,54,54,54	0
54	MG	1B	217	1/1	0.88	0.11	59,59,59,59	0
54	MG	1a	1658	1/1	0.88	0.21	62,62,62,62	0
54	MG	1A	3731	1/1	0.88	0.13	51,51,51,51	0
54	MG	2A	3455	1/1	0.89	0.23	46,46,46,46	0
54	MG	1A	3256	1/1	0.89	0.24	43,43,43,43	0
54	MG	2A	3023	1/1	0.89	0.08	32,32,32,32	0
54	MG	10	103	1/1	0.89	0.12	42,42,42,42	0
54	MG	2A	3222	1/1	0.89	0.20	66,66,66,66	0
54	MG	2A	3484	1/1	0.89	0.15	46,46,46,46	0
54	MG	1a	1677	1/1	0.89	0.13	57,57,57,57	0
54	MG	2R	202	1/1	0.89	0.18	46,46,46,46	0
54	MG	1a	1793	1/1	0.89	0.17	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1678	1/1	0.89	0.20	54,54,54,54	0
54	MG	2A	3504	1/1	0.89	0.14	52,52,52,52	0
54	MG	2A	3506	1/1	0.89	0.24	60,60,60,60	0
54	MG	2I	8001	1/1	0.89	0.27	59,59,59,59	0
54	MG	2A	3044	1/1	0.89	0.12	72,72,72,72	0
54	MG	2A	3051	1/1	0.89	0.11	54,54,54,54	0
54	MG	1A	3333	1/1	0.89	0.12	60,60,60,60	0
54	MG	2A	3535	1/1	0.89	0.20	56,56,56,56	0
54	MG	2A	3239	1/1	0.89	0.13	61,61,61,61	0
54	MG	1A	3517	1/1	0.89	0.19	56,56,56,56	0
54	MG	1A	4055	1/1	0.89	0.18	34,34,34,34	0
54	MG	2A	3561	1/1	0.89	0.20	52,52,52,52	0
54	MG	1A	3927	1/1	0.89	0.14	27,27,27,27	0
54	MG	1A	3710	1/1	0.89	0.15	36,36,36,36	0
54	MG	2A	3565	1/1	0.89	0.20	35,35,35,35	0
54	MG	2a	1613	1/1	0.89	0.09	44,44,44,44	0
54	MG	2A	3063	1/1	0.89	0.08	45,45,45,45	0
54	MG	1A	3630	1/1	0.89	0.14	44,44,44,44	0
54	MG	2A	3582	1/1	0.89	0.10	65,65,65,65	0
54	MG	2a	1619	1/1	0.89	0.23	57,57,57,57	0
54	MG	1A	3414	1/1	0.89	0.11	34,34,34,34	0
54	MG	1A	3531	1/1	0.89	0.19	61,61,61,61	0
54	MG	1B	216	1/1	0.89	0.15	43,43,43,43	0
54	MG	1a	1718	1/1	0.89	0.19	59,59,59,59	0
54	MG	1a	1613	1/1	0.89	0.10	52,52,52,52	0
54	MG	2A	3592	1/1	0.89	0.22	48,48,48,48	0
54	MG	1A	3071	1/1	0.89	0.13	35,35,35,35	0
54	MG	2A	3603	1/1	0.89	0.13	54,54,54,54	0
54	MG	2A	3604	1/1	0.89	0.23	56,56,56,56	0
54	MG	1a	1725	1/1	0.89	0.11	70,70,70,70	0
54	MG	2A	3085	1/1	0.89	0.20	68,68,68,68	0
54	MG	1a	1727	1/1	0.89	0.18	54,54,54,54	0
54	MG	2A	3616	1/1	0.89	0.10	58,58,58,58	0
54	MG	1a	1841	1/1	0.89	0.06	68,68,68,68	0
54	MG	2A	3305	1/1	0.89	0.24	41,41,41,41	0
54	MG	1A	3187	1/1	0.89	0.16	37,37,37,37	0
54	MG	2a	1659	1/1	0.89	0.12	59,59,59,59	0
54	MG	1A	3475	1/1	0.89	0.16	53,53,53,53	0
54	MG	2A	3317	1/1	0.89	0.20	55,55,55,55	0
54	MG	2A	3629	1/1	0.89	0.36	79,79,79,79	0
54	MG	1A	3046	1/1	0.89	0.26	59,59,59,59	0
54	MG	2A	3631	1/1	0.89	0.42	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3321	1/1	0.89	0.20	39,39,39,39	0
54	MG	1a	1625	1/1	0.89	0.11	55,55,55,55	0
54	MG	1a	1737	1/1	0.89	0.16	63,63,63,63	0
54	MG	1a	1742	1/1	0.89	0.11	80,80,80,80	0
54	MG	1A	3488	1/1	0.89	0.15	57,57,57,57	0
54	MG	2A	3640	1/1	0.89	0.23	68,68,68,68	0
54	MG	1a	1745	1/1	0.89	0.18	78,78,78,78	0
54	MG	1A	3362	1/1	0.89	0.10	48,48,48,48	0
54	MG	2A	3147	1/1	0.89	0.26	57,57,57,57	0
54	MG	1A	3206	1/1	0.89	0.23	43,43,43,43	0
54	MG	2A	3152	1/1	0.89	0.30	70,70,70,70	0
54	MG	1d	505	1/1	0.89	0.15	81,81,81,81	0
54	MG	2A	3158	1/1	0.89	0.14	52,52,52,52	0
54	MG	1A	3612	1/1	0.89	0.16	49,49,49,49	0
54	MG	2A	3653	1/1	0.89	0.38	50,50,50,50	0
54	MG	1f	3001	1/1	0.89	0.18	73,73,73,73	0
54	MG	1B	233	1/1	0.89	0.10	59,59,59,59	0
54	MG	2A	3657	1/1	0.89	0.05	82,82,82,82	0
54	MG	1A	3902	1/1	0.89	0.39	49,49,49,49	0
54	MG	2A	3168	1/1	0.89	0.24	65,65,65,65	0
54	MG	2A	3171	1/1	0.89	0.16	48,48,48,48	0
54	MG	2a	1748	1/1	0.89	0.12	65,65,65,65	0
54	MG	2a	1750	1/1	0.89	0.09	53,53,53,53	0
54	MG	1a	1757	1/1	0.89	0.27	68,68,68,68	0
54	MG	2A	3665	1/1	0.89	0.15	42,42,42,42	0
54	MG	1i	3001	1/1	0.89	0.11	64,64,64,64	0
54	MG	1A	3029	1/1	0.89	0.10	31,31,31,31	0
54	MG	2a	1755	1/1	0.89	0.05	66,66,66,66	0
54	MG	1A	3675	1/1	0.89	0.18	55,55,55,55	0
54	MG	1a	1768	1/1	0.89	0.10	64,64,64,64	0
54	MG	2a	1761	1/1	0.89	0.12	73,73,73,73	0
54	MG	1A	3324	1/1	0.89	0.12	31,31,31,31	0
54	MG	1A	3772	1/1	0.89	0.11	41,41,41,41	0
54	MG	2A	3414	1/1	0.89	0.17	40,40,40,40	0
54	MG	2A	3418	1/1	0.89	0.19	56,56,56,56	0
54	MG	1G	3003	1/1	0.89	0.10	60,60,60,60	0
54	MG	2A	3425	1/1	0.89	0.19	34,34,34,34	0
54	MG	2A	3426	1/1	0.89	0.20	62,62,62,62	0
54	MG	1N	203	1/1	0.89	0.07	50,50,50,50	0
54	MG	2A	3001	1/1	0.89	0.14	48,48,48,48	0
54	MG	1A	4017	1/1	0.89	0.33	52,52,52,52	0
54	MG	1a	1666	1/1	0.89	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3913	1/1	0.89	0.11	42,42,42,42	0
54	MG	2A	3444	1/1	0.89	0.18	37,37,37,37	0
54	MG	2A	3211	1/1	0.89	0.28	62,62,62,62	0
54	MG	1A	3773	1/1	0.89	0.18	31,31,31,31	0
54	MG	2A	3020	1/1	0.89	0.14	58,58,58,58	0
59	ZN	24	501	1/1	0.89	0.04	108,108,108,108	0
54	MG	1a	1854	1/1	0.90	0.26	53,53,53,53	0
54	MG	1A	3967	1/1	0.90	0.28	51,51,51,51	0
54	MG	1A	3260	1/1	0.90	0.24	51,51,51,51	0
54	MG	1D	310	1/1	0.90	0.16	64,64,64,64	0
54	MG	1A	3869	1/1	0.90	0.09	55,55,55,55	0
54	MG	1A	3769	1/1	0.90	0.08	50,50,50,50	0
54	MG	2N	8001	1/1	0.90	0.08	62,62,62,62	0
54	MG	2O	8002	1/1	0.90	0.11	57,57,57,57	0
54	MG	1A	3874	1/1	0.90	0.10	61,61,61,61	0
54	MG	2A	3206	1/1	0.90	0.14	55,55,55,55	0
54	MG	2A	3486	1/1	0.90	0.23	43,43,43,43	0
54	MG	1a	1721	1/1	0.90	0.12	66,66,66,66	0
54	MG	1a	1722	1/1	0.90	0.12	70,70,70,70	0
54	MG	1A	3580	1/1	0.90	0.18	42,42,42,42	0
54	MG	1A	3261	1/1	0.90	0.14	57,57,57,57	0
54	MG	1A	3978	1/1	0.90	0.14	65,65,65,65	0
54	MG	1H	8002	1/1	0.90	0.18	57,57,57,57	0
54	MG	2A	3520	1/1	0.90	0.15	70,70,70,70	0
54	MG	1a	1730	1/1	0.90	0.12	55,55,55,55	0
54	MG	2A	3523	1/1	0.90	0.09	75,75,75,75	0
54	MG	1A	3239	1/1	0.90	0.11	70,70,70,70	0
54	MG	1O	8001	1/1	0.90	0.08	50,50,50,50	0
54	MG	1A	3893	1/1	0.90	0.10	54,54,54,54	0
54	MG	2A	3542	1/1	0.90	0.18	62,62,62,62	0
54	MG	2A	3549	1/1	0.90	0.15	62,62,62,62	0
54	MG	1A	3417	1/1	0.90	0.13	35,35,35,35	0
54	MG	1y	3004	1/1	0.90	0.12	72,72,72,72	0
54	MG	2A	3557	1/1	0.90	0.12	60,60,60,60	0
54	MG	1a	1739	1/1	0.90	0.22	71,71,71,71	0
54	MG	1a	1741	1/1	0.90	0.11	66,66,66,66	0
54	MG	1A	3897	1/1	0.90	0.13	60,60,60,60	0
54	MG	1A	3898	1/1	0.90	0.13	61,61,61,61	0
54	MG	1A	3594	1/1	0.90	0.15	42,42,42,42	0
54	MG	1A	3780	1/1	0.90	0.20	44,44,44,44	0
54	MG	1a	1747	1/1	0.90	0.18	57,57,57,57	0
54	MG	1A	3506	1/1	0.90	0.18	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	13	101	1/1	0.90	0.19	40,40,40,40	0
54	MG	17	101	1/1	0.90	0.12	47,47,47,47	0
54	MG	2A	3039	1/1	0.90	0.15	61,61,61,61	0
54	MG	2a	1638	1/1	0.90	0.24	75,75,75,75	0
54	MG	1A	3674	1/1	0.90	0.24	56,56,56,56	0
54	MG	1A	3908	1/1	0.90	0.17	44,44,44,44	0
54	MG	2A	3594	1/1	0.90	0.17	55,55,55,55	0
54	MG	2a	1642	1/1	0.90	0.17	61,61,61,61	0
54	MG	2A	3598	1/1	0.90	0.09	51,51,51,51	0
54	MG	2a	1644	1/1	0.90	0.09	70,70,70,70	0
54	MG	1a	1758	1/1	0.90	0.12	73,73,73,73	0
54	MG	1a	1760	1/1	0.90	0.11	67,67,67,67	0
54	MG	1a	1763	1/1	0.90	0.10	53,53,53,53	0
54	MG	1A	3420	1/1	0.90	0.15	42,42,42,42	0
54	MG	1A	3266	1/1	0.90	0.09	70,70,70,70	0
54	MG	1A	3332	1/1	0.90	0.10	66,66,66,66	0
54	MG	1a	1769	1/1	0.90	0.18	60,60,60,60	0
54	MG	2A	3301	1/1	0.90	0.16	33,33,33,33	0
54	MG	1A	3697	1/1	0.90	0.12	29,29,29,29	0
54	MG	1A	3267	1/1	0.90	0.13	52,52,52,52	0
54	MG	2a	1675	1/1	0.90	0.15	57,57,57,57	0
54	MG	2A	3311	1/1	0.90	0.20	42,42,42,42	0
54	MG	2a	1678	1/1	0.90	0.18	63,63,63,63	0
54	MG	1A	3702	1/1	0.90	0.12	29,29,29,29	0
54	MG	1A	3432	1/1	0.90	0.13	23,23,23,23	0
54	MG	2a	1687	1/1	0.90	0.25	61,61,61,61	0
54	MG	2A	3318	1/1	0.90	0.26	54,54,54,54	0
54	MG	1A	4003	1/1	0.90	0.34	55,55,55,55	0
54	MG	1A	4004	1/1	0.90	0.12	47,47,47,47	0
54	MG	1A	4011	1/1	0.90	0.21	46,46,46,46	0
54	MG	1A	4015	1/1	0.90	0.12	61,61,61,61	0
54	MG	1A	3177	1/1	0.90	0.34	38,38,38,38	0
54	MG	1A	3104	1/1	0.90	0.55	42,42,42,42	0
54	MG	1A	3445	1/1	0.90	0.12	27,27,27,27	0
54	MG	2a	1721	1/1	0.90	0.10	67,67,67,67	0
54	MG	2A	3345	1/1	0.90	0.11	56,56,56,56	0
54	MG	1A	4028	1/1	0.90	0.12	59,59,59,59	0
54	MG	1A	3226	1/1	0.90	0.21	54,54,54,54	0
54	MG	1A	4032	1/1	0.90	0.09	44,44,44,44	0
54	MG	2A	3103	1/1	0.90	0.27	41,41,41,41	0
54	MG	1A	3144	1/1	0.90	0.12	40,40,40,40	0
54	MG	1A	3730	1/1	0.90	0.18	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3125	1/1	0.90	0.15	31,31,31,31	0
54	MG	2A	3374	1/1	0.90	0.13	54,54,54,54	0
54	MG	2A	3126	1/1	0.90	0.29	49,49,49,49	0
54	MG	2a	1745	1/1	0.90	0.16	64,64,64,64	0
54	MG	1A	4056	1/1	0.90	0.44	32,32,32,32	0
54	MG	2A	3139	1/1	0.90	0.18	63,63,63,63	0
54	MG	1A	4061	1/1	0.90	0.43	41,41,41,41	0
54	MG	1A	3742	1/1	0.90	0.11	73,73,73,73	0
54	MG	1A	3113	1/1	0.90	0.16	35,35,35,35	0
54	MG	2A	3662	1/1	0.90	0.17	65,65,65,65	0
54	MG	1A	3109	1/1	0.90	0.28	35,35,35,35	0
54	MG	2A	3148	1/1	0.90	0.17	60,60,60,60	0
54	MG	1A	3943	1/1	0.90	0.06	66,66,66,66	0
54	MG	1B	212	1/1	0.90	0.10	59,59,59,59	0
54	MG	1A	3307	1/1	0.90	0.15	40,40,40,40	0
54	MG	1A	3635	1/1	0.90	0.13	53,53,53,53	0
54	MG	1A	3399	1/1	0.90	0.09	60,60,60,60	0
54	MG	2A	3416	1/1	0.90	0.20	58,58,58,58	0
54	MG	2A	3163	1/1	0.90	0.15	59,59,59,59	0
54	MG	1A	3481	1/1	0.90	0.18	42,42,42,42	0
54	MG	2A	3696	1/1	0.90	0.12	34,34,34,34	0
54	MG	1a	1683	1/1	0.90	0.14	44,44,44,44	0
54	MG	1A	3857	1/1	0.90	0.18	67,67,67,67	0
54	MG	1a	1689	1/1	0.90	0.11	74,74,74,74	0
54	MG	2A	3431	1/1	0.90	0.53	53,53,53,53	0
54	MG	1A	3567	1/1	0.90	0.20	54,54,54,54	0
54	MG	2a	1784	1/1	0.90	0.14	80,80,80,80	0
54	MG	1A	3860	1/1	0.90	0.21	53,53,53,53	0
54	MG	2f	3001	1/1	0.90	0.14	52,52,52,52	0
54	MG	1a	1850	1/1	0.90	0.19	78,78,78,78	0
54	MG	1A	3570	1/1	0.90	0.23	53,53,53,53	0
57	MPD	1T	205	8/8	0.90	0.26	67,71,75,76	0
57	MPD	1a	1860	8/8	0.90	0.27	50,63,66,67	0
54	MG	1A	3966	1/1	0.90	0.12	70,70,70,70	0
54	MG	2A	3179	1/1	0.90	0.49	42,42,42,42	0
54	MG	2A	3451	1/1	0.90	0.14	70,70,70,70	0
54	MG	1A	3466	1/1	0.91	0.18	16,16,16,16	0
54	MG	2A	3352	1/1	0.91	0.42	57,57,57,57	0
54	MG	1A	3901	1/1	0.91	0.22	35,35,35,35	0
54	MG	1A	3389	1/1	0.91	0.13	47,47,47,47	0
54	MG	1A	3316	1/1	0.91	0.19	67,67,67,67	0
54	MG	1A	3777	1/1	0.91	0.14	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3158	1/1	0.91	0.10	52,52,52,52	0
54	MG	1A	3651	1/1	0.91	0.10	34,34,34,34	0
54	MG	2A	3367	1/1	0.91	0.22	49,49,49,49	0
54	MG	1A	3474	1/1	0.91	0.37	38,38,38,38	0
54	MG	1A	3569	1/1	0.91	0.22	23,23,23,23	0
54	MG	1A	4013	1/1	0.91	0.52	47,47,47,47	0
54	MG	1A	3402	1/1	0.91	0.10	41,41,41,41	0
54	MG	2A	3391	1/1	0.91	0.18	32,32,32,32	0
54	MG	1a	1781	1/1	0.91	0.09	68,68,68,68	0
