Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 04:57 PM EST

PDB ID	:	7RQE
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with protein Y, A-site deacylated tRNA analog CACCA, P-site MAI-tripeptidyl-tRNA analog ACCA-IAM, and chloramphenicol at 2.40A 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 (1)) were used in the production of this report:

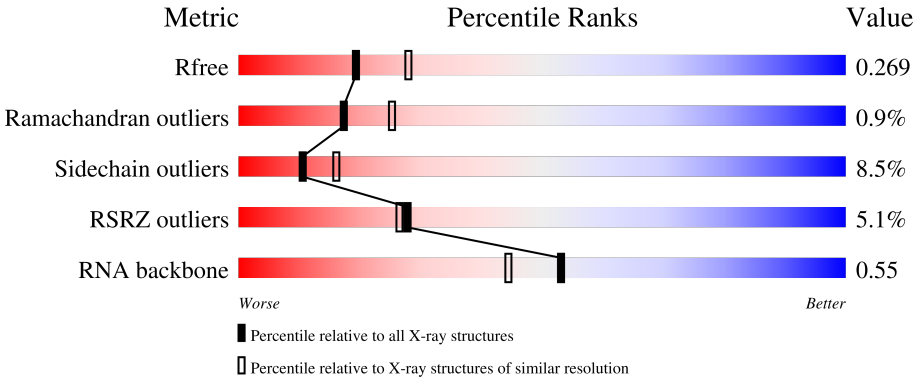
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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 <=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% 82% 15% ••
1	2A	2915	3% 81% 17% ••
2	1B	121	90% 9% •
2	2B	121	90% 9% •
3	1D	276	93% 7%

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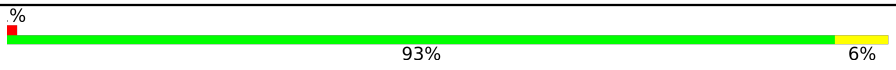
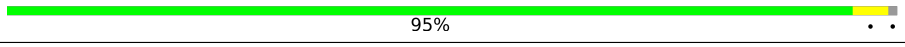
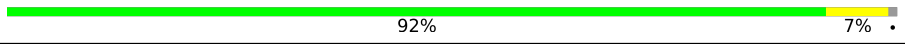
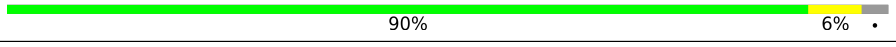
Mol	Chain	Length	Quality of chain
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
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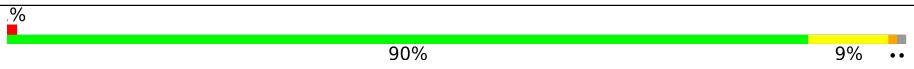
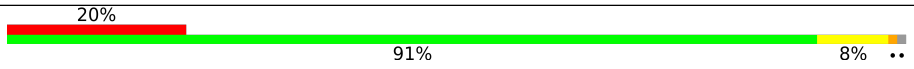
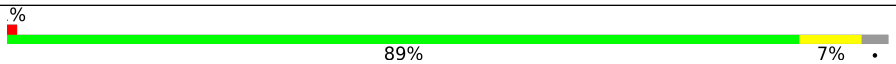
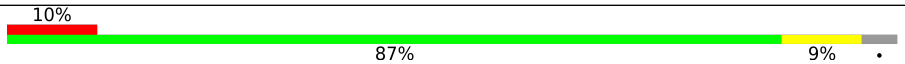
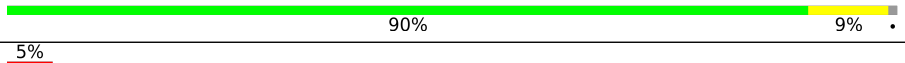
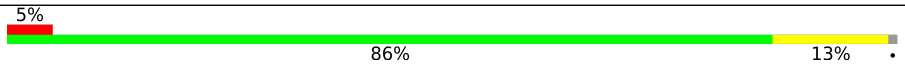
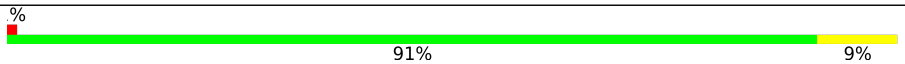
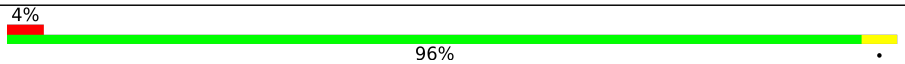
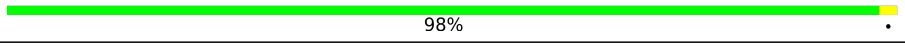
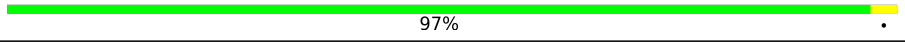
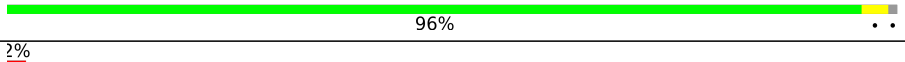
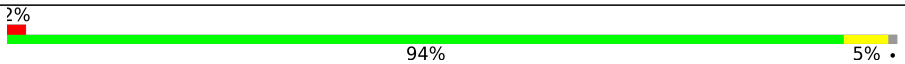
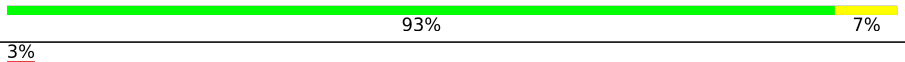
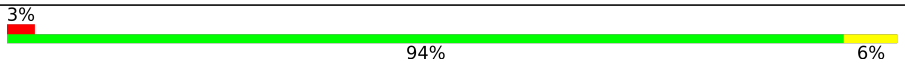
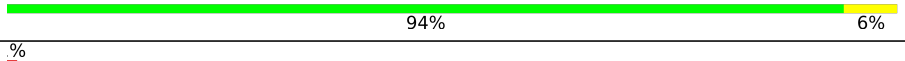
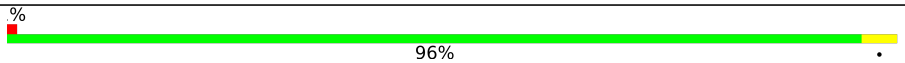
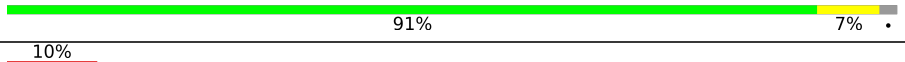
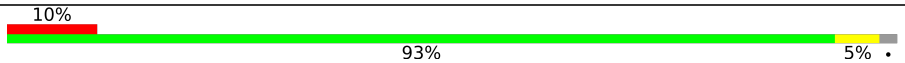
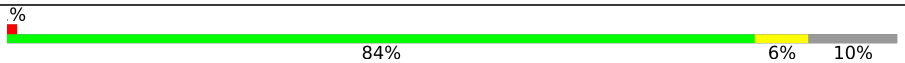
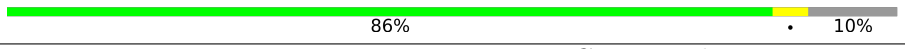
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	
15	2T	146	

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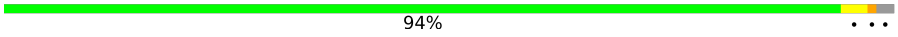
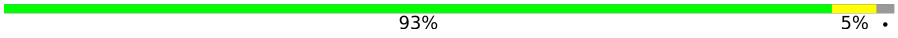
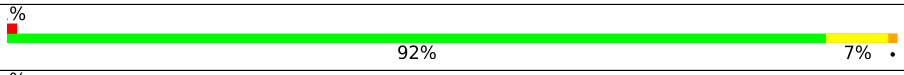
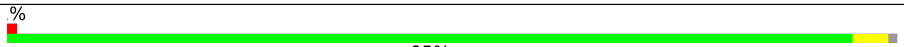
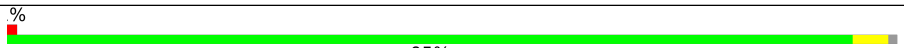
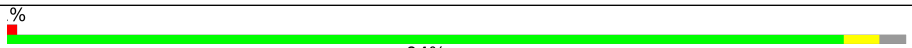
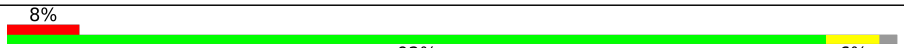
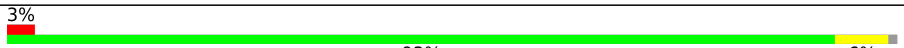
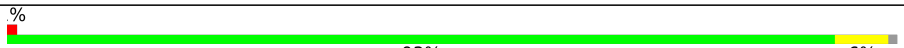
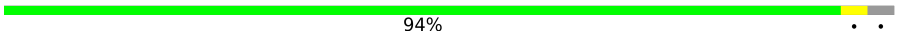
Mol	Chain	Length	Quality of chain
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
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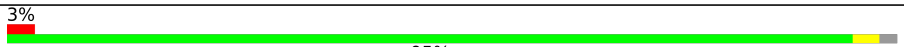
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	
28	16	54	

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Mol	Chain	Length	Quality of chain
28	26	54	2% 91% 7%
29	17	49	4% 92% 6%
29	27	49	8% 90% 8%
30	18	65	88% 11%
30	28	65	2% 88% 11%
31	19	37	100%
31	29	37	5% 95% 5%
32	1a	1521	2% 81% 17%
32	2a	1521	3% 79% 20%
33	1b	256	7% 80% 9% 10%
33	2b	256	18% 77% 12% 10%
34	1c	239	6% 83% 14%
34	2c	239	17% 77% 9% 14%
35	1d	209	7% 90% 10%
35	2d	209	8% 91% 9%
36	1e	162	3% 85% 7% 9%
36	2e	162	6% 86% 5% 9%
37	1f	101	85% 14%
37	2f	101	95%
38	1g	156	3% 94% 6%
38	2g	156	21% 88% 12%
39	1h	138	4% 91% 9%
39	2h	138	11% 91% 8%
40	1i	128	10% 89% 10%
40	2i	128	63% 89% 9%

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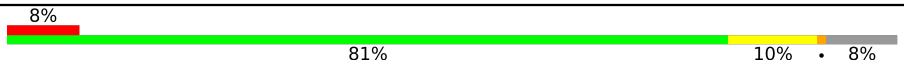
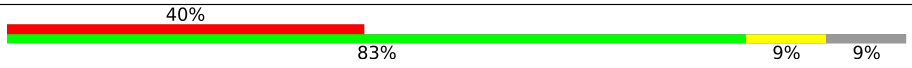
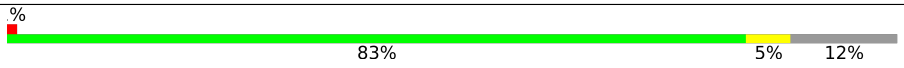
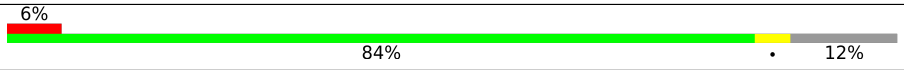
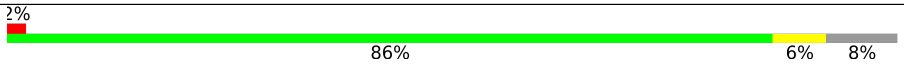
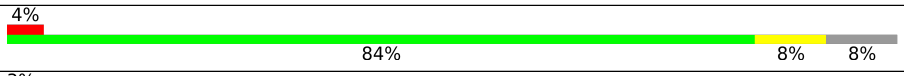
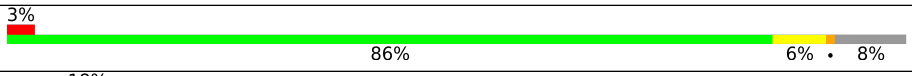
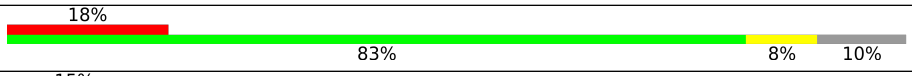
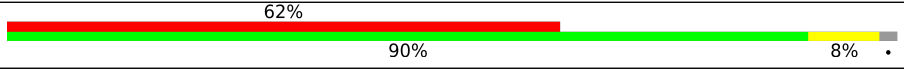
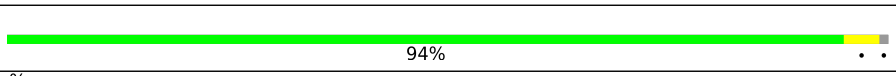
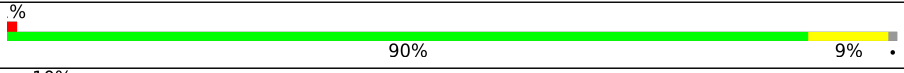
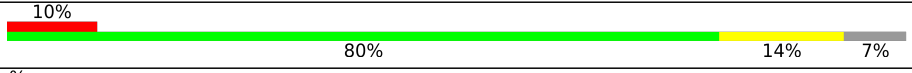
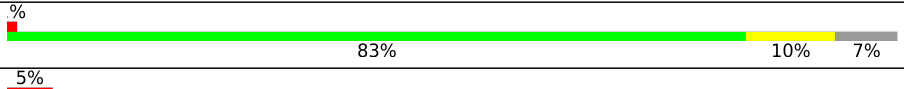
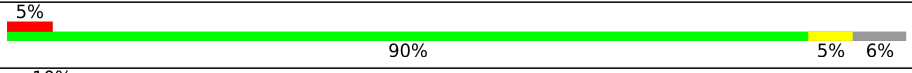
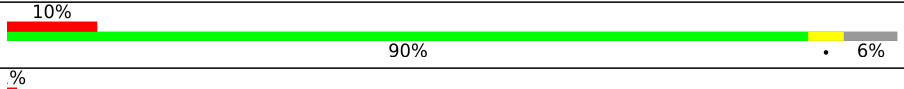
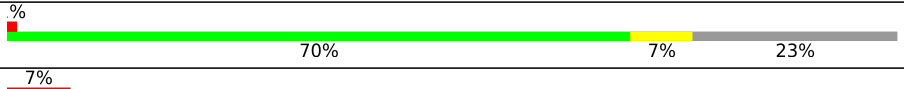
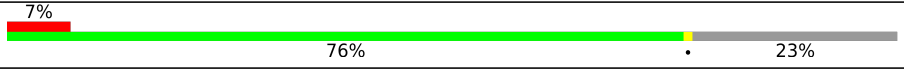
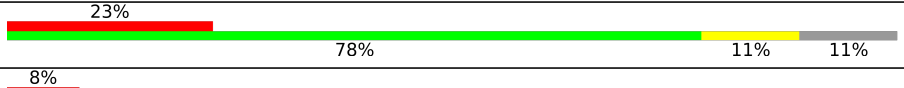
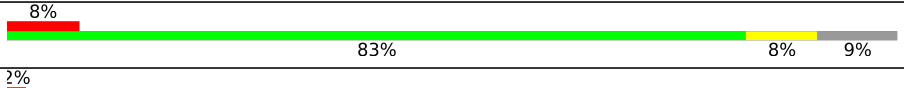
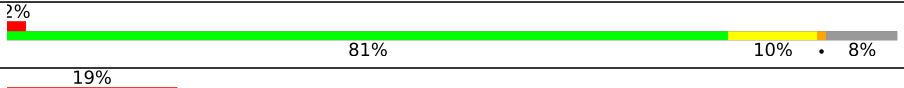
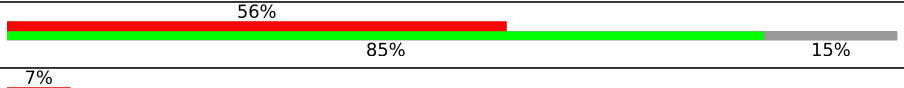
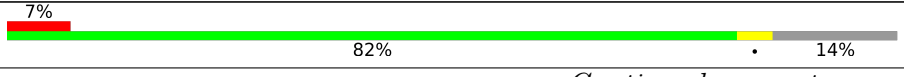
Mol	Chain	Length	Quality of chain
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	
53	1y	113	

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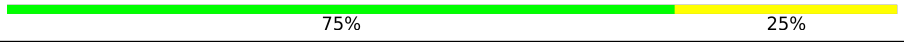
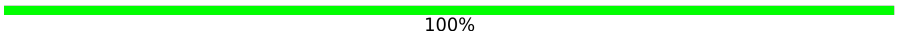
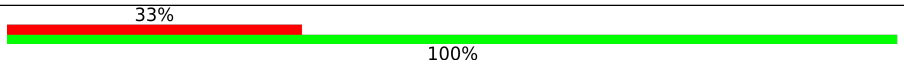
Mol	Chain	Length	Quality of chain
53	2y	113	
54	1w	5	
54	2w	5	
55	1x	4	
55	2x	4	
56	1v	3	
56	2v	3	

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	17	104	-	-	-	X
57	MG	1A	3617	-	-	-	X
57	MG	1a	1782	-	-	-	X
57	MG	2A	3065	-	-	-	X
57	MG	2A	3235	-	-	-	X
57	MG	2Q	202	-	-	-	X

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 297868 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			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 Deacylated tRNA Analog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	4	Total	C	N	O	P	0	0	1
			63	28	11	21	3			
54	2w	4	Total	C	N	O	P	0	0	1
			63	28	11	21	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
			21	14	3	3	1			
56	2v	3	Total	C	N	O	S	0	0	0
			21	14	3	3	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1016	Total	Mg	0	0
			1016	1016		
57	1B	30	Total	Mg	0	0
			30	30		
57	1D	21	Total	Mg	0	0
			21	21		
57	1E	8	Total	Mg	0	0
			8	8		
57	1F	18	Total	Mg	0	0
			18	18		

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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	5	Total Mg 5 5	0	0
57	1Q	5	Total Mg 5 5	0	0
57	1R	5	Total Mg 5 5	0	0
57	1T	7	Total Mg 7 7	0	0
57	1U	6	Total Mg 6 6	0	0
57	1V	7	Total Mg 7 7	0	0
57	1W	3	Total Mg 3 3	0	0
57	1X	1	Total Mg 1 1	0	0
57	1Y	2	Total Mg 2 2	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	7	Total Mg 7 7	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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1a	266	Total Mg 266 266	0	0
57	1b	1	Total Mg 1 1	0	0
57	1d	4	Total Mg 4 4	0	0
57	1e	2	Total Mg 2 2	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	3	Total Mg 3 3	0	0
57	1o	2	Total Mg 2 2	0	0
57	1t	2	Total Mg 2 2	0	0
57	1y	2	Total Mg 2 2	0	0
57	1x	2	Total Mg 2 2	0	0
57	2A	746	Total Mg 746 746	0	0
57	2B	19	Total Mg 19 19	0	0
57	2D	8	Total Mg 8 8	0	0
57	2E	8	Total Mg 8 8	0	0
57	2F	4	Total Mg 4 4	0	0
57	2G	3	Total Mg 3 3	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	2	Total Mg 2 2	0	0
57	2P	2	Total Mg 2 2	0	0
57	2Q	3	Total Mg 3 3	0	0
57	2R	2	Total Mg 2 2	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	3	Total Mg 3 3	0	0
57	2X	1	Total Mg 1 1	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	27	1	Total Mg 1 1	0	0
57	28	2	Total Mg 2 2	0	0
57	2a	190	Total Mg 190 190	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	1	Total Mg 1 1	0	0

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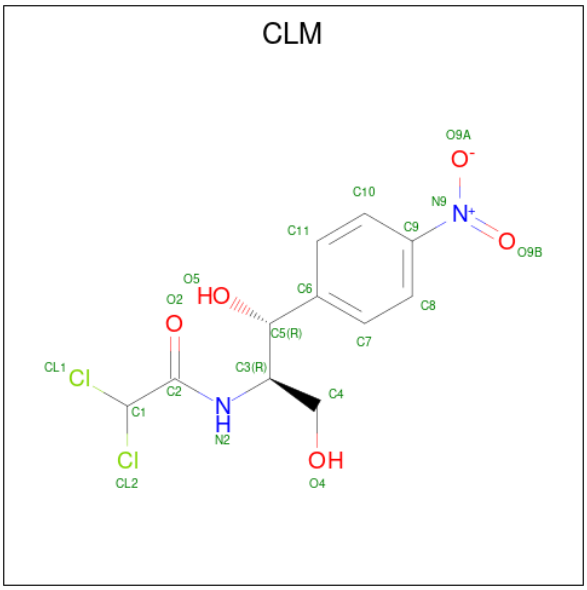
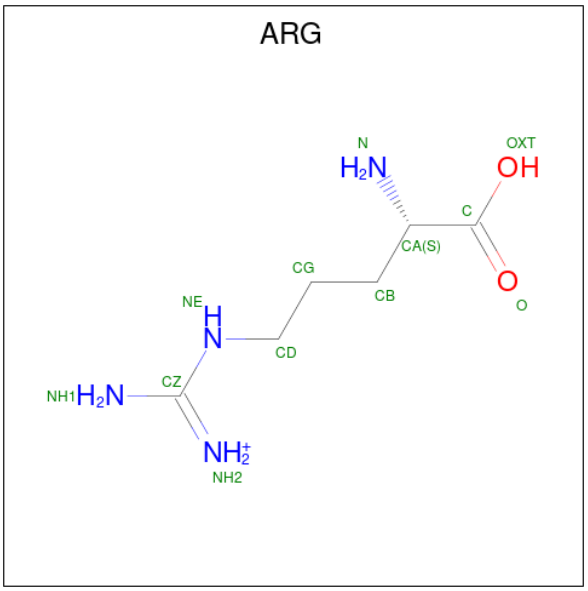
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2j	2	Total Mg 2 2	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2x	1	Total Mg 1 1	0	0

- Molecule 58 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



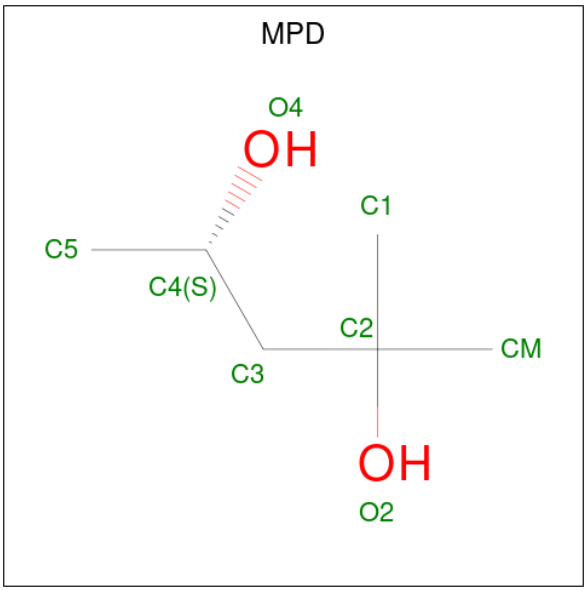
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total C Cl N O 20 11 2 2 5	0	0
58	2A	1	Total C Cl N O 20 11 2 2 5	0	0

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



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

- Molecule 60 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	1	Total C O 8 6 2	0	0

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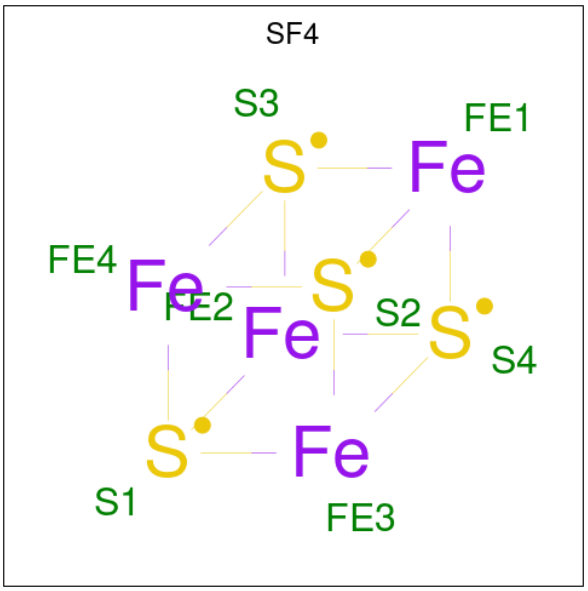
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1T	1	Total C O 8 6 2	0	0
60	18	1	Total C O 8 6 2	0	0
60	1a	1	Total C O 8 6 2	0	0
60	2A	1	Total C O 8 6 2	0	0
60	2B	1	Total C O 8 6 2	0	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1Y	1	Total Zn 1 1	0	0
61	14	1	Total Zn 1 1	0	0
61	15	1	Total Zn 1 1	0	0
61	16	1	Total Zn 1 1	0	0
61	19	1	Total Zn 1 1	0	0
61	1n	1	Total Zn 1 1	0	0
61	2Y	1	Total Zn 1 1	0	0
61	24	1	Total Zn 1 1	0	0
61	25	1	Total Zn 1 1	0	0
61	26	1	Total Zn 1 1	0	0
61	29	1	Total Zn 1 1	0	0
61	2n	1	Total Zn 1 1	0	0

- Molecule 62 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1d	1	Total Fe S 8 4 4	0	0
62	2d	1	Total Fe S 8 4 4	0	0

