



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 10:23 AM EST

PDB ID : 7RQA
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with protein Y, A-site aminoacyl-tRNA analog ACC-PMN, and P-site MTI-tripeptidyl-tRNA analog ACCA-ITM at 2.40Å resolution
Authors : Syroegin, E.A.; Flemmich, L.; Klepacki, D.; Vazquez-Laslop, N.; Micura, R.; Polikanov, Y.S.
Deposited on : 2021-08-06
Resolution : 2.40 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
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

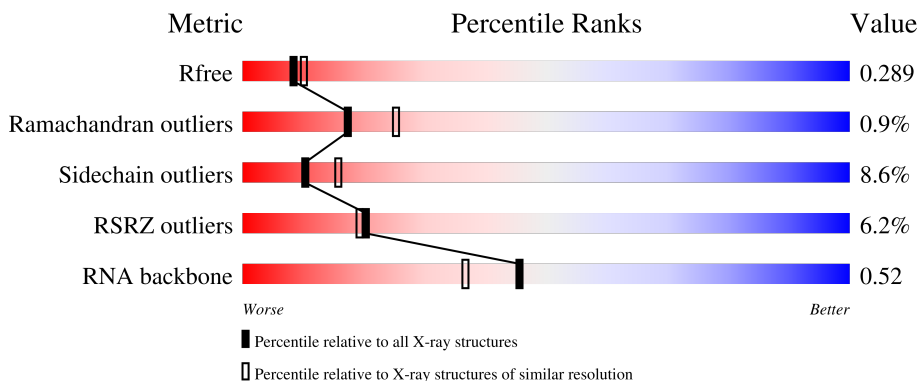
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

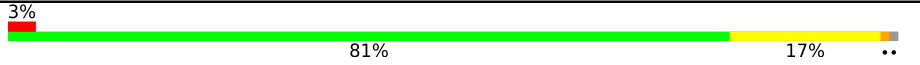



The reported resolution of this entry is 2.40 Å.

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.



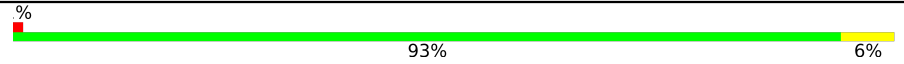
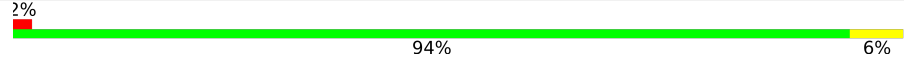
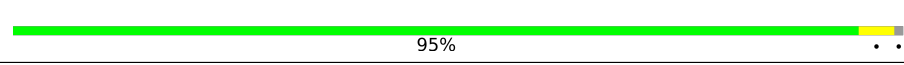
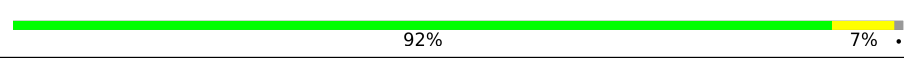
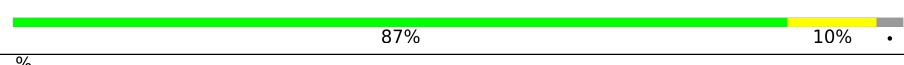
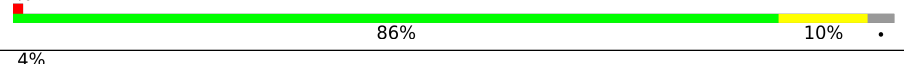
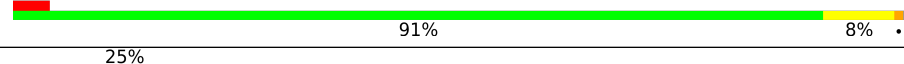
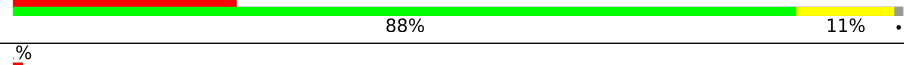
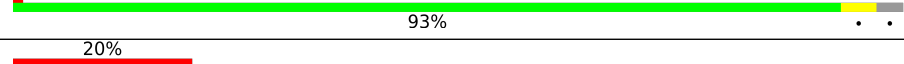
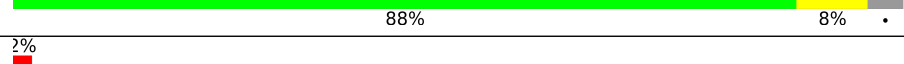
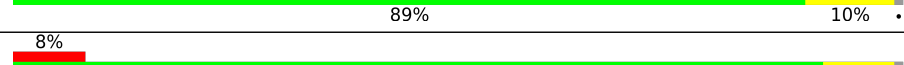
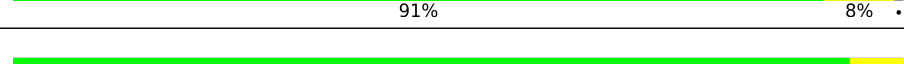
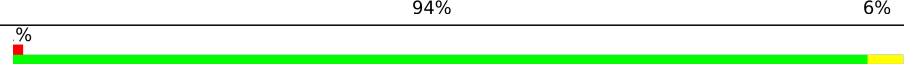
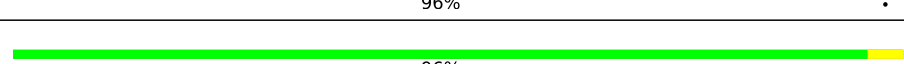
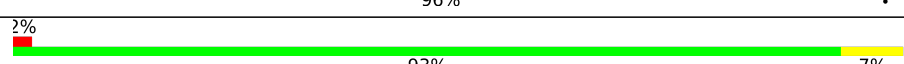
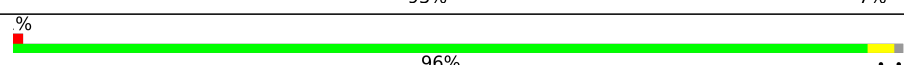
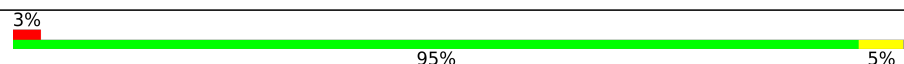
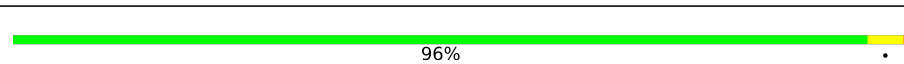
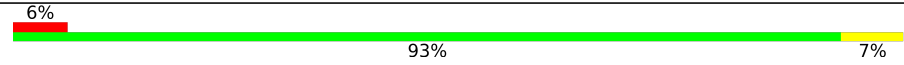
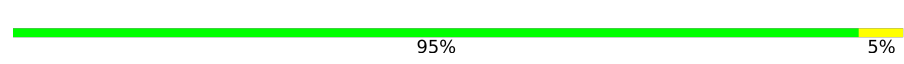
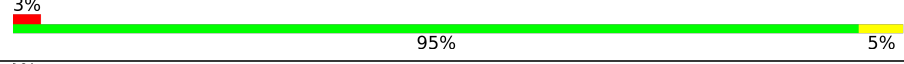
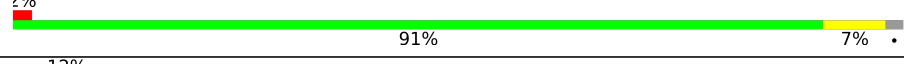
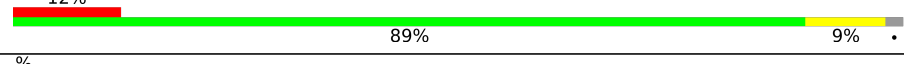


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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	 3% 81% 17% ..
1	2A	2915	 4% 80% 18% ..
2	1B	121	 84% 15% .
2	2B	121	 88% 11% .


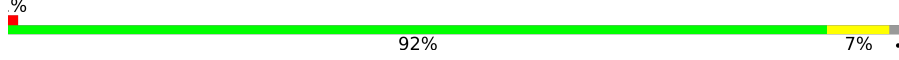
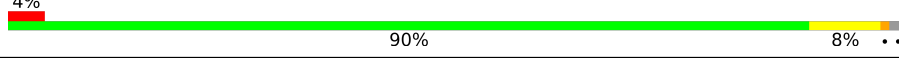
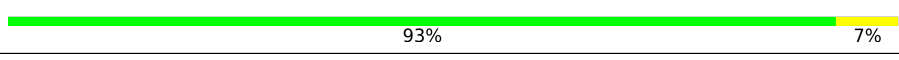
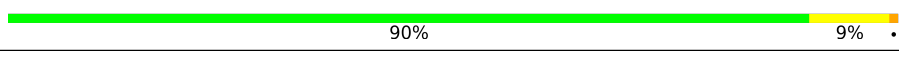
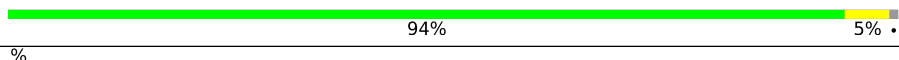
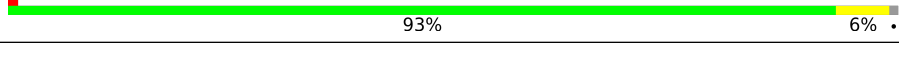
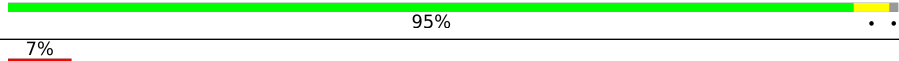
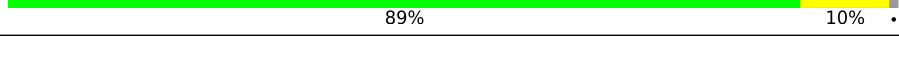
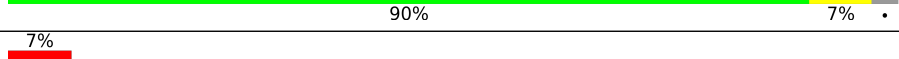
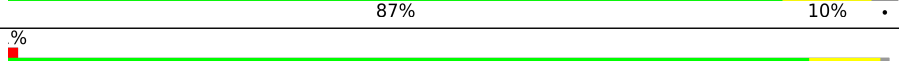
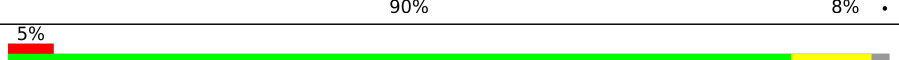
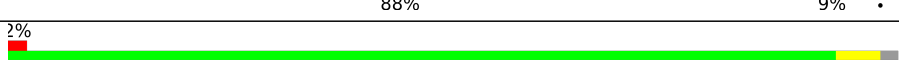
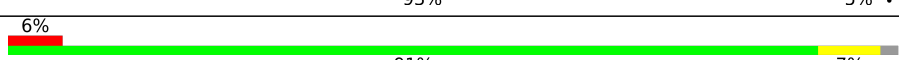
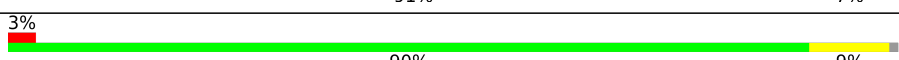
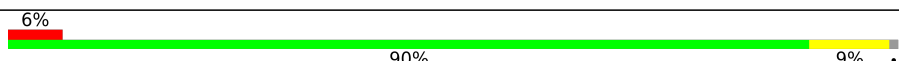
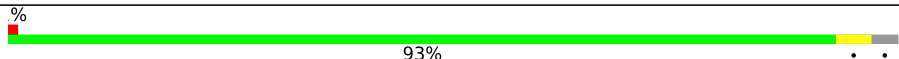
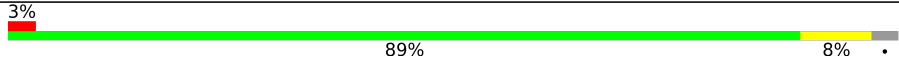
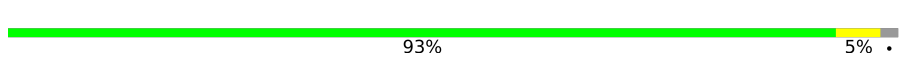
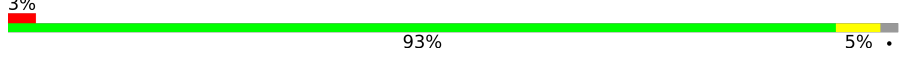

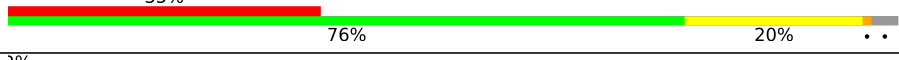
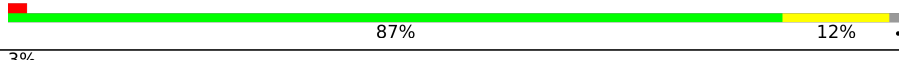
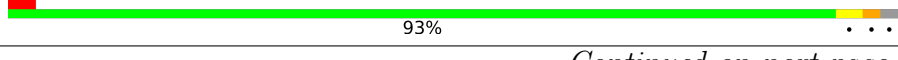

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Mol	Chain	Length	Quality of chain
3	1D	276	 93% 6%
3	2D	276	 94% 6%
4	1E	206	 95%
4	2E	206	 92% 7%
5	1F	210	 87% 10%
5	2F	210	 86% 10%
6	1G	182	 91% 8%
6	2G	182	 88% 11%
7	1H	180	 93%
7	2H	180	 88% 8%
8	1I	148	 89% 10%
8	2I	148	 91% 8%
9	1N	140	 94% 6%
9	2N	140	 96%
10	1O	122	 96%
10	2O	122	 93% 7%
11	1P	150	 96%
11	2P	150	 95% 5%
12	1Q	141	 96%
12	2Q	141	 93% 7%
13	1R	118	 95% 5%
13	2R	118	 95% 5%
14	1S	112	 91% 7%
14	2S	112	 89% 9%
15	1T	146	 84% 6% 10%

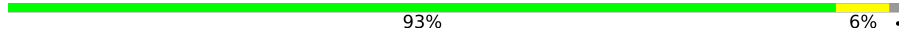

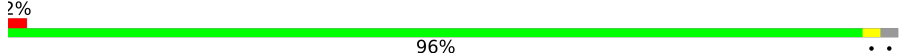

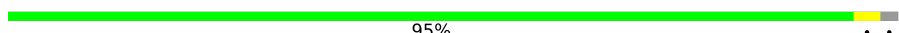

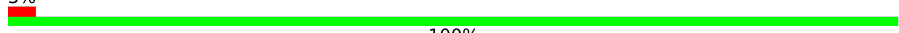





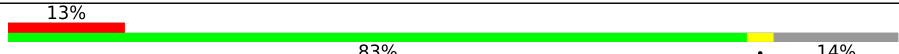
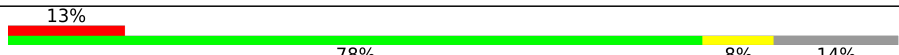
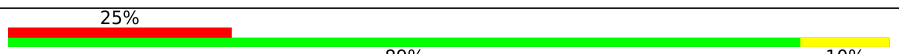
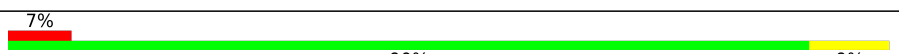
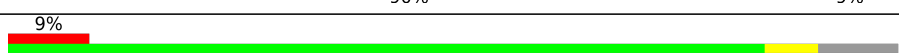




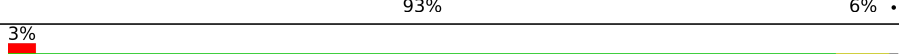
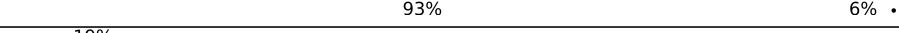

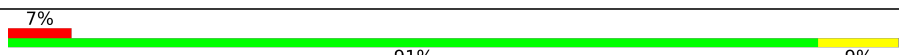
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Mol	Chain	Length	Quality of chain
15	2T	146	 %
16	1U	118	 %
16	2U	118	 4%
17	1V	101	 93% 7%
17	2V	101	 90% 9%
18	1W	113	 94% 5%
18	2W	113	 %
19	1X	96	 95%
19	2X	96	 7%
20	1Y	110	 90% 7%
20	2Y	110	 7%
21	1Z	206	 %
21	2Z	206	 5%
22	10	85	 2%
22	20	85	 6%
23	11	98	 3%
23	21	98	 6%
24	12	72	 %
24	22	72	 3%
25	13	60	 93% 5%
25	23	60	 3%
26	14	71	 15%
26	24	71	 35%
27	15	60	 2%
27	25	60	 3%

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Mol	Chain	Length	Quality of chain
28	16	54	 93% 6%
28	26	54	 4% 83% 15%
29	17	49	 2% 96%
29	27	49	 8% 86% 12%
30	18	65	 95%
30	28	65	 8% 91% 8%
31	19	37	 3% 100%
31	29	37	 5% 100%
32	1a	1521	 4% 81% 18%
32	2a	1521	 5% 79% 19%
33	1b	256	 10% 80% 9% 10%
33	2b	256	 12% 77% 13% 10%
34	1c	239	 13% 83% 14%
34	2c	239	 13% 78% 8% 14%
35	1d	209	 25% 89% 10%
35	2d	209	 7% 90% 9%
36	1e	162	 9% 85% 6% 9%
36	2e	162	 4% 84% 7% 9%
37	1f	101	 86% 13%
37	2f	101	 93% 6%
38	1g	156	 3% 93% 6%
38	2g	156	 19% 90% 9%
39	1h	138	 7% 91% 9%
39	2h	138	 6% 91% 9%
40	1i	128	 25% 91% 9%

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Mol	Chain	Length	Quality of chain
40	2i	128	38% 89% 9%
41	1j	105	24% 82% 10% 8%
41	2j	105	26% 85% 7% 9%
42	1k	129	3% 83% 5% 12%
42	2k	129	9% 83% 5% 12%
43	1l	132	5% 87% 5% 8%
43	2l	132	5% 87% 5% 8%
44	1m	126	7% 87% 6% 8%
44	2m	126	19% 79% 12% 10%
45	1n	61	25% 92% 7%
45	2n	61	39% 87% 11%
46	1o	89	3% 96%
46	2o	89	3% 94%
47	1p	88	20% 88% 6% 7%
47	2p	88	3% 82% 11% 7%
48	1q	105	16% 82% 12% 6%
48	2q	105	6% 89% 5% 6%
49	1r	88	2% 72% 6% 23%
49	2r	88	3% 76% 23%
50	1s	93	6% 86% 11%
50	2s	93	22% 78% 11% 11%
51	1t	106	25% 83% 8% 9%
51	2t	106	7% 85% 7% 8%
52	1u	27	15% 85% 15%
52	2u	27	44% 78% 7% 15%

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Mol	Chain	Length	Quality of chain
53	1y	113	
53	2y	113	
54	1w	4	
54	2w	4	
55	1x	4	
55	2x	4	
56	1v	3	
56	2v	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1A	3960	-	-	-	X
57	MG	2A	3171	-	-	-	X
57	MG	2A	3173	-	-	-	X
57	MG	2A	3231	-	-	-	X

2 Entry composition [i](#)

There are 63 unique types of molecules in this entry. The entry contains 297986 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
			Total	C	N	O	S			
21	1Z	203	Total 1587	C 1011	N 282	O 292	S 2	0	0	0
21	2Z	201	Total 1557	C 995	N 274	O 286	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	10	83	Total 653	C 404	N 139	O 109	S 1	0	0	0
22	20	83	Total 650	C 401	N 139	O 109	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	11	97	Total 754	C 475	N 148	O 130	S 1	0	0	0
23	21	97	Total 759	C 478	N 149	O 131	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	12	70	Total 588	C 365	N 118	O 103	S 2	0	0	0
24	22	70	Total 592	C 368	N 119	O 103	S 2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	14	69	Total 546	C 346	N 96	O 99	S 5	0	0	0

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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 Ribosome-associated inhibitor A.

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 a RNA chain called A-site Aminoacyl-tRNA Analog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	4	Total	C	N	O	P	0	0	1
			78	40	13	22	3			
54	2w	4	Total	C	N	O	P	0	0	1
			78	40	13	22	3			

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA Analog RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1x	4	Total	C	N	O	P	0	0	1
			63	28	12	20	3			
55	2x	4	Total	C	N	O	P	0	0	1
			63	28	12	20	3			

- Molecule 56 is a protein called P-site Peptidyl-tRNA Analog Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1v	3	Total	C	N	O	S	0	0	0
			23	15	3	4	1			
56	2v	3	Total	C	N	O	S	0	0	0
			23	15	3	4	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1028	Total	Mg	0	0
			1028	1028		
57	1B	30	Total	Mg	0	0
			30	30		
57	1D	18	Total	Mg	0	0
			18	18		
57	1E	10	Total	Mg	0	0
			10	10		
57	1F	16	Total	Mg	0	0
			16	16		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1G	4	Total Mg 4 4	0	0
57	1H	2	Total Mg 2 2	0	0
57	1N	4	Total Mg 4 4	0	0
57	1O	1	Total Mg 1 1	0	0
57	1P	4	Total Mg 4 4	0	0
57	1Q	5	Total Mg 5 5	0	0
57	1R	4	Total Mg 4 4	0	0
57	1T	4	Total Mg 4 4	0	0
57	1U	8	Total Mg 8 8	0	0
57	1V	7	Total Mg 7 7	0	0
57	1W	2	Total Mg 2 2	0	0
57	1X	1	Total Mg 1 1	0	0
57	1Z	1	Total Mg 1 1	0	0
57	10	8	Total Mg 8 8	0	0
57	11	5	Total Mg 5 5	0	0
57	13	3	Total Mg 3 3	0	0
57	15	8	Total Mg 8 8	0	0
57	17	5	Total Mg 5 5	0	0
57	18	3	Total Mg 3 3	0	0
57	19	3	Total Mg 3 3	0	0
57	1a	280	Total Mg 280 280	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1b	1	Total Mg 1 1	0	0
57	1d	6	Total Mg 6 6	0	0
57	1e	3	Total Mg 3 3	0	0
57	1f	2	Total Mg 2 2	0	0
57	1g	2	Total Mg 2 2	0	0
57	1h	2	Total Mg 2 2	0	0
57	1i	1	Total Mg 1 1	0	0
57	1l	2	Total Mg 2 2	0	0
57	1m	1	Total Mg 1 1	0	0
57	1n	1	Total Mg 1 1	0	0
57	1o	2	Total Mg 2 2	0	0
57	1t	2	Total Mg 2 2	0	0
57	1y	3	Total Mg 3 3	0	0
57	1w	1	Total Mg 1 1	0	0
57	1x	2	Total Mg 2 2	0	0
57	2A	737	Total Mg 737 737	0	0
57	2B	20	Total Mg 20 20	0	0
57	2D	11	Total Mg 11 11	0	0
57	2E	6	Total Mg 6 6	0	0
57	2F	4	Total Mg 4 4	0	0
57	2G	2	Total Mg 2 2	0	0

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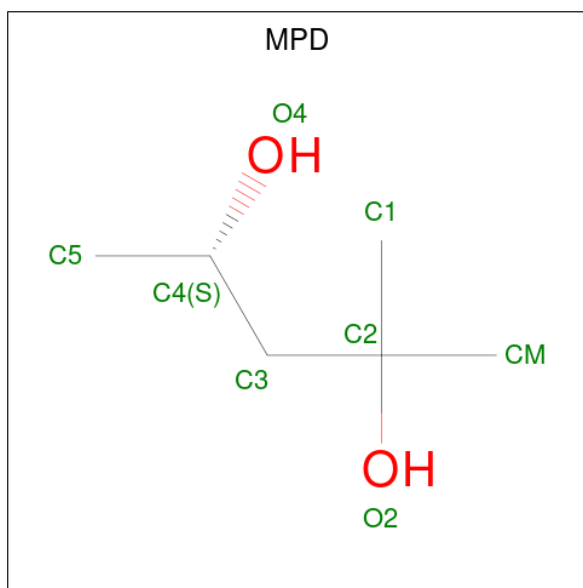
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2I	1	Total Mg 1 1	0	0
57	2N	1	Total Mg 1 1	0	0
57	2O	1	Total Mg 1 1	0	0
57	2P	3	Total Mg 3 3	0	0
57	2Q	4	Total Mg 4 4	0	0
57	2R	3	Total Mg 3 3	0	0
57	2T	4	Total Mg 4 4	0	0
57	2U	1	Total Mg 1 1	0	0
57	2V	3	Total Mg 3 3	0	0
57	2W	2	Total Mg 2 2	0	0
57	2Y	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	21	1	Total Mg 1 1	0	0
57	23	1	Total Mg 1 1	0	0
57	25	3	Total Mg 3 3	0	0
57	26	1	Total Mg 1 1	0	0
57	27	1	Total Mg 1 1	0	0
57	28	1	Total Mg 1 1	0	0
57	2a	191	Total Mg 191 191	0	0
57	2e	2	Total Mg 2 2	0	0
57	2f	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2h	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0
57	2k	2	Total Mg 2 2	0	0
57	2p	1	Total Mg 1 1	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2x	1	Total Mg 1 1	0	0

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



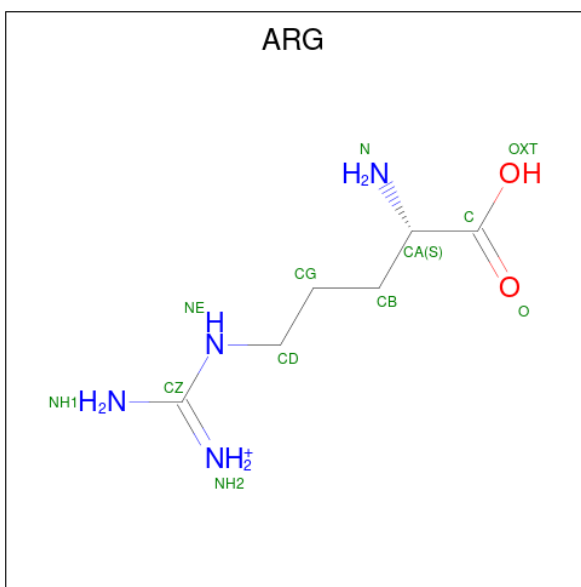
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total C O 8 6 2	0	0
58	1T	1	Total C O 8 6 2	0	0
58	18	1	Total C O 8 6 2	0	0
58	1a	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	2A	1	Total	C	O	0	0
			8	6	2		
58	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 59 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	1B	1	Total	C	N	O	0	0
			12	6	4	2		
59	1F	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

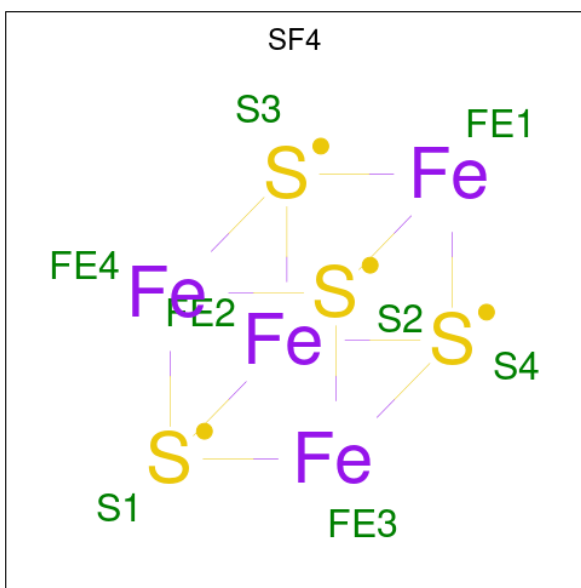
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		

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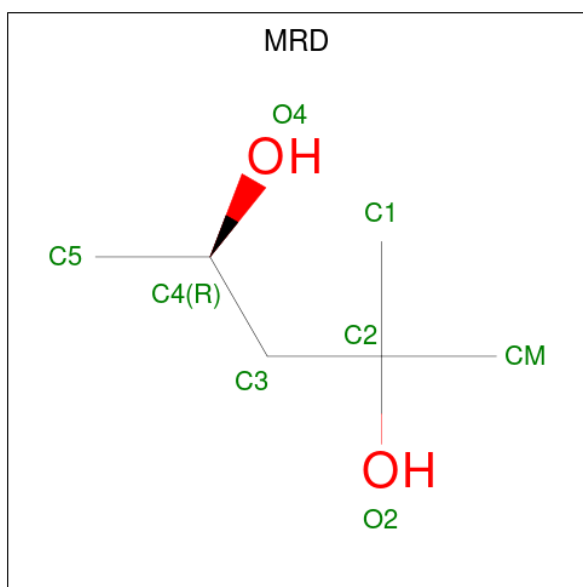
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		
60	26	1	Total	Zn	0	0
			1	1		
60	29	1	Total	Zn	0	0
			1	1		
60	2n	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	1d	1	Total	Fe	S	0	0
			8	4	4		
61	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 62 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2A	1	Total	C O	0	0
			8	6 2		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1A	3988	Total	O	0	0
			3988	3988		
63	1B	97	Total	O	0	0
			97	97		
63	1D	113	Total	O	0	0
			113	113		
63	1E	76	Total	O	0	0
			76	76		
63	1F	67	Total	O	0	0
			67	67		
63	1G	19	Total	O	0	0
			19	19		
63	1H	11	Total	O	0	0
			11	11		
63	1I	8	Total	O	0	0
			8	8		
63	1N	52	Total	O	0	0
			52	52		
63	1O	22	Total	O	0	0
			22	22		
63	1P	66	Total	O	0	0
			66	66		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1Q	36	Total 36	O 36	0	0
63	1R	32	Total 32	O 32	0	0
63	1S	12	Total 12	O 12	0	0
63	1T	34	Total 34	O 34	0	0
63	1U	47	Total 47	O 47	0	0
63	1V	40	Total 40	O 40	0	0
63	1W	33	Total 33	O 33	0	0
63	1X	26	Total 26	O 26	0	0
63	1Y	16	Total 16	O 16	0	0
63	1Z	14	Total 14	O 14	0	0
63	10	24	Total 24	O 24	0	0
63	11	27	Total 27	O 27	0	0
63	12	18	Total 18	O 18	0	0
63	13	24	Total 24	O 24	0	0
63	14	3	Total 3	O 3	0	0
63	15	24	Total 24	O 24	0	0
63	16	18	Total 18	O 18	0	0
63	17	12	Total 12	O 12	0	0
63	18	27	Total 27	O 27	0	0
63	19	6	Total 6	O 6	0	0
63	1a	511	Total 511	O 511	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1b	1	Total O 1 1	0	0
63	1d	8	Total O 8 8	0	0
63	1e	3	Total O 3 3	0	0
63	1f	2	Total O 2 2	0	0
63	1j	1	Total O 1 1	0	0
63	1k	1	Total O 1 1	0	0
63	1l	3	Total O 3 3	0	0
63	1m	1	Total O 1 1	0	0
63	1o	3	Total O 3 3	0	0
63	1p	2	Total O 2 2	0	0
63	1t	1	Total O 1 1	0	0
63	1y	7	Total O 7 7	0	0
63	1w	6	Total O 6 6	0	0
63	1x	5	Total O 5 5	0	0
63	2A	2224	Total O 2224 2224	0	0
63	2B	45	Total O 45 45	0	0
63	2D	50	Total O 50 50	0	0
63	2E	29	Total O 29 29	0	0
63	2F	22	Total O 22 22	0	0
63	2G	7	Total O 7 7	0	0
63	2H	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2I	3	Total 3	O 3	0	0
63	2N	2	Total 2	O 2	0	0
63	2O	16	Total 16	O 16	0	0
63	2P	25	Total 25	O 25	0	0
63	2Q	16	Total 16	O 16	0	0
63	2R	20	Total 20	O 20	0	0
63	2S	5	Total 5	O 5	0	0
63	2T	10	Total 10	O 10	0	0
63	2U	12	Total 12	O 12	0	0
63	2V	9	Total 9	O 9	0	0
63	2W	23	Total 23	O 23	0	0
63	2X	7	Total 7	O 7	0	0
63	2Y	6	Total 6	O 6	0	0
63	2Z	11	Total 11	O 11	0	0
63	20	14	Total 14	O 14	0	0
63	21	20	Total 20	O 20	0	0
63	22	3	Total 3	O 3	0	0
63	23	4	Total 4	O 4	0	0
63	24	2	Total 2	O 2	0	0
63	25	9	Total 9	O 9	0	0
63	26	5	Total 5	O 5	0	0

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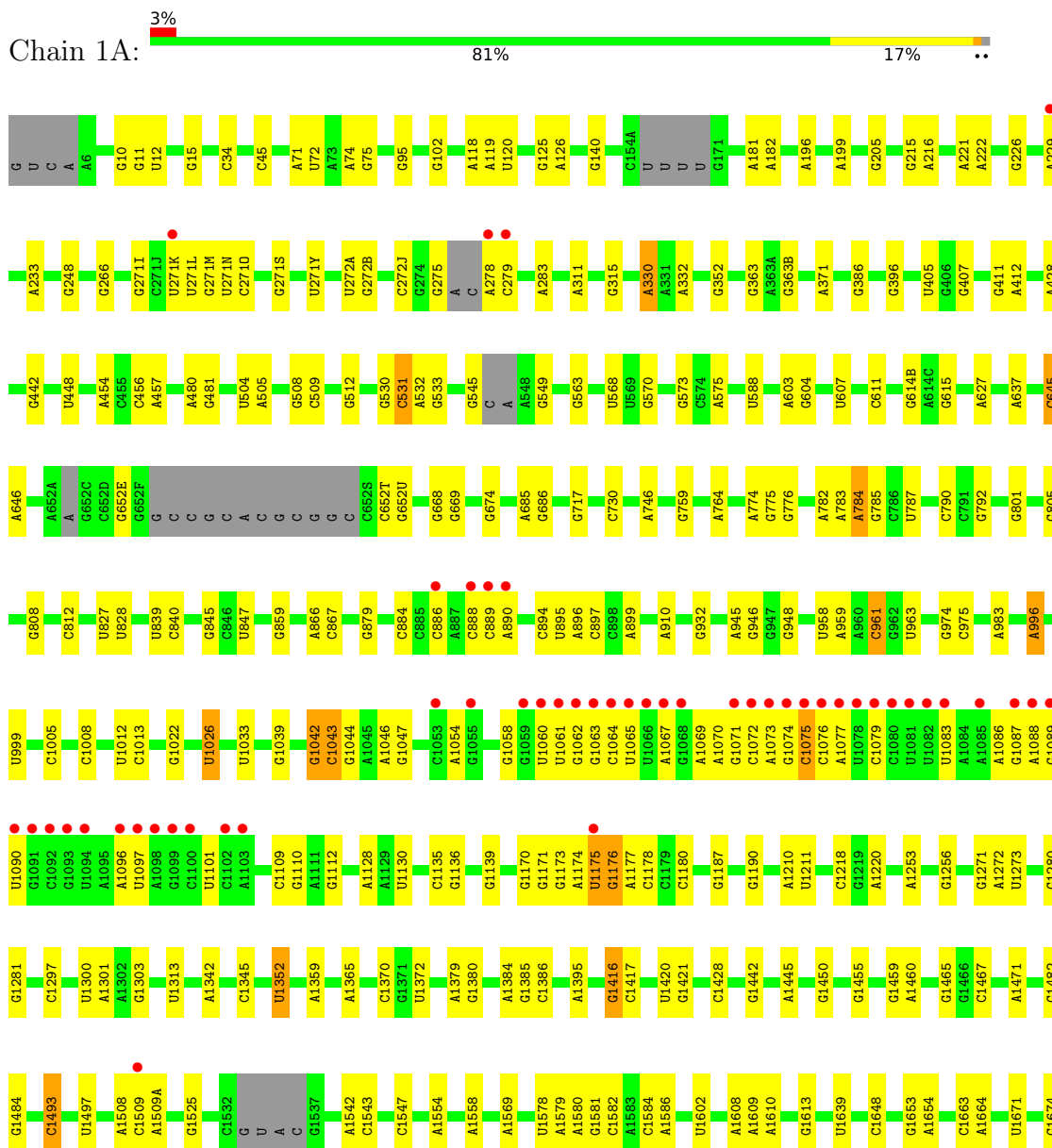
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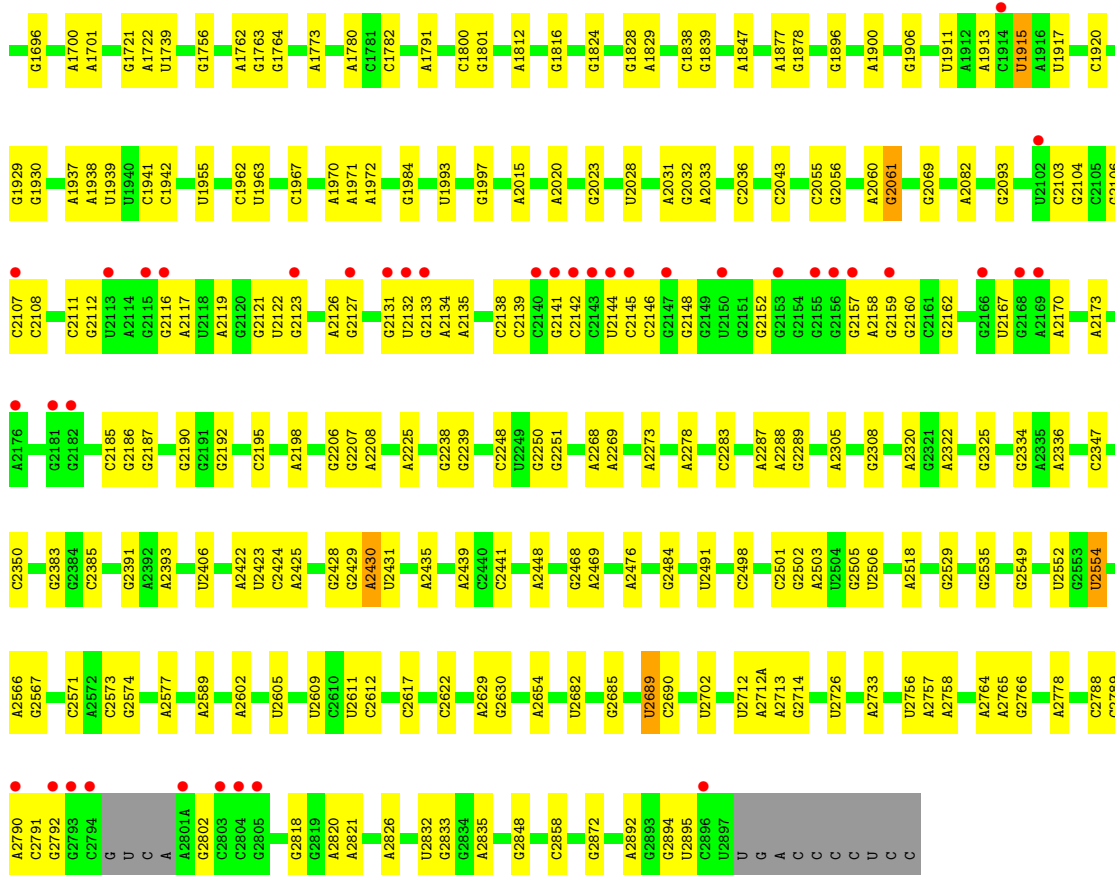
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	27	9	Total 9	O 9	0	0
63	28	12	Total 12	O 12	0	0
63	29	1	Total 1	O 1	0	0
63	2a	384	Total 384	O 384	0	0
63	2d	4	Total 4	O 4	0	0
63	2e	2	Total 2	O 2	0	0
63	2f	3	Total 3	O 3	0	0
63	2j	2	Total 2	O 2	0	0
63	2l	4	Total 4	O 4	0	0
63	2m	1	Total 1	O 1	0	0
63	2o	4	Total 4	O 4	0	0
63	2p	1	Total 1	O 1	0	0
63	2q	1	Total 1	O 1	0	0
63	2r	3	Total 3	O 3	0	0
63	2t	2	Total 2	O 2	0	0
63	2u	1	Total 1	O 1	0	0
63	2y	3	Total 3	O 3	0	0
63	2w	3	Total 3	O 3	0	0
63	2x	3	Total 3	O 3	0	0

3 Residue-property plots i

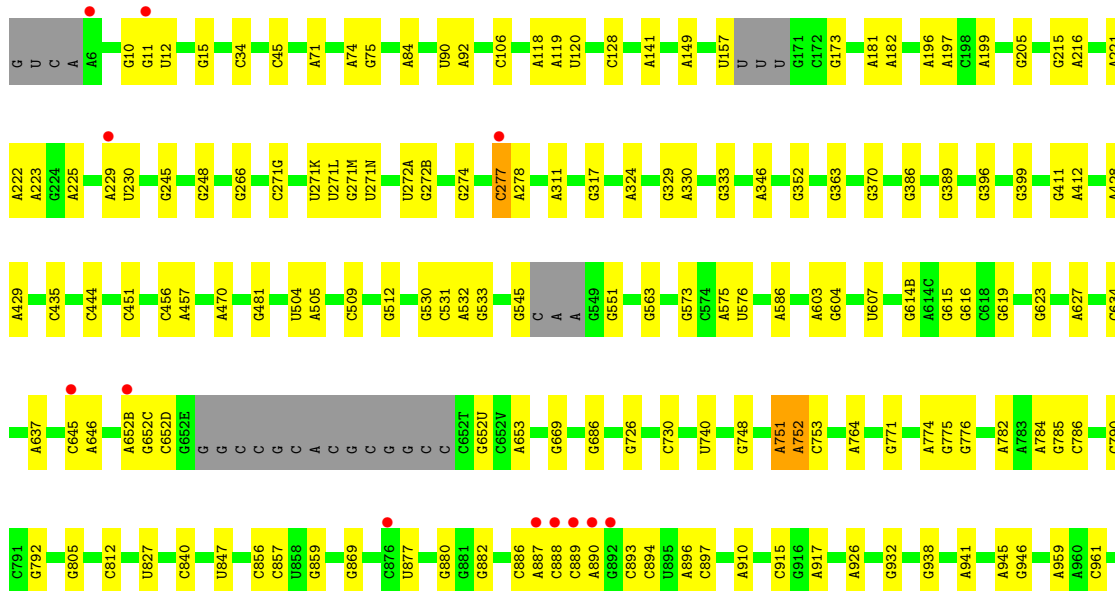
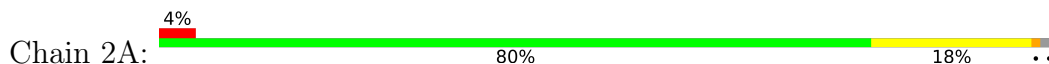
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S Ribosomal RNA



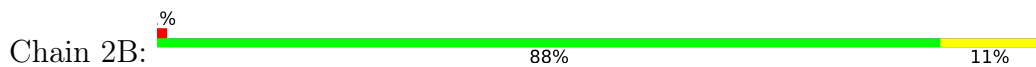


• Molecule 1: 23S Ribosomal RNA

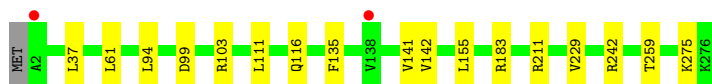




- Molecule 2: 5S Ribosomal RNA



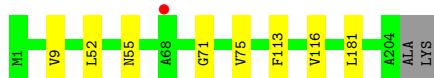
- Molecule 3: 50S ribosomal protein L2



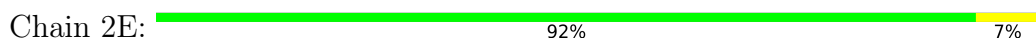
- Molecule 3: 50S ribosomal protein L2



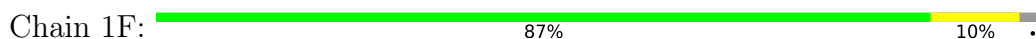
- Molecule 4: 50S ribosomal protein L3



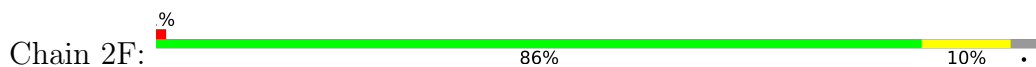
- Molecule 4: 50S ribosomal protein L3

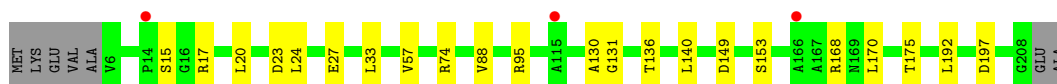


- Molecule 5: 50S ribosomal protein L4

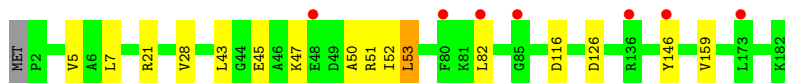
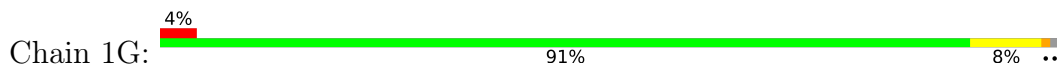


- Molecule 5: 50S ribosomal protein L4

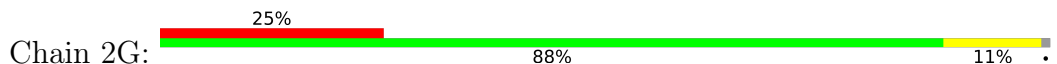




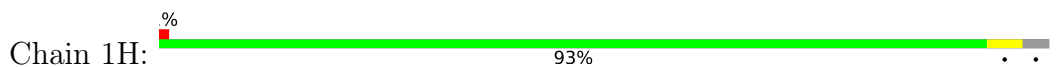
- Molecule 6: 50S ribosomal protein L5



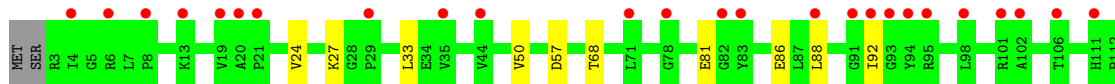
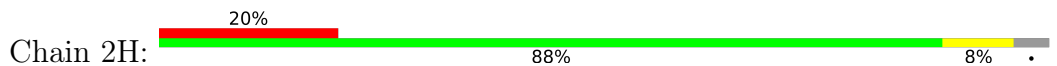
- Molecule 6: 50S ribosomal protein L5



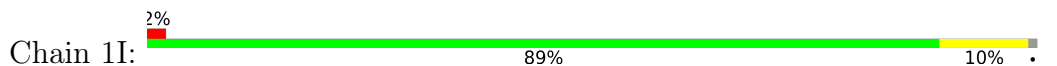
- Molecule 7: 50S ribosomal protein L6



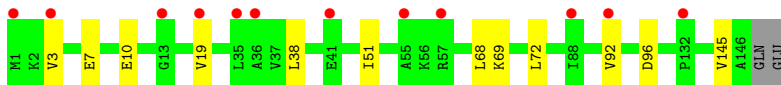
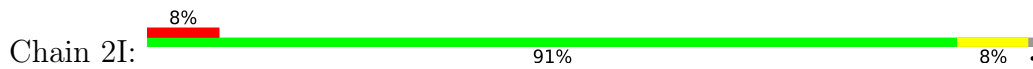
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



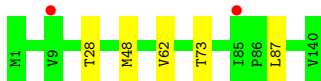
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



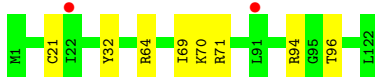
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14



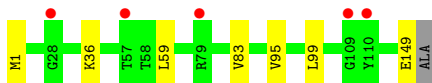
- Molecule 10: 50S ribosomal protein L14



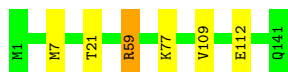
- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



• Molecule 12: 50S ribosomal protein L16



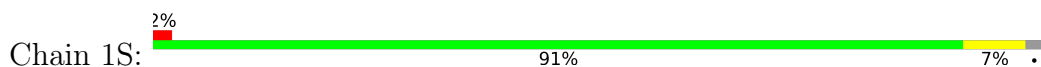
• Molecule 13: 50S ribosomal protein L17



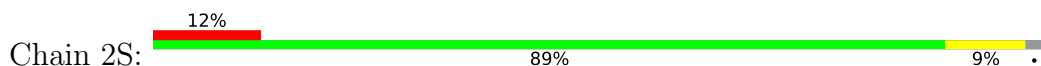
• Molecule 13: 50S ribosomal protein L17



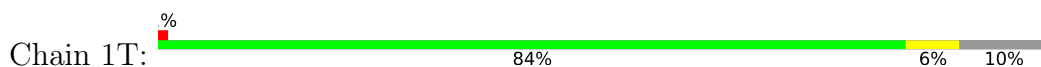
• Molecule 14: 50S ribosomal protein L18



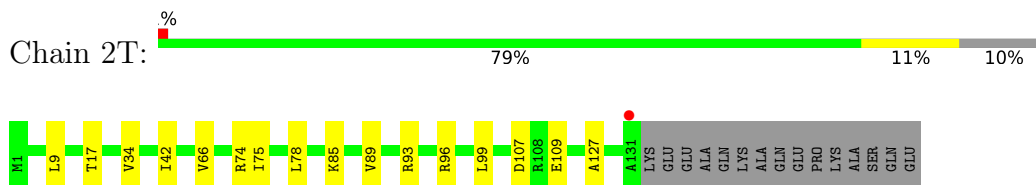
• Molecule 14: 50S ribosomal protein L18



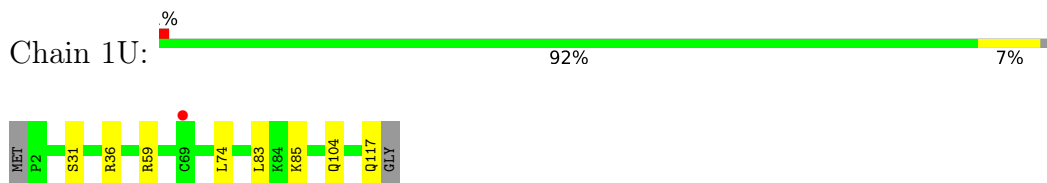
• Molecule 15: 50S ribosomal protein L19



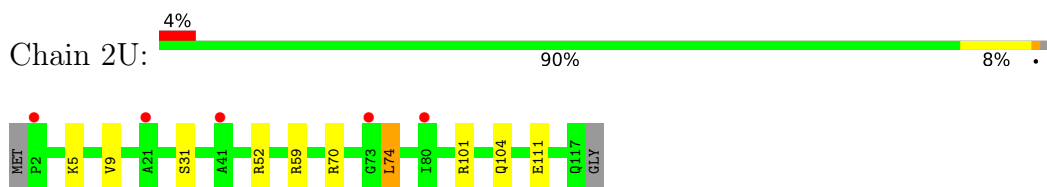
- Molecule 15: 50S ribosomal protein L19



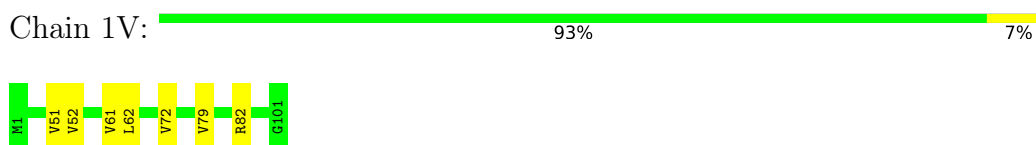
- Molecule 16: 50S ribosomal protein L20



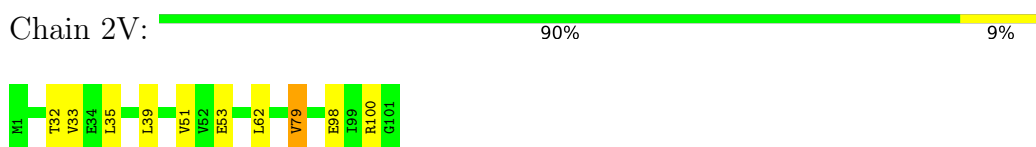
- Molecule 16: 50S ribosomal protein L20



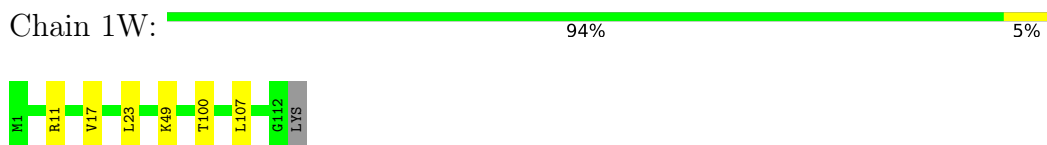
- Molecule 17: 50S ribosomal protein L21



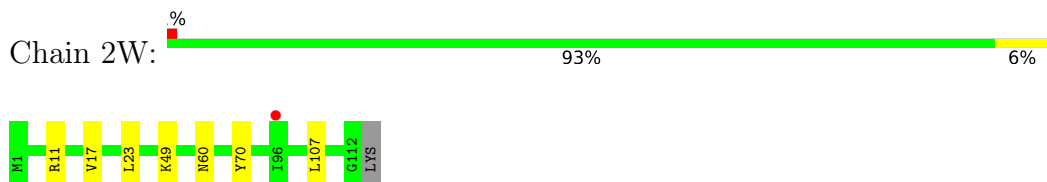
- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22

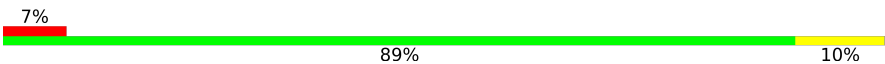


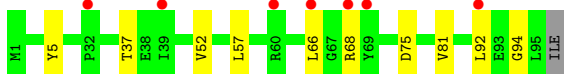
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  95%



- Molecule 19: 50S ribosomal protein L23

Chain 2X:  7% 89% 10%




- Molecule 20: 50S ribosomal protein L24

Chain 1Y:  90% 7%

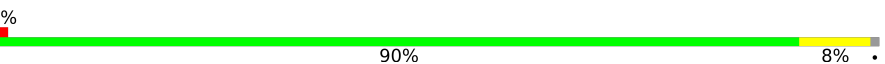


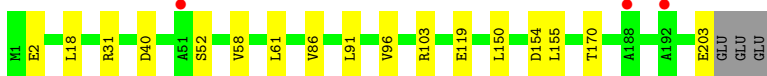
- Molecule 20: 50S ribosomal protein L24

Chain 2Y:  7% 87% 10%




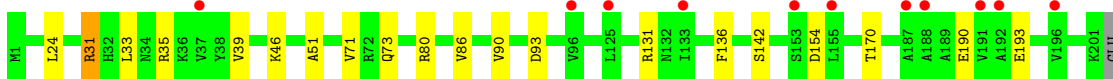
- Molecule 21: 50S ribosomal protein L25

Chain 1Z:  1% 90% 8%



- Molecule 21: 50S ribosomal protein L25

Chain 2Z:  5% 88% 9%

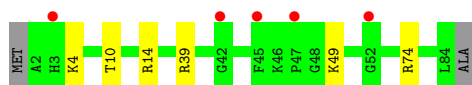


- Molecule 22: 50S ribosomal protein L27

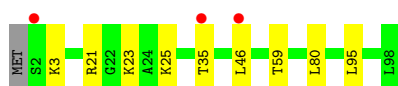
Chain 10:  2% 93% 5%



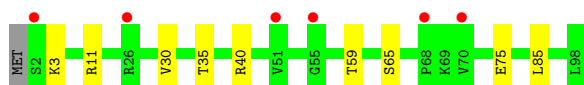
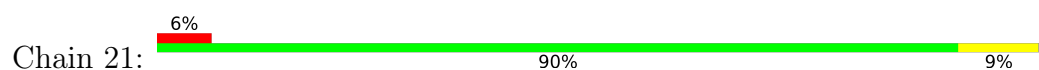
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