54	MG	2A	3099	1/1	0.91	0.37	38,38,38,38	0
54	MG	1a	1782	1/1	0.91	0.13	62,62,62,62	0
54	MG	1A	3235	1/1	0.91	0.45	27,27,27,27	0
54	MG	2A	3402	1/1	0.91	0.18	54,54,54,54	0
54	MG	1A	3575	1/1	0.91	0.11	69,69,69,69	0
54	MG	2B	215	1/1	0.91	0.14	90,90,90,90	0
54	MG	1A	4020	1/1	0.91	0.13	43,43,43,43	0
54	MG	1A	4022	1/1	0.91	0.14	37,37,37,37	0
54	MG	2B	221	1/1	0.91	0.13	62,62,62,62	0
54	MG	2D	304	1/1	0.91	0.51	52,52,52,52	0
54	MG	1A	3578	1/1	0.91	0.16	44,44,44,44	0
54	MG	1A	3922	1/1	0.91	0.14	67,67,67,67	0
54	MG	1A	3579	1/1	0.91	0.15	55,55,55,55	0
54	MG	1A	3413	1/1	0.91	0.21	15,15,15,15	0
54	MG	1A	3035	1/1	0.91	0.28	30,30,30,30	0
54	MG	1A	3801	1/1	0.91	0.16	57,57,57,57	0
54	MG	1A	3681	1/1	0.91	0.32	67,67,67,67	0
54	MG	2I	3001	1/1	0.91	0.10	60,60,60,60	0
54	MG	2A	3420	1/1	0.91	0.21	40,40,40,40	0
54	MG	2A	3424	1/1	0.91	0.16	57,57,57,57	0
54	MG	1a	1816	1/1	0.91	0.10	61,61,61,61	0
54	MG	2A	3151	1/1	0.91	0.19	61,61,61,61	0
54	MG	2A	3427	1/1	0.91	0.18	54,54,54,54	0
54	MG	2T	3002	1/1	0.91	0.09	69,69,69,69	0
54	MG	1A	3689	1/1	0.91	0.23	47,47,47,47	0
54	MG	1A	3072	1/1	0.91	0.39	34,34,34,34	0
54	MG	1A	3211	1/1	0.91	0.10	60,60,60,60	0
54	MG	1B	204	1/1	0.91	0.35	62,62,62,62	0
54	MG	1A	3212	1/1	0.91	0.19	46,46,46,46	0
54	MG	1A	3172	1/1	0.91	0.42	48,48,48,48	0
54	MG	2A	3165	1/1	0.91	0.45	50,50,50,50	0
54	MG	1A	3703	1/1	0.91	0.19	17,17,17,17	0
54	MG	2A	3448	1/1	0.91	0.38	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3707	1/1	0.91	0.21	44,44,44,44	0
54	MG	1a	1670	1/1	0.91	0.17	70,70,70,70	0
54	MG	1A	3050	1/1	0.91	0.39	40,40,40,40	0
54	MG	1a	1673	1/1	0.91	0.14	60,60,60,60	0
54	MG	1A	3838	1/1	0.91	0.09	49,49,49,49	0
54	MG	1A	3514	1/1	0.91	0.10	47,47,47,47	0
54	MG	1A	3843	1/1	0.91	0.10	48,48,48,48	0
54	MG	2A	3471	1/1	0.91	0.25	37,37,37,37	0
54	MG	2A	3472	1/1	0.91	0.18	58,58,58,58	0
54	MG	2A	3477	1/1	0.91	0.23	58,58,58,58	0
54	MG	1A	3359	1/1	0.91	0.17	20,20,20,20	0
54	MG	1a	1847	1/1	0.91	0.15	77,77,77,77	0
54	MG	2A	3182	1/1	0.91	0.08	48,48,48,48	0
54	MG	1A	3845	1/1	0.91	0.17	53,53,53,53	0
54	MG	2a	1623	1/1	0.91	0.14	70,70,70,70	0
54	MG	2a	1624	1/1	0.91	0.14	61,61,61,61	0
54	MG	1A	3715	1/1	0.91	0.23	49,49,49,49	0
54	MG	2A	3192	1/1	0.91	0.66	34,34,34,34	0
54	MG	2A	3193	1/1	0.91	0.45	39,39,39,39	0
54	MG	1a	1690	1/1	0.91	0.13	51,51,51,51	0
54	MG	2A	3507	1/1	0.91	0.30	63,63,63,63	0
54	MG	1a	1691	1/1	0.91	0.15	41,41,41,41	0
54	MG	1a	1692	1/1	0.91	0.20	60,60,60,60	0
54	MG	1A	3176	1/1	0.91	0.43	32,32,32,32	0
54	MG	1A	3136	1/1	0.91	0.14	27,27,27,27	0
54	MG	1a	1699	1/1	0.91	0.11	57,57,57,57	0
54	MG	1A	3725	1/1	0.91	0.20	61,61,61,61	0
54	MG	2A	3536	1/1	0.91	0.07	56,56,56,56	0
54	MG	1B	231	1/1	0.91	0.15	68,68,68,68	0
54	MG	1A	3521	1/1	0.91	0.13	50,50,50,50	0
54	MG	2A	3544	1/1	0.91	0.36	52,52,52,52	0
54	MG	1A	3729	1/1	0.91	0.13	31,31,31,31	0
54	MG	1f	3002	1/1	0.91	0.13	54,54,54,54	0
54	MG	1a	1711	1/1	0.91	0.18	45,45,45,45	0
54	MG	1D	311	1/1	0.91	0.18	53,53,53,53	0
54	MG	2A	3559	1/1	0.91	0.21	43,43,43,43	0
54	MG	2a	1666	1/1	0.91	0.13	67,67,67,67	0
54	MG	2a	1667	1/1	0.91	0.19	46,46,46,46	0
54	MG	1h	3001	1/1	0.91	0.19	46,46,46,46	0
54	MG	2A	3562	1/1	0.91	0.12	59,59,59,59	0
54	MG	1A	3971	1/1	0.91	0.08	65,65,65,65	0
54	MG	1a	1717	1/1	0.91	0.21	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3522	1/1	0.91	0.18	47,47,47,47	0
54	MG	2A	3573	1/1	0.91	0.23	49,49,49,49	0
54	MG	2A	3574	1/1	0.91	0.31	50,50,50,50	0
54	MG	1F	301	1/1	0.91	0.21	47,47,47,47	0
54	MG	1A	3036	1/1	0.91	0.17	50,50,50,50	0
54	MG	2a	1697	1/1	0.91	0.17	57,57,57,57	0
54	MG	2a	1700	1/1	0.91	0.23	62,62,62,62	0
54	MG	1A	3436	1/1	0.91	0.20	39,39,39,39	0
54	MG	2A	3238	1/1	0.91	0.12	57,57,57,57	0
54	MG	1A	3533	1/1	0.91	0.30	69,69,69,69	0
54	MG	2A	3585	1/1	0.91	0.24	65,65,65,65	0
54	MG	1A	3621	1/1	0.91	0.09	44,44,44,44	0
54	MG	2a	1715	1/1	0.91	0.08	75,75,75,75	0
54	MG	2A	3589	1/1	0.91	0.13	66,66,66,66	0
54	MG	1H	8001	1/1	0.91	0.20	62,62,62,62	0
54	MG	1A	3535	1/1	0.91	0.18	44,44,44,44	0
54	MG	1a	1729	1/1	0.91	0.17	63,63,63,63	0
54	MG	1H	8003	1/1	0.91	0.13	41,41,41,41	0
54	MG	1A	3626	1/1	0.91	0.17	41,41,41,41	0
54	MG	2a	1725	1/1	0.91	0.21	63,63,63,63	0
54	MG	1A	3370	1/1	0.91	0.15	40,40,40,40	0
54	MG	2A	3255	1/1	0.91	0.20	59,59,59,59	0
54	MG	2A	3257	1/1	0.91	0.25	47,47,47,47	0
54	MG	2A	3258	1/1	0.91	0.13	45,45,45,45	0
54	MG	2A	3260	1/1	0.91	0.09	41,41,41,41	0
54	MG	2a	1735	1/1	0.91	0.10	60,60,60,60	0
54	MG	2a	1736	1/1	0.91	0.22	63,63,63,63	0
54	MG	1P	201	1/1	0.91	0.38	32,32,32,32	0
54	MG	1A	3372	1/1	0.91	0.17	18,18,18,18	0
54	MG	1R	201	1/1	0.91	0.15	54,54,54,54	0
54	MG	1A	3057	1/1	0.91	0.14	42,42,42,42	0
54	MG	2A	3026	1/1	0.91	0.14	34,34,34,34	0
54	MG	1A	3634	1/1	0.91	0.23	27,27,27,27	0
54	MG	2A	3625	1/1	0.91	0.11	66,66,66,66	0
54	MG	2A	3626	1/1	0.91	0.51	69,69,69,69	0
54	MG	2A	3276	1/1	0.91	0.18	45,45,45,45	0
54	MG	2A	3628	1/1	0.91	0.24	68,68,68,68	0
54	MG	2A	3032	1/1	0.91	0.16	44,44,44,44	0
54	MG	1T	204	1/1	0.91	0.07	67,67,67,67	0
54	MG	2A	3280	1/1	0.91	0.21	61,61,61,61	0
54	MG	2A	3282	1/1	0.91	0.16	50,50,50,50	0
54	MG	1A	3989	1/1	0.91	0.15	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3294	1/1	0.91	0.15	29,29,29,29	0
54	MG	2A	3298	1/1	0.91	0.14	33,33,33,33	0
54	MG	1U	203	1/1	0.91	0.15	50,50,50,50	0
54	MG	2A	3302	1/1	0.91	0.12	67,67,67,67	0
54	MG	1W	3001	1/1	0.91	0.32	42,42,42,42	0
54	MG	2A	3306	1/1	0.91	0.16	48,48,48,48	0
54	MG	1a	1748	1/1	0.91	0.11	64,64,64,64	0
54	MG	2A	3046	1/1	0.91	0.12	40,40,40,40	0
54	MG	1X	101	1/1	0.91	0.14	67,67,67,67	0
54	MG	1a	1751	1/1	0.91	0.13	63,63,63,63	0
54	MG	1A	3895	1/1	0.91	0.14	27,27,27,27	0
54	MG	1A	3385	1/1	0.91	0.21	27,27,27,27	0
54	MG	1A	3463	1/1	0.91	0.17	17,17,17,17	0
54	MG	1A	3899	1/1	0.91	0.07	49,49,49,49	0
54	MG	13	102	1/1	0.91	0.30	59,59,59,59	0
54	MG	2A	3064	1/1	0.91	0.45	50,50,50,50	0
54	MG	2A	3337	1/1	0.91	0.18	42,42,42,42	0
54	MG	2A	3659	1/1	0.91	0.56	78,78,78,78	0
57	MPD	2A	3693	8/8	0.91	0.17	51,60,65,68	0
54	MG	1a	1759	1/1	0.91	0.30	65,65,65,65	0
54	MG	2A	3070	1/1	0.91	0.24	43,43,43,43	0
54	MG	2A	3703	1/1	0.92	0.23	41,41,41,41	0
54	MG	1A	3468	1/1	0.92	0.23	51,51,51,51	0
54	MG	2A	3197	1/1	0.92	0.14	66,66,66,66	0
54	MG	1A	3661	1/1	0.92	0.12	54,54,54,54	0
54	MG	1A	3151	1/1	0.92	0.49	37,37,37,37	0
54	MG	2B	207	1/1	0.92	0.16	56,56,56,56	0
54	MG	1A	3665	1/1	0.92	0.18	40,40,40,40	0
54	MG	1n	503	1/1	0.92	0.16	58,58,58,58	0
54	MG	10	102	1/1	0.92	0.07	45,45,45,45	0
54	MG	1A	4012	1/1	0.92	0.08	41,41,41,41	0
54	MG	2B	216	1/1	0.92	0.16	67,67,67,67	0
54	MG	1a	1738	1/1	0.92	0.06	72,72,72,72	0
54	MG	2B	219	1/1	0.92	0.11	73,73,73,73	0
54	MG	1A	3571	1/1	0.92	0.14	47,47,47,47	0
54	MG	2A	3215	1/1	0.92	0.23	55,55,55,55	0
54	MG	2A	3458	1/1	0.92	0.26	58,58,58,58	0
54	MG	2D	305	1/1	0.92	0.35	40,40,40,40	0
54	MG	2D	306	1/1	0.92	0.21	32,32,32,32	0
54	MG	1A	3793	1/1	0.92	0.17	49,49,49,49	0
54	MG	1A	3387	1/1	0.92	0.12	45,45,45,45	0
54	MG	2A	3464	1/1	0.92	0.18	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3155	1/1	0.92	0.12	58,58,58,58	0
54	MG	2A	3467	1/1	0.92	0.14	62,62,62,62	0
54	MG	2A	3221	1/1	0.92	0.15	52,52,52,52	0
54	MG	14	502	1/1	0.92	0.11	67,67,67,67	0
54	MG	2A	3475	1/1	0.92	0.28	62,62,62,62	0
54	MG	15	104	1/1	0.92	0.18	71,71,71,71	0
54	MG	2O	8001	1/1	0.92	0.12	64,64,64,64	0
54	MG	1A	4019	1/1	0.92	0.09	48,48,48,48	0
54	MG	1A	3390	1/1	0.92	0.09	54,54,54,54	0
54	MG	1A	3477	1/1	0.92	0.11	36,36,36,36	0
54	MG	2A	3488	1/1	0.92	0.35	52,52,52,52	0
54	MG	2T	3001	1/1	0.92	0.21	58,58,58,58	0
54	MG	2A	3489	1/1	0.92	0.28	54,54,54,54	0
54	MG	2A	3493	1/1	0.92	0.10	53,53,53,53	0
54	MG	1A	3157	1/1	0.92	0.32	36,36,36,36	0
54	MG	1A	3484	1/1	0.92	0.11	48,48,48,48	0
54	MG	2A	3237	1/1	0.92	0.18	49,49,49,49	0
54	MG	1A	3118	1/1	0.92	0.43	30,30,30,30	0
54	MG	1A	3694	1/1	0.92	0.09	27,27,27,27	0
54	MG	2A	3031	1/1	0.92	0.10	57,57,57,57	0
54	MG	2A	3508	1/1	0.92	0.21	53,53,53,53	0
54	MG	2A	3509	1/1	0.92	0.15	47,47,47,47	0
54	MG	1a	1609	1/1	0.92	0.18	55,55,55,55	0
54	MG	2A	3519	1/1	0.92	0.23	38,38,38,38	0
54	MG	1A	3588	1/1	0.92	0.14	49,49,49,49	0
54	MG	1A	3159	1/1	0.92	0.18	43,43,43,43	0
54	MG	1A	4043	1/1	0.92	0.35	30,30,30,30	0
54	MG	2A	3525	1/1	0.92	0.20	42,42,42,42	0
54	MG	1A	4050	1/1	0.92	0.29	27,27,27,27	0
54	MG	2A	3533	1/1	0.92	0.19	53,53,53,53	0
54	MG	1A	3489	1/1	0.92	0.19	58,58,58,58	0
54	MG	1a	1621	1/1	0.92	0.15	44,44,44,44	0
54	MG	2A	3047	1/1	0.92	0.11	55,55,55,55	0
54	MG	2A	3539	1/1	0.92	0.17	57,57,57,57	0
54	MG	1A	3406	1/1	0.92	0.09	45,45,45,45	0
54	MG	1A	3066	1/1	0.92	0.48	29,29,29,29	0
54	MG	1A	4064	1/1	0.92	0.08	40,40,40,40	0
54	MG	1B	201	1/1	0.92	0.58	38,38,38,38	0
54	MG	1A	3946	1/1	0.92	0.10	75,75,75,75	0
54	MG	2A	3554	1/1	0.92	0.15	61,61,61,61	0
54	MG	1A	3319	1/1	0.92	0.16	41,41,41,41	0
54	MG	1A	3034	1/1	0.92	0.20	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3002	1/1	0.92	0.14	44,44,44,44	0
54	MG	1A	3330	1/1	0.92	0.14	39,39,39,39	0
54	MG	1a	1783	1/1	0.92	0.13	68,68,68,68	0
54	MG	1A	3015	1/1	0.92	0.21	55,55,55,55	0
54	MG	1a	1647	1/1	0.92	0.18	51,51,51,51	0
54	MG	2A	3570	1/1	0.92	0.21	68,68,68,68	0
54	MG	2A	3075	1/1	0.92	0.20	46,46,46,46	0
54	MG	1A	3606	1/1	0.92	0.20	36,36,36,36	0
54	MG	1a	1650	1/1	0.92	0.21	35,35,35,35	0
54	MG	2a	1646	1/1	0.92	0.16	59,59,59,59	0
54	MG	1B	214	1/1	0.92	0.08	47,47,47,47	0
54	MG	1A	3055	1/1	0.92	0.28	39,39,39,39	0
54	MG	1a	1657	1/1	0.92	0.12	59,59,59,59	0
54	MG	1A	3961	1/1	0.92	0.15	61,61,61,61	0
54	MG	1a	1801	1/1	0.92	0.11	61,61,61,61	0
54	MG	2A	3586	1/1	0.92	0.22	51,51,51,51	0
54	MG	1A	3854	1/1	0.92	0.11	64,64,64,64	0
54	MG	1a	1803	1/1	0.92	0.11	78,78,78,78	0
54	MG	2A	3314	1/1	0.92	0.18	41,41,41,41	0
54	MG	1a	1663	1/1	0.92	0.20	53,53,53,53	0
54	MG	1A	3610	1/1	0.92	0.08	55,55,55,55	0
54	MG	1A	3040	1/1	0.92	0.23	51,51,51,51	0
54	MG	2a	1676	1/1	0.92	0.10	57,57,57,57	0
54	MG	2A	3595	1/1	0.92	0.19	48,48,48,48	0
54	MG	2A	3112	1/1	0.92	0.21	40,40,40,40	0
54	MG	1A	3426	1/1	0.92	0.19	43,43,43,43	0
54	MG	2a	1680	1/1	0.92	0.10	50,50,50,50	0
54	MG	2a	1681	1/1	0.92	0.12	71,71,71,71	0
54	MG	1a	1820	1/1	0.92	0.24	58,58,58,58	0
54	MG	2A	3326	1/1	0.92	0.23	44,44,44,44	0
54	MG	2a	1690	1/1	0.92	0.12	62,62,62,62	0
54	MG	2A	3605	1/1	0.92	0.13	52,52,52,52	0