- Molecule 63 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1A	4023	Total O 4023 4023	0	0
63	1B	93	Total O 93 93	0	0
63	1D	112	Total O 112 112	0	0
63	1E	81	Total O 81 81	0	0
63	1F	61	Total O 61 61	0	0
63	1G	20	Total O 20 20	0	0
63	1H	12	Total O 12 12	0	0
63	1I	6	Total O 6 6	0	0
63	1N	51	Total O 51 51	0	0
63	1O	24	Total O 24 24	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1P	71	Total O 71 71	0	0
63	1Q	41	Total O 41 41	0	0
63	1R	33	Total O 33 33	0	0
63	1S	16	Total O 16 16	0	0
63	1T	34	Total O 34 34	0	0
63	1U	54	Total O 54 54	0	0
63	1V	42	Total O 42 42	0	0
63	1W	29	Total O 29 29	0	0
63	1X	23	Total O 23 23	0	0
63	1Y	16	Total O 16 16	0	0
63	1Z	12	Total O 12 12	0	0
63	10	25	Total O 25 25	0	0
63	11	22	Total O 22 22	0	0
63	12	13	Total O 13 13	0	0
63	13	21	Total O 21 21	0	0
63	14	2	Total O 2 2	0	0
63	15	26	Total O 26 26	0	0
63	16	20	Total O 20 20	0	0
63	17	16	Total O 16 16	0	0
63	18	30	Total O 30 30	0	0
63	19	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1a	378	Total O 378 378	0	0
63	1b	1	Total O 1 1	0	0
63	1d	3	Total O 3 3	0	0
63	1e	3	Total O 3 3	0	0
63	1f	2	Total O 2 2	0	0
63	1h	1	Total O 1 1	0	0
63	1j	1	Total O 1 1	0	0
63	1l	6	Total O 6 6	0	0
63	1o	2	Total O 2 2	0	0
63	1p	3	Total O 3 3	0	0
63	1t	1	Total O 1 1	0	0
63	1y	2	Total O 2 2	0	0
63	1w	5	Total O 5 5	0	0
63	1x	3	Total O 3 3	0	0
63	2A	2284	Total O 2284 2284	0	0
63	2B	46	Total O 46 46	0	0
63	2D	57	Total O 57 57	0	0
63	2E	32	Total O 32 32	0	0
63	2F	27	Total O 27 27	0	0
63	2G	6	Total O 6 6	0	0
63	2H	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	2I	4	Total O 4 4	0	0
63	2N	6	Total O 6 6	0	0
63	2O	21	Total O 21 21	0	0
63	2P	24	Total O 24 24	0	0
63	2Q	17	Total O 17 17	0	0
63	2R	16	Total O 16 16	0	0
63	2S	5	Total O 5 5	0	0
63	2T	13	Total O 13 13	0	0
63	2U	16	Total O 16 16	0	0
63	2V	5	Total O 5 5	0	0
63	2W	17	Total O 17 17	0	0
63	2X	8	Total O 8 8	0	0
63	2Y	5	Total O 5 5	0	0
63	2Z	11	Total O 11 11	0	0
63	20	11	Total O 11 11	0	0
63	21	20	Total O 20 20	0	0
63	22	1	Total O 1 1	0	0
63	23	3	Total O 3 3	0	0
63	25	13	Total O 13 13	0	0
63	26	5	Total O 5 5	0	0
63	27	9	Total O 9 9	0	0

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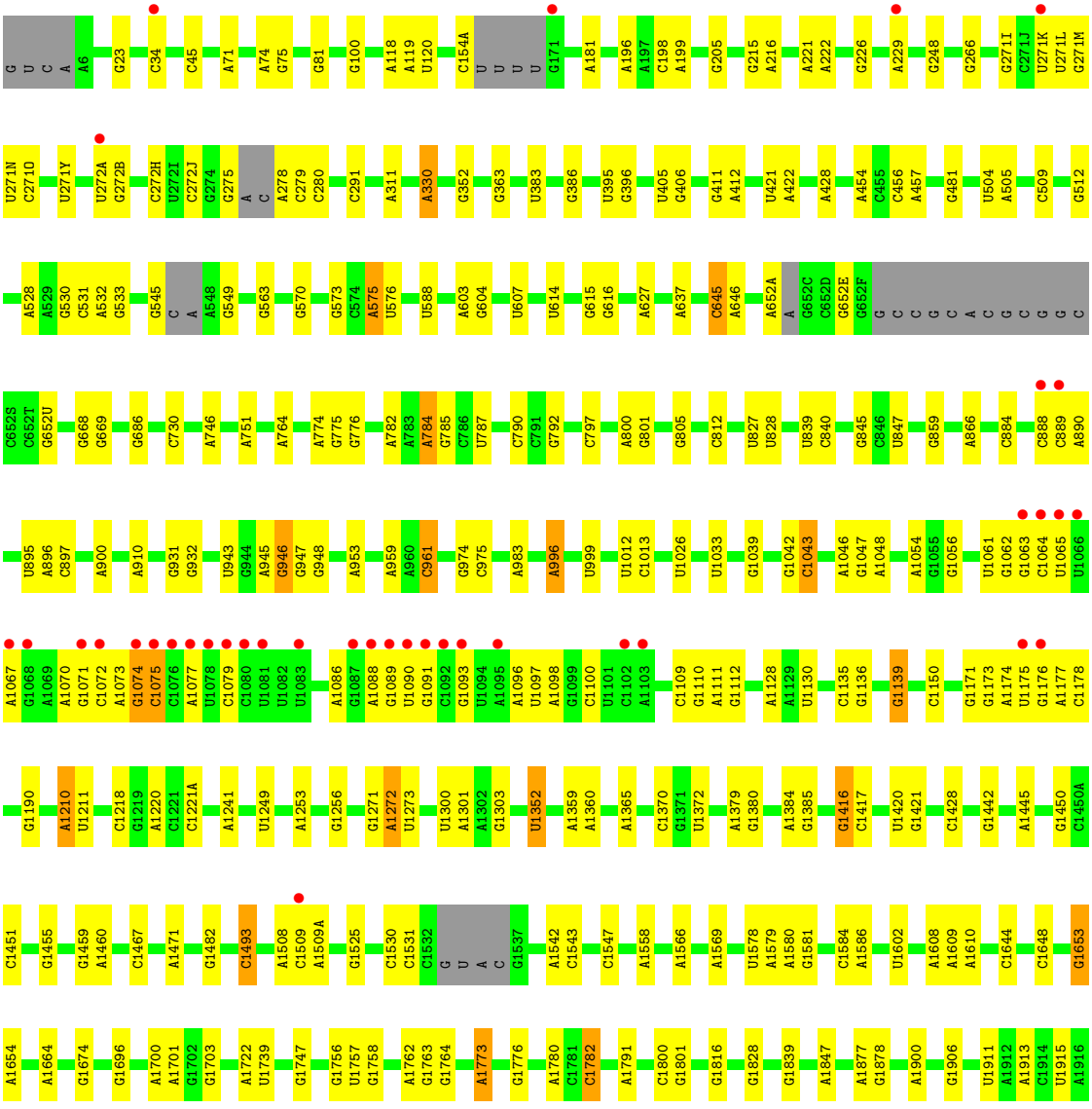
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	28	11	Total O 11 11	0	0
63	29	2	Total O 2 2	0	0
63	2a	317	Total O 317 317	0	0
63	2d	2	Total O 2 2	0	0
63	2e	1	Total O 1 1	0	0
63	2f	3	Total O 3 3	0	0
63	2j	2	Total O 2 2	0	0
63	2l	2	Total O 2 2	0	0
63	2n	2	Total O 2 2	0	0
63	2o	4	Total O 4 4	0	0
63	2p	2	Total O 2 2	0	0
63	2r	3	Total O 3 3	0	0
63	2t	2	Total O 2 2	0	0
63	2y	3	Total O 3 3	0	0
63	2w	3	Total O 3 3	0	0
63	2x	3	Total O 3 3	0	0

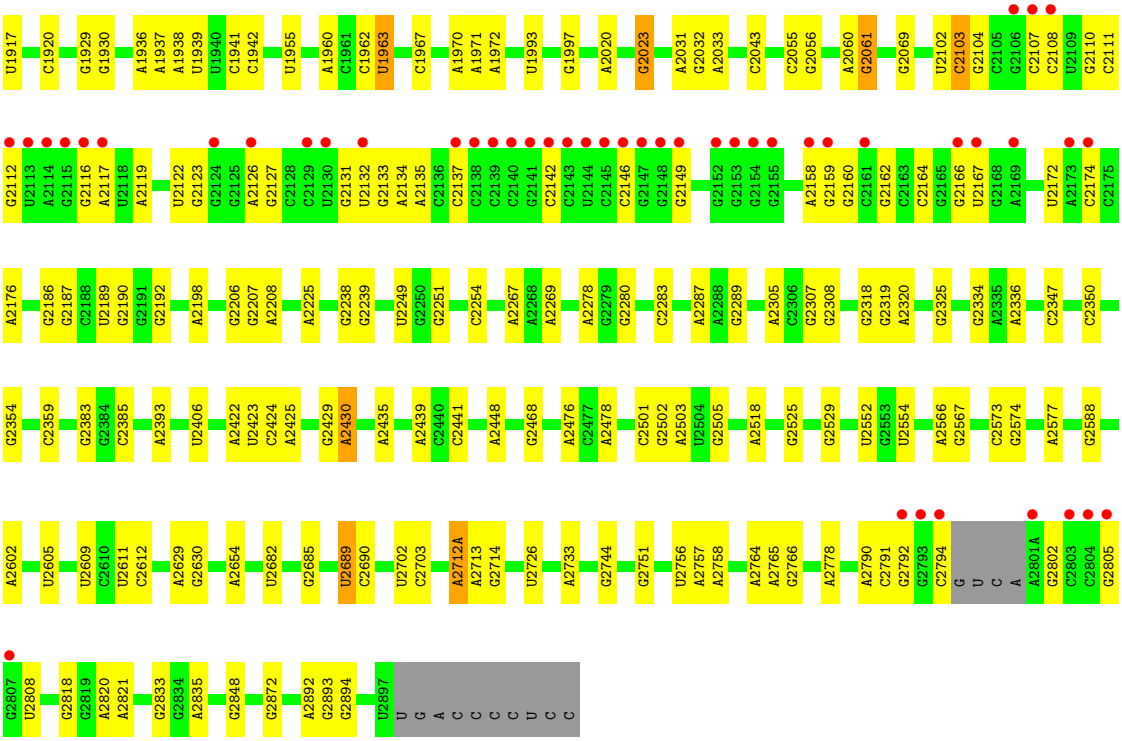
3 Residue-property plots (i)

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

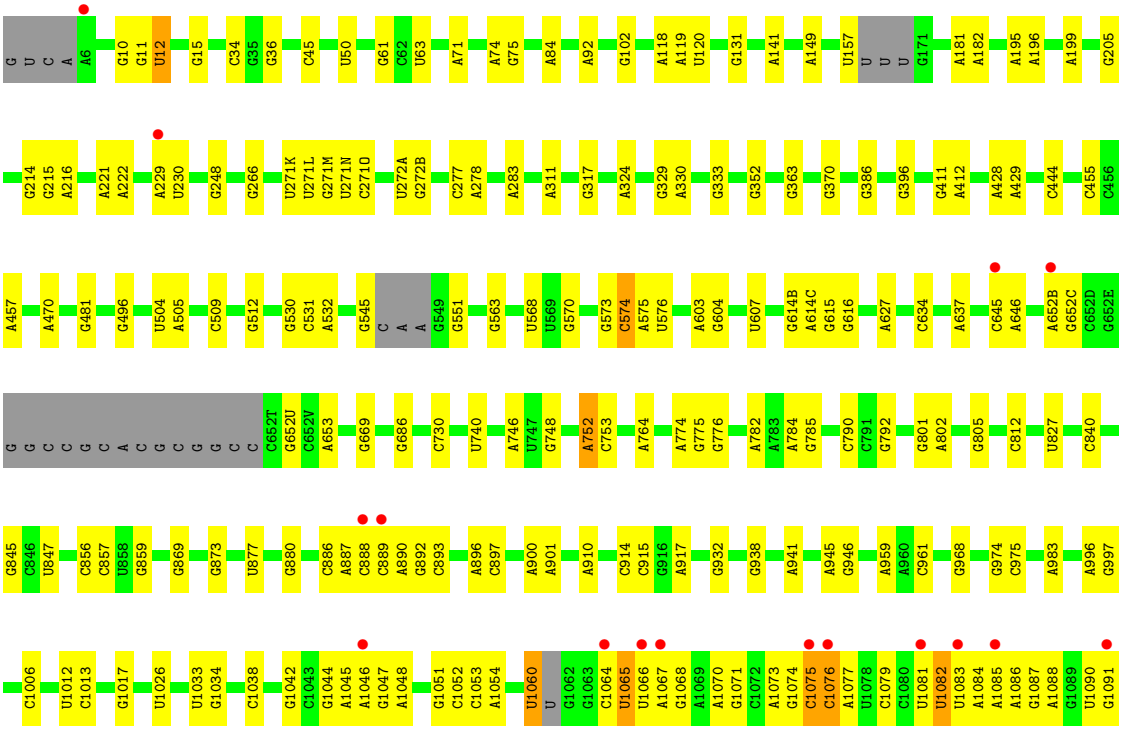
Chain 1A:

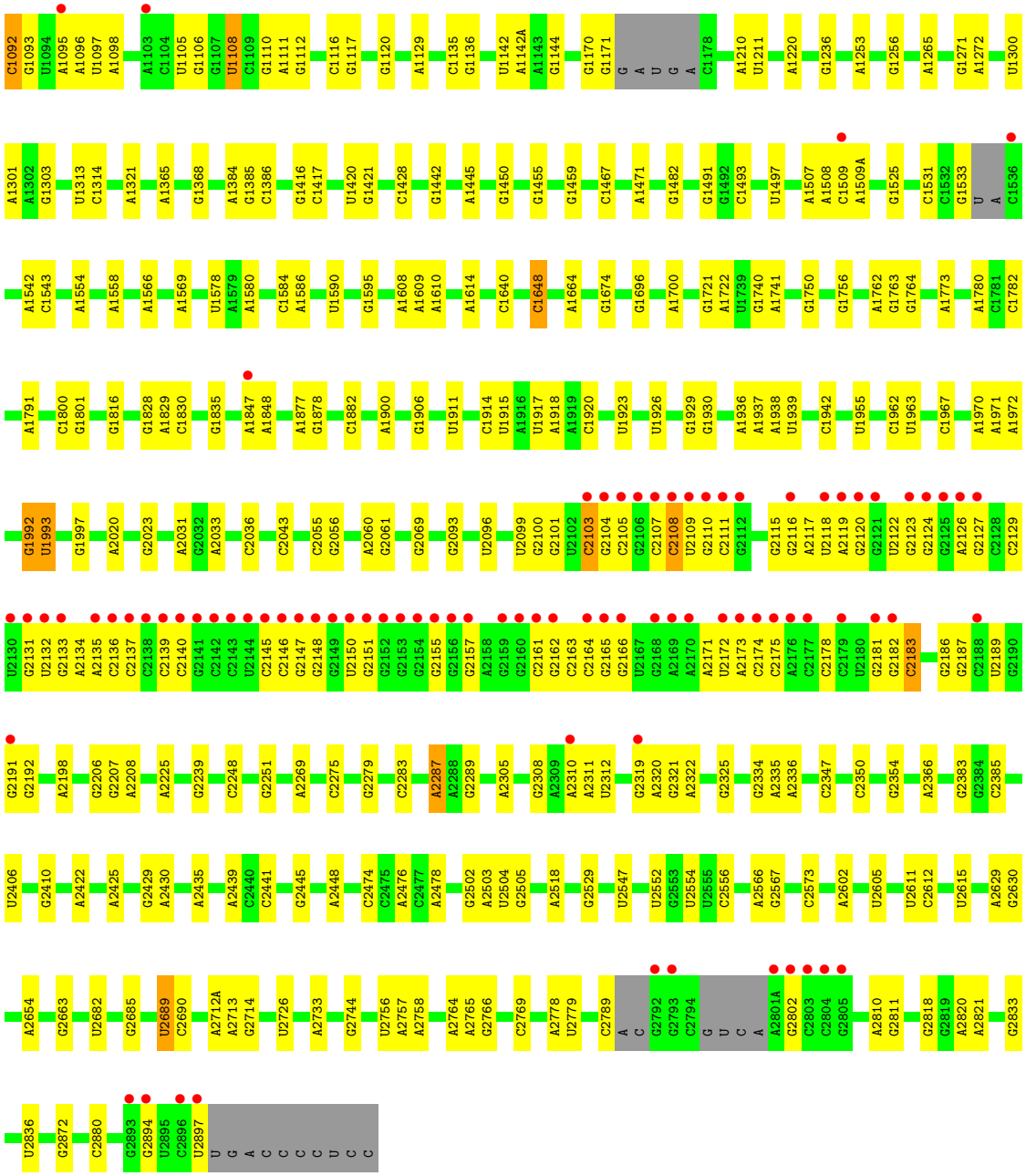




• Molecule 1: 23S Ribosomal RNA

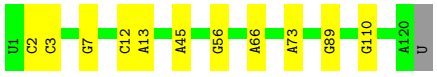
Chain 2A:





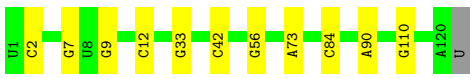
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



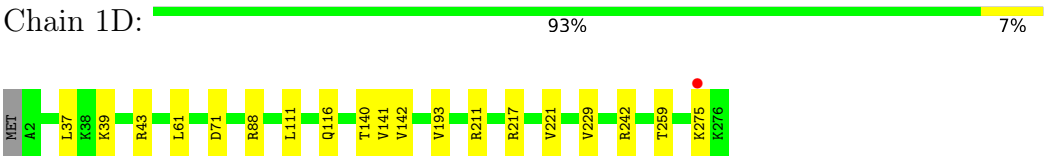
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



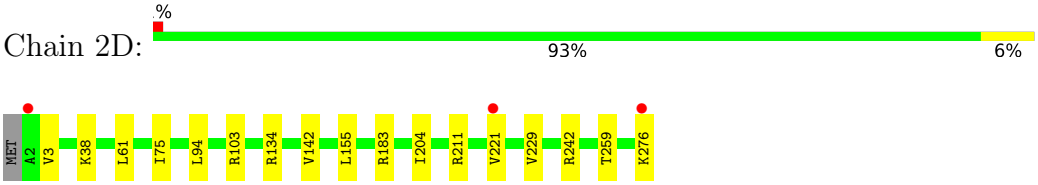
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



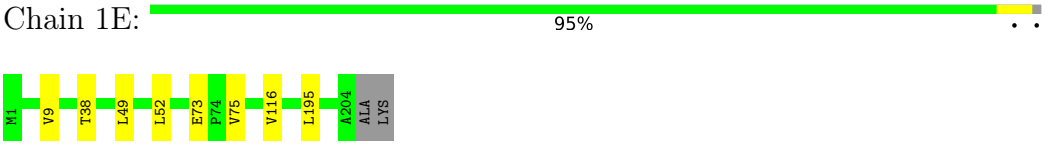
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



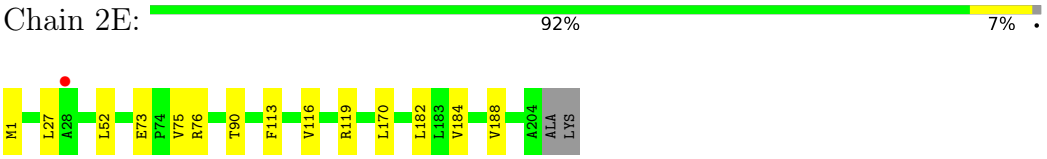
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



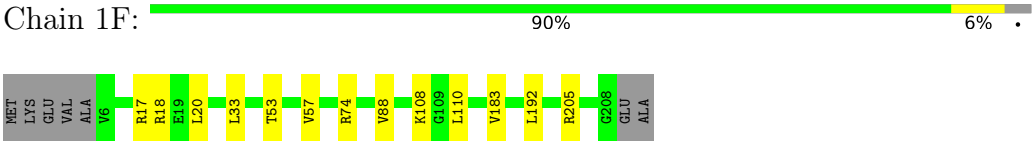
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



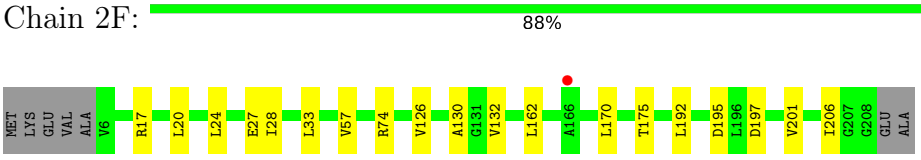
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



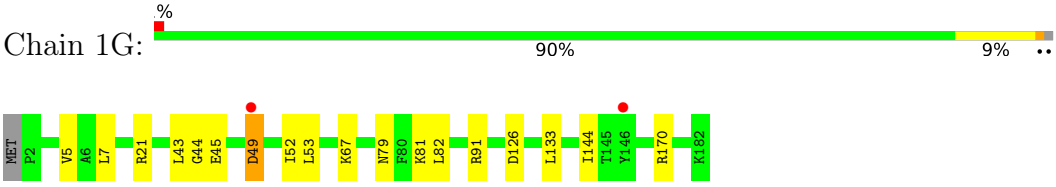
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



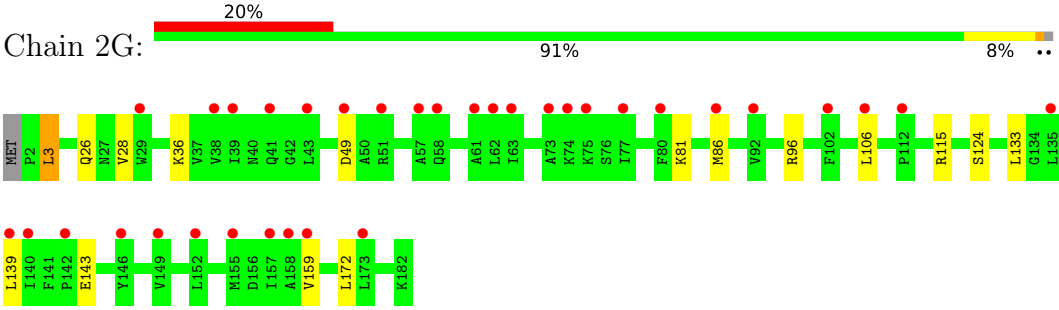
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



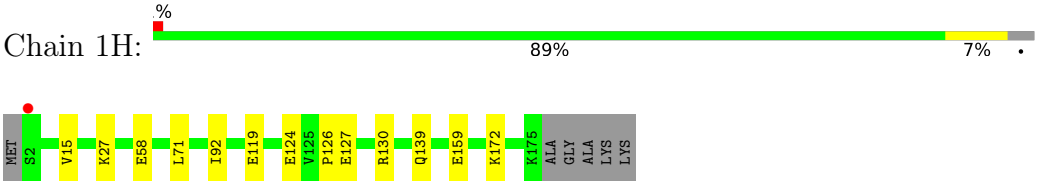
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



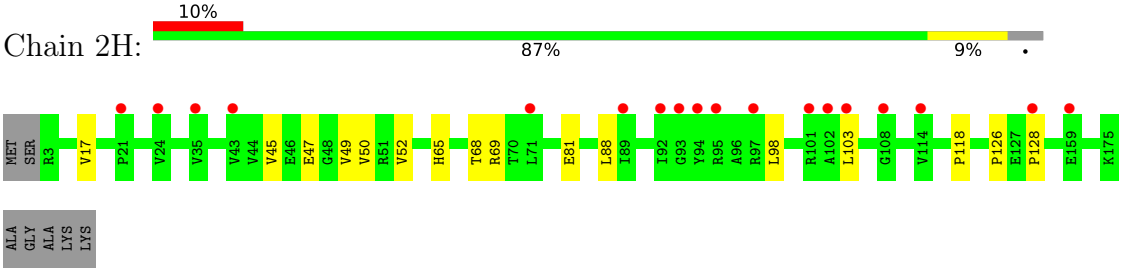
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



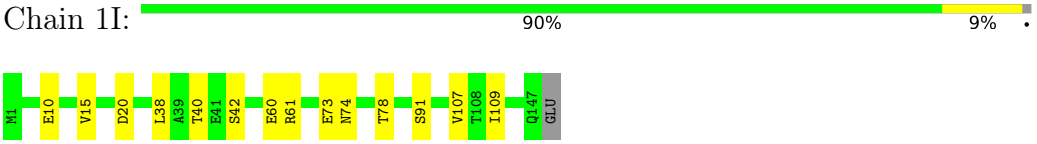
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



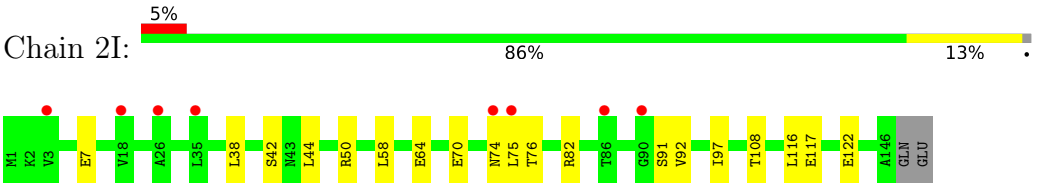
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



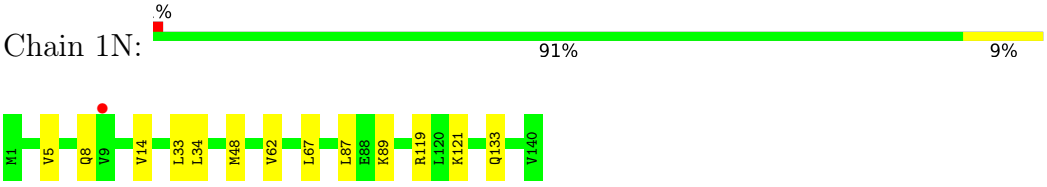
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



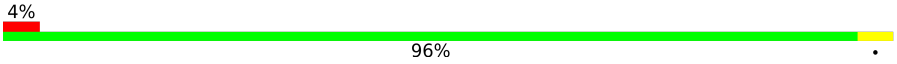
• Molecule 9: 50S ribosomal protein L13

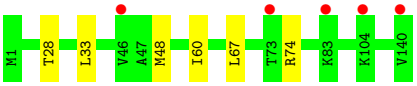
Chain 1N:



• Molecule 9: 50S ribosomal protein L13

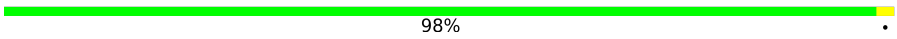
Chain 2N:





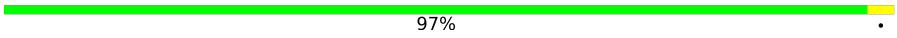
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



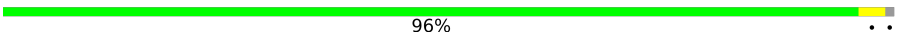
• Molecule 10: 50S ribosomal protein L14

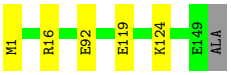
Chain 2O:



• Molecule 11: 50S ribosomal protein L15

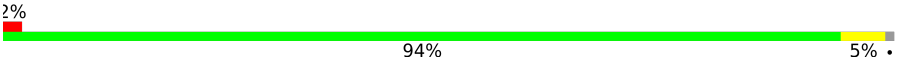
Chain 1P:

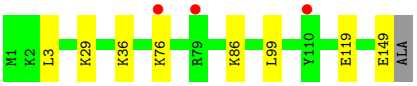




• Molecule 11: 50S ribosomal protein L15

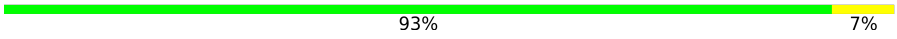
Chain 2P:

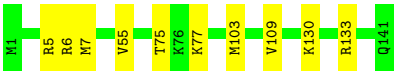




• Molecule 12: 50S ribosomal protein L16

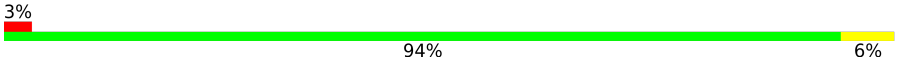
Chain 1Q:

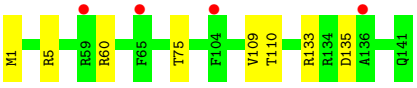




• Molecule 12: 50S ribosomal protein L16

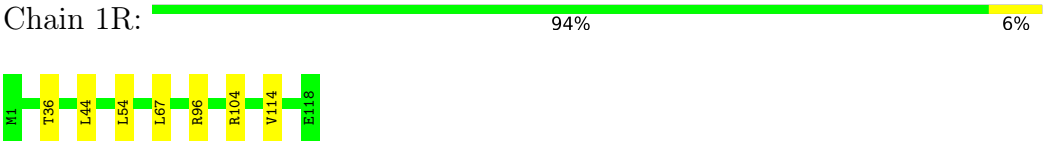
Chain 2Q:





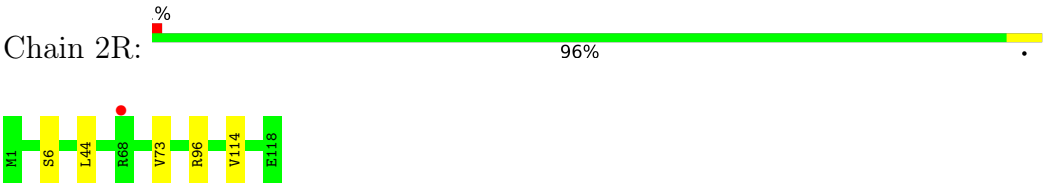
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



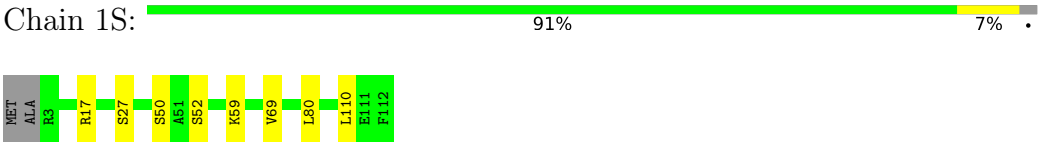
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



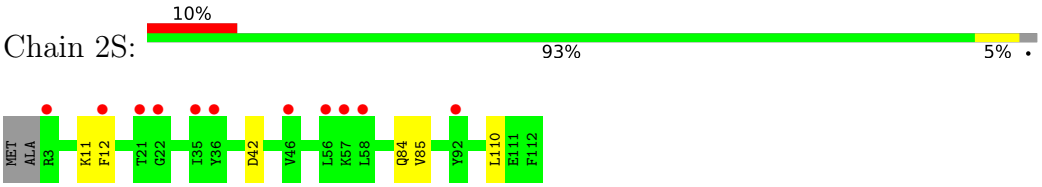
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



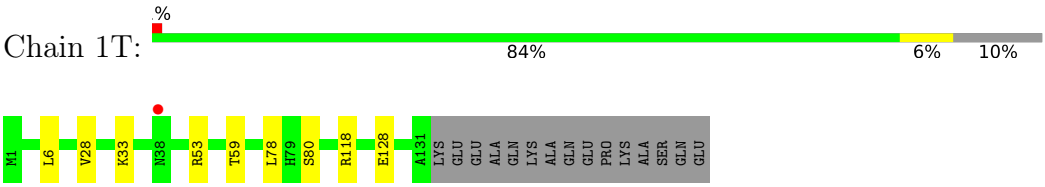
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



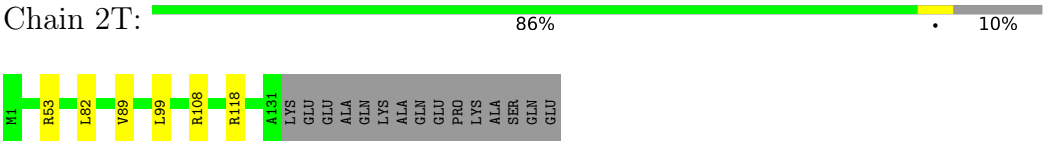
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



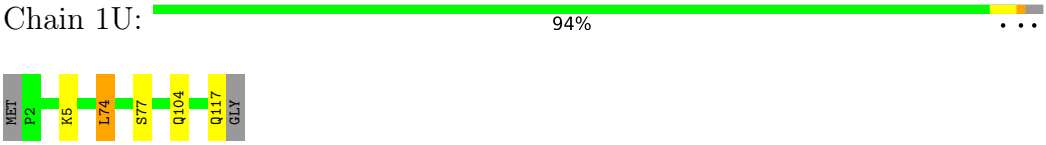
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



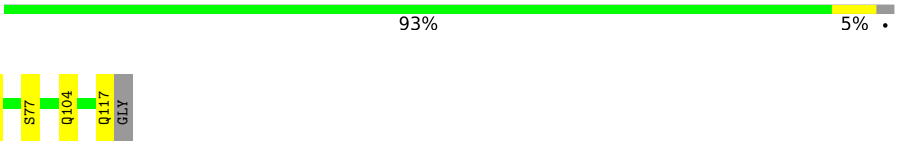
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



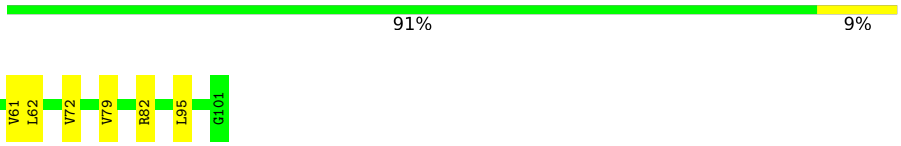
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



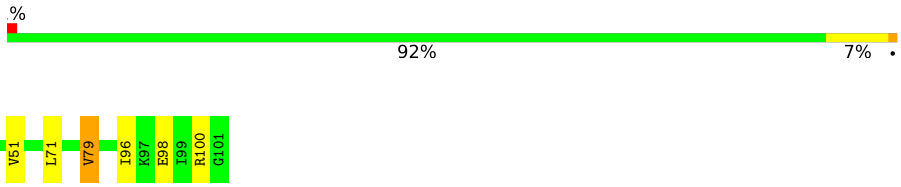
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



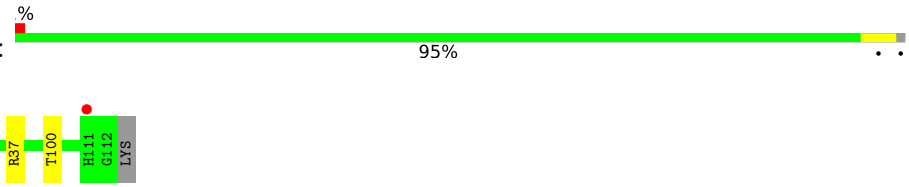
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



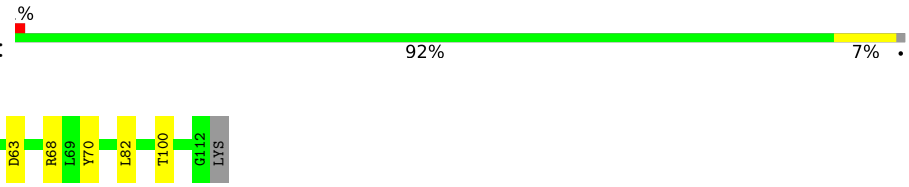
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



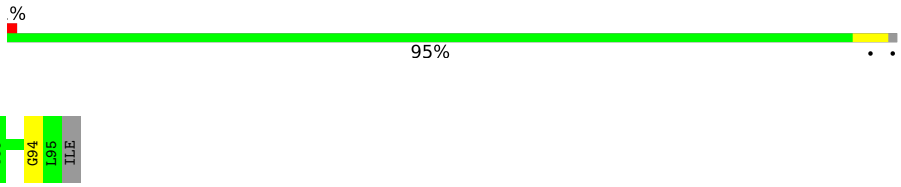
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



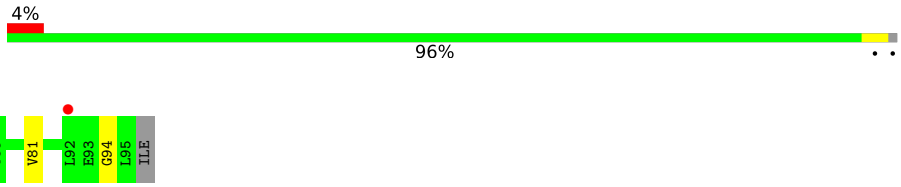
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



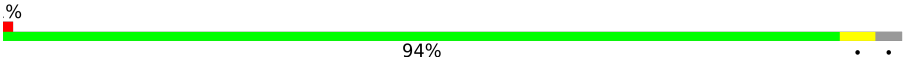
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



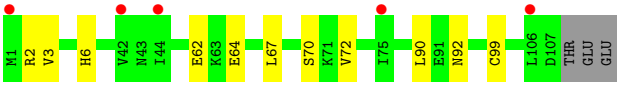
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



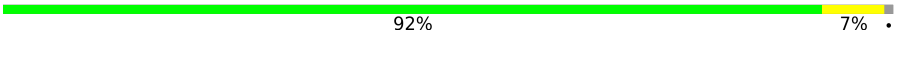
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



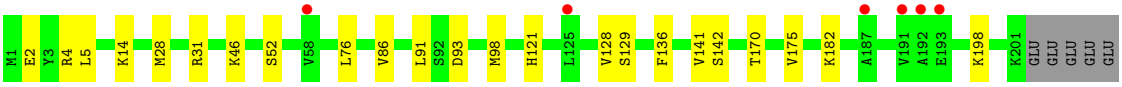
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



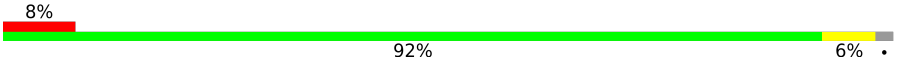
• Molecule 21: 50S ribosomal protein L25

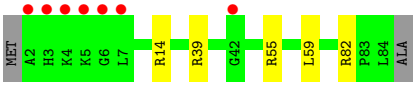
Chain 2Z:



• Molecule 22: 50S ribosomal protein L27

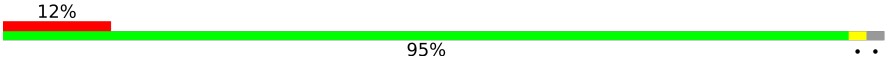
Chain 10:

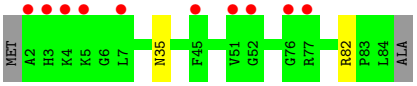




• Molecule 22: 50S ribosomal protein L27

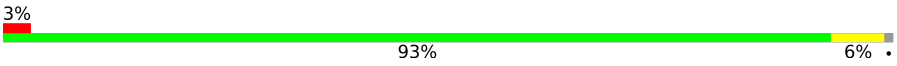
Chain 20:

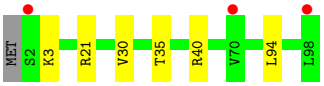




• Molecule 23: 50S ribosomal protein L28

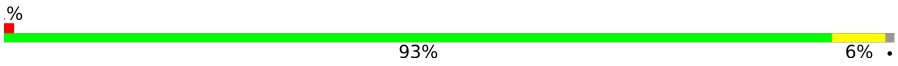
Chain 11:





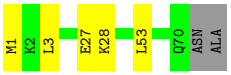
• Molecule 23: 50S ribosomal protein L28

Chain 21:



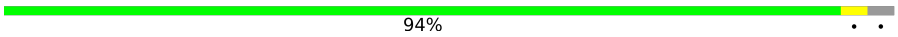
• Molecule 24: 50S ribosomal protein L29

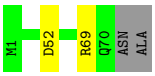
Chain 12:



• Molecule 24: 50S ribosomal protein L29

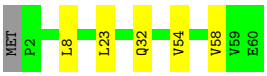
Chain 22:





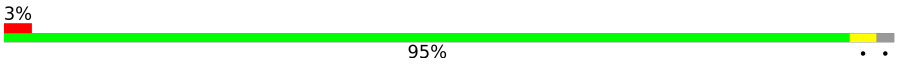
• Molecule 25: 50S ribosomal protein L30

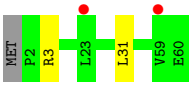
Chain 13:



• Molecule 25: 50S ribosomal protein L30

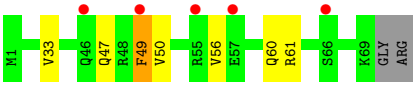
Chain 23:





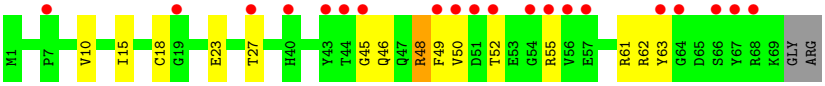
• Molecule 26: 50S ribosomal protein L31

Chain 14:

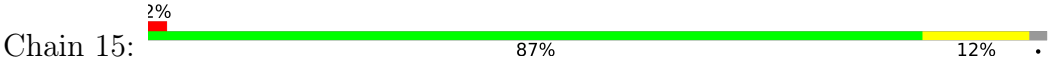


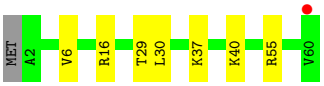
• Molecule 26: 50S ribosomal protein L31

Chain 24:

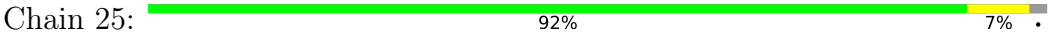


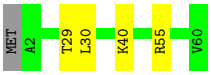
• Molecule 27: 50S ribosomal protein L32



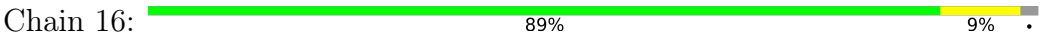


• Molecule 27: 50S ribosomal protein L32

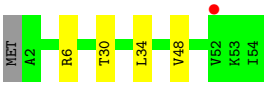




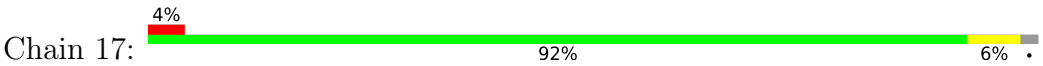
• Molecule 28: 50S ribosomal protein L33

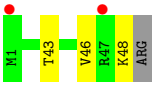


• Molecule 28: 50S ribosomal protein L33

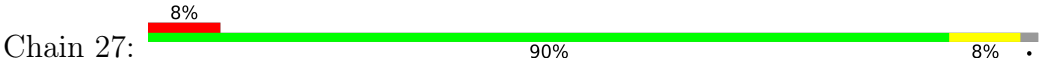


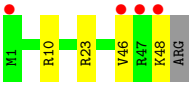
• Molecule 29: 50S ribosomal protein L34





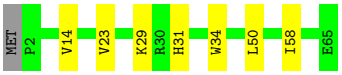
• Molecule 29: 50S ribosomal protein L34





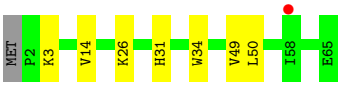
• Molecule 30: 50S ribosomal protein L35

Chain 18:



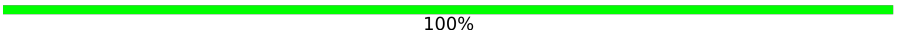
• Molecule 30: 50S ribosomal protein L35

Chain 28:



• Molecule 31: 50S ribosomal protein L36

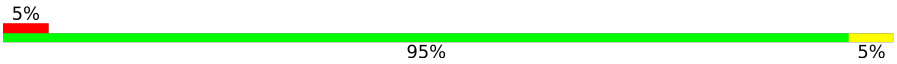
Chain 19:

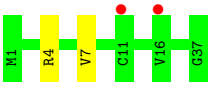


There are no outlier residues recorded for this chain.

• Molecule 31: 50S ribosomal protein L36

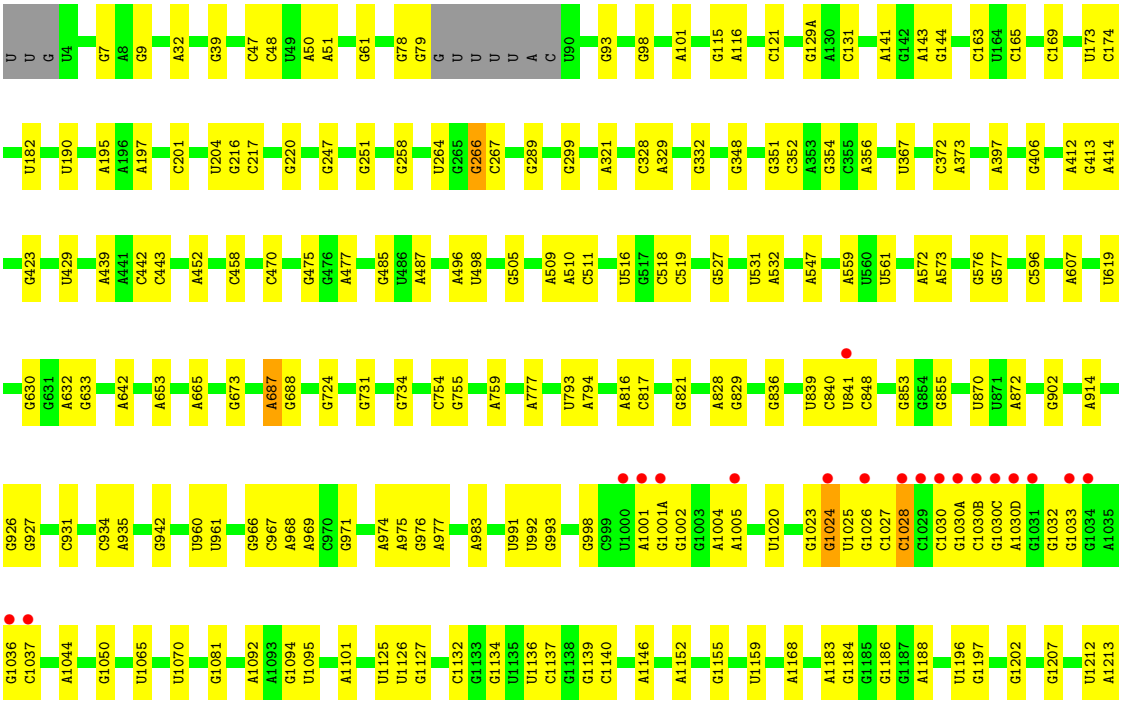
Chain 29:

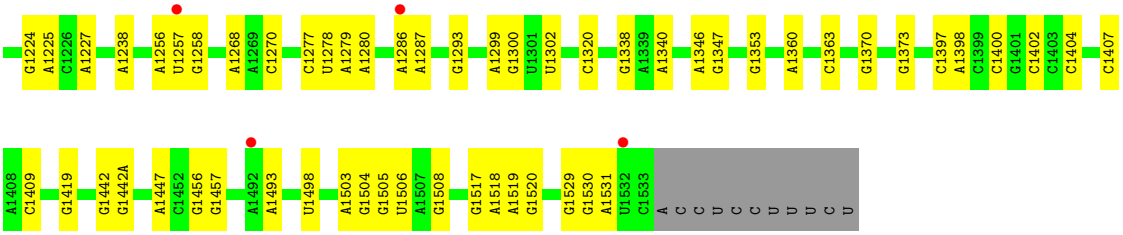




• Molecule 32: 16S Ribosomal RNA

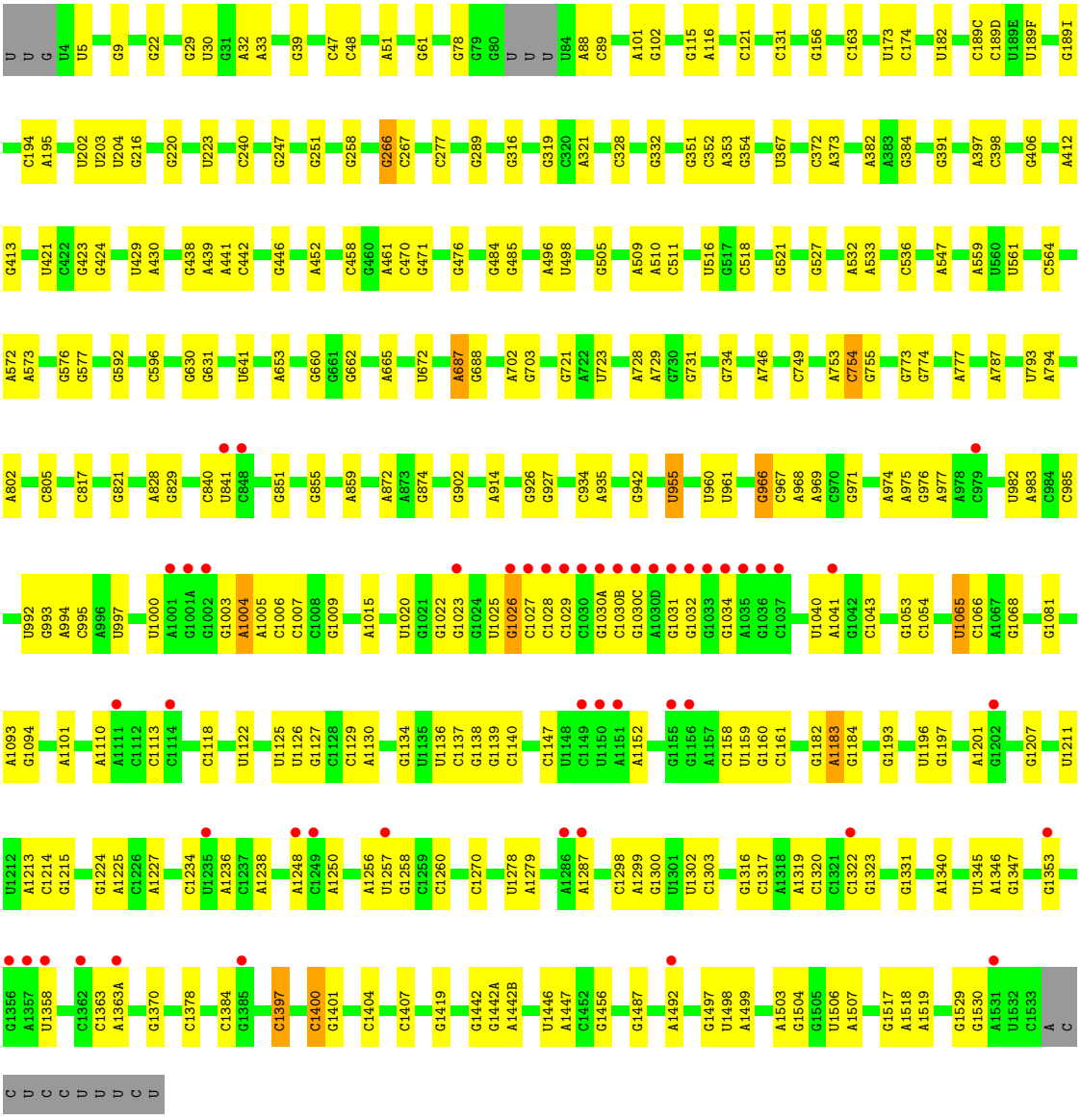
Chain 1a:





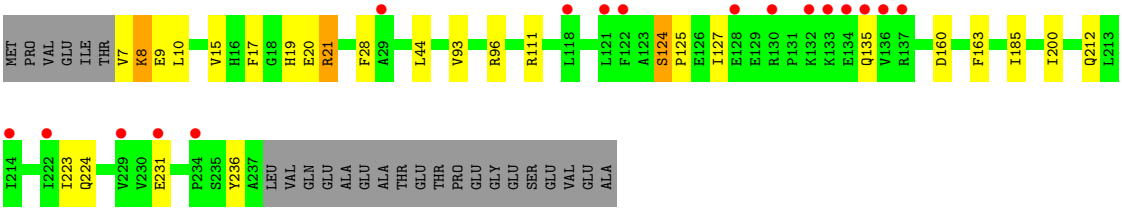
• Molecule 32: 16S Ribosomal RNA

Chain 2a:



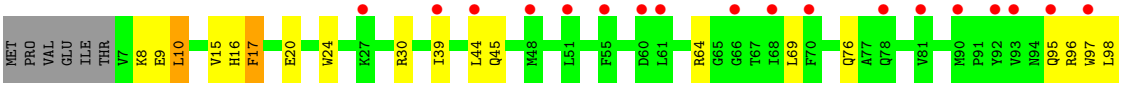
• Molecule 33: 30S ribosomal protein S2

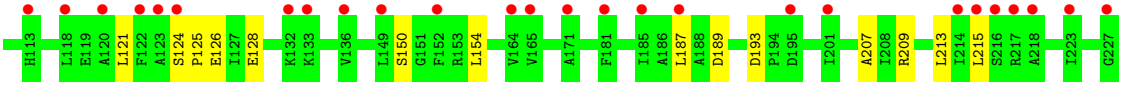
Chain 1b:

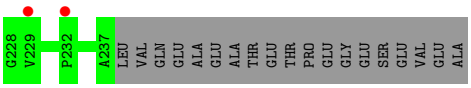


• Molecule 33: 30S ribosomal protein S2

Chain 2b:

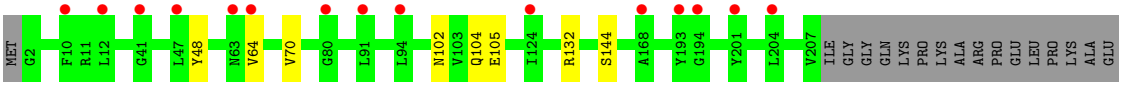






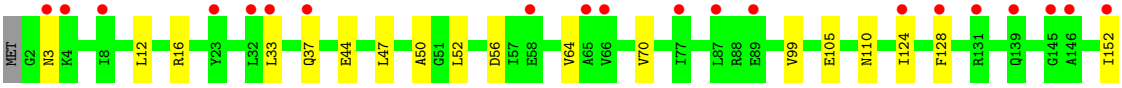
• Molecule 34: 30S ribosomal protein S3

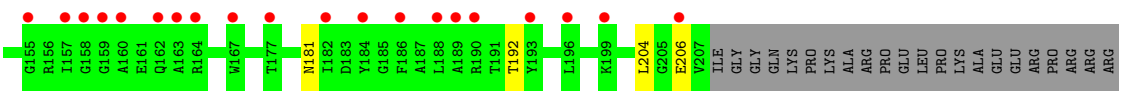
Chain 1c:



• Molecule 34: 30S ribosomal protein S3

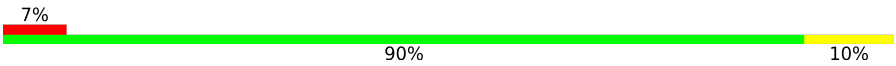
Chain 2c:





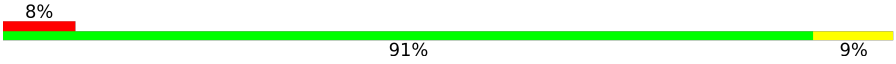
• Molecule 35: 30S ribosomal protein S4

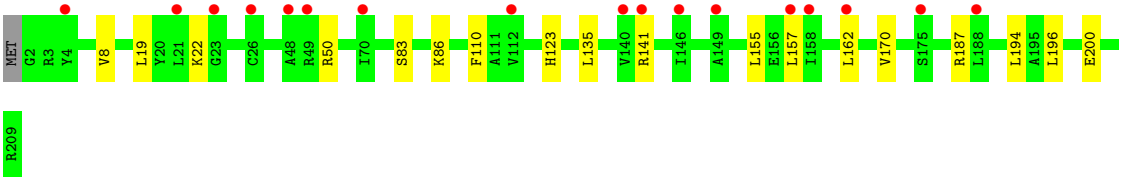
Chain 1d:



• Molecule 35: 30S ribosomal protein S4

Chain 2d:



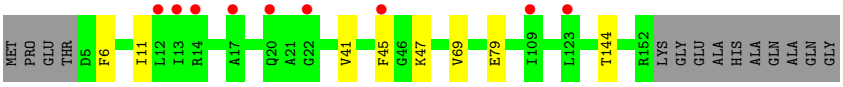


• Molecule 36: 30S ribosomal protein S5

Chain 1e:

• Molecule 36: 30S ribosomal protein S5

Chain 2e:

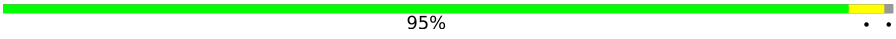


• Molecule 37: 30S ribosomal protein S6

Chain 1f:

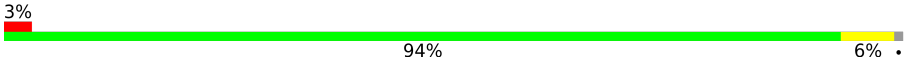
• Molecule 37: 30S ribosomal protein S6

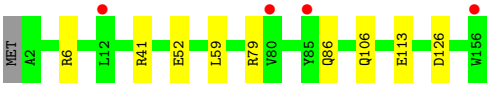
Chain 2f:



• Molecule 38: 30S ribosomal protein S7

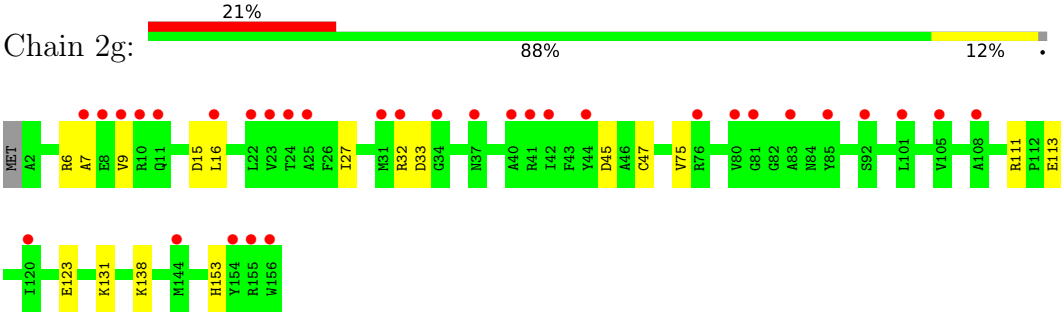
Chain 1g:





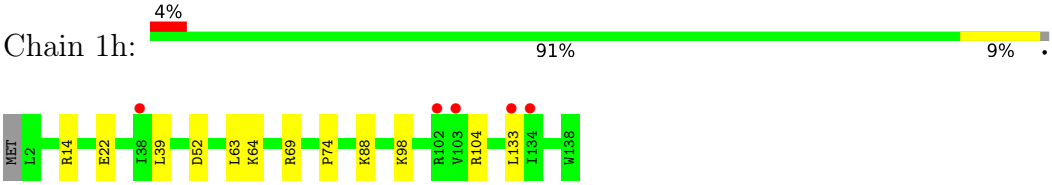
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



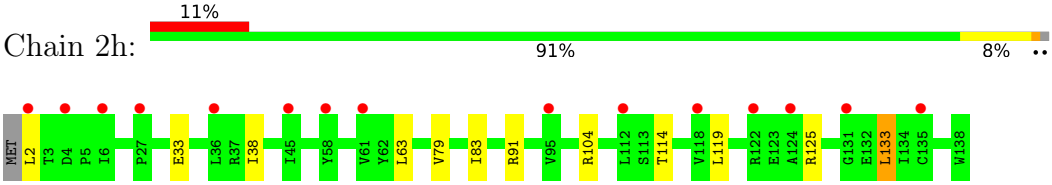
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



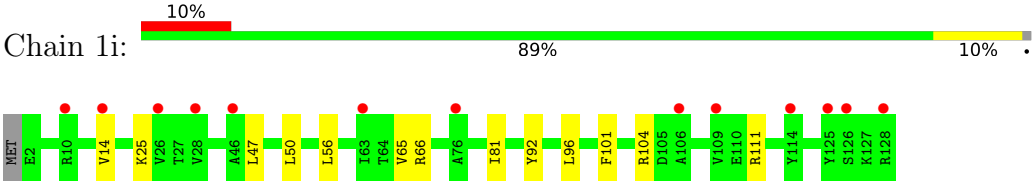
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



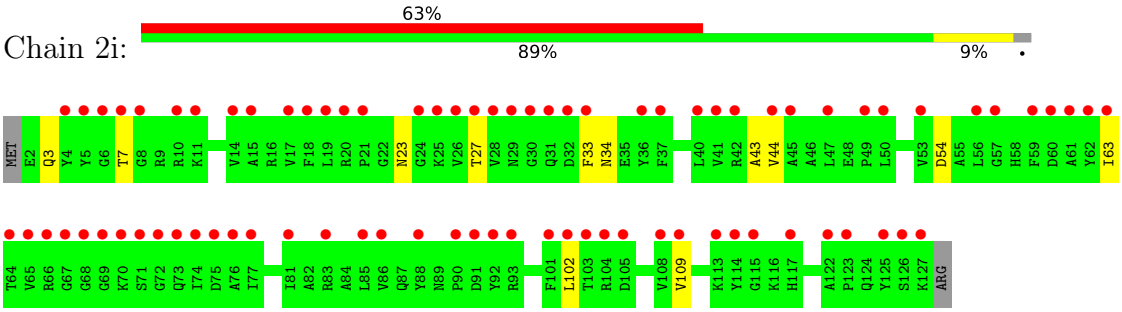
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



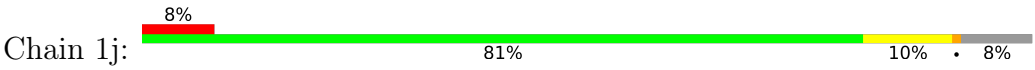
• Molecule 40: 30S ribosomal protein S9

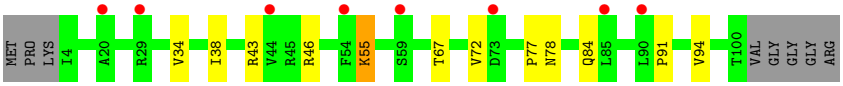
Chain 2i:



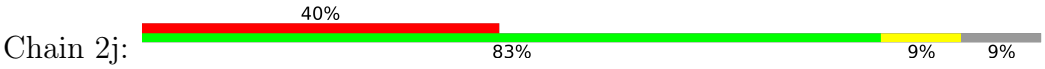
• Molecule 41: 30S ribosomal protein S10

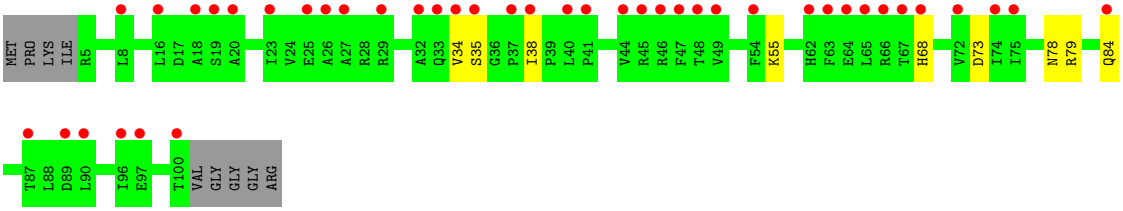
Chain 1j:



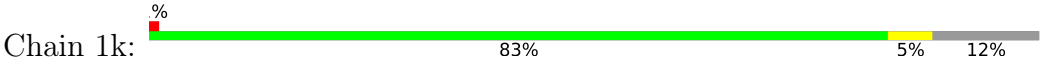


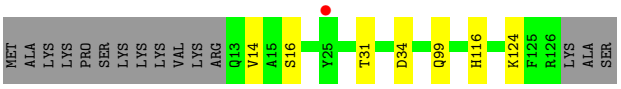
• Molecule 41: 30S ribosomal protein S10



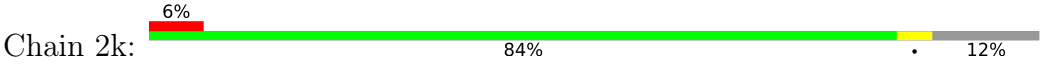


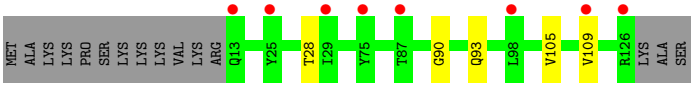
• Molecule 42: 30S ribosomal protein S11



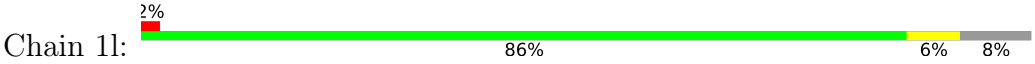


• Molecule 42: 30S ribosomal protein S11

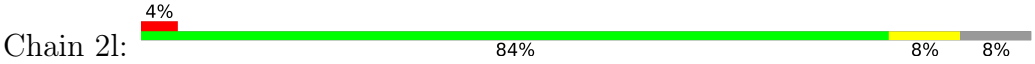




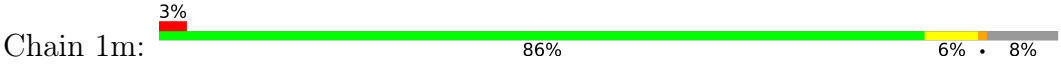
• Molecule 43: 30S ribosomal protein S12

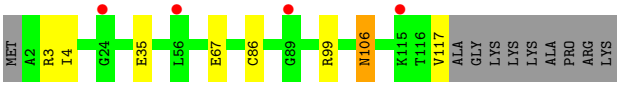


• Molecule 43: 30S ribosomal protein S12



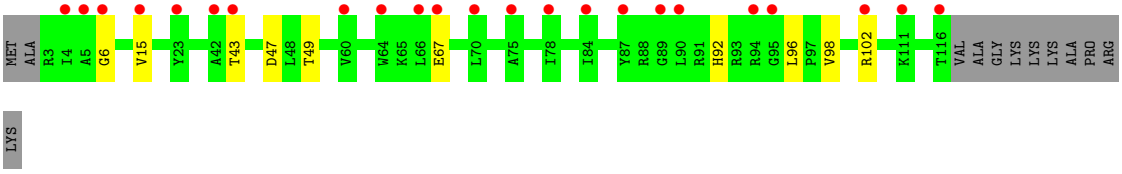
• Molecule 44: 30S ribosomal protein S13





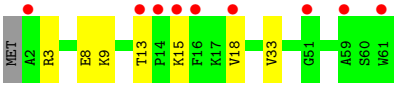
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



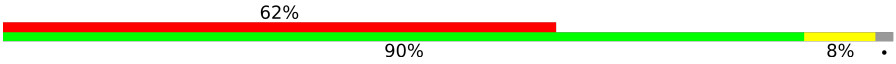
• Molecule 45: 30S ribosomal protein S14 type Z

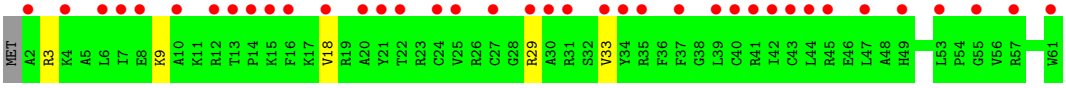
Chain 1n:



• Molecule 45: 30S ribosomal protein S14 type Z

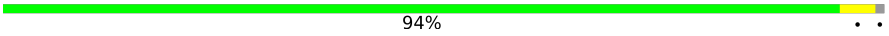
Chain 2n:

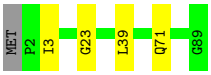




• Molecule 46: 30S ribosomal protein S15

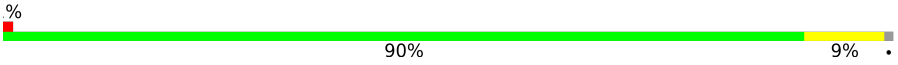
Chain 1o:

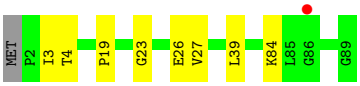




• Molecule 46: 30S ribosomal protein S15

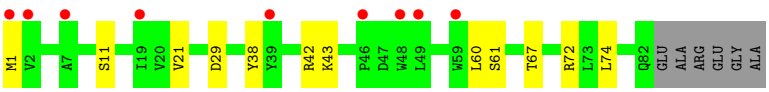
Chain 2o:





• Molecule 47: 30S ribosomal protein S16

Chain 1p:

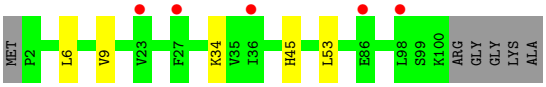


• Molecule 47: 30S ribosomal protein S16

Chain 2p:

• Molecule 48: 30S ribosomal protein S17

Chain 1q:

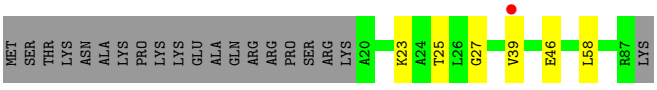


• Molecule 48: 30S ribosomal protein S17

Chain 2q:

• Molecule 49: 30S ribosomal protein S18

Chain 1r:



• Molecule 49: 30S ribosomal protein S18

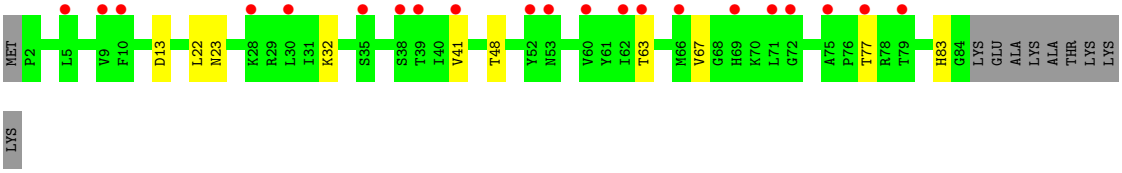
Chain 2r:

• Molecule 50: 30S ribosomal protein S19

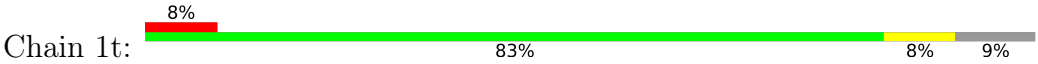
Chain 1s:

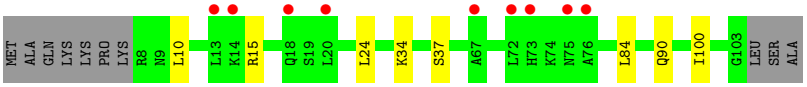
• Molecule 50: 30S ribosomal protein S19

Chain 2s:

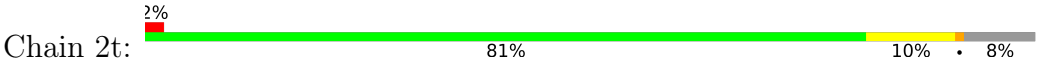


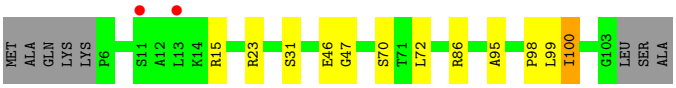
• Molecule 51: 30S ribosomal protein S20



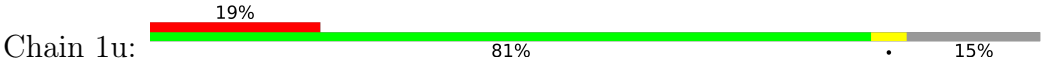


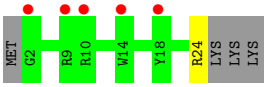
• Molecule 51: 30S ribosomal protein S20



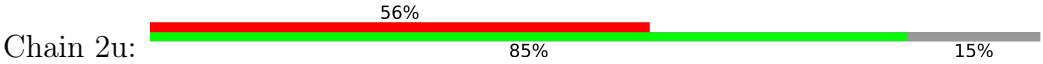


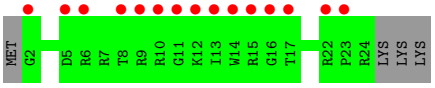
• Molecule 52: 30S ribosomal protein Thx



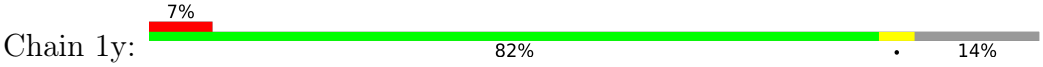


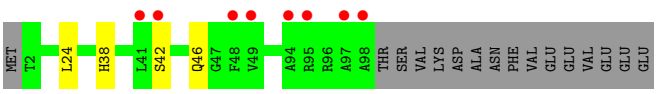
• Molecule 52: 30S ribosomal protein Thx



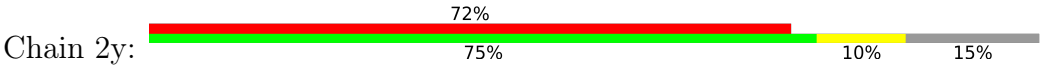


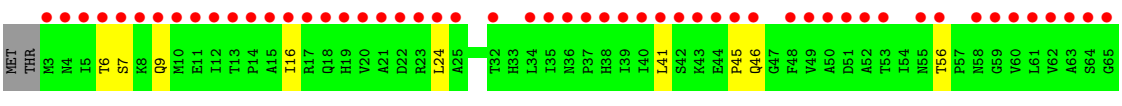
• Molecule 53: Ribosome-associated inhibitor A

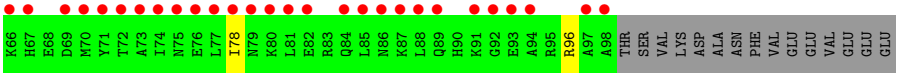




• Molecule 53: Ribosome-associated inhibitor A







• Molecule 54: A-site Deacylated tRNA Analog

Chain 1w:

• Molecule 54: A-site Deacylated tRNA Analog

Chain 2w:

• Molecule 55: P-site Peptidyl-tRNA Analog RNA

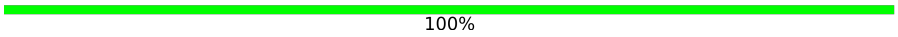
Chain 1x:

• Molecule 55: P-site Peptidyl-tRNA Analog RNA

Chain 2x:

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

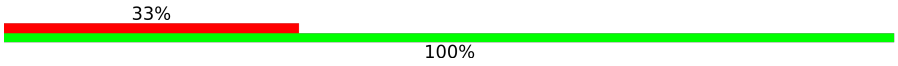
Chain 1v:



There are no outlier residues recorded for this chain.

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

Chain 2v:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.81Å 449.56Å 621.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	211.38 – 2.40 310.74 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (211.38-2.40) 99.7 (310.74-2.40)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.225 , 0.269 0.225 , 0.269	Depositor DCC
R_{free} test set	112792 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	297868	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, PSU, 2MG, 8AN, 5MC, 2MA, 0TD, CLM, OMC, 5MU, MG, 4OC, OMU, OMG, ZN, SF4, M2G, MPD, G7M, 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	0.50	0/69031	0.98	90/107754 (0.1%)
1	2A	0.39	0/68903	0.88	48/107552 (0.0%)
2	1B	0.41	0/2876	0.90	0/4486
2	2B	0.34	0/2878	0.83	0/4490
3	1D	0.34	0/2181	0.57	0/2940
3	2D	0.30	0/2186	0.53	0/2944
4	1E	0.32	0/1592	0.52	0/2149
4	2E	0.30	0/1592	0.52	0/2149
5	1F	0.33	0/1619	0.54	0/2193
5	2F	0.30	0/1615	0.51	0/2188
6	1G	0.30	0/1451	0.49	0/1961
6	2G	0.29	0/1449	0.49	0/1957
7	1H	0.30	0/1356	0.50	0/1834
7	2H	0.28	0/1350	0.47	0/1826
8	1I	0.28	0/1109	0.51	0/1512
8	2I	0.28	0/1091	0.47	0/1490
9	1N	0.33	0/1148	0.52	0/1547
9	2N	0.28	0/1144	0.46	0/1543
10	1O	0.34	0/943	0.54	0/1269
10	2O	0.31	0/943	0.54	0/1269
11	1P	0.32	0/1152	0.55	0/1533
11	2P	0.31	0/1152	0.54	0/1533
12	1Q	0.34	0/1143	0.52	0/1527
12	2Q	0.30	0/1143	0.47	0/1527
13	1R	0.31	0/982	0.56	0/1312
13	2R	0.28	0/982	0.49	0/1312
14	1S	0.31	0/887	0.52	0/1180
14	2S	0.29	0/880	0.51	0/1172
15	1T	0.32	0/1105	0.52	0/1477
15	2T	0.29	0/1097	0.48	0/1468
16	1U	0.34	0/977	0.52	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.28	0/977	0.45	0/1301
17	1V	0.37	0/786	0.58	0/1053
17	2V	0.29	0/782	0.51	0/1049
18	1W	0.37	0/897	0.53	0/1205
18	2W	0.29	0/897	0.48	0/1205
19	1X	0.36	0/764	0.54	0/1025
19	2X	0.29	0/764	0.50	0/1025
20	1Y	0.32	0/823	0.56	0/1099
20	2Y	0.29	0/823	0.50	0/1100
21	1Z	0.30	0/1620	0.49	0/2200
21	2Z	0.29	0/1590	0.48	0/2162
22	10	0.34	0/662	0.56	0/881
22	20	0.30	0/659	0.52	0/877
23	11	0.32	0/761	0.49	0/1013
23	21	0.31	0/766	0.52	0/1018
24	12	0.29	0/590	0.49	0/781
24	22	0.30	0/594	0.45	0/785
25	13	0.32	0/474	0.53	0/635
25	23	0.26	0/469	0.47	0/630
26	14	0.30	0/559	0.55	0/754
26	24	0.33	0/549	0.56	0/741
27	15	0.35	0/473	0.61	0/639
27	25	0.28	0/469	0.52	0/635
28	16	0.31	0/460	0.54	0/613
28	26	0.30	0/456	0.48	0/608
29	17	0.35	0/426	0.56	0/561
29	27	0.28	0/426	0.50	0/561
30	18	0.34	0/525	0.54	0/691
30	28	0.30	0/525	0.48	0/691
31	19	0.35	0/310	0.52	0/407
31	29	0.29	0/310	0.53	0/407
32	1a	0.35	0/35795	0.86	9/55864 (0.0%)
32	2a	0.35	0/35890	0.87	25/56012 (0.0%)
33	1b	0.30	0/1876	0.48	0/2533
33	2b	0.31	0/1860	0.51	0/2518
34	1c	0.29	0/1582	0.47	0/2137
34	2c	0.28	0/1566	0.46	0/2119
35	1d	0.28	0/1695	0.49	0/2274
35	2d	0.28	0/1698	0.47	0/2277
36	1e	0.29	0/1149	0.49	0/1548
36	2e	0.29	0/1149	0.47	0/1548
37	1f	0.29	0/827	0.47	0/1120
37	2f	0.28	0/829	0.46	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.28	0/1254	0.44	0/1683
38	2g	0.28	0/1248	0.41	0/1676
39	1h	0.27	0/1118	0.48	0/1506
39	2h	0.28	0/1108	0.46	0/1494
40	1i	0.29	0/1005	0.49	0/1351
40	2i	0.31	0/985	0.49	0/1329
41	1j	0.27	0/732	0.47	0/993
41	2j	0.28	0/723	0.50	0/984
42	1k	0.27	0/849	0.49	0/1150
42	2k	0.28	0/848	0.52	0/1149
43	1l	0.29	0/937	0.51	0/1260
43	2l	0.28	0/937	0.50	0/1260
44	1m	0.27	0/924	0.48	0/1242
44	2m	0.29	0/905	0.49	0/1217
45	1n	0.29	0/501	0.44	0/664
45	2n	0.28	0/501	0.44	0/664
46	1o	0.28	0/739	0.41	0/985
46	2o	0.27	0/739	0.40	0/985
47	1p	0.28	0/697	0.52	0/939
47	2p	0.28	0/693	0.50	0/935
48	1q	0.28	0/836	0.47	0/1117
48	2q	0.28	0/836	0.48	0/1117
49	1r	0.29	0/560	0.48	0/746
49	2r	0.29	0/560	0.47	0/746
50	1s	0.27	0/663	0.50	0/895
50	2s	0.31	0/660	0.49	0/893
51	1t	0.27	0/734	0.41	0/969
51	2t	0.28	0/736	0.43	0/976
52	1u	0.28	0/203	0.48	0/266
52	2u	0.26	0/203	0.52	0/266
53	1y	0.27	0/776	0.47	0/1048
53	2y	0.28	0/761	0.46	0/1030
54	1w	0.66	0/69	1.10	0/106
54	2w	0.34	0/69	0.90	0/106
55	1x	0.42	0/44	1.05	0/67
55	2x	0.32	0/44	0.89	0/67
56	1v	0.29	0/20	0.48	0/25
56	2v	0.22	0/20	0.40	0/25
All	All	0.38	0/310296	0.81	173/463751 (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	24	0	1
All	All	0	2

There are no bond length outliers.