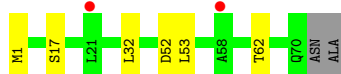
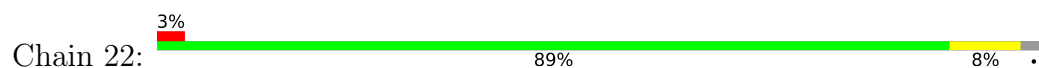
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



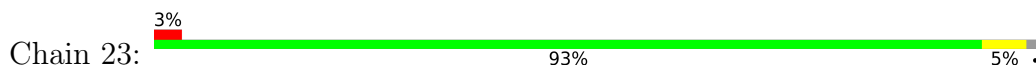
- Molecule 24: 50S ribosomal protein L29



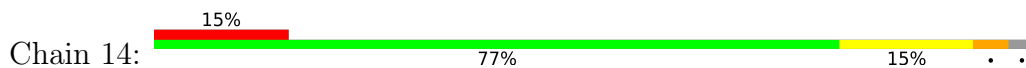
- Molecule 25: 50S ribosomal protein L30



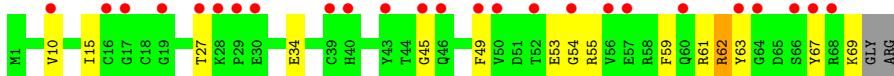
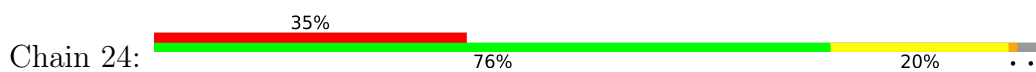
- Molecule 25: 50S ribosomal protein L30



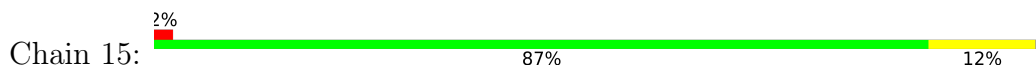
- Molecule 26: 50S ribosomal protein L31



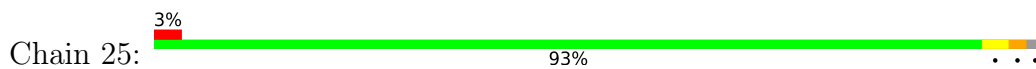
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



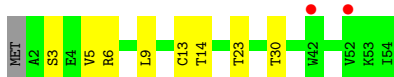
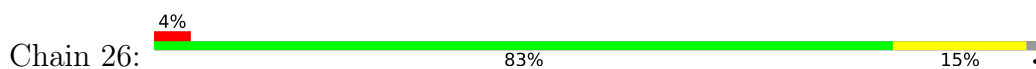
- Molecule 27: 50S ribosomal protein L32



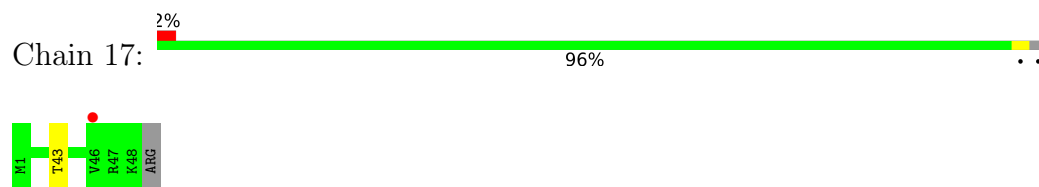
- Molecule 28: 50S ribosomal protein L33



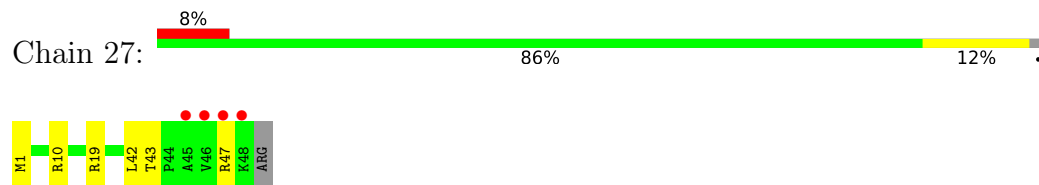
- Molecule 28: 50S ribosomal protein L33



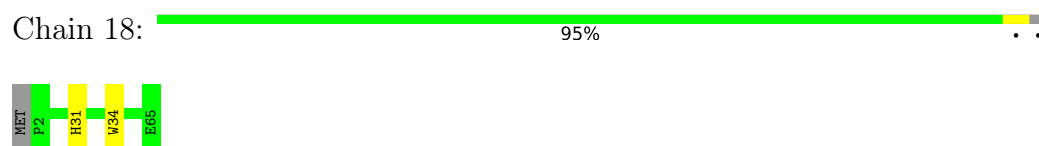
- Molecule 29: 50S ribosomal protein L34



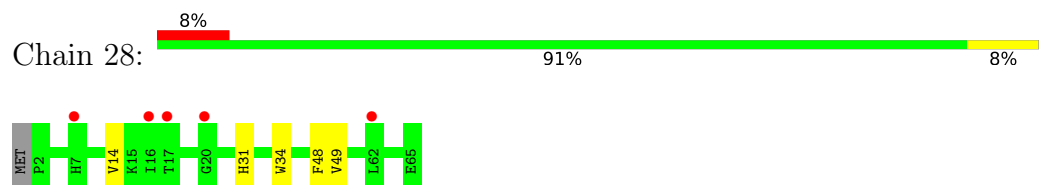
- Molecule 29: 50S ribosomal protein L34



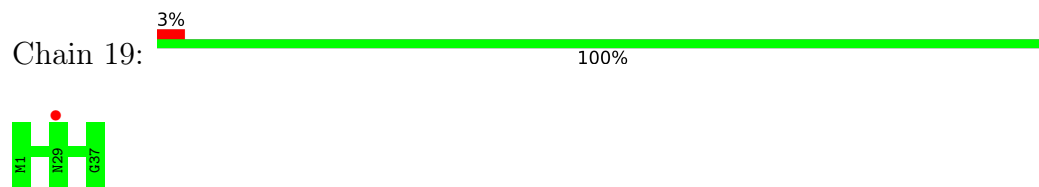
- Molecule 30: 50S ribosomal protein L35



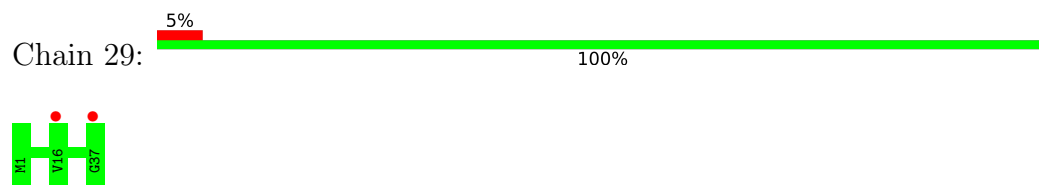
- Molecule 30: 50S ribosomal protein L35



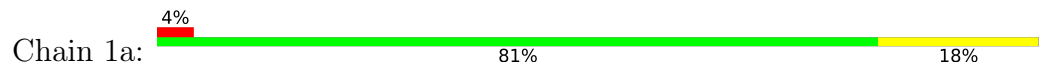
- Molecule 31: 50S ribosomal protein L36

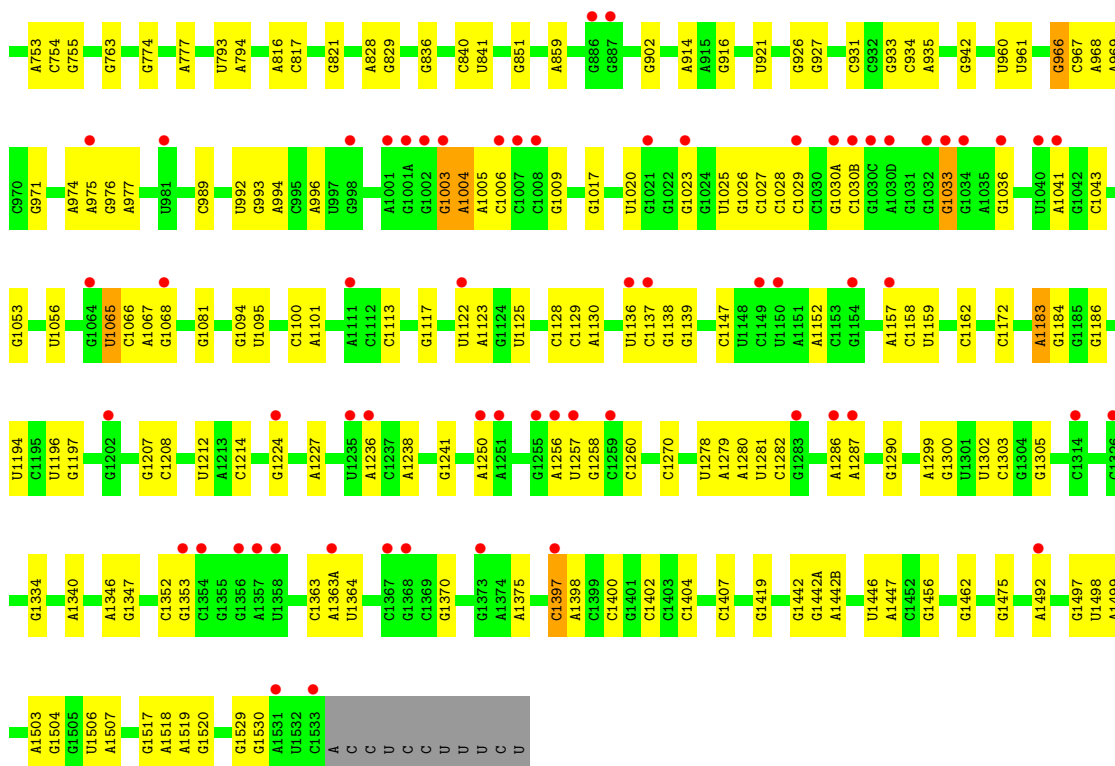


- Molecule 31: 50S ribosomal protein L36

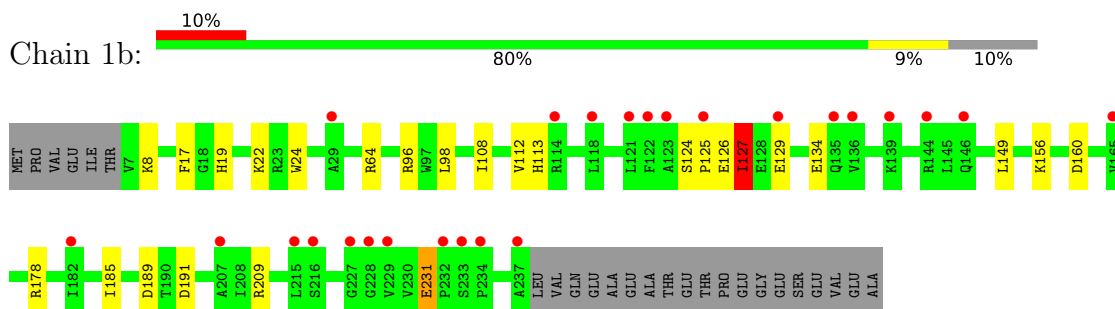


- Molecule 32: 16S Ribosomal RNA

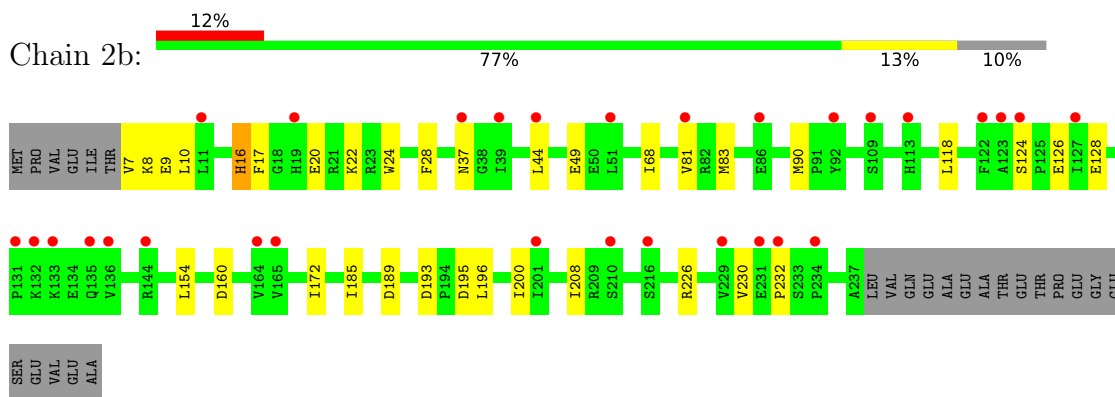




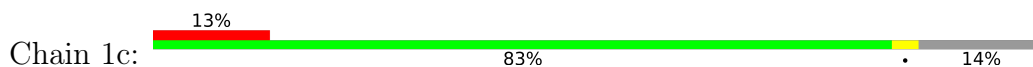
• Molecule 33: 30S ribosomal protein S2




• Molecule 33: 30S ribosomal protein S2



• Molecule 34: 30S ribosomal protein S3

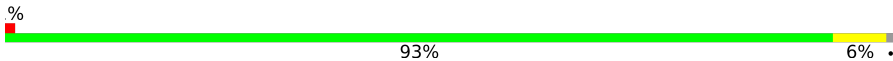


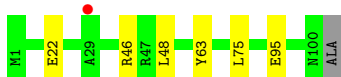
- Molecule 37: 30S ribosomal protein S6

Chain 1f:  86% 13%

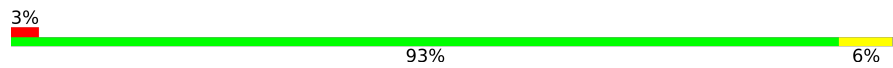


- Molecule 37: 30S ribosomal protein S6

Chain 2f:  93% 6%

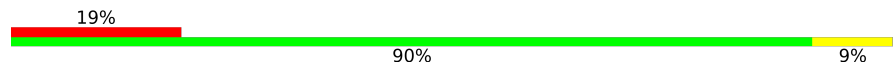


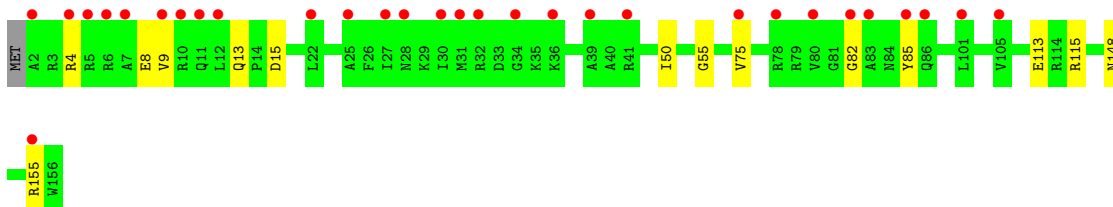
- Molecule 38: 30S ribosomal protein S7

Chain 1g:  93% 6% 3%

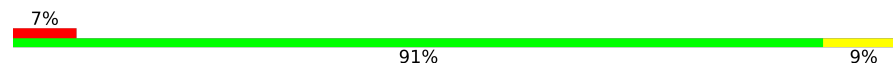


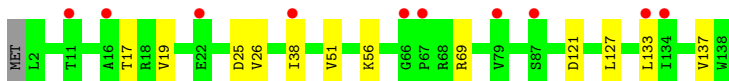
- Molecule 38: 30S ribosomal protein S7

Chain 2g:  90% 9% 19%

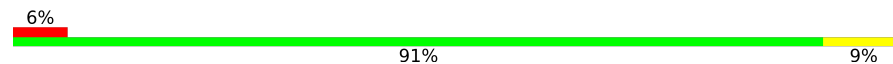


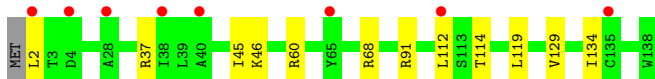
- Molecule 39: 30S ribosomal protein S8

Chain 1h:  91% 9% 7%

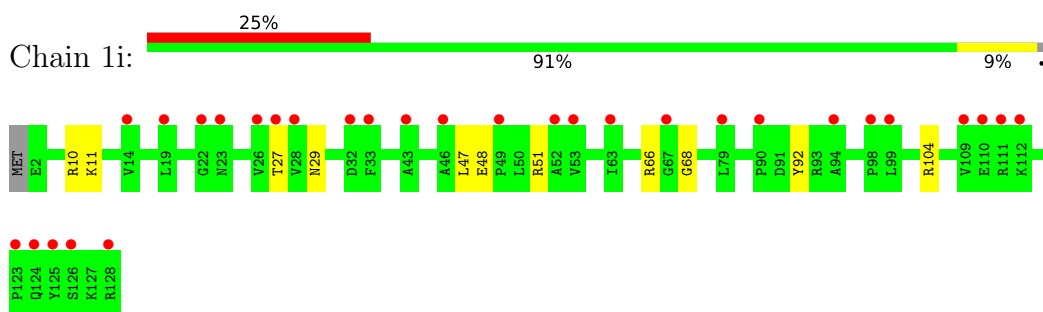


- Molecule 39: 30S ribosomal protein S8

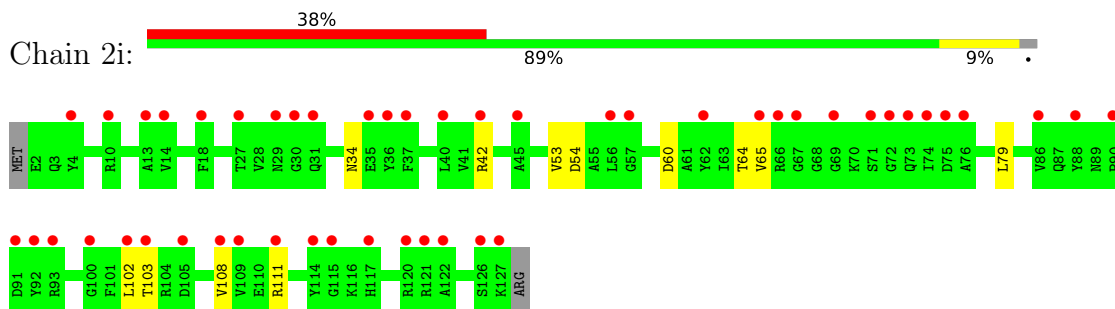
Chain 2h:  91% 9% 6%



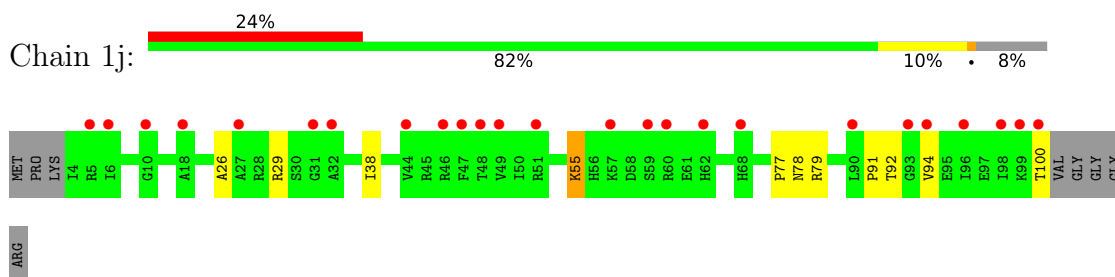
- Molecule 40: 30S ribosomal protein S9



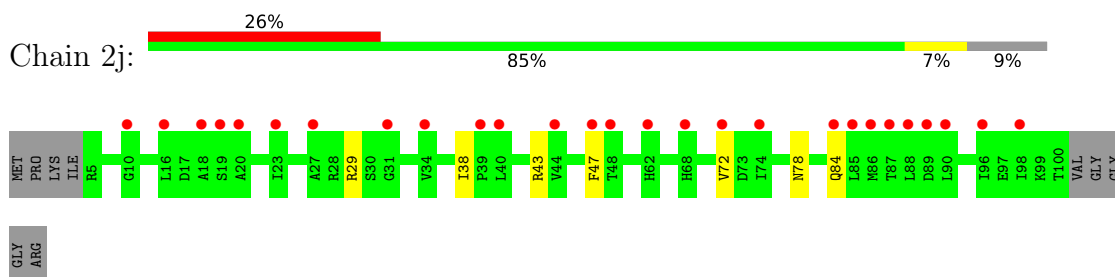
- Molecule 40: 30S ribosomal protein S9



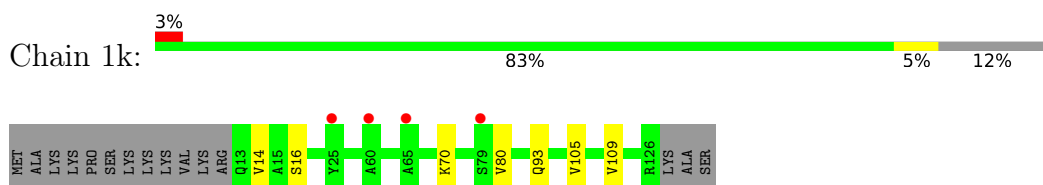
- Molecule 41: 30S ribosomal protein S10



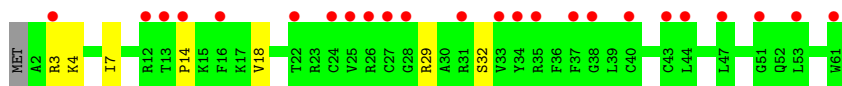
- Molecule 41: 30S ribosomal protein S10



- Molecule 42: 30S ribosomal protein S11



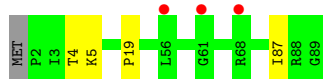
- Molecule 42: 30S ribosomal protein S11



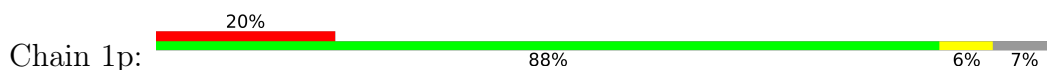
- Molecule 46: 30S ribosomal protein S15



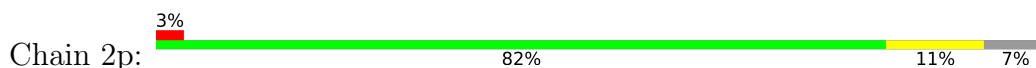
- Molecule 46: 30S ribosomal protein S15



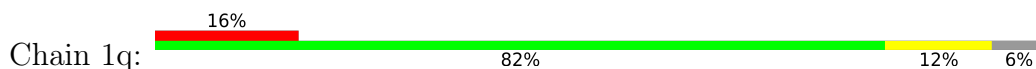
- Molecule 47: 30S ribosomal protein S16



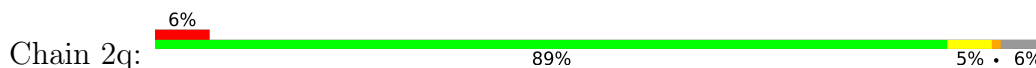
- Molecule 47: 30S ribosomal protein S16



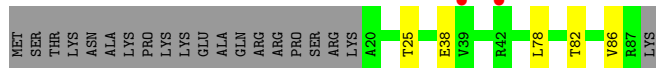
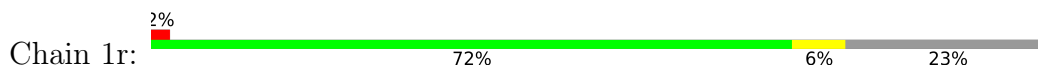
- Molecule 48: 30S ribosomal protein S17



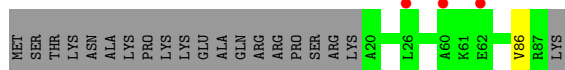
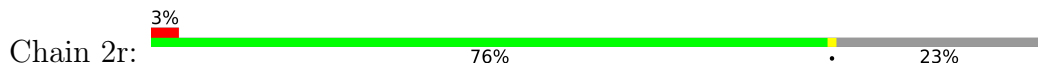
- Molecule 48: 30S ribosomal protein S17



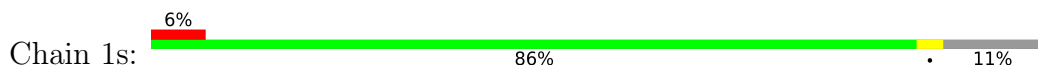
- Molecule 49: 30S ribosomal protein S18



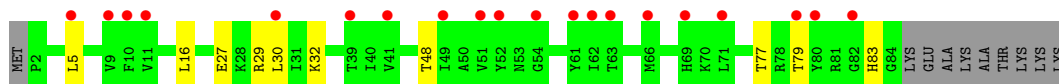
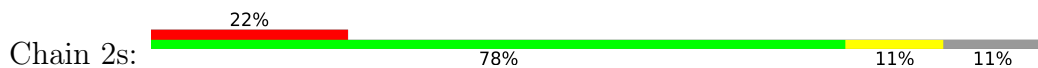
• Molecule 49: 30S ribosomal protein S18



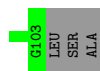
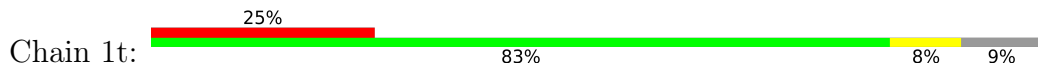
• Molecule 50: 30S ribosomal protein S19



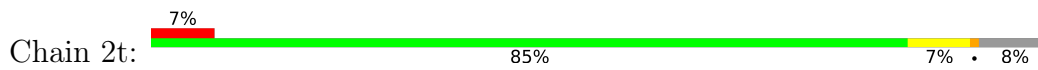
• Molecule 50: 30S ribosomal protein S19



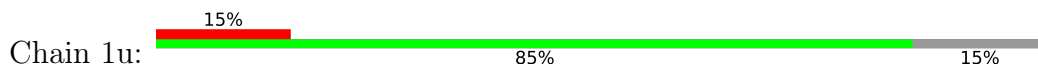
• Molecule 51: 30S ribosomal protein S20



• Molecule 51: 30S ribosomal protein S20



• Molecule 52: 30S ribosomal protein Thx



Chain 2x:  50% 50%


A73
C74
C75
A76

- Molecule 56: P-site Peptidyl-tRNA Analog Peptide

Chain 1v:  100%

There are no outlier residues recorded for this chain.

- Molecule 56: P-site Peptidyl-tRNA Analog Peptide

Chain 2v:  67% 100%


I1
I2
I3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.64Å 448.67Å 619.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	181.72 – 2.40 224.34 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (181.72-2.40) 99.7 (224.34-2.40)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.40Å)	Xtrriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.239 , 0.289 0.240 , 0.289	Depositor DCC
R_{free} test set	112220 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtrriage
Anisotropy	0.085	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	297986	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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: PPU, 2MA, 8AN, OMG, PSU, MRD, M2G, 0TD, ZN, OMC, 4OC, 2MG, 5MC, MG, G7M, UR3, 5MU, SF4, OMU, MPD, MA6

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	1/69031 (0.0%)	1.03	85/107754 (0.1%)
1	2A	0.41	2/68903 (0.0%)	0.91	74/107552 (0.1%)
2	1B	0.44	0/2876	0.97	1/4486 (0.0%)
2	2B	0.35	0/2878	0.85	0/4490
3	1D	0.35	0/2181	0.58	0/2940
3	2D	0.31	0/2186	0.52	0/2944
4	1E	0.34	0/1592	0.56	0/2149
4	2E	0.32	0/1592	0.51	0/2149
5	1F	0.34	0/1619	0.55	0/2193
5	2F	0.30	0/1615	0.51	0/2188
6	1G	0.31	0/1451	0.49	0/1961
6	2G	0.29	0/1449	0.48	0/1957
7	1H	0.32	0/1356	0.51	0/1834
7	2H	0.30	0/1350	0.49	0/1826
8	1I	0.30	0/1109	0.50	0/1512
8	2I	0.27	0/1091	0.48	0/1490
9	1N	0.35	0/1148	0.55	0/1547
9	2N	0.30	0/1144	0.46	0/1543
10	1O	0.34	0/943	0.56	0/1269
10	2O	0.32	0/943	0.52	0/1269
11	1P	0.34	0/1152	0.56	0/1533
11	2P	0.30	0/1152	0.51	0/1533
12	1Q	0.33	0/1143	0.52	0/1527
12	2Q	0.31	0/1143	0.48	0/1527
13	1R	0.33	0/982	0.56	0/1312
13	2R	0.30	0/982	0.50	0/1312
14	1S	0.31	0/887	0.51	0/1180
14	2S	0.31	0/880	0.54	0/1172
15	1T	0.35	0/1105	0.56	0/1477
15	2T	0.30	0/1097	0.50	0/1468
16	1U	0.36	0/977	0.55	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.30	0/977	0.49	1/1301 (0.1%)
17	1V	0.38	0/786	0.57	0/1053
17	2V	0.33	0/782	0.54	0/1049
18	1W	0.37	0/897	0.54	0/1205
18	2W	0.31	0/897	0.50	0/1205
19	1X	0.36	0/764	0.54	0/1025
19	2X	0.30	0/764	0.50	0/1025
20	1Y	0.33	0/823	0.53	0/1099
20	2Y	0.32	0/823	0.48	0/1100
21	1Z	0.32	0/1620	0.54	0/2200
21	2Z	0.31	0/1590	0.51	0/2162
22	10	0.36	0/662	0.56	0/881
22	20	0.31	0/659	0.54	0/877
23	11	0.33	0/761	0.54	0/1013
23	21	0.32	0/766	0.51	0/1018
24	12	0.29	0/590	0.51	0/781
24	22	0.29	0/594	0.47	0/785
25	13	0.37	0/474	0.51	0/635
25	23	0.29	0/469	0.49	0/630
26	14	0.33	0/559	0.58	0/754
26	24	0.34	0/549	0.59	0/741
27	15	0.39	0/473	0.66	1/639 (0.2%)
27	25	0.29	0/469	0.56	1/635 (0.2%)
28	16	0.35	0/460	0.58	0/613
28	26	0.30	0/456	0.50	0/608
29	17	0.38	0/426	0.61	0/561
29	27	0.29	0/426	0.47	0/561
30	18	0.35	0/525	0.56	0/691
30	28	0.29	0/525	0.48	0/691
31	19	0.37	0/310	0.54	0/407
31	29	0.28	0/310	0.54	0/407
32	1a	0.37	0/35795	0.89	16/55864 (0.0%)
32	2a	0.36	0/35890	0.89	21/56012 (0.0%)
33	1b	0.31	0/1876	0.51	0/2533
33	2b	0.31	0/1860	0.54	1/2518 (0.0%)
34	1c	0.29	0/1582	0.48	0/2137
34	2c	0.29	0/1566	0.48	0/2119
35	1d	0.29	0/1695	0.48	0/2274
35	2d	0.29	0/1698	0.47	0/2277
36	1e	0.29	0/1149	0.50	0/1548
36	2e	0.29	0/1149	0.50	0/1548
37	1f	0.30	0/827	0.48	0/1120
37	2f	0.29	0/829	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.29	0/1254	0.44	0/1683
38	2g	0.28	0/1248	0.43	0/1676
39	1h	0.29	0/1118	0.47	0/1506
39	2h	0.29	0/1108	0.48	0/1494
40	1i	0.30	0/1005	0.48	0/1351
40	2i	0.30	0/985	0.50	0/1329
41	1j	0.29	0/732	0.49	0/993
41	2j	0.28	0/723	0.48	0/984
42	1k	0.30	0/849	0.51	0/1150
42	2k	0.29	0/848	0.51	0/1149
43	1l	0.31	0/937	0.50	0/1260
43	2l	0.29	0/937	0.50	0/1260
44	1m	0.29	0/924	0.48	0/1242
44	2m	0.30	0/905	0.50	0/1217
45	1n	0.31	0/501	0.48	0/664
45	2n	0.32	0/501	0.49	0/664
46	1o	0.27	0/739	0.42	0/985
46	2o	0.26	0/739	0.43	0/985
47	1p	0.29	0/697	0.49	0/939
47	2p	0.29	0/693	0.50	0/935
48	1q	0.30	0/836	0.50	0/1117
48	2q	0.29	0/836	0.48	0/1117
49	1r	0.28	0/560	0.48	0/746
49	2r	0.28	0/560	0.47	0/746
50	1s	0.29	0/663	0.53	0/895
50	2s	0.28	0/660	0.51	0/893
51	1t	0.28	0/734	0.44	0/969
51	2t	0.28	0/736	0.40	0/976
52	1u	0.29	0/203	0.52	0/266
52	2u	0.26	0/203	0.48	0/266
53	1y	0.30	0/776	0.47	0/1048
53	2y	0.28	0/761	0.48	0/1030
54	1w	0.43	0/44	1.14	0/67
54	2w	0.34	0/44	1.07	0/67
55	1x	0.55	0/44	1.08	0/67
55	2x	0.37	0/44	0.87	0/67
56	1v	0.32	0/22	0.53	0/28
56	2v	0.32	0/22	0.53	0/28
All	All	0.41	3/310250 (0.0%)	0.85	201/463679 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
21	2Z	0	1
26	14	0	1
33	1b	0	2
33	2b	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	330	A	N9-C4	-6.38	1.34	1.37
1	2A	2104	G	N1-C2	-6.24	1.32	1.37
1	2A	2104	G	C6-N1	-5.63	1.35	1.39

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2104	G	C5-C6-O6	16.30	138.38	128.60
1	2A	2104	G	N3-C2-N2	13.41	129.28	119.90
1	2A	2104	G	N1-C2-N2	-12.20	105.22	116.20
1	1A	2577	A	O5'-P-OP1	-11.46	95.39	105.70
1	2A	2185	C	N1-C2-O2	11.36	125.71	118.90
1	1A	1042	G	OP1-P-O3'	-11.07	80.86	105.20
1	2A	576	U	O5'-P-OP1	-10.60	96.16	105.70
1	1A	801	G	O5'-P-OP2	-10.02	96.69	105.70
1	2A	2104	G	N1-C6-O6	-9.78	114.03	119.90
1	2A	1092	C	C2-N1-C1'	9.57	129.33	118.80
33	2b	232	PRO	C-N-CA	9.20	144.69	121.70
1	1A	330	A	C2-N3-C4	-9.12	106.04	110.60
1	1A	588	U	O5'-P-OP2	-9.12	97.49	105.70
1	1A	2061	G	O5'-P-OP2	-8.99	97.60	105.70
1	2A	1092	C	N1-C2-O2	8.95	124.27	118.90
1	1A	570	G	C5-C6-O6	-8.78	123.33	128.60
1	2A	1648	C	O5'-P-OP1	-8.59	97.97	105.70
1	2A	2185	C	C2-N3-C4	8.41	124.11	119.90
1	2A	2104	G	C6-N1-C2	8.24	130.04	125.10
1	1A	999	U	O5'-P-OP2	-7.96	98.53	105.70
1	2A	1092	C	C6-N1-C2	-7.95	117.12	120.30
1	2A	1092	C	N3-C2-O2	-7.91	116.36	121.90
1	2A	2104	G	C5-C6-N1	-7.84	107.58	111.50
1	1A	512	G	O4'-C1'-N9	7.79	114.43	108.20
1	2A	2154	G	C6-N1-C2	7.76	129.76	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1042	G	OP2-P-O3'	-7.76	88.14	105.20
1	2A	2186	G	C5-C6-O6	7.73	133.24	128.60
1	1A	2554	U	O5'-P-OP1	-7.67	98.79	105.70
1	1A	570	G	C5-C6-N1	7.56	115.28	111.50
1	2A	2185	C	N3-C4-N4	-7.42	112.81	118.00
1	1A	2269	A	O5'-P-OP1	-7.35	99.09	105.70
32	2a	1397	C	C2-N1-C1'	7.25	126.78	118.80
1	1A	2682	U	O5'-P-OP2	-7.19	99.23	105.70
1	2A	2105	C	C5-C6-N1	7.19	124.59	121.00
1	2A	1060	U	C2-N1-C1'	7.17	126.30	117.70
32	2a	1003	G	C8-N9-C4	-7.15	103.54	106.40
1	2A	2137	C	C5-C4-N4	7.15	125.20	120.20
1	1A	948	G	O5'-P-OP1	-7.11	99.30	105.70
1	1A	1838	C	N1-C2-O2	-7.01	114.69	118.90
1	1A	330	A	N3-C4-N9	-6.95	121.84	127.40
1	1A	1824	G	O5'-P-OP2	-6.94	99.45	105.70
1	2A	2185	C	C5-C4-N4	6.93	125.05	120.20
32	1a	1028	C	C5-C6-N1	6.89	124.45	121.00
1	1A	2501	C	C2-N1-C1'	-6.88	111.23	118.80
1	2A	512	G	O4'-C1'-N9	6.79	113.64	108.20
1	1A	996	A	O5'-P-OP1	-6.75	99.62	105.70
1	1A	1671	U	N1-C2-O2	6.75	127.52	122.80
32	2a	1033	G	C5-C6-O6	6.72	132.63	128.60
1	1A	645	C	N1-C2-O2	6.66	122.90	118.90
1	1A	961	C	O5'-P-OP2	-6.65	99.72	105.70
1	1A	1043	C	OP1-P-OP2	6.49	129.33	119.60
1	1A	330	A	N1-C2-N3	6.49	132.54	129.30
1	2A	2104	G	C4-N9-C1'	6.49	134.93	126.50
1	1A	1064	C	N1-C2-O2	6.48	122.79	118.90
32	2a	1003	G	N3-C4-C5	-6.41	125.40	128.60
1	1A	568	U	N3-C4-C5	6.39	118.43	114.60
1	1A	645	C	C2-N1-C1'	6.37	125.81	118.80
1	1A	847	U	C2-N1-C1'	6.37	125.34	117.70
1	1A	1075	C	N1-C2-O2	6.33	122.70	118.90
1	2A	1936	A	O4'-C1'-N9	6.31	113.25	108.20
1	2A	1313	U	C2-N1-C1'	6.25	125.20	117.70
1	2A	1639	U	O5'-P-OP2	-6.25	100.07	105.70
1	2A	1076	C	OP1-P-O3'	6.22	118.89	105.20
1	2A	2103	C	C5-C4-N4	6.21	124.55	120.20
1	2A	2181	G	C5-C6-O6	6.21	132.32	128.60
1	1A	568	U	C5-C4-O4	-6.20	122.18	125.90
27	15	25	LEU	C-N-CA	-6.19	106.23	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	787	U	O5'-P-OP1	-6.15	100.17	105.70
1	1A	2028	U	N3-C4-O4	-6.12	115.12	119.40
1	2A	2108	C	C2-N3-C4	6.11	122.95	119.90
1	1A	1176	G	OP1-P-O3'	6.11	118.63	105.20
1	1A	845	G	O4'-C1'-N9	6.10	113.08	108.20
32	2a	754	C	C2-N1-C1'	6.10	125.51	118.80
32	1a	1028	C	C6-N1-C2	-6.10	117.86	120.30
1	1A	2167	U	O4'-C1'-N1	6.09	113.08	108.20
1	2A	752	A	P-O3'-C3'	6.09	127.00	119.70
32	2a	1003	G	C4-N9-C1'	6.08	134.41	126.50
32	2a	266	G	P-O3'-C3'	6.08	126.99	119.70
1	2A	1092	C	C6-N1-C1'	-6.05	113.54	120.80
32	2a	754	C	N1-C2-O2	6.05	122.53	118.90
1	2A	894	C	C2-N1-C1'	6.00	125.40	118.80
1	2A	2104	G	C8-N9-C1'	-5.99	119.22	127.00
1	1A	271(Y)	U	O4'-C1'-N1	5.96	112.97	108.20
32	1a	955	U	C2-N3-C4	5.94	130.56	127.00
32	1a	1028	C	C2-N3-C4	5.90	122.85	119.90
1	2A	1060	U	C6-N1-C1'	-5.89	112.95	121.20
1	2A	2172	U	OP1-P-O3'	5.89	118.17	105.20
1	1A	1639	U	O5'-P-OP2	-5.88	100.41	105.70
1	1A	1352	U	O5'-P-OP1	-5.88	100.41	105.70
1	1A	1313	U	N3-C2-O2	-5.87	118.09	122.20
1	1A	2685	G	N1-C6-O6	-5.87	116.38	119.90
1	2A	2103	C	C2-N3-C4	5.86	122.83	119.90
1	2A	2430	A	O4'-C1'-N9	5.86	112.89	108.20
1	2A	1647	G	O4'-C1'-N9	-5.85	103.52	108.20
1	2A	2154	G	C5-C6-O6	5.85	132.11	128.60
1	1A	1493	C	N1-C2-O2	5.82	122.39	118.90
32	2a	1123	A	N1-C6-N6	-5.78	115.13	118.60
1	1A	1372	U	N3-C4-O4	5.77	123.44	119.40
1	2A	1062	G	C4-N9-C1'	5.76	133.99	126.50
1	1A	330	A	N3-C4-C5	5.73	130.81	126.80
1	1A	570	G	C8-N9-C4	5.70	108.68	106.40
1	1A	1372	U	C5-C4-O4	-5.69	122.49	125.90
32	1a	1442	G	N3-C4-C5	-5.68	125.76	128.60
1	1A	2430	A	C2-N3-C4	5.68	113.44	110.60
27	25	58	LEU	CA-CB-CG	5.68	128.36	115.30
32	1a	1054	C	N1-C2-O2	5.67	122.30	118.90
1	2A	1097	U	C2-N1-C1'	5.64	124.47	117.70
1	2A	1644	C	N1-C2-O2	5.64	122.28	118.90
32	1a	299	G	C5-C6-O6	-5.62	125.23	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	570	G	N9-C4-C5	-5.60	103.16	105.40
1	2A	1092	C	C5-C6-N1	5.59	123.79	121.00
1	2A	2147	G	C8-N9-C4	-5.58	104.17	106.40
1	1A	2250	G	N9-C4-C5	-5.57	103.17	105.40
32	2a	1003	G	N7-C8-N9	5.57	115.88	113.10
1	1A	570	G	C4-C5-N7	5.55	113.02	110.80
2	1B	1	U	C2-N1-C1'	5.53	124.33	117.70
1	1A	784	A	OP1-P-O3'	5.52	117.35	105.20
1	1A	1416	G	O4'-C1'-N9	5.52	112.61	108.20
1	1A	1671	U	N3-C2-O2	-5.49	118.36	122.20
32	2a	254	G	O5'-P-OP1	-5.47	100.78	105.70
1	2A	1992	G	P-O3'-C3'	5.46	126.25	119.70
1	1A	759	G	C5-C6-O6	-5.45	125.33	128.60
1	1A	1139	G	O5'-P-OP2	-5.45	100.80	105.70
32	1a	1137	C	C6-N1-C2	-5.44	118.12	120.30
1	2A	2154	G	C5-C6-N1	-5.44	108.78	111.50
1	2A	2723	C	C6-N1-C2	-5.44	118.12	120.30
1	1A	2015	A	C8-N9-C4	5.44	107.97	105.80
1	2A	2137	C	N3-C4-N4	-5.44	114.19	118.00
1	2A	1060	U	N1-C2-O2	5.44	126.61	122.80
1	1A	2622	C	N1-C2-O2	-5.43	115.64	118.90
1	2A	894	C	N1-C2-O2	5.42	122.15	118.90
1	2A	1255	U	N3-C2-O2	-5.42	118.41	122.20
1	1A	1026	U	N1-C2-O2	5.42	126.59	122.80
1	2A	1082	U	C2-N1-C1'	5.42	124.20	117.70
32	1a	754	C	C2-N1-C1'	5.40	124.75	118.80
1	1A	2589	A	O5'-P-OP1	-5.39	100.85	105.70
1	2A	2137	C	C2-N3-C4	5.39	122.59	119.90
1	1A	1175	U	P-O3'-C3'	5.38	126.16	119.70
32	2a	1397	C	N1-C2-O2	5.37	122.12	118.90
1	2A	2108	C	N1-C2-O2	5.36	122.12	118.90
32	2a	1065	U	P-O3'-C3'	5.36	126.13	119.70
1	1A	1176	G	P-O3'-C3'	5.35	126.12	119.70
32	2a	1397	C	C6-N1-C1'	-5.35	114.38	120.80
1	1A	808	G	O5'-P-OP2	-5.34	100.89	105.70
32	1a	955	U	C5-C4-O4	5.34	129.11	125.90
1	2A	1073	A	P-O3'-C3'	5.33	126.10	119.70
1	2A	2152	G	C8-N9-C1'	5.33	133.93	127.00
1	2A	1255	U	N1-C2-O2	5.32	126.53	122.80
1	1A	1086	A	N1-C6-N6	-5.32	115.41	118.60
1	2A	2186	G	N1-C6-O6	-5.32	116.71	119.90
1	2A	2172	U	P-O3'-C3'	5.31	126.07	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2689	U	P-O3'-C3'	5.31	126.07	119.70
32	1a	1225	A	C5-C6-N6	5.30	127.94	123.70
1	1A	2712	U	O4'-C1'-N1	5.29	112.44	108.20
32	1a	1067	A	P-O3'-C3'	5.29	126.05	119.70
32	2a	1158	C	C6-N1-C2	-5.26	118.19	120.30
1	2A	2152	G	N9-C4-C5	5.26	107.50	105.40
32	2a	754	C	N3-C2-O2	-5.26	118.22	121.90
32	2a	1004	A	O4'-C1'-N9	5.26	112.41	108.20
1	1A	2826	A	N1-C6-N6	5.24	121.75	118.60
1	2A	2161	C	C5-C4-N4	5.24	123.87	120.20
1	2A	2326	C	C6-N1-C2	-5.23	118.21	120.30
1	1A	1026	U	N3-C2-O2	-5.23	118.54	122.20
1	1A	674	G	C8-N9-C4	5.21	108.48	106.40
1	1A	2036	C	O5'-P-OP1	-5.21	101.02	105.70
1	1A	2848	G	O4'-C1'-N9	5.20	112.36	108.20
1	1A	2617	C	N3-C4-C5	-5.20	119.82	121.90
32	2a	1036	G	C4-N9-C1'	5.20	133.25	126.50
1	1A	2689	U	P-O3'-C3'	5.19	125.93	119.70
1	2A	751	A	O5'-P-OP1	-5.19	101.03	105.70
1	1A	226	G	O4'-C1'-N9	5.19	112.35	108.20
1	1A	1602	U	N3-C4-O4	-5.18	115.78	119.40
32	1a	115	G	P-O3'-C3'	5.17	125.91	119.70
32	1a	1065	U	P-O3'-C3'	5.17	125.91	119.70
32	1a	1201	A	P-O3'-C3'	5.16	125.89	119.70
1	1A	2248	C	O5'-P-OP2	-5.15	101.07	105.70
1	1A	531	C	C5-C6-N1	-5.14	118.43	121.00
1	1A	645	C	C5-C6-N1	5.13	123.56	121.00
1	2A	1899	G	N3-C4-N9	5.13	129.08	126.00
1	1A	1187	G	N1-C6-O6	-5.12	116.83	119.90
1	1A	2571	C	N1-C2-O2	-5.12	115.83	118.90
32	1a	754	C	N1-C2-O2	5.12	121.97	118.90
1	2A	1073	A	N7-C8-N9	5.11	116.36	113.80
1	1A	783	A	C2-N3-C4	5.11	113.16	110.60
32	2a	1183	A	P-O3'-C3'	5.11	125.83	119.70
1	2A	2629	A	O4'-C1'-N9	5.10	112.28	108.20
1	1A	332	A	O4'-C1'-N9	5.10	112.28	108.20
32	2a	1067	A	P-O3'-C3'	5.08	125.80	119.70
32	2a	115	G	P-O3'-C3'	5.08	125.80	119.70
1	2A	2183	C	C2-N3-C4	5.08	122.44	119.90
1	1A	2501	C	C6-N1-C1'	5.06	126.87	120.80
1	1A	1838	C	N3-C2-O2	5.05	125.44	121.90
1	2A	2185	C	N3-C2-O2	-5.05	118.37	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	748	G	C4-N9-C1'	-5.05	119.94	126.50
1	1A	1190	G	C5-N7-C8	5.04	106.82	104.30
1	2A	277	C	O4'-C1'-N1	5.04	112.23	108.20
1	2A	1076	C	P-O3'-C3'	5.04	125.75	119.70
1	1A	1297	C	OP1-P-O3'	5.04	116.28	105.20
1	2A	277	C	C2-N1-C1'	5.04	124.34	118.80
1	1A	2501	C	N3-C4-N4	-5.02	114.49	118.00
16	2U	74	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	52	THR	Peptide
33	1b	127	ILE	Peptide
33	1b	231	GLU	Peptide
21	2Z	136	PHE	Peptide
33	2b	126	GLU	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	254 (93%)	19 (7%)	0	100	100
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
4	1E	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	15	23
4	2E	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	15	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	1F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	29	41
5	2F	201/210 (96%)	189 (94%)	10 (5%)	2 (1%)	15	23
6	1G	179/182 (98%)	162 (90%)	12 (7%)	5 (3%)	5	4
6	2G	179/182 (98%)	153 (86%)	23 (13%)	3 (2%)	9	11
7	1H	172/180 (96%)	159 (92%)	11 (6%)	2 (1%)	13	19
7	2H	171/180 (95%)	150 (88%)	20 (12%)	1 (1%)	25	36
8	1I	145/148 (98%)	128 (88%)	17 (12%)	0	100	100
8	2I	144/148 (97%)	125 (87%)	18 (12%)	1 (1%)	22	32
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	127 (92%)	11 (8%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19	29
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	22	32
11	2P	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	22	32
12	1Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	32
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	17	25
14	2S	108/112 (96%)	98 (91%)	10 (9%)	0	100	100
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
15	2T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	19	29
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	23
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	1 (1%)	1 (1%)	17	25
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14	20
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	14	20
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	2Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	15	23
21	1Z	201/206 (98%)	186 (92%)	14 (7%)	1 (0%)	29	41
21	2Z	199/206 (97%)	169 (85%)	26 (13%)	4 (2%)	7	9
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	78 (96%)	2 (2%)	1 (1%)	13	19
23	11	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	14	20
23	21	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	20
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	50 (75%)	12 (18%)	5 (8%)	1	0
26	24	67/71 (94%)	43 (64%)	18 (27%)	6 (9%)	1	0
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	193 (84%)	26 (11%)	10 (4%)	2	2
33	2b	229/256 (90%)	194 (85%)	31 (14%)	4 (2%)	9	11
34	1c	204/239 (85%)	179 (88%)	25 (12%)	0	100	100
34	2c	204/239 (85%)	171 (84%)	29 (14%)	4 (2%)	7	9
35	1d	206/209 (99%)	182 (88%)	23 (11%)	1 (0%)	29	41
35	2d	206/209 (99%)	188 (91%)	17 (8%)	1 (0%)	29	41
36	1e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	11	15
36	2e	146/162 (90%)	138 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	14 (9%)	0	100	100
38	2g	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	7	9
39	1h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
39	2h	135/138 (98%)	122 (90%)	12 (9%)	1 (1%)	22	32
40	1i	125/128 (98%)	108 (86%)	13 (10%)	4 (3%)	4	3
40	2i	124/128 (97%)	102 (82%)	21 (17%)	1 (1%)	19	29
41	1j	95/105 (90%)	80 (84%)	9 (10%)	6 (6%)	1	0
41	2j	94/105 (90%)	81 (86%)	12 (13%)	1 (1%)	14	20
42	1k	112/129 (87%)	99 (88%)	12 (11%)	1 (1%)	17	25
42	2k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	17	25
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
44	1m	114/126 (90%)	100 (88%)	11 (10%)	3 (3%)	5	5
44	2m	112/126 (89%)	93 (83%)	16 (14%)	3 (3%)	5	5
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	11
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	19
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	19
47	1p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	12	17
47	2p	80/88 (91%)	68 (85%)	12 (15%)	0	100	100
48	1q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	15	23
48	2q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	15	23
49	1r	66/88 (75%)	64 (97%)	1 (2%)	1 (2%)	10	14
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	66 (82%)	15 (18%)	0	100	100
50	2s	81/93 (87%)	67 (83%)	12 (15%)	2 (2%)	5	6
51	1t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	7	8
51	2t	96/106 (91%)	87 (91%)	7 (7%)	2 (2%)	7	8
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
53	1y	95/113 (84%)	92 (97%)	3 (3%)	0	100	100
53	2y	94/113 (83%)	85 (90%)	7 (7%)	2 (2%)	7	8
56	1v	1/3 (33%)	1 (100%)	0	0	100	100
56	2v	1/3 (33%)	1 (100%)	0	0	100	100
All	All	11643/12360 (94%)	10671 (92%)	862 (7%)	110 (1%)	17	25

All (110) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	1Z	52	SER
26	14	55	ARG
33	1b	8	LYS
33	1b	17	PHE
33	1b	22	LYS
33	1b	124	SER
33	1b	125	PRO
33	1b	127	ILE
41	1j	55	LYS
42	1k	105	VAL
44	1m	3	ARG
5	2F	130	ALA
11	2P	36	LYS
26	24	62	ARG
33	2b	17	PHE
33	2b	22	LYS
40	2i	54	ASP
4	1E	71	GLY
5	1F	130	ALA
6	1G	47	LYS
6	1G	50	ALA
6	1G	126	ASP
11	1P	36	LYS
14	1S	59	LYS
19	1X	94	GLY
35	1d	173	TRP
40	1i	11	LYS
41	1j	77	PRO
44	1m	12	ASN
44	1m	67	GLU

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Mol	Chain	Res	Type
48	1q	68	ARG
51	1t	47	GLY
4	2E	71	GLY
5	2F	131	GLY
6	2G	78	SER
6	2G	124	SER
8	2I	10	GLU
17	2V	79	VAL
19	2X	94	GLY
21	2Z	131	ARG
26	24	45	GLY
34	2c	95	THR
34	2c	98	ASN
38	2g	55	GLY
41	2j	78	ASN
44	2m	7	VAL
44	2m	67	GLU
6	1G	53	LEU
7	1H	126	PRO
10	1O	29	ASN
26	14	57	GLU
33	1b	129	GLU
36	1e	97	GLY
49	1r	25	THR
23	21	3	LYS
26	24	63	TYR
33	2b	16	HIS
34	2c	204	LEU
38	2g	4	ARG
48	2q	68	ARG
4	1E	52	LEU
6	1G	51	ARG
26	14	49	PHE
26	14	61	ARG
33	1b	126	GLU
41	1j	26	ALA
4	2E	52	LEU
18	2W	60	ASN
20	2Y	103	GLY
21	2Z	31	ARG
21	2Z	193	GLU
22	20	4	LYS