54	MG	1B	224	1/1	0.92	0.17	49,49,49,49	0
54	MG	1A	3428	1/1	0.92	0.18	17,17,17,17	0
54	MG	2a	1701	1/1	0.92	0.11	63,63,63,63	0
54	MG	2A	3611	1/1	0.92	0.22	55,55,55,55	0
54	MG	2A	3336	1/1	0.92	0.16	54,54,54,54	0
54	MG	2A	3130	1/1	0.92	0.39	39,39,39,39	0
54	MG	2a	1712	1/1	0.92	0.19	63,63,63,63	0
54	MG	1A	3620	1/1	0.92	0.19	32,32,32,32	0
54	MG	2A	3619	1/1	0.92	0.18	68,68,68,68	0
54	MG	1B	228	1/1	0.92	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3344	1/1	0.92	0.21	42,42,42,42	0
54	MG	1B	229	1/1	0.92	0.12	63,63,63,63	0
54	MG	2A	3351	1/1	0.92	0.12	36,36,36,36	0
54	MG	1A	3743	1/1	0.92	0.17	26,26,26,26	0
54	MG	2A	3143	1/1	0.92	0.11	58,58,58,58	0
54	MG	1A	3523	1/1	0.92	0.16	29,29,29,29	0
54	MG	1A	3623	1/1	0.92	0.11	66,66,66,66	0
54	MG	2A	3356	1/1	0.92	0.52	45,45,45,45	0
54	MG	1D	307	1/1	0.92	0.45	66,66,66,66	0
54	MG	1A	3871	1/1	0.92	0.15	41,41,41,41	0
54	MG	1A	3337	1/1	0.92	0.12	47,47,47,47	0
54	MG	2A	3634	1/1	0.92	0.08	68,68,68,68	0
54	MG	1A	3981	1/1	0.92	0.09	53,53,53,53	0
54	MG	2A	3368	1/1	0.92	0.10	41,41,41,41	0
54	MG	2a	1737	1/1	0.92	0.10	68,68,68,68	0
54	MG	2A	3369	1/1	0.92	0.10	62,62,62,62	0
54	MG	1A	3234	1/1	0.92	0.26	26,26,26,26	0
54	MG	1a	1844	1/1	0.92	0.09	65,65,65,65	0
54	MG	2A	3161	1/1	0.92	0.19	46,46,46,46	0
54	MG	2A	3643	1/1	0.92	0.12	62,62,62,62	0
54	MG	2a	1749	1/1	0.92	0.09	69,69,69,69	0
54	MG	1A	3138	1/1	0.92	0.20	38,38,38,38	0
54	MG	1A	3272	1/1	0.92	0.18	42,42,42,42	0
54	MG	1A	3361	1/1	0.92	0.20	45,45,45,45	0
54	MG	2A	3394	1/1	0.92	0.16	51,51,51,51	0
54	MG	1A	3438	1/1	0.92	0.14	25,25,25,25	0
54	MG	1A	3542	1/1	0.92	0.10	49,49,49,49	0
54	MG	1A	3059	1/1	0.92	0.12	33,33,33,33	0
54	MG	2A	3401	1/1	0.92	0.10	55,55,55,55	0
54	MG	2a	1760	1/1	0.92	0.12	66,66,66,66	0
54	MG	1A	3771	1/1	0.92	0.11	34,34,34,34	0
54	MG	1A	3448	1/1	0.92	0.13	44,44,44,44	0
54	MG	1N	202	1/1	0.92	0.10	60,60,60,60	0
54	MG	1b	3001	1/1	0.92	0.20	68,68,68,68	0
54	MG	2a	1768	1/1	0.92	0.17	79,79,79,79	0
54	MG	1A	3114	1/1	0.92	0.17	49,49,49,49	0
54	MG	1A	3993	1/1	0.92	0.17	50,50,50,50	0
54	MG	2A	3178	1/1	0.92	0.46	54,54,54,54	0
54	MG	1A	3288	1/1	0.92	0.19	51,51,51,51	0
54	MG	1A	3291	1/1	0.92	0.14	25,25,25,25	0
54	MG	2A	3666	1/1	0.92	0.12	71,71,71,71	0
54	MG	2a	1780	1/1	0.92	0.05	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	1e	3002	1/1	0.92	0.25	58,58,58,58	0
54	MG	2A	3183	1/1	0.92	0.15	53,53,53,53	0
54	MG	1Q	203	1/1	0.92	0.17	35,35,35,35	0
54	MG	2d	301	1/1	0.92	0.08	63,63,63,63	0
54	MG	2A	3671	1/1	0.92	0.29	53,53,53,53	0
54	MG	2A	3673	1/1	0.92	0.39	72,72,72,72	0
54	MG	2A	3422	1/1	0.92	0.09	60,60,60,60	0
54	MG	2A	3185	1/1	0.92	0.12	57,57,57,57	0
54	MG	1A	3248	1/1	0.92	0.16	45,45,45,45	0
57	MPD	18	102	8/8	0.92	0.28	22,38,39,47	0
54	MG	2A	3685	1/1	0.92	0.26	42,42,42,42	0
54	MG	2A	3190	1/1	0.92	0.36	38,38,38,38	0
54	MG	1A	3295	1/1	0.92	0.18	28,28,28,28	0
57	MPD	2B	222	8/8	0.92	0.19	62,67,73,77	0
54	MG	1A	3380	1/1	0.92	0.20	23,23,23,23	0
54	MG	1A	3657	1/1	0.92	0.21	27,27,27,27	0
54	MG	2B	211	1/1	0.93	0.13	71,71,71,71	0
54	MG	1A	3618	1/1	0.93	0.43	59,59,59,59	0
54	MG	2B	214	1/1	0.93	0.12	60,60,60,60	0
54	MG	2A	3015	1/1	0.93	0.73	42,42,42,42	0
54	MG	1A	4023	1/1	0.93	0.17	35,35,35,35	0
54	MG	2A	3469	1/1	0.93	0.31	53,53,53,53	0
54	MG	1A	3924	1/1	0.93	0.14	44,44,44,44	0
54	MG	2A	3021	1/1	0.93	0.09	48,48,48,48	0
54	MG	2A	3473	1/1	0.93	0.16	41,41,41,41	0
54	MG	2A	3474	1/1	0.93	0.24	47,47,47,47	0
54	MG	1A	4027	1/1	0.93	0.43	37,37,37,37	0
54	MG	1A	3802	1/1	0.93	0.13	40,40,40,40	0
54	MG	2A	3478	1/1	0.93	0.27	50,50,50,50	0
54	MG	2A	3480	1/1	0.93	0.05	52,52,52,52	0
54	MG	2A	3025	1/1	0.93	0.18	43,43,43,43	0
54	MG	1A	3706	1/1	0.93	0.18	22,22,22,22	0
54	MG	2A	3485	1/1	0.93	0.12	50,50,50,50	0
54	MG	2A	3230	1/1	0.93	0.20	57,57,57,57	0
54	MG	1A	3805	1/1	0.93	0.16	33,33,33,33	0
54	MG	1A	3371	1/1	0.93	0.17	24,24,24,24	0
54	MG	1A	3227	1/1	0.93	0.34	39,39,39,39	0
54	MG	2A	3240	1/1	0.93	0.11	35,35,35,35	0
54	MG	1A	3485	1/1	0.93	0.22	30,30,30,30	0
54	MG	2A	3037	1/1	0.93	0.15	63,63,63,63	0
54	MG	1A	3624	1/1	0.93	0.14	64,64,64,64	0
54	MG	2A	3247	1/1	0.93	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3041	1/1	0.93	0.14	41,41,41,41	0
54	MG	1A	3813	1/1	0.93	0.14	27,27,27,27	0
54	MG	1A	3374	1/1	0.93	0.25	65,65,65,65	0
54	MG	1a	1617	1/1	0.93	0.15	45,45,45,45	0
54	MG	2X	101	1/1	0.93	0.11	56,56,56,56	0
54	MG	2A	3512	1/1	0.93	0.29	56,56,56,56	0
54	MG	2A	3045	1/1	0.93	0.21	68,68,68,68	0
54	MG	1a	1765	1/1	0.93	0.34	59,59,59,59	0
54	MG	2I	8002	1/1	0.93	0.18	81,81,81,81	0
54	MG	1a	1766	1/1	0.93	0.12	65,65,65,65	0
54	MG	2A	3259	1/1	0.93	0.14	33,33,33,33	0
54	MG	2A	3524	1/1	0.93	0.19	31,31,31,31	0
54	MG	2A	3050	1/1	0.93	0.53	49,49,49,49	0
54	MG	1A	3487	1/1	0.93	0.21	55,55,55,55	0
54	MG	2A	3531	1/1	0.93	0.12	44,44,44,44	0
54	MG	1A	3822	1/1	0.93	0.13	47,47,47,47	0
54	MG	1A	4068	1/1	0.93	0.37	35,35,35,35	0
54	MG	2a	1608	1/1	0.93	0.11	58,58,58,58	0
54	MG	1a	1770	1/1	0.93	0.17	73,73,73,73	0
54	MG	2A	3268	1/1	0.93	0.22	65,65,65,65	0
54	MG	1A	4074	1/1	0.93	0.30	38,38,38,38	0
54	MG	2A	3272	1/1	0.93	0.16	46,46,46,46	0
54	MG	1a	1772	1/1	0.93	0.09	68,68,68,68	0
54	MG	2A	3546	1/1	0.93	0.13	54,54,54,54	0
54	MG	2a	1617	1/1	0.93	0.15	45,45,45,45	0
54	MG	1a	1626	1/1	0.93	0.12	43,43,43,43	0
54	MG	1A	3944	1/1	0.93	0.35	38,38,38,38	0
54	MG	1a	1630	1/1	0.93	0.13	43,43,43,43	0
54	MG	1A	3089	1/1	0.93	0.11	43,43,43,43	0
54	MG	2A	3556	1/1	0.93	0.18	49,49,49,49	0
54	MG	2A	3071	1/1	0.93	0.17	46,46,46,46	0
54	MG	2a	1627	1/1	0.93	0.07	64,64,64,64	0
54	MG	1A	3431	1/1	0.93	0.14	29,29,29,29	0
54	MG	2A	3560	1/1	0.93	0.12	46,46,46,46	0
54	MG	1a	1633	1/1	0.93	0.13	32,32,32,32	0
54	MG	2a	1634	1/1	0.93	0.19	64,64,64,64	0
54	MG	2A	3296	1/1	0.93	0.15	48,48,48,48	0
54	MG	1A	3726	1/1	0.93	0.11	46,46,46,46	0
54	MG	1A	3090	1/1	0.93	0.16	28,28,28,28	0
54	MG	1A	3501	1/1	0.93	0.19	59,59,59,59	0
54	MG	1A	3165	1/1	0.93	0.32	43,43,43,43	0
54	MG	1A	3951	1/1	0.93	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3309	1/1	0.93	0.21	46,46,46,46	0
54	MG	1A	3232	1/1	0.93	0.18	41,41,41,41	0
54	MG	1A	3846	1/1	0.93	0.36	55,55,55,55	0
54	MG	1A	3958	1/1	0.93	0.18	54,54,54,54	0
54	MG	1a	1651	1/1	0.93	0.27	61,61,61,61	0
54	MG	2a	1647	1/1	0.93	0.11	53,53,53,53	0
54	MG	1A	3733	1/1	0.93	0.40	42,42,42,42	0
54	MG	2a	1650	1/1	0.93	0.19	57,57,57,57	0
54	MG	1A	3851	1/1	0.93	0.15	48,48,48,48	0
54	MG	1A	3963	1/1	0.93	0.10	49,49,49,49	0
54	MG	2A	3100	1/1	0.93	0.07	41,41,41,41	0
54	MG	2a	1658	1/1	0.93	0.12	58,58,58,58	0
54	MG	1A	3737	1/1	0.93	0.21	51,51,51,51	0
54	MG	1A	3388	1/1	0.93	0.11	77,77,77,77	0
54	MG	2a	1662	1/1	0.93	0.15	63,63,63,63	0
54	MG	1a	1811	1/1	0.93	0.13	57,57,57,57	0
54	MG	2A	3116	1/1	0.93	0.17	28,28,28,28	0
54	MG	2A	3330	1/1	0.93	0.09	58,58,58,58	0
54	MG	1a	1812	1/1	0.93	0.17	53,53,53,53	0
54	MG	1A	3284	1/1	0.93	0.17	23,23,23,23	0
54	MG	1A	3443	1/1	0.93	0.13	33,33,33,33	0
54	MG	2A	3600	1/1	0.93	0.08	62,62,62,62	0
54	MG	2A	3601	1/1	0.93	0.12	51,51,51,51	0
54	MG	2A	3602	1/1	0.93	0.15	51,51,51,51	0
54	MG	2A	3128	1/1	0.93	0.10	62,62,62,62	0
54	MG	1A	3039	1/1	0.93	0.17	34,34,34,34	0
54	MG	1a	1822	1/1	0.93	0.23	59,59,59,59	0
54	MG	2A	3350	1/1	0.93	0.15	46,46,46,46	0
54	MG	2A	3136	1/1	0.93	0.11	42,42,42,42	0
54	MG	2A	3137	1/1	0.93	0.19	40,40,40,40	0
54	MG	2A	3612	1/1	0.93	0.19	45,45,45,45	0
54	MG	2a	1693	1/1	0.93	0.12	57,57,57,57	0
54	MG	2a	1695	1/1	0.93	0.24	48,48,48,48	0
54	MG	2A	3613	1/1	0.93	0.18	73,73,73,73	0
54	MG	2a	1698	1/1	0.93	0.11	69,69,69,69	0
54	MG	2a	1699	1/1	0.93	0.14	58,58,58,58	0
54	MG	1A	3752	1/1	0.93	0.12	52,52,52,52	0
54	MG	1A	3972	1/1	0.93	0.20	55,55,55,55	0
54	MG	1A	3645	1/1	0.93	0.32	44,44,44,44	0
54	MG	1A	3646	1/1	0.93	0.14	60,60,60,60	0
54	MG	1a	1832	1/1	0.93	0.20	61,61,61,61	0
54	MG	2A	3146	1/1	0.93	0.20	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1674	1/1	0.93	0.11	65,65,65,65	0
54	MG	2A	3364	1/1	0.93	0.17	57,57,57,57	0
54	MG	2A	3366	1/1	0.93	0.12	59,59,59,59	0
54	MG	1A	3976	1/1	0.93	0.09	46,46,46,46	0
54	MG	1D	309	1/1	0.93	0.33	65,65,65,65	0
54	MG	1A	3755	1/1	0.93	0.16	36,36,36,36	0
54	MG	1a	1679	1/1	0.93	0.12	58,58,58,58	0
54	MG	2A	3373	1/1	0.93	0.19	53,53,53,53	0
54	MG	1a	1681	1/1	0.93	0.18	67,67,67,67	0
54	MG	2A	3378	1/1	0.93	0.12	48,48,48,48	0
54	MG	2A	3155	1/1	0.93	0.21	60,60,60,60	0
54	MG	1A	3868	1/1	0.93	0.13	22,22,22,22	0
54	MG	2A	3389	1/1	0.93	0.12	47,47,47,47	0
54	MG	1A	3584	1/1	0.93	0.47	33,33,33,33	0
54	MG	2A	3639	1/1	0.93	0.13	58,58,58,58	0
54	MG	1A	3290	1/1	0.93	0.16	16,16,16,16	0
54	MG	1E	304	1/1	0.93	0.17	26,26,26,26	0
54	MG	1A	3982	1/1	0.93	0.07	54,54,54,54	0
54	MG	2a	1742	1/1	0.93	0.05	59,59,59,59	0
54	MG	1A	3398	1/1	0.93	0.20	36,36,36,36	0
54	MG	1A	3760	1/1	0.93	0.11	29,29,29,29	0
54	MG	1A	3519	1/1	0.93	0.17	16,16,16,16	0
54	MG	1A	3592	1/1	0.93	0.16	54,54,54,54	0
54	MG	1a	1701	1/1	0.93	0.09	66,66,66,66	0
54	MG	2A	3650	1/1	0.93	0.17	82,82,82,82	0
54	MG	1A	3890	1/1	0.93	0.16	60,60,60,60	0
54	MG	1A	3458	1/1	0.93	0.11	35,35,35,35	0
54	MG	1A	3892	1/1	0.93	0.20	55,55,55,55	0
54	MG	1A	3218	1/1	0.93	0.33	30,30,30,30	0
54	MG	1A	3154	1/1	0.93	0.68	40,40,40,40	0
54	MG	1A	3188	1/1	0.93	0.58	32,32,32,32	0
54	MG	2A	3415	1/1	0.93	0.16	60,60,60,60	0
54	MG	1A	3896	1/1	0.93	0.11	49,49,49,49	0
54	MG	1A	3357	1/1	0.93	0.17	16,16,16,16	0
54	MG	1A	3532	1/1	0.93	0.10	38,38,38,38	0
54	MG	2a	1762	1/1	0.93	0.10	92,92,92,92	0
54	MG	1A	3190	1/1	0.93	0.38	30,30,30,30	0
54	MG	1A	3603	1/1	0.93	0.09	63,63,63,63	0
54	MG	2A	3664	1/1	0.93	0.13	61,61,61,61	0
54	MG	1A	3265	1/1	0.93	0.12	77,77,77,77	0
54	MG	2A	3188	1/1	0.93	0.13	67,67,67,67	0
54	MG	1A	3685	1/1	0.93	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3415	1/1	0.93	0.24	63,63,63,63	0
54	MG	2a	1774	1/1	0.93	0.06	67,67,67,67	0
54	MG	1A	3785	1/1	0.93	0.34	36,36,36,36	0
54	MG	1V	202	1/1	0.93	0.08	52,52,52,52	0
54	MG	1A	3540	1/1	0.93	0.20	43,43,43,43	0
54	MG	2A	3674	1/1	0.93	0.14	52,52,52,52	0
54	MG	1W	3002	1/1	0.93	0.18	43,43,43,43	0
54	MG	2A	3437	1/1	0.93	0.25	58,58,58,58	0
54	MG	1W	3003	1/1	0.93	0.17	48,48,48,48	0
54	MG	2A	3439	1/1	0.93	0.22	59,59,59,59	0
54	MG	1A	3242	1/1	0.93	0.11	56,56,56,56	0
54	MG	2A	3202	1/1	0.93	0.18	60,60,60,60	0