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1042	G	OP1-P-O3'	-11.70	79.46	105.20
1	1A	2577	A	O5'-P-OP1	-10.84	95.94	105.70
1	1A	751	A	O5'-P-OP1	-10.37	96.37	105.70
1	1A	1139	G	O5'-P-OP2	-10.09	96.62	105.70
1	1A	948	G	O5'-P-OP1	-9.94	96.75	105.70
1	2A	1092	C	N1-C2-O2	9.75	124.75	118.90
1	1A	512	G	O4'-C1'-N9	9.58	115.86	108.20
1	1A	1075	C	N1-C2-O2	9.26	124.46	118.90
1	1A	1086	A	N1-C6-N6	-9.22	113.07	118.60
1	1A	1372	U	C5-C4-O4	-8.47	120.82	125.90
1	1A	588	U	O5'-P-OP2	-8.44	98.11	105.70
1	2A	1092	C	N3-C2-O2	-8.40	116.02	121.90
1	2A	1092	C	C2-N1-C1'	8.30	127.94	118.80
1	1A	801	G	O5'-P-OP2	-8.19	98.33	105.70
1	1A	2682	U	O5'-P-OP2	-8.14	98.37	105.70
1	1A	787	U	O5'-P-OP1	-8.11	98.40	105.70
1	1A	570	G	C5-C6-O6	-8.07	123.76	128.60
1	1A	1042	G	OP2-P-O3'	-8.02	87.55	105.20
1	1A	1043	C	OP1-P-OP2	7.93	131.49	119.60
1	1A	2249	U	N3-C4-O4	-7.87	113.89	119.40
32	2a	1004	A	O4'-C1'-N9	7.67	114.34	108.20
1	1A	1372	U	N3-C4-O4	7.67	124.77	119.40
1	2A	576	U	O5'-P-OP1	-7.54	98.92	105.70
1	2A	2108	C	C2-N3-C4	7.52	123.66	119.90
1	1A	1782	C	O5'-P-OP1	-7.52	98.94	105.70
1	2A	801	G	O5'-P-OP2	-7.51	98.94	105.70
1	1A	570	G	C5-C6-N1	7.50	115.25	111.50
1	2A	2036	C	O5'-P-OP1	-7.48	98.97	105.70
32	2a	266	G	P-O3'-C3'	7.38	128.55	119.70
1	1A	645	C	C2-N1-C1'	7.34	126.88	118.80
32	2a	1003	G	N3-C4-C5	-7.29	124.96	128.60
1	2A	1092	C	C6-N1-C2	-7.27	117.39	120.30
1	1A	800	A	O5'-P-OP1	-7.22	99.20	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	226	G	O4'-C1'-N9	7.01	113.81	108.20
32	1a	299	G	C5-C6-O6	-6.94	124.43	128.60
1	1A	2430	A	O5'-P-OP2	-6.91	99.48	105.70
1	1A	575	A	O5'-P-OP1	-6.82	99.57	105.70
32	1a	1028	C	C5-C6-N1	6.77	124.38	121.00
1	2A	752	A	P-O3'-C3'	6.74	127.79	119.70
32	2a	1397	C	C2-N1-C1'	6.71	126.19	118.80
1	2A	1614	A	O5'-P-OP1	-6.66	99.71	105.70
1	1A	999	U	O5'-P-OP2	-6.61	99.75	105.70
1	1A	645	C	N1-C2-O2	6.60	122.86	118.90
1	1A	1249	U	O5'-P-OP1	-6.48	99.86	105.70
1	2A	2181	G	C5-C6-O6	6.45	132.47	128.60
32	2a	955	U	C5-C4-O4	6.44	129.76	125.90
1	1A	2685	G	N1-C6-O6	-6.41	116.05	119.90
1	1A	1352	U	O5'-P-OP1	-6.37	99.97	105.70
1	1A	614	U	N3-C2-O2	-6.33	117.77	122.20
1	2A	512	G	O4'-C1'-N9	6.33	113.26	108.20
1	1A	570	G	N9-C4-C5	-6.26	102.89	105.40
1	1A	1653	G	C8-N9-C4	-6.25	103.90	106.40
1	1A	946	G	O5'-P-OP1	-6.25	100.08	105.70
1	1A	943	U	O5'-P-OP2	-6.21	100.11	105.70
1	2A	1060	U	C2-N1-C1'	6.21	125.15	117.70
1	2A	574	C	N1-C2-O2	-6.20	115.18	118.90
1	2A	2689	U	N3-C2-O2	-6.19	117.86	122.20
1	1A	1963	U	C2-N1-C1'	6.16	125.09	117.70
1	1A	2689	U	P-O3'-C3'	6.14	127.07	119.70
1	2A	570	G	C5-C6-O6	-6.11	124.93	128.60
1	1A	2023	G	O5'-P-OP2	6.09	118.01	110.70
1	1A	2848	G	O4'-C1'-N9	6.09	113.08	108.20
1	2A	2108	C	N1-C2-O2	6.08	122.55	118.90
1	2A	2103	C	C2-N3-C4	6.07	122.94	119.90
1	1A	2023	G	O5'-P-OP1	-6.06	100.25	105.70
1	1A	330	A	C2-N3-C4	-6.03	107.58	110.60
1	2A	1076	C	OP1-P-O3'	6.02	118.45	105.20
1	1A	845	G	O4'-C1'-N9	6.02	113.01	108.20
1	1A	947	G	O5'-P-OP1	-5.96	100.34	105.70
32	2a	754	C	C2-N1-C1'	5.94	125.33	118.80
1	1A	2103	C	N1-C2-O2	5.93	122.46	118.90
1	2A	1993	U	O5'-P-OP1	-5.91	100.38	105.70
1	2A	2181	G	C6-N1-C2	5.89	128.63	125.10
1	1A	271(Y)	U	O4'-C1'-N1	5.86	112.89	108.20
1	2A	1313	U	C2-N1-C1'	5.85	124.72	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1074	G	N3-C2-N2	5.84	123.99	119.90
1	2A	1075	C	N1-C2-O2	5.83	122.40	118.90
1	1A	1936	A	O4'-C1'-N9	5.79	112.84	108.20
1	1A	847	U	C2-N1-C1'	5.79	124.65	117.70
1	2A	1108	U	C5-C6-N1	5.79	125.60	122.70
1	2A	1992	G	P-O3'-C3'	5.76	126.61	119.70
1	1A	751	A	O5'-P-OP2	5.74	117.59	110.70
1	1A	570	G	C8-N9-C4	5.73	108.69	106.40
32	1a	1028	C	C6-N1-C2	-5.73	118.01	120.30
1	1A	2061	G	O5'-P-OP2	-5.73	100.55	105.70
1	1A	1602	U	N3-C4-O4	-5.70	115.41	119.40
1	1A	570	G	C4-C5-N7	5.68	113.07	110.80
32	2a	1183	A	P-O3'-C3'	5.64	126.47	119.70
1	1A	1075	C	C2-N3-C4	5.63	122.72	119.90
1	2A	2191	G	C5-C6-O6	5.63	131.98	128.60
32	2a	1158	C	C2-N1-C1'	5.63	124.99	118.80
1	2A	1075	C	N3-C2-O2	-5.63	117.96	121.90
1	1A	1075	C	N3-C2-O2	-5.62	117.96	121.90
32	2a	1397	C	N1-C2-O2	5.61	122.27	118.90
1	2A	570	G	C4-C5-N7	5.61	113.04	110.80
1	1A	2359	C	C6-N1-C2	-5.56	118.08	120.30
1	2A	2287	A	O4'-C1'-N9	5.56	112.65	108.20
1	1A	784	A	OP1-P-O3'	5.56	117.43	105.20
32	2a	754	C	N1-C2-O2	5.54	122.22	118.90
1	1A	996	A	O5'-P-OP1	-5.54	100.71	105.70
1	1A	576	U	O5'-P-OP1	-5.53	100.72	105.70
1	2A	1065	U	P-O3'-C3'	5.53	126.33	119.70
32	2a	687	A	P-O3'-C3'	5.51	126.31	119.70
1	1A	2176	A	C6-N1-C2	-5.51	115.30	118.60
1	1A	2254	C	N1-C2-O2	-5.51	115.60	118.90
32	2a	1378	C	C2-N1-C1'	5.51	124.86	118.80
1	2A	845	G	O4'-C1'-N9	5.49	112.59	108.20
1	1A	1210	A	P-O3'-C3'	5.48	126.27	119.70
1	1A	797	C	C6-N1-C2	-5.47	118.11	120.30
32	2a	266	G	OP2-P-O3'	5.46	117.22	105.20
32	2a	997	U	C2-N3-C4	5.46	130.27	127.00
1	1A	961	C	O5'-P-OP2	-5.45	100.80	105.70
1	1A	1653	G	P-O3'-C3'	5.44	126.23	119.70
1	1A	1190	G	C5-N7-C8	5.43	107.02	104.30
1	1A	1493	C	C2-N1-C1'	5.43	124.77	118.80
1	1A	383	U	O4'-C1'-N1	5.42	112.54	108.20
1	2A	1648	C	O5'-P-OP1	-5.38	100.86	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2183	C	N1-C2-O2	5.38	122.13	118.90
1	1A	784	A	P-O3'-C3'	5.37	126.15	119.70
32	1a	1024	G	N3-C4-N9	5.34	129.21	126.00
1	1A	2122	U	C5-C4-O4	-5.34	122.69	125.90
1	1A	784	A	O4'-C1'-N9	5.33	112.46	108.20
1	2A	2685	G	N1-C6-O6	-5.32	116.71	119.90
1	1A	774	A	C8-N9-C4	-5.31	103.67	105.80
1	1A	330	A	N1-C2-N3	5.30	131.95	129.30
32	2a	1225	A	C6-N1-C2	5.30	121.78	118.60
1	2A	1082	U	C2-N1-C1'	5.29	124.05	117.70
1	2A	748	G	C8-N9-C1'	5.28	133.87	127.00
1	1A	395	U	O4'-C1'-N1	5.26	112.41	108.20
1	2A	1936	A	O4'-C1'-N9	5.26	112.41	108.20
1	1A	1416	G	O4'-C1'-N9	5.26	112.41	108.20
32	2a	115	G	P-O3'-C3'	5.25	126.00	119.70
1	2A	1313	U	N1-C2-O2	5.24	126.46	122.80
1	1A	1776	G	O5'-P-OP2	-5.23	100.99	105.70
1	2A	1060	U	C6-N1-C1'	-5.23	113.88	121.20
32	1a	687	A	P-O3'-C3'	5.22	125.96	119.70
1	1A	645	C	C6-N1-C1'	-5.21	114.55	120.80
1	2A	570	G	N9-C4-C5	-5.21	103.32	105.40
1	1A	1272	A	O5'-P-OP2	-5.20	101.02	105.70
16	1U	74	LEU	CA-CB-CG	5.20	127.25	115.30
32	2a	1234	C	C2-N3-C4	5.19	122.49	119.90
1	2A	1265	A	O5'-P-OP2	-5.19	101.03	105.70
32	2a	1009	G	C5-C6-O6	5.18	131.71	128.60
32	2a	1234	C	N1-C2-O2	5.17	122.00	118.90
32	2a	1065	U	P-O3'-C3'	5.17	125.90	119.70
1	1A	2319	G	N3-C4-N9	-5.17	122.90	126.00
1	1A	2685	G	C5-C6-N1	5.16	114.08	111.50
1	1A	1773	A	N9-C1'-C2'	-5.16	106.33	112.00
32	1a	266	G	P-O3'-C3'	5.15	125.88	119.70
32	2a	1331	G	O4'-C1'-N9	5.13	112.31	108.20
32	2a	1378	C	N1-C2-O2	5.13	121.98	118.90
1	2A	1092	C	C6-N1-C1'	-5.13	114.65	120.80
1	1A	2501	C	C2-N1-C1'	-5.13	113.16	118.80
1	2A	802	A	O5'-P-OP1	-5.12	101.09	105.70
1	2A	1076	C	P-O3'-C3'	5.11	125.83	119.70
1	1A	198	C	O5'-P-OP2	-5.11	101.10	105.70
32	1a	115	G	P-O3'-C3'	5.11	125.83	119.70
1	1A	2176	A	C5-C6-N6	-5.11	119.61	123.70
1	2A	2248	C	O5'-P-OP2	-5.11	101.11	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2689	U	N1-C2-O2	5.10	126.37	122.80
32	2a	1126	U	N1-C2-O2	5.10	126.37	122.80
1	2A	746	A	O4'-C1'-N9	5.09	112.28	108.20
32	1a	1050	G	N3-C4-N9	5.06	129.04	126.00
1	1A	2712(A)	A	O5'-P-OP1	-5.06	101.15	105.70
32	1a	299	G	N9-C4-C5	-5.04	103.39	105.40
1	2A	12	U	N3-C2-O2	-5.03	118.68	122.20
1	1A	2103	C	C2-N3-C4	5.03	122.41	119.90
32	2a	1026	G	C4-N9-C1'	5.02	133.03	126.50
32	2a	1158	C	N1-C2-O2	5.02	121.91	118.90
1	1A	2149	G	N3-C4-N9	-5.02	122.99	126.00
1	1A	2249	U	C4-C5-C6	-5.02	116.69	119.70
1	1A	1064	C	N1-C2-O2	5.00	121.90	118.90
1	1A	570	G	N3-C4-N9	5.00	129.00	126.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	24	18	CYS	Peptide
21	2Z	136	PHE	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%)	261 (96%)	12 (4%)	0	100	100
3	2D	273/276 (99%)	255 (93%)	18 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29 41
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	29 41
5	1F	201/210 (96%)	195 (97%)	6 (3%)	0	100 100
5	2F	201/210 (96%)	187 (93%)	13 (6%)	1 (0%)	29 41
6	1G	179/182 (98%)	155 (87%)	22 (12%)	2 (1%)	14 20
6	2G	179/182 (98%)	157 (88%)	18 (10%)	4 (2%)	6 7
7	1H	172/180 (96%)	164 (95%)	5 (3%)	3 (2%)	9 11
7	2H	171/180 (95%)	150 (88%)	17 (10%)	4 (2%)	6 7
8	1I	145/148 (98%)	126 (87%)	18 (12%)	1 (1%)	22 32
8	2I	144/148 (97%)	128 (89%)	14 (10%)	2 (1%)	11 15
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100 100
9	2N	138/140 (99%)	132 (96%)	6 (4%)	0	100 100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100 100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100 100
11	2P	147/150 (98%)	138 (94%)	6 (4%)	3 (2%)	7 9
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100 100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100 100
13	1R	116/118 (98%)	114 (98%)	2 (2%)	0	100 100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100 100
14	1S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	17 25
14	2S	108/112 (96%)	99 (92%)	9 (8%)	0	100 100
15	1T	129/146 (88%)	125 (97%)	4 (3%)	0	100 100
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100 100
16	1U	114/118 (97%)	114 (100%)	0	0	100 100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100 100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15 23
17	2V	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	7 9
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
18	2W	110/113 (97%)	110 (100%)	0	0	100 100
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14 20
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100 100
20	2Y	105/110 (96%)	98 (93%)	7 (7%)	0	100 100
21	1Z	201/206 (98%)	186 (92%)	14 (7%)	1 (0%)	29 41
21	2Z	199/206 (97%)	179 (90%)	19 (10%)	1 (0%)	29 41
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100 100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14 20
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14 20
24	12	68/72 (94%)	68 (100%)	0	0	100 100
24	22	68/72 (94%)	67 (98%)	0	1 (2%)	10 14
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
26	14	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	2 2
26	24	67/71 (94%)	49 (73%)	12 (18%)	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%)	49 (96%)	2 (4%)	0	100 100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
29	17	46/49 (94%)	46 (100%)	0	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%)	32 (91%)	3 (9%)	0	100 100
33	1b	229/256 (90%)	183 (80%)	39 (17%)	7 (3%)	4 3
33	2b	229/256 (90%)	185 (81%)	34 (15%)	10 (4%)	2 2
34	1c	204/239 (85%)	180 (88%)	24 (12%)	0	100 100
34	2c	204/239 (85%)	175 (86%)	25 (12%)	4 (2%)	7 9
35	1d	206/209 (99%)	189 (92%)	17 (8%)	0	100 100
35	2d	206/209 (99%)	185 (90%)	19 (9%)	2 (1%)	15 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
36	1e	146/162 (90%)	143 (98%)	2 (1%)	1 (1%)	22 32
36	2e	146/162 (90%)	135 (92%)	11 (8%)	0	100 100
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
38	1g	153/156 (98%)	144 (94%)	9 (6%)	0	100 100
38	2g	153/156 (98%)	136 (89%)	13 (8%)	4 (3%)	5 5
39	1h	135/138 (98%)	127 (94%)	7 (5%)	1 (1%)	22 32
39	2h	135/138 (98%)	122 (90%)	11 (8%)	2 (2%)	10 14
40	1i	125/128 (98%)	114 (91%)	11 (9%)	0	100 100
40	2i	124/128 (97%)	110 (89%)	11 (9%)	3 (2%)	6 6
41	1j	95/105 (90%)	82 (86%)	9 (10%)	4 (4%)	3 2
41	2j	94/105 (90%)	79 (84%)	11 (12%)	4 (4%)	2 2
42	1k	112/129 (87%)	100 (89%)	12 (11%)	0	100 100
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	8 10
43	1l	119/132 (90%)	110 (92%)	8 (7%)	1 (1%)	19 29
43	2l	119/132 (90%)	108 (91%)	10 (8%)	1 (1%)	19 29
44	1m	114/126 (90%)	104 (91%)	8 (7%)	2 (2%)	8 10
44	2m	112/126 (89%)	94 (84%)	17 (15%)	1 (1%)	17 25
45	1n	58/61 (95%)	57 (98%)	1 (2%)	0	100 100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
46	1o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13 19
46	2o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	6 7
47	1p	80/88 (91%)	71 (89%)	9 (11%)	0	100 100
47	2p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	12 17
48	1q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	15 23
48	2q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	15 23
49	1r	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	10 14
49	2r	66/88 (75%)	60 (91%)	6 (9%)	0	100 100
50	1s	81/93 (87%)	73 (90%)	6 (7%)	2 (2%)	5 6
50	2s	81/93 (87%)	66 (82%)	15 (18%)	0	100 100
51	1t	94/106 (89%)	83 (88%)	10 (11%)	1 (1%)	14 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	2t	96/106 (91%)	86 (90%)	6 (6%)	4 (4%)	3 2
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
53	1y	95/113 (84%)	90 (95%)	5 (5%)	0	100 100
53	2y	94/113 (83%)	82 (87%)	11 (12%)	1 (1%)	14 20
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%)	10729 (92%)	808 (7%)	106 (1%)	17 25

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	49	ASP
14	1S	59	LYS
26	14	61	ARG
33	1b	21	ARG
33	1b	124	SER
33	1b	127	ILE
41	1j	55	LYS
43	1l	91	LYS
48	1q	34	LYS
5	2F	130	ALA
6	2G	124	SER
7	2H	126	PRO
26	24	48	ARG
26	24	62	ARG
33	2b	9	GLU
33	2b	10	LEU
33	2b	17	PHE
40	2i	43	ALA
42	2k	105	VAL
43	2l	91	LYS
48	2q	34	LYS
7	1H	92	ILE
7	1H	159	GLU
19	1X	94	GLY
26	14	47	GLN
33	1b	17	PHE
44	1m	67	GLU
50	1s	27	GLU

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Mol	Chain	Res	Type
8	2I	97	ILE
11	2P	36	LYS
17	2V	100	ARG
21	2Z	52	SER
26	24	45	GLY
26	24	46	GLN
26	24	49	PHE
33	2b	128	GLU
34	2c	12	LEU
38	2g	7	ALA
38	2g	32	ARG
38	2g	33	ASP
40	2i	54	ASP
41	2j	79	ARG
47	2p	52	ASP
51	2t	95	ALA
4	1E	52	LEU
7	1H	126	PRO
41	1j	78	ASN
50	1s	12	ASP
6	2G	3	LEU
6	2G	96	ARG
17	2V	79	VAL
23	21	3	LYS
33	2b	64	ARG
33	2b	95	GLN
39	2h	83	ILE
39	2h	133	LEU
41	2j	55	LYS
51	2t	47	GLY
53	2y	45	PRO
6	1G	44	GLY
8	1I	73	GLU
21	1Z	52	SER
33	1b	8	LYS
41	1j	77	PRO
4	2E	52	LEU
6	2G	81	LYS
7	2H	65	HIS
8	2I	117	GLU
11	2P	29	LYS
11	2P	76	LYS

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Mol	Chain	Res	Type
26	24	55	ARG
33	2b	20	GLU
35	2d	22	LYS
41	2j	78	ASN
44	2m	6	GLY
17	1V	79	VAL
23	11	3	LYS
26	14	49	PHE
44	1m	106	ASN
49	1r	27	GLY
7	2H	17	VAL
19	2X	94	GLY
33	2b	125	PRO
34	2c	99	VAL
35	2d	196	LEU
38	2g	131	LYS
40	2i	44	VAL
41	2j	35	SER
24	22	69	ARG
33	2b	207	ALA
34	2c	50	ALA
42	2k	90	GLY
33	1b	231	GLU
36	1e	70	PRO
51	1t	100	ILE
46	2o	19	PRO
39	1h	74	PRO
46	1o	23	GLY
51	2t	100	ILE
7	2H	128	PRO
46	2o	23	GLY
51	2t	98	PRO
41	1j	91	PRO
33	2b	124	SER
34	2c	64	VAL
33	1b	125	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	214/218 (98%)	195 (91%)	19 (9%)	9 14
3	2D	215/218 (99%)	198 (92%)	17 (8%)	12 19
4	1E	164/166 (99%)	157 (96%)	7 (4%)	29 46
4	2E	164/166 (99%)	151 (92%)	13 (8%)	12 19
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11 18
5	2F	159/166 (96%)	141 (89%)	18 (11%)	6 8
6	1G	144/156 (92%)	127 (88%)	17 (12%)	5 7
6	2G	142/156 (91%)	129 (91%)	13 (9%)	9 13
7	1H	144/148 (97%)	134 (93%)	10 (7%)	15 25
7	2H	143/148 (97%)	131 (92%)	12 (8%)	11 16
8	1I	111/124 (90%)	98 (88%)	13 (12%)	5 7
8	2I	108/124 (87%)	91 (84%)	17 (16%)	2 3
9	1N	119/119 (100%)	106 (89%)	13 (11%)	6 8
9	2N	118/119 (99%)	112 (95%)	6 (5%)	24 39
10	1O	100/100 (100%)	98 (98%)	2 (2%)	55 74
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31 49
11	1P	115/116 (99%)	110 (96%)	5 (4%)	29 46
11	2P	115/116 (99%)	110 (96%)	5 (4%)	29 46
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	9 14
12	2Q	111/111 (100%)	103 (93%)	8 (7%)	14 23
13	1R	101/101 (100%)	94 (93%)	7 (7%)	15 25
13	2R	101/101 (100%)	96 (95%)	5 (5%)	24 40
14	1S	87/88 (99%)	80 (92%)	7 (8%)	12 18
14	2S	85/88 (97%)	79 (93%)	6 (7%)	14 23
15	1T	115/127 (91%)	106 (92%)	9 (8%)	12 19
15	2T	113/127 (89%)	107 (95%)	6 (5%)	22 37
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22 36
16	2U	93/94 (99%)	87 (94%)	6 (6%)	17 27
17	1V	81/82 (99%)	73 (90%)	8 (10%)	8 11
17	2V	80/82 (98%)	73 (91%)	7 (9%)	10 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	1W	90/92 (98%)	85 (94%)	5 (6%)	21 34
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9 14
19	1X	77/78 (99%)	74 (96%)	3 (4%)	32 50
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46 66
20	1Y	86/91 (94%)	82 (95%)	4 (5%)	26 42
20	2Y	86/91 (94%)	75 (87%)	11 (13%)	4 5
21	1Z	169/179 (94%)	156 (92%)	13 (8%)	13 20
21	2Z	165/179 (92%)	144 (87%)	21 (13%)	4 5
22	10	65/67 (97%)	60 (92%)	5 (8%)	13 20
22	20	64/67 (96%)	62 (97%)	2 (3%)	40 60
23	11	79/83 (95%)	74 (94%)	5 (6%)	18 28
23	21	81/83 (98%)	76 (94%)	5 (6%)	18 29
24	12	65/67 (97%)	60 (92%)	5 (8%)	13 20
24	22	66/67 (98%)	65 (98%)	1 (2%)	65 80
25	13	51/52 (98%)	46 (90%)	5 (10%)	8 11
25	23	50/52 (96%)	48 (96%)	2 (4%)	31 49
26	14	58/63 (92%)	53 (91%)	5 (9%)	10 16
26	24	54/63 (86%)	45 (83%)	9 (17%)	2 2
27	15	51/52 (98%)	44 (86%)	7 (14%)	3 4
27	25	50/52 (96%)	46 (92%)	4 (8%)	12 18
28	16	51/52 (98%)	46 (90%)	5 (10%)	8 11
28	26	50/52 (96%)	46 (92%)	4 (8%)	12 18
29	17	41/42 (98%)	38 (93%)	3 (7%)	14 22
29	27	41/42 (98%)	37 (90%)	4 (10%)	8 11
30	18	54/55 (98%)	47 (87%)	7 (13%)	4 4
30	28	54/55 (98%)	47 (87%)	7 (13%)	4 4
31	19	34/34 (100%)	34 (100%)	0	100 100
31	29	34/34 (100%)	32 (94%)	2 (6%)	19 32
33	1b	191/220 (87%)	168 (88%)	23 (12%)	5 6
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4 4
34	1c	144/188 (77%)	136 (94%)	8 (6%)	21 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	2c	140/188 (74%)	122 (87%)	18 (13%)	4 5
35	1d	171/181 (94%)	151 (88%)	20 (12%)	5 7
35	2d	172/181 (95%)	156 (91%)	16 (9%)	9 13
36	1e	114/123 (93%)	104 (91%)	10 (9%)	10 15
36	2e	114/123 (93%)	106 (93%)	8 (7%)	15 24
37	1f	85/90 (94%)	71 (84%)	14 (16%)	2 2
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26 42
38	1g	120/127 (94%)	111 (92%)	9 (8%)	13 21
38	2g	119/127 (94%)	105 (88%)	14 (12%)	5 7
39	1h	116/119 (98%)	105 (90%)	11 (10%)	8 12
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8 12
40	1i	91/99 (92%)	78 (86%)	13 (14%)	3 4
40	2i	88/99 (89%)	79 (90%)	9 (10%)	7 10
41	1j	68/92 (74%)	59 (87%)	9 (13%)	4 4
41	2j	68/92 (74%)	63 (93%)	5 (7%)	13 22
42	1k	83/99 (84%)	76 (92%)	7 (8%)	11 16
42	2k	83/99 (84%)	80 (96%)	3 (4%)	35 54
43	1l	96/108 (89%)	90 (94%)	6 (6%)	18 28
43	2l	96/108 (89%)	87 (91%)	9 (9%)	8 13
44	1m	90/101 (89%)	83 (92%)	7 (8%)	12 19
44	2m	87/101 (86%)	78 (90%)	9 (10%)	7 10
45	1n	49/50 (98%)	42 (86%)	7 (14%)	3 4
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7 10
46	1o	78/80 (98%)	75 (96%)	3 (4%)	33 51
46	2o	78/80 (98%)	72 (92%)	6 (8%)	13 20
47	1p	69/74 (93%)	57 (83%)	12 (17%)	2 2
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5 7
48	1q	94/97 (97%)	90 (96%)	4 (4%)	29 46
48	2q	94/97 (97%)	91 (97%)	3 (3%)	39 59
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10 16
49	2r	59/77 (77%)	58 (98%)	1 (2%)	60 78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
50	1s	68/80 (85%)	61 (90%)	7 (10%)	7 10
50	2s	67/80 (84%)	57 (85%)	10 (15%)	3 3
51	1t	71/82 (87%)	64 (90%)	7 (10%)	8 11
51	2t	70/82 (85%)	61 (87%)	9 (13%)	4 5
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21 34
52	2u	18/22 (82%)	18 (100%)	0	100 100
53	1y	82/98 (84%)	78 (95%)	4 (5%)	25 40
53	2y	79/98 (81%)	69 (87%)	10 (13%)	4 5
56	1v	2/2 (100%)	2 (100%)	0	100 100
56	2v	2/2 (100%)	2 (100%)	0	100 100
All	All	9535/10264 (93%)	8723 (92%)	812 (8%)	10 16