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Mol	Chain	Res	Type
42	2k	106	LYS
50	2s	29	ARG
50	2s	83	HIS
51	2t	45	GLN
53	2y	28	GLU
7	1H	159	GLU
33	1b	191	ASP
41	1j	78	ASN
41	1j	79	ARG
41	1j	91	PRO
47	1p	46	PRO
21	2Z	51	ALA
26	24	49	PHE
26	24	55	ARG
33	2b	20	GLU
12	1Q	59	ARG
23	11	3	LYS
26	14	47	GLN
40	1i	29	ASN
51	1t	95	ALA
7	2H	126	PRO
15	2T	127	ALA
36	1e	96	PRO
46	1o	19	PRO
26	24	54	GLY
34	2c	99	VAL
44	2m	6	GLY
33	1b	231	GLU
38	2g	82	GLY
51	2t	100	ILE
53	2y	36	ASN
40	1i	48	GLU
6	2G	177	GLY
40	1i	68	GLY
35	2d	171	GLY
39	2h	134	ILE
46	2o	19	PRO
45	2n	14	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%)	197 (92%)	17 (8%)	12	19
3	2D	215/218 (99%)	199 (93%)	16 (7%)	13	22
4	1E	164/166 (99%)	158 (96%)	6 (4%)	34	53
4	2E	164/166 (99%)	152 (93%)	12 (7%)	14	22
5	1F	160/166 (96%)	141 (88%)	19 (12%)	5	6
5	2F	159/166 (96%)	139 (87%)	20 (13%)	4	5
6	1G	144/156 (92%)	132 (92%)	12 (8%)	11	17
6	2G	142/156 (91%)	125 (88%)	17 (12%)	5	6
7	1H	144/148 (97%)	139 (96%)	5 (4%)	36	55
7	2H	143/148 (97%)	129 (90%)	14 (10%)	8	11
8	1I	111/124 (90%)	96 (86%)	15 (14%)	4	4
8	2I	108/124 (87%)	97 (90%)	11 (10%)	7	10
9	1N	119/119 (100%)	111 (93%)	8 (7%)	16	26
9	2N	118/119 (99%)	113 (96%)	5 (4%)	30	47
10	1O	100/100 (100%)	96 (96%)	4 (4%)	31	49
10	2O	100/100 (100%)	92 (92%)	8 (8%)	12	18
11	1P	115/116 (99%)	111 (96%)	4 (4%)	36	55
11	2P	115/116 (99%)	109 (95%)	6 (5%)	23	38
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	22	36
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	9	14
13	1R	101/101 (100%)	95 (94%)	6 (6%)	19	32
13	2R	101/101 (100%)	95 (94%)	6 (6%)	19	32
14	1S	87/88 (99%)	80 (92%)	7 (8%)	12	18
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	7
15	1T	115/127 (91%)	106 (92%)	9 (8%)	12	19
15	2T	113/127 (89%)	98 (87%)	15 (13%)	4	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	16
16	2U	93/94 (99%)	83 (89%)	10 (11%)	6	9
17	1V	81/82 (99%)	74 (91%)	7 (9%)	10	16
17	2V	80/82 (98%)	70 (88%)	10 (12%)	4	5
18	1W	90/92 (98%)	84 (93%)	6 (7%)	16	26
18	2W	90/92 (98%)	84 (93%)	6 (7%)	16	26
19	1X	77/78 (99%)	74 (96%)	3 (4%)	32	50
19	2X	77/78 (99%)	68 (88%)	9 (12%)	5	7
20	1Y	86/91 (94%)	78 (91%)	8 (9%)	9	13
20	2Y	86/91 (94%)	76 (88%)	10 (12%)	5	7
21	1Z	169/179 (94%)	153 (90%)	16 (10%)	8	12
21	2Z	165/179 (92%)	149 (90%)	16 (10%)	8	12
22	10	65/67 (97%)	61 (94%)	4 (6%)	18	29
22	20	64/67 (96%)	59 (92%)	5 (8%)	12	19
23	11	79/83 (95%)	71 (90%)	8 (10%)	7	11
23	21	81/83 (98%)	73 (90%)	8 (10%)	8	11
24	12	65/67 (97%)	62 (95%)	3 (5%)	27	43
24	22	66/67 (98%)	60 (91%)	6 (9%)	9	14
25	13	51/52 (98%)	48 (94%)	3 (6%)	19	32
25	23	50/52 (96%)	47 (94%)	3 (6%)	19	31
26	14	58/63 (92%)	47 (81%)	11 (19%)	1	1
26	24	54/63 (86%)	44 (82%)	10 (18%)	1	2
27	15	51/52 (98%)	45 (88%)	6 (12%)	5	7
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	31
28	16	51/52 (98%)	48 (94%)	3 (6%)	19	32
28	26	50/52 (96%)	42 (84%)	8 (16%)	2	3
29	17	41/42 (98%)	40 (98%)	1 (2%)	49	68
29	27	41/42 (98%)	35 (85%)	6 (15%)	3	3
30	18	54/55 (98%)	52 (96%)	2 (4%)	34	53
30	28	54/55 (98%)	49 (91%)	5 (9%)	9	13
31	19	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	191/220 (87%)	174 (91%)	17 (9%)	9	14
33	2b	187/220 (85%)	158 (84%)	29 (16%)	2	3
34	1c	144/188 (77%)	136 (94%)	8 (6%)	21	34
34	2c	140/188 (74%)	124 (89%)	16 (11%)	5	7
35	1d	171/181 (94%)	151 (88%)	20 (12%)	5	7
35	2d	172/181 (95%)	154 (90%)	18 (10%)	7	9
36	1e	114/123 (93%)	106 (93%)	8 (7%)	15	24
36	2e	114/123 (93%)	102 (90%)	12 (10%)	7	9
37	1f	85/90 (94%)	72 (85%)	13 (15%)	2	3
37	2f	85/90 (94%)	79 (93%)	6 (7%)	14	23
38	1g	120/127 (94%)	110 (92%)	10 (8%)	11	17
38	2g	119/127 (94%)	108 (91%)	11 (9%)	9	13
39	1h	116/119 (98%)	104 (90%)	12 (10%)	7	10
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	12
40	1i	91/99 (92%)	84 (92%)	7 (8%)	13	20
40	2i	88/99 (89%)	77 (88%)	11 (12%)	4	5
41	1j	68/92 (74%)	62 (91%)	6 (9%)	10	15
41	2j	68/92 (74%)	62 (91%)	6 (9%)	10	15
42	1k	83/99 (84%)	77 (93%)	6 (7%)	14	23
42	2k	83/99 (84%)	77 (93%)	6 (7%)	14	23
43	1l	96/108 (89%)	90 (94%)	6 (6%)	18	28
43	2l	96/108 (89%)	90 (94%)	6 (6%)	18	28
44	1m	90/101 (89%)	86 (96%)	4 (4%)	28	45
44	2m	87/101 (86%)	75 (86%)	12 (14%)	3	4
45	1n	49/50 (98%)	45 (92%)	4 (8%)	11	17
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5	6
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46	66
46	2o	78/80 (98%)	75 (96%)	3 (4%)	33	51
47	1p	69/74 (93%)	65 (94%)	4 (6%)	20	32
47	2p	68/74 (92%)	58 (85%)	10 (15%)	3	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	82 (87%)	12 (13%)	4	5
48	2q	94/97 (97%)	88 (94%)	6 (6%)	17	28
49	1r	59/77 (77%)	55 (93%)	4 (7%)	16	25
49	2r	59/77 (77%)	58 (98%)	1 (2%)	60	78
50	1s	68/80 (85%)	65 (96%)	3 (4%)	28	45
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	6
51	1t	71/82 (87%)	65 (92%)	6 (8%)	10	16
51	2t	70/82 (85%)	63 (90%)	7 (10%)	7	11
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	8
53	1y	82/98 (84%)	78 (95%)	4 (5%)	25	40
53	2y	79/98 (81%)	72 (91%)	7 (9%)	9	14
56	1v	3/3 (100%)	3 (100%)	0	100	100
56	2v	3/3 (100%)	3 (100%)	0	100	100
All	All	9537/10266 (93%)	8715 (91%)	822 (9%)	10	16

All (822) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	37	LEU
3	1D	61	LEU
3	1D	94	LEU
3	1D	99	ASP
3	1D	103	ARG
3	1D	111	LEU
3	1D	116	GLN
3	1D	135	PHE
3	1D	141	VAL
3	1D	142	VAL
3	1D	155	LEU
3	1D	183	ARG
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	275	LYS
4	1E	9	VAL

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Mol	Chain	Res	Type
4	1E	55	ASN
4	1E	75	VAL
4	1E	113	PHE
4	1E	116	VAL
4	1E	181	LEU
5	1F	12	LEU
5	1F	15	SER
5	1F	18	ARG
5	1F	24	LEU
5	1F	38	ARG
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	140	LEU
5	1F	151	SER
5	1F	158	THR
5	1F	162	LEU
5	1F	191	ARG
5	1F	192	LEU
5	1F	205	ARG
6	1G	5	VAL
6	1G	7	LEU
6	1G	21	ARG
6	1G	28	VAL
6	1G	43	LEU
6	1G	45	GLU
6	1G	52	ILE
6	1G	53	LEU
6	1G	82	LEU
6	1G	116	ASP
6	1G	146	TYR
6	1G	159	VAL
7	1H	18	GLU
7	1H	24	VAL
7	1H	104	GLU
7	1H	129	THR
7	1H	139	GLN
8	1I	1	MET

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Mol	Chain	Res	Type
8	1I	10	GLU
8	1I	12	LEU
8	1I	44	LEU
8	1I	45	LYS
8	1I	47	LEU
8	1I	51	ILE
8	1I	61	ARG
8	1I	62	LYS
8	1I	68	LEU
8	1I	82	ARG
8	1I	92	VAL
8	1I	101	LEU
8	1I	103	ARG
8	1I	109	ILE
9	1N	14	VAL
9	1N	33	LEU
9	1N	48	MET
9	1N	60	ILE
9	1N	67	LEU
9	1N	87	LEU
9	1N	89	LYS
9	1N	131	GLN
10	1O	17	ARG
10	1O	42	SER
10	1O	96	THR
10	1O	108	GLU
11	1P	6	LEU
11	1P	59	LEU
11	1P	71	VAL
11	1P	95	VAL
12	1Q	7	MET
12	1Q	21	THR
12	1Q	59	ARG
12	1Q	77	LYS
12	1Q	109	VAL
12	1Q	112	GLU
13	1R	29	LEU
13	1R	36	THR
13	1R	67	LEU
13	1R	96	ARG
13	1R	100	LEU
13	1R	114	VAL

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Mol	Chain	Res	Type
14	1S	14	VAL
14	1S	25	ARG
14	1S	43	GLU
14	1S	50	SER
14	1S	71	ARG
14	1S	83	LYS
14	1S	110	LEU
15	1T	28	VAL
15	1T	33	LYS
15	1T	49	VAL
15	1T	53	ARG
15	1T	59	THR
15	1T	85	LYS
15	1T	96	ARG
15	1T	108	ARG
15	1T	118	ARG
16	1U	31	SER
16	1U	36	ARG
16	1U	59	ARG
16	1U	74	LEU
16	1U	83	LEU
16	1U	85	LYS
16	1U	104	GLN
16	1U	117	GLN
17	1V	51	VAL
17	1V	52	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	17	VAL
18	1W	23	LEU
18	1W	49	LYS
18	1W	100	THR
18	1W	107	LEU
19	1X	52	VAL
19	1X	66	LEU
19	1X	68	ARG
20	1Y	23	ARG
20	1Y	31	LEU

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Mol	Chain	Res	Type
20	1Y	43	ASN
20	1Y	49	VAL
20	1Y	72	VAL
20	1Y	73	ARG
20	1Y	96	ILE
20	1Y	99	CYS
21	1Z	2	GLU
21	1Z	18	LEU
21	1Z	31	ARG
21	1Z	40	ASP
21	1Z	58	VAL
21	1Z	61	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	96	VAL
21	1Z	103	ARG
21	1Z	119	GLU
21	1Z	150	LEU
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	203	GLU
22	10	14	ARG
22	10	39	ARG
22	10	55	ARG
22	10	59	LEU
23	11	21	ARG
23	11	23	LYS
23	11	25	LYS
23	11	35	THR
23	11	46	LEU
23	11	59	THR
23	11	80	LEU
23	11	95	LEU
24	12	30	ARG
24	12	32	LEU
24	12	53	LEU
25	13	54	VAL
25	13	56	VAL
25	13	59	VAL
26	14	16	CYS
26	14	27	THR

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Mol	Chain	Res	Type
26	14	33	VAL
26	14	46	GLN
26	14	47	GLN
26	14	49	PHE
26	14	52	THR
26	14	56	VAL
26	14	60	GLN
26	14	67	TYR
26	14	68	ARG
27	15	16	ARG
27	15	26	THR
27	15	40	LYS
27	15	55	ARG
27	15	58	LEU
27	15	60	VAL
28	16	5	VAL
28	16	14	THR
28	16	52	VAL
29	17	43	THR
30	18	31	HIS
30	18	34	TRP
33	1b	19	HIS
33	1b	24	TRP
33	1b	64	ARG
33	1b	96	ARG
33	1b	98	LEU
33	1b	108	ILE
33	1b	112	VAL
33	1b	113	HIS
33	1b	127	ILE
33	1b	134	GLU
33	1b	149	LEU
33	1b	156	LYS
33	1b	160	ASP
33	1b	178	ARG
33	1b	185	ILE
33	1b	189	ASP
33	1b	209	ARG
34	1c	26	LYS
34	1c	37	GLN
34	1c	70	VAL
34	1c	98	ASN

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Mol	Chain	Res	Type
34	1c	101	LEU
34	1c	105	GLU
34	1c	127	ARG
34	1c	154	SER
35	1d	8	VAL
35	1d	18	LYS
35	1d	26	CYS
35	1d	58	LEU
35	1d	59	ARG
35	1d	83	SER
35	1d	108	LEU
35	1d	127	THR
35	1d	135	LEU
35	1d	138	TYR
35	1d	144	ASP
35	1d	157	LEU
35	1d	162	LEU
35	1d	166	LYS
35	1d	175	SER
35	1d	177	ASP
35	1d	188	LEU
35	1d	194	LEU
35	1d	196	LEU
35	1d	208	SER
36	1e	41	VAL
36	1e	56	GLN
36	1e	69	VAL
36	1e	75	THR
36	1e	98	THR
36	1e	101	ILE
36	1e	118	ILE
36	1e	120	THR
37	1f	10	LEU
37	1f	13	ASN
37	1f	19	LEU
37	1f	40	VAL
37	1f	41	GLU
37	1f	45	LEU
37	1f	64	GLN
37	1f	69	GLU
37	1f	70	ASP
37	1f	72	VAL

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Mol	Chain	Res	Type
37	1f	74	ASP
37	1f	86	ARG
37	1f	89	MET
38	1g	3	ARG
38	1g	6	ARG
38	1g	12	LEU
38	1g	21	VAL
38	1g	50	ILE
38	1g	63	LYS
38	1g	94	ARG
38	1g	98	SER
38	1g	143	ARG
38	1g	144	MET
39	1h	17	THR
39	1h	19	VAL
39	1h	25	ASP
39	1h	26	VAL
39	1h	38	ILE
39	1h	51	VAL
39	1h	56	LYS
39	1h	69	ARG
39	1h	121	ASP
39	1h	127	LEU
39	1h	133	LEU
39	1h	137	VAL
40	1i	10	ARG
40	1i	27	THR
40	1i	47	LEU
40	1i	51	ARG
40	1i	66	ARG
40	1i	92	TYR
40	1i	104	ARG
41	1j	29	ARG
41	1j	38	ILE
41	1j	55	LYS
41	1j	92	THR
41	1j	94	VAL
41	1j	100	THR
42	1k	14	VAL
42	1k	16	SER
42	1k	70	LYS
42	1k	80	VAL

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Mol	Chain	Res	Type
42	1k	93	GLN
42	1k	109	VAL
43	1l	22	SER
43	1l	38	THR
43	1l	55	VAL
43	1l	70	ILE
43	1l	84	LEU
43	1l	97	ARG
44	1m	11	ARG
44	1m	15	VAL
44	1m	70	LEU
44	1m	86	CYS
45	1n	4	LYS
45	1n	16	PHE
45	1n	18	VAL
45	1n	60	SER
46	1o	3	ILE
46	1o	5	LYS
47	1p	8	ARG
47	1p	42	ARG
47	1p	60	LEU
47	1p	67	THR
48	1q	11	VAL
48	1q	16	GLN
48	1q	22	LEU
48	1q	45	HIS
48	1q	57	VAL
48	1q	63	ARG
48	1q	70	ARG
48	1q	76	LEU
48	1q	81	ARG
48	1q	85	VAL
48	1q	96	GLU
48	1q	97	SER
49	1r	38	GLU
49	1r	78	LEU
49	1r	82	THR
49	1r	86	VAL
50	1s	28	LYS
50	1s	51	VAL
50	1s	56	GLN
51	1t	15	ARG

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Mol	Chain	Res	Type
51	1t	50	GLU
51	1t	62	LEU
51	1t	70	SER
51	1t	84	LEU
51	1t	100	ILE
53	1y	2	THR
53	1y	3	MET
53	1y	46	GLN
53	1y	70	MET
3	2D	3	VAL
3	2D	61	LEU
3	2D	88	ARG
3	2D	94	LEU
3	2D	103	ARG
3	2D	113	VAL
3	2D	127	VAL
3	2D	134	ARG
3	2D	142	VAL
3	2D	173	VAL
3	2D	183	ARG
3	2D	204	ILE
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
3	2D	274	ARG
4	2E	1	MET
4	2E	12	THR
4	2E	27	LEU
4	2E	38	THR
4	2E	73	GLU
4	2E	75	VAL
4	2E	89	ASP
4	2E	116	VAL
4	2E	152	LYS
4	2E	170	LEU
4	2E	181	LEU
4	2E	184	VAL
5	2F	15	SER
5	2F	17	ARG
5	2F	20	LEU
5	2F	23	ASP
5	2F	24	LEU

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Mol	Chain	Res	Type
5	2F	27	GLU
5	2F	33	LEU
5	2F	57	VAL
5	2F	74	ARG
5	2F	88	VAL
5	2F	95	ARG
5	2F	136	THR
5	2F	140	LEU
5	2F	149	ASP
5	2F	153	SER
5	2F	168	ARG
5	2F	170	LEU
5	2F	175	THR
5	2F	192	LEU
5	2F	197	ASP
6	2G	3	LEU
6	2G	5	VAL
6	2G	28	VAL
6	2G	43	LEU
6	2G	53	LEU
6	2G	62	LEU
6	2G	80	PHE
6	2G	88	ILE
6	2G	92	VAL
6	2G	103	LEU
6	2G	123	ASN
6	2G	126	ASP
6	2G	133	LEU
6	2G	138	GLN
6	2G	148	MET
6	2G	159	VAL
6	2G	173	LEU
7	2H	24	VAL
7	2H	27	LYS
7	2H	33	LEU
7	2H	50	VAL
7	2H	57	ASP
7	2H	68	THR
7	2H	81	GLU
7	2H	86	GLU
7	2H	88	LEU
7	2H	92	ILE

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Mol	Chain	Res	Type
7	2H	133	VAL
7	2H	134	SER
7	2H	137	ASP
7	2H	139	GLN
8	2I	3	VAL
8	2I	7	GLU
8	2I	19	VAL
8	2I	38	LEU
8	2I	51	ILE
8	2I	68	LEU
8	2I	69	LYS
8	2I	72	LEU
8	2I	92	VAL
8	2I	96	ASP
8	2I	145	VAL
9	2N	28	THR
9	2N	48	MET
9	2N	62	VAL
9	2N	73	THR
9	2N	87	LEU
10	2O	21	CYS
10	2O	32	TYR
10	2O	64	ARG
10	2O	69	ILE
10	2O	70	LYS
10	2O	71	ARG
10	2O	94	ARG
10	2O	96	THR
11	2P	1	MET
11	2P	59	LEU
11	2P	83	VAL
11	2P	95	VAL
11	2P	99	LEU
11	2P	149	GLU
12	2Q	6	ARG
12	2Q	7	MET
12	2Q	16	ARG
12	2Q	21	THR
12	2Q	55	VAL
12	2Q	60	ARG
12	2Q	75	THR
12	2Q	98	LYS

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Mol	Chain	Res	Type
12	2Q	109	VAL
12	2Q	133	ARG
13	2R	24	GLN
13	2R	29	LEU
13	2R	36	THR
13	2R	96	ARG
13	2R	100	LEU
13	2R	114	VAL
14	2S	10	ARG
14	2S	12	PHE
14	2S	25	ARG
14	2S	27	SER
14	2S	50	SER
14	2S	63	THR
14	2S	64	GLU
14	2S	69	VAL
14	2S	73	LEU
14	2S	110	LEU
15	2T	9	LEU
15	2T	17	THR
15	2T	34	VAL
15	2T	42	ILE
15	2T	66	VAL
15	2T	74	ARG
15	2T	75	ILE
15	2T	78	LEU
15	2T	85	LYS
15	2T	89	VAL
15	2T	93	ARG
15	2T	96	ARG
15	2T	99	LEU
15	2T	107	ASP
15	2T	109	GLU
16	2U	5	LYS
16	2U	9	VAL
16	2U	31	SER
16	2U	52	ARG
16	2U	59	ARG
16	2U	70	ARG
16	2U	74	LEU
16	2U	101	ARG
16	2U	104	GLN

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Mol	Chain	Res	Type
16	2U	111	GLU
17	2V	32	THR
17	2V	33	VAL
17	2V	35	LEU
17	2V	39	LEU
17	2V	51	VAL
17	2V	53	GLU
17	2V	62	LEU
17	2V	79	VAL
17	2V	98	GLU
17	2V	100	ARG
18	2W	11	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	49	LYS
18	2W	70	TYR
18	2W	107	LEU
19	2X	5	TYR
19	2X	37	THR
19	2X	52	VAL
19	2X	57	LEU
19	2X	66	LEU
19	2X	68	ARG
19	2X	75	ASP
19	2X	81	VAL
19	2X	92	LEU
20	2Y	3	VAL
20	2Y	6	HIS
20	2Y	14	LEU
20	2Y	31	LEU
20	2Y	44	ILE
20	2Y	55	TYR
20	2Y	64	GLU
20	2Y	67	LEU
20	2Y	73	ARG
20	2Y	76	CYS
21	2Z	24	LEU
21	2Z	31	ARG
21	2Z	33	LEU
21	2Z	35	ARG
21	2Z	39	VAL
21	2Z	46	LYS

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Mol	Chain	Res	Type
21	2Z	71	VAL
21	2Z	73	GLN
21	2Z	80	ARG
21	2Z	86	VAL
21	2Z	90	VAL
21	2Z	93	ASP
21	2Z	142	SER
21	2Z	154	ASP
21	2Z	170	THR
21	2Z	190	GLU
22	20	10	THR
22	20	14	ARG
22	20	39	ARG
22	20	49	LYS
22	20	74	ARG
23	21	11	ARG
23	21	30	VAL
23	21	35	THR
23	21	40	ARG
23	21	59	THR
23	21	65	SER
23	21	75	GLU
23	21	85	LEU
24	22	1	MET
24	22	17	SER
24	22	32	LEU
24	22	52	ASP
24	22	53	LEU
24	22	62	THR
25	23	18	ASP
25	23	31	LEU
25	23	35	ARG
26	24	10	VAL
26	24	15	ILE
26	24	27	THR
26	24	34	GLU
26	24	53	GLU
26	24	59	PHE
26	24	61	ARG
26	24	62	ARG
26	24	67	TYR
26	24	69	LYS

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Mol	Chain	Res	Type
27	25	29	THR
27	25	58	LEU
27	25	60	VAL
28	26	3	SER
28	26	5	VAL
28	26	6	ARG
28	26	9	LEU
28	26	13	CYS
28	26	14	THR
28	26	23	THR
28	26	30	THR
29	27	1	MET
29	27	10	ARG
29	27	19	ARG
29	27	42	LEU
29	27	43	THR
29	27	47	ARG
30	28	14	VAL
30	28	31	HIS
30	28	34	TRP
30	28	48	PHE
30	28	49	VAL
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	10	LEU
33	2b	16	HIS
33	2b	24	TRP
33	2b	28	PHE
33	2b	37	ASN
33	2b	44	LEU
33	2b	49	GLU
33	2b	68	ILE
33	2b	81	VAL
33	2b	83	MET
33	2b	90	MET
33	2b	118	LEU
33	2b	124	SER
33	2b	128	GLU
33	2b	154	LEU
33	2b	160	ASP
33	2b	172	ILE

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Mol	Chain	Res	Type
33	2b	185	ILE
33	2b	189	ASP
33	2b	193	ASP
33	2b	195	ASP
33	2b	196	LEU
33	2b	200	ILE
33	2b	208	ILE
33	2b	226	ARG
33	2b	230	VAL
34	2c	3	ASN
34	2c	8	ILE
34	2c	15	THR
34	2c	16	ARG
34	2c	30	ARG
34	2c	56	ASP
34	2c	58	GLU
34	2c	98	ASN
34	2c	105	GLU
34	2c	115	LEU
34	2c	130	VAL
34	2c	152	ILE
34	2c	178	LEU
34	2c	188	LEU
34	2c	206	GLU
34	2c	207	VAL
35	2d	5	ILE
35	2d	8	VAL
35	2d	31	CYS
35	2d	34	GLU
35	2d	58	LEU
35	2d	59	ARG
35	2d	108	LEU
35	2d	122	ARG
35	2d	127	THR
35	2d	135	LEU
35	2d	146	ILE
35	2d	150	GLU
35	2d	155	LEU
35	2d	158	ILE
35	2d	162	LEU
35	2d	166	LYS
35	2d	175	SER

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Mol	Chain	Res	Type
35	2d	200	GLU
36	2e	10	MET
36	2e	11	ILE
36	2e	34	VAL
36	2e	41	VAL
36	2e	45	PHE
36	2e	56	GLN
36	2e	75	THR
36	2e	81	GLU
36	2e	118	ILE
36	2e	120	THR
36	2e	121	LYS
36	2e	145	LYS
37	2f	22	GLU
37	2f	46	ARG
37	2f	48	LEU
37	2f	63	TYR
37	2f	75	LEU
37	2f	95	GLU
38	2g	8	GLU
38	2g	9	VAL
38	2g	13	GLN
38	2g	15	ASP
38	2g	50	ILE
38	2g	75	VAL
38	2g	85	TYR
38	2g	113	GLU
38	2g	115	ARG
38	2g	148	ASN
38	2g	155	ARG
39	2h	2	LEU
39	2h	37	ARG
39	2h	45	ILE
39	2h	46	LYS
39	2h	60	ARG
39	2h	68	ARG
39	2h	91	ARG
39	2h	112	LEU
39	2h	114	THR
39	2h	119	LEU
39	2h	129	VAL
40	2i	34	ASN

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Mol	Chain	Res	Type
40	2i	42	ARG
40	2i	53	VAL
40	2i	60	ASP
40	2i	64	THR
40	2i	65	VAL
40	2i	79	LEU
40	2i	102	LEU
40	2i	103	THR
40	2i	108	VAL
40	2i	111	ARG
41	2j	29	ARG
41	2j	38	ILE
41	2j	43	ARG
41	2j	47	PHE
41	2j	72	VAL
41	2j	84	GLN
42	2k	47	VAL
42	2k	53	SER
42	2k	80	VAL
42	2k	103	LEU
42	2k	107	SER
42	2k	109	VAL
43	2l	23	LYS
43	2l	28	LYS
43	2l	34	ARG
43	2l	38	THR
43	2l	57	LYS
43	2l	89	ARG
44	2m	8	GLU
44	2m	11	ARG
44	2m	27	LYS
44	2m	32	GLU
44	2m	47	ASP
44	2m	48	LEU
44	2m	62	ASN
44	2m	88	ARG
44	2m	102	ARG
44	2m	106	ASN
44	2m	109	THR
44	2m	116	THR
45	2n	3	ARG
45	2n	4	LYS

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Mol	Chain	Res	Type
45	2n	7	ILE
45	2n	18	VAL
45	2n	29	ARG
45	2n	32	SER
46	2o	4	THR
46	2o	5	LYS
46	2o	87	ILE
47	2p	1	MET
47	2p	3	LYS
47	2p	20	VAL
47	2p	33	ILE
47	2p	45	THR
47	2p	47	ASP
47	2p	62	VAL
47	2p	67	THR
47	2p	69	THR
47	2p	76	GLN
48	2q	16	GLN
48	2q	53	LEU
48	2q	57	VAL
48	2q	68	ARG
48	2q	70	ARG
48	2q	76	LEU
49	2r	86	VAL
50	2s	5	LEU
50	2s	16	LEU
50	2s	27	GLU
50	2s	30	LEU
50	2s	32	LYS
50	2s	48	THR
50	2s	77	THR
50	2s	79	THR
51	2t	10	LEU
51	2t	15	ARG
51	2t	24	LEU
51	2t	71	THR
51	2t	72	LEU
51	2t	84	LEU
51	2t	100	ILE
52	2u	7	ARG
52	2u	24	ARG
53	2y	8	LYS

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Mol	Chain	Res	Type
53	2y	11	GLU
53	2y	16	ILE
53	2y	38	HIS
53	2y	49	VAL
53	2y	62	VAL
53	2y	78	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	253	GLN
4	1E	48	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
7	1H	139	GLN
9	1N	69	GLN
10	1O	3	GLN
12	1Q	12	GLN
13	1R	71	GLN
13	1R	91	GLN
15	1T	58	ASN
15	1T	123	GLN
16	1U	117	GLN
19	1X	31	HIS
20	1Y	92	ASN
21	1Z	55	HIS
21	1Z	73	GLN
22	10	35	ASN
25	13	32	GLN
26	14	47	GLN
26	14	60	GLN
33	1b	40	HIS
34	1c	6	HIS
34	1c	102	ASN
34	1c	162	GLN
35	1d	45	GLN
35	1d	77	ASN
35	1d	119	GLN
35	1d	123	HIS
35	1d	129	ASN
36	1e	141	GLN

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Mol	Chain	Res	Type
38	1g	28	ASN
38	1g	37	ASN
38	1g	64	GLN
38	1g	86	GLN
40	1i	3	GLN
40	1i	34	ASN
40	1i	73	GLN
41	1j	56	HIS
41	1j	84	GLN
42	1k	93	GLN
46	1o	28	GLN
46	1o	50	HIS
48	1q	94	ASN
50	1s	83	HIS
51	1t	18	GLN
51	1t	73	HIS
53	1y	38	HIS
53	1y	79	ASN
3	2D	126	GLN
3	2D	143	HIS
3	2D	253	GLN
4	2E	143	ASN
5	2F	69	HIS
5	2F	75	HIS
5	2F	203	GLN
6	2G	79	ASN
6	2G	130	ASN
8	2I	43	ASN
8	2I	139	GLN
9	2N	94	HIS
10	2O	3	GLN
10	2O	5	GLN
11	2P	70	GLN
12	2Q	57	HIS
12	2Q	89	ASN
13	2R	71	GLN
13	2R	91	GLN
15	2T	38	ASN
16	2U	94	ASN
16	2U	104	GLN
18	2W	60	ASN
19	2X	31	HIS

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Mol	Chain	Res	Type
19	2X	82	GLN
20	2Y	6	HIS
24	22	70	GLN
25	23	32	GLN
31	29	29	ASN
33	2b	40	HIS
33	2b	76	GLN
33	2b	78	GLN
33	2b	135	GLN
33	2b	140	HIS
33	2b	212	GLN
34	2c	69	HIS
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	201	GLN
36	2e	65	ASN
37	2f	94	GLN
38	2g	13	GLN
38	2g	64	GLN
38	2g	106	GLN
38	2g	148	ASN
40	2i	3	GLN
40	2i	31	GLN
40	2i	58	HIS
40	2i	73	GLN
41	2j	69	ASN
41	2j	84	GLN
42	2k	22	HIS
42	2k	99	GLN
42	2k	117	ASN
43	2l	99	HIS
44	2m	62	ASN
44	2m	77	ASN
46	2o	28	GLN
47	2p	76	GLN
50	2s	14	HIS
50	2s	83	HIS
53	2y	89	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	447 (15%)	32 (1%)
1	2A	2857/2915 (98%)	498 (17%)	32 (1%)
2	1B	119/121 (98%)	17 (14%)	0
2	2B	119/121 (98%)	13 (10%)	0
32	1a	1494/1521 (98%)	253 (16%)	0
32	2a	1498/1521 (98%)	280 (18%)	0
54	1w	2/4 (50%)	0	0
54	2w	2/4 (50%)	1 (50%)	0
55	1x	2/4 (50%)	1 (50%)	0
55	2x	2/4 (50%)	1 (50%)	0
All	All	8959/9130 (98%)	1511 (16%)	64 (0%)

All (1511) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	11	G
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	72	U
1	1A	74	A
1	1A	75	G
1	1A	95	G
1	1A	102	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	126	A
1	1A	140	G
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A

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Mol	Chain	Res	Type
1	1A	222	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	266	G
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(J)	C
1	1A	275	G
1	1A	279	C
1	1A	283	A
1	1A	311	A
1	1A	315	G
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	371	A
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	407	G
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	442	G
1	1A	448	U
1	1A	454	A
1	1A	456	C
1	1A	457	A
1	1A	480	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	508	G

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Mol	Chain	Res	Type
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	611	C
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	652(U)	G
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	867	C

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Mol	Chain	Res	Type
1	1A	879	G
1	1A	884	C
1	1A	886	C
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	894	C
1	1A	896	A
1	1A	897	C
1	1A	899	A
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	958	U
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1005	C
1	1A	1008	C
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1039	G
1	1A	1042	G
1	1A	1043	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1058	G
1	1A	1060	U
1	1A	1061	U
1	1A	1062	G
1	1A	1063	G
1	1A	1065	U

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Mol	Chain	Res	Type
1	1A	1067	A
1	1A	1069	A
1	1A	1070	A
1	1A	1071	G
1	1A	1072	C
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1079	C
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1096	A
1	1A	1097	U
1	1A	1101	U
1	1A	1109	C
1	1A	1110	G
1	1A	1112	G
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1180	C
1	1A	1210	A
1	1A	1211	U
1	1A	1218	C
1	1A	1220	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G

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Mol	Chain	Res	Type
1	1A	1272	A
1	1A	1273	U
1	1A	1280	G
1	1A	1281	G
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1342	A
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1365	A
1	1A	1370	C
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1395	A
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1459	G
1	1A	1460	A
1	1A	1465	G
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G
1	1A	1484	G
1	1A	1493	C
1	1A	1497	U
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1525	G
1	1A	1542	A
1	1A	1543	C
1	1A	1547	C

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Mol	Chain	Res	Type
1	1A	1554	A
1	1A	1558	A
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
1	1A	1580	A
1	1A	1581	G
1	1A	1582	C
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1613	G
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1721	G
1	1A	1722	A
1	1A	1739	U
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G

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Mol	Chain	Res	Type
1	1A	1896	G
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1915	5MU
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1941	C
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1984	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2082	A
1	1A	2093	G
1	1A	2103	C
1	1A	2104	G
1	1A	2106	G
1	1A	2107	C
1	1A	2108	C
1	1A	2111	C
1	1A	2112	G
1	1A	2116	G
1	1A	2117	A
1	1A	2119	A

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Mol	Chain	Res	Type
1	1A	2121	G
1	1A	2122	U
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2138	C
1	1A	2139	C
1	1A	2141	G
1	1A	2142	C
1	1A	2144	U
1	1A	2145	C
1	1A	2146	C
1	1A	2148	G
1	1A	2152	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2160	G
1	1A	2162	G
1	1A	2170	A
1	1A	2173	A
1	1A	2185	C
1	1A	2186	G
1	1A	2187	G
1	1A	2190	G
1	1A	2192	G
1	1A	2195	C
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2273	A
1	1A	2278	A

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Mol	Chain	Res	Type
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2322	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2383	G
1	1A	2385	C
1	1A	2391	G
1	1A	2393	A
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2424	C
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2469	A
1	1A	2476	A
1	1A	2484	G
1	1A	2491	U
1	1A	2498	C
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G

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Mol	Chain	Res	Type
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2788	C
1	1A	2789	C
1	1A	2790	A
1	1A	2791	C
1	1A	2792	G
1	1A	2802	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2832	U
1	1A	2833	G
1	1A	2835	A
1	1A	2858	C
1	1A	2872	G
1	1A	2892	A
1	1A	2894	G

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Mol	Chain	Res	Type
1	1A	2895	U
2	1B	2	C
2	1B	3	C
2	1B	7	G
2	1B	12	C
2	1B	13	A
2	1B	24	G
2	1B	32	C
2	1B	42	C
2	1B	45	A
2	1B	53	A
2	1B	56	G
2	1B	63	G
2	1B	65	C
2	1B	67	G
2	1B	73	A
2	1B	84	C
2	1B	110	G
32	1a	6	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	59	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	116	A
32	1a	121	C
32	1a	123	C
32	1a	131	C
32	1a	132	C
32	1a	143	A
32	1a	144	G
32	1a	145	G
32	1a	151	A
32	1a	160	A
32	1a	163	C
32	1a	167	G

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Mol	Chain	Res	Type
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	189(F)	U
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	226	G
32	1a	231	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	259	G
32	1a	262	A
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	397	A
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A

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Mol	Chain	Res	Type
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	475	G
32	1a	477	A
32	1a	485	G
32	1a	487	A
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	514	C
32	1a	518	C
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	572	A
32	1a	573	A
32	1a	575	G
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	616	G
32	1a	619	U
32	1a	630	G
32	1a	633	G
32	1a	634	C
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	697	U
32	1a	723	U

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Mol	Chain	Res	Type
32	1a	728	A
32	1a	731	G
32	1a	747	C
32	1a	755	G
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	855	G
32	1a	872	A
32	1a	874	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	929	G
32	1a	934	C
32	1a	935	A
32	1a	936	C
32	1a	960	U
32	1a	961	U
32	1a	963	G
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	996	A

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Mol	Chain	Res	Type
32	1a	997	U
32	1a	998	G
32	1a	1001	A
32	1a	1001(A)	G
32	1a	1005	A
32	1a	1006	C
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	1033	G
32	1a	1037	C
32	1a	1040	U
32	1a	1042	G
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1086	U
32	1a	1089	G
32	1a	1092	A
32	1a	1094	G
32	1a	1095	U
32	1a	1096	C
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A
32	1a	1124	G
32	1a	1126	U
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C

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Mol	Chain	Res	Type
32	1a	1139	G
32	1a	1152	A
32	1a	1154	G
32	1a	1159	U
32	1a	1166	G
32	1a	1168	A
32	1a	1178	G
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1208	C
32	1a	1213	A
32	1a	1214	C
32	1a	1224	G
32	1a	1227	A
32	1a	1238	A
32	1a	1248	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1262	C
32	1a	1270	C
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1301	U
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1347	G
32	1a	1353	G
32	1a	1370	G
32	1a	1381	U
32	1a	1397	C
32	1a	1400	5MC
32	1a	1410	G

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Mol	Chain	Res	Type
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1493	A
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
55	1x	74	C
1	2A	10	G
1	2A	11	G
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	92	A
1	2A	106	C
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	128	C
1	2A	141	A
1	2A	149	A
1	2A	157	U
1	2A	173	G
1	2A	181	A

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Mol	Chain	Res	Type
1	2A	182	A
1	2A	196	A
1	2A	197	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	223	A
1	2A	225	A
1	2A	229	A
1	2A	230	U
1	2A	245	G
1	2A	248	G
1	2A	271(G)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	274	G
1	2A	277	C
1	2A	278	A
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	346	A
1	2A	352	G
1	2A	363	G
1	2A	370	G
1	2A	386	G
1	2A	389	G
1	2A	396	G
1	2A	399	G
1	2A	411	G
1	2A	412	A
1	2A	428	A

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Mol	Chain	Res	Type
1	2A	429	A
1	2A	435	C
1	2A	444	C
1	2A	451	C
1	2A	456	C
1	2A	457	A
1	2A	470	A
1	2A	481	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	551	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	619	G
1	2A	623	G
1	2A	627	A
1	2A	634	C
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(D)	C
1	2A	652(U)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	726	G

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Mol	Chain	Res	Type
1	2A	730	C
1	2A	740	U
1	2A	751	A
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	786	C
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	869	G
1	2A	877	U
1	2A	880	G
1	2A	882	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	897	C
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	926	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	959	A

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Mol	Chain	Res	Type
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1020	A
1	2A	1026	U
1	2A	1033	U
1	2A	1034	G
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1049	C
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A
1	2A	1058	G
1	2A	1060	U
1	2A	1063	G
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	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
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

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Mol	Chain	Res	Type
1	2A	1086	A
1	2A	1088	A
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	1109	C
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1114	G
1	2A	1116	C
1	2A	1117	G
1	2A	1135	C
1	2A	1136	G
1	2A	1171	G
1	2A	1181	C
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1229	G
1	2A	1236	G
1	2A	1244	G
1	2A	1247	A
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1275	A
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1342	A
1	2A	1345	C

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Mol	Chain	Res	Type
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1419	A
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1459	G
1	2A	1460	A
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	1514	U
1	2A	1520	G
1	2A	1531	C
1	2A	1533	G
1	2A	1539	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	1584	C

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Mol	Chain	Res	Type
1	2A	1586	A
1	2A	1593	G
1	2A	1594	G
1	2A	1595	G
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1639	U
1	2A	1640	C
1	2A	1648	C
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1750	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1817	G
1	2A	1829	A
1	2A	1835	G
1	2A	1836	C
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A

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Mol	Chain	Res	Type
1	2A	1904	G
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	1960	A
1	2A	1963	U
1	2A	1966	A
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2093	G
1	2A	2096	U
1	2A	2099	U
1	2A	2100	G
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	2110	G
1	2A	2112	G
1	2A	2114	A
1	2A	2115	G

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Mol	Chain	Res	Type
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	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2136	C
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2163	C
1	2A	2164	C
1	2A	2165	G
1	2A	2168	G
1	2A	2170	A
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2184	G
1	2A	2186	G
1	2A	2189	U
1	2A	2192	G
1	2A	2193	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G

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Mol	Chain	Res	Type
1	2A	2208	A
1	2A	2225	A
1	2A	2232	U
1	2A	2238	G
1	2A	2239	G
1	2A	2269	A
1	2A	2275	C
1	2A	2279	G
1	2A	2280	G
1	2A	2283	C
1	2A	2286	A
1	2A	2289	G
1	2A	2293	C
1	2A	2294	C
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2312	U
1	2A	2314	C
1	2A	2315	G
1	2A	2316	C
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2326	C
1	2A	2334	G
1	2A	2336	A
1	2A	2342	C
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2410	G
1	2A	2414	G
1	2A	2422	A
1	2A	2423	U
1	2A	2425	A
1	2A	2429	G

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Mol	Chain	Res	Type
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2458	G
1	2A	2465	C
1	2A	2468	G
1	2A	2474	C
1	2A	2476	A
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2529	G
1	2A	2536	G
1	2A	2549	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2582	G
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2630	G
1	2A	2654	A
1	2A	2669	G
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2757	A
1	2A	2758	A

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Mol	Chain	Res	Type
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2802	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	30	C
2	2B	32	C
2	2B	33	G
2	2B	41	U
2	2B	45	A
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	91	C
2	2B	110	G
32	2a	5	U
32	2a	6	G
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	51	A
32	2a	54	C
32	2a	61	G
32	2a	66	G
32	2a	69	G
32	2a	70	G

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Mol	Chain	Res	Type
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	105	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	156	G
32	2a	163	C
32	2a	170	U
32	2a	174	C
32	2a	182	U
32	2a	189(D)	C
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	195	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	220	G
32	2a	232	G
32	2a	237	C
32	2a	245	C
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	281	G
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	342	C
32	2a	345	C
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A

Continued on next page...

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Mol	Chain	Res	Type
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	381	C
32	2a	392	G
32	2a	397	A
32	2a	398	C
32	2a	404	U
32	2a	406	G
32	2a	411	A
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	446	G
32	2a	452	A
32	2a	458	C
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	508	C
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	560	U
32	2a	561	U

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Mol	Chain	Res	Type
32	2a	562	C
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	592	G
32	2a	596	C
32	2a	608	A
32	2a	630	G
32	2a	632	A
32	2a	639	G
32	2a	651	C
32	2a	653	A
32	2a	661	G
32	2a	665	A
32	2a	685	G
32	2a	687	A
32	2a	688	G
32	2a	703	G
32	2a	712	A
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	729	A
32	2a	731	G
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	763	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	836	G
32	2a	840	C
32	2a	841	U

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Mol	Chain	Res	Type
32	2a	851	G
32	2a	859	A
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	921	U
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	933	G
32	2a	934	C
32	2a	935	A
32	2a	942	G
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	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	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1017	G
32	2a	1020	U
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030(A)	G

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Mol	Chain	Res	Type
32	2a	1030(B)	C
32	2a	1033	G
32	2a	1041	A
32	2a	1043	C
32	2a	1053	G
32	2a	1056	U
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	1100	C
32	2a	1101	A
32	2a	1113	C
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1128	C
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1162	C
32	2a	1172	C
32	2a	1183	A
32	2a	1184	G
32	2a	1186	G
32	2a	1194	U
32	2a	1196	U
32	2a	1197	G
32	2a	1208	C
32	2a	1212	U
32	2a	1214	C
32	2a	1224	G
32	2a	1227	A

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Mol	Chain	Res	Type
32	2a	1236	A
32	2a	1238	A
32	2a	1241	G
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1282	C
32	2a	1286	A
32	2a	1287	A
32	2a	1290	G
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1334	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1352	C
32	2a	1353	G
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1364	U
32	2a	1370	G
32	2a	1375	A
32	2a	1397	C
32	2a	1398	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1446	U
32	2a	1447	A
32	2a	1456	G

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Mol	Chain	Res	Type
32	2a	1462	G
32	2a	1475	G
32	2a	1492	A
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
54	2w	74	C
55	2x	74	C

All (64) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	685	A
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	839	U
1	1A	840	C
1	1A	888	C
1	1A	895	U
1	1A	974	G
1	1A	1065	U
1	1A	1067	A
1	1A	1089	G
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1379	A
1	1A	1442	G
1	1A	1608	A
1	1A	1653	G

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Mol	Chain	Res	Type
1	1A	1663	C
1	1A	2126	A
1	1A	2238	G
1	1A	2288	A
1	1A	2406	U
1	1A	2430	A
1	1A	2439	A
1	1A	2689	U
1	1A	2756	U
1	2A	196	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	752	A
1	2A	764	A
1	2A	774	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	1004	C
1	2A	1047	G
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1076	C
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1493	C
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2321	G
1	2A	2406	U
1	2A	2689	U
1	2A	2756	U

5.4 Non-standard residues in protein, DNA, RNA chains

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	2MG	2a	1207	32	18,26,27	0.93	1 (5%)	16,38,41	1.04	1 (6%)
32	G7M	2a	527	32	20,26,27	1.17	2 (10%)	17,39,42	0.66	0
32	UR3	2a	1498	57,32	19,22,23	1.02	1 (5%)	26,32,35	1.33	2 (7%)
1	OMC	1A	1920	1	19,22,23	0.84	0	26,31,34	0.98	1 (3%)
1	5MC	2A	1942	1	18,22,23	0.95	2 (11%)	26,32,35	1.17	2 (7%)
1	OMG	2A	2251	55,1,57	18,26,27	0.97	1 (5%)	19,38,41	1.08	2 (10%)
32	5MC	2a	1400	32	18,22,23	0.98	2 (11%)	26,32,35	1.23	3 (11%)
32	PSU	2a	516	57,32	18,21,22	1.34	3 (16%)	22,30,33	1.91	4 (18%)
32	G7M	1a	527	57,32	20,26,27	1.23	2 (10%)	17,39,42	0.56	0
1	5MC	1A	1942	1	18,22,23	0.96	2 (11%)	26,32,35	1.17	3 (11%)
1	PSU	2A	2605	1	18,21,22	1.33	3 (16%)	22,30,33	1.88	4 (18%)
32	2MG	1a	1207	32	18,26,27	0.95	1 (5%)	16,38,41	1.40	3 (18%)
1	5MC	2A	1962	1,57	18,22,23	1.01	2 (11%)	26,32,35	1.14	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.87	0	26,31,34	1.02	2 (7%)
1	PSU	1A	1917	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
32	5MC	2a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.03	2 (7%)
54	PPU	1w	76	1,54	32,40,41	0.92	1 (3%)	33,57,60	1.39	5 (15%)
1	PSU	1A	2605	1	18,21,22	1.40	3 (16%)	22,30,33	1.77	4 (18%)
32	4OC	2a	1402	32	20,23,24	0.76	1 (5%)	26,32,35	0.92	1 (3%)
32	MA6	2a	1519	32	19,26,27	0.82	0	18,38,41	1.60	2 (11%)
32	5MC	2a	1407	32	18,22,23	0.96	2 (11%)	26,32,35	1.23	3 (11%)
1	OMU	2A	2552	1,57	19,22,23	1.17	2 (10%)	26,31,34	1.84	5 (19%)
32	MA6	1a	1518	32	19,26,27	0.81	0	18,38,41	1.29	2 (11%)
55	8AN	1x	76	55,57	19,24,25	1.17	3 (15%)	13,35,38	1.87	2 (15%)
32	MA6	2a	1518	32	19,26,27	0.81	0	18,38,41	1.46	2 (11%)
1	5MU	1A	1915	1	19,22,23	1.39	5 (26%)	28,32,35	2.29	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	2A	1915	1	19,22,23	1.42	4 (21%)	28,32,35	2.15	7 (25%)
54	PPU	2w	76	1,54	32,40,41	0.89	1 (3%)	33,57,60	1.35	6 (18%)
32	5MC	2a	1404	32	18,22,23	1.01	2 (11%)	26,32,35	1.21	2 (7%)
55	8AN	2x	76	55,57,56	19,24,25	1.18	3 (15%)	13,35,38	1.81	2 (15%)
1	OMU	1A	2552	1,57	19,22,23	1.25	2 (10%)	26,31,34	1.80	6 (23%)
32	4OC	1a	1402	32	20,23,24	0.77	0	26,32,35	0.84	1 (3%)
1	PSU	2A	1917	1	18,21,22	1.31	2 (11%)	22,30,33	1.82	3 (13%)
1	5MC	1A	1962	1,57	18,22,23	1.00	2 (11%)	26,32,35	1.16	3 (11%)
32	UR3	1a	1498	32	19,22,23	0.99	2 (10%)	26,32,35	1.49	3 (11%)
32	M2G	2a	966	32	20,27,28	1.49	3 (15%)	22,40,43	0.90	2 (9%)
1	OMG	1A	2251	55,1,57	18,26,27	0.97	1 (5%)	19,38,41	1.07	2 (10%)
43	0TD	1l	92	43	7,9,10	4.85	1 (14%)	6,11,13	6.78	3 (50%)
1	2MA	2A	2503	1,57	17,25,26	0.97	1 (5%)	17,37,40	1.03	2 (11%)
32	5MC	1a	1400	32	18,22,23	1.01	2 (11%)	26,32,35	1.22	2 (7%)
1	5MU	1A	1939	1,57	19,22,23	1.43	5 (26%)	28,32,35	2.19	7 (25%)
32	PSU	1a	516	57,32	18,21,22	1.36	2 (11%)	22,30,33	1.88	5 (22%)
1	5MU	2A	1939	1,57	19,22,23	1.44	3 (15%)	28,32,35	2.14	6 (21%)
1	PSU	1A	1911	1	18,21,22	1.33	2 (11%)	22,30,33	1.85	3 (13%)
32	M2G	1a	966	32	20,27,28	1.39	3 (15%)	22,40,43	1.00	2 (9%)
32	5MC	1a	1404	32	18,22,23	0.99	2 (11%)	26,32,35	1.17	2 (7%)
32	5MC	1a	1407	32	18,22,23	0.96	1 (5%)	26,32,35	1.09	2 (7%)
1	2MA	1A	2503	1,57	17,25,26	1.04	1 (5%)	17,37,40	0.99	2 (11%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	22,30,33	1.80	3 (13%)
43	0TD	2l	92	43	7,9,10	4.87	1 (14%)	6,11,13	5.00	3 (50%)
32	MA6	1a	1519	32	19,26,27	0.79	0	18,38,41	1.45	2 (11%)
32	5MC	1a	967	32	18,22,23	0.95	2 (11%)	26,32,35	1.16	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MG	2a	1207	32	-	2/5/27/28	0/3/3/3
32	G7M	2a	527	32	-	1/3/25/26	0/3/3/3
32	UR3	2a	1498	57,32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1,57	-	0/5/27/28	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	57,32	-	2/7/25/26	0/2/2/2
32	G7M	1a	527	57,32	-	2/3/25/26	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/5/27/28	0/3/3/3
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	PPU	1w	76	1,54	-	2/21/43/44	0/4/4/4
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
32	MA6	2a	1519	32	-	2/7/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
55	8AN	1x	76	55,57	-	3/3/25/26	0/3/3/3
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	4/7/25/26	0/2/2/2
54	PPU	2w	76	1,54	-	0/21/43/44	0/4/4/4
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
55	8AN	2x	76	55,57,56	-	3/3/25/26	0/3/3/3
1	OMU	1A	2552	1,57	-	0/9/27/28	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,57	-	2/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
1	OMG	1A	2251	55,1,57	-	1/5/27/28	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
1	2MA	2A	2503	1,57	-	1/3/25/26	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	57,32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,57	-	1/3/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.53	1.69	1.82
43	1l	92	0TD	CB-SB	-12.47	1.69	1.82
32	2a	966	M2G	C2-N3	4.84	1.36	1.30
32	1a	966	M2G	C2-N3	4.38	1.36	1.30
32	1a	527	G7M	C5-C4	3.76	1.46	1.39
32	2a	527	G7M	C5-C4	3.46	1.46	1.39
32	1a	516	PSU	C6-C5	3.41	1.39	1.35
1	2A	1911	PSU	C6-C5	3.33	1.39	1.35
1	2A	1939	5MU	C6-C5	3.21	1.39	1.34
1	1A	1917	PSU	C6-C5	3.19	1.39	1.35
1	1A	1911	PSU	C6-C5	3.12	1.39	1.35
32	2a	516	PSU	C6-C5	3.08	1.38	1.35
1	2A	1962	5MC	C6-C5	3.07	1.39	1.34
1	1A	2605	PSU	C6-C5	3.05	1.38	1.35
1	1A	1939	5MU	C6-C5	3.02	1.39	1.34
1	1A	2605	PSU	C4-N3	-3.02	1.33	1.38
1	2A	1917	PSU	C6-C5	3.02	1.38	1.35
32	1a	1407	5MC	C6-C5	2.98	1.39	1.34
32	2a	967	5MC	C6-C5	2.95	1.39	1.34
1	2A	1915	5MU	C6-C5	2.89	1.39	1.34
32	1a	1404	5MC	C6-C5	2.89	1.39	1.34
1	1A	1939	5MU	C4-C5	2.84	1.49	1.44
32	2a	1404	5MC	C6-C5	2.84	1.39	1.34
1	2A	2251	OMG	C6-N1	-2.83	1.33	1.37
1	2A	2605	PSU	C6-C5	2.80	1.38	1.35
32	2a	1400	5MC	C6-C5	2.77	1.39	1.34
1	2A	1942	5MC	C6-C5	2.75	1.39	1.34
32	2a	1407	5MC	C6-C5	2.73	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1939	5MU	C4-N3	-2.72	1.33	1.38
1	1A	1915	5MU	C2-N1	2.72	1.42	1.38
32	1a	1400	5MC	C6-C5	2.71	1.39	1.34
1	2A	1915	5MU	C2-N1	2.71	1.42	1.38
1	1A	1962	5MC	C6-C5	2.67	1.39	1.34
32	2a	966	M2G	C6-N1	-2.67	1.33	1.37
1	2A	1939	5MU	C4-C5	2.66	1.49	1.44
1	1A	2251	OMG	C6-N1	-2.63	1.34	1.37
1	1A	1942	5MC	C6-C5	2.61	1.38	1.34
32	2a	966	M2G	C2-N2	2.61	1.40	1.35
1	1A	1917	PSU	C4-N3	-2.60	1.34	1.38
55	2x	76	8AN	C5-C4	-2.59	1.34	1.40
55	2x	76	8AN	C6-C5	-2.58	1.33	1.43
55	1x	76	8AN	C5-C4	-2.56	1.34	1.40
1	2A	1911	PSU	C4-N3	-2.56	1.34	1.38
1	1A	1915	5MU	C6-C5	2.54	1.38	1.34
1	1A	1911	PSU	C4-N3	-2.54	1.34	1.38
55	1x	76	8AN	C6-C5	-2.53	1.33	1.43
32	1a	516	PSU	C4-N3	-2.53	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.49	1.33	1.38
32	1a	966	M2G	C6-N1	-2.49	1.34	1.37
32	2a	516	PSU	C4-N3	-2.48	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.47	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.47	1.34	1.38
32	1a	966	M2G	C2-N2	2.47	1.39	1.35
32	1a	967	5MC	C6-C5	2.46	1.38	1.34
54	2w	76	PPU	C5-C4	2.46	1.47	1.40
54	1w	76	PPU	C5-C4	2.45	1.47	1.40
1	1A	1915	5MU	C4-C5	2.44	1.48	1.44
1	2A	1917	PSU	C4-N3	-2.44	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.44	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.43	1.34	1.37
1	1A	1942	5MC	C6-N1	-2.43	1.33	1.38
1	1A	2552	OMU	C5-C4	2.43	1.49	1.43
1	2A	2552	OMU	C5-C4	2.40	1.49	1.43
32	2a	1404	5MC	C6-N1	-2.40	1.33	1.38
1	1A	2552	OMU	C4-N3	-2.37	1.34	1.38
55	2x	76	8AN	C5-N7	-2.33	1.31	1.39
32	1a	1207	2MG	C6-N1	-2.30	1.34	1.37
32	2a	527	G7M	C6-N1	-2.30	1.34	1.37
32	1a	527	G7M	C6-N1	-2.29	1.34	1.37
1	1A	2605	PSU	C2-N3	-2.28	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C2-N1	2.27	1.42	1.38
1	1A	1915	5MU	C4-N3	-2.26	1.34	1.38
1	2A	1915	5MU	C4-C5	2.24	1.48	1.44
1	1A	1939	5MU	C6-N1	-2.24	1.34	1.38
32	1a	1498	UR3	C2-N1	2.23	1.41	1.38
32	1a	967	5MC	C6-N1	-2.20	1.34	1.38
1	1A	2503	2MA	C2-N3	2.20	1.35	1.31
1	2A	2552	OMU	C4-N3	-2.18	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.15	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.15	1.33	1.37
32	2a	1407	5MC	C6-N1	-2.14	1.34	1.38
32	1a	1498	UR3	C6-C5	2.14	1.40	1.35
32	1a	1404	5MC	C6-N1	-2.13	1.34	1.38
32	2a	1498	UR3	C6-C5	2.12	1.39	1.35
55	1x	76	8AN	C5-N7	-2.11	1.32	1.39
32	2a	516	PSU	O4'-C1'	-2.10	1.40	1.43
1	2A	1962	5MC	C6-N1	-2.09	1.34	1.38
1	2A	2503	2MA	C2-N3	2.09	1.35	1.31
1	2A	1942	5MC	C6-N1	-2.09	1.34	1.38
1	1A	1939	5MU	C4-N3	-2.07	1.35	1.38
32	2a	967	5MC	C6-N1	-2.04	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.01	1.34	1.38
32	2a	1402	4OC	C6-C5	2.01	1.39	1.35