54	MG	1A	3695	1/1	0.93	0.17	59,59,59,59	0
54	MG	2A	3447	1/1	0.93	0.15	44,44,44,44	0
54	MG	1A	3912	1/1	0.93	0.34	50,50,50,50	0
54	MG	1A	3696	1/1	0.93	0.16	50,50,50,50	0
54	MG	1y	3002	1/1	0.93	0.12	56,56,56,56	0
54	MG	10	105	1/1	0.93	0.13	64,64,64,64	0
54	MG	1A	3792	1/1	0.93	0.12	36,36,36,36	0
54	MG	1A	3246	1/1	0.93	0.52	40,40,40,40	0
54	MG	1A	3312	1/1	0.93	0.18	17,17,17,17	0
54	MG	1A	3269	1/1	0.93	0.22	45,45,45,45	0
54	MG	2A	3383	1/1	0.94	0.25	54,54,54,54	0
54	MG	2A	3384	1/1	0.94	0.11	43,43,43,43	0
54	MG	2A	3386	1/1	0.94	0.09	61,61,61,61	0
54	MG	19	103	1/1	0.94	0.09	62,62,62,62	0
54	MG	1A	3379	1/1	0.94	0.17	45,45,45,45	0
54	MG	1A	3076	1/1	0.94	0.43	35,35,35,35	0
54	MG	1A	3585	1/1	0.94	0.18	58,58,58,58	0
54	MG	1A	3473	1/1	0.94	0.14	19,19,19,19	0
54	MG	2A	3124	1/1	0.94	0.11	54,54,54,54	0
54	MG	1A	3720	1/1	0.94	0.26	65,65,65,65	0
54	MG	1A	3384	1/1	0.94	0.14	52,52,52,52	0
54	MG	1A	3872	1/1	0.94	0.11	54,54,54,54	0
54	MG	1a	1788	1/1	0.94	0.06	66,66,66,66	0
54	MG	2A	3680	1/1	0.94	0.10	23,23,23,23	0
54	MG	2A	3403	1/1	0.94	0.13	41,41,41,41	0
54	MG	2A	3135	1/1	0.94	0.07	63,63,63,63	0
54	MG	1a	1611	1/1	0.94	0.14	55,55,55,55	0
54	MG	2A	3694	1/1	0.94	0.54	38,38,38,38	0
54	MG	1A	4006	1/1	0.94	0.33	28,28,28,28	0
54	MG	2A	3697	1/1	0.94	0.54	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3408	1/1	0.94	0.11	31,31,31,31	0
54	MG	2A	3702	1/1	0.94	0.27	37,37,37,37	0
54	MG	2A	3138	1/1	0.94	0.13	46,46,46,46	0
54	MG	1a	1791	1/1	0.94	0.06	67,67,67,67	0
54	MG	1A	4007	1/1	0.94	0.35	25,25,25,25	0
54	MG	1A	4009	1/1	0.94	0.14	17,17,17,17	0
54	MG	1A	3183	1/1	0.94	0.77	42,42,42,42	0
54	MG	1a	1798	1/1	0.94	0.08	59,59,59,59	0
54	MG	2B	208	1/1	0.94	0.15	61,61,61,61	0
54	MG	1a	1799	1/1	0.94	0.19	49,49,49,49	0
54	MG	1A	3293	1/1	0.94	0.17	31,31,31,31	0
54	MG	1A	3881	1/1	0.94	0.10	44,44,44,44	0
54	MG	2B	212	1/1	0.94	0.22	65,65,65,65	0
54	MG	2A	3149	1/1	0.94	0.09	51,51,51,51	0
54	MG	1A	3185	1/1	0.94	0.19	43,43,43,43	0
54	MG	1a	1805	1/1	0.94	0.27	52,52,52,52	0
54	MG	1a	1806	1/1	0.94	0.24	63,63,63,63	0
54	MG	2A	3153	1/1	0.94	0.11	49,49,49,49	0
54	MG	1A	3889	1/1	0.94	0.18	54,54,54,54	0
54	MG	1A	3044	1/1	0.94	0.34	22,22,22,22	0
54	MG	2A	3432	1/1	0.94	0.12	56,56,56,56	0
54	MG	1A	3146	1/1	0.94	0.39	47,47,47,47	0
54	MG	2A	3434	1/1	0.94	0.23	44,44,44,44	0
54	MG	1A	3241	1/1	0.94	0.12	31,31,31,31	0
54	MG	2E	302	1/1	0.94	0.16	52,52,52,52	0
54	MG	1a	1815	1/1	0.94	0.09	70,70,70,70	0
54	MG	1A	3038	1/1	0.94	0.11	43,43,43,43	0
54	MG	1a	1817	1/1	0.94	0.20	62,62,62,62	0
54	MG	1A	3020	1/1	0.94	0.39	40,40,40,40	0
54	MG	1A	3601	1/1	0.94	0.21	17,17,17,17	0
54	MG	1A	3740	1/1	0.94	0.22	44,44,44,44	0
54	MG	1A	3401	1/1	0.94	0.16	53,53,53,53	0
54	MG	2A	3169	1/1	0.94	0.14	52,52,52,52	0
54	MG	2A	3449	1/1	0.94	0.09	59,59,59,59	0
54	MG	2A	3450	1/1	0.94	0.20	60,60,60,60	0
54	MG	1a	1635	1/1	0.94	0.07	69,69,69,69	0
54	MG	2Q	3002	1/1	0.94	0.21	54,54,54,54	0
54	MG	1A	3309	1/1	0.94	0.17	28,28,28,28	0
54	MG	1A	3491	1/1	0.94	0.24	48,48,48,48	0
54	MG	1a	1639	1/1	0.94	0.24	59,59,59,59	0
54	MG	2A	3456	1/1	0.94	0.32	58,58,58,58	0
54	MG	1a	1834	1/1	0.94	0.09	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	1a	1640	1/1	0.94	0.19	43,43,43,43	0
54	MG	2A	3460	1/1	0.94	0.11	32,32,32,32	0
54	MG	1A	3495	1/1	0.94	0.14	35,35,35,35	0
54	MG	1A	3499	1/1	0.94	0.10	34,34,34,34	0
54	MG	1a	1645	1/1	0.94	0.14	43,43,43,43	0
54	MG	1A	4041	1/1	0.94	0.58	38,38,38,38	0
54	MG	1A	3086	1/1	0.94	0.14	35,35,35,35	0
54	MG	1a	1649	1/1	0.94	0.06	70,70,70,70	0
54	MG	28	101	1/1	0.94	0.12	59,59,59,59	0
54	MG	1A	4045	1/1	0.94	0.24	32,32,32,32	0
54	MG	1A	3611	1/1	0.94	0.17	37,37,37,37	0
54	MG	1A	3504	1/1	0.94	0.10	56,56,56,56	0
54	MG	1a	1654	1/1	0.94	0.07	64,64,64,64	0
54	MG	1A	3408	1/1	0.94	0.19	37,37,37,37	0
54	MG	1A	4058	1/1	0.94	0.27	37,37,37,37	0
54	MG	2a	1606	1/1	0.94	0.16	59,59,59,59	0
54	MG	1A	3615	1/1	0.94	0.17	58,58,58,58	0
54	MG	1A	4062	1/1	0.94	0.19	40,40,40,40	0
54	MG	2A	3482	1/1	0.94	0.27	46,46,46,46	0
54	MG	2A	3198	1/1	0.94	0.20	43,43,43,43	0
54	MG	1a	1660	1/1	0.94	0.16	60,60,60,60	0
54	MG	1A	3193	1/1	0.94	0.22	29,29,29,29	0
54	MG	2A	3487	1/1	0.94	0.20	46,46,46,46	0
54	MG	1a	1665	1/1	0.94	0.26	51,51,51,51	0
54	MG	2A	3205	1/1	0.94	0.09	44,44,44,44	0
54	MG	2A	3491	1/1	0.94	0.26	43,43,43,43	0
54	MG	1A	3195	1/1	0.94	0.51	34,34,34,34	0
54	MG	1a	1857	1/1	0.94	0.10	50,50,50,50	0
54	MG	1A	3197	1/1	0.94	0.36	38,38,38,38	0
54	MG	2A	3499	1/1	0.94	0.38	54,54,54,54	0
54	MG	2A	3209	1/1	0.94	0.15	49,49,49,49	0
54	MG	2A	3210	1/1	0.94	0.16	45,45,45,45	0
54	MG	1A	3764	1/1	0.94	0.15	52,52,52,52	0
54	MG	2a	1629	1/1	0.94	0.19	66,66,66,66	0
54	MG	2a	1630	1/1	0.94	0.15	78,78,78,78	0
54	MG	1d	503	1/1	0.94	0.12	67,67,67,67	0
54	MG	1A	3917	1/1	0.94	0.13	52,52,52,52	0
54	MG	1B	203	1/1	0.94	0.12	61,61,61,61	0
54	MG	1A	3918	1/1	0.94	0.17	57,57,57,57	0
54	MG	2a	1636	1/1	0.94	0.11	55,55,55,55	0
54	MG	1A	3766	1/1	0.94	0.19	45,45,45,45	0
54	MG	2A	3513	1/1	0.94	0.14	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3517	1/1	0.94	0.21	46,46,46,46	0
54	MG	1A	3198	1/1	0.94	0.24	31,31,31,31	0
54	MG	1B	208	1/1	0.94	0.31	53,53,53,53	0
54	MG	1B	210	1/1	0.94	0.25	49,49,49,49	0
54	MG	1A	3067	1/1	0.94	0.33	30,30,30,30	0
54	MG	1a	1680	1/1	0.94	0.12	55,55,55,55	0
54	MG	1A	3207	1/1	0.94	0.58	39,39,39,39	0
54	MG	2A	3527	1/1	0.94	0.23	70,70,70,70	0
54	MG	1A	3923	1/1	0.94	0.06	42,42,42,42	0
54	MG	1A	3331	1/1	0.94	0.09	35,35,35,35	0
54	MG	1A	3926	1/1	0.94	0.09	47,47,47,47	0
54	MG	1n	502	1/1	0.94	0.12	71,71,71,71	0
54	MG	2A	3235	1/1	0.94	0.14	55,55,55,55	0
54	MG	1A	3518	1/1	0.94	0.30	40,40,40,40	0
54	MG	2a	1657	1/1	0.94	0.14	62,62,62,62	0
54	MG	1A	3421	1/1	0.94	0.18	44,44,44,44	0
54	MG	1A	3014	1/1	0.94	0.45	31,31,31,31	0
54	MG	1A	3041	1/1	0.94	0.26	26,26,26,26	0
54	MG	1A	3262	1/1	0.94	0.43	76,76,76,76	0
54	MG	1A	3524	1/1	0.94	0.20	54,54,54,54	0
54	MG	2A	3550	1/1	0.94	0.14	58,58,58,58	0
54	MG	2A	3244	1/1	0.94	0.13	34,34,34,34	0
54	MG	1A	3525	1/1	0.94	0.15	60,60,60,60	0
54	MG	2a	1670	1/1	0.94	0.16	68,68,68,68	0
54	MG	2A	3553	1/1	0.94	0.18	51,51,51,51	0
54	MG	1B	226	1/1	0.94	0.08	46,46,46,46	0
54	MG	1A	3526	1/1	0.94	0.21	19,19,19,19	0
54	MG	1A	3784	1/1	0.94	0.25	43,43,43,43	0
54	MG	2A	3558	1/1	0.94	0.24	63,63,63,63	0
54	MG	1A	3427	1/1	0.94	0.22	48,48,48,48	0
54	MG	1A	3530	1/1	0.94	0.37	37,37,37,37	0
54	MG	2A	3009	1/1	0.94	0.15	71,71,71,71	0
54	MG	2a	1682	1/1	0.94	0.14	57,57,57,57	0
54	MG	2a	1684	1/1	0.94	0.12	68,68,68,68	0
54	MG	2A	3011	1/1	0.94	0.15	47,47,47,47	0
54	MG	2A	3013	1/1	0.94	0.18	51,51,51,51	0
54	MG	2a	1688	1/1	0.94	0.20	63,63,63,63	0
54	MG	1A	3787	1/1	0.94	0.18	26,26,26,26	0
54	MG	2A	3017	1/1	0.94	0.18	46,46,46,46	0
54	MG	1A	3214	1/1	0.94	0.10	38,38,38,38	0
54	MG	2a	1694	1/1	0.94	0.21	72,72,72,72	0
54	MG	1A	3264	1/1	0.94	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1D	308	1/1	0.94	0.19	37,37,37,37	0
54	MG	1a	1719	1/1	0.94	0.10	52,52,52,52	0
54	MG	1A	3345	1/1	0.94	0.27	34,34,34,34	0
54	MG	2A	3577	1/1	0.94	0.11	48,48,48,48	0
54	MG	2A	3579	1/1	0.94	0.28	56,56,56,56	0
54	MG	2A	3024	1/1	0.94	0.13	55,55,55,55	0
54	MG	1A	3647	1/1	0.94	0.21	32,32,32,32	0
54	MG	1A	3648	1/1	0.94	0.16	34,34,34,34	0
54	MG	1A	3216	1/1	0.94	0.29	42,42,42,42	0
54	MG	2A	3028	1/1	0.94	0.14	62,62,62,62	0
54	MG	2A	3029	1/1	0.94	0.14	63,63,63,63	0
54	MG	1E	301	1/1	0.94	0.07	37,37,37,37	0
54	MG	1A	3536	1/1	0.94	0.14	42,42,42,42	0
54	MG	1A	3160	1/1	0.94	0.22	26,26,26,26	0
54	MG	1A	3539	1/1	0.94	0.17	20,20,20,20	0
54	MG	1F	306	1/1	0.94	0.91	48,48,48,48	0
54	MG	1A	3434	1/1	0.94	0.22	24,24,24,24	0
54	MG	2A	3299	1/1	0.94	0.30	68,68,68,68	0
54	MG	1A	3959	1/1	0.94	0.12	48,48,48,48	0
54	MG	1A	3221	1/1	0.94	0.11	52,52,52,52	0
54	MG	1A	3806	1/1	0.94	0.16	36,36,36,36	0
54	MG	1A	3128	1/1	0.94	0.09	62,62,62,62	0
54	MG	1A	3129	1/1	0.94	0.14	29,29,29,29	0
54	MG	1A	3439	1/1	0.94	0.18	17,17,17,17	0
54	MG	2A	3048	1/1	0.94	0.12	50,50,50,50	0
54	MG	2A	3312	1/1	0.94	0.21	69,69,69,69	0
54	MG	2A	3313	1/1	0.94	0.24	51,51,51,51	0
54	MG	2a	1738	1/1	0.94	0.18	66,66,66,66	0
54	MG	2a	1739	1/1	0.94	0.16	66,66,66,66	0
54	MG	2a	1740	1/1	0.94	0.17	64,64,64,64	0
54	MG	2A	3610	1/1	0.94	0.11	57,57,57,57	0
54	MG	2A	3049	1/1	0.94	0.15	36,36,36,36	0
54	MG	1A	3669	1/1	0.94	0.11	39,39,39,39	0
54	MG	1A	3671	1/1	0.94	0.08	36,36,36,36	0
54	MG	1a	1744	1/1	0.94	0.17	66,66,66,66	0
54	MG	1A	3547	1/1	0.94	0.11	35,35,35,35	0
54	MG	1A	3816	1/1	0.94	0.13	46,46,46,46	0
54	MG	1A	3363	1/1	0.94	0.13	21,21,21,21	0
54	MG	2A	3620	1/1	0.94	0.48	68,68,68,68	0
54	MG	1A	3364	1/1	0.94	0.20	59,59,59,59	0
54	MG	2A	3327	1/1	0.94	0.20	48,48,48,48	0
54	MG	2A	3060	1/1	0.94	0.22	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	2A	3062	1/1	0.94	0.24	47,47,47,47	0
54	MG	1A	3823	1/1	0.94	0.16	29,29,29,29	0
54	MG	2a	1757	1/1	0.94	0.11	74,74,74,74	0
54	MG	2A	3332	1/1	0.94	0.28	52,52,52,52	0
54	MG	1A	3825	1/1	0.94	0.16	16,16,16,16	0
54	MG	1A	3678	1/1	0.94	0.21	24,24,24,24	0
54	MG	1A	3558	1/1	0.94	0.20	27,27,27,27	0
54	MG	2A	3341	1/1	0.94	0.14	35,35,35,35	0
54	MG	1A	3834	1/1	0.94	0.14	12,12,12,12	0
54	MG	1A	3980	1/1	0.94	0.12	47,47,47,47	0
54	MG	1A	3447	1/1	0.94	0.20	47,47,47,47	0
54	MG	1A	3073	1/1	0.94	0.28	33,33,33,33	0
54	MG	1A	3449	1/1	0.94	0.09	45,45,45,45	0
54	MG	2A	3077	1/1	0.94	0.15	71,71,71,71	0
54	MG	1A	3691	1/1	0.94	0.15	23,23,23,23	0
54	MG	2A	3079	1/1	0.94	0.15	66,66,66,66	0
54	MG	1A	3566	1/1	0.94	0.20	42,42,42,42	0
54	MG	2A	3082	1/1	0.94	0.15	40,40,40,40	0
54	MG	1A	3693	1/1	0.94	0.24	60,60,60,60	0
54	MG	1A	3169	1/1	0.94	0.21	37,37,37,37	0
54	MG	1A	3275	1/1	0.94	0.38	40,40,40,40	0
54	MG	1A	3132	1/1	0.94	0.34	48,48,48,48	0
54	MG	1A	3074	1/1	0.94	0.45	45,45,45,45	0
54	MG	1A	3462	1/1	0.94	0.16	49,49,49,49	0
54	MG	2A	3091	1/1	0.94	0.11	48,48,48,48	0
54	MG	2A	3092	1/1	0.94	0.10	60,60,60,60	0
54	MG	1A	3056	1/1	0.94	0.29	43,43,43,43	0
54	MG	2A	3372	1/1	0.94	0.18	55,55,55,55	0
54	MG	1A	3376	1/1	0.94	0.08	60,60,60,60	0
54	MG	1A	3377	1/1	0.94	0.22	23,23,23,23	0
54	MG	2A	3375	1/1	0.94	0.18	52,52,52,52	0
54	MG	1A	3106	1/1	0.94	0.28	30,30,30,30	0
54	MG	2A	3380	1/1	0.94	0.22	60,60,60,60	0
58	ARG	1B	232	12/12	0.94	0.26	29,45,53,55	0