All (812) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	37	LEU
3	1D	39	LYS
3	1D	43	ARG
3	1D	61	LEU
3	1D	71	ASP
3	1D	88	ARG
3	1D	111	LEU
3	1D	116	GLN
3	1D	140	THR
3	1D	141	VAL
3	1D	142	VAL
3	1D	193	VAL
3	1D	211	ARG
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	275	LYS
4	1E	9	VAL
4	1E	38	THR
4	1E	49	LEU
4	1E	73	GLU

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Mol	Chain	Res	Type
4	1E	75	VAL
4	1E	116	VAL
4	1E	195	LEU
5	1F	17	ARG
5	1F	18	ARG
5	1F	20	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	108	LYS
5	1F	110	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	205	ARG
6	1G	5	VAL
6	1G	7	LEU
6	1G	21	ARG
6	1G	43	LEU
6	1G	45	GLU
6	1G	49	ASP
6	1G	52	ILE
6	1G	53	LEU
6	1G	67	LYS
6	1G	79	ASN
6	1G	81	LYS
6	1G	82	LEU
6	1G	91	ARG
6	1G	126	ASP
6	1G	133	LEU
6	1G	144	ILE
6	1G	170	ARG
7	1H	15	VAL
7	1H	27	LYS
7	1H	58	GLU
7	1H	71	LEU
7	1H	119	GLU
7	1H	124	GLU
7	1H	127	GLU
7	1H	130	ARG
7	1H	139	GLN

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Mol	Chain	Res	Type
7	1H	172	LYS
8	1I	10	GLU
8	1I	15	VAL
8	1I	20	ASP
8	1I	38	LEU
8	1I	40	THR
8	1I	42	SER
8	1I	60	GLU
8	1I	61	ARG
8	1I	74	ASN
8	1I	78	THR
8	1I	91	SER
8	1I	107	VAL
8	1I	109	ILE
9	1N	5	VAL
9	1N	8	GLN
9	1N	14	VAL
9	1N	33	LEU
9	1N	34	LEU
9	1N	48	MET
9	1N	62	VAL
9	1N	67	LEU
9	1N	87	LEU
9	1N	89	LYS
9	1N	119	ARG
9	1N	121	LYS
9	1N	133	GLN
10	1O	92	GLU
10	1O	112	MET
11	1P	1	MET
11	1P	16	ARG
11	1P	92	GLU
11	1P	119	GLU
11	1P	124	LYS
12	1Q	5	ARG
12	1Q	6	ARG
12	1Q	7	MET
12	1Q	55	VAL
12	1Q	75	THR
12	1Q	77	LYS
12	1Q	103	MET
12	1Q	109	VAL

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Mol	Chain	Res	Type
12	1Q	130	LYS
12	1Q	133	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	67	LEU
13	1R	96	ARG
13	1R	104	ARG
13	1R	114	VAL
14	1S	17	ARG
14	1S	27	SER
14	1S	50	SER
14	1S	52	SER
14	1S	69	VAL
14	1S	80	LEU
14	1S	110	LEU
15	1T	6	LEU
15	1T	28	VAL
15	1T	33	LYS
15	1T	53	ARG
15	1T	59	THR
15	1T	78	LEU
15	1T	80	SER
15	1T	118	ARG
15	1T	128	GLU
16	1U	5	LYS
16	1U	74	LEU
16	1U	77	SER
16	1U	104	GLN
16	1U	117	GLN
17	1V	21	ARG
17	1V	26	ASP
17	1V	46	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	82	ARG
17	1V	95	LEU
18	1W	11	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	37	ARG

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Mol	Chain	Res	Type
18	1W	100	THR
19	1X	49	VAL
19	1X	66	LEU
19	1X	68	ARG
20	1Y	23	ARG
20	1Y	43	ASN
20	1Y	72	VAL
20	1Y	107	ASP
21	1Z	41	LEU
21	1Z	76	LEU
21	1Z	80	ARG
21	1Z	86	VAL
21	1Z	107	THR
21	1Z	138	GLU
21	1Z	156	LYS
21	1Z	161	VAL
21	1Z	171	ILE
21	1Z	185	GLU
21	1Z	198	LYS
21	1Z	202	GLU
21	1Z	203	GLU
22	10	14	ARG
22	10	39	ARG
22	10	55	ARG
22	10	59	LEU
22	10	82	ARG
23	11	21	ARG
23	11	30	VAL
23	11	35	THR
23	11	40	ARG
23	11	94	LEU
24	12	1	MET
24	12	3	LEU
24	12	27	GLU
24	12	28	LYS
24	12	53	LEU
25	13	8	LEU
25	13	23	LEU
25	13	32	GLN
25	13	54	VAL
25	13	58	VAL
26	14	33	VAL

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Mol	Chain	Res	Type
26	14	49	PHE
26	14	50	VAL
26	14	56	VAL
26	14	60	GLN
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	30	LEU
27	15	37	LYS
27	15	40	LYS
27	15	55	ARG
28	16	6	ARG
28	16	14	THR
28	16	44	ARG
28	16	48	VAL
28	16	52	VAL
29	17	43	THR
29	17	46	VAL
29	17	48	LYS
30	18	14	VAL
30	18	23	VAL
30	18	29	LYS
30	18	31	HIS
30	18	34	TRP
30	18	50	LEU
30	18	58	ILE
33	1b	7	VAL
33	1b	8	LYS
33	1b	9	GLU
33	1b	10	LEU
33	1b	15	VAL
33	1b	19	HIS
33	1b	20	GLU
33	1b	21	ARG
33	1b	28	PHE
33	1b	44	LEU
33	1b	93	VAL
33	1b	96	ARG
33	1b	111	ARG
33	1b	124	SER
33	1b	135	GLN
33	1b	160	ASP

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Mol	Chain	Res	Type
33	1b	163	PHE
33	1b	185	ILE
33	1b	200	ILE
33	1b	212	GLN
33	1b	223	ILE
33	1b	224	GLN
33	1b	236	TYR
34	1c	48	TYR
34	1c	64	VAL
34	1c	70	VAL
34	1c	102	ASN
34	1c	104	GLN
34	1c	105	GLU
34	1c	132	ARG
34	1c	144	SER
35	1d	3	ARG
35	1d	18	LYS
35	1d	19	LEU
35	1d	28	SER
35	1d	58	LEU
35	1d	70	ILE
35	1d	77	ASN
35	1d	83	SER
35	1d	135	LEU
35	1d	137	SER
35	1d	150	GLU
35	1d	162	LEU
35	1d	166	LYS
35	1d	168	ARG
35	1d	179	GLU
35	1d	187	ARG
35	1d	193	ASP
35	1d	194	LEU
35	1d	196	LEU
35	1d	208	SER
36	1e	5	ASP
36	1e	41	VAL
36	1e	47	LYS
36	1e	53	LEU
36	1e	69	VAL
36	1e	120	THR
36	1e	144	THR

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Mol	Chain	Res	Type
36	1e	147	ASP
36	1e	150	ARG
36	1e	151	LEU
37	1f	10	LEU
37	1f	15	ASP
37	1f	21	LEU
37	1f	36	ARG
37	1f	40	VAL
37	1f	42	GLU
37	1f	67	MET
37	1f	69	GLU
37	1f	70	ASP
37	1f	71	ARG
37	1f	72	VAL
37	1f	74	ASP
37	1f	81	ILE
37	1f	89	MET
38	1g	6	ARG
38	1g	41	ARG
38	1g	52	GLU
38	1g	59	LEU
38	1g	79	ARG
38	1g	86	GLN
38	1g	106	GLN
38	1g	113	GLU
38	1g	126	ASP
39	1h	14	ARG
39	1h	22	GLU
39	1h	39	LEU
39	1h	52	ASP
39	1h	63	LEU
39	1h	64	LYS
39	1h	69	ARG
39	1h	88	LYS
39	1h	98	LYS
39	1h	104	ARG
39	1h	133	LEU
40	1i	14	VAL
40	1i	25	LYS
40	1i	47	LEU
40	1i	50	LEU
40	1i	56	LEU

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Mol	Chain	Res	Type
40	1i	65	VAL
40	1i	66	ARG
40	1i	81	ILE
40	1i	92	TYR
40	1i	96	LEU
40	1i	101	PHE
40	1i	104	ARG
40	1i	111	ARG
41	1j	34	VAL
41	1j	38	ILE
41	1j	43	ARG
41	1j	46	ARG
41	1j	55	LYS
41	1j	67	THR
41	1j	72	VAL
41	1j	84	GLN
41	1j	94	VAL
42	1k	14	VAL
42	1k	16	SER
42	1k	31	THR
42	1k	34	ASP
42	1k	99	GLN
42	1k	116	HIS
42	1k	124	LYS
43	1l	22	SER
43	1l	33	ARG
43	1l	79	GLU
43	1l	83	VAL
43	1l	106	ASP
43	1l	123	LYS
44	1m	3	ARG
44	1m	4	ILE
44	1m	35	GLU
44	1m	86	CYS
44	1m	99	ARG
44	1m	106	ASN
44	1m	117	VAL
45	1n	3	ARG
45	1n	8	GLU
45	1n	9	LYS
45	1n	13	THR
45	1n	15	LYS

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Mol	Chain	Res	Type
45	1n	18	VAL
45	1n	33	VAL
46	1o	3	ILE
46	1o	39	LEU
46	1o	71	GLN
47	1p	1	MET
47	1p	11	SER
47	1p	21	VAL
47	1p	29	ASP
47	1p	38	TYR
47	1p	42	ARG
47	1p	43	LYS
47	1p	60	LEU
47	1p	61	SER
47	1p	67	THR
47	1p	72	ARG
47	1p	74	LEU
48	1q	6	LEU
48	1q	9	VAL
48	1q	45	HIS
48	1q	53	LEU
49	1r	23	LYS
49	1r	25	THR
49	1r	39	VAL
49	1r	46	GLU
49	1r	58	LEU
50	1s	12	ASP
50	1s	28	LYS
50	1s	35	SER
50	1s	37	ARG
50	1s	40	ILE
50	1s	48	THR
50	1s	66	MET
51	1t	10	LEU
51	1t	15	ARG
51	1t	24	LEU
51	1t	34	LYS
51	1t	37	SER
51	1t	84	LEU
51	1t	90	GLN
52	1u	24	ARG
53	1y	24	LEU

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Mol	Chain	Res	Type
53	1y	38	HIS
53	1y	42	SER
53	1y	46	GLN
3	2D	3	VAL
3	2D	38	LYS
3	2D	61	LEU
3	2D	75	ILE
3	2D	94	LEU
3	2D	103	ARG
3	2D	134	ARG
3	2D	142	VAL
3	2D	155	LEU
3	2D	183	ARG
3	2D	204	ILE
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	276	LYS
4	2E	1	MET
4	2E	27	LEU
4	2E	73	GLU
4	2E	75	VAL
4	2E	76	ARG
4	2E	90	THR
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	170	LEU
4	2E	182	LEU
4	2E	184	VAL
4	2E	188	VAL
5	2F	17	ARG
5	2F	20	LEU
5	2F	24	LEU
5	2F	27	GLU
5	2F	28	ILE
5	2F	33	LEU
5	2F	57	VAL
5	2F	74	ARG
5	2F	126	VAL

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Mol	Chain	Res	Type
5	2F	132	VAL
5	2F	162	LEU
5	2F	170	LEU
5	2F	175	THR
5	2F	192	LEU
5	2F	195	ASP
5	2F	197	ASP
5	2F	201	VAL
5	2F	206	ILE
6	2G	3	LEU
6	2G	26	GLN
6	2G	28	VAL
6	2G	36	LYS
6	2G	49	ASP
6	2G	86	MET
6	2G	106	LEU
6	2G	115	ARG
6	2G	133	LEU
6	2G	139	LEU
6	2G	143	GLU
6	2G	159	VAL
6	2G	172	LEU
7	2H	45	VAL
7	2H	47	GLU
7	2H	49	VAL
7	2H	50	VAL
7	2H	52	VAL
7	2H	68	THR
7	2H	69	ARG
7	2H	81	GLU
7	2H	88	LEU
7	2H	98	LEU
7	2H	103	LEU
7	2H	118	PRO
8	2I	7	GLU
8	2I	38	LEU
8	2I	42	SER
8	2I	44	LEU
8	2I	50	ARG
8	2I	58	LEU
8	2I	64	GLU
8	2I	70	GLU

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Mol	Chain	Res	Type
8	2I	74	ASN
8	2I	75	LEU
8	2I	76	THR
8	2I	82	ARG
8	2I	91	SER
8	2I	92	VAL
8	2I	108	THR
8	2I	116	LEU
8	2I	122	GLU
9	2N	28	THR
9	2N	33	LEU
9	2N	48	MET
9	2N	60	ILE
9	2N	67	LEU
9	2N	74	ARG
10	2O	35	VAL
10	2O	64	ARG
10	2O	78	ARG
10	2O	94	ARG
11	2P	3	LEU
11	2P	86	LYS
11	2P	99	LEU
11	2P	119	GLU
11	2P	149	GLU
12	2Q	1	MET
12	2Q	5	ARG
12	2Q	60	ARG
12	2Q	75	THR
12	2Q	109	VAL
12	2Q	110	THR
12	2Q	133	ARG
12	2Q	135	ASP
13	2R	6	SER
13	2R	44	LEU
13	2R	73	VAL
13	2R	96	ARG
13	2R	114	VAL
14	2S	11	LYS
14	2S	12	PHE
14	2S	42	ASP
14	2S	84	GLN
14	2S	85	VAL

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Mol	Chain	Res	Type
14	2S	110	LEU
15	2T	53	ARG
15	2T	82	LEU
15	2T	89	VAL
15	2T	99	LEU
15	2T	108	ARG
15	2T	118	ARG
16	2U	5	LYS
16	2U	31	SER
16	2U	74	LEU
16	2U	77	SER
16	2U	104	GLN
16	2U	117	GLN
17	2V	32	THR
17	2V	46	VAL
17	2V	51	VAL
17	2V	71	LEU
17	2V	79	VAL
17	2V	96	ILE
17	2V	98	GLU
18	2W	1	MET
18	2W	11	ARG
18	2W	17	VAL
18	2W	63	ASP
18	2W	68	ARG
18	2W	70	TYR
18	2W	82	LEU
18	2W	100	THR
19	2X	45	THR
19	2X	81	VAL
20	2Y	2	ARG
20	2Y	3	VAL
20	2Y	6	HIS
20	2Y	62	GLU
20	2Y	64	GLU
20	2Y	67	LEU
20	2Y	70	SER
20	2Y	72	VAL
20	2Y	90	LEU
20	2Y	92	ASN
20	2Y	99	CYS
21	2Z	2	GLU

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Mol	Chain	Res	Type
21	2Z	4	ARG
21	2Z	5	LEU
21	2Z	14	LYS
21	2Z	28	MET
21	2Z	31	ARG
21	2Z	46	LYS
21	2Z	76	LEU
21	2Z	86	VAL
21	2Z	91	LEU
21	2Z	93	ASP
21	2Z	98	MET
21	2Z	121	HIS
21	2Z	128	VAL
21	2Z	129	SER
21	2Z	141	VAL
21	2Z	142	SER
21	2Z	170	THR
21	2Z	175	VAL
21	2Z	182	LYS
21	2Z	198	LYS
22	20	35	ASN
22	20	82	ARG
23	21	21	ARG
23	21	35	THR
23	21	40	ARG
23	21	85	LEU
23	21	95	LEU
24	22	52	ASP
25	23	3	ARG
25	23	31	LEU
26	24	10	VAL
26	24	15	ILE
26	24	23	GLU
26	24	27	THR
26	24	48	ARG
26	24	50	VAL
26	24	52	THR
26	24	61	ARG
26	24	63	TYR
27	25	29	THR
27	25	30	LEU
27	25	40	LYS

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Mol	Chain	Res	Type
27	25	55	ARG
28	26	6	ARG
28	26	30	THR
28	26	34	LEU
28	26	48	VAL
29	27	10	ARG
29	27	23	ARG
29	27	46	VAL
29	27	48	LYS
30	28	3	LYS
30	28	14	VAL
30	28	26	LYS
30	28	31	HIS
30	28	34	TRP
30	28	49	VAL
30	28	50	LEU
31	29	4	ARG
31	29	7	VAL
33	2b	8	LYS
33	2b	10	LEU
33	2b	15	VAL
33	2b	16	HIS
33	2b	17	PHE
33	2b	24	TRP
33	2b	30	ARG
33	2b	39	ILE
33	2b	44	LEU
33	2b	45	GLN
33	2b	69	LEU
33	2b	76	GLN
33	2b	96	ARG
33	2b	97	TRP
33	2b	98	LEU
33	2b	121	LEU
33	2b	126	GLU
33	2b	150	SER
33	2b	154	LEU
33	2b	187	LEU
33	2b	189	ASP
33	2b	193	ASP
33	2b	209	ARG
33	2b	213	LEU

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Mol	Chain	Res	Type
33	2b	215	LEU
34	2c	3	ASN
34	2c	16	ARG
34	2c	33	LEU
34	2c	37	GLN
34	2c	44	GLU
34	2c	47	LEU
34	2c	52	LEU
34	2c	56	ASP
34	2c	70	VAL
34	2c	105	GLU
34	2c	110	ASN
34	2c	124	ILE
34	2c	128	PHE
34	2c	152	ILE
34	2c	181	ASN
34	2c	192	THR
34	2c	204	LEU
34	2c	206	GLU
35	2d	8	VAL
35	2d	19	LEU
35	2d	50	ARG
35	2d	83	SER
35	2d	86	LYS
35	2d	110	PHE
35	2d	123	HIS
35	2d	135	LEU
35	2d	141	ARG
35	2d	155	LEU
35	2d	157	LEU
35	2d	162	LEU
35	2d	170	VAL
35	2d	187	ARG
35	2d	194	LEU
35	2d	200	GLU
36	2e	6	PHE
36	2e	11	ILE
36	2e	41	VAL
36	2e	45	PHE
36	2e	47	LYS
36	2e	69	VAL
36	2e	79	GLU

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Mol	Chain	Res	Type
36	2e	144	THR
37	2f	40	VAL
37	2f	45	LEU
37	2f	57	GLN
37	2f	72	VAL
38	2g	6	ARG
38	2g	9	VAL
38	2g	15	ASP
38	2g	16	LEU
38	2g	27	ILE
38	2g	45	ASP
38	2g	47	CYS
38	2g	75	VAL
38	2g	111	ARG
38	2g	113	GLU
38	2g	115	ARG
38	2g	123	GLU
38	2g	138	LYS
38	2g	153	HIS
39	2h	2	LEU
39	2h	33	GLU
39	2h	38	ILE
39	2h	63	LEU
39	2h	79	VAL
39	2h	91	ARG
39	2h	104	ARG
39	2h	114	THR
39	2h	119	LEU
39	2h	125	ARG
39	2h	133	LEU
40	2i	3	GLN
40	2i	7	THR
40	2i	23	ASN
40	2i	27	THR
40	2i	33	PHE
40	2i	34	ASN
40	2i	63	ILE
40	2i	102	LEU
40	2i	109	VAL
41	2j	34	VAL
41	2j	38	ILE
41	2j	68	HIS

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Mol	Chain	Res	Type
41	2j	73	ASP
41	2j	84	GLN
42	2k	28	THR
42	2k	93	GLN
42	2k	109	VAL
43	2l	10	LEU
43	2l	13	LYS
43	2l	28	LYS
43	2l	33	ARG
43	2l	39	VAL
43	2l	58	VAL
43	2l	67	THR
43	2l	83	VAL
43	2l	123	LYS
44	2m	15	VAL
44	2m	43	THR
44	2m	47	ASP
44	2m	49	THR
44	2m	67	GLU
44	2m	92	HIS
44	2m	96	LEU
44	2m	98	VAL
44	2m	102	ARG
45	2n	3	ARG
45	2n	9	LYS
45	2n	18	VAL
45	2n	29	ARG
45	2n	33	VAL
46	2o	3	ILE
46	2o	4	THR
46	2o	26	GLU
46	2o	27	VAL
46	2o	39	LEU
46	2o	84	LYS
47	2p	5	ARG
47	2p	11	SER
47	2p	12	LYS
47	2p	20	VAL
47	2p	21	VAL
47	2p	28	ARG
47	2p	45	THR
47	2p	69	THR

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Mol	Chain	Res	Type
48	2q	6	LEU
48	2q	13	ASP
48	2q	99	SER
49	2r	84	LYS
50	2s	13	ASP
50	2s	22	LEU
50	2s	23	ASN
50	2s	32	LYS
50	2s	41	VAL
50	2s	48	THR
50	2s	63	THR
50	2s	67	VAL
50	2s	77	THR
50	2s	83	HIS
51	2t	15	ARG
51	2t	23	ARG
51	2t	31	SER
51	2t	46	GLU
51	2t	70	SER
51	2t	72	LEU
51	2t	86	ARG
51	2t	99	LEU
51	2t	100	ILE
53	2y	6	THR
53	2y	7	SER
53	2y	9	GLN
53	2y	16	ILE
53	2y	24	LEU
53	2y	41	LEU
53	2y	46	GLN
53	2y	56	THR
53	2y	78	ILE
53	2y	96	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	253	GLN
4	1E	48	GLN
5	1F	69	HIS
5	1F	133	ASN

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Mol	Chain	Res	Type
6	1G	26	GLN
8	1I	43	ASN
9	1N	133	GLN
10	1O	3	GLN
11	1P	70	GLN
12	1Q	89	ASN
14	1S	68	GLN
15	1T	123	GLN
16	1U	81	HIS
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	73	GLN
22	10	35	ASN
23	11	56	GLN
24	12	9	GLN
25	13	32	GLN
26	14	47	GLN
26	14	60	GLN
33	1b	76	GLN
33	1b	212	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	69	HIS
34	1c	102	ASN
34	1c	104	GLN
34	1c	139	GLN
35	1d	45	GLN
35	1d	77	ASN
35	1d	123	HIS
35	1d	129	ASN
36	1e	56	GLN
36	1e	141	GLN
37	1f	32	ASN
37	1f	84	ASN
38	1g	28	ASN
38	1g	56	GLN
38	1g	64	GLN
38	1g	86	GLN
38	1g	148	ASN
40	1i	3	GLN

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Mol	Chain	Res	Type
40	1i	73	GLN
41	1j	56	HIS
41	1j	84	GLN
42	1k	93	GLN
42	1k	117	ASN
43	1l	99	HIS
45	1n	49	HIS
46	1o	28	GLN
46	1o	71	GLN
47	1p	16	HIS
48	1q	16	GLN
50	1s	56	GLN
50	1s	57	HIS
50	1s	69	HIS
50	1s	83	HIS
53	1y	38	HIS
3	2D	253	GLN
4	2E	48	GLN
5	2F	69	HIS
7	2H	74	ASN
8	2I	43	ASN
8	2I	104	GLN
9	2N	131	GLN
10	2O	88	ASN
13	2R	31	HIS
13	2R	71	GLN
15	2T	58	ASN
17	2V	64	HIS
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
20	2Y	92	ASN
21	2Z	73	GLN
24	22	9	GLN
25	23	32	GLN
26	24	20	ASN
26	24	60	GLN
30	28	35	GLN
33	2b	40	HIS
33	2b	76	GLN
33	2b	78	GLN
33	2b	212	GLN

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Mol	Chain	Res	Type
34	2c	102	ASN
34	2c	110	ASN
34	2c	176	HIS
34	2c	181	ASN
35	2d	77	ASN
35	2d	116	GLN
35	2d	123	HIS
36	2e	20	GLN
36	2e	56	GLN
37	2f	13	ASN
37	2f	100	ASN
38	2g	56	GLN
38	2g	64	GLN
39	2h	15	ASN
40	2i	3	GLN
40	2i	58	HIS
41	2j	33	GLN
41	2j	62	HIS
41	2j	68	HIS
41	2j	69	ASN
41	2j	84	GLN
42	2k	22	HIS
43	2l	99	HIS
44	2m	62	ASN
44	2m	77	ASN
45	2n	49	HIS
46	2o	9	GLN
46	2o	28	GLN
46	2o	71	GLN
48	2q	26	GLN
50	2s	14	HIS
50	2s	23	ASN
53	2y	46	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	410 (14%)	30 (1%)
1	2A	2857/2915 (98%)	474 (16%)	29 (1%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	119/121 (98%)	11 (9%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	1a	1494/1521 (98%)	246 (16%)	0
32	2a	1498/1521 (98%)	289 (19%)	0
54	1w	3/5 (60%)	1 (33%)	0
54	2w	3/5 (60%)	1 (33%)	0
55	1x	1/4 (25%)	0	0
55	2x	1/4 (25%)	0	0
All	All	8959/9132 (98%)	1443 (16%)	59 (0%)

All (1443) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	23	G
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	81	G
1	1A	100	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	154(A)	C
1	1A	181	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
1	1A	222	A
1	1A	229	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	272(A)	U
1	1A	272(B)	G

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Mol	Chain	Res	Type
1	1A	272(H)	C
1	1A	272(J)	C
1	1A	275	G
1	1A	279	C
1	1A	280	C
1	1A	291	C
1	1A	311	A
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	406	G
1	1A	411	G
1	1A	412	A
1	1A	421	U
1	1A	422	A
1	1A	428	A
1	1A	454	A
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	615	G
1	1A	616	G
1	1A	627	A

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Mol	Chain	Res	Type
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(A)	A
1	1A	652(E)	G
1	1A	652(U)	G
1	1A	668	G
1	1A	669	G
1	1A	686	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	884	C
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	896	A
1	1A	897	C
1	1A	900	A
1	1A	910	A
1	1A	931	G
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A