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-16.07	73.36	102.44
43	2l	92	0TD	CSB-SB-CB	-11.68	81.31	102.44
32	1a	1498	UR3	C4-N3-C2	-6.06	118.86	124.56
55	1x	76	8AN	N3-C2-N1	-5.94	119.39	128.68
32	2a	516	PSU	N1-C2-N3	5.91	121.82	115.13
1	1A	1917	PSU	N1-C2-N3	5.86	121.77	115.13
1	1A	1911	PSU	N1-C2-N3	5.82	121.73	115.13
32	1a	516	PSU	N1-C2-N3	5.72	121.61	115.13
1	1A	2605	PSU	N1-C2-N3	5.72	121.61	115.13
1	2A	1911	PSU	N1-C2-N3	5.69	121.58	115.13
1	2A	2605	PSU	N1-C2-N3	5.63	121.50	115.13
1	2A	1939	5MU	N3-C2-N1	5.59	122.31	114.89
1	2A	1917	PSU	N1-C2-N3	5.53	121.40	115.13
55	2x	76	8AN	N3-C2-N1	-5.53	120.04	128.68
1	1A	1939	5MU	C4-N3-C2	-5.46	120.29	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1498	UR3	C4-N3-C2	-5.35	119.53	124.56
1	2A	1939	5MU	C4-N3-C2	-5.33	120.45	127.35
1	2A	2552	OMU	N3-C2-N1	5.23	121.83	114.89
1	1A	2552	OMU	N3-C2-N1	5.03	121.57	114.89
32	2a	1518	MA6	N3-C2-N1	-4.94	120.96	128.68
1	1A	1939	5MU	C5-C4-N3	4.93	119.52	115.31
1	1A	1915	5MU	C1 [?] -N1-C2	4.79	126.24	117.57
32	2a	1519	MA6	N3-C2-N1	-4.67	121.38	128.68
1	2A	1915	5MU	N3-C2-N1	4.62	121.03	114.89
1	2A	1915	5MU	C4-N3-C2	-4.58	121.42	127.35
32	1a	1519	MA6	N3-C2-N1	-4.57	121.54	128.68
1	1A	1915	5MU	C4-N3-C2	-4.51	121.51	127.35
1	1A	1939	5MU	N3-C2-N1	4.51	120.88	114.89
1	1A	1915	5MU	N3-C2-N1	4.49	120.85	114.89
1	2A	2552	OMU	C4-N3-C2	-4.34	120.85	126.58
1	1A	1939	5MU	O4-C4-C5	-4.33	119.88	124.90
1	2A	1915	5MU	C5-C4-N3	4.32	119.00	115.31
1	1A	1915	5MU	C1 [?] -N1-C6	-4.32	113.94	121.12
1	1A	1915	5MU	O4-C4-C5	-4.27	119.95	124.90
32	1a	1518	MA6	N3-C2-N1	-4.25	122.04	128.68
1	2A	1939	5MU	C5-C4-N3	4.25	118.94	115.31
1	2A	1915	5MU	O4-C4-C5	-4.15	120.09	124.90
1	2A	2605	PSU	C4-N3-C2	-4.08	120.47	126.34
1	1A	2552	OMU	C4-N3-C2	-4.06	121.22	126.58
32	1a	516	PSU	C4-N3-C2	-4.03	120.53	126.34
1	2A	2552	OMU	O2-C2-N1	-4.01	117.45	122.79
32	1a	1400	5MC	C5-C6-N1	-4.01	119.22	123.34
32	2a	1400	5MC	C5-C6-N1	-3.99	119.23	123.34
1	1A	1915	5MU	C5-C4-N3	3.99	118.71	115.31
1	1A	1939	5MU	C5-C6-N1	-3.98	119.25	123.34
1	1A	1942	5MC	C5-C6-N1	-3.97	119.25	123.34
32	2a	516	PSU	C4-N3-C2	-3.96	120.64	126.34
54	1w	76	PPU	N1-C6-N6	3.92	121.18	117.06
1	2A	1939	5MU	C5-C6-N1	-3.91	119.31	123.34
1	1A	1917	PSU	C4-N3-C2	-3.89	120.73	126.34
1	2A	1942	5MC	C5-C6-N1	-3.89	119.33	123.34
1	1A	1911	PSU	C4-N3-C2	-3.83	120.82	126.34
32	2a	1519	MA6	C4-C5-N7	-3.77	105.47	109.40
1	2A	1917	PSU	C4-N3-C2	-3.73	120.97	126.34
1	1A	2605	PSU	C4-N3-C2	-3.70	121.00	126.34
32	2a	967	5MC	C5-C6-N1	-3.70	119.53	123.34
1	2A	1917	PSU	O2-C2-N1	-3.68	118.74	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1917	PSU	O2-C2-N1	-3.66	118.76	122.79
1	2A	1915	5MU	C1'-N1-C2	3.65	124.17	117.57
1	2A	1939	5MU	O2-C2-N1	-3.64	117.95	122.79
1	1A	1962	5MC	C5-C6-N1	-3.56	119.68	123.34
32	2a	1404	5MC	C5-C6-N1	-3.55	119.69	123.34
1	2A	1911	PSU	C4-N3-C2	-3.52	121.26	126.34
1	1A	1911	PSU	O2-C2-N1	-3.37	119.08	122.79
54	2w	76	PPU	C4-C5-N7	-3.37	105.89	109.40
1	2A	1962	5MC	C5-C6-N1	-3.36	119.88	123.34
32	2a	1407	5MC	C5-C6-N1	-3.33	119.91	123.34
1	2A	1939	5MU	O4-C4-C5	-3.33	121.05	124.90
32	1a	1404	5MC	C5-C6-N1	-3.32	119.93	123.34
32	2a	516	PSU	O2-C2-N1	-3.32	119.14	122.79
1	2A	1911	PSU	O2-C2-N1	-3.24	119.22	122.79
32	1a	516	PSU	O2-C2-N1	-3.23	119.23	122.79
54	2w	76	PPU	N3-C2-N1	-3.22	123.64	128.68
1	1A	2552	OMU	O2-C2-N1	-3.20	118.54	122.79
43	1l	92	0TD	OD2-CG-CB	3.16	119.98	113.15
32	1a	1519	MA6	C4-C5-N7	-3.12	106.15	109.40
32	1a	967	5MC	C5-C6-N1	-3.09	120.16	123.34
1	2A	1915	5MU	C1'-N1-C6	-3.05	116.05	121.12
32	1a	1404	5MC	C5-C4-N3	-3.05	118.39	121.67
1	2A	2605	PSU	O2-C2-N1	-3.01	119.48	122.79
55	2x	76	8AN	O4'-C1'-C2'	-3.01	102.53	106.93
32	2a	1404	5MC	C5-C4-N3	-3.00	118.44	121.67
54	1w	76	PPU	N3-C2-N1	-2.98	124.01	128.68
1	1A	1939	5MU	O2-C2-N1	-2.96	118.85	122.79
32	2a	1518	MA6	C4-C5-N7	-2.90	106.38	109.40
1	1A	2552	OMU	C2'-C1'-N1	-2.89	108.61	114.22
43	2l	92	0TD	OD2-CG-CB	2.84	119.29	113.15
1	1A	2251	OMG	C8-N7-C5	2.84	108.40	102.99
32	1a	1407	5MC	C5-C6-N1	-2.81	120.45	123.34
54	1w	76	PPU	C4-C5-N7	-2.79	106.50	109.40
1	2A	2552	OMU	O4-C4-C5	-2.74	120.34	125.16
32	2a	1407	5MC	O2-C2-N3	-2.73	117.90	122.33
32	1a	1407	5MC	C5-C4-N3	-2.71	118.75	121.67
1	2A	2503	2MA	C8-N7-C5	2.68	108.09	102.99
32	1a	1400	5MC	C5-C4-N3	-2.67	118.79	121.67
32	1a	1518	MA6	C4-C5-N7	-2.66	106.62	109.40
32	1a	1207	2MG	C8-N7-C5	2.60	107.94	102.99
1	2A	2251	OMG	C5-C6-N1	2.56	118.47	113.95
54	2w	76	PPU	N1-C6-N6	2.53	119.72	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1962	5MC	C5-C4-N3	-2.53	118.94	121.67
54	2w	76	PPU	CG-CB-CA	-2.48	108.97	114.13
1	1A	1915	5MU	C5M-C5-C4	2.47	121.49	118.77
1	2A	1920	OMC	O2-C2-N3	-2.47	118.32	122.33
32	2a	1407	5MC	C5-C4-N3	-2.45	119.03	121.67
54	1w	76	PPU	C3'-N3'-C	-2.45	119.52	123.21
1	2A	1915	5MU	C5-C6-N1	-2.44	120.83	123.34
1	1A	1962	5MC	C5-C4-N3	-2.44	119.05	121.67
1	2A	2503	2MA	C5-C6-N1	2.43	118.21	114.02
1	1A	2552	OMU	O4-C4-C5	-2.41	120.93	125.16
32	1a	967	5MC	C5-C4-N3	-2.41	119.08	121.67
1	1A	2503	2MA	C8-N7-C5	2.40	107.56	102.99
32	2a	516	PSU	O4'-C1'-C2'	2.34	108.45	105.14
1	1A	1939	5MU	C5M-C5-C4	2.34	121.34	118.77
32	2a	1402	4OC	C6-C5-C4	2.33	119.81	116.96
43	1l	92	0TD	OD1-CG-CB	-2.31	117.61	122.44
1	1A	2552	OMU	C5-C4-N3	2.29	118.27	114.84
32	1a	966	M2G	C8-N7-C5	2.29	107.35	102.99
1	2A	1920	OMC	C1'-N1-C2	2.28	123.51	118.42
54	1w	76	PPU	C10-N6-C6	-2.27	112.63	119.51
55	1x	76	8AN	O4'-C1'-C2'	-2.27	103.61	106.93
1	1A	1920	OMC	O2-C2-N3	-2.27	118.64	122.33
1	2A	2552	OMU	C5-C4-N3	2.26	118.23	114.84
32	2a	1400	5MC	C5-C4-N3	-2.26	119.24	121.67
54	2w	76	PPU	C10-N6-C6	-2.25	112.69	119.51
32	1a	1207	2MG	C5-C6-N1	2.25	117.92	113.95
1	1A	1915	5MU	C5-C6-N1	-2.24	121.03	123.34
1	2A	1942	5MC	C5-C4-N3	-2.24	119.26	121.67
1	1A	2605	PSU	C5-C6-N1	-2.24	118.75	122.11
1	2A	2251	OMG	O6-C6-C5	-2.24	120.00	124.37
1	1A	2605	PSU	O2-C2-N3	-2.22	117.63	121.82
32	1a	967	5MC	C1'-N1-C6	-2.20	117.46	121.12
32	2a	1400	5MC	O2-C2-N3	-2.20	118.75	122.33
32	2a	1207	2MG	C8-N7-C5	2.19	107.16	102.99
32	1a	516	PSU	O4'-C1'-C2'	2.18	108.21	105.14
32	1a	1498	UR3	C6-N1-C2	-2.18	119.84	121.79
32	1a	966	M2G	C5-C6-N1	2.18	117.79	113.95
32	2a	966	M2G	C5-C6-N1	2.16	117.77	113.95
1	1A	2251	OMG	C5-C6-N1	2.16	117.77	113.95
32	2a	1498	UR3	C3U-N3-C2	2.14	121.06	117.31
32	2a	966	M2G	C8-N7-C5	2.13	107.05	102.99
32	2a	967	5MC	C5-C4-N3	-2.11	119.40	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1207	2MG	O3'-C3'-C2'	2.10	118.62	111.82
1	1A	2503	2MA	C5-C6-N1	2.09	117.62	114.02
32	1a	516	PSU	C5-C6-N1	-2.08	118.99	122.11
1	2A	2605	PSU	C5-C6-N1	-2.07	119.01	122.11
1	1A	1942	5MC	C5-C4-N3	-2.06	119.45	121.67
54	2w	76	PPU	C3'-N3'-C	-2.06	120.11	123.21
43	2l	92	0TD	OD1-CG-CB	-2.03	118.19	122.44
32	1a	1498	UR3	C3U-N3-C4	2.03	120.79	117.89
32	1a	1402	4OC	C6-C5-C4	2.02	119.44	116.96
1	1A	1962	5MC	CM5-C5-C6	-2.02	120.15	122.85
1	1A	1942	5MC	CM5-C5-C6	-2.01	120.16	122.85

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
1	1A	2251	OMG	C1'-C2'-O2'-CM2
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
32	2a	1207	2MG	N1-C2-N2-CM2
32	2a	1207	2MG	N3-C2-N2-CM2
55	1x	76	8AN	O4'-C4'-C5'-O5'
55	1x	76	8AN	C3'-C4'-C5'-O5'
55	2x	76	8AN	C3'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
1	2A	1915	5MU	O4'-C4'-C5'-O5'
55	2x	76	8AN	O4'-C4'-C5'-O5'
55	2x	76	8AN	C4'-C5'-O5'-P
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
55	1x	76	8AN	C4'-C5'-O5'-P
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	1920	OMC	C3'-C2'-O2'-CM2
54	1w	76	PPU	C2'-C3'-N3'-C
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	2a	516	PSU	O4'-C1'-C5-C4
1	1A	1962	5MC	C2'-C1'-N1-C6
1	2A	1915	5MU	C3'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
32	1a	1519	MA6	C4'-C5'-O5'-P
54	1w	76	PPU	CA-C-N3'-C3'
1	1A	1962	5MC	O4'-C1'-N1-C6
32	2a	516	PSU	O4'-C1'-C5-C6
43	2l	92	0TD	CG-CB-SB-CSB
1	1A	1920	OMC	C2'-C1'-N1-C2
43	2l	92	0TD	SB-CB-CG-OD1
1	1A	2503	2MA	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	527	G7M	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 2534 ligands modelled in this entry, 2523 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	ARG	1B	231	57	10,11,11	0.79	1 (10%)	11,13,13	1.13	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	ARG	1F	317	-	10,11,11	0.74	1 (10%)	11,13,13	1.11	2 (18%)
58	MPD	18	104	-	7,7,7	0.36	0	9,10,10	0.34	0
58	MPD	1T	205	-	7,7,7	0.23	0	9,10,10	0.30	0
61	SF4	1d	307	35	0,12,12	-	-	-	-	-
58	MPD	2B	221	-	7,7,7	0.29	0	9,10,10	0.15	0
58	MPD	2A	3739	-	7,7,7	0.26	0	9,10,10	0.21	0
58	MPD	1a	1881	-	7,7,7	0.33	0	9,10,10	0.29	0
58	MPD	1A	4029	-	7,7,7	0.38	0	9,10,10	0.37	0
61	SF4	2d	501	35	0,12,12	-	-	-	-	-
62	MRD	2A	3738	-	7,7,7	0.28	0	9,10,10	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	ARG	1B	231	57	-	0/11/11/11	-
59	ARG	1F	317	-	-	1/11/11/11	-
58	MPD	18	104	-	-	1/5/5/5	-
58	MPD	1T	205	-	-	5/5/5/5	-
61	SF4	1d	307	35	-	-	0/6/5/5
58	MPD	2B	221	-	-	2/5/5/5	-
58	MPD	2A	3739	-	-	5/5/5/5	-
58	MPD	1a	1881	-	-	2/5/5/5	-
58	MPD	1A	4029	-	-	2/5/5/5	-
61	SF4	2d	501	35	-	-	0/6/5/5
62	MRD	2A	3738	-	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1B	231	ARG	OXT-C	-2.28	1.23	1.30
59	1F	317	ARG	OXT-C	-2.12	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1B	231	ARG	OXT-C-O	-2.89	117.52	124.09
59	1F	317	ARG	OXT-C-O	-2.83	117.66	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1F	317	ARG	OXT-C-CA	2.24	121.01	113.38
59	1B	231	ARG	OXT-C-CA	2.11	120.59	113.38

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1T	205	MPD	C1-C2-C3-C4
58	2A	3739	MPD	C2-C3-C4-O4
58	1T	205	MPD	O2-C2-C3-C4
58	1a	1881	MPD	O2-C2-C3-C4
58	2A	3739	MPD	O2-C2-C3-C4
58	18	104	MPD	C2-C3-C4-C5
58	1a	1881	MPD	C2-C3-C4-C5
58	2B	221	MPD	C2-C3-C4-C5
58	1T	205	MPD	CM-C2-C3-C4
58	2A	3739	MPD	C1-C2-C3-C4
58	2A	3739	MPD	CM-C2-C3-C4
58	1A	4029	MPD	C2-C3-C4-C5
58	1T	205	MPD	C2-C3-C4-C5
58	2A	3739	MPD	C2-C3-C4-C5
62	2A	3738	MRD	C2-C3-C4-C5
59	1F	317	ARG	CG-CD-NE-CZ
58	1A	4029	MPD	C2-C3-C4-O4
58	1T	205	MPD	C2-C3-C4-O4
58	2B	221	MPD	C2-C3-C4-O4
62	2A	3738	MRD	C2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2861/2915 (98%)	0.78	90 (3%) 49 47	19, 36, 80, 92	0
1	2A	2856/2915 (97%)	0.59	120 (4%) 36 35	33, 53, 81, 91	0
2	1B	120/121 (99%)	0.46	0 100 100	28, 49, 63, 76	0
2	2B	120/121 (99%)	0.35	1 (0%) 86 84	52, 68, 73, 78	0
3	1D	275/276 (99%)	0.71	2 (0%) 87 86	22, 38, 48, 62	0
3	2D	275/276 (99%)	0.68	5 (1%) 68 66	34, 48, 58, 68	0
4	1E	204/206 (99%)	0.71	1 (0%) 91 89	20, 40, 57, 68	0
4	2E	204/206 (99%)	0.57	1 (0%) 91 89	32, 54, 64, 79	0
5	1F	203/210 (96%)	0.67	0 100 100	18, 39, 63, 74	0
5	2F	203/210 (96%)	0.54	3 (1%) 73 72	37, 58, 68, 75	0
6	1G	181/182 (99%)	0.59	7 (3%) 39 38	42, 59, 67, 73	0
6	2G	181/182 (99%)	1.38	45 (24%) 0 0	60, 70, 75, 82	0
7	1H	174/180 (96%)	0.47	1 (0%) 89 88	34, 50, 59, 64	0
7	2H	173/180 (96%)	1.13	36 (20%) 1 0	59, 69, 74, 77	0
8	1I	147/148 (99%)	0.35	3 (2%) 65 63	41, 64, 71, 75	0
8	2I	146/148 (98%)	0.64	12 (8%) 11 10	50, 66, 73, 77	0
9	1N	140/140 (100%)	0.73	0 100 100	24, 36, 53, 64	0
9	2N	140/140 (100%)	0.57	2 (1%) 75 73	42, 57, 67, 71	0
10	1O	122/122 (100%)	0.56	0 100 100	29, 42, 56, 63	0
10	2O	122/122 (100%)	0.54	2 (1%) 72 70	44, 52, 62, 66	0
11	1P	149/150 (99%)	0.64	1 (0%) 87 86	20, 44, 59, 65	0
11	2P	149/150 (99%)	0.55	5 (3%) 45 44	36, 59, 70, 80	0
12	1Q	141/141 (100%)	0.70	0 100 100	26, 40, 50, 61	0
12	2Q	141/141 (100%)	0.67	9 (6%) 19 18	41, 56, 65, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.73	0 100 100	26, 35, 47, 57	0
13	2R	118/118 (100%)	0.59	4 (3%) 45 44	39, 50, 58, 60	0
14	1S	110/112 (98%)	0.61	2 (1%) 68 66	36, 49, 58, 61	0
14	2S	110/112 (98%)	0.82	14 (12%) 3 3	56, 62, 70, 72	0
15	1T	131/146 (89%)	0.56	1 (0%) 86 84	34, 44, 60, 70	0
15	2T	131/146 (89%)	0.45	1 (0%) 86 84	45, 55, 65, 73	0
16	1U	116/118 (98%)	0.86	1 (0%) 84 82	20, 29, 42, 53	0
16	2U	116/118 (98%)	0.72	5 (4%) 35 33	38, 53, 64, 69	0
17	1V	101/101 (100%)	0.68	0 100 100	21, 38, 52, 59	0
17	2V	101/101 (100%)	0.39	0 100 100	37, 60, 67, 71	0
18	1W	112/113 (99%)	0.79	0 100 100	22, 30, 50, 66	0
18	2W	112/113 (99%)	0.67	1 (0%) 84 82	41, 49, 58, 71	0
19	1X	95/96 (98%)	0.80	0 100 100	28, 38, 56, 65	0
19	2X	95/96 (98%)	0.75	7 (7%) 14 13	47, 55, 63, 67	0
20	1Y	107/110 (97%)	0.61	0 100 100	34, 46, 59, 67	0
20	2Y	107/110 (97%)	0.76	8 (7%) 14 13	52, 62, 69, 75	0
21	1Z	203/206 (98%)	0.58	3 (1%) 73 72	34, 52, 64, 70	0
21	2Z	201/206 (97%)	0.66	11 (5%) 25 24	54, 65, 71, 77	0
22	10	83/85 (97%)	0.78	2 (2%) 59 57	26, 37, 45, 54	0
22	20	83/85 (97%)	0.89	5 (6%) 21 20	41, 55, 62, 66	0
23	11	97/98 (98%)	0.72	3 (3%) 49 47	28, 43, 64, 66	0
23	21	97/98 (98%)	0.70	6 (6%) 20 19	41, 52, 63, 68	0
24	12	70/72 (97%)	0.55	1 (1%) 75 73	36, 47, 57, 71	0
24	22	70/72 (97%)	0.56	2 (2%) 51 50	51, 61, 67, 70	0
25	13	59/60 (98%)	0.66	0 100 100	24, 34, 57, 63	0
25	23	59/60 (98%)	0.64	2 (3%) 45 44	46, 54, 68, 75	0
26	14	69/71 (97%)	0.87	11 (15%) 1 1	56, 70, 76, 80	0
26	24	69/71 (97%)	1.73	25 (36%) 0 0	65, 75, 82, 83	0
27	15	59/60 (98%)	0.94	1 (1%) 70 68	21, 34, 48, 54	0
27	25	59/60 (98%)	0.63	2 (3%) 45 44	37, 47, 62, 72	0
28	16	53/54 (98%)	0.64	0 100 100	35, 41, 52, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.42	2 (3%) 40 39	49, 56, 62, 65	0
29	17	48/49 (97%)	0.96	1 (2%) 63 61	21, 28, 53, 60	0
29	27	48/49 (97%)	0.99	4 (8%) 11 10	34, 43, 58, 65	0
30	18	64/65 (98%)	0.78	0 100 100	27, 33, 42, 49	0
30	28	64/65 (98%)	0.83	5 (7%) 13 11	42, 52, 57, 61	0
31	19	37/37 (100%)	0.85	1 (2%) 54 52	28, 39, 50, 59	0
31	29	37/37 (100%)	0.92	2 (5%) 25 24	53, 59, 64, 66	0
32	1a	1488/1521 (97%)	0.57	64 (4%) 35 33	37, 65, 80, 90	0
32	2a	1492/1521 (98%)	0.56	72 (4%) 30 29	47, 67, 80, 88	0
33	1b	231/256 (90%)	0.76	25 (10%) 5 5	58, 69, 76, 79	0
33	2b	231/256 (90%)	0.92	30 (12%) 3 3	61, 71, 76, 81	0
34	1c	206/239 (86%)	0.96	31 (15%) 2 1	56, 68, 75, 80	0
34	2c	206/239 (86%)	1.07	32 (15%) 2 1	60, 71, 76, 79	0
35	1d	208/209 (99%)	1.31	52 (25%) 0 0	54, 66, 72, 76	0
35	2d	208/209 (99%)	0.76	15 (7%) 15 14	55, 64, 70, 73	0
36	1e	148/162 (91%)	0.87	15 (10%) 7 6	45, 61, 67, 72	0
36	2e	148/162 (91%)	0.67	7 (4%) 31 30	52, 63, 71, 78	0
37	1f	100/101 (99%)	0.38	0 100 100	52, 62, 67, 71	0
37	2f	100/101 (99%)	0.38	1 (1%) 82 80	52, 62, 68, 70	0
38	1g	155/156 (99%)	0.44	4 (2%) 56 54	58, 65, 72, 77	0
38	2g	155/156 (99%)	0.99	30 (19%) 1 0	60, 69, 73, 77	0
39	1h	137/138 (99%)	0.80	10 (7%) 15 13	53, 62, 68, 71	0
39	2h	137/138 (99%)	0.62	8 (5%) 23 22	57, 63, 68, 72	0
40	1i	127/128 (99%)	1.20	32 (25%) 0 0	58, 69, 74, 78	0
40	2i	126/128 (98%)	1.96	49 (38%) 0 0	64, 71, 76, 79	0
41	1j	97/105 (92%)	1.21	25 (25%) 0 0	57, 69, 76, 78	0
41	2j	96/105 (91%)	1.34	27 (28%) 0 0	63, 72, 75, 78	0
42	1k	114/129 (88%)	0.50	4 (3%) 44 43	45, 59, 66, 70	0
42	2k	114/129 (88%)	0.85	11 (9%) 8 7	54, 63, 70, 72	0
43	1l	121/132 (91%)	0.75	7 (5%) 23 22	50, 58, 64, 67	0
43	2l	121/132 (91%)	0.59	6 (4%) 28 27	52, 62, 68, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.65	9 (7%) 13 11	56, 67, 71, 76	0
44	2m	114/126 (90%)	1.25	24 (21%) 1 0	64, 70, 75, 77	0
45	1n	60/61 (98%)	1.67	15 (25%) 0 0	60, 67, 71, 72	0
45	2n	60/61 (98%)	2.21	24 (40%) 0 0	63, 70, 76, 79	0
46	1o	88/89 (98%)	0.50	3 (3%) 45 44	47, 59, 68, 75	0
46	2o	88/89 (98%)	0.53	3 (3%) 45 44	54, 63, 69, 72	0
47	1p	82/88 (93%)	1.36	18 (21%) 0 0	57, 66, 72, 73	0
47	2p	82/88 (93%)	0.65	3 (3%) 41 41	56, 62, 68, 71	0
48	1q	99/105 (94%)	1.09	17 (17%) 1 1	53, 63, 69, 72	0
48	2q	99/105 (94%)	0.78	6 (6%) 21 20	54, 62, 68, 73	0
49	1r	68/88 (77%)	0.52	2 (2%) 51 50	54, 61, 69, 75	0
49	2r	68/88 (77%)	0.52	3 (4%) 34 33	56, 62, 69, 71	0
50	1s	83/93 (89%)	0.78	6 (7%) 15 14	53, 68, 73, 78	0
50	2s	83/93 (89%)	1.30	20 (24%) 0 0	66, 72, 76, 79	0
51	1t	96/106 (90%)	1.39	26 (27%) 0 0	56, 66, 72, 75	0
51	2t	98/106 (92%)	0.74	7 (7%) 16 14	53, 63, 70, 74	0
52	1u	23/27 (85%)	1.31	4 (17%) 1 1	63, 67, 70, 71	0
52	2u	23/27 (85%)	1.91	12 (52%) 0 0	65, 69, 72, 74	0
53	1y	97/113 (85%)	0.69	2 (2%) 63 61	50, 60, 67, 71	0
53	2y	96/113 (84%)	2.49	54 (56%) 0 0	62, 68, 74, 75	0
54	1w	3/4 (75%)	0.27	0 100 100	28, 28, 36, 40	0
54	2w	3/4 (75%)	-0.23	0 100 100	44, 44, 47, 53	0
55	1x	3/4 (75%)	0.72	0 100 100	27, 27, 29, 44	0
55	2x	3/4 (75%)	0.50	0 100 100	43, 43, 46, 52	0
56	1v	3/3 (100%)	0.98	0 100 100	22, 22, 23, 26	0
56	2v	3/3 (100%)	2.22	2 (66%) 0 0	46, 46, 49, 52	0
All	All	20796/21490 (96%)	0.73	1296 (6%) 20 19	18, 58, 76, 92	0

All (1296) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1091	G	9.5
34	2c	160	ALA	8.5

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Mol	Chain	Res	Type	RSRZ
33	1b	228	GLY	8.2
53	2y	40	ILE	8.0
1	2A	2138	C	7.8
53	2y	88	LEU	7.6
33	2b	231	GLU	7.2
1	2A	2141	G	7.1
1	2A	2147	G	6.9
45	2n	13	THR	6.8
1	1A	1090	U	6.8
48	1q	98	LEU	6.7
1	2A	2140	C	6.6
1	1A	1076	C	6.5
44	1m	2	ALA	6.4
1	2A	229	A	6.3
1	1A	1065	U	6.2
53	2y	52	ALA	6.2
1	2A	2139	C	6.1
1	1A	1066	U	6.1
45	2n	43	CYS	6.1
45	2n	38	GLY	6.1
1	2A	2142	C	6.0
41	2j	19	SER	6.0
1	1A	1089	G	5.9
32	2a	1030(B)	C	5.9
38	2g	5	ARG	5.8
1	2A	2146	C	5.7
1	2A	2153	G	5.6
1	2A	2154	G	5.6
1	2A	2107	C	5.6
40	2i	45	ALA	5.5
1	1A	1075	C	5.5
34	2c	157	ILE	5.5
32	1a	1028	C	5.5
26	24	49	PHE	5.4
31	29	16	VAL	5.4
43	2l	18	VAL	5.4
32	1a	1257	U	5.4
33	2b	216	SER	5.4
42	2k	74	ALA	5.3
1	2A	2106	G	5.3
26	14	18	CYS	5.3
34	1c	180	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
53	2y	42	SER	5.2
1	2A	2179	C	5.2
33	2b	123	ALA	5.2
1	1A	1074	G	5.2
26	24	50	VAL	5.1
6	2G	135	LEU	5.1
45	2n	44	LEU	5.1
26	24	63	TYR	5.1
41	1j	47	PHE	5.1
53	2y	63	ALA	5.1
1	2A	2136	C	5.1
1	2A	2162	G	5.0
51	1t	76	ALA	5.0
1	2A	2110	G	5.0
1	2A	2151	G	5.0
50	2s	49	ILE	5.0
1	1A	1080	C	5.0
32	1a	1031	G	5.0
35	1d	69	GLY	5.0
53	2y	9	GLN	5.0
1	2A	2168	G	4.9
32	2a	1286	A	4.9
51	1t	73	HIS	4.9
26	24	52	THR	4.9
53	2y	45	PRO	4.9
1	2A	2120	G	4.9
32	2a	1257	U	4.9
34	1c	81	GLY	4.9
45	2n	12	ARG	4.8
45	1n	34	TYR	4.8
48	1q	27	PHE	4.8
35	1d	32	ALA	4.8
53	2y	74	ILE	4.8
32	1a	1001(A)	G	4.8
50	2s	9	VAL	4.8
1	1A	1087	G	4.8
1	1A	1072	C	4.8
53	2y	15	ALA	4.8
53	2y	71	TYR	4.7
32	1a	1001	A	4.7
51	1t	70	SER	4.7
1	2A	2174	C	4.7

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Mol	Chain	Res	Type	RSRZ
6	2G	146	TYR	4.7
1	1A	2141	G	4.7
1	2A	2124	G	4.7
53	2y	11	GLU	4.7
33	2b	124	SER	4.7
20	2Y	1	MET	4.7
40	2i	115	GLY	4.7
21	2Z	191	VAL	4.7
1	2A	1076	C	4.6
1	1A	1092	C	4.6
1	2A	2116	G	4.6
7	2H	82	GLY	4.6
44	2m	15	VAL	4.6
53	2y	48	PHE	4.6
1	2A	2176	A	4.6
1	1A	1068	G	4.6
1	2A	2155	G	4.6
40	2i	72	GLY	4.6
40	2i	27	THR	4.5
26	14	49	PHE	4.5
7	2H	93	GLY	4.5
40	2i	73	GLN	4.5
7	2H	19	VAL	4.5
1	2A	1509	C	4.5
33	1b	123	ALA	4.4
1	1A	1064	C	4.4
1	2A	2805	G	4.4
47	1p	19	ILE	4.4
1	2A	2132	U	4.4
52	2u	15	ARG	4.4
40	2i	18	PHE	4.4
39	1h	134	ILE	4.4
1	2A	1046	A	4.4
1	2A	2792	G	4.4
45	2n	35	ARG	4.3
40	2i	108	VAL	4.3
35	1d	87	GLY	4.3
52	2u	14	TRP	4.3
1	2A	2125	G	4.3
53	2y	77	LEU	4.3
32	1a	999	C	4.3
6	2G	58	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
45	1n	33	VAL	4.3
40	2i	10	ARG	4.3
1	2A	2793	G	4.3
1	2A	2804	C	4.2
34	2c	177	THR	4.2
50	2s	63	THR	4.2
1	2A	2169	A	4.2
45	2n	61	TRP	4.2
45	1n	25	VAL	4.2
40	2i	122	ALA	4.2
1	1A	1088	A	4.2
41	2j	89	ASP	4.2
1	2A	888	C	4.2
32	1a	1030	C	4.2
6	2G	85	GLY	4.2
21	2Z	192	ALA	4.2
53	2y	79	ASN	4.2
1	1A	2132	U	4.2
1	1A	2142	C	4.2
1	1A	1093	G	4.1
45	1n	14	PRO	4.1
1	2A	2802	G	4.1
7	2H	165	ALA	4.1
34	2c	23	TYR	4.1
53	2y	72	THR	4.1
23	21	51	VAL	4.1
45	2n	25	VAL	4.1
15	1T	38	ASN	4.1
33	2b	136	VAL	4.1
1	2A	2165	G	4.1
40	2i	62	TYR	4.1
40	2i	126	SER	4.0
1	1A	1067	A	4.0
1	1A	1079	C	4.0
1	1A	2805	G	4.0
41	1j	49	VAL	4.0
7	2H	102	ALA	4.0
26	24	66	SER	4.0
35	1d	4	TYR	4.0
35	1d	3	ARG	4.0
41	1j	46	ARG	4.0
14	2S	22	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
35	1d	186	LEU	3.9
32	2a	1001(A)	G	3.9
6	2G	61	ALA	3.9
45	2n	24	CYS	3.9
34	1c	87	LEU	3.9
40	1i	26	VAL	3.9
53	2y	78	ILE	3.9
1	1A	1077	A	3.9
32	2a	1531	A	3.9
32	2a	1030(A)	G	3.9
40	1i	28	VAL	3.9
1	2A	2126	A	3.9
32	1a	1492	A	3.9
1	2A	2123	G	3.9
33	1b	121	LEU	3.9
34	2c	87	LEU	3.9
40	2i	103	THR	3.9
1	1A	888	C	3.9
40	2i	109	VAL	3.9
1	2A	6	A	3.9
6	2G	62	LEU	3.9
32	2a	1001	A	3.9
33	1b	233	SER	3.9
45	1n	24	CYS	3.9
53	2y	49	VAL	3.9
50	2s	79	THR	3.8
1	1A	2113	U	3.8
1	2A	2803	C	3.8
6	2G	152	LEU	3.8
41	2j	98	ILE	3.8
3	2D	272	ALA	3.8
45	1n	10	ALA	3.8
1	2A	1085	A	3.8
1	2A	2108	C	3.8
45	2n	34	TYR	3.8
42	2k	69	ALA	3.8
53	2y	39	ILE	3.8
12	2Q	59	ARG	3.8
6	2G	138	GLN	3.8
1	1A	1059	G	3.8
1	1A	1102	C	3.8
34	1c	41	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
52	2u	9	ARG	3.8
40	2i	74	ILE	3.8
53	2y	73	ALA	3.8
1	1A	2794	C	3.8
29	27	47	ARG	3.7
51	1t	67	ALA	3.7
30	28	20	GLY	3.7
1	2A	2152	G	3.7
7	2H	98	LEU	3.7
47	1p	73	LEU	3.7
23	11	2	SER	3.7
38	2g	6	ARG	3.7
1	2A	2801(A)	A	3.7
26	24	64	GLY	3.7
40	2i	30	GLY	3.7
1	1A	1509	C	3.7
1	1A	2159	G	3.7
6	1G	82	LEU	3.7
35	1d	58	LEU	3.7
34	1c	80	GLY	3.7
40	2i	127	LYS	3.7
7	2H	95	ARG	3.7
40	2i	66	ARG	3.7
45	2n	26	ARG	3.7
33	2b	44	LEU	3.7
40	2i	105	ASP	3.7
35	1d	67	ILE	3.7
1	1A	1078	U	3.7
1	1A	2155	G	3.7
6	2G	7	LEU	3.7
26	24	29	PRO	3.7
53	2y	64	SER	3.7
53	2y	23	ARG	3.7
40	2i	14	VAL	3.7
34	1c	60	ALA	3.7
33	1b	227	GLY	3.6
1	1A	2147	G	3.6
6	2G	39	ILE	3.6
23	21	2	SER	3.6
39	2h	2	LEU	3.6
47	1p	29	ASP	3.6
44	2m	5	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
53	2y	50	ALA	3.6
1	2A	2104	G	3.6
1	2A	2131	G	3.6
40	2i	67	GLY	3.6
53	2y	51	ASP	3.6
35	1d	112	VAL	3.6
1	2A	2149	G	3.6
50	2s	10	PHE	3.6
1	1A	2140	C	3.6
32	1a	1000	U	3.6
26	14	52	THR	3.6
50	2s	41	VAL	3.6
33	2b	127	ILE	3.6
53	2y	12	ILE	3.6
1	2A	2118	U	3.6
52	2u	23	PRO	3.6
1	2A	2181	G	3.6
29	27	45	ALA	3.6
38	2g	83	ALA	3.6
45	1n	22	THR	3.6
1	1A	1103	A	3.6
53	2y	91	LYS	3.6
1	1A	2803	C	3.6
53	2y	41	LEU	3.6
40	2i	36	TYR	3.6
35	2d	146	ILE	3.5
41	2j	68	HIS	3.5
38	2g	25	ALA	3.5
1	2A	652(B)	A	3.5
26	24	28	LYS	3.5
33	1b	118	LEU	3.5
1	1A	1071	G	3.5
38	2g	30	ILE	3.5
40	1i	33	PHE	3.5
1	1A	2144	U	3.5
32	2a	1040	U	3.5
40	2i	102	LEU	3.5
45	2n	53	LEU	3.5
53	2y	75	ASN	3.5
45	1n	13	THR	3.5
48	1q	7	THR	3.5
53	2y	25	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
26	24	10	VAL	3.5
42	2k	14	VAL	3.5
6	2G	140	ILE	3.5
1	1A	1063	G	3.5
1	2A	2105	C	3.5
34	2c	155	GLY	3.5
32	1a	198	G	3.5
26	24	45	GLY	3.5
1	2A	2164	C	3.5
32	2a	1150	U	3.5
1	1A	1098	A	3.4
6	2G	139	LEU	3.4
38	2g	22	LEU	3.4
35	2d	48	ALA	3.4
36	1e	134	ALA	3.4
35	2d	166	LYS	3.4
44	2m	64	TRP	3.4
53	2y	10	MET	3.4
1	2A	2190	G	3.4
1	1A	2123	G	3.4
34	2c	60	ALA	3.4
1	2A	1075	C	3.4
1	2A	2143	C	3.4
51	1t	17	ARG	3.4
52	1u	14	TRP	3.4
7	2H	71	LEU	3.4
47	1p	60	LEU	3.4
50	2s	80	TYR	3.4
36	2e	16	THR	3.4
1	2A	2173	A	3.4
1	2A	2159	G	3.4
40	2i	75	ASP	3.4
7	2H	166	GLY	3.4
45	1n	61	TRP	3.4
45	2n	14	PRO	3.4
29	27	46	VAL	3.4
32	2a	1030(C)	G	3.4
44	2m	93	ARG	3.4
34	2c	145	GLY	3.3
40	1i	67	GLY	3.3
34	1c	193	TYR	3.3
40	2i	76	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
29	17	46	VAL	3.3
38	2g	80	VAL	3.3
32	1a	1029	C	3.3
32	1a	1023	G	3.3
32	2a	1036	G	3.3
6	2G	43	LEU	3.3
41	1j	96	ILE	3.3
40	2i	90	PRO	3.3
33	2b	113	HIS	3.3
40	1i	117	HIS	3.3
53	2y	38	HIS	3.3
52	1u	2	GLY	3.3
35	1d	11	LEU	3.3
26	24	27	THR	3.3
44	2m	26	GLY	3.3
19	2X	92	LEU	3.3
33	2b	122	PHE	3.3
32	1a	1040	U	3.3
34	1c	182	ILE	3.3
34	2c	8	ILE	3.3
35	1d	138	TYR	3.3
40	1i	125	TYR	3.3
44	2m	7	VAL	3.3
33	1b	122	PHE	3.3
1	1A	2804	C	3.3
51	1t	12	ALA	3.3
41	1j	10	GLY	3.3
1	1A	2153	G	3.3
38	2g	41	ARG	3.3
7	2H	128	PRO	3.3
53	2y	19	HIS	3.3
26	24	68	ARG	3.3
32	1a	1030(C)	G	3.2
35	1d	37	PRO	3.2
34	1c	204	LEU	3.2
34	2c	61	ALA	3.2
39	1h	16	ALA	3.2
45	2n	28	GLY	3.2
51	1t	32	ALA	3.2
1	1A	1082	U	3.2
38	2g	4	ARG	3.2
45	1n	18	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
47	1p	59	TRP	3.2
50	2s	71	LEU	3.2
33	2b	39	ILE	3.2
1	2A	645	C	3.2
47	1p	38	TYR	3.2
34	1c	47	LEU	3.2
44	2m	116	THR	3.2
1	2A	2121	G	3.2
26	24	56	VAL	3.2
40	2i	13	ALA	3.2
47	1p	7	ALA	3.2
1	2A	1083	U	3.2
7	2H	101	ARG	3.2
14	2S	20	ARG	3.2
40	2i	42	ARG	3.2
1	2A	2148	G	3.2
50	2s	82	GLY	3.2
1	2A	1079	C	3.2
53	2y	53	THR	3.2
7	2H	92	ILE	3.2
56	2v	1	MET	3.2
22	20	42	GLY	3.2
41	2j	10	GLY	3.2
1	2A	2115	G	3.2
1	2A	2319	G	3.2
32	2a	1068	G	3.2
38	2g	105	VAL	3.2
43	1l	24	VAL	3.2
34	1c	39	ILE	3.2
44	2m	84	ILE	3.2
45	2n	37	PHE	3.2
6	2G	3	LEU	3.2
20	2Y	42	VAL	3.2
35	2d	56	VAL	3.2
35	1d	70	ILE	3.1
48	1q	36	ILE	3.1
53	2y	65	GLY	3.1
53	2y	80	LYS	3.1
14	2S	54	LEU	3.1
26	24	30	GLU	3.1
35	1d	157	LEU	3.1
38	2g	7	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
35	1d	38	TYR	3.1
26	14	46	GLN	3.1
12	2Q	19	GLY	3.1
6	2G	87	PRO	3.1
7	2H	8	PRO	3.1
33	2b	131	PRO	3.1
40	1i	94	ALA	3.1
50	2s	11	VAL	3.1
1	2A	2172	U	3.1
32	2a	1358	U	3.1
34	1c	128	PHE	3.1
32	1a	1043	C	3.1
32	1a	1286	A	3.1
40	1i	14	VAL	3.1
40	1i	99	LEU	3.1
12	2Q	89	ASN	3.1
42	1k	25	TYR	3.1
44	1m	25	ILE	3.1
1	2A	2127	G	3.1
35	1d	19	LEU	3.1
41	1j	18	ALA	3.1
48	2q	6	LEU	3.1
36	1e	6	PHE	3.1
39	2h	65	TYR	3.1
46	1o	19	PRO	3.1
1	2A	889	C	3.1
7	2H	20	ALA	3.1
12	2Q	114	ALA	3.1
34	2c	4	LYS	3.1
53	2y	16	ILE	3.1
43	2l	19	ARG	3.1
11	2P	109	GLY	3.1
44	1m	115	LYS	3.1
40	1i	19	LEU	3.1
41	2j	44	VAL	3.1
34	1c	8	ILE	3.0
38	1g	156	TRP	3.0
6	2G	11	TYR	3.0
11	2P	110	TYR	3.0
26	24	67	TYR	3.0
32	1a	76	C	3.0
1	2A	2117	A	3.0

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Mol	Chain	Res	Type	RSRZ
6	2G	20	ILE	3.0
48	1q	90	ILE	3.0
20	2Y	55	TYR	3.0
47	1p	17	TYR	3.0
32	1a	70	G	3.0
53	2y	92	GLY	3.0
35	2d	58	LEU	3.0
40	1i	126	SER	3.0
1	2A	2191	G	3.0
10	2O	91	LEU	3.0
32	1a	1368	G	3.0
53	2y	98	ALA	3.0
1	2A	2111	C	3.0
38	2g	27	ILE	3.0
32	1a	1030(D)	A	3.0
47	1p	61	SER	3.0
14	2S	5	THR	3.0
51	2t	35	THR	3.0
34	1c	206	GLU	3.0
46	2o	61	GLY	3.0
1	1A	1081	U	3.0
40	2i	121	ARG	3.0
1	2A	1067	A	3.0
1	2A	2170	A	3.0
6	2G	151	ALA	3.0
51	1t	72	LEU	3.0
53	2y	94	ALA	3.0
33	1b	125	PRO	3.0
40	2i	111	ARG	3.0
51	1t	47	GLY	3.0
1	2A	2163	C	3.0
1	2A	2175	C	3.0
26	24	46	GLN	3.0
34	2c	162	GLN	3.0
35	1d	2	GLY	3.0
35	1d	132	ARG	3.0
38	2g	32	ARG	3.0
6	2G	149	VAL	2.9
1	2A	2167	U	2.9
32	1a	1036	G	2.9
32	2a	216	G	2.9
35	1d	10	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
5	2F	14	PRO	2.9
39	2h	28	ALA	2.9
21	2Z	96	VAL	2.9
35	1d	178	VAL	2.9
32	1a	1212	U	2.9
36	1e	118	ILE	2.9
34	1c	139	GLN	2.9
51	1t	79	ARG	2.9
32	2a	1008	C	2.9
1	1A	2181	G	2.9
21	2Z	187	ALA	2.9
32	1a	1033	G	2.9
39	1h	67	PRO	2.9
45	1n	55	GLY	2.9
51	1t	66	ALA	2.9
8	2I	19	VAL	2.9
32	2a	975	A	2.9
50	2s	69	HIS	2.9
14	2S	12	PHE	2.9
1	1A	1053	C	2.9
1	1A	2792	G	2.9
33	1b	165	VAL	2.9
42	2k	109	VAL	2.9
1	1A	229	A	2.9
1	2A	2119	A	2.9
32	2a	1041	A	2.9
51	1t	55	ILE	2.9
26	14	45	GLY	2.9
34	2c	159	GLY	2.9
48	1q	37	LYS	2.9
33	1b	232	PRO	2.9
40	2i	91	ASP	2.9
41	2j	40	LEU	2.9
44	2m	72	ALA	2.9
1	2A	2145	C	2.9
29	27	48	LYS	2.9
47	2p	11	SER	2.9
1	1A	1175	U	2.9
31	29	37	GLY	2.9
35	2d	5	ILE	2.9
41	2j	20	ALA	2.9
32	2a	1006	C	2.9

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Mol	Chain	Res	Type	RSRZ
32	2a	1259	C	2.9
35	1d	124	GLY	2.9
51	2t	9	ASN	2.9
41	2j	74	ILE	2.9
26	24	54	GLY	2.8
32	1a	401	C	2.8
40	1i	32	ASP	2.8
41	1j	44	VAL	2.8
43	1l	18	VAL	2.8
41	1j	59	SER	2.8
52	2u	11	GLY	2.8
33	2b	229	VAL	2.8
51	1t	18	GLN	2.8
6	2G	157	ILE	2.8
7	2H	159	GLU	2.8
50	2s	5	LEU	2.8
35	1d	152	SER	2.8
6	2G	5	VAL	2.8
7	2H	35	VAL	2.8
19	2X	69	TYR	2.8
1	2A	1041	C	2.8
32	1a	1030(B)	C	2.8
40	2i	29	ASN	2.8
33	1b	135	GLN	2.8
1	1A	2127	G	2.8
1	1A	2793	G	2.8
7	2H	44	VAL	2.8
32	2a	1033	G	2.8
32	2a	1202	G	2.8
8	1I	89	TYR	2.8
1	2A	2177	C	2.8
44	1m	28	ALA	2.8
49	1r	42	ARG	2.8
7	2H	113	VAL	2.8
7	2H	115	VAL	2.8
47	1p	48	TRP	2.8
49	2r	60	ALA	2.8
44	2m	68	GLY	2.8
41	1j	62	HIS	2.8
6	2G	117	PHE	2.8
6	2G	144	ILE	2.8
34	2c	158	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
36	1e	95	ALA	2.8
45	1n	2	ALA	2.8
45	1n	7	ILE	2.8
32	2a	1283	G	2.8
35	2d	188	LEU	2.8
35	1d	166	LYS	2.8
32	2a	1367	C	2.8
51	1t	64	ASP	2.8
26	24	57	GLU	2.7
48	1q	86	GLU	2.7
1	2A	2144	U	2.7
36	2e	29	GLY	2.7
51	1t	75	ASN	2.7
8	2I	55	ALA	2.7
32	1a	1447	A	2.7
36	1e	94	ALA	2.7
21	2Z	153	SER	2.7
1	2A	11	G	2.7
32	2a	1034	G	2.7
33	1b	136	VAL	2.7
33	2b	133	LYS	2.7
35	1d	133	VAL	2.7
41	1j	31	GLY	2.7
46	1o	86	GLY	2.7
1	1A	1083	U	2.7
12	2Q	110	THR	2.7
34	1c	124	ILE	2.7
36	1e	131	ILE	2.7
36	1e	132	ALA	2.7
40	1i	52	ALA	2.7
44	2m	11	ARG	2.7
53	2y	7	SER	2.7
1	2A	2178	C	2.7
6	2G	142	PRO	2.7
32	1a	1030(A)	G	2.7
32	2a	1023	G	2.7
40	1i	121	ARG	2.7
6	1G	80	PHE	2.7
50	2s	39	THR	2.7
41	2j	16	LEU	2.7
38	2g	36	LYS	2.7
35	2d	23	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2161	C	2.7
41	2j	72	VAL	2.7
1	2A	2833	G	2.7
32	1a	306	G	2.7
32	1a	1021	G	2.7
1	1A	271(K)	U	2.7
14	1S	6	ALA	2.7
35	1d	21	LEU	2.7
51	1t	45	GLN	2.7
34	2c	22	TRP	2.7
1	2A	1095	A	2.7
33	2b	86	GLU	2.7
48	1q	2	PRO	2.7
1	1A	889	C	2.7
1	1A	2143	C	2.7
6	2G	49	ASP	2.7
32	1a	1037	C	2.7
40	2i	65	VAL	2.7
6	2G	110	ALA	2.7
7	1H	2	SER	2.7
26	14	59	PHE	2.7
32	2a	998	G	2.7
12	2Q	33	GLY	2.7
40	1i	22	GLY	2.7
40	2i	100	GLY	2.7
32	2a	1157	A	2.7
26	14	66	SER	2.7
32	2a	202	U	2.7
44	2m	20	THR	2.7
6	2G	23	PHE	2.7
7	2H	4	ILE	2.7
7	2H	111	HIS	2.7
1	2A	2166	G	2.7
26	24	19	GLY	2.7
44	2m	87	TYR	2.7
6	2G	29	TRP	2.7
32	2a	1492	A	2.6
34	1c	146	ALA	2.6
53	1y	95	ARG	2.6
6	2G	127	GLY	2.6
7	2H	142	GLY	2.6
27	15	60	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	1A	1073	A	2.6
1	2A	2134	A	2.6
32	1a	270	A	2.6
26	24	39	CYS	2.6
34	2c	63	ASN	2.6
38	2g	101	LEU	2.6
44	1m	89	GLY	2.6
51	2t	55	ILE	2.6
53	2y	5	ILE	2.6
1	1A	2107	C	2.6
32	1a	623	C	2.6
40	1i	98	PRO	2.6
19	2X	68	ARG	2.6
41	1j	60	ARG	2.6
1	2A	2156	G	2.6
1	2A	890	A	2.6
32	2a	981	U	2.6
33	2b	132	LYS	2.6
40	2i	92	TYR	2.6
31	19	29	ASN	2.6
8	2I	3	VAL	2.6
34	2c	165	THR	2.6
40	1i	27	THR	2.6
1	1A	2166	G	2.6
32	1a	1034	G	2.6
35	1d	97	LEU	2.6
40	1i	90	PRO	2.6
45	1n	12	ARG	2.6
43	1l	64	TYR	2.6
34	2c	71	ALA	2.6
35	1d	73	ARG	2.6
1	2A	2150	U	2.6
7	2H	21	PRO	2.6
49	2r	26	LEU	2.6
1	1A	2168	G	2.6
1	2A	2187	G	2.6
32	2a	1003	G	2.6
1	1A	1085	A	2.6
1	2A	2137	C	2.6
1	2A	2896	C	2.6
8	2I	13	GLY	2.6
36	2e	22	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
40	2i	117	HIS	2.6
38	2g	10	ARG	2.6
40	2i	93	ARG	2.6
33	1b	207	ALA	2.6
41	2j	27	ALA	2.6
33	1b	229	VAL	2.6
48	1q	85	VAL	2.6
21	2Z	125	LEU	2.6
1	1A	1061	U	2.6
1	1A	1097	U	2.6
1	1A	278	A	2.6
1	1A	1099	G	2.6
7	2H	155	SER	2.6
41	1j	68	HIS	2.6
6	2G	57	ALA	2.5
30	28	17	THR	2.5
19	2X	66	LEU	2.5
36	1e	91	LEU	2.5
26	24	17	GLY	2.5
33	2b	19	HIS	2.5
50	2s	66	MET	2.5
52	1u	18	TYR	2.5
14	2S	21	THR	2.5
38	2g	39	ALA	2.5
23	21	68	PRO	2.5
32	2a	1533	C	2.5
6	2G	51	ARG	2.5
32	2a	1136	U	2.5
7	2H	121	ILE	2.5
34	1c	203	PHE	2.5
36	2e	84	PHE	2.5
50	2s	54	GLY	2.5
7	2H	83	TYR	2.5
26	24	60	GLN	2.5
40	2i	88	TYR	2.5
40	2i	114	TYR	2.5
41	2j	87	THR	2.5
51	1t	40	ALA	2.5
6	2G	103	LEU	2.5
24	22	21	LEU	2.5
32	2a	1029	C	2.5
32	2a	1032	G	2.5