54	MG	2A	3381	1/1	0.94	0.17	29,29,29,29	0
59	ZN	2Y	501	1/1	0.94	0.12	79,79,79,79	0
54	MG	2A	3106	1/1	0.94	0.16	74,74,74,74	0
59	ZN	2n	501	1/1	0.94	0.05	89,89,89,89	0
54	MG	2A	3682	1/1	0.95	0.16	58,58,58,58	0
54	MG	1A	3286	1/1	0.95	0.19	22,22,22,22	0
54	MG	1A	3247	1/1	0.95	0.19	31,31,31,31	0
54	MG	1A	4070	1/1	0.95	0.54	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3423	1/1	0.95	0.37	56,56,56,56	0
54	MG	2A	3695	1/1	0.95	0.37	50,50,50,50	0
54	MG	2A	3170	1/1	0.95	0.07	67,67,67,67	0
54	MG	1A	3529	1/1	0.95	0.22	35,35,35,35	0
54	MG	2A	3698	1/1	0.95	0.15	57,57,57,57	0
54	MG	1A	3761	1/1	0.95	0.22	31,31,31,31	0
54	MG	1A	3135	1/1	0.95	0.15	27,27,27,27	0
54	MG	1A	3365	1/1	0.95	0.15	19,19,19,19	0
54	MG	2B	201	1/1	0.95	0.22	72,72,72,72	0
54	MG	2A	3430	1/1	0.95	0.51	39,39,39,39	0
54	MG	1A	3088	1/1	0.95	0.11	50,50,50,50	0
54	MG	1a	1852	1/1	0.95	0.31	72,72,72,72	0
54	MG	1A	3444	1/1	0.95	0.10	55,55,55,55	0
54	MG	1A	3030	1/1	0.95	0.13	13,13,13,13	0
54	MG	1A	3770	1/1	0.95	0.17	27,27,27,27	0
54	MG	1A	3251	1/1	0.95	0.27	37,37,37,37	0
54	MG	1a	1861	1/1	0.95	0.08	66,66,66,66	0
54	MG	1A	3252	1/1	0.95	0.28	29,29,29,29	0
54	MG	1A	3296	1/1	0.95	0.12	49,49,49,49	0
54	MG	2A	3441	1/1	0.95	0.27	55,55,55,55	0
54	MG	2A	3443	1/1	0.95	0.13	36,36,36,36	0
54	MG	2A	3187	1/1	0.95	0.14	52,52,52,52	0
54	MG	1A	3451	1/1	0.95	0.14	61,61,61,61	0
54	MG	2A	3189	1/1	0.95	0.17	60,60,60,60	0
54	MG	1a	1676	1/1	0.95	0.14	54,54,54,54	0
54	MG	1A	3644	1/1	0.95	0.16	39,39,39,39	0
54	MG	1A	3175	1/1	0.95	0.69	35,35,35,35	0
54	MG	2D	302	1/1	0.95	1.17	44,44,44,44	0
54	MG	2D	303	1/1	0.95	0.25	39,39,39,39	0
54	MG	1A	3457	1/1	0.95	0.15	39,39,39,39	0
54	MG	1e	3003	1/1	0.95	0.39	53,53,53,53	0
54	MG	1A	3375	1/1	0.95	0.14	22,22,22,22	0
54	MG	1A	3459	1/1	0.95	0.14	22,22,22,22	0
54	MG	1A	3299	1/1	0.95	0.23	37,37,37,37	0
54	MG	2A	3457	1/1	0.95	0.18	47,47,47,47	0
54	MG	1A	3301	1/1	0.95	0.16	45,45,45,45	0
54	MG	2A	3201	1/1	0.95	0.12	53,53,53,53	0
54	MG	1A	3938	1/1	0.95	0.14	59,59,59,59	0
54	MG	2A	3203	1/1	0.95	0.15	57,57,57,57	0
54	MG	1A	3655	1/1	0.95	0.19	48,48,48,48	0
54	MG	1A	3302	1/1	0.95	0.13	57,57,57,57	0
54	MG	2A	3466	1/1	0.95	0.29	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3554	1/1	0.95	0.14	48,48,48,48	0
54	MG	2A	3468	1/1	0.95	0.22	56,56,56,56	0
54	MG	2P	8001	1/1	0.95	0.12	52,52,52,52	0
54	MG	2Q	3001	1/1	0.95	0.10	49,49,49,49	0
54	MG	1A	3557	1/1	0.95	0.12	36,36,36,36	0
54	MG	2A	3470	1/1	0.95	0.25	44,44,44,44	0
54	MG	1A	3305	1/1	0.95	0.12	49,49,49,49	0
54	MG	1a	1695	1/1	0.95	0.13	54,54,54,54	0
54	MG	1o	3001	1/1	0.95	0.22	48,48,48,48	0
54	MG	1a	1698	1/1	0.95	0.14	32,32,32,32	0
54	MG	1A	3663	1/1	0.95	0.21	31,31,31,31	0
54	MG	1A	3791	1/1	0.95	0.12	43,43,43,43	0
54	MG	1A	3139	1/1	0.95	0.16	48,48,48,48	0
54	MG	1D	306	1/1	0.95	0.12	43,43,43,43	0
54	MG	1A	3058	1/1	0.95	0.23	48,48,48,48	0
54	MG	1A	3666	1/1	0.95	0.13	28,28,28,28	0
54	MG	1a	1710	1/1	0.95	0.16	59,59,59,59	0
54	MG	1A	3257	1/1	0.95	0.15	48,48,48,48	0
54	MG	1A	3798	1/1	0.95	0.16	27,27,27,27	0
54	MG	1A	3799	1/1	0.95	0.17	29,29,29,29	0
54	MG	1D	312	1/1	0.95	0.50	50,50,50,50	0
54	MG	1A	3952	1/1	0.95	0.17	43,43,43,43	0
54	MG	2A	3490	1/1	0.95	0.28	50,50,50,50	0
54	MG	1A	3117	1/1	0.95	0.12	40,40,40,40	0
54	MG	1E	302	1/1	0.95	0.22	22,22,22,22	0
54	MG	2A	3231	1/1	0.95	0.17	21,21,21,21	0
54	MG	2A	3495	1/1	0.95	0.19	32,32,32,32	0
54	MG	2A	3496	1/1	0.95	0.22	54,54,54,54	0
54	MG	2A	3232	1/1	0.95	0.88	41,41,41,41	0
54	MG	2A	3498	1/1	0.95	0.12	52,52,52,52	0
54	MG	2A	3233	1/1	0.95	0.82	53,53,53,53	0
54	MG	2A	3234	1/1	0.95	0.29	59,59,59,59	0
54	MG	1A	3954	1/1	0.95	0.14	48,48,48,48	0
54	MG	2a	1615	1/1	0.95	0.17	55,55,55,55	0
54	MG	1A	3471	1/1	0.95	0.08	49,49,49,49	0
54	MG	1A	3025	1/1	0.95	0.21	24,24,24,24	0
54	MG	1F	303	1/1	0.95	0.11	35,35,35,35	0
54	MG	1A	3093	1/1	0.95	0.23	51,51,51,51	0
54	MG	1F	307	1/1	0.95	0.10	44,44,44,44	0
54	MG	2a	1621	1/1	0.95	0.12	58,58,58,58	0
54	MG	1F	309	1/1	0.95	0.41	42,42,42,42	0
54	MG	2A	3243	1/1	0.95	0.08	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3095	1/1	0.95	0.27	32,32,32,32	0
54	MG	2a	1625	1/1	0.95	0.11	37,37,37,37	0
54	MG	1a	1731	1/1	0.95	0.16	60,60,60,60	0
54	MG	1A	3122	1/1	0.95	0.43	45,45,45,45	0
54	MG	1a	1733	1/1	0.95	0.13	62,62,62,62	0
54	MG	1A	3962	1/1	0.95	0.23	65,65,65,65	0
54	MG	2A	3030	1/1	0.95	0.17	49,49,49,49	0
54	MG	1A	3395	1/1	0.95	0.11	38,38,38,38	0
54	MG	1A	3965	1/1	0.95	0.14	52,52,52,52	0
54	MG	1A	3680	1/1	0.95	0.12	54,54,54,54	0
54	MG	1A	3577	1/1	0.95	0.07	44,44,44,44	0
54	MG	2A	3532	1/1	0.95	0.24	61,61,61,61	0
54	MG	2A	3038	1/1	0.95	0.13	52,52,52,52	0
54	MG	1A	3682	1/1	0.95	0.13	35,35,35,35	0
54	MG	1A	3684	1/1	0.95	0.20	33,33,33,33	0
54	MG	1A	3479	1/1	0.95	0.16	20,20,20,20	0
54	MG	1A	3687	1/1	0.95	0.17	30,30,30,30	0
54	MG	2A	3540	1/1	0.95	0.28	61,61,61,61	0
54	MG	1A	3322	1/1	0.95	0.16	64,64,64,64	0
54	MG	1A	3323	1/1	0.95	0.15	36,36,36,36	0
54	MG	2A	3545	1/1	0.95	0.20	64,64,64,64	0
54	MG	1Q	204	1/1	0.95	0.20	47,47,47,47	0
54	MG	1A	3062	1/1	0.95	0.09	57,57,57,57	0
54	MG	1A	3975	1/1	0.95	0.10	65,65,65,65	0
54	MG	2A	3275	1/1	0.95	0.16	28,28,28,28	0
54	MG	1A	3583	1/1	0.95	0.23	55,55,55,55	0
54	MG	1A	3327	1/1	0.95	0.11	57,57,57,57	0
54	MG	1A	3829	1/1	0.95	0.10	25,25,25,25	0
54	MG	1A	3830	1/1	0.95	0.16	14,14,14,14	0
54	MG	1A	3405	1/1	0.95	0.16	20,20,20,20	0
54	MG	2A	3288	1/1	0.95	0.13	44,44,44,44	0
54	MG	2A	3291	1/1	0.95	0.14	32,32,32,32	0
54	MG	2a	1663	1/1	0.95	0.11	44,44,44,44	0
54	MG	1V	203	1/1	0.95	0.11	54,54,54,54	0
54	MG	2A	3055	1/1	0.95	0.14	53,53,53,53	0
54	MG	2A	3295	1/1	0.95	0.19	34,34,34,34	0
54	MG	1A	3835	1/1	0.95	0.08	38,38,38,38	0
54	MG	2a	1669	1/1	0.95	0.11	54,54,54,54	0
54	MG	1A	3051	1/1	0.95	0.34	38,38,38,38	0
54	MG	2a	1673	1/1	0.95	0.18	67,67,67,67	0
54	MG	1a	1762	1/1	0.95	0.07	66,66,66,66	0
54	MG	2A	3567	1/1	0.95	0.13	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	1A	3587	1/1	0.95	0.17	34,34,34,34	0
54	MG	2A	3571	1/1	0.95	0.13	53,53,53,53	0
54	MG	2A	3572	1/1	0.95	0.07	66,66,66,66	0
54	MG	1A	3102	1/1	0.95	0.24	34,34,34,34	0
54	MG	2A	3303	1/1	0.95	0.17	40,40,40,40	0
54	MG	1X	102	1/1	0.95	0.17	34,34,34,34	0
54	MG	10	101	1/1	0.95	0.13	46,46,46,46	0
54	MG	2A	3066	1/1	0.95	0.17	45,45,45,45	0
54	MG	2A	3068	1/1	0.95	0.34	41,41,41,41	0
54	MG	2A	3069	1/1	0.95	0.54	45,45,45,45	0
54	MG	1A	3008	1/1	0.95	0.14	34,34,34,34	0
54	MG	1A	3591	1/1	0.95	0.19	47,47,47,47	0
54	MG	1A	3705	1/1	0.95	0.17	36,36,36,36	0
54	MG	1A	3847	1/1	0.95	0.14	31,31,31,31	0
54	MG	11	101	1/1	0.95	0.10	41,41,41,41	0
54	MG	1A	3410	1/1	0.95	0.17	54,54,54,54	0
54	MG	1A	3849	1/1	0.95	0.10	36,36,36,36	0
54	MG	2A	3320	1/1	0.95	0.20	60,60,60,60	0
54	MG	1a	1775	1/1	0.95	0.17	60,60,60,60	0
54	MG	2A	3323	1/1	0.95	0.16	58,58,58,58	0
54	MG	1A	3593	1/1	0.95	0.13	64,64,64,64	0
54	MG	2A	3596	1/1	0.95	0.21	47,47,47,47	0
54	MG	2a	1704	1/1	0.95	0.32	59,59,59,59	0
54	MG	1A	3494	1/1	0.95	0.11	33,33,33,33	0
54	MG	2A	3081	1/1	0.95	0.16	54,54,54,54	0
54	MG	1A	3412	1/1	0.95	0.14	35,35,35,35	0
54	MG	1A	3497	1/1	0.95	0.18	40,40,40,40	0
54	MG	19	101	1/1	0.95	0.08	59,59,59,59	0
54	MG	1A	3713	1/1	0.95	0.19	53,53,53,53	0
54	MG	2A	3333	1/1	0.95	0.21	38,38,38,38	0
54	MG	1A	3856	1/1	0.95	0.10	58,58,58,58	0
54	MG	2a	1719	1/1	0.95	0.08	66,66,66,66	0
54	MG	2A	3606	1/1	0.95	0.36	55,55,55,55	0
54	MG	1A	3162	1/1	0.95	0.42	36,36,36,36	0
54	MG	2A	3338	1/1	0.95	0.17	43,43,43,43	0
54	MG	1A	3999	1/1	0.95	0.27	44,44,44,44	0
54	MG	1A	3717	1/1	0.95	0.18	28,28,28,28	0
54	MG	1A	3238	1/1	0.95	0.38	42,42,42,42	0
54	MG	2A	3093	1/1	0.95	0.12	67,67,67,67	0
54	MG	2a	1728	1/1	0.95	0.17	56,56,56,56	0
54	MG	2a	1729	1/1	0.95	0.20	53,53,53,53	0
54	MG	1A	3334	1/1	0.95	0.16	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3346	1/1	0.95	0.22	52,52,52,52	0
54	MG	2A	3347	1/1	0.95	0.20	32,32,32,32	0
54	MG	2A	3095	1/1	0.95	0.13	57,57,57,57	0
54	MG	2A	3098	1/1	0.95	0.18	42,42,42,42	0
54	MG	1A	3863	1/1	0.95	0.16	54,54,54,54	0
54	MG	1A	3131	1/1	0.95	0.15	62,62,62,62	0
54	MG	1A	3866	1/1	0.95	0.12	24,24,24,24	0
54	MG	1A	3867	1/1	0.95	0.17	26,26,26,26	0
54	MG	2A	3110	1/1	0.95	0.27	52,52,52,52	0
54	MG	2A	3111	1/1	0.95	0.17	59,59,59,59	0
54	MG	1a	1796	1/1	0.95	0.17	61,61,61,61	0
54	MG	1a	1797	1/1	0.95	0.22	63,63,63,63	0
54	MG	1A	3723	1/1	0.95	0.17	61,61,61,61	0
54	MG	2a	1747	1/1	0.95	0.14	73,73,73,73	0
54	MG	2A	3119	1/1	0.95	0.20	49,49,49,49	0
54	MG	1A	3028	1/1	0.95	0.15	32,32,32,32	0
54	MG	1A	3340	1/1	0.95	0.18	34,34,34,34	0
54	MG	1A	3512	1/1	0.95	0.15	48,48,48,48	0
54	MG	1A	3605	1/1	0.95	0.13	52,52,52,52	0
54	MG	2A	3127	1/1	0.95	0.12	58,58,58,58	0
54	MG	1A	3013	1/1	0.95	0.17	17,17,17,17	0
54	MG	2A	3638	1/1	0.95	0.08	53,53,53,53	0
54	MG	1A	3875	1/1	0.95	0.07	48,48,48,48	0
54	MG	1A	3343	1/1	0.95	0.15	17,17,17,17	0
54	MG	2A	3376	1/1	0.95	0.12	57,57,57,57	0
54	MG	2a	1759	1/1	0.95	0.14	68,68,68,68	0
54	MG	2A	3133	1/1	0.95	0.44	48,48,48,48	0
54	MG	1A	3732	1/1	0.95	0.10	56,56,56,56	0
54	MG	1a	1809	1/1	0.95	0.12	50,50,50,50	0
54	MG	1A	3344	1/1	0.95	0.14	20,20,20,20	0
54	MG	1A	3734	1/1	0.95	0.19	73,73,73,73	0
54	MG	1a	1814	1/1	0.95	0.19	56,56,56,56	0
54	MG	2A	3385	1/1	0.95	0.23	61,61,61,61	0
54	MG	1A	3166	1/1	0.95	0.28	38,38,38,38	0
54	MG	1A	4026	1/1	0.95	0.31	48,48,48,48	0
54	MG	1A	3738	1/1	0.95	0.14	45,45,45,45	0
54	MG	1A	3348	1/1	0.95	0.20	21,21,21,21	0
54	MG	1A	3741	1/1	0.95	0.18	44,44,44,44	0
54	MG	1A	3279	1/1	0.95	0.16	20,20,20,20	0
54	MG	2A	3395	1/1	0.95	0.16	29,29,29,29	0
54	MG	1a	1823	1/1	0.95	0.11	65,65,65,65	0
54	MG	1A	3352	1/1	0.95	0.14	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	4037	1/1	0.95	0.30	32,32,32,32	0
54	MG	1a	1641	1/1	0.95	0.19	46,46,46,46	0
54	MG	1A	3745	1/1	0.95	0.24	36,36,36,36	0
54	MG	1A	3520	1/1	0.95	0.22	51,51,51,51	0
54	MG	1A	3750	1/1	0.95	0.11	19,19,19,19	0
54	MG	1A	3617	1/1	0.95	0.20	22,22,22,22	0
54	MG	2t	3001	1/1	0.95	0.15	54,54,54,54	0
56	EZM	2A	3691	24/24	0.95	0.36	38,42,48,51	0
54	MG	2A	3667	1/1	0.95	0.19	62,62,62,62	0
54	MG	2A	3157	1/1	0.95	0.23	66,66,66,66	0
54	MG	1A	3430	1/1	0.95	0.16	14,14,14,14	0
54	MG	2A	3160	1/1	0.95	0.53	54,54,54,54	0
54	MG	1A	3356	1/1	0.95	0.16	18,18,18,18	0
54	MG	2A	3412	1/1	0.95	0.11	57,57,57,57	0