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Mol	Chain	Res	Type
1	1A	1012	U
1	1A	1013	C
1	1A	1026	U
1	1A	1033	U
1	1A	1039	G
1	1A	1043	C
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1056	G
1	1A	1061	U
1	1A	1062	G
1	1A	1063	G
1	1A	1065	U
1	1A	1067	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	1077	A
1	1A	1079	C
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1096	A
1	1A	1097	U
1	1A	1098	A
1	1A	1100	C
1	1A	1109	C
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1139	G

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Mol	Chain	Res	Type
1	1A	1150	C
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	1210	A
1	1A	1211	U
1	1A	1218	C
1	1A	1220	A
1	1A	1221(A)	C
1	1A	1241	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
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	1451	C
1	1A	1455	G
1	1A	1459	G
1	1A	1460	A
1	1A	1467	C

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Mol	Chain	Res	Type
1	1A	1471	A
1	1A	1482	G
1	1A	1493	C
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1525	G
1	1A	1530	C
1	1A	1531	C
1	1A	1542	A
1	1A	1543	C
1	1A	1547	C
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1644	C
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	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1747	G
1	1A	1756	G
1	1A	1757	U
1	1A	1758	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G

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Mol	Chain	Res	Type
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	1816	G
1	1A	1828	G
1	1A	1839	G
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
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	1960	A
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	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	2102	U
1	1A	2103	C

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Mol	Chain	Res	Type
1	1A	2104	G
1	1A	2107	C
1	1A	2108	C
1	1A	2110	G
1	1A	2111	C
1	1A	2112	G
1	1A	2116	G
1	1A	2117	A
1	1A	2119	A
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	2137	C
1	1A	2142	C
1	1A	2146	C
1	1A	2158	A
1	1A	2159	G
1	1A	2160	G
1	1A	2162	G
1	1A	2164	C
1	1A	2166	G
1	1A	2167	U
1	1A	2172	U
1	1A	2174	C
1	1A	2186	G
1	1A	2187	G
1	1A	2189	U
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2267	A

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Mol	Chain	Res	Type
1	1A	2269	A
1	1A	2278	A
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2307	G
1	1A	2308	G
1	1A	2318	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2383	G
1	1A	2385	C
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	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2525	G
1	1A	2529	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G

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Mol	Chain	Res	Type
1	1A	2573	C
1	1A	2574	G
1	1A	2588	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	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2744	G
1	1A	2751	G
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	2790	A
1	1A	2791	C
1	1A	2792	G
1	1A	2794	C
1	1A	2802	G
1	1A	2805	G
1	1A	2808	U
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2892	A
1	1A	2893	G

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Mol	Chain	Res	Type
1	1A	2894	G
2	1B	2	C
2	1B	3	C
2	1B	7	G
2	1B	12	C
2	1B	13	A
2	1B	45	A
2	1B	56	G
2	1B	66	A
2	1B	73	A
2	1B	89	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	93	G
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	129(A)	G
32	1a	131	C
32	1a	141	A
32	1a	143	A
32	1a	144	G
32	1a	163	C
32	1a	165	C
32	1a	169	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	190	U
32	1a	195	A
32	1a	197	A

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Mol	Chain	Res	Type
32	1a	201	C
32	1a	204	U
32	1a	216	G
32	1a	217	C
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	264	U
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	354	G
32	1a	356	A
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	414	A
32	1a	423	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	443	C
32	1a	452	A
32	1a	458	C
32	1a	470	C
32	1a	475	G
32	1a	477	A
32	1a	485	G
32	1a	487	A
32	1a	496	A

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Mol	Chain	Res	Type
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	519	C
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	619	U
32	1a	630	G
32	1a	632	A
32	1a	633	G
32	1a	642	A
32	1a	653	A
32	1a	665	A
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	724	G
32	1a	731	G
32	1a	734	G
32	1a	754	C
32	1a	755	G
32	1a	759	A
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G

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Mol	Chain	Res	Type
32	1a	836	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	853	G
32	1a	855	G
32	1a	870	U
32	1a	872	A
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	931	C
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	983	A
32	1a	991	U
32	1a	992	U
32	1a	993	G
32	1a	998	G
32	1a	1001	A
32	1a	1001(A)	G
32	1a	1002	G
32	1a	1004	A
32	1a	1005	A
32	1a	1020	U
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C

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Mol	Chain	Res	Type
32	1a	1028	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1032	G
32	1a	1033	G
32	1a	1036	G
32	1a	1037	C
32	1a	1044	A
32	1a	1065	U
32	1a	1070	U
32	1a	1081	G
32	1a	1092	A
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1125	U
32	1a	1126	U
32	1a	1127	G
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1155	G
32	1a	1159	U
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1186	G
32	1a	1188	A
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1224	G

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Mol	Chain	Res	Type
32	1a	1225	A
32	1a	1227	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1268	A
32	1a	1270	C
32	1a	1277	C
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1293	G
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1360	A
32	1a	1363	C
32	1a	1370	G
32	1a	1373	G
32	1a	1397	C
32	1a	1398	A
32	1a	1409	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1447	A
32	1a	1456	G
32	1a	1457	G
32	1a	1493	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U

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Mol	Chain	Res	Type
32	1a	1508	G
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
54	1w	74	C
1	2A	10	G
1	2A	11	G
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	36	G
1	2A	45	C
1	2A	50	U
1	2A	61	G
1	2A	63	U
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	92	A
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	149	A
1	2A	157	U
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	229	A
1	2A	230	U

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Mol	Chain	Res	Type
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	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	352	G
1	2A	363	G
1	2A	370	G
1	2A	386	G
1	2A	396	G
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	429	A
1	2A	444	C
1	2A	455	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	496	G
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	545	G
1	2A	551	G
1	2A	563	G
1	2A	568	U

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Mol	Chain	Res	Type
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	730	C
1	2A	740	U
1	2A	752	A
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	869	G
1	2A	873	G
1	2A	877	U
1	2A	880	G

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Mol	Chain	Res	Type
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	892	G
1	2A	893	C
1	2A	896	A
1	2A	897	C
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	959	A
1	2A	961	C
1	2A	968	G
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1026	U
1	2A	1033	U
1	2A	1034	G
1	2A	1038	C
1	2A	1042	G
1	2A	1044	G
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1052	C

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Mol	Chain	Res	Type
1	2A	1054	A
1	2A	1060	U
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1070	A
1	2A	1071	G
1	2A	1073	A
1	2A	1074	G
1	2A	1075	C
1	2A	1076	C
1	2A	1077	A
1	2A	1079	C
1	2A	1081	U
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1087	G
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	1105	U
1	2A	1106	G
1	2A	1108	U
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1117	G
1	2A	1120	G
1	2A	1129	A
1	2A	1135	C

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Mol	Chain	Res	Type
1	2A	1136	G
1	2A	1142	U
1	2A	1142(A)	A
1	2A	1144	G
1	2A	1170	G
1	2A	1171	G
1	2A	1211	U
1	2A	1220	A
1	2A	1236	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1321	A
1	2A	1365	A
1	2A	1368	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1497	U
1	2A	1507	A
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1525	G

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Mol	Chain	Res	Type
1	2A	1531	C
1	2A	1533	G
1	2A	1542	A
1	2A	1543	C
1	2A	1554	A
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1590	U
1	2A	1595	G
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1648	C
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1741	A
1	2A	1750	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1830	C

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Mol	Chain	Res	Type
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1882	C
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1918	A
1	2A	1923	U
1	2A	1926	U
1	2A	1929	G
1	2A	1930	G
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	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	2101	G
1	2A	2103	C
1	2A	2104	G
1	2A	2105	C

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Mol	Chain	Res	Type
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2123	G
1	2A	2124	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2139	C
1	2A	2140	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	2155	G
1	2A	2157	G
1	2A	2161	C
1	2A	2162	G
1	2A	2163	C
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G
1	2A	2172	U
1	2A	2173	A

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Mol	Chain	Res	Type
1	2A	2174	C
1	2A	2175	C
1	2A	2178	C
1	2A	2182	G
1	2A	2183	C
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2239	G
1	2A	2269	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2308	G
1	2A	2310	A
1	2A	2311	A
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2366	A
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2410	G

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Mol	Chain	Res	Type
1	2A	2422	A
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2518	A
1	2A	2529	G
1	2A	2547	U
1	2A	2554	U
1	2A	2556	C
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
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	2769	C
1	2A	2778	A
1	2A	2779	U
1	2A	2789	C
1	2A	2802	G
1	2A	2810	A
1	2A	2811	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2836	U
1	2A	2872	G
1	2A	2880	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	7	G
2	2B	9	G
2	2B	12	C
2	2B	33	G
2	2B	42	C
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	90	A
2	2B	110	G
32	2a	5	U
32	2a	9	G
32	2a	22	G
32	2a	29	G
32	2a	30	U
32	2a	32	A
32	2a	33	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	61	G

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Mol	Chain	Res	Type
32	2a	78	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	102	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	156	G
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(C)	C
32	2a	189(D)	C
32	2a	189(F)	U
32	2a	189(I)	G
32	2a	194	C
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	223	U
32	2a	240	C
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	277	C
32	2a	289	G
32	2a	316	G
32	2a	319	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G

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Mol	Chain	Res	Type
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	382	A
32	2a	384	G
32	2a	391	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	438	G
32	2a	439	A
32	2a	441	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	476	G
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	532	A
32	2a	533	A
32	2a	536	C
32	2a	547	A
32	2a	559	A

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Mol	Chain	Res	Type
32	2a	561	U
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	630	G
32	2a	631	G
32	2a	641	U
32	2a	653	A
32	2a	660	G
32	2a	662	G
32	2a	665	A
32	2a	672	U
32	2a	687	A
32	2a	688	G
32	2a	702	A
32	2a	703	G
32	2a	721	G
32	2a	723	U
32	2a	728	A
32	2a	729	A
32	2a	731	G
32	2a	734	G
32	2a	746	A
32	2a	749	C
32	2a	753	A
32	2a	754	C
32	2a	755	G
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	787	A
32	2a	793	U
32	2a	794	A
32	2a	802	A
32	2a	805	C
32	2a	817	C
32	2a	821	G
32	2a	828	A

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Mol	Chain	Res	Type
32	2a	829	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	855	G
32	2a	859	A
32	2a	872	A
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	955	U
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	982	U
32	2a	983	A
32	2a	985	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	1000	U
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1007	C
32	2a	1015	A
32	2a	1020	U
32	2a	1022	G
32	2a	1023	G

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Mol	Chain	Res	Type
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
32	2a	1030(B)	C
32	2a	1030(C)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1034	G
32	2a	1040	U
32	2a	1041	A
32	2a	1043	C
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1093	A
32	2a	1094	G
32	2a	1101	A
32	2a	1110	A
32	2a	1113	C
32	2a	1118	C
32	2a	1122	U
32	2a	1125	U
32	2a	1127	G
32	2a	1129	C
32	2a	1130	A
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1147	C
32	2a	1152	A
32	2a	1159	U
32	2a	1160	G
32	2a	1161	C

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Mol	Chain	Res	Type
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1211	U
32	2a	1213	A
32	2a	1214	C
32	2a	1215	G
32	2a	1224	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1248	A
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	1287	A
32	2a	1298	C
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1316	G
32	2a	1317	C
32	2a	1319	A
32	2a	1320	C
32	2a	1322	C
32	2a	1323	G
32	2a	1340	A
32	2a	1345	U
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U

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Mol	Chain	Res	Type
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1370	G
32	2a	1384	C
32	2a	1397	C
32	2a	1400	5MC
32	2a	1401	G
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
32	2a	1487	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	1529	G
32	2a	1530	G
54	2w	74	C

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	199	A
1	1A	266	G
1	1A	278	A
1	1A	573	G
1	1A	746	A
1	1A	764	A
1	1A	839	U
1	1A	840	C
1	1A	888	C
1	1A	895	U
1	1A	974	G

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Mol	Chain	Res	Type
1	1A	1047	G
1	1A	1089	G
1	1A	1175	U
1	1A	1210	A
1	1A	1301	A
1	1A	1379	A
1	1A	1442	G
1	1A	1608	A
1	1A	1653	G
1	1A	2126	A
1	1A	2238	G
1	1A	2406	U
1	1A	2422	A
1	1A	2439	A
1	1A	2611	U
1	1A	2689	U
1	1A	2756	U
1	1A	2893	G
1	2A	195	A
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	900	A
1	2A	1051	G
1	2A	1053	C
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1076	C
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1992	G
1	2A	2126	A

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Mol	Chain	Res	Type
1	2A	2171	A
1	2A	2172	U
1	2A	2321	G
1	2A	2689	U
1	2A	2756	U

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

50 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	MA6	1a	1519	32	19,26,27	0.81	0	18,38,41	1.45	2 (11%)
1	5MU	1A	1939	57,1	19,22,23	1.44	5 (26%)	28,32,35	2.17	8 (28%)
32	UR3	1a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.48	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.75	1 (5%)	26,32,35	1.00	1 (3%)
32	5MC	1a	1407	32	18,22,23	0.98	1 (5%)	26,32,35	1.16	3 (11%)
32	G7M	2a	527	32	20,26,27	1.23	2 (10%)	17,39,42	0.69	0
32	M2G	2a	966	57,32	20,27,28	1.49	3 (15%)	22,40,43	0.89	1 (4%)
32	MA6	2a	1518	32	19,26,27	0.80	0	18,38,41	1.43	2 (11%)
32	PSU	1a	516	32	18,21,22	1.34	2 (11%)	22,30,33	1.81	5 (22%)
1	PSU	2A	1917	57,1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	OMU	1A	2552	57,1	19,22,23	1.29	3 (15%)	26,31,34	1.74	6 (23%)
32	5MC	2a	1407	32	18,22,23	0.97	1 (5%)	26,32,35	1.11	3 (11%)
1	5MC	1A	1942	1	18,22,23	0.97	2 (11%)	26,32,35	1.12	2 (7%)
43	0TD	2l	92	43	7,9,10	4.73	1 (14%)	6,11,13	5.94	3 (50%)
1	OMG	2A	2251	55,57,1	18,26,27	0.95	1 (5%)	19,38,41	1.12	3 (15%)
1	OMU	2A	2552	57,1	19,22,23	1.22	3 (15%)	26,31,34	1.81	6 (23%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
1	5MU	2A	1915	1	19,22,23	1.44	4 (21%)	28,32,35	2.09	8 (28%)
32	PSU	2a	516	57,32	18,21,22	1.31	2 (11%)	22,30,33	1.94	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	5MC	2a	967	32	18,22,23	0.98	2 (11%)	26,32,35	1.08	2 (7%)
55	8AN	1x	76	55,57	19,24,25	1.19	3 (15%)	13,35,38	1.85	3 (23%)
32	5MC	2a	1404	32	18,22,23	1.00	2 (11%)	26,32,35	1.22	3 (11%)
1	5MC	1A	1962	57,1	18,22,23	0.95	2 (11%)	26,32,35	1.13	4 (15%)
1	5MU	1A	1915	1	19,22,23	1.44	4 (21%)	28,32,35	2.16	9 (32%)
32	G7M	1a	527	57,32	20,26,27	1.18	2 (10%)	17,39,42	0.56	0
32	5MC	2a	1400	32	18,22,23	0.96	1 (5%)	26,32,35	1.25	3 (11%)
32	2MG	1a	1207	32	18,26,27	0.97	1 (5%)	16,38,41	1.13	3 (18%)
55	8AN	2x	76	55,57	19,24,25	1.22	3 (15%)	13,35,38	1.77	2 (15%)
1	PSU	1A	2605	1	18,21,22	1.45	4 (22%)	22,30,33	1.84	4 (18%)
32	4OC	2a	1402	32	20,23,24	0.76	0	26,32,35	0.95	0
32	MA6	2a	1519	32	19,26,27	0.86	0	18,38,41	1.59	2 (11%)
1	OMC	2A	1920	1	19,22,23	0.84	0	26,31,34	1.05	2 (7%)
32	2MG	2a	1207	32	18,26,27	0.92	1 (5%)	16,38,41	1.08	2 (12%)
1	5MC	2A	1942	1	18,22,23	0.93	2 (11%)	26,32,35	1.17	2 (7%)
32	M2G	1a	966	32	20,27,28	1.39	3 (15%)	22,40,43	1.01	2 (9%)
32	MA6	1a	1518	32	19,26,27	0.79	0	18,38,41	1.33	2 (11%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	22,30,33	1.87	4 (18%)
32	5MC	1a	967	32	18,22,23	0.98	2 (11%)	26,32,35	1.12	2 (7%)
32	UR3	2a	1498	32	19,22,23	1.01	2 (10%)	26,32,35	1.36	1 (3%)
1	OMC	1A	1920	1	19,22,23	0.85	0	26,31,34	0.96	1 (3%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	22,30,33	1.94	4 (18%)
1	OMG	1A	2251	55,57,1	18,26,27	1.01	1 (5%)	19,38,41	1.07	2 (10%)
1	PSU	2A	2605	1	18,21,22	1.33	2 (11%)	22,30,33	1.79	3 (13%)
1	5MU	2A	1939	1	19,22,23	1.48	5 (26%)	28,32,35	2.14	8 (28%)
32	5MC	1a	1404	32	18,22,23	0.96	2 (11%)	26,32,35	1.13	2 (7%)
1	2MA	2A	2503	57,1	17,25,26	1.00	1 (5%)	17,37,40	1.08	2 (11%)
32	5MC	1a	1400	32	18,22,23	1.00	2 (11%)	26,32,35	1.12	2 (7%)
1	5MC	2A	1962	57,1	18,22,23	0.97	2 (11%)	26,32,35	1.14	2 (7%)
43	0TD	1l	92	43	7,9,10	4.78	1 (14%)	6,11,13	2.74	3 (50%)
1	2MA	1A	2503	57,1	17,25,26	0.99	1 (5%)	17,37,40	0.95	2 (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	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	2/3/25/26	0/3/3/3
32	M2G	2a	966	57,32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	PSU	1a	516	32	-	1/7/25/26	0/2/2/2
1	PSU	2A	1917	57,1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
1	OMG	2A	2251	55,57,1	-	0/5/27/28	0/3/3/3
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	PSU	2a	516	57,32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	55,57	-	1/3/25/26	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
32	G7M	1a	527	57,32	-	2/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
55	8AN	2x	76	55,57	-	1/3/25/26	0/3/3/3
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
32	MA6	2a	1519	32	-	2/7/29/30	0/3/3/3
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
32	2MG	2a	1207	32	-	2/5/27/28	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1A	2251	55,57,1	-	0/5/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	57,1	-	1/3/25/26	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	57,1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
1	2MA	1A	2503	57,1	-	2/3/25/26	0/3/3/3

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.17	1.69	1.82
43	2l	92	0TD	CB-SB	-12.16	1.69	1.82
32	2a	966	M2G	C2-N3	4.78	1.36	1.30
32	1a	966	M2G	C2-N3	4.10	1.35	1.30
32	2a	527	G7M	C5-C4	3.64	1.46	1.39
32	1a	527	G7M	C5-C4	3.61	1.46	1.39
1	2A	1911	PSU	C6-C5	3.52	1.39	1.35
32	1a	516	PSU	C6-C5	3.33	1.39	1.35
1	1A	1911	PSU	C6-C5	3.28	1.39	1.35
1	1A	2605	PSU	C4-N3	-3.27	1.32	1.38
1	1A	1917	PSU	C6-C5	3.26	1.39	1.35
1	2A	1917	PSU	C6-C5	3.17	1.39	1.35
1	2A	1915	5MU	C6-C5	3.10	1.39	1.34
1	2A	1939	5MU	C4-C5	3.02	1.49	1.44
32	2a	516	PSU	C6-C5	2.98	1.38	1.35
32	1a	1400	5MC	C6-C5	2.98	1.39	1.34
32	2a	966	M2G	C2-N2	2.97	1.40	1.35
32	2a	1400	5MC	C6-C5	2.96	1.39	1.34
32	2a	1404	5MC	C6-C5	2.95	1.39	1.34
32	1a	1407	5MC	C6-C5	2.94	1.39	1.34
32	2a	967	5MC	C6-C5	2.89	1.39	1.34
1	1A	1939	5MU	C6-C5	2.87	1.39	1.34
1	1A	1915	5MU	C2-N1	2.86	1.43	1.38
1	2A	2605	PSU	C6-C5	2.85	1.38	1.35
1	1A	1939	5MU	C4-C5	2.84	1.49	1.44
32	2a	1407	5MC	C6-C5	2.84	1.39	1.34
32	1a	967	5MC	C6-C5	2.83	1.39	1.34
55	1x	76	8AN	C6-C5	-2.83	1.32	1.43
1	2A	1915	5MU	C2-N1	2.80	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1404	5MC	C6-C5	2.79	1.39	1.34
1	1A	2605	PSU	C6-C5	2.79	1.38	1.35
55	2x	76	8AN	C5-C4	-2.77	1.33	1.40
1	2A	1962	5MC	C6-C5	2.77	1.39	1.34
1	1A	2251	OMG	C6-N1	-2.77	1.33	1.37
1	2A	1939	5MU	C4-N3	-2.75	1.33	1.38
1	1A	1915	5MU	C6-C5	2.73	1.39	1.34
1	2A	2605	PSU	C4-N3	-2.65	1.33	1.38
1	1A	2552	OMU	C2-N1	2.64	1.42	1.38
1	2A	1939	5MU	C6-C5	2.64	1.38	1.34
1	1A	1917	PSU	C4-N3	-2.63	1.34	1.38
1	1A	1942	5MC	C6-C5	2.62	1.38	1.34
55	2x	76	8AN	C6-C5	-2.61	1.33	1.43
1	2A	1917	PSU	C4-N3	-2.56	1.34	1.38
32	1a	966	M2G	C6-N1	-2.55	1.34	1.37
32	1a	966	M2G	C2-N2	2.55	1.39	1.35
1	2A	1942	5MC	C6-C5	2.55	1.38	1.34
1	1A	2605	PSU	C2-N3	-2.53	1.33	1.37
1	1A	1911	PSU	C4-N3	-2.52	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.52	1.33	1.38
1	1A	1942	5MC	C6-N1	-2.51	1.33	1.38
1	1A	1939	5MU	C4-N3	-2.51	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.49	1.34	1.38
1	1A	1962	5MC	C6-C5	2.47	1.38	1.34
1	2A	1911	PSU	C4-N3	-2.46	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.45	1.33	1.38
32	1a	1207	2MG	C6-N1	-2.45	1.34	1.37
1	1A	1915	5MU	C4-C5	2.43	1.48	1.44
1	1A	1915	5MU	C4-N3	-2.42	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.42	1.34	1.37
1	2A	1915	5MU	C4-C5	2.41	1.48	1.44
1	1A	2552	OMU	C5-C4	2.40	1.48	1.43
1	2A	2552	OMU	C5-C4	2.38	1.48	1.43
32	2a	527	G7M	C6-N1	-2.36	1.34	1.37
32	2a	516	PSU	C4-N3	-2.34	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.32	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.31	1.34	1.37
1	2A	1962	5MC	C6-N1	-2.31	1.34	1.38
32	1a	516	PSU	C4-N3	-2.30	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.27	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.26	1.34	1.38
55	1x	76	8AN	C5-N7	-2.23	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	C4-N3	-2.23	1.34	1.38
32	2a	1498	UR3	C2-N1	2.21	1.41	1.38
1	2A	1939	5MU	C2-N1	2.21	1.42	1.38
55	1x	76	8AN	C5-C4	-2.20	1.35	1.40
1	1A	2552	OMU	C4-N3	-2.20	1.34	1.38
1	1A	2503	2MA	C2-N3	2.19	1.35	1.31
32	2a	966	M2G	C6-N1	-2.16	1.34	1.37
1	1A	1939	5MU	C6-N1	-2.16	1.34	1.38
32	1a	1498	UR3	C6-C5	2.15	1.40	1.35
32	1a	967	5MC	C6-N1	-2.13	1.34	1.38
32	1a	527	G7M	C6-N1	-2.12	1.34	1.37
32	1a	1404	5MC	C6-N1	-2.11	1.34	1.38
32	2a	1498	UR3	C6-C5	2.07	1.39	1.35
1	1A	2605	PSU	C2-N1	-2.04	1.34	1.36
55	2x	76	8AN	C5-N7	-2.03	1.32	1.39
1	1A	1939	5MU	C2-N3	-2.03	1.34	1.38
1	2A	2552	OMU	C2-N1	2.03	1.41	1.38
32	1a	1402	4OC	C6-C5	2.02	1.39	1.35
32	2a	967	5MC	C6-N1	-2.02	1.34	1.38
1	2A	2503	2MA	C2-N3	2.00	1.35	1.31