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Mol	Chain	Res	Type	RSRZ
33	2b	164	VAL	2.5
34	2c	196	LEU	2.5
45	2n	33	VAL	2.5
48	1q	73	VAL	2.5
50	2s	51	VAL	2.5
1	2A	2109	U	2.5
34	2c	3	ASN	2.5
35	1d	130	GLY	2.5
39	1h	38	ILE	2.5
39	1h	66	GLY	2.5
39	1h	87	SER	2.5
7	2H	106	THR	2.5
11	2P	57	THR	2.5
39	2h	40	ALA	2.5
41	1j	32	ALA	2.5
1	1A	890	A	2.5
1	1A	2169	A	2.5
3	2D	3	VAL	2.5
7	2H	88	LEU	2.5
32	1a	913	A	2.5
35	2d	203	VAL	2.5
1	1A	1055	G	2.5
1	1A	2182	G	2.5
48	1q	99	SER	2.5
4	1E	68	ALA	2.5
7	2H	145	ALA	2.5
34	2c	199	LYS	2.5
43	1l	61	THR	2.5
35	2d	69	GLY	2.5
36	2e	12	LEU	2.5
32	2a	1357	A	2.5
16	2U	80	ILE	2.5
32	2a	1007	C	2.5
34	1c	179	ARG	2.5
48	2q	86	GLU	2.5
1	1A	2156	G	2.5
21	1Z	192	ALA	2.5
35	2d	147	ALA	2.5
33	1b	215	LEU	2.5
2	2B	90	A	2.5
9	2N	85	ILE	2.5
35	1d	86	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
32	1a	1032	G	2.5
32	1a	1186	G	2.5
41	2j	18	ALA	2.5
44	2m	69	GLU	2.5
47	1p	37	GLY	2.5
53	2y	6	THR	2.5
33	1b	139	LYS	2.4
39	2h	38	ILE	2.4
41	2j	47	PHE	2.4
32	1a	307	C	2.4
32	2a	1326	C	2.4
8	2I	36	ALA	2.4
35	2d	180	GLY	2.4
35	1d	168	ARG	2.4
38	2g	86	GLN	2.4
32	1a	61	G	2.4
32	1a	78	G	2.4
32	2a	1021	G	2.4
32	2a	1353	G	2.4
25	23	59	VAL	2.4
33	2b	81	VAL	2.4
42	2k	75	TYR	2.4
52	2u	5	ASP	2.4
35	1d	93	PHE	2.4
50	1s	72	GLY	2.4
1	2A	1847	A	2.4
32	2a	1030(D)	A	2.4
3	2D	119	ALA	2.4
6	2G	145	THR	2.4
44	2m	63	THR	2.4
47	2p	45	THR	2.4
34	2c	89	GLU	2.4
1	2A	2182	G	2.4
52	1u	21	TYR	2.4
41	2j	96	ILE	2.4
38	2g	11	GLN	2.4
53	2y	70	MET	2.4
44	2m	89	GLY	2.4
26	24	40	HIS	2.4
45	2n	22	THR	2.4
32	1a	1027	C	2.4
6	2G	133	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
38	1g	16	LEU	2.4
40	2i	40	LEU	2.4
41	1j	94	VAL	2.4
41	1j	51	ARG	2.4
6	1G	85	GLY	2.4
34	1c	158	GLY	2.4
45	2n	51	GLY	2.4
1	2A	2184	G	2.4
15	2T	131	ALA	2.4
24	22	58	ALA	2.4
34	1c	168	ALA	2.4
51	1t	78	ALA	2.4
14	2S	17	ARG	2.4
32	2a	91	C	2.4
35	1d	170	VAL	2.4
50	1s	58	VAL	2.4
52	2u	16	GLY	2.4
26	24	43	TYR	2.4
39	2h	4	ASP	2.4
42	1k	60	ALA	2.4
1	1A	2131	G	2.4
1	2A	1099	G	2.4
1	2A	2133	G	2.4
32	1a	1024	G	2.4
41	2j	48	THR	2.4
45	2n	47	LEU	2.4
1	1A	2790	A	2.4
38	2g	9	VAL	2.4
40	2i	69	GLY	2.4
1	1A	1094	U	2.4
1	1A	2150	U	2.4
12	2Q	32	TYR	2.4
20	2Y	5	MET	2.4
33	2b	201	ILE	2.4
35	1d	126	ILE	2.4
51	1t	63	ILE	2.4
20	2Y	89	PHE	2.4
21	1Z	51	ALA	2.4
34	2c	144	SER	2.4
21	2Z	155	LEU	2.4
30	28	62	LEU	2.4
34	2c	52	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
38	1g	12	LEU	2.4
40	2i	35	GLU	2.4
47	1p	49	LEU	2.4
1	1A	2116	G	2.3
14	2S	19	LYS	2.3
26	14	17	GLY	2.3
40	2i	57	GLY	2.3
23	2l	70	VAL	2.3
43	1l	104	VAL	2.3
32	1a	841	U	2.3
32	1a	1020	U	2.3
32	2a	1287	A	2.3
34	1c	134	ILE	2.3
40	1i	123	PRO	2.3
53	2y	67	HIS	2.3
41	2j	86	MET	2.3
40	2i	4	TYR	2.3
21	1Z	188	ALA	2.3
35	1d	179	GLU	2.3
51	2t	11	SER	2.3
35	1d	61	LYS	2.3
41	2j	31	GLY	2.3
43	2l	93	LEU	2.3
11	2P	79	ARG	2.3
32	2a	1356	G	2.3
6	2G	150	ASP	2.3
6	2G	166	ASP	2.3
16	2U	2	PRO	2.3
33	1b	146	GLN	2.3
20	2Y	78	ALA	2.3
21	2Z	188	ALA	2.3
34	2c	184	TYR	2.3
23	2l	55	GLY	2.3
35	1d	16	GLY	2.3
34	1c	91	LEU	2.3
35	1d	78	LEU	2.3
51	1t	22	ARG	2.3
41	2j	62	HIS	2.3
51	2t	73	HIS	2.3
33	2b	165	VAL	2.3
47	1p	20	VAL	2.3
1	1A	1914	C	2.3

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Mol	Chain	Res	Type	RSRZ
1	1A	2133	G	2.3
1	2A	277	C	2.3
1	2A	1104	C	2.3
32	1a	1006	C	2.3
32	2a	1236	A	2.3
36	2e	48	ALA	2.3
43	2l	118	SER	2.3
8	2I	35	LEU	2.3
25	23	30	ARG	2.3
41	1j	5	ARG	2.3
41	2j	85	LEU	2.3
52	2u	6	ARG	2.3
6	2G	67	LYS	2.3
7	2H	154	PRO	2.3
8	1I	19	VAL	2.3
34	2c	18	TRP	2.3
38	1g	112	PRO	2.3
46	1o	87	ILE	2.3
35	1d	12	CYS	2.3
37	2f	29	ALA	2.3
40	1i	43	ALA	2.3
42	2k	89	ALA	2.3
43	1l	22	SER	2.3
45	2n	27	CYS	2.3
19	2X	60	ARG	2.3
32	1a	1285	A	2.3
32	2a	79	G	2.3
32	2a	1064	G	2.3
3	2D	38	LYS	2.3
13	2R	18	LEU	2.3
35	1d	201	GLN	2.3
41	2j	88	LEU	2.3
42	2k	13	GLN	2.3
44	2m	90	LEU	2.3
38	2g	75	VAL	2.3
38	2g	34	GLY	2.3
40	1i	111	ARG	2.3
45	1n	11	LYS	2.3
51	2t	28	ALA	2.3
39	1h	11	THR	2.3
41	1j	100	THR	2.3
32	2a	1137	C	2.3

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Mol	Chain	Res	Type	RSRZ
35	1d	20	TYR	2.3
50	2s	52	TYR	2.3
1	2A	1087	G	2.3
32	2a	1154	G	2.3
32	2a	1255	G	2.3
22	20	47	PRO	2.3
50	1s	29	ARG	2.3
33	2b	210	SER	2.3
36	1e	103	GLY	2.3
38	2g	82	GLY	2.3
11	1P	127	ALA	2.3
16	2U	21	ALA	2.3
36	2e	54	ALA	2.3
6	2G	165	THR	2.3
6	1G	146	TYR	2.3
12	2Q	137	TYR	2.3
1	1A	2896	C	2.3
1	2A	2183	C	2.3
32	2a	311	C	2.3
8	2I	132	PRO	2.2
32	1a	1041	A	2.2
33	2b	144	ARG	2.2
32	1a	998	G	2.2
48	2q	23	VAL	2.2
53	2y	20	VAL	2.2
1	2A	2189	U	2.2
36	1e	117	ASP	2.2
51	1t	31	SER	2.2
27	25	14	ALA	2.2
38	2g	2	ALA	2.2
22	10	43	THR	2.2
40	2i	37	PHE	2.2
33	1b	129	GLU	2.2
14	2S	58	LEU	2.2
33	1b	114	ARG	2.2
33	2b	11	LEU	2.2
34	2c	85	ARG	2.2
51	1t	20	LEU	2.2
53	2y	87	LYS	2.2
16	1U	69	CYS	2.2
6	2G	116	ASP	2.2
32	1a	1046	A	2.2