54	MG	1A	3243	1/1	0.95	0.16	60,60,60,60	0
54	MG	1A	3903	1/1	0.95	0.30	38,38,38,38	0
54	MG	1A	3167	1/1	0.95	0.15	53,53,53,53	0
54	MG	1A	3285	1/1	0.95	0.16	57,57,57,57	0
54	MG	1a	1655	1/1	0.95	0.34	61,61,61,61	0
54	MG	2A	3681	1/1	0.95	0.20	37,37,37,37	0
54	MG	2A	3005	1/1	0.96	0.12	43,43,43,43	0
54	MG	2A	3454	1/1	0.96	0.18	58,58,58,58	0
54	MG	2A	3007	1/1	0.96	0.26	44,44,44,44	0
54	MG	1A	3255	1/1	0.96	0.26	51,51,51,51	0
54	MG	1A	3140	1/1	0.96	0.16	26,26,26,26	0
54	MG	2A	3010	1/1	0.96	0.27	37,37,37,37	0
54	MG	1A	3440	1/1	0.96	0.11	46,46,46,46	0
54	MG	1A	3441	1/1	0.96	0.14	18,18,18,18	0
54	MG	1A	3217	1/1	0.96	0.15	42,42,42,42	0
54	MG	2A	3016	1/1	0.96	0.50	45,45,45,45	0
54	MG	1A	3258	1/1	0.96	0.11	47,47,47,47	0
54	MG	2A	3018	1/1	0.96	0.46	54,54,54,54	0
54	MG	1A	3092	1/1	0.96	0.36	35,35,35,35	0
54	MG	1A	3736	1/1	0.96	0.15	26,26,26,26	0
54	MG	1A	3174	1/1	0.96	0.34	40,40,40,40	0
54	MG	1A	3311	1/1	0.96	0.11	26,26,26,26	0
54	MG	1A	3077	1/1	0.96	0.34	30,30,30,30	0
54	MG	1A	3865	1/1	0.96	0.10	22,22,22,22	0
54	MG	1A	3031	1/1	0.96	0.12	46,46,46,46	0
54	MG	1A	3452	1/1	0.96	0.12	36,36,36,36	0
54	MG	1T	203	1/1	0.96	0.07	59,59,59,59	0
54	MG	2A	3476	1/1	0.96	0.20	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3453	1/1	0.96	0.16	38,38,38,38	0
54	MG	1a	1740	1/1	0.96	0.13	66,66,66,66	0
54	MG	1A	3744	1/1	0.96	0.36	30,30,30,30	0
54	MG	1A	3454	1/1	0.96	0.12	44,44,44,44	0
54	MG	1V	201	1/1	0.96	0.14	47,47,47,47	0
54	MG	2A	3483	1/1	0.96	0.23	62,62,62,62	0
54	MG	2A	3033	1/1	0.96	0.07	27,27,27,27	0
54	MG	1A	3631	1/1	0.96	0.25	48,48,48,48	0
54	MG	2A	3036	1/1	0.96	0.14	55,55,55,55	0
54	MG	1A	3047	1/1	0.96	0.13	19,19,19,19	0
54	MG	1A	3873	1/1	0.96	0.09	57,57,57,57	0
54	MG	1A	3381	1/1	0.96	0.17	25,25,25,25	0
54	MG	2A	3249	1/1	0.96	0.18	51,51,51,51	0
54	MG	1A	3179	1/1	0.96	0.16	41,41,41,41	0
54	MG	2A	3492	1/1	0.96	0.14	48,48,48,48	0
54	MG	1a	1749	1/1	0.96	0.20	61,61,61,61	0
54	MG	2A	3252	1/1	0.96	0.14	51,51,51,51	0
54	MG	1A	3877	1/1	0.96	0.11	62,62,62,62	0
54	MG	2A	3254	1/1	0.96	0.12	43,43,43,43	0
54	MG	1A	3080	1/1	0.96	0.19	51,51,51,51	0
54	MG	2W	8002	1/1	0.96	0.23	66,66,66,66	0
54	MG	1Z	8001	1/1	0.96	0.12	54,54,54,54	0
54	MG	1a	1753	1/1	0.96	0.21	57,57,57,57	0
54	MG	2A	3500	1/1	0.96	0.21	43,43,43,43	0
54	MG	2A	3501	1/1	0.96	0.22	38,38,38,38	0
54	MG	2A	3502	1/1	0.96	0.13	61,61,61,61	0
54	MG	23	101	1/1	0.96	0.15	55,55,55,55	0
54	MG	1A	3880	1/1	0.96	0.25	44,44,44,44	0
54	MG	1A	3124	1/1	0.96	0.16	19,19,19,19	0
54	MG	1A	3184	1/1	0.96	0.51	31,31,31,31	0
54	MG	1A	3883	1/1	0.96	0.13	38,38,38,38	0
54	MG	1A	3544	1/1	0.96	0.19	48,48,48,48	0
54	MG	2A	3264	1/1	0.96	0.20	50,50,50,50	0
54	MG	2A	3265	1/1	0.96	0.15	37,37,37,37	0
54	MG	1A	4010	1/1	0.96	0.10	18,18,18,18	0
54	MG	1a	1761	1/1	0.96	0.23	56,56,56,56	0
54	MG	2A	3515	1/1	0.96	0.21	45,45,45,45	0
54	MG	1A	3268	1/1	0.96	0.24	31,31,31,31	0
54	MG	1A	3758	1/1	0.96	0.19	27,27,27,27	0
54	MG	1A	3546	1/1	0.96	0.18	39,39,39,39	0
54	MG	1A	4014	1/1	0.96	0.30	34,34,34,34	0
54	MG	1A	3328	1/1	0.96	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3061	1/1	0.96	0.48	47,47,47,47	0
54	MG	1A	3548	1/1	0.96	0.14	41,41,41,41	0
54	MG	2A	3526	1/1	0.96	0.22	54,54,54,54	0
54	MG	18	101	1/1	0.96	0.22	48,48,48,48	0
54	MG	1A	3762	1/1	0.96	0.14	41,41,41,41	0
54	MG	2A	3285	1/1	0.96	0.16	30,30,30,30	0
54	MG	2A	3286	1/1	0.96	0.17	54,54,54,54	0
54	MG	1A	3464	1/1	0.96	0.20	16,16,16,16	0
54	MG	2A	3290	1/1	0.96	0.16	33,33,33,33	0
54	MG	1A	3650	1/1	0.96	0.15	51,51,51,51	0
54	MG	2A	3292	1/1	0.96	0.25	55,55,55,55	0
54	MG	1A	3550	1/1	0.96	0.14	40,40,40,40	0
54	MG	2a	1626	1/1	0.96	0.14	66,66,66,66	0
54	MG	1A	3551	1/1	0.96	0.22	47,47,47,47	0
54	MG	1a	1774	1/1	0.96	0.14	51,51,51,51	0
54	MG	1A	3156	1/1	0.96	0.38	41,41,41,41	0
54	MG	1A	3393	1/1	0.96	0.15	50,50,50,50	0
54	MG	1a	1778	1/1	0.96	0.11	57,57,57,57	0
54	MG	1A	3099	1/1	0.96	0.17	55,55,55,55	0
54	MG	1A	3469	1/1	0.96	0.15	18,18,18,18	0
54	MG	1A	3904	1/1	0.96	0.31	66,66,66,66	0
54	MG	1A	3397	1/1	0.96	0.17	20,20,20,20	0
54	MG	1A	4033	1/1	0.96	0.09	48,48,48,48	0
54	MG	1A	3774	1/1	0.96	0.09	31,31,31,31	0
54	MG	1A	3907	1/1	0.96	0.18	59,59,59,59	0
54	MG	1A	4038	1/1	0.96	0.25	50,50,50,50	0
54	MG	1a	1619	1/1	0.96	0.17	53,53,53,53	0
54	MG	1A	3101	1/1	0.96	0.25	25,25,25,25	0
54	MG	1A	3563	1/1	0.96	0.17	23,23,23,23	0
54	MG	1A	3049	1/1	0.96	0.25	34,34,34,34	0
54	MG	1a	1623	1/1	0.96	0.10	46,46,46,46	0
54	MG	2A	3088	1/1	0.96	0.15	29,29,29,29	0
54	MG	1a	1624	1/1	0.96	0.10	63,63,63,63	0
54	MG	1a	1794	1/1	0.96	0.23	61,61,61,61	0
54	MG	2A	3566	1/1	0.96	0.18	27,27,27,27	0
54	MG	1A	4044	1/1	0.96	0.15	25,25,25,25	0
54	MG	1A	3400	1/1	0.96	0.25	62,62,62,62	0
54	MG	1a	1627	1/1	0.96	0.18	57,57,57,57	0
54	MG	2A	3325	1/1	0.96	0.14	63,63,63,63	0
54	MG	1A	3236	1/1	0.96	0.55	43,43,43,43	0
54	MG	1A	4053	1/1	0.96	0.41	34,34,34,34	0
54	MG	2a	1660	1/1	0.96	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3914	1/1	0.96	0.11	48,48,48,48	0
54	MG	1A	3276	1/1	0.96	0.22	28,28,28,28	0
54	MG	2A	3101	1/1	0.96	0.30	51,51,51,51	0
54	MG	2A	3331	1/1	0.96	0.15	55,55,55,55	0
54	MG	2A	3580	1/1	0.96	0.22	40,40,40,40	0
54	MG	1A	4057	1/1	0.96	0.45	29,29,29,29	0
54	MG	2A	3105	1/1	0.96	0.09	61,61,61,61	0
54	MG	2A	3335	1/1	0.96	0.21	53,53,53,53	0
54	MG	1a	1804	1/1	0.96	0.07	52,52,52,52	0
54	MG	2a	1671	1/1	0.96	0.08	68,68,68,68	0
54	MG	2a	1672	1/1	0.96	0.18	70,70,70,70	0
54	MG	2A	3108	1/1	0.96	0.16	57,57,57,57	0
54	MG	1A	3237	1/1	0.96	0.11	55,55,55,55	0
54	MG	2A	3588	1/1	0.96	0.13	42,42,42,42	0
54	MG	1A	3783	1/1	0.96	0.08	46,46,46,46	0
54	MG	1A	3085	1/1	0.96	0.42	33,33,33,33	0
54	MG	2A	3113	1/1	0.96	0.13	59,59,59,59	0
54	MG	2A	3114	1/1	0.96	0.16	41,41,41,41	0
54	MG	2A	3593	1/1	0.96	0.13	39,39,39,39	0
54	MG	1A	4063	1/1	0.96	0.30	39,39,39,39	0
54	MG	1A	3480	1/1	0.96	0.13	58,58,58,58	0
54	MG	2a	1683	1/1	0.96	0.17	56,56,56,56	0
54	MG	1A	4065	1/1	0.96	0.18	29,29,29,29	0
54	MG	1A	4066	1/1	0.96	0.30	33,33,33,33	0
54	MG	2a	1686	1/1	0.96	0.20	57,57,57,57	0
54	MG	1a	1642	1/1	0.96	0.10	51,51,51,51	0
54	MG	1A	3339	1/1	0.96	0.18	44,44,44,44	0
54	MG	1A	4069	1/1	0.96	0.14	28,28,28,28	0
54	MG	1A	3676	1/1	0.96	0.14	50,50,50,50	0
54	MG	1A	4072	1/1	0.96	0.27	36,36,36,36	0
54	MG	2A	3129	1/1	0.96	0.36	47,47,47,47	0
54	MG	2A	3357	1/1	0.96	0.16	45,45,45,45	0
54	MG	2A	3358	1/1	0.96	0.13	41,41,41,41	0
54	MG	2A	3607	1/1	0.96	0.10	72,72,72,72	0
54	MG	1A	3482	1/1	0.96	0.12	21,21,21,21	0
54	MG	1A	3161	1/1	0.96	0.31	35,35,35,35	0
54	MG	2A	3362	1/1	0.96	0.11	51,51,51,51	0
54	MG	2a	1702	1/1	0.96	0.09	69,69,69,69	0
54	MG	1A	3281	1/1	0.96	0.16	39,39,39,39	0
54	MG	2A	3134	1/1	0.96	0.14	40,40,40,40	0
54	MG	2a	1705	1/1	0.96	0.33	58,58,58,58	0
54	MG	2a	1709	1/1	0.96	0.23	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	1a	1824	1/1	0.96	0.09	42,42,42,42	0
54	MG	1A	3282	1/1	0.96	0.17	49,49,49,49	0
54	MG	1a	1826	1/1	0.96	0.14	47,47,47,47	0
54	MG	1a	1827	1/1	0.96	0.06	65,65,65,65	0
54	MG	1a	1652	1/1	0.96	0.20	58,58,58,58	0
54	MG	1A	3929	1/1	0.96	0.16	58,58,58,58	0
54	MG	2A	3141	1/1	0.96	0.19	53,53,53,53	0
54	MG	1B	205	1/1	0.96	0.15	47,47,47,47	0
54	MG	1A	3581	1/1	0.96	0.25	32,32,32,32	0
54	MG	2a	1720	1/1	0.96	0.12	66,66,66,66	0
54	MG	1A	3683	1/1	0.96	0.11	40,40,40,40	0
54	MG	2A	3145	1/1	0.96	0.12	62,62,62,62	0
54	MG	1A	3283	1/1	0.96	0.26	58,58,58,58	0
54	MG	1A	3796	1/1	0.96	0.24	24,24,24,24	0
54	MG	1A	3004	1/1	0.96	0.24	47,47,47,47	0
54	MG	1A	3347	1/1	0.96	0.15	27,27,27,27	0
54	MG	1a	1661	1/1	0.96	0.26	55,55,55,55	0
54	MG	1a	1662	1/1	0.96	0.17	63,63,63,63	0
54	MG	1A	3037	1/1	0.96	0.12	48,48,48,48	0
54	MG	2a	1730	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	3350	1/1	0.96	0.20	19,19,19,19	0
54	MG	2A	3388	1/1	0.96	0.20	56,56,56,56	0
54	MG	1A	3493	1/1	0.96	0.12	27,27,27,27	0
54	MG	2A	3390	1/1	0.96	0.16	66,66,66,66	0
54	MG	1a	1667	1/1	0.96	0.27	56,56,56,56	0
54	MG	1A	3418	1/1	0.96	0.09	50,50,50,50	0
54	MG	1a	1846	1/1	0.96	0.17	51,51,51,51	0
54	MG	2A	3159	1/1	0.96	0.14	45,45,45,45	0
54	MG	1A	3060	1/1	0.96	0.12	40,40,40,40	0
54	MG	2a	1741	1/1	0.96	0.24	47,47,47,47	0
54	MG	1A	3590	1/1	0.96	0.12	29,29,29,29	0
54	MG	2A	3644	1/1	0.96	0.15	53,53,53,53	0
54	MG	1A	3112	1/1	0.96	0.17	28,28,28,28	0
54	MG	2A	3400	1/1	0.96	0.23	50,50,50,50	0
54	MG	1A	3353	1/1	0.96	0.21	34,34,34,34	0
54	MG	1A	3423	1/1	0.96	0.16	29,29,29,29	0
54	MG	1A	3701	1/1	0.96	0.13	41,41,41,41	0
54	MG	1A	3502	1/1	0.96	0.23	48,48,48,48	0
54	MG	1A	3503	1/1	0.96	0.17	31,31,31,31	0
54	MG	1A	3201	1/1	0.96	0.29	58,58,58,58	0
54	MG	1a	1856	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	3817	1/1	0.96	0.23	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1858	1/1	0.96	0.18	59,59,59,59	0
54	MG	2A	3411	1/1	0.96	0.15	47,47,47,47	0
54	MG	1a	1859	1/1	0.96	0.12	57,57,57,57	0
54	MG	1A	3202	1/1	0.96	0.51	35,35,35,35	0
54	MG	1A	3358	1/1	0.96	0.15	17,17,17,17	0
54	MG	1A	3956	1/1	0.96	0.11	48,48,48,48	0
54	MG	1D	305	1/1	0.96	0.16	30,30,30,30	0
54	MG	1A	3708	1/1	0.96	0.13	33,33,33,33	0
54	MG	1A	3824	1/1	0.96	0.09	11,11,11,11	0
54	MG	1A	3012	1/1	0.96	0.15	43,43,43,43	0
54	MG	2a	1764	1/1	0.96	0.07	63,63,63,63	0
54	MG	1A	3509	1/1	0.96	0.17	58,58,58,58	0
54	MG	1A	3065	1/1	0.96	0.42	41,41,41,41	0
54	MG	2a	1767	1/1	0.96	0.24	72,72,72,72	0
54	MG	1A	3712	1/1	0.96	0.13	51,51,51,51	0
54	MG	1A	3208	1/1	0.96	0.15	31,31,31,31	0
54	MG	1a	1697	1/1	0.96	0.09	66,66,66,66	0
54	MG	1A	3833	1/1	0.96	0.10	50,50,50,50	0
54	MG	2a	1773	1/1	0.96	0.08	59,59,59,59	0
54	MG	1A	3168	1/1	0.96	0.38	48,48,48,48	0
54	MG	1a	1700	1/1	0.96	0.28	31,31,31,31	0
54	MG	1A	3716	1/1	0.96	0.18	42,42,42,42	0
54	MG	1A	3297	1/1	0.96	0.10	35,35,35,35	0
54	MG	1A	3718	1/1	0.96	0.24	41,41,41,41	0
54	MG	1a	1704	1/1	0.96	0.12	56,56,56,56	0
54	MG	1a	1706	1/1	0.96	0.12	59,59,59,59	0
54	MG	2a	1783	1/1	0.96	0.14	49,49,49,49	0
54	MG	2A	3683	1/1	0.96	0.15	27,27,27,27	0
54	MG	2A	3684	1/1	0.96	0.07	53,53,53,53	0
54	MG	1E	305	1/1	0.96	0.17	57,57,57,57	0
54	MG	1A	3116	1/1	0.96	0.09	46,46,46,46	0
54	MG	1A	3607	1/1	0.96	0.25	42,42,42,42	0
54	MG	2A	3689	1/1	0.96	0.20	59,59,59,59	0
54	MG	1A	3366	1/1	0.96	0.11	35,35,35,35	0
54	MG	1t	3001	1/1	0.96	0.10	63,63,63,63	0