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Mol	Chain	Res	Type	RSRZ
34	1c	2	GLY	2.2
52	2u	2	GLY	2.2
35	1d	104	VAL	2.2
50	1s	13	ASP	2.2
1	1A	1062	G	2.2
6	1G	48	GLU	2.2
32	2a	232	G	2.2
3	1D	2	ALA	2.2
40	1i	63	ILE	2.2
35	1d	206	PHE	2.2
44	2m	103	THR	2.2
14	2S	3	ARG	2.2
44	1m	91	ARG	2.2
45	2n	3	ARG	2.2
33	2b	51	LEU	2.2
14	2S	92	TYR	2.2
19	2X	32	PRO	2.2
33	2b	92	TYR	2.2
8	2I	41	GLU	2.2
32	1a	218	C	2.2
9	2N	9	VAL	2.2
26	14	56	VAL	2.2
33	2b	109	SER	2.2
40	1i	109	VAL	2.2
53	2y	62	VAL	2.2
32	1a	1319	A	2.2
32	1a	1532	U	2.2
33	1b	182	ILE	2.2
38	2g	78	ARG	2.2
42	2k	64	ALA	2.2
44	2m	75	ALA	2.2
36	1e	84	PHE	2.2
1	1A	2115	G	2.2
35	2d	96	LEU	2.2
28	26	42	TRP	2.2
53	2y	44	GLU	2.2
44	1m	24	GLY	2.2
48	1q	13	ASP	2.2
21	2Z	196	VAL	2.2
32	2a	1314	C	2.2
38	2g	155	ARG	2.2
48	2q	10	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
52	2u	10	ARG	2.2
1	1A	2176	A	2.2
1	2A	2135	A	2.2
27	25	2	ALA	2.2
32	2a	329	A	2.2
22	20	45	PHE	2.2
43	1l	67	THR	2.2
23	11	46	LEU	2.2
34	1c	196	LEU	2.2
40	1i	79	LEU	2.2
47	1p	15	PRO	2.2
1	2A	2186	G	2.2
32	2a	1224	G	2.2
7	2H	94	TYR	2.2
40	2i	120	ARG	2.2
46	2o	68	ARG	2.2
34	2c	207	VAL	2.2
36	1e	55	VAL	2.2
41	2j	34	VAL	2.2
1	2A	2103	C	2.2
5	2F	115	ALA	2.2
32	1a	1366	C	2.2
32	2a	1354	C	2.2
40	1i	110	GLU	2.2
42	2k	104	GLN	2.2
3	2D	50	THR	2.2
1	1A	1096	A	2.2
11	2P	28	GLY	2.2
33	1b	234	PRO	2.2
33	2b	234	PRO	2.2
39	1h	133	LEU	2.2
40	2i	56	LEU	2.2
1	1A	2157	G	2.2
1	2A	2206	G	2.2
26	14	63	TYR	2.2
50	2s	61	TYR	2.2
53	2y	82	GLU	2.2
12	2Q	102	VAL	2.2
24	12	70	GLN	2.2
48	1q	82	MET	2.2
34	2c	163	ALA	2.2
40	1i	46	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
53	1y	94	ALA	2.2
1	2A	1476	C	2.2
34	1c	177	THR	2.2
41	1j	48	THR	2.2
8	2I	57	ARG	2.2
35	1d	50	ARG	2.2
44	2m	6	GLY	2.2
45	2n	16	PHE	2.2
47	1p	9	PHE	2.2
1	2A	887	A	2.2
14	2S	4	LEU	2.2
32	2a	1251	A	2.2
49	2r	62	GLU	2.2
7	2H	13	LYS	2.1
38	2g	31	MET	2.1
1	1A	2102	U	2.1
1	2A	2180	U	2.1
33	1b	29	ALA	2.1
51	1t	59	ALA	2.1
20	2Y	44	ILE	2.1
22	20	52	GLY	2.1
41	1j	93	GLY	2.1
41	1j	98	ILE	2.1
48	1q	33	GLY	2.1
40	1i	49	PRO	2.1
35	1d	94	LEU	2.1
41	1j	90	LEU	2.1
44	2m	96	LEU	2.1
20	2Y	52	SER	2.1
32	2a	1363(A)	A	2.1
41	2j	84	GLN	2.1
4	2E	58	ARG	2.1
23	2I	26	ARG	2.1
36	1e	10	MET	2.1
34	1c	63	ASN	2.1
34	1c	85	ARG	2.1
47	1p	1	MET	2.1
38	2g	28	ASN	2.1
39	1h	79	VAL	2.1
48	2q	92	ARG	2.1
1	1A	1060	U	2.1
13	2R	25	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
39	1h	22	GLU	2.1
44	2m	50	GLU	2.1
51	2t	12	ALA	2.1
8	2I	88	ILE	2.1
32	2a	1373	G	2.1
34	2c	57	ILE	2.1
43	2l	13	LYS	2.1
44	1m	97	PRO	2.1
47	1p	36	ILE	2.1
50	1s	59	PRO	2.1
35	1d	64	LEU	2.1
35	1d	96	LEU	2.1
38	2g	12	LEU	2.1
41	2j	90	LEU	2.1
1	1A	1100	C	2.1
1	2A	2129	C	2.1
33	1b	144	ARG	2.1
26	24	16	CYS	2.1
35	1d	8	VAL	2.1
35	2d	8	VAL	2.1
36	1e	34	VAL	2.1
38	2g	85	TYR	2.1
44	2m	95	GLY	2.1
14	1S	37	ALA	2.1
18	2W	96	ILE	2.1
21	2Z	133	ILE	2.1
41	2j	39	PRO	2.1
42	2k	35	PRO	2.1
6	1G	173	LEU	2.1
6	2G	94	LEU	2.1
46	2o	56	LEU	2.1
32	2a	886	G	2.1
32	2a	1002	G	2.1
1	1A	2145	C	2.1
32	1a	194	C	2.1
45	2n	31	ARG	2.1
48	1q	94	ASN	2.1
32	1a	134	A	2.1
32	2a	1256	A	2.1
5	2F	166	ALA	2.1
8	1I	100	ALA	2.1
13	2R	21	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
32	2a	1235	U	2.1
33	2b	135	GLN	2.1
34	2c	65	ALA	2.1
43	2l	43	VAL	2.1
51	1t	44	ALA	2.1
53	2y	46	GLN	2.1
30	28	16	ILE	2.1
13	2R	70	LEU	2.1
35	1d	76	ARG	2.1
53	2y	24	LEU	2.1
30	28	7	HIS	2.1
1	1A	886	C	2.1
1	2A	892	G	2.1
1	2A	1816	G	2.1
1	2A	2053	G	2.1
6	2G	65	GLY	2.1
22	10	52	GLY	2.1
32	1a	386	C	2.1
32	1a	1003	G	2.1
32	2a	150	C	2.1
32	2a	887	G	2.1
32	2a	1397	C	2.1
34	1c	74	GLY	2.1
53	2y	47	GLY	2.1
40	1i	124	GLN	2.1
1	2A	2897	U	2.1
7	2H	29	PRO	2.1
32	1a	1111	A	2.1
34	2c	143	GLU	2.1
6	1G	136	ARG	2.1
52	2u	17	THR	2.1
35	2d	135	LEU	2.1
39	2h	135	CYS	2.1
45	2n	40	CYS	2.1
51	1t	62	LEU	2.1
7	2H	78	GLY	2.1
35	1d	62	GLN	2.1
32	2a	174	C	2.1
32	2a	1149	C	2.1
53	2y	68	GLU	2.1
16	2U	41	ALA	2.1
51	1t	68	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
8	2I	92	VAL	2.1
32	1a	202	U	2.1
32	2a	1250	A	2.1
41	1j	6	ILE	2.1
44	2m	70	LEU	2.1
50	2s	30	LEU	2.1
53	2y	85	LEU	2.1
7	2H	91	GLY	2.1
34	1c	205	GLY	2.1
36	1e	74	GLY	2.1
40	1i	112	LYS	2.1
35	1d	33	MET	2.0
32	1a	135	C	2.0
23	11	35	THR	2.0
28	26	52	VAL	2.0
47	2p	53	VAL	2.0
49	1r	39	VAL	2.0
52	2u	8	THR	2.0
56	2v	2	THR	2.0
1	2A	1115	G	2.0
32	2a	1368	G	2.0
6	2G	52	ILE	2.0
41	2j	23	ILE	2.0
42	1k	79	SER	2.0
48	2q	90	ILE	2.0
39	2h	112	LEU	2.0
48	1q	84	LEU	2.0
14	2S	81	GLY	2.0
34	1c	155	GLY	2.0
50	1s	10	PHE	2.0
6	2G	122	PRO	2.0
33	2b	232	PRO	2.0
42	1k	65	ALA	2.0
1	1A	279	C	2.0
6	2G	48	GLU	2.0
21	2Z	37	VAL	2.0
22	20	3	HIS	2.0
32	1a	219	C	2.0
32	1a	1362	C	2.0
32	2a	1122	U	2.0
40	1i	53	VAL	2.0
40	2i	86	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
47	1p	62	VAL	2.0
53	2y	60	VAL	2.0
33	1b	216	SER	2.0
33	2b	37	ASN	2.0
40	1i	23	ASN	2.0
40	2i	71	SER	2.0
19	2X	39	ILE	2.0
44	1m	22	ILE	2.0
50	2s	62	ILE	2.0
40	1i	128	ARG	2.0
1	2A	1042	G	2.0
32	2a	1111	A	2.0
8	2I	1	MET	2.0
6	2G	100	TRP	2.0
33	1b	237	ALA	2.0
41	1j	27	ALA	2.0
41	1j	57	LYS	2.0
41	1j	99	LYS	2.0
3	1D	138	VAL	2.0
35	1d	140	VAL	2.0
7	2H	6	ARG	2.0
1	2A	876	C	2.0
16	2U	73	GLY	2.0
10	2O	22	ILE	2.0
26	14	14	ILE	2.0
32	1a	1260	C	2.0
35	1d	174	LEU	2.0
14	2S	36	TYR	2.0
1	1A	2801(A)	A	2.0
32	1a	42	G	2.0
32	1a	542	G	2.0
40	2i	31	GLN	2.0
42	2k	77	MET	2.0
48	1q	28	PRO	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(\AA^2)	Q<0.9
43	0TD	2l	92	10/11	0.77	0.16	59,63,66,74	0
32	2MG	2a	1207	24/25	0.82	0.22	70,78,81,86	0
32	M2G	2a	966	25/26	0.83	0.23	55,68,78,84	0
1	5MU	2A	1915	21/22	0.86	0.20	69,74,81,90	0
1	PSU	2A	1911	20/21	0.87	0.15	61,67,79,80	0
1	PSU	1A	1917	20/21	0.88	0.18	58,67,76,76	0
32	2MG	1a	1207	24/25	0.89	0.19	61,67,72,75	0
43	0TD	1l	92	10/11	0.89	0.18	51,58,60,75	0
1	PSU	2A	1917	20/21	0.89	0.20	59,73,81,83	0
1	5MU	1A	1915	21/22	0.90	0.16	66,72,75,80	0
32	5MC	2a	967	21/22	0.90	0.19	60,67,70,78	0
1	OMC	2A	1920	21/22	0.91	0.16	57,62,65,66	0
32	5MC	2a	1404	21/22	0.92	0.20	54,58,61,62	0
32	5MC	1a	967	21/22	0.92	0.23	59,66,70,74	0
32	5MC	2a	1400	21/22	0.93	0.25	56,63,67,67	0
32	4OC	2a	1402	22/23	0.93	0.19	57,63,65,66	0
32	G7M	2a	527	24/25	0.93	0.18	52,63,66,68	0
32	MA6	2a	1518	24/25	0.93	0.19	56,60,64,67	0
32	PSU	2a	516	20/21	0.93	0.15	66,71,77,78	0
32	UR3	1a	1498	21/22	0.94	0.22	40,53,56,66	0
32	PSU	1a	516	20/21	0.94	0.19	55,60,66,67	0
32	5MC	2a	1407	21/22	0.94	0.16	52,57,62,63	0
32	G7M	1a	527	24/25	0.94	0.21	43,55,59,61	0
32	MA6	2a	1519	24/25	0.94	0.26	46,58,62,63	0
32	5MC	1a	1404	21/22	0.94	0.21	47,54,59,66	0
32	M2G	1a	966	25/26	0.95	0.21	57,63,68,71	0
1	PSU	1A	1911	20/21	0.95	0.15	52,63,68,72	0
1	5MC	2A	1942	21/22	0.95	0.19	47,54,57,58	0
1	OMU	2A	2552	21/22	0.95	0.22	33,40,43,53	0
32	MA6	1a	1518	24/25	0.95	0.21	45,48,51,57	0
32	UR3	2a	1498	21/22	0.95	0.25	52,62,65,67	0
1	OMC	1A	1920	21/22	0.95	0.23	44,56,61,62	0
32	5MC	1a	1400	21/22	0.95	0.19	51,57,63,66	0
32	4OC	1a	1402	22/23	0.95	0.18	46,54,57,66	0
55	8AN	2x	76	22/23	0.95	0.24	34,41,51,60	0
1	PSU	2A	2605	20/21	0.96	0.24	33,38,45,48	0
32	5MC	1a	1407	21/22	0.96	0.17	43,52,57,61	0
32	MA6	1a	1519	24/25	0.96	0.23	44,48,53,53	0
1	5MC	2A	1962	21/22	0.96	0.18	35,46,49,52	0
54	PPU	2w	76	37/38	0.96	0.22	29,38,43,44	0
1	5MU	1A	1939	21/22	0.96	0.19	25,30,38,43	0
1	5MC	1A	1962	21/22	0.97	0.20	30,41,45,47	0
1	2MA	1A	2503	23/24	0.97	0.24	17,22,25,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OMG	2A	2251	24/25	0.97	0.20	33,38,44,44	0
1	2MA	2A	2503	23/24	0.97	0.22	22,36,41,43	0
1	PSU	1A	2605	20/21	0.97	0.20	18,28,32,34	0
54	PPU	1w	76	37/38	0.97	0.25	15,24,31,33	0
1	5MC	1A	1942	21/22	0.97	0.20	28,40,44,46	0
55	8AN	1x	76	22/23	0.97	0.24	18,24,29,40	0
1	5MU	2A	1939	21/22	0.97	0.18	34,43,48,49	0
1	OMG	1A	2251	24/25	0.98	0.23	18,25,29,35	0
1	OMU	1A	2552	21/22	0.98	0.22	25,28,30,31	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	4024	1/1	0.03	0.19	60,60,60,60	0
57	MG	2A	3698	1/1	0.14	0.16	58,58,58,58	0
57	MG	2B	218	1/1	0.29	0.18	61,61,61,61	0
57	MG	1A	3578	1/1	0.30	0.10	62,62,62,62	0
57	MG	2A	3489	1/1	0.34	0.15	48,48,48,48	0
57	MG	2A	3681	1/1	0.35	0.30	64,64,64,64	0
57	MG	1A	3900	1/1	0.36	0.19	58,58,58,58	0
57	MG	2a	3170	1/1	0.40	0.16	76,76,76,76	0
57	MG	2a	3100	1/1	0.41	0.18	68,68,68,68	0
57	MG	1A	3944	1/1	0.41	0.31	59,59,59,59	0
57	MG	2A	3654	1/1	0.44	0.15	63,63,63,63	0
57	MG	2A	3633	1/1	0.44	0.18	67,67,67,67	0
57	MG	2A	3558	1/1	0.46	0.13	62,62,62,62	0
57	MG	2A	3252	1/1	0.47	0.22	63,63,63,63	0
57	MG	2A	3606	1/1	0.47	0.13	57,57,57,57	0
57	MG	1a	1608	1/1	0.47	0.22	70,70,70,70	0
57	MG	2A	3199	1/1	0.49	0.19	64,64,64,64	0
57	MG	1a	1856	1/1	0.50	0.09	64,64,64,64	0
57	MG	2a	3010	1/1	0.50	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1P	204	1/1	0.51	0.14	73,73,73,73	0
57	MG	1a	1730	1/1	0.51	0.12	53,53,53,53	0
57	MG	2A	3511	1/1	0.53	0.10	67,67,67,67	0
57	MG	2A	3556	1/1	0.53	0.24	72,72,72,72	0
57	MG	1A	3463	1/1	0.53	0.23	70,70,70,70	0
57	MG	2A	3596	1/1	0.54	0.10	61,61,61,61	0
57	MG	1y	203	1/1	0.55	0.25	73,73,73,73	0
57	MG	2A	3364	1/1	0.55	0.12	57,57,57,57	0
57	MG	1A	3947	1/1	0.56	0.11	43,43,43,43	0
57	MG	1A	3936	1/1	0.56	0.13	55,55,55,55	0
57	MG	1A	3898	1/1	0.56	0.13	34,34,34,34	0
57	MG	2a	3169	1/1	0.57	0.17	65,65,65,65	0
57	MG	1d	306	1/1	0.57	0.18	79,79,79,79	0
57	MG	1a	1778	1/1	0.58	0.10	82,82,82,82	0
57	MG	1a	1792	1/1	0.58	0.28	78,78,78,78	0
57	MG	2A	3726	1/1	0.58	0.25	65,65,65,65	0
57	MG	2A	3549	1/1	0.58	0.12	74,74,74,74	0
57	MG	1a	1787	1/1	0.59	0.08	71,71,71,71	0
57	MG	2A	3231	1/1	0.59	0.41	53,53,53,53	0
57	MG	2A	3153	1/1	0.59	0.15	60,60,60,60	0
57	MG	1A	3960	1/1	0.60	0.53	81,81,81,81	0
57	MG	1a	1749	1/1	0.60	0.08	68,68,68,68	0
57	MG	2B	207	1/1	0.61	0.19	68,68,68,68	0
57	MG	1A	3932	1/1	0.61	0.11	48,48,48,48	0
57	MG	2A	3173	1/1	0.61	0.65	60,60,60,60	0
57	MG	1A	3313	1/1	0.62	0.18	79,79,79,79	0
57	MG	1A	3997	1/1	0.62	0.19	62,62,62,62	0
57	MG	2A	3216	1/1	0.62	0.15	57,57,57,57	0
57	MG	2A	3676	1/1	0.63	0.17	63,63,63,63	0
57	MG	1A	3377	1/1	0.63	0.13	47,47,47,47	0
57	MG	1A	3440	1/1	0.63	0.18	43,43,43,43	0
57	MG	2a	3123	1/1	0.63	0.09	61,61,61,61	0
57	MG	2a	3138	1/1	0.63	0.09	65,65,65,65	0
57	MG	1A	3581	1/1	0.63	0.14	63,63,63,63	0
57	MG	1A	3933	1/1	0.63	0.10	48,48,48,48	0
57	MG	1a	1777	1/1	0.64	0.14	69,69,69,69	0
57	MG	1a	1723	1/1	0.64	0.16	52,52,52,52	0
57	MG	2A	3700	1/1	0.64	0.15	61,61,61,61	0
57	MG	2a	3179	1/1	0.64	0.13	65,65,65,65	0
57	MG	1H	202	1/1	0.65	0.14	58,58,58,58	0
57	MG	2A	3665	1/1	0.65	0.08	66,66,66,66	0
57	MG	1a	1729	1/1	0.65	0.12	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1a	1636	1/1	0.65	0.16	71,71,71,71	0
57	MG	1a	1690	1/1	0.65	0.09	60,60,60,60	0
57	MG	2A	3160	1/1	0.65	0.13	56,56,56,56	0
57	MG	2A	3441	1/1	0.65	0.23	58,58,58,58	0
57	MG	1a	1797	1/1	0.65	0.19	61,61,61,61	0
57	MG	1A	3812	1/1	0.66	0.21	55,55,55,55	0
57	MG	2a	3025	1/1	0.66	0.14	64,64,64,64	0
57	MG	2B	213	1/1	0.66	0.16	56,56,56,56	0
57	MG	1A	3733	1/1	0.66	0.10	51,51,51,51	0
57	MG	10	105	1/1	0.67	0.19	58,58,58,58	0
57	MG	2a	3132	1/1	0.67	0.15	56,56,56,56	0
57	MG	1a	1678	1/1	0.67	0.16	64,64,64,64	0
57	MG	2A	3272	1/1	0.67	0.24	51,51,51,51	0
57	MG	2a	3094	1/1	0.67	0.13	59,59,59,59	0
57	MG	2A	3495	1/1	0.67	0.08	51,51,51,51	0
57	MG	2A	3342	1/1	0.68	0.10	53,53,53,53	0
57	MG	2a	3142	1/1	0.68	0.10	55,55,55,55	0
57	MG	1A	3946	1/1	0.68	0.17	46,46,46,46	0
57	MG	2A	3117	1/1	0.68	0.20	59,59,59,59	0
57	MG	2A	3171	1/1	0.68	0.41	65,65,65,65	0
60	ZN	24	501	1/1	0.68	0.14	122,122,122,122	0
57	MG	1a	1722	1/1	0.69	0.16	77,77,77,77	0
57	MG	2A	3279	1/1	0.69	0.16	62,62,62,62	0
57	MG	2a	3128	1/1	0.69	0.14	60,60,60,60	0
57	MG	1A	3705	1/1	0.69	0.16	61,61,61,61	0
57	MG	1A	3959	1/1	0.69	0.17	53,53,53,53	0
57	MG	1E	305	1/1	0.69	0.11	52,52,52,52	0
57	MG	2a	3161	1/1	0.69	0.16	47,47,47,47	0
57	MG	1a	1870	1/1	0.69	0.07	64,64,64,64	0
57	MG	1a	1675	1/1	0.69	0.21	68,68,68,68	0
57	MG	1A	3448	1/1	0.69	0.24	29,29,29,29	0
57	MG	1A	3969	1/1	0.69	0.13	63,63,63,63	0
57	MG	2a	3162	1/1	0.70	0.15	67,67,67,67	0
57	MG	1B	224	1/1	0.70	0.15	44,44,44,44	0
57	MG	2A	3672	1/1	0.70	0.07	61,61,61,61	0
57	MG	2A	3652	1/1	0.70	0.09	49,49,49,49	0
57	MG	1A	3697	1/1	0.70	0.08	75,75,75,75	0
57	MG	1a	1789	1/1	0.71	0.14	75,75,75,75	0
57	MG	2B	204	1/1	0.71	0.14	65,65,65,65	0
57	MG	1a	1671	1/1	0.71	0.11	68,68,68,68	0
57	MG	2a	3140	1/1	0.71	0.17	61,61,61,61	0
57	MG	2A	3659	1/1	0.71	0.19	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3148	1/1	0.71	0.16	51,51,51,51	0
57	MG	1a	1603	1/1	0.71	0.11	66,66,66,66	0
57	MG	1B	223	1/1	0.71	0.08	55,55,55,55	0
57	MG	2A	3230	1/1	0.71	0.17	56,56,56,56	0
57	MG	1A	3902	1/1	0.71	0.16	41,41,41,41	0
57	MG	2A	3476	1/1	0.71	0.09	53,53,53,53	0
57	MG	2A	3240	1/1	0.71	0.17	57,57,57,57	0
57	MG	1A	4007	1/1	0.72	0.14	73,73,73,73	0
57	MG	1a	1751	1/1	0.72	0.14	72,72,72,72	0
57	MG	1A	3533	1/1	0.72	0.18	64,64,64,64	0
57	MG	2A	3383	1/1	0.72	0.14	78,78,78,78	0
57	MG	1A	3212	1/1	0.72	0.25	51,51,51,51	0
57	MG	1A	3097	1/1	0.72	0.17	61,61,61,61	0
57	MG	1A	3170	1/1	0.72	0.20	49,49,49,49	0
57	MG	1a	1647	1/1	0.72	0.20	60,60,60,60	0
57	MG	1A	4003	1/1	0.72	0.16	54,54,54,54	0
57	MG	2a	3135	1/1	0.72	0.21	61,61,61,61	0
62	MRD	2A	3738	8/8	0.72	0.32	46,55,58,59	0
57	MG	2a	3028	1/1	0.73	0.15	64,64,64,64	0
57	MG	2A	3082	1/1	0.73	0.15	64,64,64,64	0
57	MG	1a	1609	1/1	0.73	0.17	68,68,68,68	0
57	MG	1a	1630	1/1	0.73	0.16	52,52,52,52	0
57	MG	1A	3949	1/1	0.73	0.12	61,61,61,61	0
57	MG	2A	3668	1/1	0.73	0.08	63,63,63,63	0
57	MG	1A	3382	1/1	0.73	0.25	67,67,67,67	0
57	MG	1a	1822	1/1	0.73	0.09	68,68,68,68	0
57	MG	1a	1832	1/1	0.73	0.17	61,61,61,61	0
57	MG	1A	3763	1/1	0.73	0.23	55,55,55,55	0
57	MG	1a	1861	1/1	0.73	0.12	57,57,57,57	0
57	MG	1A	3223	1/1	0.73	0.13	65,65,65,65	0
57	MG	1A	3311	1/1	0.73	0.34	67,67,67,67	0
57	MG	1E	304	1/1	0.73	0.14	34,34,34,34	0
57	MG	2A	3045	1/1	0.73	0.14	48,48,48,48	0
57	MG	2A	3061	1/1	0.73	0.23	56,56,56,56	0
57	MG	2A	3636	1/1	0.73	0.09	64,64,64,64	0
57	MG	2A	3647	1/1	0.73	0.08	60,60,60,60	0
57	MG	2a	3035	1/1	0.74	0.17	69,69,69,69	0
57	MG	2A	3667	1/1	0.74	0.11	63,63,63,63	0
57	MG	1A	3034	1/1	0.74	0.32	56,56,56,56	0
57	MG	1A	3107	1/1	0.74	0.25	37,37,37,37	0
57	MG	2A	3096	1/1	0.74	0.23	68,68,68,68	0
57	MG	1a	1703	1/1	0.74	0.11	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3692	1/1	0.74	0.13	54,54,54,54	0
57	MG	2A	3632	1/1	0.74	0.16	63,63,63,63	0
57	MG	1a	1808	1/1	0.74	0.15	70,70,70,70	0
57	MG	2a	3004	1/1	0.75	0.20	60,60,60,60	0
57	MG	1A	3803	1/1	0.75	0.18	53,53,53,53	0
57	MG	1R	202	1/1	0.75	0.39	48,48,48,48	0
57	MG	2A	3161	1/1	0.75	0.23	55,55,55,55	0
57	MG	2A	3592	1/1	0.75	0.12	50,50,50,50	0
57	MG	2A	3717	1/1	0.75	0.11	65,65,65,65	0
57	MG	2A	3450	1/1	0.75	0.18	57,57,57,57	0
57	MG	1A	3916	1/1	0.75	0.06	54,54,54,54	0
57	MG	1a	1695	1/1	0.75	0.18	61,61,61,61	0
57	MG	1A	3676	1/1	0.75	0.15	52,52,52,52	0
57	MG	1A	3951	1/1	0.75	0.09	51,51,51,51	0
57	MG	2A	3323	1/1	0.76	0.17	70,70,70,70	0
57	MG	2a	3038	1/1	0.76	0.14	58,58,58,58	0
57	MG	2a	3059	1/1	0.76	0.27	67,67,67,67	0
57	MG	1A	3392	1/1	0.76	0.15	53,53,53,53	0
57	MG	2A	3678	1/1	0.76	0.18	41,41,41,41	0
57	MG	2A	3205	1/1	0.76	0.18	52,52,52,52	0
57	MG	1d	301	1/1	0.76	0.20	73,73,73,73	0
57	MG	2A	3394	1/1	0.76	0.28	60,60,60,60	0
57	MG	2A	3619	1/1	0.76	0.10	60,60,60,60	0
57	MG	2A	3422	1/1	0.76	0.13	50,50,50,50	0
57	MG	1A	3937	1/1	0.76	0.11	53,53,53,53	0
57	MG	2a	3141	1/1	0.76	0.08	61,61,61,61	0
57	MG	2A	3442	1/1	0.76	0.18	44,44,44,44	0
57	MG	1A	3850	1/1	0.76	0.08	43,43,43,43	0
57	MG	2a	3158	1/1	0.76	0.06	69,69,69,69	0
57	MG	2A	3454	1/1	0.76	0.10	60,60,60,60	0
57	MG	1a	1845	1/1	0.76	0.19	73,73,73,73	0
57	MG	2A	3247	1/1	0.76	0.25	77,77,77,77	0
57	MG	1R	204	1/1	0.76	0.33	52,52,52,52	0
57	MG	2a	3013	1/1	0.76	0.13	63,63,63,63	0
57	MG	1Z	301	1/1	0.76	0.20	52,52,52,52	0
57	MG	2A	3197	1/1	0.76	0.17	73,73,73,73	0
57	MG	1A	4020	1/1	0.77	0.07	54,54,54,54	0
57	MG	1Q	205	1/1	0.77	0.24	51,51,51,51	0
57	MG	1A	3246	1/1	0.77	0.26	64,64,64,64	0
57	MG	1A	3824	1/1	0.77	0.14	71,71,71,71	0
57	MG	1A	3109	1/1	0.77	0.34	64,64,64,64	0
57	MG	2A	3532	1/1	0.77	0.10	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3329	1/1	0.77	0.17	53,53,53,53	0
57	MG	1a	1803	1/1	0.77	0.16	67,67,67,67	0
57	MG	2A	3035	1/1	0.77	0.22	49,49,49,49	0
57	MG	2A	3569	1/1	0.77	0.18	44,44,44,44	0
57	MG	1A	3863	1/1	0.77	0.16	56,56,56,56	0
57	MG	2A	3060	1/1	0.77	0.11	47,47,47,47	0
57	MG	1A	3876	1/1	0.77	0.09	45,45,45,45	0
57	MG	2a	3176	1/1	0.77	0.19	51,51,51,51	0
57	MG	1a	1688	1/1	0.77	0.31	68,68,68,68	0
57	MG	2h	201	1/1	0.77	0.19	73,73,73,73	0
57	MG	1A	3660	1/1	0.77	0.21	56,56,56,56	0
57	MG	2A	3115	1/1	0.77	0.11	60,60,60,60	0
57	MG	2A	3680	1/1	0.78	0.09	51,51,51,51	0
57	MG	2a	3114	1/1	0.78	0.12	63,63,63,63	0
57	MG	1A	3691	1/1	0.78	0.32	43,43,43,43	0
57	MG	1A	3887	1/1	0.78	0.11	38,38,38,38	0
57	MG	2A	3068	1/1	0.78	0.14	52,52,52,52	0
57	MG	2A	3403	1/1	0.78	0.10	48,48,48,48	0
57	MG	2A	3075	1/1	0.78	0.30	46,46,46,46	0
57	MG	1B	230	1/1	0.78	0.12	56,56,56,56	0
57	MG	1a	1683	1/1	0.78	0.23	69,69,69,69	0
57	MG	1l	104	1/1	0.78	0.14	47,47,47,47	0
57	MG	2A	3116	1/1	0.78	0.20	66,66,66,66	0
57	MG	2A	3650	1/1	0.78	0.11	49,49,49,49	0
57	MG	1A	3806	1/1	0.78	0.22	57,57,57,57	0
57	MG	1A	3342	1/1	0.78	0.19	41,41,41,41	0
57	MG	1A	3593	1/1	0.78	0.26	40,40,40,40	0
57	MG	2A	3498	1/1	0.78	0.10	62,62,62,62	0
57	MG	2A	3313	1/1	0.78	0.10	44,44,44,44	0
57	MG	2A	3314	1/1	0.78	0.12	36,36,36,36	0
57	MG	1A	3914	1/1	0.78	0.12	50,50,50,50	0
58	MPD	2B	221	8/8	0.78	0.25	52,63,69,73	0
57	MG	1A	3186	1/1	0.78	0.16	42,42,42,42	0
57	MG	1A	3334	1/1	0.78	0.19	55,55,55,55	0
57	MG	2A	3455	1/1	0.79	0.22	78,78,78,78	0
57	MG	2A	3464	1/1	0.79	0.29	65,65,65,65	0
57	MG	1a	1794	1/1	0.79	0.27	55,55,55,55	0
57	MG	2A	3477	1/1	0.79	0.10	57,57,57,57	0
57	MG	1A	3664	1/1	0.79	0.19	54,54,54,54	0
57	MG	1A	3296	1/1	0.79	0.25	49,49,49,49	0
57	MG	2A	3162	1/1	0.79	0.15	63,63,63,63	0
57	MG	1a	1805	1/1	0.79	0.19	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3292	1/1	0.79	0.19	74,74,74,74	0
57	MG	1a	1679	1/1	0.79	0.14	52,52,52,52	0
57	MG	2A	3357	1/1	0.79	0.14	64,64,64,64	0
57	MG	1A	3413	1/1	0.79	0.14	36,36,36,36	0
57	MG	2A	3200	1/1	0.79	0.15	57,57,57,57	0
57	MG	1a	1614	1/1	0.79	0.14	67,67,67,67	0
57	MG	2A	3396	1/1	0.79	0.12	49,49,49,49	0
57	MG	2a	3154	1/1	0.79	0.17	67,67,67,67	0
57	MG	1a	1852	1/1	0.79	0.15	60,60,60,60	0
57	MG	2a	3160	1/1	0.79	0.10	48,48,48,48	0
57	MG	2A	3612	1/1	0.79	0.16	50,50,50,50	0
57	MG	2A	3093	1/1	0.79	0.23	67,67,67,67	0
57	MG	1A	3606	1/1	0.79	0.18	63,63,63,63	0
57	MG	2F	302	1/1	0.79	0.14	43,43,43,43	0
57	MG	2T	201	1/1	0.79	0.16	56,56,56,56	0
57	MG	1A	3612	1/1	0.79	0.11	40,40,40,40	0
57	MG	1A	3435	1/1	0.79	0.15	80,80,80,80	0
57	MG	2A	3451	1/1	0.79	0.16	65,65,65,65	0
57	MG	2A	3452	1/1	0.79	0.09	61,61,61,61	0
57	MG	1a	1664	1/1	0.79	0.35	72,72,72,72	0
57	MG	1A	4000	1/1	0.80	0.39	51,51,51,51	0
57	MG	2A	3608	1/1	0.80	0.20	49,49,49,49	0
57	MG	2A	3453	1/1	0.80	0.12	51,51,51,51	0
57	MG	1A	3014	1/1	0.80	0.22	55,55,55,55	0
57	MG	2A	3005	1/1	0.80	0.17	57,57,57,57	0
57	MG	2A	3210	1/1	0.80	0.13	52,52,52,52	0
57	MG	1A	3683	1/1	0.80	0.12	42,42,42,42	0
57	MG	2A	3641	1/1	0.80	0.13	49,49,49,49	0
57	MG	2A	3219	1/1	0.80	0.17	53,53,53,53	0
57	MG	2A	3135	1/1	0.80	0.13	57,57,57,57	0
57	MG	2A	3389	1/1	0.80	0.21	59,59,59,59	0
57	MG	2T	203	1/1	0.80	0.15	55,55,55,55	0
57	MG	1a	1661	1/1	0.80	0.11	62,62,62,62	0
57	MG	1A	3345	1/1	0.80	0.13	55,55,55,55	0
57	MG	2A	3529	1/1	0.80	0.20	67,67,67,67	0
57	MG	1P	203	1/1	0.80	0.16	36,36,36,36	0
57	MG	1A	3406	1/1	0.80	0.17	52,52,52,52	0
57	MG	2a	3175	1/1	0.80	0.26	68,68,68,68	0
57	MG	2A	3423	1/1	0.80	0.17	67,67,67,67	0
57	MG	1A	3211	1/1	0.80	0.14	40,40,40,40	0
57	MG	2a	3182	1/1	0.80	0.14	68,68,68,68	0
57	MG	2a	3185	1/1	0.80	0.12	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3894	1/1	0.80	0.20	60,60,60,60	0
57	MG	2a	3086	1/1	0.80	0.10	65,65,65,65	0
57	MG	2A	3285	1/1	0.80	0.14	53,53,53,53	0
57	MG	1a	1736	1/1	0.80	0.10	66,66,66,66	0
57	MG	2A	3239	1/1	0.81	0.23	43,43,43,43	0
57	MG	1A	3609	1/1	0.81	0.22	51,51,51,51	0
57	MG	1A	3967	1/1	0.81	0.30	59,59,59,59	0
57	MG	2a	3067	1/1	0.81	0.11	74,74,74,74	0
57	MG	2A	3106	1/1	0.81	0.21	69,69,69,69	0
57	MG	2A	3656	1/1	0.81	0.09	65,65,65,65	0
57	MG	1A	3541	1/1	0.81	0.13	47,47,47,47	0
57	MG	2a	3105	1/1	0.81	0.17	63,63,63,63	0
57	MG	1a	1851	1/1	0.81	0.20	62,62,62,62	0
57	MG	2A	3282	1/1	0.81	0.21	66,66,66,66	0
57	MG	1a	1659	1/1	0.81	0.26	47,47,47,47	0
57	MG	2A	3295	1/1	0.81	0.20	56,56,56,56	0
57	MG	1A	3977	1/1	0.81	0.20	52,52,52,52	0
57	MG	1A	3623	1/1	0.81	0.11	53,53,53,53	0
57	MG	2A	3520	1/1	0.81	0.17	43,43,43,43	0
57	MG	1a	1668	1/1	0.81	0.19	62,62,62,62	0
57	MG	2A	3683	1/1	0.81	0.09	55,55,55,55	0
57	MG	1a	1762	1/1	0.81	0.10	75,75,75,75	0
57	MG	2A	3538	1/1	0.81	0.30	68,68,68,68	0
57	MG	1a	1670	1/1	0.81	0.12	58,58,58,58	0
57	MG	1A	3714	1/1	0.81	0.17	49,49,49,49	0
57	MG	2A	3001	1/1	0.81	0.17	66,66,66,66	0
57	MG	2A	3186	1/1	0.81	0.59	62,62,62,62	0
57	MG	2A	3580	1/1	0.81	0.10	59,59,59,59	0
57	MG	1A	3627	1/1	0.81	0.20	30,30,30,30	0
57	MG	1A	3892	1/1	0.81	0.19	50,50,50,50	0
57	MG	1A	3945	1/1	0.81	0.27	55,55,55,55	0
57	MG	1A	3087	1/1	0.81	0.23	38,38,38,38	0
57	MG	1A	3801	1/1	0.81	0.09	52,52,52,52	0
57	MG	2A	3215	1/1	0.81	0.11	53,53,53,53	0
57	MG	1A	3372	1/1	0.81	0.14	28,28,28,28	0
57	MG	2A	3070	1/1	0.81	0.20	49,49,49,49	0
57	MG	1A	3506	1/1	0.81	0.12	42,42,42,42	0
57	MG	1A	3218	1/1	0.81	0.30	67,67,67,67	0
57	MG	1A	3150	1/1	0.82	0.12	41,41,41,41	0
57	MG	1A	3854	1/1	0.82	0.10	38,38,38,38	0
57	MG	2A	3163	1/1	0.82	0.17	56,56,56,56	0
57	MG	2A	3470	1/1	0.82	0.13	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3472	1/1	0.82	0.18	61,61,61,61	0
57	MG	1A	3721	1/1	0.82	0.26	51,51,51,51	0
57	MG	2a	3072	1/1	0.82	0.16	62,62,62,62	0
57	MG	2a	3077	1/1	0.82	0.17	64,64,64,64	0
57	MG	2A	3049	1/1	0.82	0.11	55,55,55,55	0
57	MG	1A	3521	1/1	0.82	0.11	49,49,49,49	0
57	MG	1N	204	1/1	0.82	0.05	52,52,52,52	0
57	MG	2A	3331	1/1	0.82	0.12	57,57,57,57	0
57	MG	2a	3109	1/1	0.82	0.10	52,52,52,52	0
57	MG	1A	3987	1/1	0.82	0.20	45,45,45,45	0
57	MG	2a	3116	1/1	0.82	0.10	60,60,60,60	0
57	MG	1A	3990	1/1	0.82	0.14	55,55,55,55	0
57	MG	1A	3301	1/1	0.82	0.16	36,36,36,36	0
57	MG	2A	3375	1/1	0.82	0.12	59,59,59,59	0
57	MG	1a	1737	1/1	0.82	0.07	69,69,69,69	0
57	MG	2A	3539	1/1	0.82	0.29	60,60,60,60	0
57	MG	1A	3791	1/1	0.82	0.14	37,37,37,37	0
57	MG	1a	1853	1/1	0.82	0.08	53,53,53,53	0
57	MG	1A	3059	1/1	0.82	0.19	52,52,52,52	0
57	MG	2A	3560	1/1	0.82	0.07	60,60,60,60	0
57	MG	2A	3566	1/1	0.82	0.22	66,66,66,66	0
57	MG	2A	3226	1/1	0.82	0.18	49,49,49,49	0
57	MG	1T	202	1/1	0.82	0.15	55,55,55,55	0
57	MG	2B	203	1/1	0.82	0.12	63,63,63,63	0
57	MG	2A	3590	1/1	0.82	0.16	45,45,45,45	0
57	MG	1A	3086	1/1	0.82	0.20	43,43,43,43	0
57	MG	1A	3408	1/1	0.82	0.21	31,31,31,31	0
57	MG	2A	3118	1/1	0.82	0.27	46,46,46,46	0
57	MG	2A	3133	1/1	0.82	0.17	46,46,46,46	0
57	MG	2A	3610	1/1	0.82	0.28	53,53,53,53	0
57	MG	1A	3703	1/1	0.82	0.15	64,64,64,64	0
57	MG	2I	101	1/1	0.82	0.11	59,59,59,59	0
57	MG	1A	3909	1/1	0.82	0.19	39,39,39,39	0
57	MG	2A	3621	1/1	0.82	0.11	63,63,63,63	0
57	MG	1A	3640	1/1	0.82	0.18	21,21,21,21	0
57	MG	2a	3021	1/1	0.82	0.13	70,70,70,70	0
57	MG	2a	3033	1/1	0.83	0.13	57,57,57,57	0
57	MG	2A	3496	1/1	0.83	0.13	66,66,66,66	0
57	MG	1a	1839	1/1	0.83	0.12	71,71,71,71	0
57	MG	2a	3049	1/1	0.83	0.18	62,62,62,62	0
57	MG	2A	3504	1/1	0.83	0.12	66,66,66,66	0
57	MG	2a	3062	1/1	0.83	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3752	1/1	0.83	0.12	56,56,56,56	0
57	MG	1a	1848	1/1	0.83	0.09	52,52,52,52	0
57	MG	1A	3291	1/1	0.83	0.23	49,49,49,49	0
57	MG	1a	1765	1/1	0.83	0.14	53,53,53,53	0
57	MG	2A	3669	1/1	0.83	0.13	52,52,52,52	0
57	MG	2A	3218	1/1	0.83	0.16	43,43,43,43	0
57	MG	1F	308	1/1	0.83	0.18	52,52,52,52	0
57	MG	1A	3202	1/1	0.83	0.16	39,39,39,39	0
57	MG	2A	3421	1/1	0.83	0.33	47,47,47,47	0
57	MG	1a	1779	1/1	0.83	0.10	65,65,65,65	0
57	MG	2A	3682	1/1	0.83	0.14	54,54,54,54	0
57	MG	1a	1869	1/1	0.83	0.09	65,65,65,65	0
57	MG	2A	3437	1/1	0.83	0.16	72,72,72,72	0
57	MG	1A	3994	1/1	0.83	0.18	39,39,39,39	0
57	MG	2a	3137	1/1	0.83	0.15	65,65,65,65	0
57	MG	1A	3458	1/1	0.83	0.19	60,60,60,60	0
57	MG	2A	3585	1/1	0.83	0.17	46,46,46,46	0
57	MG	2A	3447	1/1	0.83	0.19	55,55,55,55	0
57	MG	1d	305	1/1	0.83	0.14	57,57,57,57	0
57	MG	1A	3153	1/1	0.83	0.16	54,54,54,54	0
57	MG	2A	3141	1/1	0.83	0.16	55,55,55,55	0
57	MG	1A	3633	1/1	0.83	0.08	39,39,39,39	0
57	MG	1A	3639	1/1	0.83	0.20	46,46,46,46	0
57	MG	2D	305	1/1	0.83	0.24	46,46,46,46	0
57	MG	1A	3355	1/1	0.83	0.14	57,57,57,57	0
57	MG	2G	3302	1/1	0.83	0.11	70,70,70,70	0
57	MG	2A	3034	1/1	0.83	0.12	64,64,64,64	0
57	MG	1A	3715	1/1	0.83	0.18	47,47,47,47	0
57	MG	2A	3630	1/1	0.83	0.15	59,59,59,59	0
57	MG	1A	3599	1/1	0.83	0.21	50,50,50,50	0
57	MG	1a	1817	1/1	0.83	0.17	78,78,78,78	0
57	MG	1A	3860	1/1	0.83	0.14	36,36,36,36	0
57	MG	2a	3191	1/1	0.83	0.12	73,73,73,73	0
57	MG	2A	3478	1/1	0.83	0.12	34,34,34,34	0
57	MG	1A	3438	1/1	0.83	0.27	32,32,32,32	0
57	MG	2A	3067	1/1	0.83	0.13	49,49,49,49	0
57	MG	2a	3031	1/1	0.83	0.15	54,54,54,54	0
57	MG	1A	3988	1/1	0.84	0.25	50,50,50,50	0
57	MG	1a	1644	1/1	0.84	0.16	49,49,49,49	0
57	MG	1A	3725	1/1	0.84	0.19	58,58,58,58	0
57	MG	1a	1738	1/1	0.84	0.15	86,86,86,86	0
57	MG	1a	1648	1/1	0.84	0.27	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3043	1/1	0.84	0.19	60,60,60,60	0
57	MG	2a	3047	1/1	0.84	0.10	63,63,63,63	0
57	MG	2A	3283	1/1	0.84	0.13	58,58,58,58	0
57	MG	1A	3993	1/1	0.84	0.11	29,29,29,29	0
57	MG	2A	3484	1/1	0.84	0.22	55,55,55,55	0
57	MG	2a	3066	1/1	0.84	0.29	74,74,74,74	0
57	MG	1a	1759	1/1	0.84	0.14	57,57,57,57	0
57	MG	1A	3002	1/1	0.84	0.15	40,40,40,40	0
57	MG	2A	3150	1/1	0.84	0.09	52,52,52,52	0
57	MG	1a	1662	1/1	0.84	0.12	55,55,55,55	0
57	MG	2a	3088	1/1	0.84	0.12	65,65,65,65	0
57	MG	1A	3210	1/1	0.84	0.49	50,50,50,50	0
57	MG	1i	201	1/1	0.84	0.15	65,65,65,65	0
57	MG	2A	3341	1/1	0.84	0.09	43,43,43,43	0
57	MG	1A	3390	1/1	0.84	0.22	35,35,35,35	0
57	MG	1w	101	1/1	0.84	0.16	54,54,54,54	0
57	MG	1A	3344	1/1	0.84	0.24	28,28,28,28	0
57	MG	1A	3579	1/1	0.84	0.13	43,43,43,43	0
57	MG	2a	3125	1/1	0.84	0.19	68,68,68,68	0
57	MG	2A	3014	1/1	0.84	0.19	61,61,61,61	0
57	MG	1A	3454	1/1	0.84	0.28	62,62,62,62	0
57	MG	1A	4023	1/1	0.84	0.09	53,53,53,53	0
57	MG	1A	3968	1/1	0.84	0.30	68,68,68,68	0
57	MG	2A	3399	1/1	0.84	0.13	58,58,58,58	0
57	MG	1A	3172	1/1	0.84	0.21	41,41,41,41	0
57	MG	2A	3571	1/1	0.84	0.10	58,58,58,58	0
57	MG	1a	1687	1/1	0.84	0.16	64,64,64,64	0
57	MG	2A	3581	1/1	0.84	0.07	63,63,63,63	0
57	MG	2a	3152	1/1	0.84	0.18	69,69,69,69	0
57	MG	2A	3582	1/1	0.84	0.16	64,64,64,64	0
57	MG	2a	3156	1/1	0.84	0.32	77,77,77,77	0
57	MG	2B	210	1/1	0.84	0.21	68,68,68,68	0
57	MG	15	106	1/1	0.84	0.14	38,38,38,38	0
57	MG	1A	3972	1/1	0.84	0.14	58,58,58,58	0
57	MG	1a	1692	1/1	0.84	0.15	49,49,49,49	0
57	MG	1B	226	1/1	0.84	0.13	53,53,53,53	0
57	MG	2A	3221	1/1	0.84	0.24	56,56,56,56	0
57	MG	1A	3260	1/1	0.84	0.17	55,55,55,55	0
57	MG	1A	3981	1/1	0.84	0.16	46,46,46,46	0
57	MG	1a	1629	1/1	0.84	0.21	50,50,50,50	0
57	MG	26	101	1/1	0.84	0.19	56,56,56,56	0
57	MG	2A	3235	1/1	0.84	0.19	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3127	1/1	0.84	0.23	46,46,46,46	0
57	MG	2A	3624	1/1	0.84	0.11	64,64,64,64	0
57	MG	2A	3629	1/1	0.84	0.07	64,64,64,64	0
59	ARG	1F	317	12/12	0.84	0.24	42,62,67,68	0
57	MG	2A	3099	1/1	0.84	0.16	52,52,52,52	0
57	MG	2a	3026	1/1	0.84	0.23	69,69,69,69	0
57	MG	1A	3617	1/1	0.85	0.15	42,42,42,42	0
57	MG	2D	308	1/1	0.85	0.23	44,44,44,44	0
57	MG	1a	1828	1/1	0.85	0.15	70,70,70,70	0
57	MG	2A	3308	1/1	0.85	0.20	38,38,38,38	0
57	MG	1a	1691	1/1	0.85	0.22	53,53,53,53	0
57	MG	1a	1837	1/1	0.85	0.11	63,63,63,63	0
57	MG	2A	3550	1/1	0.85	0.11	58,58,58,58	0
57	MG	2A	3319	1/1	0.85	0.19	50,50,50,50	0
57	MG	2A	3320	1/1	0.85	0.17	68,68,68,68	0
57	MG	1A	4002	1/1	0.85	0.13	38,38,38,38	0
57	MG	1A	3035	1/1	0.85	0.25	44,44,44,44	0
57	MG	2a	3016	1/1	0.85	0.21	60,60,60,60	0
57	MG	1A	3214	1/1	0.85	0.28	38,38,38,38	0
57	MG	2A	3339	1/1	0.85	0.15	44,44,44,44	0
57	MG	1A	3877	1/1	0.85	0.25	47,47,47,47	0
57	MG	1A	3128	1/1	0.85	0.16	62,62,62,62	0
57	MG	2A	3346	1/1	0.85	0.16	62,62,62,62	0
57	MG	1a	1726	1/1	0.85	0.13	62,62,62,62	0
57	MG	2A	3586	1/1	0.85	0.11	48,48,48,48	0
57	MG	2a	3037	1/1	0.85	0.20	59,59,59,59	0
57	MG	2A	3588	1/1	0.85	0.11	58,58,58,58	0
57	MG	2A	3363	1/1	0.85	0.19	69,69,69,69	0
57	MG	1A	3555	1/1	0.85	0.17	45,45,45,45	0
57	MG	2A	3154	1/1	0.85	0.20	44,44,44,44	0
57	MG	2a	3057	1/1	0.85	0.08	57,57,57,57	0
57	MG	2A	3376	1/1	0.85	0.11	47,47,47,47	0
57	MG	1a	1622	1/1	0.85	0.14	51,51,51,51	0
57	MG	1B	205	1/1	0.85	0.27	50,50,50,50	0
57	MG	1A	3570	1/1	0.85	0.21	51,51,51,51	0
57	MG	2a	3068	1/1	0.85	0.13	65,65,65,65	0
57	MG	1A	3896	1/1	0.85	0.17	28,28,28,28	0
57	MG	2A	3170	1/1	0.85	0.24	68,68,68,68	0
57	MG	2A	3623	1/1	0.85	0.19	45,45,45,45	0
57	MG	1A	3644	1/1	0.85	0.13	42,42,42,42	0
57	MG	2a	3089	1/1	0.85	0.13	52,52,52,52	0
57	MG	2A	3412	1/1	0.85	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1645	1/1	0.85	0.15	59,59,59,59	0
57	MG	2A	3182	1/1	0.85	0.15	61,61,61,61	0
57	MG	1A	3302	1/1	0.85	0.14	33,33,33,33	0
57	MG	2a	3112	1/1	0.85	0.11	76,76,76,76	0
57	MG	1y	201	1/1	0.85	0.21	56,56,56,56	0
57	MG	1D	316	1/1	0.85	0.13	51,51,51,51	0
57	MG	1D	318	1/1	0.85	0.18	51,51,51,51	0
57	MG	2A	3444	1/1	0.85	0.11	52,52,52,52	0
57	MG	1A	3075	1/1	0.85	0.16	41,41,41,41	0
57	MG	1A	3450	1/1	0.85	0.11	36,36,36,36	0
57	MG	1A	3088	1/1	0.85	0.15	42,42,42,42	0
57	MG	1a	1780	1/1	0.85	0.12	75,75,75,75	0
57	MG	1A	3165	1/1	0.85	0.35	50,50,50,50	0
57	MG	2A	3038	1/1	0.85	0.12	52,52,52,52	0
57	MG	1A	3982	1/1	0.85	0.20	44,44,44,44	0
57	MG	2A	3223	1/1	0.85	0.23	69,69,69,69	0
57	MG	1a	1790	1/1	0.85	0.14	62,62,62,62	0
57	MG	1A	3921	1/1	0.85	0.16	37,37,37,37	0
57	MG	2a	3153	1/1	0.85	0.13	65,65,65,65	0
57	MG	1A	3927	1/1	0.85	0.27	22,22,22,22	0
57	MG	2A	3065	1/1	0.85	0.21	60,60,60,60	0
57	MG	1a	1795	1/1	0.85	0.12	64,64,64,64	0
57	MG	1A	3462	1/1	0.85	0.21	44,44,44,44	0
57	MG	2A	3244	1/1	0.85	0.15	55,55,55,55	0
57	MG	2A	3490	1/1	0.85	0.18	58,58,58,58	0
57	MG	2a	3166	1/1	0.85	0.21	60,60,60,60	0
57	MG	1A	3828	1/1	0.85	0.21	44,44,44,44	0
57	MG	1A	3272	1/1	0.85	0.42	67,67,67,67	0
57	MG	1A	3995	1/1	0.85	0.16	66,66,66,66	0
57	MG	2A	3084	1/1	0.85	0.17	53,53,53,53	0
57	MG	2a	3177	1/1	0.85	0.15	72,72,72,72	0
57	MG	2A	3731	1/1	0.85	0.23	59,59,59,59	0
57	MG	2A	3732	1/1	0.85	0.12	71,71,71,71	0
57	MG	2A	3735	1/1	0.85	0.18	69,69,69,69	0
57	MG	2a	3187	1/1	0.85	0.12	68,68,68,68	0
57	MG	2A	3508	1/1	0.85	0.18	56,56,56,56	0
57	MG	1a	1812	1/1	0.85	0.08	63,63,63,63	0
57	MG	2A	3512	1/1	0.85	0.18	47,47,47,47	0
57	MG	1A	3167	1/1	0.85	0.23	30,30,30,30	0
57	MG	2A	3521	1/1	0.85	0.10	57,57,57,57	0
57	MG	2A	3525	1/1	0.85	0.22	42,42,42,42	0
57	MG	2A	3081	1/1	0.86	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
57	MG	2A	3626	1/1	0.86	0.17	59,59,59,59	0
57	MG	1a	1682	1/1	0.86	0.14	66,66,66,66	0
57	MG	2A	3241	1/1	0.86	0.14	63,63,63,63	0
57	MG	1A	3788	1/1	0.86	0.12	47,47,47,47	0
57	MG	1a	1685	1/1	0.86	0.12	59,59,59,59	0
57	MG	2A	3094	1/1	0.86	0.19	45,45,45,45	0
57	MG	2A	3253	1/1	0.86	0.37	50,50,50,50	0
57	MG	1A	3012	1/1	0.86	0.17	40,40,40,40	0
57	MG	2a	3050	1/1	0.86	0.08	60,60,60,60	0
57	MG	1A	3249	1/1	0.86	0.15	51,51,51,51	0
57	MG	1A	3582	1/1	0.86	0.20	44,44,44,44	0
57	MG	1A	3591	1/1	0.86	0.18	61,61,61,61	0
57	MG	1A	3810	1/1	0.86	0.18	73,73,73,73	0
57	MG	2A	3658	1/1	0.86	0.07	49,49,49,49	0
57	MG	2A	3286	1/1	0.86	0.15	42,42,42,42	0
57	MG	1A	3682	1/1	0.86	0.10	52,52,52,52	0
57	MG	2A	3666	1/1	0.86	0.09	48,48,48,48	0
57	MG	1a	1696	1/1	0.86	0.26	70,70,70,70	0
57	MG	2A	3309	1/1	0.86	0.17	51,51,51,51	0
57	MG	1A	3813	1/1	0.86	0.09	61,61,61,61	0
57	MG	2a	3092	1/1	0.86	0.12	53,53,53,53	0
57	MG	1A	4010	1/1	0.86	0.21	55,55,55,55	0
57	MG	2A	3673	1/1	0.86	0.13	66,66,66,66	0
57	MG	1A	3399	1/1	0.86	0.16	47,47,47,47	0
57	MG	2A	3146	1/1	0.86	0.17	60,60,60,60	0
57	MG	1A	3105	1/1	0.86	0.23	29,29,29,29	0
57	MG	1a	1621	1/1	0.86	0.28	52,52,52,52	0
57	MG	1A	3695	1/1	0.86	0.05	57,57,57,57	0
57	MG	2A	3526	1/1	0.86	0.45	55,55,55,55	0
57	MG	1A	3602	1/1	0.86	0.24	35,35,35,35	0
57	MG	1A	3106	1/1	0.86	0.17	30,30,30,30	0
57	MG	1A	3483	1/1	0.86	0.18	41,41,41,41	0
57	MG	2A	3705	1/1	0.86	0.13	53,53,53,53	0
57	MG	2A	3706	1/1	0.86	0.19	60,60,60,60	0
57	MG	1a	1640	1/1	0.86	0.17	53,53,53,53	0
57	MG	2A	3718	1/1	0.86	0.12	53,53,53,53	0
57	MG	1a	1641	1/1	0.86	0.18	68,68,68,68	0
57	MG	2A	3361	1/1	0.86	0.12	47,47,47,47	0
57	MG	1a	1643	1/1	0.86	0.34	64,64,64,64	0
57	MG	1A	3276	1/1	0.86	0.24	58,58,58,58	0
57	MG	2A	3367	1/1	0.86	0.15	41,41,41,41	0
57	MG	1A	3423	1/1	0.86	0.12	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3184	1/1	0.86	0.12	41,41,41,41	0
57	MG	2a	3157	1/1	0.86	0.32	63,63,63,63	0
57	MG	1D	315	1/1	0.86	0.19	63,63,63,63	0
57	MG	1A	3883	1/1	0.86	0.12	39,39,39,39	0
57	MG	1a	1657	1/1	0.86	0.13	51,51,51,51	0
57	MG	1A	3885	1/1	0.86	0.14	72,72,72,72	0
57	MG	1A	3720	1/1	0.86	0.07	38,38,38,38	0
57	MG	2A	3040	1/1	0.86	0.22	58,58,58,58	0
57	MG	1A	3430	1/1	0.86	0.16	37,37,37,37	0
57	MG	2a	3174	1/1	0.86	0.10	61,61,61,61	0
57	MG	2A	3048	1/1	0.86	0.09	53,53,53,53	0
57	MG	1A	3367	1/1	0.86	0.15	29,29,29,29	0
57	MG	1G	201	1/1	0.86	0.18	65,65,65,65	0
57	MG	2A	3597	1/1	0.86	0.07	63,63,63,63	0
57	MG	1A	3729	1/1	0.86	0.11	39,39,39,39	0
57	MG	2a	3009	1/1	0.86	0.19	55,55,55,55	0
57	MG	1A	3235	1/1	0.86	0.24	51,51,51,51	0
57	MG	2a	3189	1/1	0.86	0.15	59,59,59,59	0
57	MG	1a	1674	1/1	0.86	0.24	56,56,56,56	0
57	MG	2A	3227	1/1	0.86	0.23	55,55,55,55	0
57	MG	1A	3320	1/1	0.86	0.12	41,41,41,41	0
57	MG	1A	3324	1/1	0.86	0.22	40,40,40,40	0
57	MG	1A	3764	1/1	0.86	0.27	64,64,64,64	0
57	MG	2a	3027	1/1	0.86	0.22	65,65,65,65	0
57	MG	1A	3758	1/1	0.87	0.24	42,42,42,42	0
57	MG	2A	3392	1/1	0.87	0.09	40,40,40,40	0
57	MG	1A	4021	1/1	0.87	0.16	39,39,39,39	0
57	MG	2A	3107	1/1	0.87	0.23	56,56,56,56	0
57	MG	1A	3479	1/1	0.87	0.16	59,59,59,59	0
57	MG	1a	1784	1/1	0.87	0.12	52,52,52,52	0
57	MG	1h	202	1/1	0.87	0.13	67,67,67,67	0
57	MG	1A	3826	1/1	0.87	0.16	32,32,32,32	0
57	MG	1A	3938	1/1	0.87	0.09	50,50,50,50	0
57	MG	1A	3939	1/1	0.87	0.08	47,47,47,47	0
57	MG	2A	3426	1/1	0.87	0.21	56,56,56,56	0
57	MG	2A	3433	1/1	0.87	0.12	57,57,57,57	0
57	MG	1A	3630	1/1	0.87	0.16	58,58,58,58	0
57	MG	2A	3438	1/1	0.87	0.13	57,57,57,57	0
57	MG	1a	1651	1/1	0.87	0.23	55,55,55,55	0
57	MG	1a	1698	1/1	0.87	0.25	62,62,62,62	0
57	MG	2A	3730	1/1	0.87	0.07	57,57,57,57	0
57	MG	2A	3011	1/1	0.87	0.41	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1655	1/1	0.87	0.07	60,60,60,60	0
57	MG	2A	3733	1/1	0.87	0.12	65,65,65,65	0
57	MG	1a	1716	1/1	0.87	0.21	41,41,41,41	0
57	MG	2B	201	1/1	0.87	0.37	68,68,68,68	0
57	MG	1a	1721	1/1	0.87	0.10	58,58,58,58	0
57	MG	2A	3287	1/1	0.87	0.28	56,56,56,56	0
57	MG	1A	3832	1/1	0.87	0.19	49,49,49,49	0
57	MG	2A	3601	1/1	0.87	0.12	66,66,66,66	0
57	MG	1A	3842	1/1	0.87	0.19	35,35,35,35	0
57	MG	1A	3422	1/1	0.87	0.15	53,53,53,53	0
57	MG	1A	3234	1/1	0.87	0.17	38,38,38,38	0
57	MG	2A	3465	1/1	0.87	0.11	54,54,54,54	0
57	MG	2A	3617	1/1	0.87	0.10	38,38,38,38	0
57	MG	1a	1607	1/1	0.87	0.11	50,50,50,50	0
57	MG	2Q	203	1/1	0.87	0.30	50,50,50,50	0
57	MG	2A	3620	1/1	0.87	0.20	46,46,46,46	0
57	MG	2A	3058	1/1	0.87	0.23	56,56,56,56	0
57	MG	1A	3131	1/1	0.87	0.30	49,49,49,49	0
57	MG	2A	3185	1/1	0.87	0.20	53,53,53,53	0
57	MG	2a	3003	1/1	0.87	0.22	57,57,57,57	0
57	MG	1A	3315	1/1	0.87	0.30	46,46,46,46	0
57	MG	2a	3163	1/1	0.87	0.14	60,60,60,60	0
57	MG	1A	3205	1/1	0.87	0.31	46,46,46,46	0
57	MG	2A	3334	1/1	0.87	0.08	54,54,54,54	0
57	MG	1A	3738	1/1	0.87	0.17	49,49,49,49	0
57	MG	2A	3493	1/1	0.87	0.12	50,50,50,50	0
57	MG	1A	3417	1/1	0.87	0.21	21,21,21,21	0
57	MG	1A	3884	1/1	0.87	0.11	33,33,33,33	0
57	MG	1N	203	1/1	0.87	0.13	50,50,50,50	0
57	MG	1a	1635	1/1	0.87	0.15	63,63,63,63	0
57	MG	2a	3181	1/1	0.87	0.14	74,74,74,74	0
57	MG	1a	1770	1/1	0.87	0.12	51,51,51,51	0
57	MG	1a	1858	1/1	0.87	0.18	63,63,63,63	0
57	MG	2A	3090	1/1	0.87	0.19	70,70,70,70	0
57	MG	2A	3091	1/1	0.87	0.21	42,42,42,42	0
57	MG	1a	1774	1/1	0.87	0.07	67,67,67,67	0
57	MG	2A	3522	1/1	0.87	0.25	56,56,56,56	0
57	MG	2t	201	1/1	0.87	0.13	51,51,51,51	0
57	MG	2A	3524	1/1	0.87	0.16	50,50,50,50	0
57	MG	1a	1868	1/1	0.87	0.17	46,46,46,46	0
60	ZN	14	501	1/1	0.87	0.08	101,101,101,101	0
57	MG	1A	4019	1/1	0.87	0.10	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3527	1/1	0.87	0.10	52,52,52,52	0
57	MG	1B	219	1/1	0.88	0.15	45,45,45,45	0
57	MG	2A	3431	1/1	0.88	0.08	77,77,77,77	0
57	MG	2A	3605	1/1	0.88	0.13	64,64,64,64	0
57	MG	2A	3432	1/1	0.88	0.17	47,47,47,47	0
57	MG	1a	1617	1/1	0.88	0.13	54,54,54,54	0
57	MG	1B	222	1/1	0.88	0.21	35,35,35,35	0
57	MG	1A	3901	1/1	0.88	0.10	40,40,40,40	0
57	MG	2A	3439	1/1	0.88	0.18	64,64,64,64	0
57	MG	2A	3232	1/1	0.88	0.18	64,64,64,64	0
57	MG	1A	3616	1/1	0.88	0.16	40,40,40,40	0
57	MG	1A	3971	1/1	0.88	0.18	65,65,65,65	0
57	MG	1A	3833	1/1	0.88	0.15	60,60,60,60	0
57	MG	1A	3912	1/1	0.88	0.16	31,31,31,31	0
57	MG	1A	3464	1/1	0.88	0.17	60,60,60,60	0
57	MG	2A	3627	1/1	0.88	0.16	48,48,48,48	0
57	MG	1D	317	1/1	0.88	0.18	38,38,38,38	0
57	MG	2A	3248	1/1	0.88	0.16	51,51,51,51	0
57	MG	1A	3189	1/1	0.88	0.18	59,59,59,59	0
57	MG	1a	1733	1/1	0.88	0.08	65,65,65,65	0
57	MG	2A	3456	1/1	0.88	0.10	61,61,61,61	0
57	MG	2a	3056	1/1	0.88	0.11	60,60,60,60	0
57	MG	2A	3460	1/1	0.88	0.24	44,44,44,44	0
57	MG	2A	3643	1/1	0.88	0.11	74,74,74,74	0
57	MG	2a	3061	1/1	0.88	0.16	54,54,54,54	0
57	MG	1A	3446	1/1	0.88	0.31	45,45,45,45	0
57	MG	1A	3770	1/1	0.88	0.31	44,44,44,44	0
57	MG	2A	3280	1/1	0.88	0.15	47,47,47,47	0
57	MG	2A	3112	1/1	0.88	0.14	47,47,47,47	0
57	MG	2a	3070	1/1	0.88	0.19	56,56,56,56	0
57	MG	2a	3071	1/1	0.88	0.20	68,68,68,68	0
57	MG	2A	3655	1/1	0.88	0.17	49,49,49,49	0
57	MG	1E	310	1/1	0.88	0.17	40,40,40,40	0
57	MG	1a	1748	1/1	0.88	0.07	63,63,63,63	0
57	MG	1A	3772	1/1	0.88	0.13	50,50,50,50	0
57	MG	1a	1872	1/1	0.88	0.16	70,70,70,70	0
57	MG	2A	3487	1/1	0.88	0.10	59,59,59,59	0
57	MG	2A	3292	1/1	0.88	0.20	59,59,59,59	0
57	MG	2A	3128	1/1	0.88	0.21	47,47,47,47	0
57	MG	1F	314	1/1	0.88	0.31	60,60,60,60	0
57	MG	1A	3867	1/1	0.88	0.11	40,40,40,40	0
57	MG	1G	202	1/1	0.88	0.16	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1f	201	1/1	0.88	0.36	68,68,68,68	0
57	MG	1h	201	1/1	0.88	0.24	57,57,57,57	0
57	MG	1A	3868	1/1	0.88	0.11	45,45,45,45	0
57	MG	1A	3871	1/1	0.88	0.16	55,55,55,55	0
57	MG	2a	3127	1/1	0.88	0.29	54,54,54,54	0
57	MG	1A	3494	1/1	0.88	0.17	27,27,27,27	0
57	MG	2a	3129	1/1	0.88	0.20	68,68,68,68	0
57	MG	2A	3513	1/1	0.88	0.14	60,60,60,60	0
57	MG	1A	3583	1/1	0.88	0.15	40,40,40,40	0
57	MG	2A	3694	1/1	0.88	0.43	59,59,59,59	0
57	MG	2A	3697	1/1	0.88	0.13	54,54,54,54	0
57	MG	1A	3708	1/1	0.88	0.10	48,48,48,48	0
57	MG	1A	3637	1/1	0.88	0.16	38,38,38,38	0
57	MG	1A	4005	1/1	0.88	0.11	45,45,45,45	0
57	MG	1A	3371	1/1	0.88	0.21	27,27,27,27	0
57	MG	2A	3708	1/1	0.88	0.20	51,51,51,51	0
57	MG	2A	3172	1/1	0.88	0.17	78,78,78,78	0
57	MG	1A	3078	1/1	0.88	0.16	56,56,56,56	0
57	MG	2A	3722	1/1	0.88	0.22	61,61,61,61	0
57	MG	2A	3725	1/1	0.88	0.14	67,67,67,67	0
57	MG	2A	3017	1/1	0.88	0.26	52,52,52,52	0
57	MG	2A	3030	1/1	0.88	0.14	38,38,38,38	0
57	MG	1a	1788	1/1	0.88	0.09	69,69,69,69	0
57	MG	1A	4011	1/1	0.88	0.30	53,53,53,53	0
57	MG	1A	3376	1/1	0.88	0.19	42,42,42,42	0
57	MG	2A	3198	1/1	0.88	0.20	46,46,46,46	0
57	MG	10	106	1/1	0.88	0.10	46,46,46,46	0
57	MG	2A	3387	1/1	0.88	0.10	46,46,46,46	0
57	MG	1a	1793	1/1	0.88	0.11	68,68,68,68	0
57	MG	2A	3047	1/1	0.88	0.25	51,51,51,51	0
57	MG	2B	208	1/1	0.88	0.21	59,59,59,59	0
57	MG	2A	3208	1/1	0.88	0.39	53,53,53,53	0
57	MG	2a	3178	1/1	0.88	0.14	53,53,53,53	0
57	MG	2B	212	1/1	0.88	0.09	58,58,58,58	0
57	MG	1A	3950	1/1	0.88	0.16	43,43,43,43	0
57	MG	2A	3578	1/1	0.88	0.07	55,55,55,55	0
57	MG	1A	3433	1/1	0.88	0.19	28,28,28,28	0
57	MG	2a	3186	1/1	0.88	0.07	52,52,52,52	0
57	MG	2A	3400	1/1	0.88	0.10	55,55,55,55	0
57	MG	1A	3261	1/1	0.88	0.26	46,46,46,46	0
57	MG	2A	3408	1/1	0.88	0.18	59,59,59,59	0
57	MG	2Q	202	1/1	0.88	0.28	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3115	1/1	0.88	0.21	41,41,41,41	0
58	MPD	1a	1881	8/8	0.88	0.23	54,63,67,70	0
57	MG	1A	3575	1/1	0.88	0.15	59,59,59,59	0
57	MG	1B	213	1/1	0.88	0.17	47,47,47,47	0
57	MG	1a	1611	1/1	0.88	0.27	51,51,51,51	0
57	MG	2A	3424	1/1	0.88	0.19	53,53,53,53	0
57	MG	28	101	1/1	0.88	0.21	54,54,54,54	0
57	MG	2a	3012	1/1	0.89	0.23	58,58,58,58	0
57	MG	2A	3616	1/1	0.89	0.20	66,66,66,66	0
57	MG	1A	3057	1/1	0.89	0.16	47,47,47,47	0
57	MG	2a	3017	1/1	0.89	0.15	56,56,56,56	0
57	MG	2a	3018	1/1	0.89	0.23	63,63,63,63	0
57	MG	2A	3076	1/1	0.89	0.21	61,61,61,61	0
57	MG	1a	1704	1/1	0.89	0.17	57,57,57,57	0
57	MG	2A	3237	1/1	0.89	0.13	48,48,48,48	0
57	MG	1A	3985	1/1	0.89	0.22	32,32,32,32	0
57	MG	1a	1842	1/1	0.89	0.12	62,62,62,62	0
57	MG	1a	1632	1/1	0.89	0.21	47,47,47,47	0
57	MG	1A	3701	1/1	0.89	0.12	37,37,37,37	0
57	MG	1E	301	1/1	0.89	0.20	42,42,42,42	0
57	MG	1A	3453	1/1	0.89	0.10	58,58,58,58	0
57	MG	1a	1727	1/1	0.89	0.25	63,63,63,63	0
57	MG	2a	3041	1/1	0.89	0.16	61,61,61,61	0
57	MG	1A	3618	1/1	0.89	0.22	33,33,33,33	0
57	MG	2A	3266	1/1	0.89	0.36	52,52,52,52	0
57	MG	2A	3638	1/1	0.89	0.07	63,63,63,63	0
57	MG	2A	3104	1/1	0.89	0.14	63,63,63,63	0
57	MG	2A	3274	1/1	0.89	0.23	47,47,47,47	0
57	MG	1A	3284	1/1	0.89	0.26	37,37,37,37	0
57	MG	2A	3461	1/1	0.89	0.15	60,60,60,60	0
57	MG	1A	3173	1/1	0.89	0.16	49,49,49,49	0
57	MG	1A	3577	1/1	0.89	0.17	51,51,51,51	0
57	MG	2a	3064	1/1	0.89	0.25	42,42,42,42	0
57	MG	1A	3461	1/1	0.89	0.12	35,35,35,35	0
57	MG	2A	3471	1/1	0.89	0.12	62,62,62,62	0
57	MG	1A	3156	1/1	0.89	0.12	47,47,47,47	0
57	MG	1a	1744	1/1	0.89	0.10	60,60,60,60	0
57	MG	1a	1873	1/1	0.89	0.12	57,57,57,57	0
57	MG	1A	3338	1/1	0.89	0.25	42,42,42,42	0
57	MG	2A	3293	1/1	0.89	0.16	54,54,54,54	0
57	MG	2A	3132	1/1	0.89	0.14	70,70,70,70	0
57	MG	2A	3297	1/1	0.89	0.18	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3298	1/1	0.89	0.09	61,61,61,61	0
57	MG	2A	3492	1/1	0.89	0.12	61,61,61,61	0
57	MG	1A	3726	1/1	0.89	0.13	48,48,48,48	0
57	MG	1a	1750	1/1	0.89	0.40	74,74,74,74	0
57	MG	2a	3102	1/1	0.89	0.15	74,74,74,74	0
57	MG	1A	3123	1/1	0.89	0.13	36,36,36,36	0
57	MG	1A	3469	1/1	0.89	0.25	64,64,64,64	0
57	MG	1A	3736	1/1	0.89	0.14	33,33,33,33	0
57	MG	1A	3646	1/1	0.89	0.12	53,53,53,53	0
57	MG	1l	201	1/1	0.89	0.18	55,55,55,55	0
57	MG	2A	3155	1/1	0.89	0.18	37,37,37,37	0
57	MG	2A	3695	1/1	0.89	0.17	55,55,55,55	0
57	MG	1a	1663	1/1	0.89	0.11	70,70,70,70	0
57	MG	1A	3740	1/1	0.89	0.17	38,38,38,38	0
57	MG	2A	3699	1/1	0.89	0.13	51,51,51,51	0
57	MG	1a	1665	1/1	0.89	0.14	62,62,62,62	0
57	MG	1A	3477	1/1	0.89	0.22	23,23,23,23	0
57	MG	2A	3165	1/1	0.89	0.31	48,48,48,48	0
57	MG	1A	3253	1/1	0.89	0.24	30,30,30,30	0
57	MG	2A	3715	1/1	0.89	0.07	72,72,72,72	0
57	MG	1A	3672	1/1	0.89	0.13	38,38,38,38	0
57	MG	1A	3395	1/1	0.89	0.20	42,42,42,42	0
57	MG	2a	3147	1/1	0.89	0.08	70,70,70,70	0
57	MG	2A	3016	1/1	0.89	0.17	54,54,54,54	0
57	MG	2A	3723	1/1	0.89	0.20	56,56,56,56	0
57	MG	1A	4026	1/1	0.89	0.16	46,46,46,46	0
57	MG	2A	3025	1/1	0.89	0.15	54,54,54,54	0
57	MG	2A	3373	1/1	0.89	0.10	42,42,42,42	0
57	MG	2A	3541	1/1	0.89	0.12	49,49,49,49	0
57	MG	2A	3374	1/1	0.89	0.08	58,58,58,58	0
57	MG	1a	1676	1/1	0.89	0.10	56,56,56,56	0
57	MG	2A	3033	1/1	0.89	0.18	54,54,54,54	0
57	MG	2A	3381	1/1	0.89	0.15	58,58,58,58	0
57	MG	2A	3188	1/1	0.89	0.25	67,67,67,67	0
57	MG	1A	3083	1/1	0.89	0.24	32,32,32,32	0
57	MG	1B	207	1/1	0.89	0.35	49,49,49,49	0
57	MG	17	105	1/1	0.89	0.18	34,34,34,34	0
57	MG	2A	3393	1/1	0.89	0.12	33,33,33,33	0
57	MG	1B	212	1/1	0.89	0.10	54,54,54,54	0
57	MG	1A	3443	1/1	0.89	0.19	28,28,28,28	0
57	MG	1A	3778	1/1	0.89	0.29	63,63,63,63	0
57	MG	2D	303	1/1	0.89	0.52	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3687	1/1	0.89	0.11	61,61,61,61	0
57	MG	1A	3790	1/1	0.89	0.26	47,47,47,47	0
57	MG	2A	3404	1/1	0.89	0.19	69,69,69,69	0
57	MG	2A	3589	1/1	0.89	0.06	48,48,48,48	0
57	MG	2P	201	1/1	0.89	0.15	54,54,54,54	0
57	MG	1A	3152	1/1	0.89	0.13	63,63,63,63	0
57	MG	2A	3410	1/1	0.89	0.18	37,37,37,37	0
57	MG	1A	3800	1/1	0.89	0.12	31,31,31,31	0
57	MG	1a	1693	1/1	0.89	0.13	57,57,57,57	0
57	MG	2r	101	1/1	0.89	0.13	64,64,64,64	0
57	MG	2A	3220	1/1	0.89	0.21	47,47,47,47	0
57	MG	2A	3602	1/1	0.89	0.15	35,35,35,35	0
57	MG	1A	3694	1/1	0.89	0.14	58,58,58,58	0
57	MG	1A	3228	1/1	0.89	0.11	39,39,39,39	0
57	MG	1a	1623	1/1	0.89	0.11	57,57,57,57	0
57	MG	1a	1829	1/1	0.89	0.17	73,73,73,73	0
57	MG	2A	3073	1/1	0.89	0.23	54,54,54,54	0
57	MG	1A	3312	1/1	0.90	0.20	40,40,40,40	0
57	MG	1a	1624	1/1	0.90	0.09	41,41,41,41	0
57	MG	1a	1628	1/1	0.90	0.21	57,57,57,57	0
57	MG	1A	3277	1/1	0.90	0.30	63,63,63,63	0
57	MG	2B	205	1/1	0.90	0.19	49,49,49,49	0
57	MG	1a	1754	1/1	0.90	0.14	66,66,66,66	0
57	MG	1A	3547	1/1	0.90	0.17	47,47,47,47	0
57	MG	2A	3507	1/1	0.90	0.23	60,60,60,60	0
57	MG	1A	3774	1/1	0.90	0.13	36,36,36,36	0
57	MG	2A	3046	1/1	0.90	0.20	50,50,50,50	0
57	MG	2B	215	1/1	0.90	0.17	62,62,62,62	0
57	MG	1A	3915	1/1	0.90	0.17	52,52,52,52	0
57	MG	2A	3256	1/1	0.90	0.36	54,54,54,54	0
57	MG	1a	1769	1/1	0.90	0.30	66,66,66,66	0
57	MG	1A	3775	1/1	0.90	0.10	42,42,42,42	0
57	MG	2E	304	1/1	0.90	0.14	57,57,57,57	0
57	MG	2F	301	1/1	0.90	0.24	42,42,42,42	0
57	MG	2A	3055	1/1	0.90	0.21	62,62,62,62	0
57	MG	2A	3057	1/1	0.90	0.22	62,62,62,62	0
57	MG	1A	3657	1/1	0.90	0.10	50,50,50,50	0
57	MG	1B	206	1/1	0.90	0.40	56,56,56,56	0
57	MG	1a	1642	1/1	0.90	0.12	57,57,57,57	0
57	MG	2Q	204	1/1	0.90	0.12	46,46,46,46	0
57	MG	1A	3922	1/1	0.90	0.07	37,37,37,37	0
57	MG	1B	210	1/1	0.90	0.34	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3533	1/1	0.90	0.48	66,66,66,66	0
57	MG	1A	3779	1/1	0.90	0.20	41,41,41,41	0
57	MG	1A	3783	1/1	0.90	0.15	27,27,27,27	0
57	MG	1A	3280	1/1	0.90	0.14	52,52,52,52	0
57	MG	1A	3561	1/1	0.90	0.28	46,46,46,46	0
57	MG	1A	3379	1/1	0.90	0.12	42,42,42,42	0
57	MG	2A	3078	1/1	0.90	0.20	57,57,57,57	0
57	MG	2A	3307	1/1	0.90	0.10	49,49,49,49	0
57	MG	1A	3281	1/1	0.90	0.35	48,48,48,48	0
57	MG	1a	1658	1/1	0.90	0.08	71,71,71,71	0
57	MG	1A	3678	1/1	0.90	0.10	40,40,40,40	0
57	MG	2A	3570	1/1	0.90	0.13	42,42,42,42	0
57	MG	1A	3680	1/1	0.90	0.16	29,29,29,29	0
57	MG	2a	3024	1/1	0.90	0.17	46,46,46,46	0
57	MG	2A	3573	1/1	0.90	0.15	46,46,46,46	0
57	MG	1A	3383	1/1	0.90	0.26	40,40,40,40	0
57	MG	2A	3092	1/1	0.90	0.19	63,63,63,63	0
57	MG	1A	3384	1/1	0.90	0.15	31,31,31,31	0
57	MG	1A	3811	1/1	0.90	0.22	54,54,54,54	0
57	MG	1a	1806	1/1	0.90	0.06	66,66,66,66	0
57	MG	1A	3187	1/1	0.90	0.21	31,31,31,31	0
57	MG	2A	3103	1/1	0.90	0.19	42,42,42,42	0
57	MG	1a	1809	1/1	0.90	0.10	70,70,70,70	0
57	MG	1A	3580	1/1	0.90	0.16	47,47,47,47	0
57	MG	1A	3693	1/1	0.90	0.18	57,57,57,57	0
57	MG	2A	3351	1/1	0.90	0.21	47,47,47,47	0
57	MG	1A	3391	1/1	0.90	0.14	37,37,37,37	0
57	MG	2A	3599	1/1	0.90	0.15	49,49,49,49	0
57	MG	2a	3055	1/1	0.90	0.10	66,66,66,66	0
57	MG	2A	3113	1/1	0.90	0.48	45,45,45,45	0
57	MG	2A	3362	1/1	0.90	0.08	40,40,40,40	0
57	MG	1A	3327	1/1	0.90	0.13	42,42,42,42	0
57	MG	2a	3060	1/1	0.90	0.14	64,64,64,64	0
57	MG	1A	3966	1/1	0.90	0.21	47,47,47,47	0
57	MG	1A	3394	1/1	0.90	0.17	43,43,43,43	0
57	MG	1a	1836	1/1	0.90	0.13	57,57,57,57	0
57	MG	1A	3289	1/1	0.90	0.11	33,33,33,33	0
57	MG	1A	3834	1/1	0.90	0.14	27,27,27,27	0
57	MG	1A	3290	1/1	0.90	0.26	52,52,52,52	0
57	MG	2A	3378	1/1	0.90	0.15	64,64,64,64	0
57	MG	1a	1843	1/1	0.90	0.16	65,65,65,65	0
57	MG	2A	3137	1/1	0.90	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
57	MG	2A	3139	1/1	0.90	0.18	53,53,53,53	0
57	MG	2a	3082	1/1	0.90	0.14	61,61,61,61	0
57	MG	1A	3227	1/1	0.90	0.34	42,42,42,42	0
57	MG	2a	3087	1/1	0.90	0.12	60,60,60,60	0
57	MG	2A	3145	1/1	0.90	0.18	55,55,55,55	0
57	MG	1a	1846	1/1	0.90	0.20	59,59,59,59	0
57	MG	2A	3148	1/1	0.90	0.26	42,42,42,42	0
57	MG	2A	3395	1/1	0.90	0.22	59,59,59,59	0
57	MG	1a	1684	1/1	0.90	0.24	48,48,48,48	0
57	MG	2A	3397	1/1	0.90	0.21	42,42,42,42	0
57	MG	1A	3255	1/1	0.90	0.20	43,43,43,43	0
57	MG	1A	3604	1/1	0.90	0.24	44,44,44,44	0
57	MG	2A	3640	1/1	0.90	0.34	68,68,68,68	0
57	MG	1A	3411	1/1	0.90	0.29	25,25,25,25	0
57	MG	2A	3642	1/1	0.90	0.12	49,49,49,49	0
57	MG	2a	3120	1/1	0.90	0.14	60,60,60,60	0
57	MG	2A	3156	1/1	0.90	0.22	60,60,60,60	0
57	MG	2A	3644	1/1	0.90	0.12	54,54,54,54	0
57	MG	1A	3471	1/1	0.90	0.21	50,50,50,50	0
57	MG	1a	1857	1/1	0.90	0.05	64,64,64,64	0
57	MG	1A	3610	1/1	0.90	0.16	43,43,43,43	0
57	MG	1A	3723	1/1	0.90	0.16	39,39,39,39	0
57	MG	1A	3130	1/1	0.90	0.16	33,33,33,33	0
57	MG	1V	204	1/1	0.90	0.19	45,45,45,45	0
57	MG	1A	3992	1/1	0.90	0.08	45,45,45,45	0
57	MG	1A	3198	1/1	0.90	0.21	63,63,63,63	0
57	MG	2A	3660	1/1	0.90	0.10	50,50,50,50	0
57	MG	2A	3429	1/1	0.90	0.17	52,52,52,52	0
57	MG	2a	3145	1/1	0.90	0.17	56,56,56,56	0
57	MG	2a	3146	1/1	0.90	0.18	56,56,56,56	0
57	MG	1a	1700	1/1	0.90	0.23	65,65,65,65	0
57	MG	2A	3174	1/1	0.90	0.24	58,58,58,58	0
57	MG	1a	1874	1/1	0.90	0.21	74,74,74,74	0
57	MG	1a	1876	1/1	0.90	0.12	69,69,69,69	0
57	MG	1A	3361	1/1	0.90	0.16	50,50,50,50	0
57	MG	1A	3493	1/1	0.90	0.19	23,23,23,23	0
57	MG	1a	1709	1/1	0.90	0.22	53,53,53,53	0
57	MG	2A	3192	1/1	0.90	0.14	45,45,45,45	0
57	MG	1e	201	1/1	0.90	0.25	62,62,62,62	0
57	MG	1e	203	1/1	0.90	0.26	49,49,49,49	0
57	MG	1A	3181	1/1	0.90	0.24	46,46,46,46	0
57	MG	1a	1718	1/1	0.90	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3164	1/1	0.90	0.21	54,54,54,54	0
57	MG	2A	3685	1/1	0.90	0.16	43,43,43,43	0
57	MG	2A	3691	1/1	0.90	0.13	43,43,43,43	0
57	MG	1A	3425	1/1	0.90	0.16	19,19,19,19	0
57	MG	1A	3508	1/1	0.90	0.14	33,33,33,33	0
57	MG	1A	3744	1/1	0.90	0.12	41,41,41,41	0
57	MG	2A	3211	1/1	0.90	0.18	41,41,41,41	0
57	MG	1m	201	1/1	0.90	0.06	65,65,65,65	0
57	MG	1n	101	1/1	0.90	0.06	58,58,58,58	0
57	MG	2A	3217	1/1	0.90	0.24	60,60,60,60	0
57	MG	1A	4004	1/1	0.90	0.21	47,47,47,47	0
57	MG	1A	3748	1/1	0.90	0.13	43,43,43,43	0
57	MG	2a	3183	1/1	0.90	0.07	65,65,65,65	0
57	MG	2a	3184	1/1	0.90	0.07	47,47,47,47	0
57	MG	1A	4006	1/1	0.90	0.17	29,29,29,29	0
57	MG	2A	3711	1/1	0.90	0.14	53,53,53,53	0
57	MG	1A	3509	1/1	0.90	0.12	29,29,29,29	0
57	MG	1a	1616	1/1	0.90	0.18	56,56,56,56	0
57	MG	2A	3473	1/1	0.90	0.13	54,54,54,54	0
57	MG	2f	201	1/1	0.90	0.09	54,54,54,54	0
57	MG	1A	3011	1/1	0.90	0.23	50,50,50,50	0
57	MG	1a	1620	1/1	0.90	0.15	56,56,56,56	0
57	MG	1A	3525	1/1	0.90	0.16	42,42,42,42	0
57	MG	2x	101	1/1	0.90	0.08	42,42,42,42	0
58	MPD	1A	4029	8/8	0.90	0.17	37,50,57,60	0
57	MG	2A	3480	1/1	0.90	0.24	69,69,69,69	0
58	MPD	2A	3739	8/8	0.90	0.19	46,56,63,64	0
57	MG	2A	3728	1/1	0.90	0.16	52,52,52,52	0
57	MG	1a	1742	1/1	0.90	0.15	63,63,63,63	0
57	MG	1A	4013	1/1	0.90	0.12	44,44,44,44	0
57	MG	2A	3234	1/1	0.90	0.17	50,50,50,50	0
57	MG	2A	3029	1/1	0.90	0.14	63,63,63,63	0
57	MG	1A	4008	1/1	0.91	0.13	55,55,55,55	0
57	MG	2A	3178	1/1	0.91	0.18	53,53,53,53	0
57	MG	2V	203	1/1	0.91	0.23	53,53,53,53	0
57	MG	2A	3181	1/1	0.91	0.13	57,57,57,57	0
57	MG	1a	1673	1/1	0.91	0.12	56,56,56,56	0
57	MG	1A	3934	1/1	0.91	0.19	22,22,22,22	0
57	MG	2A	3390	1/1	0.91	0.16	52,52,52,52	0
57	MG	2A	3024	1/1	0.91	0.12	63,63,63,63	0
57	MG	1A	3558	1/1	0.91	0.19	20,20,20,20	0
57	MG	1A	3015	1/1	0.91	0.23	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1677	1/1	0.91	0.28	57,57,57,57	0
57	MG	2A	3193	1/1	0.91	0.09	60,60,60,60	0
57	MG	1A	3190	1/1	0.91	0.21	53,53,53,53	0
57	MG	2A	3398	1/1	0.91	0.12	46,46,46,46	0
57	MG	1A	3849	1/1	0.91	0.08	50,50,50,50	0
57	MG	1A	3295	1/1	0.91	0.09	67,67,67,67	0
57	MG	2a	3023	1/1	0.91	0.11	54,54,54,54	0
57	MG	2A	3037	1/1	0.91	0.16	39,39,39,39	0
57	MG	1A	3240	1/1	0.91	0.27	36,36,36,36	0
57	MG	2A	3207	1/1	0.91	0.07	55,55,55,55	0
57	MG	1A	3621	1/1	0.91	0.27	35,35,35,35	0
57	MG	2A	3044	1/1	0.91	0.23	66,66,66,66	0
57	MG	2A	3419	1/1	0.91	0.14	39,39,39,39	0
57	MG	2a	3032	1/1	0.91	0.10	60,60,60,60	0
57	MG	1a	1601	1/1	0.91	0.19	46,46,46,46	0
57	MG	1A	3622	1/1	0.91	0.15	30,30,30,30	0
57	MG	2A	3625	1/1	0.91	0.12	64,64,64,64	0
57	MG	1B	204	1/1	0.91	0.23	53,53,53,53	0
57	MG	1A	3866	1/1	0.91	0.14	44,44,44,44	0
57	MG	2A	3628	1/1	0.91	0.08	64,64,64,64	0
57	MG	1A	3768	1/1	0.91	0.16	57,57,57,57	0
57	MG	2a	3048	1/1	0.91	0.20	61,61,61,61	0
57	MG	1A	3299	1/1	0.91	0.24	31,31,31,31	0
57	MG	2A	3056	1/1	0.91	0.10	65,65,65,65	0
57	MG	1A	3957	1/1	0.91	0.14	61,61,61,61	0
57	MG	1a	1826	1/1	0.91	0.23	59,59,59,59	0
57	MG	2A	3434	1/1	0.91	0.13	58,58,58,58	0
57	MG	2A	3435	1/1	0.91	0.14	36,36,36,36	0
57	MG	2A	3059	1/1	0.91	0.23	41,41,41,41	0
57	MG	1a	1615	1/1	0.91	0.17	58,58,58,58	0
57	MG	1A	3010	1/1	0.91	0.24	39,39,39,39	0
57	MG	2a	3063	1/1	0.91	0.22	63,63,63,63	0
57	MG	1A	3698	1/1	0.91	0.20	19,19,19,19	0
57	MG	1a	1834	1/1	0.91	0.11	71,71,71,71	0
57	MG	1a	1835	1/1	0.91	0.14	57,57,57,57	0
57	MG	1a	1619	1/1	0.91	0.27	59,59,59,59	0
57	MG	1A	3183	1/1	0.91	0.17	31,31,31,31	0
57	MG	1a	1838	1/1	0.91	0.13	65,65,65,65	0
57	MG	1A	3882	1/1	0.91	0.11	40,40,40,40	0
57	MG	2a	3076	1/1	0.91	0.13	54,54,54,54	0
57	MG	1A	3203	1/1	0.91	0.17	47,47,47,47	0
57	MG	2a	3078	1/1	0.91	0.21	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3079	1/1	0.91	0.12	51,51,51,51	0
57	MG	1a	1714	1/1	0.91	0.21	58,58,58,58	0
57	MG	2A	3662	1/1	0.91	0.16	44,44,44,44	0
57	MG	1a	1715	1/1	0.91	0.17	38,38,38,38	0
57	MG	1A	3520	1/1	0.91	0.14	44,44,44,44	0
57	MG	1A	3385	1/1	0.91	0.20	27,27,27,27	0
57	MG	2A	3462	1/1	0.91	0.12	62,62,62,62	0
57	MG	1A	3710	1/1	0.91	0.12	72,72,72,72	0
57	MG	2a	3101	1/1	0.91	0.08	65,65,65,65	0
57	MG	2A	3671	1/1	0.91	0.10	59,59,59,59	0
57	MG	2A	3259	1/1	0.91	0.23	56,56,56,56	0
57	MG	2A	3261	1/1	0.91	0.18	62,62,62,62	0
57	MG	2A	3262	1/1	0.91	0.41	49,49,49,49	0
57	MG	2a	3113	1/1	0.91	0.13	58,58,58,58	0
57	MG	1D	303	1/1	0.91	0.27	48,48,48,48	0
57	MG	1D	313	1/1	0.91	0.19	48,48,48,48	0
57	MG	1a	1631	1/1	0.91	0.20	50,50,50,50	0
57	MG	2a	3121	1/1	0.91	0.12	60,60,60,60	0
57	MG	2A	3277	1/1	0.91	0.09	54,54,54,54	0
57	MG	1A	3889	1/1	0.91	0.16	28,28,28,28	0
57	MG	2A	3684	1/1	0.91	0.10	69,69,69,69	0
57	MG	2A	3098	1/1	0.91	0.14	49,49,49,49	0
57	MG	2A	3687	1/1	0.91	0.16	49,49,49,49	0
57	MG	1A	3586	1/1	0.91	0.13	53,53,53,53	0
57	MG	1A	3524	1/1	0.91	0.15	39,39,39,39	0
57	MG	2a	3136	1/1	0.91	0.16	50,50,50,50	0
57	MG	1a	1864	1/1	0.91	0.07	59,59,59,59	0
57	MG	1a	1866	1/1	0.91	0.16	46,46,46,46	0
57	MG	2A	3491	1/1	0.91	0.07	56,56,56,56	0
57	MG	1a	1867	1/1	0.91	0.14	52,52,52,52	0
57	MG	2A	3290	1/1	0.91	0.28	48,48,48,48	0
57	MG	2A	3291	1/1	0.91	0.12	37,37,37,37	0
57	MG	2A	3701	1/1	0.91	0.11	50,50,50,50	0
57	MG	2A	3111	1/1	0.91	0.18	63,63,63,63	0
57	MG	1a	1731	1/1	0.91	0.10	55,55,55,55	0
57	MG	1A	3793	1/1	0.91	0.15	44,44,44,44	0
57	MG	1A	3718	1/1	0.91	0.14	60,60,60,60	0
57	MG	1A	3592	1/1	0.91	0.13	29,29,29,29	0
57	MG	1A	3655	1/1	0.91	0.17	39,39,39,39	0
57	MG	1A	3804	1/1	0.91	0.17	51,51,51,51	0
57	MG	1a	1743	1/1	0.91	0.20	50,50,50,50	0
57	MG	2A	3312	1/1	0.91	0.16	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1877	1/1	0.91	0.23	67,67,67,67	0
57	MG	1b	301	1/1	0.91	0.14	67,67,67,67	0
57	MG	2A	3727	1/1	0.91	0.08	54,54,54,54	0
57	MG	1A	3351	1/1	0.91	0.23	37,37,37,37	0
57	MG	1F	310	1/1	0.91	0.12	31,31,31,31	0
57	MG	1A	3132	1/1	0.91	0.49	41,41,41,41	0
57	MG	1a	1650	1/1	0.91	0.14	53,53,53,53	0
57	MG	2a	3171	1/1	0.91	0.15	59,59,59,59	0
57	MG	1F	316	1/1	0.91	0.11	32,32,32,32	0
57	MG	1A	3259	1/1	0.91	0.21	61,61,61,61	0
57	MG	1a	1758	1/1	0.91	0.09	66,66,66,66	0
57	MG	2B	202	1/1	0.91	0.15	59,59,59,59	0
57	MG	2A	3534	1/1	0.91	0.13	55,55,55,55	0
57	MG	2A	3536	1/1	0.91	0.11	71,71,71,71	0
57	MG	1A	3666	1/1	0.91	0.19	42,42,42,42	0
57	MG	1A	3731	1/1	0.91	0.16	35,35,35,35	0
57	MG	1A	3920	1/1	0.91	0.19	25,25,25,25	0
57	MG	2A	3542	1/1	0.91	0.16	54,54,54,54	0
57	MG	1A	3817	1/1	0.91	0.10	59,59,59,59	0
57	MG	1O	201	1/1	0.91	0.16	45,45,45,45	0
57	MG	2A	3555	1/1	0.91	0.09	56,56,56,56	0
57	MG	1a	1773	1/1	0.91	0.12	63,63,63,63	0
57	MG	1A	3393	1/1	0.91	0.16	56,56,56,56	0
57	MG	1A	3735	1/1	0.91	0.19	34,34,34,34	0
57	MG	1Q	202	1/1	0.91	0.20	43,43,43,43	0
57	MG	2D	309	1/1	0.91	0.21	64,64,64,64	0
57	MG	2A	3002	1/1	0.91	0.11	54,54,54,54	0
57	MG	2A	3369	1/1	0.91	0.10	51,51,51,51	0
57	MG	2A	3370	1/1	0.91	0.19	60,60,60,60	0
57	MG	2G	3301	1/1	0.91	0.14	68,68,68,68	0
57	MG	2A	3372	1/1	0.91	0.14	61,61,61,61	0
57	MG	2A	3003	1/1	0.91	0.27	58,58,58,58	0
57	MG	2P	203	1/1	0.91	0.21	64,64,64,64	0
57	MG	1A	3551	1/1	0.91	0.20	36,36,36,36	0
57	MG	2A	3006	1/1	0.91	0.15	43,43,43,43	0
57	MG	1A	3144	1/1	0.91	0.21	35,35,35,35	0
57	MG	1A	3336	1/1	0.92	0.39	65,65,65,65	0
57	MG	2A	3579	1/1	0.92	0.08	44,44,44,44	0
57	MG	1A	3199	1/1	0.92	0.34	56,56,56,56	0
57	MG	1a	1775	1/1	0.92	0.13	57,57,57,57	0
57	MG	2U	201	1/1	0.92	0.14	48,48,48,48	0
57	MG	1a	1776	1/1	0.92	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3583	1/1	0.92	0.10	50,50,50,50	0
57	MG	2A	3584	1/1	0.92	0.10	43,43,43,43	0
57	MG	1A	3628	1/1	0.92	0.13	45,45,45,45	0
57	MG	2a	3001	1/1	0.92	0.30	50,50,50,50	0
57	MG	1A	3839	1/1	0.92	0.22	59,59,59,59	0
57	MG	2A	3587	1/1	0.92	0.12	60,60,60,60	0
57	MG	2a	3008	1/1	0.92	0.19	60,60,60,60	0
57	MG	2A	3382	1/1	0.92	0.13	65,65,65,65	0
57	MG	1A	3841	1/1	0.92	0.32	34,34,34,34	0
57	MG	2A	3385	1/1	0.92	0.15	44,44,44,44	0
57	MG	1A	3952	1/1	0.92	0.17	55,55,55,55	0
57	MG	1A	3953	1/1	0.92	0.24	53,53,53,53	0
57	MG	1A	3629	1/1	0.92	0.20	39,39,39,39	0
57	MG	2A	3027	1/1	0.92	0.16	50,50,50,50	0
57	MG	1A	3441	1/1	0.92	0.29	34,34,34,34	0
57	MG	1E	308	1/1	0.92	0.16	48,48,48,48	0
57	MG	2A	3032	1/1	0.92	0.20	51,51,51,51	0
57	MG	1A	3632	1/1	0.92	0.09	53,53,53,53	0
57	MG	1A	3852	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	3542	1/1	0.92	0.14	24,24,24,24	0
57	MG	2A	3611	1/1	0.92	0.07	36,36,36,36	0
57	MG	1A	3858	1/1	0.92	0.19	49,49,49,49	0
57	MG	2A	3613	1/1	0.92	0.17	50,50,50,50	0
57	MG	1A	3125	1/1	0.92	0.32	58,58,58,58	0
57	MG	2A	3401	1/1	0.92	0.09	57,57,57,57	0
57	MG	2A	3209	1/1	0.92	0.25	56,56,56,56	0
57	MG	1A	3970	1/1	0.92	0.14	48,48,48,48	0
57	MG	2a	3040	1/1	0.92	0.15	57,57,57,57	0
57	MG	1a	1800	1/1	0.92	0.13	60,60,60,60	0
57	MG	1a	1801	1/1	0.92	0.08	52,52,52,52	0
57	MG	2a	3045	1/1	0.92	0.17	65,65,65,65	0
57	MG	1A	3861	1/1	0.92	0.16	53,53,53,53	0
57	MG	2A	3415	1/1	0.92	0.18	56,56,56,56	0
57	MG	1G	203	1/1	0.92	0.09	58,58,58,58	0
57	MG	1A	3090	1/1	0.92	0.14	42,42,42,42	0
57	MG	1A	3278	1/1	0.92	0.14	42,42,42,42	0
57	MG	1A	3978	1/1	0.92	0.17	55,55,55,55	0
57	MG	1A	3346	1/1	0.92	0.14	33,33,33,33	0
57	MG	2a	3058	1/1	0.92	0.08	67,67,67,67	0
57	MG	1a	1816	1/1	0.92	0.12	58,58,58,58	0
57	MG	2A	3225	1/1	0.92	0.19	54,54,54,54	0
57	MG	2A	3635	1/1	0.92	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3742	1/1	0.92	0.22	39,39,39,39	0
57	MG	1A	3452	1/1	0.92	0.16	30,30,30,30	0
57	MG	1a	1824	1/1	0.92	0.16	68,68,68,68	0
57	MG	2a	3065	1/1	0.92	0.09	62,62,62,62	0
57	MG	1A	3651	1/1	0.92	0.31	37,37,37,37	0
57	MG	2A	3064	1/1	0.92	0.14	37,37,37,37	0
57	MG	1Q	204	1/1	0.92	0.22	53,53,53,53	0
57	MG	1A	3750	1/1	0.92	0.08	49,49,49,49	0
57	MG	1A	3881	1/1	0.92	0.20	34,34,34,34	0
57	MG	1A	3991	1/1	0.92	0.10	52,52,52,52	0
57	MG	2a	3073	1/1	0.92	0.19	44,44,44,44	0
57	MG	1A	3310	1/1	0.92	0.18	34,34,34,34	0
57	MG	1T	204	1/1	0.92	0.07	60,60,60,60	0
57	MG	2A	3446	1/1	0.92	0.37	64,64,64,64	0
57	MG	1A	3174	1/1	0.92	0.18	38,38,38,38	0
57	MG	1V	206	1/1	0.92	0.29	56,56,56,56	0
57	MG	1A	3659	1/1	0.92	0.21	30,30,30,30	0
57	MG	2A	3249	1/1	0.92	0.56	49,49,49,49	0
57	MG	1A	3576	1/1	0.92	0.18	43,43,43,43	0
57	MG	1A	3091	1/1	0.92	0.12	35,35,35,35	0
57	MG	2A	3255	1/1	0.92	0.16	39,39,39,39	0
57	MG	2a	3095	1/1	0.92	0.17	64,64,64,64	0
57	MG	1a	1844	1/1	0.92	0.07	64,64,64,64	0
57	MG	2A	3258	1/1	0.92	0.12	47,47,47,47	0
57	MG	1A	3404	1/1	0.92	0.12	31,31,31,31	0
57	MG	1l	105	1/1	0.92	0.13	28,28,28,28	0
57	MG	2a	3107	1/1	0.92	0.10	57,57,57,57	0
57	MG	1A	3405	1/1	0.92	0.16	41,41,41,41	0
57	MG	1A	3363	1/1	0.92	0.21	38,38,38,38	0
57	MG	2A	3674	1/1	0.92	0.15	44,44,44,44	0
57	MG	2A	3468	1/1	0.92	0.12	61,61,61,61	0
57	MG	1a	1710	1/1	0.92	0.28	52,52,52,52	0
57	MG	1A	3050	1/1	0.92	0.18	38,38,38,38	0
57	MG	1A	3159	1/1	0.92	0.20	35,35,35,35	0
57	MG	1A	3470	1/1	0.92	0.11	60,60,60,60	0
57	MG	2A	3475	1/1	0.92	0.45	70,70,70,70	0
57	MG	2A	3100	1/1	0.92	0.09	53,53,53,53	0
57	MG	2A	3101	1/1	0.92	0.13	50,50,50,50	0
57	MG	2A	3686	1/1	0.92	0.09	41,41,41,41	0
57	MG	1A	3316	1/1	0.92	0.28	33,33,33,33	0
57	MG	1A	3686	1/1	0.92	0.14	36,36,36,36	0
57	MG	2A	3482	1/1	0.92	0.20	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3907	1/1	0.92	0.19	34,34,34,34	0
57	MG	1A	3588	1/1	0.92	0.17	42,42,42,42	0
57	MG	2A	3696	1/1	0.92	0.13	53,53,53,53	0
57	MG	1A	3910	1/1	0.92	0.12	45,45,45,45	0
57	MG	1A	3416	1/1	0.92	0.19	18,18,18,18	0
57	MG	1A	3373	1/1	0.92	0.17	21,21,21,21	0
57	MG	2A	3114	1/1	0.92	0.15	55,55,55,55	0
57	MG	1A	3374	1/1	0.92	0.19	25,25,25,25	0
57	MG	2A	3296	1/1	0.92	0.16	60,60,60,60	0
57	MG	1A	3160	1/1	0.92	0.19	37,37,37,37	0
57	MG	1A	3099	1/1	0.92	0.16	43,43,43,43	0
57	MG	2A	3299	1/1	0.92	0.16	38,38,38,38	0
57	MG	2A	3506	1/1	0.92	0.13	57,57,57,57	0
57	MG	2A	3304	1/1	0.92	0.08	49,49,49,49	0
57	MG	1A	3502	1/1	0.92	0.20	24,24,24,24	0
57	MG	2A	3123	1/1	0.92	0.28	49,49,49,49	0
57	MG	2A	3127	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	3504	1/1	0.92	0.15	25,25,25,25	0
57	MG	2A	3516	1/1	0.92	0.08	65,65,65,65	0
57	MG	1A	3923	1/1	0.92	0.16	26,26,26,26	0
57	MG	1a	1878	1/1	0.92	0.13	57,57,57,57	0
57	MG	1A	3808	1/1	0.92	0.12	48,48,48,48	0
57	MG	1A	3809	1/1	0.92	0.14	64,64,64,64	0
57	MG	1B	208	1/1	0.92	0.15	41,41,41,41	0
57	MG	2a	3173	1/1	0.92	0.12	63,63,63,63	0
57	MG	2A	3328	1/1	0.92	0.14	54,54,54,54	0
57	MG	1A	3426	1/1	0.92	0.17	41,41,41,41	0
57	MG	1A	3427	1/1	0.92	0.30	39,39,39,39	0
57	MG	1a	1634	1/1	0.92	0.13	47,47,47,47	0
57	MG	1A	3117	1/1	0.92	0.21	31,31,31,31	0
57	MG	2A	3149	1/1	0.92	0.27	53,53,53,53	0
57	MG	1g	3101	1/1	0.92	0.22	52,52,52,52	0
57	MG	1a	1753	1/1	0.92	0.12	60,60,60,60	0
57	MG	2A	3349	1/1	0.92	0.16	44,44,44,44	0
57	MG	1A	3512	1/1	0.92	0.11	40,40,40,40	0
57	MG	1A	3431	1/1	0.92	0.21	37,37,37,37	0
57	MG	2A	3548	1/1	0.92	0.11	44,44,44,44	0
57	MG	2A	3360	1/1	0.92	0.11	63,63,63,63	0
57	MG	1A	3331	1/1	0.92	0.21	59,59,59,59	0
57	MG	2A	3552	1/1	0.92	0.13	50,50,50,50	0
57	MG	2A	3554	1/1	0.92	0.13	52,52,52,52	0
57	MG	1a	1761	1/1	0.92	0.09	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2p	101	1/1	0.92	0.13	37,37,37,37	0
57	MG	1A	3942	1/1	0.92	0.17	49,49,49,49	0
57	MG	2D	310	1/1	0.92	0.14	42,42,42,42	0
57	MG	1A	3522	1/1	0.92	0.16	27,27,27,27	0
57	MG	2A	3365	1/1	0.92	0.13	65,65,65,65	0
57	MG	1y	202	1/1	0.92	0.19	51,51,51,51	0
57	MG	2A	3368	1/1	0.92	0.16	37,37,37,37	0
57	MG	1a	1767	1/1	0.92	0.13	56,56,56,56	0
57	MG	1B	229	1/1	0.92	0.22	58,58,58,58	0
57	MG	2P	202	1/1	0.92	0.08	41,41,41,41	0
57	MG	1A	3064	1/1	0.92	0.17	35,35,35,35	0
57	MG	2A	3576	1/1	0.92	0.15	51,51,51,51	0
57	MG	1A	3702	1/1	0.93	0.07	41,41,41,41	0
57	MG	2A	3391	1/1	0.93	0.17	58,58,58,58	0
57	MG	1A	3498	1/1	0.93	0.14	42,42,42,42	0
57	MG	2A	3201	1/1	0.93	0.07	54,54,54,54	0
57	MG	1A	3831	1/1	0.93	0.21	40,40,40,40	0
57	MG	2A	3595	1/1	0.93	0.13	46,46,46,46	0
57	MG	1A	3704	1/1	0.93	0.18	51,51,51,51	0
57	MG	1A	3258	1/1	0.93	0.34	42,42,42,42	0
57	MG	1A	3503	1/1	0.93	0.12	44,44,44,44	0
57	MG	1A	3835	1/1	0.93	0.28	37,37,37,37	0
57	MG	2A	3042	1/1	0.93	0.15	53,53,53,53	0
57	MG	2A	3212	1/1	0.93	0.16	47,47,47,47	0
57	MG	2A	3214	1/1	0.93	0.20	71,71,71,71	0
57	MG	2A	3607	1/1	0.93	0.06	56,56,56,56	0
57	MG	1A	3709	1/1	0.93	0.32	42,42,42,42	0
57	MG	1a	1667	1/1	0.93	0.18	74,74,74,74	0
57	MG	1A	3029	1/1	0.93	0.20	30,30,30,30	0
57	MG	1A	3077	1/1	0.93	0.31	28,28,28,28	0
57	MG	1A	3965	1/1	0.93	0.20	47,47,47,47	0
57	MG	1A	3507	1/1	0.93	0.16	49,49,49,49	0
57	MG	1A	3614	1/1	0.93	0.13	51,51,51,51	0
57	MG	2a	3030	1/1	0.93	0.11	63,63,63,63	0
57	MG	1A	3340	1/1	0.93	0.10	32,32,32,32	0
57	MG	1A	3388	1/1	0.93	0.12	49,49,49,49	0
57	MG	1A	3341	1/1	0.93	0.21	36,36,36,36	0
57	MG	1A	3859	1/1	0.93	0.20	15,15,15,15	0
57	MG	1a	1819	1/1	0.93	0.14	57,57,57,57	0
57	MG	1a	1821	1/1	0.93	0.15	73,73,73,73	0
57	MG	1A	3230	1/1	0.93	0.20	29,29,29,29	0
57	MG	2A	3233	1/1	0.93	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3268	1/1	0.93	0.13	31,31,31,31	0
57	MG	1A	3862	1/1	0.93	0.14	40,40,40,40	0
57	MG	1A	3270	1/1	0.93	0.16	27,27,27,27	0
57	MG	1A	3626	1/1	0.93	0.23	35,35,35,35	0
57	MG	2A	3072	1/1	0.93	0.23	32,32,32,32	0
57	MG	1a	1831	1/1	0.93	0.20	59,59,59,59	0
57	MG	1A	3983	1/1	0.93	0.16	39,39,39,39	0
57	MG	1A	3305	1/1	0.93	0.17	39,39,39,39	0
57	MG	1A	3348	1/1	0.93	0.23	43,43,43,43	0
57	MG	1A	3451	1/1	0.93	0.11	57,57,57,57	0
57	MG	1A	3737	1/1	0.93	0.15	27,27,27,27	0
57	MG	2A	3448	1/1	0.93	0.06	51,51,51,51	0
57	MG	1A	3535	1/1	0.93	0.09	53,53,53,53	0
57	MG	1A	3537	1/1	0.93	0.24	40,40,40,40	0
57	MG	1A	3397	1/1	0.93	0.17	38,38,38,38	0
57	MG	1a	1697	1/1	0.93	0.19	55,55,55,55	0
57	MG	1U	203	1/1	0.93	0.39	55,55,55,55	0
57	MG	1A	3743	1/1	0.93	0.23	38,38,38,38	0
57	MG	1a	1701	1/1	0.93	0.26	51,51,51,51	0
57	MG	1A	3231	1/1	0.93	0.18	40,40,40,40	0
57	MG	1a	1849	1/1	0.93	0.12	63,63,63,63	0
57	MG	1A	3051	1/1	0.93	0.18	35,35,35,35	0
57	MG	2A	3661	1/1	0.93	0.14	38,38,38,38	0
57	MG	1A	3999	1/1	0.93	0.15	23,23,23,23	0
57	MG	2A	3278	1/1	0.93	0.09	55,55,55,55	0
57	MG	2A	3467	1/1	0.93	0.09	60,60,60,60	0
57	MG	1A	3056	1/1	0.93	0.19	41,41,41,41	0
57	MG	2A	3102	1/1	0.93	0.26	50,50,50,50	0
57	MG	2a	3084	1/1	0.93	0.26	54,54,54,54	0
57	MG	2A	3281	1/1	0.93	0.21	56,56,56,56	0
57	MG	2A	3670	1/1	0.93	0.07	41,41,41,41	0
57	MG	1a	1711	1/1	0.93	0.14	44,44,44,44	0
57	MG	1A	4001	1/1	0.93	0.16	28,28,28,28	0
57	MG	2a	3091	1/1	0.93	0.21	70,70,70,70	0
57	MG	1A	3137	1/1	0.93	0.24	30,30,30,30	0
57	MG	1A	3557	1/1	0.93	0.18	31,31,31,31	0
57	MG	1A	3365	1/1	0.93	0.21	33,33,33,33	0
57	MG	2A	3289	1/1	0.93	0.14	46,46,46,46	0
57	MG	19	103	1/1	0.93	0.11	55,55,55,55	0
57	MG	1A	3652	1/1	0.93	0.22	41,41,41,41	0
57	MG	1A	3767	1/1	0.93	0.17	29,29,29,29	0
57	MG	1a	1606	1/1	0.93	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3366	1/1	0.93	0.12	60,60,60,60	0
57	MG	2a	3111	1/1	0.93	0.23	63,63,63,63	0
57	MG	1a	1871	1/1	0.93	0.09	63,63,63,63	0
57	MG	1A	3568	1/1	0.93	0.16	52,52,52,52	0
57	MG	2A	3122	1/1	0.93	0.12	41,41,41,41	0
57	MG	1A	3569	1/1	0.93	0.23	34,34,34,34	0
57	MG	2a	3117	1/1	0.93	0.08	65,65,65,65	0
57	MG	2a	3119	1/1	0.93	0.14	60,60,60,60	0
57	MG	1A	3191	1/1	0.93	0.23	56,56,56,56	0
57	MG	1A	3248	1/1	0.93	0.17	39,39,39,39	0
57	MG	2A	3130	1/1	0.93	0.22	45,45,45,45	0
57	MG	1A	3194	1/1	0.93	0.31	46,46,46,46	0
57	MG	2A	3505	1/1	0.93	0.12	47,47,47,47	0
57	MG	2A	3311	1/1	0.93	0.13	52,52,52,52	0
57	MG	1A	3670	1/1	0.93	0.13	52,52,52,52	0
57	MG	1a	1880	1/1	0.93	0.16	66,66,66,66	0
57	MG	2A	3510	1/1	0.93	0.10	61,61,61,61	0
57	MG	2A	3703	1/1	0.93	0.16	56,56,56,56	0
57	MG	2A	3704	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3913	1/1	0.93	0.07	43,43,43,43	0
57	MG	1a	1739	1/1	0.93	0.12	56,56,56,56	0
57	MG	1a	1741	1/1	0.93	0.10	52,52,52,52	0
57	MG	1a	1618	1/1	0.93	0.18	56,56,56,56	0
57	MG	1A	3065	1/1	0.93	0.13	53,53,53,53	0
57	MG	1A	3472	1/1	0.93	0.18	42,42,42,42	0
57	MG	1a	1746	1/1	0.93	0.09	63,63,63,63	0
57	MG	2A	3721	1/1	0.93	0.15	59,59,59,59	0
57	MG	2A	3333	1/1	0.93	0.17	42,42,42,42	0
57	MG	1A	3475	1/1	0.93	0.14	29,29,29,29	0
57	MG	2A	3724	1/1	0.93	0.18	59,59,59,59	0
57	MG	2A	3338	1/1	0.93	0.14	46,46,46,46	0
57	MG	1B	202	1/1	0.93	0.22	63,63,63,63	0
57	MG	2A	3528	1/1	0.93	0.10	54,54,54,54	0
57	MG	2a	3159	1/1	0.93	0.12	58,58,58,58	0
57	MG	1B	203	1/1	0.93	0.37	52,52,52,52	0
57	MG	2A	3530	1/1	0.93	0.19	55,55,55,55	0
57	MG	1A	3918	1/1	0.93	0.20	21,21,21,21	0
57	MG	1A	3476	1/1	0.93	0.22	22,22,22,22	0
57	MG	2A	3348	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3158	1/1	0.93	0.27	51,51,51,51	0
57	MG	1A	3681	1/1	0.93	0.11	58,58,58,58	0
57	MG	2A	3353	1/1	0.93	0.16	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3540	1/1	0.93	0.10	64,64,64,64	0
57	MG	2A	3356	1/1	0.93	0.14	46,46,46,46	0
57	MG	1A	3254	1/1	0.93	0.21	33,33,33,33	0
57	MG	1A	3424	1/1	0.93	0.19	55,55,55,55	0
57	MG	1A	3481	1/1	0.93	0.13	43,43,43,43	0
57	MG	1A	3585	1/1	0.93	0.15	36,36,36,36	0
57	MG	1a	1764	1/1	0.93	0.12	41,41,41,41	0
57	MG	1A	3690	1/1	0.93	0.09	42,42,42,42	0
57	MG	1A	3328	1/1	0.93	0.18	34,34,34,34	0
57	MG	2A	3366	1/1	0.93	0.15	37,37,37,37	0
57	MG	1a	1638	1/1	0.93	0.07	71,71,71,71	0
57	MG	1B	220	1/1	0.93	0.15	37,37,37,37	0
57	MG	2A	3562	1/1	0.93	0.20	48,48,48,48	0
57	MG	2A	3564	1/1	0.93	0.08	61,61,61,61	0
57	MG	1B	221	1/1	0.93	0.18	27,27,27,27	0
57	MG	1A	3485	1/1	0.93	0.17	44,44,44,44	0
57	MG	1A	3486	1/1	0.93	0.17	19,19,19,19	0
57	MG	2A	3015	1/1	0.93	0.16	34,34,34,34	0
57	MG	1A	3164	1/1	0.93	0.21	29,29,29,29	0
57	MG	1B	225	1/1	0.93	0.25	60,60,60,60	0
57	MG	2A	3577	1/1	0.93	0.16	47,47,47,47	0
57	MG	2A	3187	1/1	0.93	0.12	57,57,57,57	0
57	MG	1A	3332	1/1	0.93	0.14	37,37,37,37	0
57	MG	2A	3191	1/1	0.93	0.24	55,55,55,55	0
58	MPD	18	104	8/8	0.93	0.26	25,36,38,39	0
57	MG	1A	3497	1/1	0.93	0.29	32,32,32,32	0
57	MG	1A	3700	1/1	0.93	0.17	33,33,33,33	0
57	MG	2A	3196	1/1	0.93	0.16	51,51,51,51	0
57	MG	2A	3386	1/1	0.93	0.23	35,35,35,35	0
57	MG	1A	3600	1/1	0.93	0.07	35,35,35,35	0
57	MG	2V	202	1/1	0.93	0.21	46,46,46,46	0
57	MG	1D	306	1/1	0.93	0.23	38,38,38,38	0
57	MG	1W	202	1/1	0.94	0.26	40,40,40,40	0
57	MG	2A	3242	1/1	0.94	0.12	61,61,61,61	0
57	MG	1X	101	1/1	0.94	0.15	40,40,40,40	0
57	MG	2A	3246	1/1	0.94	0.20	68,68,68,68	0
57	MG	2A	3737	1/1	0.94	0.16	47,47,47,47	0
57	MG	1A	3974	1/1	0.94	0.17	45,45,45,45	0
57	MG	1A	3114	1/1	0.94	0.17	30,30,30,30	0
57	MG	1A	3251	1/1	0.94	0.25	38,38,38,38	0
57	MG	10	107	1/1	0.94	0.21	50,50,50,50	0
57	MG	1A	3061	1/1	0.94	0.32	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3031	1/1	0.94	0.20	16,16,16,16	0
57	MG	15	102	1/1	0.94	0.15	27,27,27,27	0
57	MG	2B	209	1/1	0.94	0.24	60,60,60,60	0
57	MG	2A	3257	1/1	0.94	0.18	41,41,41,41	0
57	MG	1A	3596	1/1	0.94	0.18	53,53,53,53	0
57	MG	17	103	1/1	0.94	0.18	33,33,33,33	0
57	MG	2B	214	1/1	0.94	0.14	58,58,58,58	0
57	MG	2A	3260	1/1	0.94	0.24	57,57,57,57	0
57	MG	1A	3984	1/1	0.94	0.16	25,25,25,25	0
57	MG	2B	219	1/1	0.94	0.10	59,59,59,59	0
57	MG	2D	301	1/1	0.94	0.31	42,42,42,42	0
57	MG	18	103	1/1	0.94	0.11	53,53,53,53	0
57	MG	2A	3265	1/1	0.94	0.19	27,27,27,27	0
57	MG	2D	306	1/1	0.94	0.23	38,38,38,38	0
57	MG	2D	307	1/1	0.94	0.15	42,42,42,42	0
57	MG	1A	3122	1/1	0.94	0.22	27,27,27,27	0
57	MG	1A	3986	1/1	0.94	0.17	46,46,46,46	0
57	MG	1A	3256	1/1	0.94	0.29	35,35,35,35	0
57	MG	2E	302	1/1	0.94	0.28	43,43,43,43	0
57	MG	2A	3275	1/1	0.94	0.15	48,48,48,48	0
57	MG	2A	3276	1/1	0.94	0.30	59,59,59,59	0
57	MG	1a	1605	1/1	0.94	0.13	62,62,62,62	0
57	MG	2A	3523	1/1	0.94	0.10	41,41,41,41	0
57	MG	1a	1766	1/1	0.94	0.11	62,62,62,62	0
57	MG	2N	201	1/1	0.94	0.24	55,55,55,55	0
57	MG	2A	3054	1/1	0.94	0.11	38,38,38,38	0
57	MG	1A	3163	1/1	0.94	0.16	36,36,36,36	0
57	MG	1A	3847	1/1	0.94	0.18	44,44,44,44	0
57	MG	1A	3706	1/1	0.94	0.28	45,45,45,45	0
57	MG	1A	3054	1/1	0.94	0.51	33,33,33,33	0
57	MG	1a	1610	1/1	0.94	0.16	58,58,58,58	0
57	MG	1A	3206	1/1	0.94	0.20	58,58,58,58	0
57	MG	1A	3510	1/1	0.94	0.14	37,37,37,37	0
57	MG	1A	3857	1/1	0.94	0.16	50,50,50,50	0
57	MG	1A	3711	1/1	0.94	0.18	38,38,38,38	0
57	MG	2A	3066	1/1	0.94	0.20	53,53,53,53	0
57	MG	2W	201	1/1	0.94	0.16	44,44,44,44	0
57	MG	1A	3066	1/1	0.94	0.27	40,40,40,40	0
57	MG	25	101	1/1	0.94	0.71	51,51,51,51	0
57	MG	25	103	1/1	0.94	0.18	48,48,48,48	0
57	MG	1A	3611	1/1	0.94	0.14	41,41,41,41	0
57	MG	1a	1781	1/1	0.94	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1782	1/1	0.94	0.14	54,54,54,54	0
57	MG	2a	3002	1/1	0.94	0.35	52,52,52,52	0
57	MG	1A	3717	1/1	0.94	0.15	38,38,38,38	0
57	MG	1A	3387	1/1	0.94	0.25	50,50,50,50	0
57	MG	1A	3613	1/1	0.94	0.17	57,57,57,57	0
57	MG	2A	3300	1/1	0.94	0.15	40,40,40,40	0
57	MG	2A	3302	1/1	0.94	0.14	50,50,50,50	0
57	MG	2a	3011	1/1	0.94	0.09	65,65,65,65	0
57	MG	1A	3093	1/1	0.94	0.19	34,34,34,34	0
57	MG	1A	3722	1/1	0.94	0.16	38,38,38,38	0
57	MG	2a	3015	1/1	0.94	0.26	55,55,55,55	0
57	MG	1A	3067	1/1	0.94	0.23	40,40,40,40	0
57	MG	2A	3559	1/1	0.94	0.09	45,45,45,45	0
57	MG	1a	1626	1/1	0.94	0.14	74,74,74,74	0
57	MG	1A	3129	1/1	0.94	0.22	31,31,31,31	0
57	MG	2A	3085	1/1	0.94	0.17	49,49,49,49	0
57	MG	2A	3565	1/1	0.94	0.10	59,59,59,59	0
57	MG	1A	3098	1/1	0.94	0.16	33,33,33,33	0
57	MG	1A	3728	1/1	0.94	0.14	28,28,28,28	0
57	MG	1a	1799	1/1	0.94	0.09	63,63,63,63	0
57	MG	1A	3529	1/1	0.94	0.20	22,22,22,22	0
57	MG	2A	3572	1/1	0.94	0.14	44,44,44,44	0
57	MG	2A	3322	1/1	0.94	0.23	36,36,36,36	0
57	MG	1A	3531	1/1	0.94	0.17	60,60,60,60	0
57	MG	2A	3324	1/1	0.94	0.19	64,64,64,64	0
57	MG	2a	3034	1/1	0.94	0.19	52,52,52,52	0
57	MG	1A	4014	1/1	0.94	0.10	57,57,57,57	0
57	MG	2A	3097	1/1	0.94	0.10	68,68,68,68	0
57	MG	1A	3055	1/1	0.94	0.17	27,27,27,27	0
57	MG	1A	3534	1/1	0.94	0.09	44,44,44,44	0
57	MG	1A	3456	1/1	0.94	0.14	51,51,51,51	0
57	MG	2A	3336	1/1	0.94	0.15	48,48,48,48	0
57	MG	1a	1639	1/1	0.94	0.14	60,60,60,60	0
57	MG	2a	3046	1/1	0.94	0.13	65,65,65,65	0
57	MG	1A	4022	1/1	0.94	0.11	47,47,47,47	0
57	MG	1A	3225	1/1	0.94	0.16	20,20,20,20	0
57	MG	1A	3540	1/1	0.94	0.28	48,48,48,48	0
57	MG	1a	1818	1/1	0.94	0.16	45,45,45,45	0
57	MG	2a	3051	1/1	0.94	0.18	52,52,52,52	0
57	MG	2a	3052	1/1	0.94	0.26	43,43,43,43	0
57	MG	2a	3053	1/1	0.94	0.18	48,48,48,48	0
57	MG	1A	3890	1/1	0.94	0.44	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	2A	3109	1/1	0.94	0.15	49,49,49,49	0
57	MG	2A	3350	1/1	0.94	0.19	31,31,31,31	0
57	MG	1A	4028	1/1	0.94	0.14	46,46,46,46	0
57	MG	1A	3891	1/1	0.94	0.22	55,55,55,55	0
57	MG	1A	3176	1/1	0.94	0.19	39,39,39,39	0
57	MG	1A	3741	1/1	0.94	0.20	38,38,38,38	0
57	MG	2A	3359	1/1	0.94	0.06	51,51,51,51	0
57	MG	1a	1827	1/1	0.94	0.21	62,62,62,62	0
57	MG	2A	3604	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3179	1/1	0.94	0.19	52,52,52,52	0
57	MG	1A	3897	1/1	0.94	0.13	47,47,47,47	0
57	MG	1A	3544	1/1	0.94	0.14	52,52,52,52	0
57	MG	1A	3635	1/1	0.94	0.21	20,20,20,20	0
57	MG	2A	3609	1/1	0.94	0.13	42,42,42,42	0
57	MG	1a	1833	1/1	0.94	0.13	68,68,68,68	0
57	MG	2A	3125	1/1	0.94	0.07	53,53,53,53	0
57	MG	2A	3126	1/1	0.94	0.35	45,45,45,45	0
57	MG	1A	3343	1/1	0.94	0.21	44,44,44,44	0
57	MG	1A	3282	1/1	0.94	0.14	38,38,38,38	0
57	MG	1A	3553	1/1	0.94	0.16	48,48,48,48	0
57	MG	2a	3080	1/1	0.94	0.12	55,55,55,55	0
57	MG	1B	215	1/1	0.94	0.18	58,58,58,58	0
57	MG	1B	217	1/1	0.94	0.21	56,56,56,56	0
57	MG	1B	218	1/1	0.94	0.17	52,52,52,52	0
57	MG	1a	1840	1/1	0.94	0.14	62,62,62,62	0
57	MG	1A	3908	1/1	0.94	0.09	41,41,41,41	0
57	MG	1a	1666	1/1	0.94	0.15	52,52,52,52	0
57	MG	1A	3753	1/1	0.94	0.11	44,44,44,44	0
57	MG	1A	3468	1/1	0.94	0.19	18,18,18,18	0
57	MG	2a	3093	1/1	0.94	0.17	62,62,62,62	0
57	MG	2A	3147	1/1	0.94	0.17	50,50,50,50	0
57	MG	2A	3384	1/1	0.94	0.19	58,58,58,58	0
57	MG	2a	3099	1/1	0.94	0.06	63,63,63,63	0
57	MG	1a	1669	1/1	0.94	0.27	45,45,45,45	0
57	MG	2A	3631	1/1	0.94	0.26	53,53,53,53	0
57	MG	1a	1847	1/1	0.94	0.14	64,64,64,64	0
57	MG	1A	3100	1/1	0.94	0.39	36,36,36,36	0
57	MG	2A	3634	1/1	0.94	0.12	59,59,59,59	0
57	MG	2a	3108	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	3040	1/1	0.94	0.24	33,33,33,33	0
57	MG	1A	3232	1/1	0.94	0.24	37,37,37,37	0
57	MG	1A	3563	1/1	0.94	0.23	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3769	1/1	0.94	0.19	35,35,35,35	0
57	MG	2A	3157	1/1	0.94	0.46	55,55,55,55	0
57	MG	1B	228	1/1	0.94	0.20	53,53,53,53	0
57	MG	1A	3656	1/1	0.94	0.23	52,52,52,52	0
57	MG	1A	3771	1/1	0.94	0.24	36,36,36,36	0
57	MG	1a	1860	1/1	0.94	0.10	55,55,55,55	0
57	MG	1A	3564	1/1	0.94	0.10	51,51,51,51	0
57	MG	2A	3651	1/1	0.94	0.12	50,50,50,50	0
57	MG	2A	3164	1/1	0.94	0.23	39,39,39,39	0
57	MG	1a	1863	1/1	0.94	0.14	50,50,50,50	0
57	MG	2A	3169	1/1	0.94	0.11	56,56,56,56	0
57	MG	1a	1681	1/1	0.94	0.20	48,48,48,48	0
57	MG	1A	3658	1/1	0.94	0.18	46,46,46,46	0
57	MG	1A	3565	1/1	0.94	0.26	41,41,41,41	0
57	MG	1A	3233	1/1	0.94	0.12	34,34,34,34	0
57	MG	1A	3663	1/1	0.94	0.10	44,44,44,44	0
57	MG	1A	3782	1/1	0.94	0.25	36,36,36,36	0
57	MG	2A	3418	1/1	0.94	0.10	62,62,62,62	0
57	MG	1A	3140	1/1	0.94	0.13	39,39,39,39	0
57	MG	1A	3784	1/1	0.94	0.19	40,40,40,40	0
57	MG	1A	3414	1/1	0.94	0.18	17,17,17,17	0
57	MG	1A	3789	1/1	0.94	0.16	34,34,34,34	0
57	MG	1a	1875	1/1	0.94	0.13	61,61,61,61	0
57	MG	2A	3425	1/1	0.94	0.07	55,55,55,55	0
57	MG	1A	3573	1/1	0.94	0.18	38,38,38,38	0
57	MG	2A	3428	1/1	0.94	0.22	45,45,45,45	0
57	MG	1A	3940	1/1	0.94	0.14	50,50,50,50	0
57	MG	2A	3675	1/1	0.94	0.10	42,42,42,42	0
57	MG	1A	3574	1/1	0.94	0.19	47,47,47,47	0
57	MG	1A	3360	1/1	0.94	0.17	38,38,38,38	0
57	MG	2A	3679	1/1	0.94	0.14	56,56,56,56	0
57	MG	1F	313	1/1	0.94	0.15	31,31,31,31	0
57	MG	1A	3795	1/1	0.94	0.17	33,33,33,33	0
57	MG	1A	3045	1/1	0.94	0.19	34,34,34,34	0
57	MG	1A	3480	1/1	0.94	0.10	37,37,37,37	0
57	MG	1A	3418	1/1	0.94	0.20	21,21,21,21	0
57	MG	1A	3482	1/1	0.94	0.21	59,59,59,59	0
57	MG	2a	3167	1/1	0.94	0.09	63,63,63,63	0
57	MG	1A	3236	1/1	0.94	0.21	27,27,27,27	0
57	MG	1N	202	1/1	0.94	0.14	42,42,42,42	0
57	MG	2A	3690	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3685	1/1	0.94	0.26	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3147	1/1	0.94	0.28	49,49,49,49	0
57	MG	2A	3693	1/1	0.94	0.12	35,35,35,35	0
57	MG	1A	3954	1/1	0.94	0.07	47,47,47,47	0
57	MG	1A	3245	1/1	0.94	0.30	61,61,61,61	0
57	MG	1l	202	1/1	0.94	0.25	55,55,55,55	0
57	MG	1a	1719	1/1	0.94	0.12	42,42,42,42	0
57	MG	1A	3689	1/1	0.94	0.16	54,54,54,54	0
57	MG	1o	102	1/1	0.94	0.27	57,57,57,57	0
57	MG	1A	3491	1/1	0.94	0.19	24,24,24,24	0
57	MG	1A	3962	1/1	0.94	0.11	36,36,36,36	0
57	MG	1A	3584	1/1	0.94	0.22	17,17,17,17	0
57	MG	1A	3814	1/1	0.94	0.07	50,50,50,50	0
57	MG	1x	101	1/1	0.94	0.12	46,46,46,46	0
57	MG	2a	3188	1/1	0.94	0.12	58,58,58,58	0
57	MG	1a	1728	1/1	0.94	0.15	39,39,39,39	0
57	MG	2a	3190	1/1	0.94	0.24	58,58,58,58	0
57	MG	1A	3816	1/1	0.94	0.07	36,36,36,36	0
57	MG	2e	201	1/1	0.94	0.32	70,70,70,70	0
57	MG	2e	202	1/1	0.94	0.12	65,65,65,65	0
57	MG	2A	3710	1/1	0.94	0.07	53,53,53,53	0
57	MG	1A	3692	1/1	0.94	0.20	59,59,59,59	0
57	MG	2A	3713	1/1	0.94	0.26	47,47,47,47	0
57	MG	2A	3004	1/1	0.94	0.17	38,38,38,38	0
57	MG	1T	203	1/1	0.94	0.12	43,43,43,43	0
57	MG	2A	3469	1/1	0.94	0.13	57,57,57,57	0
57	MG	1A	3818	1/1	0.94	0.17	36,36,36,36	0
57	MG	2A	3007	1/1	0.94	0.16	45,45,45,45	0
57	MG	1a	1734	1/1	0.94	0.11	47,47,47,47	0
57	MG	1A	3016	1/1	0.94	0.14	32,32,32,32	0
57	MG	1U	206	1/1	0.94	0.15	28,28,28,28	0
57	MG	1A	3060	1/1	0.94	0.25	36,36,36,36	0
57	MG	1A	3587	1/1	0.94	0.33	36,36,36,36	0
57	MG	2A	3019	1/1	0.94	0.22	40,40,40,40	0
57	MG	1a	1740	1/1	0.94	0.08	55,55,55,55	0
57	MG	1A	3943	1/1	0.95	0.12	29,29,29,29	0
57	MG	1A	3478	1/1	0.95	0.29	53,53,53,53	0
57	MG	2D	302	1/1	0.95	0.29	46,46,46,46	0
57	MG	2A	3517	1/1	0.95	0.18	59,59,59,59	0
57	MG	1a	1807	1/1	0.95	0.12	69,69,69,69	0
57	MG	1a	1649	1/1	0.95	0.15	35,35,35,35	0
57	MG	1A	3273	1/1	0.95	0.18	40,40,40,40	0
57	MG	1a	1811	1/1	0.95	0.11	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3005	1/1	0.95	0.25	21,21,21,21	0
57	MG	2A	3284	1/1	0.95	0.18	45,45,45,45	0
57	MG	1a	1813	1/1	0.95	0.20	61,61,61,61	0
57	MG	1a	1814	1/1	0.95	0.08	68,68,68,68	0
57	MG	1D	304	1/1	0.95	0.10	49,49,49,49	0
57	MG	2A	3288	1/1	0.95	0.14	52,52,52,52	0
57	MG	2F	303	1/1	0.95	0.22	44,44,44,44	0
57	MG	1A	3039	1/1	0.95	0.26	41,41,41,41	0
57	MG	2A	3086	1/1	0.95	0.21	50,50,50,50	0
57	MG	2I	201	1/1	0.95	0.12	52,52,52,52	0
57	MG	2A	3088	1/1	0.95	0.13	38,38,38,38	0
57	MG	2O	201	1/1	0.95	0.17	47,47,47,47	0
57	MG	2A	3089	1/1	0.95	0.23	48,48,48,48	0
57	MG	1D	311	1/1	0.95	0.18	42,42,42,42	0
57	MG	2A	3537	1/1	0.95	0.17	52,52,52,52	0
57	MG	1A	3948	1/1	0.95	0.23	53,53,53,53	0