54	MG	1A	3213	1/1	0.96	0.53	30,30,30,30	0
54	MG	2A	3204	1/1	0.96	0.39	38,38,38,38	0
54	MG	2A	3445	1/1	0.96	0.16	38,38,38,38	0
54	MG	1a	1715	1/1	0.96	0.12	67,67,67,67	0
54	MG	2A	3701	1/1	0.96	0.27	46,46,46,46	0
54	MG	1F	308	1/1	0.96	0.24	52,52,52,52	0
54	MG	1A	3724	1/1	0.96	0.21	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3170	1/1	0.96	0.23	40,40,40,40	0
59	ZN	14	501	1/1	0.96	0.13	82,82,82,82	0
54	MG	1A	3437	1/1	0.96	0.18	25,25,25,25	0
54	MG	2A	3003	1/1	0.96	0.12	31,31,31,31	0
54	MG	1A	3727	1/1	0.96	0.20	30,30,30,30	0
54	MG	1a	1735	1/1	0.97	0.13	54,54,54,54	0
54	MG	1A	3815	1/1	0.97	0.21	29,29,29,29	0
54	MG	13	103	1/1	0.97	0.14	39,39,39,39	0
54	MG	2A	3156	1/1	0.97	0.20	61,61,61,61	0
54	MG	1A	4049	1/1	0.97	0.16	35,35,35,35	0
54	MG	2A	3541	1/1	0.97	0.27	56,56,56,56	0
54	MG	2V	201	1/1	0.97	0.15	57,57,57,57	0
54	MG	15	101	1/1	0.97	0.09	44,44,44,44	0
54	MG	2A	3543	1/1	0.97	0.15	40,40,40,40	0
54	MG	15	103	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3556	1/1	0.97	0.25	29,29,29,29	0
54	MG	2A	3349	1/1	0.97	0.13	49,49,49,49	0
54	MG	2A	3548	1/1	0.97	0.15	34,34,34,34	0
54	MG	1A	4051	1/1	0.97	0.17	34,34,34,34	0
54	MG	1A	3632	1/1	0.97	0.28	48,48,48,48	0
54	MG	1A	4054	1/1	0.97	0.24	34,34,34,34	0
54	MG	1A	3818	1/1	0.97	0.15	24,24,24,24	0
54	MG	28	103	1/1	0.97	0.08	46,46,46,46	0
54	MG	1A	3819	1/1	0.97	0.11	46,46,46,46	0
54	MG	1A	3932	1/1	0.97	0.08	53,53,53,53	0
54	MG	1A	3633	1/1	0.97	0.43	50,50,50,50	0
54	MG	1A	3934	1/1	0.97	0.04	76,76,76,76	0
54	MG	2A	3006	1/1	0.97	0.13	45,45,45,45	0
54	MG	1A	3821	1/1	0.97	0.10	40,40,40,40	0
54	MG	1a	1607	1/1	0.97	0.10	49,49,49,49	0
54	MG	1A	3315	1/1	0.97	0.12	45,45,45,45	0
54	MG	1A	3196	1/1	0.97	0.52	33,33,33,33	0
54	MG	2a	1610	1/1	0.97	0.12	48,48,48,48	0
54	MG	1a	1610	1/1	0.97	0.12	49,49,49,49	0
54	MG	2A	3365	1/1	0.97	0.15	38,38,38,38	0
54	MG	1A	3070	1/1	0.97	0.23	25,25,25,25	0
54	MG	2A	3014	1/1	0.97	0.39	42,42,42,42	0
54	MG	1a	1756	1/1	0.97	0.18	49,49,49,49	0
54	MG	2A	3568	1/1	0.97	0.17	43,43,43,43	0
54	MG	2A	3569	1/1	0.97	0.16	24,24,24,24	0
54	MG	1A	3318	1/1	0.97	0.18	13,13,13,13	0
54	MG	2A	3181	1/1	0.97	0.42	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	2A	3371	1/1	0.97	0.18	48,48,48,48	0
54	MG	1A	4067	1/1	0.97	0.27	33,33,33,33	0
54	MG	1A	3562	1/1	0.97	0.11	39,39,39,39	0
54	MG	1A	3033	1/1	0.97	0.13	41,41,41,41	0
54	MG	1A	3564	1/1	0.97	0.19	18,18,18,18	0
54	MG	1a	1618	1/1	0.97	0.09	52,52,52,52	0
54	MG	2A	3578	1/1	0.97	0.21	54,54,54,54	0
54	MG	1A	3320	1/1	0.97	0.20	15,15,15,15	0
54	MG	1A	4073	1/1	0.97	0.27	36,36,36,36	0
54	MG	2A	3581	1/1	0.97	0.13	44,44,44,44	0
54	MG	1A	3831	1/1	0.97	0.14	39,39,39,39	0
54	MG	1A	3832	1/1	0.97	0.20	22,22,22,22	0
54	MG	2A	3191	1/1	0.97	0.12	57,57,57,57	0
54	MG	1A	3199	1/1	0.97	0.35	25,25,25,25	0
54	MG	1A	3141	1/1	0.97	0.11	23,23,23,23	0
54	MG	2A	3194	1/1	0.97	0.06	53,53,53,53	0
54	MG	1A	3735	1/1	0.97	0.18	48,48,48,48	0
54	MG	1A	3836	1/1	0.97	0.40	32,32,32,32	0
54	MG	1A	3568	1/1	0.97	0.20	47,47,47,47	0
54	MG	1a	1628	1/1	0.97	0.14	58,58,58,58	0
54	MG	1A	3839	1/1	0.97	0.19	24,24,24,24	0
54	MG	1A	3498	1/1	0.97	0.13	28,28,28,28	0
54	MG	1B	209	1/1	0.97	0.12	35,35,35,35	0
54	MG	2A	3035	1/1	0.97	0.11	53,53,53,53	0
54	MG	1A	3842	1/1	0.97	0.23	50,50,50,50	0
54	MG	1A	3083	1/1	0.97	0.15	34,34,34,34	0
54	MG	2A	3398	1/1	0.97	0.14	42,42,42,42	0
54	MG	1A	3500	1/1	0.97	0.21	33,33,33,33	0
54	MG	2a	1649	1/1	0.97	0.19	50,50,50,50	0
54	MG	1A	3652	1/1	0.97	0.14	39,39,39,39	0
54	MG	2a	1651	1/1	0.97	0.11	68,68,68,68	0
54	MG	2a	1652	1/1	0.97	0.09	71,71,71,71	0
54	MG	2A	3040	1/1	0.97	0.16	39,39,39,39	0
54	MG	1A	3325	1/1	0.97	0.16	22,22,22,22	0
54	MG	1B	215	1/1	0.97	0.17	39,39,39,39	0
54	MG	1A	3654	1/1	0.97	0.14	24,24,24,24	0
54	MG	1A	3574	1/1	0.97	0.20	21,21,21,21	0
54	MG	2A	3406	1/1	0.97	0.21	63,63,63,63	0
54	MG	1B	218	1/1	0.97	0.19	39,39,39,39	0
54	MG	1A	3326	1/1	0.97	0.18	27,27,27,27	0
54	MG	2A	3214	1/1	0.97	0.31	38,38,38,38	0
54	MG	1A	3850	1/1	0.97	0.07	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	1A	3203	1/1	0.97	0.33	35,35,35,35	0
54	MG	2a	1665	1/1	0.97	0.12	58,58,58,58	0
54	MG	1A	3749	1/1	0.97	0.20	30,30,30,30	0
54	MG	1A	3098	1/1	0.97	0.22	25,25,25,25	0
54	MG	1A	3442	1/1	0.97	0.18	16,16,16,16	0
54	MG	1A	3662	1/1	0.97	0.08	39,39,39,39	0
54	MG	2A	3618	1/1	0.97	0.10	66,66,66,66	0
54	MG	1A	3245	1/1	0.97	0.21	12,12,12,12	0
54	MG	2A	3417	1/1	0.97	0.21	61,61,61,61	0
54	MG	1A	3507	1/1	0.97	0.17	32,32,32,32	0
54	MG	1A	3145	1/1	0.97	0.20	37,37,37,37	0
54	MG	2A	3623	1/1	0.97	0.12	64,64,64,64	0
54	MG	2A	3056	1/1	0.97	0.34	39,39,39,39	0
54	MG	1A	3084	1/1	0.97	0.14	36,36,36,36	0
54	MG	1A	3510	1/1	0.97	0.11	47,47,47,47	0
54	MG	1A	3862	1/1	0.97	0.12	39,39,39,39	0
54	MG	1a	1800	1/1	0.97	0.16	50,50,50,50	0
54	MG	1D	301	1/1	0.97	0.20	12,12,12,12	0
54	MG	1D	304	1/1	0.97	0.22	41,41,41,41	0
54	MG	2A	3428	1/1	0.97	0.15	35,35,35,35	0
54	MG	1A	3511	1/1	0.97	0.16	24,24,24,24	0
54	MG	1A	3148	1/1	0.97	0.32	26,26,26,26	0
54	MG	1A	3672	1/1	0.97	0.18	55,55,55,55	0
54	MG	1A	3054	1/1	0.97	0.31	25,25,25,25	0
54	MG	1A	3123	1/1	0.97	0.22	35,35,35,35	0
54	MG	1A	3450	1/1	0.97	0.11	16,16,16,16	0
54	MG	2a	1691	1/1	0.97	0.18	68,68,68,68	0
54	MG	2A	3435	1/1	0.97	0.17	60,60,60,60	0
54	MG	1a	1664	1/1	0.97	0.14	56,56,56,56	0
54	MG	1A	3287	1/1	0.97	0.17	22,22,22,22	0
54	MG	2A	3073	1/1	0.97	0.25	61,61,61,61	0
54	MG	1A	3178	1/1	0.97	0.30	27,27,27,27	0
54	MG	1A	3338	1/1	0.97	0.16	48,48,48,48	0
54	MG	1A	3396	1/1	0.97	0.14	46,46,46,46	0
54	MG	1A	3061	1/1	0.97	0.13	26,26,26,26	0
54	MG	1A	3181	1/1	0.97	0.31	24,24,24,24	0
54	MG	2A	3647	1/1	0.97	0.07	55,55,55,55	0
54	MG	1a	1818	1/1	0.97	0.11	51,51,51,51	0
54	MG	1A	3341	1/1	0.97	0.13	24,24,24,24	0
54	MG	1A	3292	1/1	0.97	0.18	28,28,28,28	0
54	MG	2a	1707	1/1	0.97	0.16	48,48,48,48	0
54	MG	2a	1708	1/1	0.97	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1821	1/1	0.97	0.11	58,58,58,58	0
54	MG	1A	3087	1/1	0.97	0.15	17,17,17,17	0
54	MG	1F	302	1/1	0.97	0.42	33,33,33,33	0
54	MG	1A	3686	1/1	0.97	0.20	36,36,36,36	0
54	MG	2A	3655	1/1	0.97	0.23	79,79,79,79	0
54	MG	1F	305	1/1	0.97	0.33	30,30,30,30	0
54	MG	1A	3219	1/1	0.97	0.34	31,31,31,31	0
54	MG	1A	3688	1/1	0.97	0.14	46,46,46,46	0
54	MG	1A	3220	1/1	0.97	0.24	32,32,32,32	0
54	MG	2a	1718	1/1	0.97	0.20	46,46,46,46	0
54	MG	1A	3884	1/1	0.97	0.10	25,25,25,25	0
54	MG	1a	1830	1/1	0.97	0.19	60,60,60,60	0
54	MG	1a	1682	1/1	0.97	0.14	54,54,54,54	0
54	MG	1A	3886	1/1	0.97	0.08	51,51,51,51	0
54	MG	1a	1684	1/1	0.97	0.23	46,46,46,46	0
54	MG	2A	3096	1/1	0.97	0.21	50,50,50,50	0
54	MG	2A	3463	1/1	0.97	0.30	48,48,48,48	0
54	MG	2A	3270	1/1	0.97	0.08	55,55,55,55	0
54	MG	1A	3887	1/1	0.97	0.12	37,37,37,37	0
54	MG	1a	1686	1/1	0.97	0.10	46,46,46,46	0
54	MG	1a	1687	1/1	0.97	0.20	34,34,34,34	0
54	MG	2A	3274	1/1	0.97	0.18	46,46,46,46	0
54	MG	1A	3690	1/1	0.97	0.25	37,37,37,37	0
54	MG	2A	3102	1/1	0.97	0.37	36,36,36,36	0
54	MG	1A	3009	1/1	0.97	0.12	24,24,24,24	0
54	MG	2A	3104	1/1	0.97	0.14	65,65,65,65	0
54	MG	2A	3279	1/1	0.97	0.14	51,51,51,51	0
54	MG	1A	3407	1/1	0.97	0.17	47,47,47,47	0
54	MG	2A	3281	1/1	0.97	0.14	32,32,32,32	0
54	MG	1A	3108	1/1	0.97	0.23	34,34,34,34	0
54	MG	2A	3283	1/1	0.97	0.20	29,29,29,29	0
54	MG	2A	3284	1/1	0.97	0.15	27,27,27,27	0
54	MG	2A	3479	1/1	0.97	0.24	53,53,53,53	0
54	MG	1A	3063	1/1	0.97	0.20	53,53,53,53	0
54	MG	2A	3109	1/1	0.97	0.11	60,60,60,60	0
54	MG	1N	201	1/1	0.97	0.16	36,36,36,36	0
54	MG	2A	3690	1/1	0.97	0.31	37,37,37,37	0
54	MG	2A	3289	1/1	0.97	0.17	53,53,53,53	0
54	MG	1A	3110	1/1	0.97	0.08	33,33,33,33	0
54	MG	1a	1696	1/1	0.97	0.23	56,56,56,56	0
54	MG	1A	4005	1/1	0.97	0.06	57,57,57,57	0
54	MG	1A	3018	1/1	0.97	0.24	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3699	1/1	0.97	0.65	47,47,47,47	0
54	MG	1A	3608	1/1	0.97	0.12	36,36,36,36	0
54	MG	1A	3019	1/1	0.97	0.46	35,35,35,35	0
54	MG	2A	3117	1/1	0.97	0.38	49,49,49,49	0
54	MG	1A	3700	1/1	0.97	0.13	27,27,27,27	0
54	MG	1A	3354	1/1	0.97	0.19	17,17,17,17	0
54	MG	2A	3300	1/1	0.97	0.14	47,47,47,47	0
54	MG	2A	3121	1/1	0.97	0.12	59,59,59,59	0
54	MG	1A	3355	1/1	0.97	0.18	16,16,16,16	0
54	MG	2B	205	1/1	0.97	0.11	67,67,67,67	0
54	MG	2A	3123	1/1	0.97	0.15	38,38,38,38	0
54	MG	2A	3304	1/1	0.97	0.18	60,60,60,60	0
54	MG	1A	3189	1/1	0.97	0.51	33,33,33,33	0
54	MG	2A	3125	1/1	0.97	0.16	52,52,52,52	0
54	MG	1A	3704	1/1	0.97	0.20	38,38,38,38	0
54	MG	1T	202	1/1	0.97	0.16	58,58,58,58	0
54	MG	1a	1708	1/1	0.97	0.15	31,31,31,31	0
54	MG	1A	3794	1/1	0.97	0.16	18,18,18,18	0
54	MG	2a	1770	1/1	0.97	0.06	67,67,67,67	0
54	MG	1A	3001	1/1	0.97	0.14	31,31,31,31	0
54	MG	2A	3505	1/1	0.97	0.12	44,44,44,44	0
54	MG	1A	3231	1/1	0.97	0.23	29,29,29,29	0
54	MG	1U	202	1/1	0.97	0.12	46,46,46,46	0
54	MG	2a	1775	1/1	0.97	0.13	78,78,78,78	0
54	MG	2B	218	1/1	0.97	0.14	60,60,60,60	0
54	MG	1A	3476	1/1	0.97	0.15	19,19,19,19	0
54	MG	1A	3191	1/1	0.97	0.34	35,35,35,35	0
54	MG	2A	3510	1/1	0.97	0.15	36,36,36,36	0
54	MG	1A	3478	1/1	0.97	0.06	38,38,38,38	0
54	MG	1A	3800	1/1	0.97	0.19	21,21,21,21	0
54	MG	1A	3360	1/1	0.97	0.15	18,18,18,18	0
54	MG	1A	3068	1/1	0.97	0.14	36,36,36,36	0
54	MG	1A	3622	1/1	0.97	0.14	27,27,27,27	0
54	MG	1A	3310	1/1	0.97	0.18	16,16,16,16	0
54	MG	1A	3915	1/1	0.97	0.13	17,17,17,17	0
54	MG	1A	3714	1/1	0.97	0.10	32,32,32,32	0
54	MG	2E	306	1/1	0.97	0.34	42,42,42,42	0
56	EZM	1A	4035	24/24	0.97	0.34	21,31,39,44	0
54	MG	2A	3522	1/1	0.97	0.12	53,53,53,53	0
54	MG	1A	3424	1/1	0.97	0.05	42,42,42,42	0
54	MG	2F	3003	1/1	0.97	0.41	43,43,43,43	0
54	MG	1A	3483	1/1	0.97	0.22	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3137	1/1	0.97	0.24	28,28,28,28	0
54	MG	1A	3115	1/1	0.97	0.31	26,26,26,26	0
54	MG	1A	3811	1/1	0.97	0.17	28,28,28,28	0
54	MG	2A	3528	1/1	0.97	0.18	54,54,54,54	0
54	MG	2A	3529	1/1	0.97	0.33	64,64,64,64	0
54	MG	1k	3001	1/1	0.97	0.16	42,42,42,42	0
54	MG	1A	3812	1/1	0.97	0.15	42,42,42,42	0
54	MG	1A	3313	1/1	0.97	0.20	23,23,23,23	0
54	MG	1A	3314	1/1	0.97	0.10	22,22,22,22	0
59	ZN	29	501	1/1	0.97	0.15	68,68,68,68	0
54	MG	2A	3534	1/1	0.97	0.24	60,60,60,60	0
60	SF4	1d	501	8/8	0.97	0.15	50,59,66,73	0
54	MG	1A	3552	1/1	0.98	0.27	35,35,35,35	0
54	MG	1A	3446	1/1	0.98	0.15	22,22,22,22	0
54	MG	1A	3209	1/1	0.98	0.25	36,36,36,36	0