57	MG	1D	314	1/1	0.95	0.20	38,38,38,38	0
57	MG	1A	3239	1/1	0.95	0.51	39,39,39,39	0
57	MG	1a	1823	1/1	0.95	0.08	64,64,64,64	0
57	MG	2A	3095	1/1	0.95	0.15	51,51,51,51	0
57	MG	2A	3546	1/1	0.95	0.21	37,37,37,37	0
57	MG	2V	201	1/1	0.95	0.25	67,67,67,67	0
57	MG	1A	3820	1/1	0.95	0.12	52,52,52,52	0
57	MG	1A	3279	1/1	0.95	0.21	38,38,38,38	0
57	MG	1A	3484	1/1	0.95	0.11	43,43,43,43	0
57	MG	2Y	201	1/1	0.95	0.26	45,45,45,45	0
57	MG	20	102	1/1	0.95	0.19	58,58,58,58	0
57	MG	2A	3551	1/1	0.95	0.08	63,63,63,63	0
57	MG	1A	3329	1/1	0.95	0.19	43,43,43,43	0
57	MG	1A	3330	1/1	0.95	0.16	37,37,37,37	0
57	MG	1A	3636	1/1	0.95	0.16	38,38,38,38	0
57	MG	27	101	1/1	0.95	0.28	40,40,40,40	0
57	MG	2A	3310	1/1	0.95	0.08	52,52,52,52	0
57	MG	1A	3488	1/1	0.95	0.20	51,51,51,51	0
57	MG	1A	3208	1/1	0.95	0.14	50,50,50,50	0
57	MG	1F	302	1/1	0.95	0.14	23,23,23,23	0
57	MG	1a	1672	1/1	0.95	0.22	57,57,57,57	0
57	MG	2A	3318	1/1	0.95	0.16	68,68,68,68	0
57	MG	1F	304	1/1	0.95	0.31	36,36,36,36	0
57	MG	1A	3571	1/1	0.95	0.22	41,41,41,41	0
57	MG	1A	3642	1/1	0.95	0.15	51,51,51,51	0
57	MG	1F	311	1/1	0.95	0.25	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3434	1/1	0.95	0.20	33,33,33,33	0
57	MG	2a	3014	1/1	0.95	0.27	54,54,54,54	0
57	MG	1A	3645	1/1	0.95	0.21	28,28,28,28	0
57	MG	1A	3009	1/1	0.95	0.15	22,22,22,22	0
57	MG	1A	3647	1/1	0.95	0.18	39,39,39,39	0
57	MG	1A	3649	1/1	0.95	0.21	41,41,41,41	0
57	MG	1A	3851	1/1	0.95	0.15	32,32,32,32	0
57	MG	2A	3335	1/1	0.95	0.15	34,34,34,34	0
57	MG	2A	3119	1/1	0.95	0.19	43,43,43,43	0
57	MG	2A	3120	1/1	0.95	0.13	57,57,57,57	0
57	MG	1G	204	1/1	0.95	0.18	45,45,45,45	0
57	MG	1A	3436	1/1	0.95	0.16	26,26,26,26	0
57	MG	2A	3124	1/1	0.95	0.19	54,54,54,54	0
57	MG	2A	3344	1/1	0.95	0.15	32,32,32,32	0
57	MG	1A	3973	1/1	0.95	0.15	55,55,55,55	0
57	MG	1a	1850	1/1	0.95	0.13	59,59,59,59	0
57	MG	1A	3739	1/1	0.95	0.25	31,31,31,31	0
57	MG	1A	3856	1/1	0.95	0.15	41,41,41,41	0
57	MG	1A	3182	1/1	0.95	0.42	36,36,36,36	0
57	MG	2a	3036	1/1	0.95	0.12	46,46,46,46	0
57	MG	1a	1855	1/1	0.95	0.07	51,51,51,51	0
57	MG	2A	3354	1/1	0.95	0.11	39,39,39,39	0
57	MG	2a	3039	1/1	0.95	0.08	71,71,71,71	0
57	MG	1A	3653	1/1	0.95	0.15	28,28,28,28	0
57	MG	1A	3386	1/1	0.95	0.20	24,24,24,24	0
57	MG	1A	3335	1/1	0.95	0.21	23,23,23,23	0
57	MG	2a	3044	1/1	0.95	0.23	56,56,56,56	0
57	MG	1a	1859	1/1	0.95	0.18	49,49,49,49	0
57	MG	2A	3140	1/1	0.95	0.19	47,47,47,47	0
57	MG	1A	3094	1/1	0.95	0.22	25,25,25,25	0
57	MG	2A	3143	1/1	0.95	0.21	56,56,56,56	0
57	MG	1A	3746	1/1	0.95	0.15	48,48,48,48	0
57	MG	1A	3747	1/1	0.95	0.16	34,34,34,34	0
57	MG	1R	203	1/1	0.95	0.24	45,45,45,45	0
57	MG	1a	1865	1/1	0.95	0.33	66,66,66,66	0
57	MG	1A	3161	1/1	0.95	0.15	22,22,22,22	0
57	MG	2a	3054	1/1	0.95	0.23	38,38,38,38	0
57	MG	1A	3749	1/1	0.95	0.14	47,47,47,47	0
57	MG	2A	3151	1/1	0.95	0.11	53,53,53,53	0
57	MG	2A	3152	1/1	0.95	0.17	46,46,46,46	0
57	MG	1A	3250	1/1	0.95	0.22	35,35,35,35	0
57	MG	1a	1707	1/1	0.95	0.16	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	1708	1/1	0.95	0.23	52,52,52,52	0
57	MG	1A	3870	1/1	0.95	0.12	19,19,19,19	0
57	MG	2A	3377	1/1	0.95	0.10	36,36,36,36	0
57	MG	1U	201	1/1	0.95	0.15	27,27,27,27	0
57	MG	1A	3062	1/1	0.95	0.16	33,33,33,33	0
57	MG	1A	3220	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3293	1/1	0.95	0.08	76,76,76,76	0
57	MG	1A	3759	1/1	0.95	0.14	50,50,50,50	0
57	MG	1a	1717	1/1	0.95	0.17	67,67,67,67	0
57	MG	1V	207	1/1	0.95	0.20	46,46,46,46	0
57	MG	1a	1879	1/1	0.95	0.14	65,65,65,65	0
57	MG	2A	3167	1/1	0.95	0.18	43,43,43,43	0
57	MG	1W	201	1/1	0.95	0.35	45,45,45,45	0
57	MG	2a	3074	1/1	0.95	0.22	53,53,53,53	0
57	MG	1A	3761	1/1	0.95	0.28	47,47,47,47	0
57	MG	1A	3998	1/1	0.95	0.10	38,38,38,38	0
57	MG	1d	303	1/1	0.95	0.10	56,56,56,56	0
57	MG	1A	3762	1/1	0.95	0.34	59,59,59,59	0
57	MG	2a	3081	1/1	0.95	0.12	54,54,54,54	0
57	MG	2A	3637	1/1	0.95	0.14	59,59,59,59	0
57	MG	1a	1725	1/1	0.95	0.12	74,74,74,74	0
57	MG	2A	3176	1/1	0.95	0.25	44,44,44,44	0
57	MG	2A	3177	1/1	0.95	0.19	50,50,50,50	0
57	MG	10	101	1/1	0.95	0.20	31,31,31,31	0
57	MG	10	103	1/1	0.95	0.18	36,36,36,36	0
57	MG	1A	3511	1/1	0.95	0.21	48,48,48,48	0
57	MG	2A	3645	1/1	0.95	0.11	34,34,34,34	0
57	MG	2A	3183	1/1	0.95	0.13	46,46,46,46	0
57	MG	2A	3402	1/1	0.95	0.22	48,48,48,48	0
57	MG	1f	202	1/1	0.95	0.15	52,52,52,52	0
57	MG	1A	3082	1/1	0.95	0.25	41,41,41,41	0
57	MG	2A	3405	1/1	0.95	0.23	61,61,61,61	0
57	MG	2A	3406	1/1	0.95	0.16	39,39,39,39	0
57	MG	1A	3766	1/1	0.95	0.18	34,34,34,34	0
57	MG	2A	3657	1/1	0.95	0.10	51,51,51,51	0
57	MG	11	102	1/1	0.95	0.17	52,52,52,52	0
57	MG	1A	3518	1/1	0.95	0.10	53,53,53,53	0
57	MG	2A	3413	1/1	0.95	0.12	42,42,42,42	0
57	MG	2A	3414	1/1	0.95	0.06	52,52,52,52	0
57	MG	2A	3189	1/1	0.95	0.10	49,49,49,49	0
57	MG	2A	3416	1/1	0.95	0.24	50,50,50,50	0
57	MG	2A	3190	1/1	0.95	0.17	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3519	1/1	0.95	0.18	39,39,39,39	0
57	MG	13	101	1/1	0.95	0.17	26,26,26,26	0
57	MG	2a	3118	1/1	0.95	0.18	60,60,60,60	0
57	MG	1A	3224	1/1	0.95	0.14	53,53,53,53	0
57	MG	1A	3142	1/1	0.95	0.19	39,39,39,39	0
57	MG	15	108	1/1	0.95	0.17	47,47,47,47	0
57	MG	1A	3166	1/1	0.95	0.30	49,49,49,49	0
57	MG	1A	3895	1/1	0.95	0.10	43,43,43,43	0
57	MG	18	102	1/1	0.95	0.22	42,42,42,42	0
57	MG	1A	4009	1/1	0.95	0.15	43,43,43,43	0
57	MG	2A	3430	1/1	0.95	0.16	55,55,55,55	0
57	MG	2a	3130	1/1	0.95	0.12	68,68,68,68	0
57	MG	19	101	1/1	0.95	0.26	46,46,46,46	0
57	MG	2A	3206	1/1	0.95	0.14	40,40,40,40	0
57	MG	1A	3594	1/1	0.95	0.25	23,23,23,23	0
57	MG	1A	3143	1/1	0.95	0.26	18,18,18,18	0
57	MG	1A	3597	1/1	0.95	0.26	33,33,33,33	0
57	MG	1A	3777	1/1	0.95	0.23	39,39,39,39	0
57	MG	1A	4017	1/1	0.95	0.16	51,51,51,51	0
57	MG	1A	4018	1/1	0.95	0.13	41,41,41,41	0
57	MG	2a	3143	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3598	1/1	0.95	0.27	45,45,45,45	0
57	MG	1A	3303	1/1	0.95	0.21	31,31,31,31	0
57	MG	2A	3013	1/1	0.95	0.17	27,27,27,27	0
57	MG	1A	3903	1/1	0.95	0.16	45,45,45,45	0
57	MG	2a	3149	1/1	0.95	0.09	52,52,52,52	0
57	MG	1A	3526	1/1	0.95	0.15	22,22,22,22	0
57	MG	1A	3359	1/1	0.95	0.13	30,30,30,30	0
57	MG	1A	3409	1/1	0.95	0.19	20,20,20,20	0
57	MG	1A	3786	1/1	0.95	0.20	24,24,24,24	0
57	MG	2A	3020	1/1	0.95	0.13	45,45,45,45	0
57	MG	1A	3787	1/1	0.95	0.12	35,35,35,35	0
57	MG	1A	3466	1/1	0.95	0.18	39,39,39,39	0
57	MG	2A	3026	1/1	0.95	0.18	46,46,46,46	0
57	MG	2A	3229	1/1	0.95	0.15	43,43,43,43	0
57	MG	2A	3458	1/1	0.95	0.17	47,47,47,47	0
57	MG	1a	1768	1/1	0.95	0.10	64,64,64,64	0
57	MG	1A	3607	1/1	0.95	0.22	59,59,59,59	0
57	MG	2a	3165	1/1	0.95	0.11	53,53,53,53	0
57	MG	1A	3197	1/1	0.95	0.26	45,45,45,45	0
57	MG	1a	1771	1/1	0.95	0.20	51,51,51,51	0
57	MG	2A	3707	1/1	0.95	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3412	1/1	0.95	0.17	33,33,33,33	0
57	MG	1A	3792	1/1	0.95	0.23	17,17,17,17	0
57	MG	2a	3172	1/1	0.95	0.07	62,62,62,62	0
57	MG	1A	3696	1/1	0.95	0.07	55,55,55,55	0
57	MG	2A	3712	1/1	0.95	0.13	62,62,62,62	0
57	MG	1A	3307	1/1	0.95	0.11	34,34,34,34	0
57	MG	1A	3797	1/1	0.95	0.18	38,38,38,38	0
57	MG	1a	1627	1/1	0.95	0.19	50,50,50,50	0
57	MG	1B	211	1/1	0.95	0.29	42,42,42,42	0
57	MG	2A	3720	1/1	0.95	0.10	40,40,40,40	0
57	MG	1A	3063	1/1	0.95	0.09	44,44,44,44	0
57	MG	2A	3245	1/1	0.95	0.11	60,60,60,60	0
57	MG	1A	3262	1/1	0.95	0.27	28,28,28,28	0
57	MG	1B	214	1/1	0.95	0.20	37,37,37,37	0
57	MG	1A	3930	1/1	0.95	0.12	38,38,38,38	0
57	MG	1a	1785	1/1	0.95	0.14	63,63,63,63	0
57	MG	2A	3481	1/1	0.95	0.15	57,57,57,57	0
57	MG	1A	3802	1/1	0.95	0.17	25,25,25,25	0
57	MG	2A	3051	1/1	0.95	0.23	57,57,57,57	0
57	MG	2A	3486	1/1	0.95	0.19	53,53,53,53	0
57	MG	1A	3473	1/1	0.95	0.13	51,51,51,51	0
57	MG	1A	3041	1/1	0.95	0.26	47,47,47,47	0
57	MG	1a	1637	1/1	0.95	0.17	43,43,43,43	0
57	MG	1A	3021	1/1	0.95	0.16	36,36,36,36	0
57	MG	1A	3550	1/1	0.95	0.15	44,44,44,44	0
57	MG	2j	3201	1/1	0.95	0.07	60,60,60,60	0
57	MG	2k	201	1/1	0.95	0.12	61,61,61,61	0
57	MG	1A	3619	1/1	0.95	0.18	52,52,52,52	0
57	MG	1A	3620	1/1	0.95	0.12	48,48,48,48	0
57	MG	1A	3047	1/1	0.95	0.22	37,37,37,37	0
57	MG	2A	3264	1/1	0.95	0.16	48,48,48,48	0
57	MG	2A	3499	1/1	0.95	0.17	53,53,53,53	0
58	MPD	1T	205	8/8	0.95	0.19	52,60,64,64	0
57	MG	2A	3062	1/1	0.95	0.12	48,48,48,48	0
57	MG	1A	3941	1/1	0.95	0.09	46,46,46,46	0
57	MG	2A	3267	1/1	0.95	0.18	51,51,51,51	0
57	MG	2A	3268	1/1	0.95	0.26	21,21,21,21	0
59	ARG	1B	231	12/12	0.95	0.24	24,39,48,53	0
57	MG	1A	3552	1/1	0.95	0.12	47,47,47,47	0
57	MG	1B	227	1/1	0.95	0.14	52,52,52,52	0
57	MG	1a	1802	1/1	0.95	0.11	55,55,55,55	0
57	MG	1a	1646	1/1	0.95	0.12	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3716	1/1	0.96	0.11	38,38,38,38	0
57	MG	2A	3028	1/1	0.96	0.09	38,38,38,38	0
57	MG	2A	3236	1/1	0.96	0.11	39,39,39,39	0
57	MG	1a	1752	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3420	1/1	0.96	0.20	32,32,32,32	0
57	MG	2A	3031	1/1	0.96	0.18	36,36,36,36	0
57	MG	2B	206	1/1	0.96	0.22	42,42,42,42	0
57	MG	1A	3855	1/1	0.96	0.26	34,34,34,34	0
57	MG	1a	1756	1/1	0.96	0.21	47,47,47,47	0
57	MG	2A	3479	1/1	0.96	0.17	53,53,53,53	0
57	MG	2A	3243	1/1	0.96	0.18	49,49,49,49	0
57	MG	1a	1757	1/1	0.96	0.12	57,57,57,57	0
57	MG	15	107	1/1	0.96	0.14	54,54,54,54	0
57	MG	1A	3204	1/1	0.96	0.18	40,40,40,40	0
57	MG	1a	1760	1/1	0.96	0.16	57,57,57,57	0
57	MG	2B	216	1/1	0.96	0.21	54,54,54,54	0
57	MG	17	101	1/1	0.96	0.21	38,38,38,38	0
57	MG	2A	3488	1/1	0.96	0.21	31,31,31,31	0
57	MG	1A	3162	1/1	0.96	0.23	32,32,32,32	0
57	MG	2A	3250	1/1	0.96	0.35	55,55,55,55	0
57	MG	2A	3251	1/1	0.96	0.12	41,41,41,41	0
57	MG	1a	1763	1/1	0.96	0.14	62,62,62,62	0
57	MG	17	104	1/1	0.96	0.12	46,46,46,46	0
57	MG	2A	3254	1/1	0.96	0.21	52,52,52,52	0
57	MG	1A	3071	1/1	0.96	0.17	27,27,27,27	0
57	MG	1A	3615	1/1	0.96	0.13	41,41,41,41	0
57	MG	1A	3514	1/1	0.96	0.19	49,49,49,49	0
57	MG	2A	3500	1/1	0.96	0.15	31,31,31,31	0
57	MG	2E	303	1/1	0.96	0.07	45,45,45,45	0
57	MG	2A	3501	1/1	0.96	0.07	48,48,48,48	0
57	MG	2E	305	1/1	0.96	0.18	36,36,36,36	0
57	MG	1A	3207	1/1	0.96	0.19	39,39,39,39	0
57	MG	19	102	1/1	0.96	0.23	46,46,46,46	0
57	MG	1A	3058	1/1	0.96	0.26	25,25,25,25	0
57	MG	2F	304	1/1	0.96	0.23	49,49,49,49	0
57	MG	1A	3727	1/1	0.96	0.17	39,39,39,39	0
57	MG	1a	1772	1/1	0.96	0.27	65,65,65,65	0
57	MG	2A	3263	1/1	0.96	0.13	38,38,38,38	0
57	MG	1A	3864	1/1	0.96	0.13	25,25,25,25	0
57	MG	1a	1604	1/1	0.96	0.23	48,48,48,48	0
57	MG	1A	3266	1/1	0.96	0.12	34,34,34,34	0
57	MG	1A	3428	1/1	0.96	0.16	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3429	1/1	0.96	0.31	59,59,59,59	0
57	MG	2A	3271	1/1	0.96	0.19	26,26,26,26	0
57	MG	1A	3869	1/1	0.96	0.11	34,34,34,34	0
57	MG	2A	3063	1/1	0.96	0.15	60,60,60,60	0
57	MG	2R	201	1/1	0.96	0.17	46,46,46,46	0
57	MG	2R	202	1/1	0.96	0.17	44,44,44,44	0
57	MG	1A	3209	1/1	0.96	0.30	44,44,44,44	0
57	MG	1A	3023	1/1	0.96	0.17	33,33,33,33	0
57	MG	1A	3874	1/1	0.96	0.19	40,40,40,40	0
57	MG	1a	1612	1/1	0.96	0.19	60,60,60,60	0
57	MG	1a	1613	1/1	0.96	0.30	37,37,37,37	0
57	MG	1A	3875	1/1	0.96	0.17	47,47,47,47	0
57	MG	2A	3071	1/1	0.96	0.15	56,56,56,56	0
57	MG	2W	202	1/1	0.96	0.12	51,51,51,51	0
57	MG	1A	3624	1/1	0.96	0.25	55,55,55,55	0
57	MG	1A	3271	1/1	0.96	0.14	50,50,50,50	0
57	MG	1A	3878	1/1	0.96	0.18	31,31,31,31	0
57	MG	1A	3879	1/1	0.96	0.07	37,37,37,37	0
57	MG	25	102	1/1	0.96	0.18	41,41,41,41	0
57	MG	2A	3535	1/1	0.96	0.12	55,55,55,55	0
57	MG	1A	3049	1/1	0.96	0.15	36,36,36,36	0
57	MG	1A	3079	1/1	0.96	0.21	41,41,41,41	0
57	MG	2A	3080	1/1	0.96	0.16	50,50,50,50	0
57	MG	1A	3349	1/1	0.96	0.20	24,24,24,24	0
57	MG	1A	3350	1/1	0.96	0.19	24,24,24,24	0
57	MG	1A	3631	1/1	0.96	0.25	24,24,24,24	0
57	MG	1B	201	1/1	0.96	0.23	46,46,46,46	0
57	MG	2a	3005	1/1	0.96	0.16	52,52,52,52	0
57	MG	2a	3007	1/1	0.96	0.14	62,62,62,62	0
57	MG	2A	3543	1/1	0.96	0.09	39,39,39,39	0
57	MG	2A	3544	1/1	0.96	0.11	43,43,43,43	0
57	MG	1a	1625	1/1	0.96	0.17	42,42,42,42	0
57	MG	2A	3294	1/1	0.96	0.16	34,34,34,34	0
57	MG	2A	3087	1/1	0.96	0.14	41,41,41,41	0
57	MG	1A	3274	1/1	0.96	0.14	26,26,26,26	0
57	MG	1A	3353	1/1	0.96	0.18	37,37,37,37	0
57	MG	1A	3538	1/1	0.96	0.13	45,45,45,45	0
57	MG	1A	3213	1/1	0.96	0.14	36,36,36,36	0
57	MG	1A	3168	1/1	0.96	0.14	52,52,52,52	0
57	MG	2A	3301	1/1	0.96	0.20	21,21,21,21	0
57	MG	2a	3019	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3557	1/1	0.96	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3447	1/1	0.96	0.17	49,49,49,49	0
57	MG	1A	3215	1/1	0.96	0.22	27,27,27,27	0
57	MG	2A	3305	1/1	0.96	0.12	47,47,47,47	0
57	MG	1B	209	1/1	0.96	0.21	48,48,48,48	0
57	MG	2A	3563	1/1	0.96	0.12	49,49,49,49	0
57	MG	1a	1810	1/1	0.96	0.13	60,60,60,60	0
57	MG	1A	3216	1/1	0.96	0.18	38,38,38,38	0
57	MG	1A	3643	1/1	0.96	0.17	32,32,32,32	0
57	MG	2A	3567	1/1	0.96	0.10	55,55,55,55	0
57	MG	2A	3568	1/1	0.96	0.10	52,52,52,52	0
57	MG	1A	3548	1/1	0.96	0.18	43,43,43,43	0
57	MG	1A	3101	1/1	0.96	0.17	26,26,26,26	0
57	MG	1A	3171	1/1	0.96	0.18	24,24,24,24	0
57	MG	1A	3221	1/1	0.96	0.15	29,29,29,29	0
57	MG	2A	3315	1/1	0.96	0.09	36,36,36,36	0
57	MG	2A	3574	1/1	0.96	0.07	58,58,58,58	0
57	MG	2A	3575	1/1	0.96	0.17	39,39,39,39	0
57	MG	2A	3317	1/1	0.96	0.15	37,37,37,37	0
57	MG	1A	3102	1/1	0.96	0.16	46,46,46,46	0
57	MG	1A	3368	1/1	0.96	0.20	32,32,32,32	0
57	MG	2A	3105	1/1	0.96	0.22	45,45,45,45	0
57	MG	1A	3765	1/1	0.96	0.14	21,21,21,21	0
57	MG	1A	3457	1/1	0.96	0.13	34,34,34,34	0
57	MG	1A	3285	1/1	0.96	0.38	39,39,39,39	0
57	MG	2A	3325	1/1	0.96	0.17	58,58,58,58	0
57	MG	1A	3654	1/1	0.96	0.24	28,28,28,28	0
57	MG	1A	3288	1/1	0.96	0.16	23,23,23,23	0
57	MG	1A	3562	1/1	0.96	0.25	38,38,38,38	0
57	MG	1A	3136	1/1	0.96	0.18	33,33,33,33	0
57	MG	1A	3080	1/1	0.96	0.21	35,35,35,35	0
57	MG	1a	1830	1/1	0.96	0.09	57,57,57,57	0
57	MG	1A	3773	1/1	0.96	0.14	32,32,32,32	0
57	MG	2A	3337	1/1	0.96	0.12	45,45,45,45	0
57	MG	2A	3593	1/1	0.96	0.16	48,48,48,48	0
57	MG	2A	3594	1/1	0.96	0.14	34,34,34,34	0
57	MG	1a	1652	1/1	0.96	0.08	64,64,64,64	0
57	MG	1a	1654	1/1	0.96	0.20	42,42,42,42	0
57	MG	2A	3340	1/1	0.96	0.13	59,59,59,59	0
57	MG	2A	3598	1/1	0.96	0.10	48,48,48,48	0
57	MG	1A	3226	1/1	0.96	0.22	31,31,31,31	0
57	MG	2A	3600	1/1	0.96	0.12	41,41,41,41	0
57	MG	2A	3121	1/1	0.96	0.22	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3566	1/1	0.96	0.12	18,18,18,18	0
57	MG	2A	3603	1/1	0.96	0.13	39,39,39,39	0
57	MG	2a	3069	1/1	0.96	0.17	57,57,57,57	0
57	MG	1A	3776	1/1	0.96	0.15	35,35,35,35	0
57	MG	1A	3661	1/1	0.96	0.17	40,40,40,40	0
57	MG	1a	1660	1/1	0.96	0.16	61,61,61,61	0
57	MG	1A	3924	1/1	0.96	0.17	28,28,28,28	0
57	MG	1D	305	1/1	0.96	0.17	28,28,28,28	0
57	MG	2A	3352	1/1	0.96	0.23	57,57,57,57	0
57	MG	1a	1841	1/1	0.96	0.06	54,54,54,54	0
57	MG	1A	3926	1/1	0.96	0.18	39,39,39,39	0
57	MG	2a	3079	1/1	0.96	0.18	55,55,55,55	0
57	MG	2A	3355	1/1	0.96	0.12	35,35,35,35	0
57	MG	1D	308	1/1	0.96	0.19	14,14,14,14	0
57	MG	2A	3615	1/1	0.96	0.20	48,48,48,48	0
57	MG	1D	310	1/1	0.96	0.12	31,31,31,31	0
57	MG	2A	3358	1/1	0.96	0.14	38,38,38,38	0
57	MG	2A	3134	1/1	0.96	0.24	62,62,62,62	0
57	MG	1A	3662	1/1	0.96	0.16	34,34,34,34	0
57	MG	2A	3136	1/1	0.96	0.17	63,63,63,63	0
57	MG	2a	3090	1/1	0.96	0.25	50,50,50,50	0
57	MG	1A	3929	1/1	0.96	0.20	12,12,12,12	0
57	MG	1A	3465	1/1	0.96	0.13	36,36,36,36	0
57	MG	1A	3931	1/1	0.96	0.30	33,33,33,33	0
57	MG	1A	3781	1/1	0.96	0.15	57,57,57,57	0
57	MG	1A	3175	1/1	0.96	0.16	19,19,19,19	0
57	MG	2a	3097	1/1	0.96	0.25	60,60,60,60	0
57	MG	2A	3144	1/1	0.96	0.17	47,47,47,47	0
57	MG	1A	3665	1/1	0.96	0.14	28,28,28,28	0
57	MG	1A	3935	1/1	0.96	0.13	30,30,30,30	0
57	MG	1E	302	1/1	0.96	0.27	36,36,36,36	0
57	MG	2a	3103	1/1	0.96	0.14	47,47,47,47	0
57	MG	2a	3104	1/1	0.96	0.14	55,55,55,55	0
57	MG	1A	3138	1/1	0.96	0.13	31,31,31,31	0
57	MG	1A	3667	1/1	0.96	0.21	42,42,42,42	0
57	MG	1A	3669	1/1	0.96	0.26	56,56,56,56	0
57	MG	1E	309	1/1	0.96	0.17	32,32,32,32	0
57	MG	1A	3139	1/1	0.96	0.27	45,45,45,45	0
57	MG	1A	3024	1/1	0.96	0.18	14,14,14,14	0
57	MG	1A	3675	1/1	0.96	0.22	12,12,12,12	0
57	MG	2A	3639	1/1	0.96	0.20	50,50,50,50	0
57	MG	2A	3379	1/1	0.96	0.19	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1F	305	1/1	0.96	0.23	29,29,29,29	0
57	MG	1A	3038	1/1	0.96	0.27	34,34,34,34	0
57	MG	1A	3677	1/1	0.96	0.21	27,27,27,27	0
57	MG	1A	3052	1/1	0.96	0.16	26,26,26,26	0
57	MG	2A	3159	1/1	0.96	0.21	33,33,33,33	0
57	MG	2a	3122	1/1	0.96	0.11	57,57,57,57	0
57	MG	1A	3679	1/1	0.96	0.13	47,47,47,47	0
57	MG	2a	3124	1/1	0.96	0.19	73,73,73,73	0
57	MG	1a	1689	1/1	0.96	0.24	58,58,58,58	0
57	MG	1A	3111	1/1	0.96	0.17	26,26,26,26	0
57	MG	1F	315	1/1	0.96	0.10	46,46,46,46	0
57	MG	2A	3653	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3113	1/1	0.96	0.26	26,26,26,26	0
57	MG	2a	3131	1/1	0.96	0.10	54,54,54,54	0
57	MG	1A	3304	1/1	0.96	0.17	37,37,37,37	0
57	MG	2a	3134	1/1	0.96	0.11	66,66,66,66	0
57	MG	1A	3389	1/1	0.96	0.23	46,46,46,46	0
57	MG	2A	3168	1/1	0.96	0.11	36,36,36,36	0
57	MG	1A	3684	1/1	0.96	0.21	34,34,34,34	0
57	MG	1A	3188	1/1	0.96	0.14	32,32,32,32	0
57	MG	1A	3148	1/1	0.96	0.23	28,28,28,28	0
57	MG	1N	201	1/1	0.96	0.23	43,43,43,43	0
57	MG	1A	3309	1/1	0.96	0.27	33,33,33,33	0
57	MG	2A	3663	1/1	0.96	0.07	38,38,38,38	0
57	MG	1A	3688	1/1	0.96	0.28	33,33,33,33	0
57	MG	1A	3955	1/1	0.96	0.18	20,20,20,20	0
57	MG	1a	1705	1/1	0.96	0.14	59,59,59,59	0
57	MG	1a	1706	1/1	0.96	0.16	64,64,64,64	0
57	MG	2A	3179	1/1	0.96	0.14	49,49,49,49	0
57	MG	2A	3180	1/1	0.96	0.15	37,37,37,37	0
57	MG	1A	3026	1/1	0.96	0.18	25,25,25,25	0
57	MG	2A	3407	1/1	0.96	0.11	37,37,37,37	0
57	MG	1d	304	1/1	0.96	0.15	62,62,62,62	0
57	MG	1P	201	1/1	0.96	0.16	29,29,29,29	0
57	MG	1P	202	1/1	0.96	0.15	25,25,25,25	0
57	MG	1A	3241	1/1	0.96	0.23	31,31,31,31	0
57	MG	1e	202	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3244	1/1	0.96	0.24	63,63,63,63	0
57	MG	1a	1713	1/1	0.96	0.08	69,69,69,69	0
57	MG	2A	3417	1/1	0.96	0.15	33,33,33,33	0
57	MG	1A	3006	1/1	0.96	0.21	35,35,35,35	0
57	MG	1A	3963	1/1	0.96	0.18	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3192	1/1	0.96	0.18	32,32,32,32	0
57	MG	1A	3402	1/1	0.96	0.22	18,18,18,18	0
57	MG	2a	3168	1/1	0.96	0.28	56,56,56,56	0
57	MG	1A	3590	1/1	0.96	0.24	59,59,59,59	0
57	MG	2A	3195	1/1	0.96	0.18	48,48,48,48	0
57	MG	1A	3247	1/1	0.96	0.17	25,25,25,25	0
57	MG	1A	3489	1/1	0.96	0.24	46,46,46,46	0
57	MG	1A	3821	1/1	0.96	0.20	41,41,41,41	0
57	MG	1A	3116	1/1	0.96	0.14	32,32,32,32	0
57	MG	1o	101	1/1	0.96	0.18	59,59,59,59	0
57	MG	1A	3321	1/1	0.96	0.14	27,27,27,27	0
57	MG	1U	202	1/1	0.96	0.20	27,27,27,27	0
57	MG	1A	3196	1/1	0.96	0.26	44,44,44,44	0
57	MG	1A	3325	1/1	0.96	0.15	32,32,32,32	0
57	MG	2a	3180	1/1	0.96	0.09	63,63,63,63	0
57	MG	1U	208	1/1	0.96	0.15	30,30,30,30	0
57	MG	2A	3436	1/1	0.96	0.17	58,58,58,58	0
57	MG	1A	3007	1/1	0.96	0.24	28,28,28,28	0
57	MG	1x	102	1/1	0.96	0.16	26,26,26,26	0
57	MG	1V	205	1/1	0.96	0.13	46,46,46,46	0
57	MG	1A	3499	1/1	0.96	0.15	32,32,32,32	0
57	MG	2A	3213	1/1	0.96	0.14	38,38,38,38	0
57	MG	2A	3443	1/1	0.96	0.11	39,39,39,39	0
57	MG	1A	3501	1/1	0.96	0.19	23,23,23,23	0
57	MG	2A	3445	1/1	0.96	0.09	48,48,48,48	0
57	MG	1a	1735	1/1	0.96	0.09	49,49,49,49	0
57	MG	1A	3157	1/1	0.96	0.20	37,37,37,37	0
57	MG	1A	3836	1/1	0.96	0.17	33,33,33,33	0
57	MG	2A	3449	1/1	0.96	0.13	49,49,49,49	0
57	MG	2A	3716	1/1	0.96	0.12	55,55,55,55	0
57	MG	1A	3837	1/1	0.96	0.17	34,34,34,34	0
57	MG	2A	3008	1/1	0.96	0.23	45,45,45,45	0
57	MG	2A	3719	1/1	0.96	0.14	58,58,58,58	0
57	MG	1A	3707	1/1	0.96	0.23	45,45,45,45	0
57	MG	1A	3603	1/1	0.96	0.12	48,48,48,48	0
57	MG	2A	3222	1/1	0.96	0.14	59,59,59,59	0
57	MG	1A	3252	1/1	0.96	0.15	44,44,44,44	0
57	MG	2A	3224	1/1	0.96	0.11	51,51,51,51	0
57	MG	1A	3844	1/1	0.96	0.13	43,43,43,43	0
57	MG	1A	3989	1/1	0.96	0.16	41,41,41,41	0
57	MG	1A	3032	1/1	0.96	0.23	44,44,44,44	0
57	MG	2A	3228	1/1	0.96	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1a	1745	1/1	0.96	0.14	59,59,59,59	0
57	MG	1l	101	1/1	0.96	0.18	37,37,37,37	0
57	MG	1A	3201	1/1	0.96	0.18	46,46,46,46	0
57	MG	1A	3069	1/1	0.96	0.18	32,32,32,32	0
57	MG	1A	3124	1/1	0.96	0.26	36,36,36,36	0
57	MG	1A	3757	1/1	0.97	0.20	37,37,37,37	0
57	MG	1A	3294	1/1	0.97	0.17	31,31,31,31	0
57	MG	1A	3872	1/1	0.97	0.21	36,36,36,36	0
57	MG	1A	3126	1/1	0.97	0.16	34,34,34,34	0
57	MG	2A	3427	1/1	0.97	0.24	52,52,52,52	0
57	MG	1A	3760	1/1	0.97	0.23	42,42,42,42	0
57	MG	1A	3154	1/1	0.97	0.24	28,28,28,28	0
57	MG	1V	202	1/1	0.97	0.24	29,29,29,29	0
57	MG	1A	3298	1/1	0.97	0.20	14,14,14,14	0
57	MG	2A	3622	1/1	0.97	0.16	43,43,43,43	0
57	MG	1A	3490	1/1	0.97	0.23	45,45,45,45	0
57	MG	1a	1699	1/1	0.97	0.19	50,50,50,50	0
57	MG	1A	3419	1/1	0.97	0.17	29,29,29,29	0
57	MG	1A	3880	1/1	0.97	0.20	28,28,28,28	0
57	MG	1A	3492	1/1	0.97	0.16	45,45,45,45	0
57	MG	2a	3020	1/1	0.97	0.15	46,46,46,46	0
57	MG	1A	3155	1/1	0.97	0.23	31,31,31,31	0
57	MG	2a	3022	1/1	0.97	0.12	49,49,49,49	0
57	MG	1A	3421	1/1	0.97	0.16	45,45,45,45	0
57	MG	1A	3300	1/1	0.97	0.19	32,32,32,32	0
57	MG	2A	3440	1/1	0.97	0.15	34,34,34,34	0
57	MG	1A	3356	1/1	0.97	0.24	29,29,29,29	0
57	MG	10	102	1/1	0.97	0.13	34,34,34,34	0
57	MG	1A	3886	1/1	0.97	0.10	22,22,22,22	0
57	MG	2a	3029	1/1	0.97	0.11	51,51,51,51	0
57	MG	1A	3673	1/1	0.97	0.21	20,20,20,20	0
57	MG	1A	3888	1/1	0.97	0.15	33,33,33,33	0
57	MG	1a	1712	1/1	0.97	0.21	44,44,44,44	0
57	MG	1A	3674	1/1	0.97	0.19	55,55,55,55	0
57	MG	2A	3269	1/1	0.97	0.15	52,52,52,52	0
57	MG	1A	3358	1/1	0.97	0.25	23,23,23,23	0
57	MG	2A	3108	1/1	0.97	0.24	58,58,58,58	0
57	MG	1A	4016	1/1	0.97	0.20	42,42,42,42	0
57	MG	1l	103	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3027	1/1	0.97	0.26	51,51,51,51	0
57	MG	1A	3257	1/1	0.97	0.19	40,40,40,40	0
57	MG	1A	3073	1/1	0.97	0.21	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3042	1/1	0.97	0.28	60,60,60,60	0
57	MG	1a	1720	1/1	0.97	0.09	62,62,62,62	0
57	MG	1A	3362	1/1	0.97	0.14	41,41,41,41	0
57	MG	15	105	1/1	0.97	0.23	28,28,28,28	0
57	MG	1A	3158	1/1	0.97	0.33	34,34,34,34	0
57	MG	1A	3108	1/1	0.97	0.16	29,29,29,29	0
57	MG	2A	3463	1/1	0.97	0.14	32,32,32,32	0
57	MG	1A	3595	1/1	0.97	0.20	29,29,29,29	0
57	MG	1A	3780	1/1	0.97	0.18	32,32,32,32	0
57	MG	1A	3033	1/1	0.97	0.25	29,29,29,29	0
57	MG	1A	3432	1/1	0.97	0.10	33,33,33,33	0
57	MG	1A	3076	1/1	0.97	0.31	29,29,29,29	0
57	MG	18	101	1/1	0.97	0.19	31,31,31,31	0
57	MG	1A	3905	1/1	0.97	0.24	35,35,35,35	0
57	MG	1A	3263	1/1	0.97	0.17	33,33,33,33	0
57	MG	1A	3369	1/1	0.97	0.13	60,60,60,60	0
57	MG	2A	3474	1/1	0.97	0.21	46,46,46,46	0
57	MG	1A	3601	1/1	0.97	0.19	40,40,40,40	0
57	MG	1A	3513	1/1	0.97	0.24	20,20,20,20	0
57	MG	1A	3911	1/1	0.97	0.16	44,44,44,44	0
57	MG	1A	3195	1/1	0.97	0.23	60,60,60,60	0
57	MG	1d	302	1/1	0.97	0.12	57,57,57,57	0
57	MG	1A	3516	1/1	0.97	0.17	48,48,48,48	0
57	MG	1A	3605	1/1	0.97	0.26	44,44,44,44	0
57	MG	2A	3138	1/1	0.97	0.19	29,29,29,29	0
57	MG	2A	3483	1/1	0.97	0.11	54,54,54,54	0
57	MG	1A	3229	1/1	0.97	0.24	27,27,27,27	0
57	MG	1A	3439	1/1	0.97	0.16	37,37,37,37	0
57	MG	1A	3794	1/1	0.97	0.22	35,35,35,35	0
57	MG	1A	3269	1/1	0.97	0.23	31,31,31,31	0
57	MG	1A	3796	1/1	0.97	0.17	43,43,43,43	0
57	MG	1a	1747	1/1	0.97	0.26	52,52,52,52	0
57	MG	1A	3314	1/1	0.97	0.29	33,33,33,33	0
57	MG	2a	3075	1/1	0.97	0.18	48,48,48,48	0
57	MG	1A	3798	1/1	0.97	0.14	44,44,44,44	0
57	MG	1A	3112	1/1	0.97	0.24	29,29,29,29	0
57	MG	2A	3494	1/1	0.97	0.18	33,33,33,33	0
57	MG	1A	3925	1/1	0.97	0.21	21,21,21,21	0
57	MG	2A	3689	1/1	0.97	0.12	55,55,55,55	0
57	MG	1A	3134	1/1	0.97	0.18	34,34,34,34	0
57	MG	2A	3497	1/1	0.97	0.10	41,41,41,41	0
57	MG	1A	3699	1/1	0.97	0.11	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3085	1/1	0.97	0.38	53,53,53,53	0
57	MG	1A	3378	1/1	0.97	0.23	11,11,11,11	0
57	MG	2A	3316	1/1	0.97	0.08	34,34,34,34	0
57	MG	1a	1755	1/1	0.97	0.14	64,64,64,64	0
57	MG	2A	3502	1/1	0.97	0.08	39,39,39,39	0
57	MG	2A	3503	1/1	0.97	0.13	52,52,52,52	0
57	MG	1A	3317	1/1	0.97	0.25	31,31,31,31	0
57	MG	1A	3805	1/1	0.97	0.12	22,22,22,22	0
57	MG	1A	3527	1/1	0.97	0.27	22,22,22,22	0
57	MG	1t	201	1/1	0.97	0.13	56,56,56,56	0
57	MG	1t	202	1/1	0.97	0.13	56,56,56,56	0
57	MG	2a	3096	1/1	0.97	0.31	48,48,48,48	0
57	MG	1A	3449	1/1	0.97	0.20	40,40,40,40	0
57	MG	2a	3098	1/1	0.97	0.36	50,50,50,50	0
57	MG	1A	3380	1/1	0.97	0.17	22,22,22,22	0
57	MG	2A	3326	1/1	0.97	0.20	41,41,41,41	0
57	MG	2A	3327	1/1	0.97	0.12	56,56,56,56	0
57	MG	2A	3514	1/1	0.97	0.11	66,66,66,66	0
57	MG	2A	3709	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3319	1/1	0.97	0.21	29,29,29,29	0
57	MG	1A	3135	1/1	0.97	0.22	32,32,32,32	0
57	MG	2a	3106	1/1	0.97	0.18	53,53,53,53	0
57	MG	2A	3518	1/1	0.97	0.16	49,49,49,49	0
57	MG	2A	3519	1/1	0.97	0.13	46,46,46,46	0
57	MG	2A	3714	1/1	0.97	0.16	42,42,42,42	0
57	MG	2a	3110	1/1	0.97	0.17	52,52,52,52	0
57	MG	1D	301	1/1	0.97	0.12	27,27,27,27	0
57	MG	1A	3013	1/1	0.97	0.24	18,18,18,18	0
57	MG	1A	3042	1/1	0.97	0.22	29,29,29,29	0
57	MG	2A	3166	1/1	0.97	0.14	42,42,42,42	0
57	MG	1A	3044	1/1	0.97	0.18	22,22,22,22	0
57	MG	1A	3539	1/1	0.97	0.23	19,19,19,19	0
57	MG	1A	3030	1/1	0.97	0.19	21,21,21,21	0
57	MG	1A	3712	1/1	0.97	0.10	31,31,31,31	0
57	MG	1A	3625	1/1	0.97	0.19	29,29,29,29	0
57	MG	1a	1633	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	3237	1/1	0.97	0.17	31,31,31,31	0
57	MG	2A	3343	1/1	0.97	0.17	37,37,37,37	0
57	MG	1A	3081	1/1	0.97	0.19	32,32,32,32	0
57	MG	2A	3175	1/1	0.97	0.23	43,43,43,43	0
57	MG	2a	3126	1/1	0.97	0.10	60,60,60,60	0
57	MG	2A	3012	1/1	0.97	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3825	1/1	0.97	0.15	24,24,24,24	0
57	MG	1A	3141	1/1	0.97	0.18	35,35,35,35	0
57	MG	1A	3545	1/1	0.97	0.26	45,45,45,45	0
57	MG	1A	3829	1/1	0.97	0.10	37,37,37,37	0
57	MG	1A	3546	1/1	0.97	0.15	25,25,25,25	0
57	MG	2a	3133	1/1	0.97	0.16	63,63,63,63	0
57	MG	2A	3018	1/1	0.97	0.38	37,37,37,37	0
57	MG	1A	3119	1/1	0.97	0.21	28,28,28,28	0
57	MG	1A	3120	1/1	0.97	0.27	17,17,17,17	0
57	MG	2A	3023	1/1	0.97	0.20	60,60,60,60	0
57	MG	2A	3545	1/1	0.97	0.19	34,34,34,34	0
57	MG	2a	3139	1/1	0.97	0.08	59,59,59,59	0
57	MG	1A	3333	1/1	0.97	0.18	19,19,19,19	0
57	MG	1E	306	1/1	0.97	0.12	38,38,38,38	0
57	MG	1a	1783	1/1	0.97	0.13	55,55,55,55	0
57	MG	1A	3634	1/1	0.97	0.20	16,16,16,16	0
57	MG	2a	3144	1/1	0.97	0.15	60,60,60,60	0
57	MG	1A	3283	1/1	0.97	0.20	38,38,38,38	0
57	MG	2B	211	1/1	0.97	0.17	57,57,57,57	0
57	MG	1a	1786	1/1	0.97	0.14	63,63,63,63	0
57	MG	1A	3956	1/1	0.97	0.15	41,41,41,41	0
57	MG	1F	301	1/1	0.97	0.18	26,26,26,26	0
57	MG	2a	3150	1/1	0.97	0.19	60,60,60,60	0
57	MG	2A	3194	1/1	0.97	0.31	40,40,40,40	0
57	MG	1A	3467	1/1	0.97	0.20	24,24,24,24	0
57	MG	2B	217	1/1	0.97	0.14	57,57,57,57	0
57	MG	1A	3838	1/1	0.97	0.16	26,26,26,26	0
57	MG	1A	3121	1/1	0.97	0.24	25,25,25,25	0
57	MG	1F	307	1/1	0.97	0.19	25,25,25,25	0
57	MG	2A	3036	1/1	0.97	0.24	41,41,41,41	0
57	MG	1A	3840	1/1	0.97	0.16	15,15,15,15	0
57	MG	1A	3396	1/1	0.97	0.23	40,40,40,40	0
57	MG	2A	3202	1/1	0.97	0.21	56,56,56,56	0
57	MG	2A	3203	1/1	0.97	0.33	56,56,56,56	0
57	MG	2A	3204	1/1	0.97	0.18	51,51,51,51	0
57	MG	2A	3039	1/1	0.97	0.17	48,48,48,48	0
57	MG	1a	1656	1/1	0.97	0.21	45,45,45,45	0
57	MG	2D	311	1/1	0.97	0.07	55,55,55,55	0
57	MG	2A	3380	1/1	0.97	0.10	60,60,60,60	0
57	MG	2A	3041	1/1	0.97	0.19	37,37,37,37	0
57	MG	1a	1798	1/1	0.97	0.10	52,52,52,52	0
57	MG	1A	3964	1/1	0.97	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1F	312	1/1	0.97	0.32	42,42,42,42	0
57	MG	1A	3046	1/1	0.97	0.24	12,12,12,12	0
57	MG	1A	3641	1/1	0.97	0.21	42,42,42,42	0
57	MG	1A	3734	1/1	0.97	0.55	40,40,40,40	0
57	MG	1A	3848	1/1	0.97	0.17	32,32,32,32	0
57	MG	1A	3398	1/1	0.97	0.22	49,49,49,49	0
57	MG	1A	3560	1/1	0.97	0.16	32,32,32,32	0
57	MG	1A	3286	1/1	0.97	0.14	25,25,25,25	0
57	MG	1A	3401	1/1	0.97	0.28	31,31,31,31	0
57	MG	1A	3853	1/1	0.97	0.26	36,36,36,36	0
57	MG	1A	3474	1/1	0.97	0.20	55,55,55,55	0
57	MG	1A	3976	1/1	0.97	0.11	32,32,32,32	0
57	MG	2Q	201	1/1	0.97	0.13	46,46,46,46	0
57	MG	1A	3339	1/1	0.97	0.22	23,23,23,23	0
57	MG	1A	3648	1/1	0.97	0.15	40,40,40,40	0
57	MG	1A	3980	1/1	0.97	0.12	21,21,21,21	0
57	MG	1A	3287	1/1	0.97	0.20	27,27,27,27	0
57	MG	1A	3037	1/1	0.97	0.20	34,34,34,34	0
57	MG	2R	203	1/1	0.97	0.28	51,51,51,51	0
57	MG	2A	3591	1/1	0.97	0.15	52,52,52,52	0
57	MG	1A	3567	1/1	0.97	0.13	30,30,30,30	0
57	MG	2T	204	1/1	0.97	0.19	45,45,45,45	0
57	MG	1a	1820	1/1	0.97	0.11	62,62,62,62	0
57	MG	1A	3745	1/1	0.97	0.17	28,28,28,28	0
57	MG	1A	3178	1/1	0.97	0.20	19,19,19,19	0
57	MG	2A	3069	1/1	0.97	0.26	38,38,38,38	0
57	MG	2k	202	1/1	0.97	0.10	58,58,58,58	0
57	MG	1A	3084	1/1	0.97	0.14	41,41,41,41	0
57	MG	1A	3180	1/1	0.97	0.13	28,28,28,28	0
57	MG	1a	1825	1/1	0.97	0.07	49,49,49,49	0
57	MG	20	101	1/1	0.97	0.17	46,46,46,46	0
57	MG	2A	3411	1/1	0.97	0.12	56,56,56,56	0
57	MG	1a	1680	1/1	0.97	0.21	48,48,48,48	0
57	MG	1R	201	1/1	0.97	0.21	32,32,32,32	0
57	MG	1A	3410	1/1	0.97	0.19	26,26,26,26	0
57	MG	2A	3077	1/1	0.97	0.30	47,47,47,47	0
57	MG	1A	3151	1/1	0.97	0.20	33,33,33,33	0
57	MG	1A	3004	1/1	0.97	0.23	45,45,45,45	0
57	MG	1T	201	1/1	0.97	0.19	36,36,36,36	0
60	ZN	1Y	501	1/1	0.97	0.16	55,55,55,55	0
57	MG	1A	3347	1/1	0.97	0.19	20,20,20,20	0
60	ZN	2Y	202	1/1	0.97	0.13	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3755	1/1	0.97	0.11	38,38,38,38	0
60	ZN	29	501	1/1	0.97	0.14	57,57,57,57	0
60	ZN	2n	501	1/1	0.97	0.06	85,85,85,85	0
57	MG	2A	3083	1/1	0.97	0.13	59,59,59,59	0
57	MG	1A	3219	1/1	0.98	0.14	25,25,25,25	0
57	MG	2A	3553	1/1	0.98	0.16	63,63,63,63	0
57	MG	1A	3403	1/1	0.98	0.22	23,23,23,23	0
57	MG	1a	1796	1/1	0.98	0.11	45,45,45,45	0
57	MG	1A	3318	1/1	0.98	0.21	16,16,16,16	0
57	MG	2A	3409	1/1	0.98	0.24	53,53,53,53	0
57	MG	1A	3505	1/1	0.98	0.19	27,27,27,27	0
57	MG	10	104	1/1	0.98	0.21	39,39,39,39	0
57	MG	2A	3270	1/1	0.98	0.19	44,44,44,44	0
57	MG	2A	3561	1/1	0.98	0.16	26,26,26,26	0
57	MG	2A	3009	1/1	0.98	0.15	41,41,41,41	0
57	MG	2A	3010	1/1	0.98	0.14	52,52,52,52	0
57	MG	2A	3142	1/1	0.98	0.20	40,40,40,40	0
57	MG	1A	3169	1/1	0.98	0.21	25,25,25,25	0
57	MG	1B	216	1/1	0.98	0.29	45,45,45,45	0
57	MG	1A	3149	1/1	0.98	0.29	33,33,33,33	0
57	MG	1a	1686	1/1	0.98	0.20	52,52,52,52	0
57	MG	2A	3420	1/1	0.98	0.15	40,40,40,40	0
57	MG	1a	1804	1/1	0.98	0.15	67,67,67,67	0
57	MG	10	108	1/1	0.98	0.19	32,32,32,32	0
57	MG	1A	3110	1/1	0.98	0.20	25,25,25,25	0
57	MG	1A	3572	1/1	0.98	0.10	45,45,45,45	0
57	MG	1A	3323	1/1	0.98	0.27	16,16,16,16	0
57	MG	1A	3364	1/1	0.98	0.21	20,20,20,20	0
57	MG	1A	3638	1/1	0.98	0.10	33,33,33,33	0
57	MG	1A	3459	1/1	0.98	0.11	50,50,50,50	0
57	MG	2A	3734	1/1	0.98	0.12	61,61,61,61	0
57	MG	13	102	1/1	0.98	0.13	58,58,58,58	0
57	MG	2a	3083	1/1	0.98	0.28	48,48,48,48	0
57	MG	2A	3736	1/1	0.98	0.16	59,59,59,59	0
57	MG	13	103	1/1	0.98	0.18	41,41,41,41	0
57	MG	15	101	1/1	0.98	0.14	29,29,29,29	0
57	MG	1A	3865	1/1	0.98	0.15	28,28,28,28	0
57	MG	1A	3460	1/1	0.98	0.15	23,23,23,23	0
57	MG	1A	3022	1/1	0.98	0.18	49,49,49,49	0
57	MG	1A	3958	1/1	0.98	0.17	48,48,48,48	0
57	MG	1a	1702	1/1	0.98	0.33	48,48,48,48	0
57	MG	1A	3048	1/1	0.98	0.16	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3326	1/1	0.98	0.24	35,35,35,35	0
57	MG	17	102	1/1	0.98	0.19	28,28,28,28	0
57	MG	1A	3517	1/1	0.98	0.15	46,46,46,46	0
57	MG	1A	3785	1/1	0.98	0.15	52,52,52,52	0
57	MG	1D	302	1/1	0.98	0.20	32,32,32,32	0
57	MG	1A	3096	1/1	0.98	0.10	46,46,46,46	0
57	MG	1A	3873	1/1	0.98	0.16	36,36,36,36	0
57	MG	2A	3303	1/1	0.98	0.18	37,37,37,37	0
57	MG	1A	3415	1/1	0.98	0.19	26,26,26,26	0
57	MG	1A	3713	1/1	0.98	0.24	32,32,32,32	0
57	MG	2A	3043	1/1	0.98	0.17	24,24,24,24	0
57	MG	1D	307	1/1	0.98	0.22	41,41,41,41	0
57	MG	1A	3200	1/1	0.98	0.15	27,27,27,27	0
57	MG	1D	309	1/1	0.98	0.21	36,36,36,36	0
57	MG	1a	1602	1/1	0.98	0.23	41,41,41,41	0
57	MG	2D	304	1/1	0.98	0.12	37,37,37,37	0
57	MG	1A	3017	1/1	0.98	0.20	28,28,28,28	0
57	MG	1A	3068	1/1	0.98	0.27	33,33,33,33	0
57	MG	1A	3650	1/1	0.98	0.25	37,37,37,37	0
57	MG	2A	3052	1/1	0.98	0.10	51,51,51,51	0
57	MG	2A	3053	1/1	0.98	0.13	42,42,42,42	0
57	MG	2A	3459	1/1	0.98	0.16	48,48,48,48	0
57	MG	2a	3115	1/1	0.98	0.20	51,51,51,51	0
57	MG	1A	3523	1/1	0.98	0.15	56,56,56,56	0
57	MG	2E	301	1/1	0.98	0.16	59,59,59,59	0
57	MG	1A	3719	1/1	0.98	0.23	38,38,38,38	0
57	MG	1A	3036	1/1	0.98	0.25	28,28,28,28	0
57	MG	1A	3975	1/1	0.98	0.14	39,39,39,39	0
57	MG	1a	1724	1/1	0.98	0.13	55,55,55,55	0
57	MG	1A	3070	1/1	0.98	0.19	22,22,22,22	0
57	MG	2A	3466	1/1	0.98	0.18	48,48,48,48	0
57	MG	1A	3589	1/1	0.98	0.13	30,30,30,30	0
57	MG	1A	3118	1/1	0.98	0.17	21,21,21,21	0
57	MG	1A	3799	1/1	0.98	0.17	43,43,43,43	0
57	MG	1A	3724	1/1	0.98	0.20	25,25,25,25	0
57	MG	1A	3043	1/1	0.98	0.21	13,13,13,13	0
57	MG	1A	3072	1/1	0.98	0.23	30,30,30,30	0
57	MG	2A	3330	1/1	0.98	0.20	51,51,51,51	0
57	MG	1A	3530	1/1	0.98	0.24	37,37,37,37	0
57	MG	2A	3332	1/1	0.98	0.10	59,59,59,59	0
57	MG	1A	3297	1/1	0.98	0.17	23,23,23,23	0
57	MG	1A	3532	1/1	0.98	0.18	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3730	1/1	0.98	0.15	26,26,26,26	0
57	MG	1a	1854	1/1	0.98	0.14	49,49,49,49	0
57	MG	1F	303	1/1	0.98	0.19	27,27,27,27	0
57	MG	1A	3807	1/1	0.98	0.17	29,29,29,29	0
57	MG	1A	3337	1/1	0.98	0.18	22,22,22,22	0
57	MG	2A	3074	1/1	0.98	0.16	30,30,30,30	0
57	MG	1A	3381	1/1	0.98	0.20	13,13,13,13	0
57	MG	2T	202	1/1	0.98	0.11	65,65,65,65	0
57	MG	1A	3264	1/1	0.98	0.25	32,32,32,32	0
57	MG	1F	309	1/1	0.98	0.16	35,35,35,35	0
57	MG	1A	3899	1/1	0.98	0.24	37,37,37,37	0
57	MG	2A	3345	1/1	0.98	0.16	35,35,35,35	0
57	MG	1a	1862	1/1	0.98	0.13	46,46,46,46	0
57	MG	2A	3347	1/1	0.98	0.19	37,37,37,37	0
57	MG	1A	3536	1/1	0.98	0.16	23,23,23,23	0
57	MG	1A	3103	1/1	0.98	0.25	32,32,32,32	0
57	MG	2a	3151	1/1	0.98	0.08	68,68,68,68	0
57	MG	1A	3267	1/1	0.98	0.13	43,43,43,43	0
57	MG	1A	3996	1/1	0.98	0.15	38,38,38,38	0
57	MG	1A	3185	1/1	0.98	0.24	37,37,37,37	0
57	MG	2a	3155	1/1	0.98	0.23	60,60,60,60	0
57	MG	2A	3646	1/1	0.98	0.15	35,35,35,35	0
57	MG	23	101	1/1	0.98	0.17	48,48,48,48	0
57	MG	1A	3815	1/1	0.98	0.18	32,32,32,32	0
57	MG	2A	3649	1/1	0.98	0.26	49,49,49,49	0
57	MG	1A	3906	1/1	0.98	0.19	42,42,42,42	0
57	MG	1A	3668	1/1	0.98	0.32	61,61,61,61	0
57	MG	1A	3104	1/1	0.98	0.19	29,29,29,29	0
57	MG	1A	3238	1/1	0.98	0.21	35,35,35,35	0
57	MG	1H	201	1/1	0.98	0.30	34,34,34,34	0
57	MG	1A	3819	1/1	0.98	0.21	46,46,46,46	0
57	MG	1A	3671	1/1	0.98	0.08	29,29,29,29	0
57	MG	1A	3019	1/1	0.98	0.22	20,20,20,20	0
57	MG	1A	3543	1/1	0.98	0.23	31,31,31,31	0
57	MG	2a	3006	1/1	0.98	0.14	51,51,51,51	0
57	MG	1A	3053	1/1	0.98	0.24	29,29,29,29	0
57	MG	1A	3020	1/1	0.98	0.19	31,31,31,31	0
57	MG	2A	3509	1/1	0.98	0.11	39,39,39,39	0
57	MG	1A	3827	1/1	0.98	0.18	23,23,23,23	0
57	MG	1A	3917	1/1	0.98	0.16	39,39,39,39	0
57	MG	2A	3664	1/1	0.98	0.19	38,38,38,38	0
57	MG	1A	3242	1/1	0.98	0.23	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3919	1/1	0.98	0.22	13,13,13,13	0
57	MG	1Q	201	1/1	0.98	0.15	29,29,29,29	0
57	MG	1A	3487	1/1	0.98	0.17	25,25,25,25	0
57	MG	2A	3371	1/1	0.98	0.18	49,49,49,49	0
57	MG	1Q	203	1/1	0.98	0.21	27,27,27,27	0
57	MG	1A	3830	1/1	0.98	0.18	26,26,26,26	0
57	MG	1A	3275	1/1	0.98	0.17	25,25,25,25	0
57	MG	1A	3549	1/1	0.98	0.20	25,25,25,25	0
57	MG	1A	3751	1/1	0.98	0.20	30,30,30,30	0
57	MG	1A	3243	1/1	0.98	0.18	24,24,24,24	0
57	MG	2A	3238	1/1	0.98	0.31	45,45,45,45	0
57	MG	2A	3677	1/1	0.98	0.35	65,65,65,65	0
57	MG	1A	3146	1/1	0.98	0.24	35,35,35,35	0
57	MG	2A	3110	1/1	0.98	0.19	31,31,31,31	0
57	MG	1A	3754	1/1	0.98	0.21	31,31,31,31	0
57	MG	1g	3102	1/1	0.98	0.15	54,54,54,54	0
57	MG	1A	3003	1/1	0.98	0.26	28,28,28,28	0
57	MG	1A	3756	1/1	0.98	0.19	17,17,17,17	0
57	MG	2A	3531	1/1	0.98	0.10	48,48,48,48	0
57	MG	1A	4025	1/1	0.98	0.37	45,45,45,45	0
57	MG	1A	3442	1/1	0.98	0.20	21,21,21,21	0
57	MG	1A	4027	1/1	0.98	0.24	47,47,47,47	0
57	MG	2A	3688	1/1	0.98	0.16	56,56,56,56	0
57	MG	1A	3352	1/1	0.98	0.22	13,13,13,13	0
57	MG	1A	3556	1/1	0.98	0.14	17,17,17,17	0
57	MG	1U	207	1/1	0.98	0.21	32,32,32,32	0
57	MG	1A	3444	1/1	0.98	0.18	26,26,26,26	0
57	MG	1V	201	1/1	0.98	0.31	28,28,28,28	0
57	MG	1A	3495	1/1	0.98	0.17	24,24,24,24	0
57	MG	1A	3845	1/1	0.98	0.15	41,41,41,41	0
57	MG	1A	3559	1/1	0.98	0.18	29,29,29,29	0
57	MG	1A	3496	1/1	0.98	0.16	27,27,27,27	0
57	MG	1A	3092	1/1	0.98	0.15	28,28,28,28	0
57	MG	1A	3354	1/1	0.98	0.20	25,25,25,25	0
57	MG	2A	3129	1/1	0.98	0.20	64,64,64,64	0
57	MG	2A	3547	1/1	0.98	0.15	44,44,44,44	0
60	ZN	15	109	1/1	0.98	0.18	38,38,38,38	0
60	ZN	19	104	1/1	0.98	0.18	38,38,38,38	0
57	MG	2A	3702	1/1	0.98	0.14	53,53,53,53	0
57	MG	1a	1791	1/1	0.98	0.10	55,55,55,55	0
60	ZN	25	104	1/1	0.98	0.18	51,51,51,51	0
60	ZN	26	102	1/1	0.98	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3131	1/1	0.98	0.19	45,45,45,45	0
57	MG	1A	3217	1/1	0.98	0.20	30,30,30,30	0
61	SF4	1d	307	8/8	0.98	0.10	58,62,71,72	0
61	SF4	2d	501	8/8	0.98	0.10	65,72,77,83	0
57	MG	1A	3193	1/1	0.98	0.20	30,30,30,30	0
57	MG	1A	3437	1/1	0.99	0.15	45,45,45,45	0
57	MG	2A	3618	1/1	0.99	0.14	60,60,60,60	0
57	MG	1A	3028	1/1	0.99	0.19	22,22,22,22	0
57	MG	2B	220	1/1	0.99	0.17	43,43,43,43	0
57	MG	1A	3515	1/1	0.99	0.18	31,31,31,31	0
57	MG	1A	3095	1/1	0.99	0.20	14,14,14,14	0
57	MG	1U	204	1/1	0.99	0.20	32,32,32,32	0
57	MG	1a	1653	1/1	0.99	0.12	51,51,51,51	0
57	MG	1a	1815	1/1	0.99	0.13	55,55,55,55	0
57	MG	2A	3306	1/1	0.99	0.28	37,37,37,37	0
57	MG	1U	205	1/1	0.99	0.17	35,35,35,35	0
57	MG	1A	3961	1/1	0.99	0.17	22,22,22,22	0
57	MG	1A	3074	1/1	0.99	0.16	32,32,32,32	0
57	MG	1A	3133	1/1	0.99	0.19	28,28,28,28	0
57	MG	1A	3177	1/1	0.99	0.15	18,18,18,18	0
57	MG	1F	306	1/1	0.99	0.18	24,24,24,24	0
57	MG	2A	3021	1/1	0.99	0.22	37,37,37,37	0
57	MG	2A	3022	1/1	0.99	0.24	42,42,42,42	0
57	MG	1V	203	1/1	0.99	0.19	35,35,35,35	0
57	MG	1A	3357	1/1	0.99	0.17	37,37,37,37	0
57	MG	2E	306	1/1	0.99	0.20	44,44,44,44	0
57	MG	1A	3018	1/1	0.99	0.22	23,23,23,23	0
57	MG	1A	3928	1/1	0.99	0.17	45,45,45,45	0
57	MG	1A	3608	1/1	0.99	0.20	21,21,21,21	0
57	MG	1A	3822	1/1	0.99	0.23	32,32,32,32	0
57	MG	2A	3321	1/1	0.99	0.23	47,47,47,47	0
57	MG	1A	3893	1/1	0.99	0.21	35,35,35,35	0
57	MG	1A	3823	1/1	0.99	0.16	43,43,43,43	0
57	MG	1A	4012	1/1	0.99	0.26	15,15,15,15	0
57	MG	1A	3445	1/1	0.99	0.23	12,12,12,12	0
57	MG	1A	3400	1/1	0.99	0.25	27,27,27,27	0
57	MG	2A	3388	1/1	0.99	0.15	46,46,46,46	0
57	MG	2A	3515	1/1	0.99	0.13	42,42,42,42	0
57	MG	2A	3648	1/1	0.99	0.19	51,51,51,51	0
57	MG	1A	4015	1/1	0.99	0.31	29,29,29,29	0
57	MG	1A	3322	1/1	0.99	0.20	27,27,27,27	0
57	MG	1A	3732	1/1	0.99	0.16	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3145	1/1	0.99	0.20	27,27,27,27	0
57	MG	1A	3554	1/1	0.99	0.12	21,21,21,21	0
57	MG	1A	3306	1/1	0.99	0.19	40,40,40,40	0
57	MG	2A	3457	1/1	0.99	0.20	48,48,48,48	0
57	MG	1A	3979	1/1	0.99	0.19	41,41,41,41	0
57	MG	2A	3273	1/1	0.99	0.23	31,31,31,31	0
57	MG	1A	3500	1/1	0.99	0.25	25,25,25,25	0
57	MG	1a	1732	1/1	0.99	0.14	64,64,64,64	0
57	MG	1A	3528	1/1	0.99	0.16	29,29,29,29	0
57	MG	2A	3729	1/1	0.99	0.13	38,38,38,38	0
57	MG	1A	3904	1/1	0.99	0.20	33,33,33,33	0
57	MG	1A	3089	1/1	0.99	0.24	34,34,34,34	0
57	MG	1A	3308	1/1	0.99	0.21	29,29,29,29	0
57	MG	1A	3025	1/1	0.99	0.18	35,35,35,35	0
57	MG	1D	312	1/1	0.99	0.21	23,23,23,23	0
57	MG	1A	3407	1/1	0.99	0.19	35,35,35,35	0
57	MG	2A	3050	1/1	0.99	0.05	43,43,43,43	0
57	MG	1A	3008	1/1	0.99	0.19	29,29,29,29	0
57	MG	15	103	1/1	0.99	0.20	29,29,29,29	0
57	MG	15	104	1/1	0.99	0.22	33,33,33,33	0
57	MG	1A	3455	1/1	0.99	0.15	14,14,14,14	0
57	MG	1A	3222	1/1	0.99	0.14	22,22,22,22	0
57	MG	1A	3265	1/1	0.99	0.14	54,54,54,54	0
57	MG	1A	3001	1/1	0.99	0.20	25,25,25,25	0
60	ZN	16	501	1/1	0.99	0.23	39,39,39,39	0
57	MG	1A	3184	1/1	0.99	0.17	28,28,28,28	0
60	ZN	1n	102	1/1	0.99	0.10	68,68,68,68	0
57	MG	1a	1694	1/1	0.99	0.25	39,39,39,39	0
57	MG	1A	3843	1/1	0.99	0.20	21,21,21,21	0
57	MG	1E	303	1/1	0.99	0.26	32,32,32,32	0
57	MG	1A	3370	1/1	0.99	0.15	27,27,27,27	0
57	MG	1A	3085	1/1	0.99	0.25	29,29,29,29	0
57	MG	1A	3846	1/1	0.99	0.14	34,34,34,34	0
57	MG	2A	3614	1/1	0.99	0.10	26,26,26,26	0
57	MG	1E	307	1/1	0.99	0.20	25,25,25,25	0
57	MG	2A	3485	1/1	0.99	0.14	33,33,33,33	0
57	MG	1A	3375	1/1	1.00	0.21	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.