54	MG	1A	3555	1/1	0.98	0.23	34,34,34,34	0
54	MG	1A	3273	1/1	0.98	0.26	33,33,33,33	0
54	MG	1D	302	1/1	0.98	0.18	33,33,33,33	0
54	MG	1D	303	1/1	0.98	0.38	40,40,40,40	0
54	MG	2A	3089	1/1	0.98	0.21	64,64,64,64	0
54	MG	1A	3274	1/1	0.98	0.25	34,34,34,34	0
54	MG	1A	3210	1/1	0.98	0.15	49,49,49,49	0
54	MG	2A	3218	1/1	0.98	0.17	40,40,40,40	0
54	MG	2A	3361	1/1	0.98	0.14	30,30,30,30	0
54	MG	1A	3619	1/1	0.98	0.08	40,40,40,40	0
54	MG	2A	3220	1/1	0.98	0.20	48,48,48,48	0
54	MG	2a	1655	1/1	0.98	0.20	61,61,61,61	0
54	MG	1A	3403	1/1	0.98	0.10	47,47,47,47	0
54	MG	1A	3837	1/1	0.98	0.07	41,41,41,41	0
54	MG	2A	3223	1/1	0.98	0.25	55,55,55,55	0
54	MG	1A	4008	1/1	0.98	0.17	11,11,11,11	0
54	MG	1A	3560	1/1	0.98	0.13	30,30,30,30	0
54	MG	2A	3097	1/1	0.98	0.23	46,46,46,46	0
54	MG	2A	3514	1/1	0.98	0.29	43,43,43,43	0
54	MG	1A	3404	1/1	0.98	0.17	18,18,18,18	0
54	MG	2A	3516	1/1	0.98	0.09	26,26,26,26	0
54	MG	1a	1637	1/1	0.98	0.14	51,51,51,51	0
54	MG	2A	3518	1/1	0.98	0.27	60,60,60,60	0
54	MG	1A	3840	1/1	0.98	0.12	46,46,46,46	0
54	MG	1A	3180	1/1	0.98	0.18	22,22,22,22	0
54	MG	1A	3925	1/1	0.98	0.09	46,46,46,46	0
54	MG	1A	3765	1/1	0.98	0.14	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3676	1/1	0.98	0.14	40,40,40,40	0
54	MG	1g	3003	1/1	0.98	0.10	52,52,52,52	0
54	MG	2A	3377	1/1	0.98	0.14	63,63,63,63	0
54	MG	1A	3082	1/1	0.98	0.20	33,33,33,33	0
54	MG	2A	3379	1/1	0.98	0.15	55,55,55,55	0
54	MG	1A	3928	1/1	0.98	0.17	62,62,62,62	0
54	MG	2A	3107	1/1	0.98	0.20	27,27,27,27	0
54	MG	1A	3455	1/1	0.98	0.16	57,57,57,57	0
54	MG	1A	3768	1/1	0.98	0.06	36,36,36,36	0
54	MG	2A	3686	1/1	0.98	0.11	43,43,43,43	0
54	MG	1a	1646	1/1	0.98	0.18	49,49,49,49	0
54	MG	1A	3244	1/1	0.98	0.17	18,18,18,18	0
54	MG	1A	3048	1/1	0.98	0.32	43,43,43,43	0
54	MG	1F	304	1/1	0.98	0.37	24,24,24,24	0
54	MG	1A	3023	1/1	0.98	0.23	18,18,18,18	0
54	MG	1A	4024	1/1	0.98	0.29	27,27,27,27	0
54	MG	2A	3246	1/1	0.98	0.32	44,44,44,44	0
54	MG	2A	3538	1/1	0.98	0.21	60,60,60,60	0
54	MG	2a	1689	1/1	0.98	0.18	58,58,58,58	0
54	MG	1A	3698	1/1	0.98	0.22	41,41,41,41	0
54	MG	1A	3629	1/1	0.98	0.21	49,49,49,49	0
54	MG	2A	3393	1/1	0.98	0.10	57,57,57,57	0
54	MG	1A	3936	1/1	0.98	0.15	63,63,63,63	0
54	MG	1A	3215	1/1	0.98	0.13	59,59,59,59	0
54	MG	1A	3411	1/1	0.98	0.19	42,42,42,42	0
54	MG	2a	1696	1/1	0.98	0.21	52,52,52,52	0
54	MG	1A	4030	1/1	0.98	0.15	33,33,33,33	0
54	MG	1A	4031	1/1	0.98	0.34	38,38,38,38	0
54	MG	2A	3547	1/1	0.98	0.16	31,31,31,31	0
54	MG	1G	3004	1/1	0.98	0.15	37,37,37,37	0
54	MG	1A	3776	1/1	0.98	0.20	26,26,26,26	0
54	MG	2A	3256	1/1	0.98	0.19	30,30,30,30	0
54	MG	1A	3007	1/1	0.98	0.18	32,32,32,32	0
54	MG	1A	3100	1/1	0.98	0.43	28,28,28,28	0
54	MG	1a	1777	1/1	0.98	0.14	64,64,64,64	0
54	MG	2a	1706	1/1	0.98	0.27	63,63,63,63	0
54	MG	1A	3572	1/1	0.98	0.13	25,25,25,25	0
54	MG	2A	3555	1/1	0.98	0.24	55,55,55,55	0
54	MG	1A	3119	1/1	0.98	0.50	25,25,25,25	0
54	MG	2A	3131	1/1	0.98	0.16	65,65,65,65	0
54	MG	1A	3636	1/1	0.98	0.25	36,36,36,36	0
54	MG	1A	3005	1/1	0.98	0.20	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3052	1/1	0.98	0.14	28,28,28,28	0
54	MG	1A	3639	1/1	0.98	0.10	27,27,27,27	0
54	MG	2A	3012	1/1	0.98	0.31	39,39,39,39	0
54	MG	1a	1784	1/1	0.98	0.16	59,59,59,59	0
54	MG	1Q	201	1/1	0.98	0.16	49,49,49,49	0
54	MG	1A	3027	1/1	0.98	0.40	30,30,30,30	0
54	MG	2D	301	1/1	0.98	0.56	52,52,52,52	0
54	MG	1a	1671	1/1	0.98	0.43	58,58,58,58	0
54	MG	1A	4046	1/1	0.98	0.14	20,20,20,20	0
54	MG	1A	4047	1/1	0.98	0.26	24,24,24,24	0
54	MG	1A	4048	1/1	0.98	0.15	31,31,31,31	0
54	MG	1A	3289	1/1	0.98	0.13	20,20,20,20	0
54	MG	2E	301	1/1	0.98	0.18	35,35,35,35	0
54	MG	2A	3421	1/1	0.98	0.13	72,72,72,72	0
54	MG	1A	3642	1/1	0.98	0.19	40,40,40,40	0
54	MG	2E	304	1/1	0.98	0.14	26,26,26,26	0
54	MG	1A	3419	1/1	0.98	0.23	45,45,45,45	0
54	MG	1A	4052	1/1	0.98	0.27	30,30,30,30	0
54	MG	1A	3064	1/1	0.98	0.24	34,34,34,34	0
54	MG	1A	3223	1/1	0.98	0.21	27,27,27,27	0
54	MG	1A	3224	1/1	0.98	0.50	26,26,26,26	0
54	MG	1A	3955	1/1	0.98	0.11	50,50,50,50	0
54	MG	1A	3143	1/1	0.98	0.38	40,40,40,40	0
54	MG	1A	3043	1/1	0.98	0.32	29,29,29,29	0
54	MG	2A	3287	1/1	0.98	0.22	42,42,42,42	0
54	MG	1A	4059	1/1	0.98	0.23	28,28,28,28	0
54	MG	1A	4060	1/1	0.98	0.26	38,38,38,38	0
54	MG	1A	3719	1/1	0.98	0.17	26,26,26,26	0
54	MG	2O	8003	1/1	0.98	0.11	64,64,64,64	0
54	MG	1a	1688	1/1	0.98	0.17	36,36,36,36	0
54	MG	1A	3649	1/1	0.98	0.15	21,21,21,21	0
54	MG	1A	3006	1/1	0.98	0.21	25,25,25,25	0
54	MG	1A	3335	1/1	0.98	0.08	46,46,46,46	0
54	MG	1A	3876	1/1	0.98	0.30	62,62,62,62	0
54	MG	1A	3528	1/1	0.98	0.16	19,19,19,19	0
54	MG	2A	3297	1/1	0.98	0.20	39,39,39,39	0
54	MG	2A	3442	1/1	0.98	0.20	37,37,37,37	0
54	MG	1a	1810	1/1	0.98	0.10	60,60,60,60	0
54	MG	1A	3964	1/1	0.98	0.09	68,68,68,68	0
54	MG	1A	3194	1/1	0.98	0.49	29,29,29,29	0
54	MG	2W	8001	1/1	0.98	0.30	44,44,44,44	0
54	MG	1A	3879	1/1	0.98	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3597	1/1	0.98	0.29	43,43,43,43	0
54	MG	1A	3127	1/1	0.98	0.26	29,29,29,29	0
54	MG	1A	4071	1/1	0.98	0.35	33,33,33,33	0
54	MG	1A	3147	1/1	0.98	0.32	26,26,26,26	0
54	MG	1A	3171	1/1	0.98	0.35	35,35,35,35	0
54	MG	1A	3300	1/1	0.98	0.08	30,30,30,30	0
54	MG	2A	3307	1/1	0.98	0.20	37,37,37,37	0
54	MG	2A	3308	1/1	0.98	0.16	29,29,29,29	0
54	MG	1A	3804	1/1	0.98	0.09	60,60,60,60	0
54	MG	1A	3885	1/1	0.98	0.15	28,28,28,28	0
54	MG	1A	3658	1/1	0.98	0.22	48,48,48,48	0
54	MG	1a	1705	1/1	0.98	0.13	61,61,61,61	0
54	MG	2A	3177	1/1	0.98	0.42	43,43,43,43	0
54	MG	1A	3534	1/1	0.98	0.14	44,44,44,44	0
54	MG	2A	3315	1/1	0.98	0.19	40,40,40,40	0
54	MG	1A	3888	1/1	0.98	0.17	24,24,24,24	0
54	MG	2A	3462	1/1	0.98	0.22	22,22,22,22	0
54	MG	2A	3614	1/1	0.98	0.20	52,52,52,52	0
54	MG	1A	3660	1/1	0.98	0.11	28,28,28,28	0
54	MG	1A	3016	1/1	0.98	0.19	30,30,30,30	0
54	MG	1A	3595	1/1	0.98	0.10	25,25,25,25	0
54	MG	1A	3386	1/1	0.98	0.14	29,29,29,29	0
54	MG	2a	1778	1/1	0.98	0.08	56,56,56,56	0
54	MG	2A	3058	1/1	0.98	0.20	30,30,30,30	0
54	MG	1A	3149	1/1	0.98	0.24	28,28,28,28	0
54	MG	1a	1714	1/1	0.98	0.11	67,67,67,67	0
54	MG	1a	1603	1/1	0.98	0.12	44,44,44,44	0
54	MG	1A	3304	1/1	0.98	0.07	41,41,41,41	0
54	MG	1A	3150	1/1	0.98	0.14	45,45,45,45	0
54	MG	1A	3022	1/1	0.98	0.19	26,26,26,26	0
54	MG	1A	3346	1/1	0.98	0.21	38,38,38,38	0
54	MG	1A	3670	1/1	0.98	0.18	45,45,45,45	0
54	MG	2A	3067	1/1	0.98	0.14	56,56,56,56	0
54	MG	1A	3392	1/1	0.98	0.15	12,12,12,12	0
54	MG	1A	3152	1/1	0.98	0.18	28,28,28,28	0
54	MG	2A	3334	1/1	0.98	0.21	45,45,45,45	0
54	MG	1A	3394	1/1	0.98	0.13	37,37,37,37	0
54	MG	1A	3492	1/1	0.98	0.13	24,24,24,24	0
54	MG	1a	1726	1/1	0.98	0.13	55,55,55,55	0
54	MG	1A	3153	1/1	0.98	0.28	32,32,32,32	0
54	MG	1a	1614	1/1	0.98	0.11	63,63,63,63	0
54	MG	2a	1631	1/1	0.98	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3748	1/1	0.98	0.13	12,12,12,12	0
54	MG	1A	3349	1/1	0.98	0.18	16,16,16,16	0
54	MG	2A	3343	1/1	0.98	0.22	45,45,45,45	0
54	MG	1A	3094	1/1	0.98	0.53	28,28,28,28	0
59	ZN	15	102	1/1	0.98	0.20	38,38,38,38	0
59	ZN	1n	501	1/1	0.98	0.11	59,59,59,59	0
54	MG	1A	3496	1/1	0.98	0.12	34,34,34,34	0
54	MG	1A	3069	1/1	0.98	0.12	27,27,27,27	0
59	ZN	25	501	1/1	0.98	0.20	52,52,52,52	0
59	ZN	26	501	1/1	0.98	0.18	58,58,58,58	0
54	MG	1A	3827	1/1	0.98	0.21	49,49,49,49	0
54	MG	2A	3348	1/1	0.98	0.18	70,70,70,70	0
54	MG	1A	3997	1/1	0.98	0.16	48,48,48,48	0
60	SF4	2d	302	8/8	0.98	0.12	59,71,73,91	0
54	MG	1A	3303	1/1	0.99	0.20	18,18,18,18	0
54	MG	1A	3103	1/1	0.99	0.33	27,27,27,27	0
54	MG	1A	3537	1/1	0.99	0.12	41,41,41,41	0
54	MG	1A	3746	1/1	0.99	0.39	27,27,27,27	0
54	MG	2A	3322	1/1	0.99	0.23	49,49,49,49	0
54	MG	1A	3024	1/1	0.99	0.29	30,30,30,30	0
54	MG	1A	3382	1/1	0.99	0.21	12,12,12,12	0
54	MG	1a	1723	1/1	0.99	0.14	49,49,49,49	0
54	MG	1A	4016	1/1	0.99	0.13	14,14,14,14	0
54	MG	1A	3383	1/1	0.99	0.16	28,28,28,28	0
54	MG	2A	3672	1/1	0.99	0.19	54,54,54,54	0
54	MG	1A	3200	1/1	0.99	0.24	24,24,24,24	0
54	MG	1a	1833	1/1	0.99	0.12	29,29,29,29	0
54	MG	1A	3677	1/1	0.99	0.08	21,21,21,21	0
54	MG	2a	1734	1/1	0.99	0.24	46,46,46,46	0
54	MG	1A	3321	1/1	0.99	0.13	12,12,12,12	0
54	MG	1Q	202	1/1	0.99	0.17	22,22,22,22	0
54	MG	1A	4021	1/1	0.99	0.14	36,36,36,36	0
54	MG	2A	3679	1/1	0.99	0.14	58,58,58,58	0
54	MG	1A	3367	1/1	0.99	0.16	21,21,21,21	0
54	MG	1A	3858	1/1	0.99	0.20	19,19,19,19	0
54	MG	1A	3105	1/1	0.99	0.35	36,36,36,36	0
54	MG	1A	3003	1/1	0.99	0.13	19,19,19,19	0
54	MG	2A	3176	1/1	0.99	0.23	51,51,51,51	0
55	K	1A	3278	1/1	0.99	0.10	22,22,22,22	0
55	K	2A	3236	1/1	0.99	0.11	28,28,28,28	0
54	MG	1A	3465	1/1	0.99	0.17	22,22,22,22	0
54	MG	2A	3340	1/1	0.99	0.17	33,33,33,33	0

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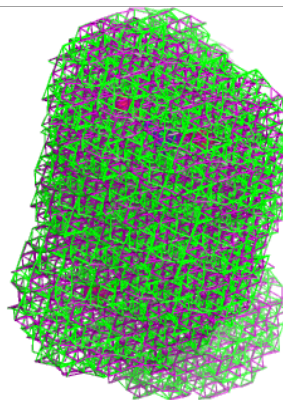
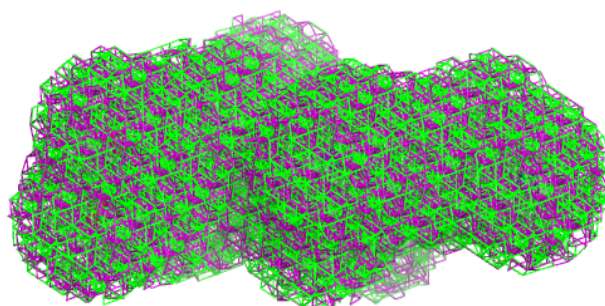
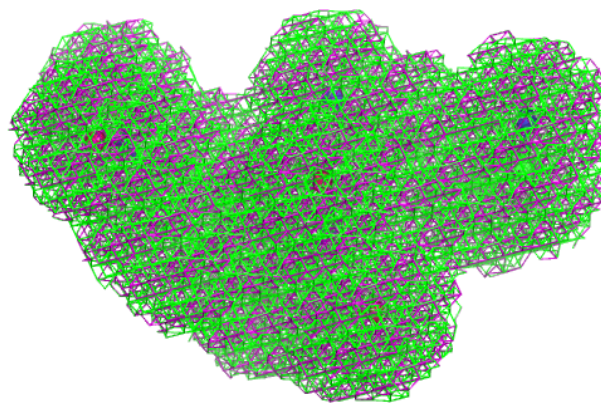
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3107	1/1	0.99	0.18	27,27,27,27	0
54	MG	1A	3613	1/1	0.99	0.19	59,59,59,59	0
54	MG	1A	3204	1/1	0.99	0.40	30,30,30,30	0
54	MG	1A	3205	1/1	0.99	0.42	25,25,25,25	0
54	MG	1A	3373	1/1	0.99	0.20	20,20,20,20	0
54	MG	1B	222	1/1	0.99	0.14	30,30,30,30	0
54	MG	1A	3045	1/1	0.99	0.21	11,11,11,11	0
54	MG	1a	1813	1/1	0.99	0.09	53,53,53,53	0
54	MG	1A	3134	1/1	0.99	0.42	37,37,37,37	0
59	ZN	1Y	501	1/1	0.99	0.19	46,46,46,46	0
54	MG	2A	3266	1/1	0.99	0.09	19,19,19,19	0
54	MG	1A	3017	1/1	0.99	0.23	21,21,21,21	0
59	ZN	16	501	1/1	0.99	0.24	39,39,39,39	0
59	ZN	19	102	1/1	0.99	0.24	41,41,41,41	0
54	MG	1A	3739	1/1	0.99	0.09	30,30,30,30	0
54	MG	2A	3269	1/1	0.99	0.20	34,34,34,34	0
54	MG	1A	3126	1/1	0.99	0.18	25,25,25,25	0
54	MG	1A	4039	1/1	0.99	0.21	31,31,31,31	0
54	MG	1a	1713	1/1	0.99	0.15	52,52,52,52	0
54	MG	1A	3576	1/1	0.99	0.11	36,36,36,36	0
54	MG	1A	3042	1/1	0.99	0.17	12,12,12,12	0
54	MG	1A	4042	1/1	0.99	0.31	31,31,31,31	0
54	MG	2A	3118	1/1	0.99	0.16	46,46,46,46	0
54	MG	1A	3668	1/1	1.00	0.24	13,13,13,13	0
54	MG	1A	3911	1/1	1.00	0.16	20,20,20,20	0

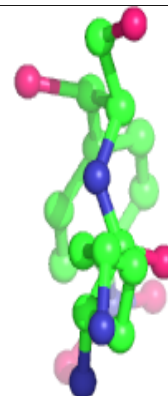
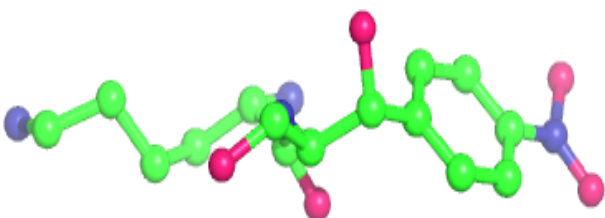
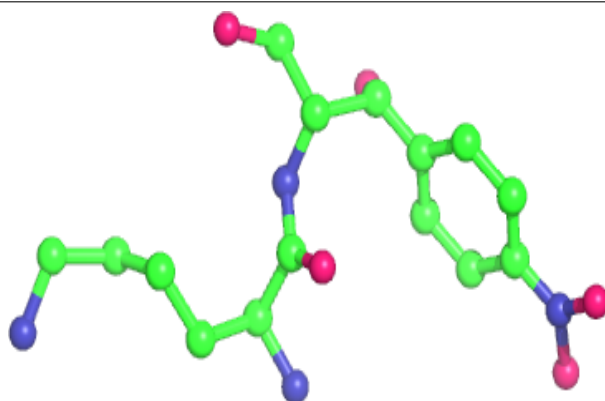
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EZM 2A 3691:

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

**Electron density around EZM 1A 4035:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.