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-13.82	77.44	102.44
1	1A	1911	PSU	N1-C2-N3	6.15	122.10	115.13
32	1a	1498	UR3	C4-N3-C2	-6.13	118.79	124.56
32	2a	516	PSU	N1-C2-N3	5.97	121.89	115.13
1	2A	1917	PSU	N1-C2-N3	5.91	121.82	115.13
1	1A	1917	PSU	N1-C2-N3	5.83	121.74	115.13
1	2A	1911	PSU	N1-C2-N3	5.83	121.73	115.13
1	1A	2605	PSU	N1-C2-N3	5.69	121.58	115.13
55	2x	76	8AN	N3-C2-N1	-5.68	119.81	128.68
55	1x	76	8AN	N3-C2-N1	-5.60	119.92	128.68
32	2a	1498	UR3	C4-N3-C2	-5.48	119.40	124.56
1	2A	1939	5MU	N3-C2-N1	5.48	122.16	114.89
1	2A	1939	5MU	C4-N3-C2	-5.42	120.34	127.35
1	2A	2605	PSU	N1-C2-N3	5.34	121.18	115.13
1	1A	1939	5MU	C4-N3-C2	-5.32	120.47	127.35
1	2A	2552	OMU	N3-C2-N1	5.10	121.66	114.89
32	1a	516	PSU	N1-C2-N3	5.07	120.88	115.13
43	1l	92	0TD	CSB-SB-CB	-5.05	93.30	102.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1915	5MU	N3-C2-N1	4.95	121.47	114.89
1	1A	1939	5MU	N3-C2-N1	4.91	121.41	114.89
32	2a	1519	MA6	N3-C2-N1	-4.79	121.19	128.68
1	1A	1915	5MU	C4-N3-C2	-4.77	121.18	127.35
32	1a	1519	MA6	N3-C2-N1	-4.74	121.26	128.68
1	2A	1915	5MU	C4-N3-C2	-4.71	121.25	127.35
32	2a	1518	MA6	N3-C2-N1	-4.69	121.35	128.68
1	1A	1915	5MU	C5-C4-N3	4.62	119.25	115.31
1	1A	1939	5MU	C5-C4-N3	4.61	119.24	115.31
1	1A	1915	5MU	N3-C2-N1	4.58	120.97	114.89
32	1a	1518	MA6	N3-C2-N1	-4.48	121.68	128.68
1	2A	2552	OMU	C4-N3-C2	-4.44	120.72	126.58
1	1A	2552	OMU	N3-C2-N1	4.39	120.72	114.89
1	1A	1939	5MU	C5-C6-N1	-4.13	119.09	123.34
32	2a	516	PSU	C4-N3-C2	-4.04	120.51	126.34
1	2A	1915	5MU	C5-C4-N3	4.04	118.76	115.31
1	1A	2552	OMU	C4-N3-C2	-4.02	121.27	126.58
1	1A	1917	PSU	C4-N3-C2	-3.99	120.59	126.34
1	1A	1915	5MU	O4-C4-C5	-3.97	120.30	124.90
1	2A	1939	5MU	C5-C4-N3	3.96	118.69	115.31
32	2a	516	PSU	O2-C2-N1	-3.95	118.44	122.79
1	1A	1911	PSU	C4-N3-C2	-3.91	120.71	126.34
1	2A	1942	5MC	C5-C6-N1	-3.91	119.32	123.34
1	2A	1911	PSU	C4-N3-C2	-3.88	120.75	126.34
1	1A	2605	PSU	C4-N3-C2	-3.87	120.77	126.34
32	1a	516	PSU	C4-N3-C2	-3.84	120.81	126.34
32	1a	967	5MC	C5-C6-N1	-3.82	119.41	123.34
32	1a	1404	5MC	C5-C6-N1	-3.78	119.45	123.34
1	2A	2605	PSU	C4-N3-C2	-3.77	120.90	126.34
1	2A	1917	PSU	O2-C2-N1	-3.77	118.64	122.79
1	2A	1962	5MC	C5-C6-N1	-3.74	119.49	123.34
1	1A	1939	5MU	O2-C2-N1	-3.71	117.85	122.79
1	2A	1939	5MU	C5-C6-N1	-3.71	119.52	123.34
1	2A	1917	PSU	C4-N3-C2	-3.65	121.08	126.34
1	2A	1915	5MU	O4-C4-C5	-3.65	120.67	124.90
1	1A	1915	5MU	C1'-N1-C2	3.64	124.16	117.57
32	1a	1400	5MC	C5-C6-N1	-3.63	119.61	123.34
1	1A	1911	PSU	O2-C2-N1	-3.60	118.82	122.79
32	2a	1519	MA6	C4-C5-N7	-3.51	105.75	109.40
1	2A	1915	5MU	C1'-N1-C2	3.48	123.87	117.57
1	1A	1962	5MC	C5-C6-N1	-3.48	119.76	123.34
1	1A	1942	5MC	C5-C6-N1	-3.47	119.77	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1404	5MC	C5-C6-N1	-3.46	119.78	123.34
43	2l	92	0TD	OD2-CG-CB	3.44	120.59	113.15
43	1l	92	0TD	OD2-CG-CB	3.39	120.48	113.15
32	2a	1404	5MC	C5-C4-N3	-3.35	118.06	121.67
1	1A	1939	5MU	O4-C4-C5	-3.35	121.02	124.90
32	1a	1407	5MC	C5-C6-N1	-3.34	119.90	123.34
1	2A	2605	PSU	O2-C2-N1	-3.26	119.20	122.79
32	2a	967	5MC	C5-C6-N1	-3.22	120.03	123.34
1	1A	2552	OMU	C2'-C1'-N1	-3.19	108.03	114.22
1	1A	1915	5MU	C1'-N1-C6	-3.19	115.82	121.12
1	1A	1917	PSU	O2-C2-N1	-3.16	119.31	122.79
1	2A	1911	PSU	O2-C2-N1	-3.07	119.42	122.79
32	1a	1402	4OC	C6-C5-C4	3.02	120.66	116.96
32	2a	1518	MA6	C4-C5-N7	-3.00	106.27	109.40
32	1a	1519	MA6	C4-C5-N7	-3.00	106.27	109.40
1	1A	2552	OMU	O4-C4-C5	-2.98	119.91	125.16
1	2A	1939	5MU	O2-C2-N1	-2.90	118.93	122.79
32	2a	1407	5MC	C5-C6-N1	-2.87	120.38	123.34
1	2A	2552	OMU	C2'-C1'-N1	-2.81	108.77	114.22
32	2a	1407	5MC	C5-C4-N3	-2.80	118.65	121.67
1	2A	2552	OMU	C5-C4-N3	2.80	119.03	114.84
32	2a	1400	5MC	C5-C6-N1	-2.79	120.47	123.34
32	1a	1400	5MC	C5-C4-N3	-2.79	118.66	121.67
32	1a	516	PSU	O2-C2-N1	-2.78	119.73	122.79
1	2A	2503	2MA	C8-N7-C5	2.74	108.20	102.99
1	2A	1939	5MU	C5M-C5-C4	2.73	121.77	118.77
1	2A	1915	5MU	C5-C6-N1	-2.72	120.54	123.34
1	2A	2552	OMU	O4-C4-C5	-2.71	120.39	125.16
1	2A	1915	5MU	C1'-N1-C6	-2.71	116.61	121.12
1	2A	1939	5MU	C5M-C5-C6	-2.66	119.29	122.85
1	1A	1939	5MU	C5M-C5-C4	2.64	121.67	118.77
1	2A	2552	OMU	O2-C2-N1	-2.59	119.34	122.79
32	1a	1518	MA6	C4-C5-N7	-2.59	106.70	109.40
1	1A	1915	5MU	C5-C6-N1	-2.59	120.68	123.34
1	1A	2605	PSU	O2-C2-N1	-2.58	119.95	122.79
1	2A	1920	OMC	O2-C2-N3	-2.58	118.14	122.33
32	1a	1407	5MC	C5-C4-N3	-2.53	118.94	121.67
1	2A	1939	5MU	O4-C4-C5	-2.53	121.97	124.90
32	1a	516	PSU	C6-C5-C4	-2.52	116.43	118.20
32	2a	1400	5MC	C5-C4-N3	-2.52	118.96	121.67
1	1A	2251	OMG	C5-C6-N1	2.51	118.39	113.95
43	2l	92	0TD	OD1-CG-CB	-2.51	117.18	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	967	5MC	C5-C4-N3	-2.50	118.98	121.67
1	1A	2251	OMG	C8-N7-C5	2.48	107.72	102.99
1	1A	2552	OMU	C5-C4-N3	2.46	118.52	114.84
32	1a	1407	5MC	O2-C2-N3	-2.46	118.33	122.33
32	1a	1404	5MC	C5-C4-N3	-2.43	119.05	121.67
32	2a	1207	2MG	C8-N7-C5	2.39	107.55	102.99
1	2A	2503	2MA	C5-C6-N1	2.39	118.14	114.02
55	1x	76	8AN	C4-C5-N7	-2.38	106.92	109.40
32	1a	1498	UR3	C3U-N3-C2	2.37	121.46	117.31
1	1A	2503	2MA	C8-N7-C5	2.36	107.48	102.99
1	2A	2251	OMG	C8-N7-C5	2.35	107.47	102.99
32	1a	1207	2MG	C8-N7-C5	2.33	107.42	102.99
1	2A	1962	5MC	C5-C4-N3	-2.31	119.18	121.67
32	2a	967	5MC	C5-C4-N3	-2.30	119.19	121.67
32	1a	966	M2G	C5-C6-N1	2.25	117.92	113.95
1	1A	1920	OMC	O2-C2-N3	-2.24	118.69	122.33
55	1x	76	8AN	O4'-C1'-C2'	-2.24	103.66	106.93
32	2a	1400	5MC	O2-C2-N3	-2.22	118.72	122.33
1	2A	1942	5MC	C5-C4-N3	-2.20	119.30	121.67
32	1a	1207	2MG	C5-C6-N1	2.18	117.80	113.95
32	1a	966	M2G	C8-N7-C5	2.18	107.14	102.99
32	2a	966	M2G	C8-N7-C5	2.17	107.13	102.99
55	2x	76	8AN	O4'-C1'-C2'	-2.17	103.75	106.93
1	1A	2605	PSU	C5-C6-N1	-2.15	118.88	122.11
1	1A	2503	2MA	C5-C6-N1	2.15	117.72	114.02
1	1A	1939	5MU	C5M-C5-C6	-2.14	119.99	122.85
1	1A	1962	5MC	CM5-C5-C6	-2.14	120.00	122.85
1	2A	2251	OMG	C5-C6-N1	2.13	117.72	113.95
1	1A	1915	5MU	O2-C2-N3	-2.13	117.53	121.50
32	2a	516	PSU	O4'-C1'-C2'	2.13	108.14	105.14
1	1A	1942	5MC	C5-C4-N3	-2.13	119.38	121.67
1	1A	1915	5MU	C5M-C5-C4	2.12	121.10	118.77
32	2a	1407	5MC	O2-C2-N3	-2.11	118.89	122.33
1	2A	1911	PSU	C6-C5-C4	-2.10	116.73	118.20
1	2A	1920	OMC	C1'-N1-C2	2.09	123.08	118.42
32	1a	516	PSU	O4'-C1'-C2'	2.09	108.08	105.14
1	1A	1962	5MC	C5-C4-N3	-2.08	119.43	121.67
32	2a	1207	2MG	CM2-N2-C2	-2.08	119.28	123.86
1	2A	2251	OMG	CM2-O2'-C2'	-2.07	109.08	114.52
1	2A	1915	5MU	O2-C2-N3	-2.07	117.64	121.50
43	1l	92	0TD	OD1-CG-CB	-2.07	118.11	122.44
1	1A	1911	PSU	O4'-C1'-C2'	2.06	108.05	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2552	OMU	O2-C2-N1	-2.05	120.06	122.79
32	2a	1404	5MC	CM5-C5-C6	-2.04	120.13	122.85
32	2a	516	PSU	C5-C6-N1	-2.04	119.06	122.11
32	1a	1207	2MG	CM2-N2-C2	-2.03	119.37	123.86
1	1A	1962	5MC	C1'-N1-C6	-2.03	117.75	121.12

There are no chirality outliers.

All (28) 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
43	1l	92	0TD	CG-CB-SB-CSB
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
43	2l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
55	1x	76	8AN	C4'-C5'-O5'-P
32	1a	1519	MA6	O4'-C4'-C5'-O5'
55	2x	76	8AN	C4'-C5'-O5'-P
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	516	PSU	O4'-C1'-C5-C4
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
1	2A	1920	OMC	C2'-C1'-N1-C2
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
1	1A	1920	OMC	C2'-C1'-N1-C2
1	1A	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 2517 ligands modelled in this entry, 2505 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
62	SF4	1d	305	35	0,12,12	-	-	-		
60	MPD	2B	220	-	7,7,7	0.29	0	9,10,10	0.17	0
60	MPD	1T	208	-	7,7,7	0.28	0	9,10,10	0.24	0
62	SF4	2d	501	35	0,12,12	-	-	-		
59	ARG	1B	231	-	10,11,11	0.76	1 (10%)	11,13,13	1.10	2 (18%)
58	CLM	2A	3747	-	19,20,20	0.85	0	23,27,27	1.25	2 (8%)
58	CLM	1A	4017	-	19,20,20	1.10	2 (10%)	23,27,27	2.12	7 (30%)
60	MPD	1A	4019	-	7,7,7	0.29	0	9,10,10	0.18	0
60	MPD	18	104	-	7,7,7	0.26	0	9,10,10	0.20	0
60	MPD	2A	3748	-	7,7,7	0.26	0	9,10,10	0.21	0
60	MPD	1a	1867	-	7,7,7	0.33	0	9,10,10	0.40	0
59	ARG	1A	4018	57	10,11,11	0.74	1 (10%)	11,13,13	1.01	1 (9%)

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
62	SF4	1d	305	35	-	-	0/6/5/5
60	MPD	2B	220	-	-	3/5/5/5	-
60	MPD	1T	208	-	-	2/5/5/5	-
62	SF4	2d	501	35	-	-	0/6/5/5
59	ARG	1B	231	-	-	3/11/11/11	-
58	CLM	2A	3747	-	-	0/20/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	CLM	1A	4017	-	-	2/20/22/22	0/1/1/1
60	MPD	1A	4019	-	-	1/5/5/5	-
60	MPD	18	104	-	-	2/5/5/5	-
60	MPD	2A	3748	-	-	2/5/5/5	-
60	MPD	1a	1867	-	-	3/5/5/5	-
59	ARG	1A	4018	57	-	2/11/11/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4017	CLM	C6-C5	-2.95	1.47	1.51
58	1A	4017	CLM	C9-N9	-2.41	1.39	1.45
59	1B	231	ARG	OXT-C	-2.17	1.23	1.30
59	1A	4018	ARG	OXT-C	-2.06	1.23	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	1A	4017	CLM	C10-C9-N9	-5.34	115.35	119.38
58	1A	4017	CLM	C8-C9-N9	5.26	123.33	119.38
58	1A	4017	CLM	C6-C5-C3	3.55	117.89	111.64
58	2A	3747	CLM	C6-C5-C3	3.14	117.17	111.64
58	1A	4017	CLM	O5-C5-C6	-2.70	105.30	111.19
59	1A	4018	ARG	OXT-C-O	-2.54	118.33	124.09
59	1B	231	ARG	OXT-C-O	-2.51	118.40	124.09
58	2A	3747	CLM	C3-N2-C2	-2.39	118.86	123.07
58	1A	4017	CLM	C11-C6-C5	-2.26	117.36	120.73
58	1A	4017	CLM	C11-C6-C7	2.11	120.93	118.29
59	1B	231	ARG	OXT-C-CA	2.06	120.39	113.38
58	1A	4017	CLM	O9B-N9-C9	2.05	121.70	118.80

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1B	231	ARG	O-C-CA-N
60	1A	4019	MPD	C2-C3-C4-O4
59	1B	231	ARG	CA-CB-CG-CD
59	1A	4018	ARG	NE-CD-CG-CB
59	1B	231	ARG	OXT-C-CA-N

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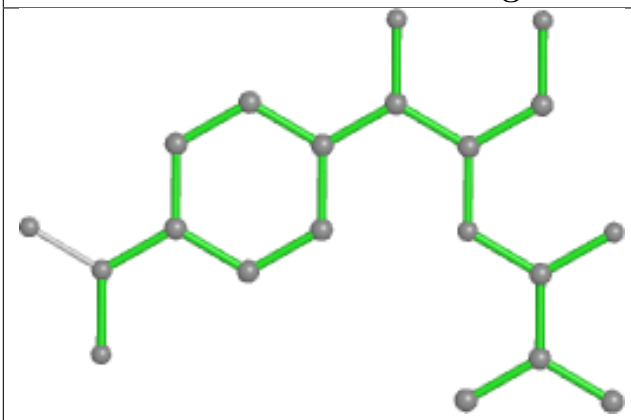
Mol	Chain	Res	Type	Atoms
59	1A	4018	ARG	CA-CB-CG-CD
58	1A	4017	CLM	C5-C3-C4-O4
60	1a	1867	MPD	C2-C3-C4-C5
60	2B	220	MPD	C2-C3-C4-C5
60	1a	1867	MPD	CM-C2-C3-C4
60	2A	3748	MPD	C1-C2-C3-C4
60	2B	220	MPD	C1-C2-C3-C4
58	1A	4017	CLM	N2-C3-C4-O4
60	1T	208	MPD	C2-C3-C4-C5
60	18	104	MPD	C2-C3-C4-C5
60	2A	3748	MPD	C2-C3-C4-C5
60	1T	208	MPD	C2-C3-C4-O4
60	18	104	MPD	C2-C3-C4-O4
60	1a	1867	MPD	C2-C3-C4-O4
60	2B	220	MPD	C2-C3-C4-O4

There are no ring outliers.

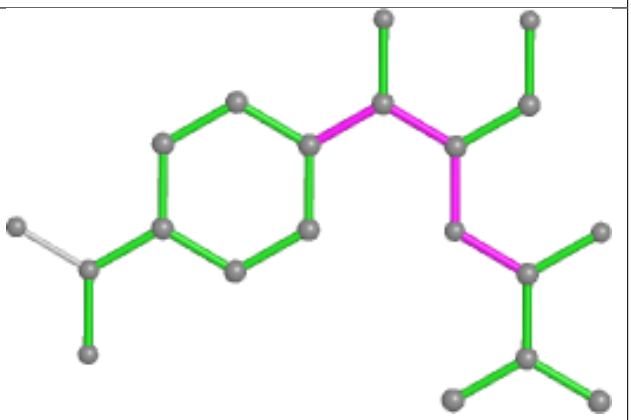
No monomer is involved in short contacts.

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

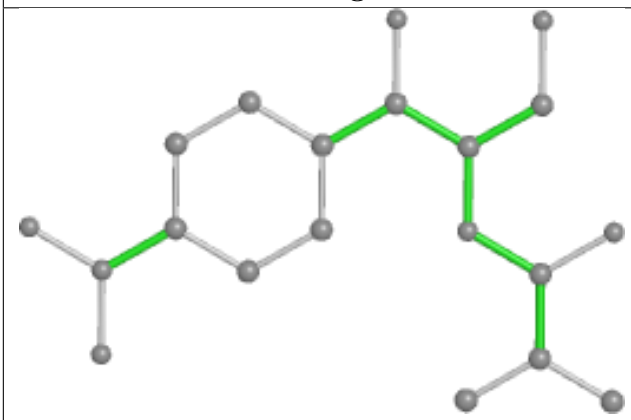
Ligand CLM 2A 3747



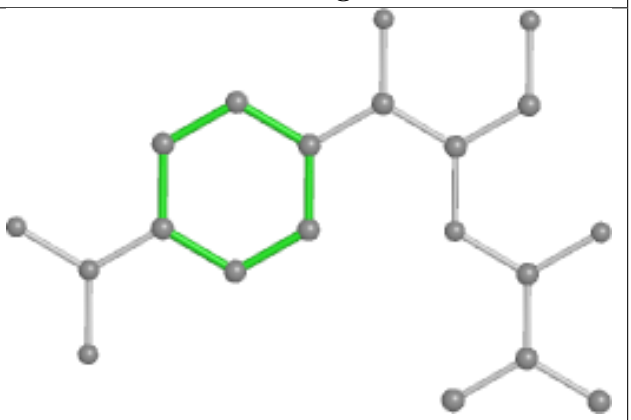
Bond lengths



Bond angles

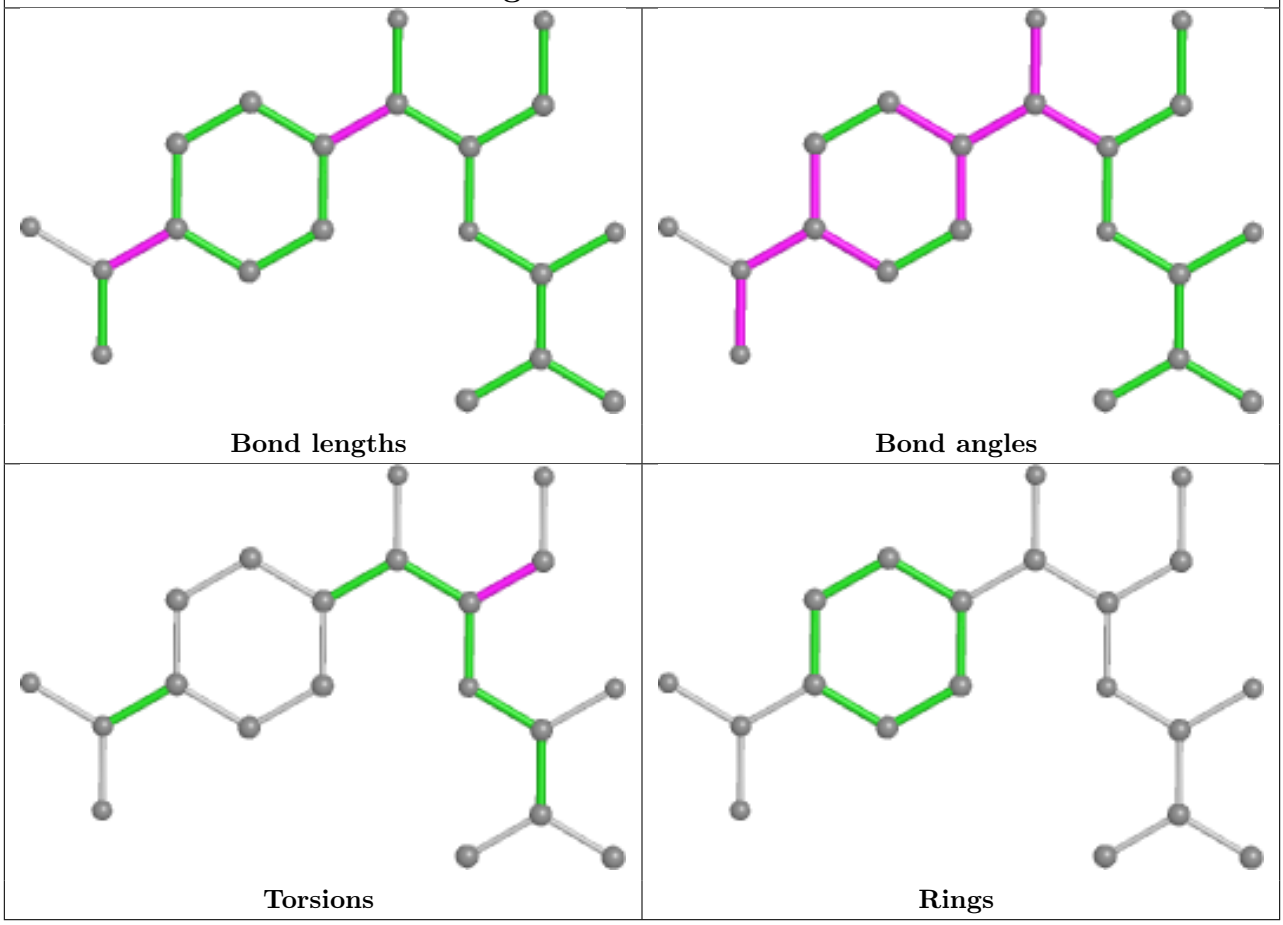


Torsions



Rings

Ligand CLM 1A 4017



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1A	2861/2915 (98%)	0.31	84 (2%) 51 50	19, 36, 84, 95	0
1	2A	2856/2915 (97%)	0.12	102 (3%) 42 42	32, 53, 85, 95	0
2	1B	120/121 (99%)	0.01	0 100 100	30, 48, 62, 74	0
2	2B	120/121 (99%)	-0.01	0 100 100	58, 70, 78, 82	0
3	1D	275/276 (99%)	0.40	1 (0%) 92 91	21, 36, 49, 61	0
3	2D	275/276 (99%)	0.45	3 (1%) 80 79	29, 48, 60, 71	0
4	1E	204/206 (99%)	0.44	0 100 100	18, 40, 57, 66	0
4	2E	204/206 (99%)	0.33	1 (0%) 91 89	32, 53, 66, 75	0
5	1F	203/210 (96%)	0.33	0 100 100	19, 41, 64, 77	0
5	2F	203/210 (96%)	0.26	1 (0%) 91 89	31, 62, 71, 78	0
6	1G	181/182 (99%)	0.12	2 (1%) 80 79	45, 59, 70, 79	0
6	2G	181/182 (99%)	1.11	37 (20%) 1 0	63, 73, 80, 84	0
7	1H	174/180 (96%)	0.30	1 (0%) 89 88	37, 52, 62, 66	0
7	2H	173/180 (96%)	0.72	18 (10%) 6 6	58, 71, 77, 80	0
8	1I	147/148 (99%)	0.08	0 100 100	41, 66, 73, 78	0
8	2I	146/148 (98%)	0.34	8 (5%) 25 24	54, 68, 77, 84	0
9	1N	140/140 (100%)	0.48	1 (0%) 87 86	25, 38, 57, 72	0
9	2N	140/140 (100%)	0.35	5 (3%) 42 42	44, 60, 69, 71	0
10	1O	122/122 (100%)	0.37	0 100 100	28, 41, 56, 64	0
10	2O	122/122 (100%)	0.22	0 100 100	42, 51, 62, 68	0
11	1P	149/150 (99%)	0.25	0 100 100	19, 45, 65, 74	0
11	2P	149/150 (99%)	0.43	3 (2%) 65 63	37, 61, 72, 78	0
12	1Q	141/141 (100%)	0.37	0 100 100	25, 39, 50, 60	0
12	2Q	141/141 (100%)	0.52	4 (2%) 53 51	43, 60, 68, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.39	0 100 100	25, 34, 48, 54	0
13	2R	118/118 (100%)	0.27	1 (0%) 86 84	37, 49, 58, 65	0
14	1S	110/112 (98%)	0.24	0 100 100	37, 48, 59, 63	0
14	2S	110/112 (98%)	0.68	11 (10%) 7 6	59, 66, 71, 71	0
15	1T	131/146 (89%)	0.34	1 (0%) 86 84	33, 45, 64, 80	0
15	2T	131/146 (89%)	0.20	0 100 100	42, 55, 68, 77	0
16	1U	116/118 (98%)	0.45	0 100 100	21, 30, 45, 59	0
16	2U	116/118 (98%)	0.44	0 100 100	40, 56, 67, 72	0
17	1V	101/101 (100%)	0.34	0 100 100	22, 40, 55, 63	0
17	2V	101/101 (100%)	0.33	1 (0%) 82 80	40, 64, 71, 77	0
18	1W	112/113 (99%)	0.44	1 (0%) 84 82	24, 31, 50, 72	0
18	2W	112/113 (99%)	0.45	1 (0%) 84 82	35, 49, 63, 81	0
19	1X	95/96 (98%)	0.37	1 (1%) 80 79	27, 38, 57, 64	0
19	2X	95/96 (98%)	0.46	4 (4%) 36 35	45, 56, 68, 75	0
20	1Y	107/110 (97%)	0.34	1 (0%) 84 82	34, 47, 59, 71	0
20	2Y	107/110 (97%)	0.59	5 (4%) 31 30	55, 65, 73, 78	0
21	1Z	203/206 (98%)	0.13	1 (0%) 91 89	39, 55, 67, 75	0
21	2Z	201/206 (97%)	0.42	6 (2%) 50 49	61, 69, 76, 80	0
22	10	83/85 (97%)	0.59	7 (8%) 11 10	27, 36, 55, 69	0
22	20	83/85 (97%)	0.95	10 (12%) 4 3	45, 58, 68, 70	0
23	11	97/98 (98%)	0.53	3 (3%) 49 47	27, 43, 63, 68	0
23	21	97/98 (98%)	0.45	1 (1%) 82 80	38, 52, 68, 73	0
24	12	70/72 (97%)	0.29	0 100 100	37, 48, 58, 68	0
24	22	70/72 (97%)	0.27	0 100 100	55, 64, 69, 71	0
25	13	59/60 (98%)	0.33	0 100 100	24, 35, 57, 63	0
25	23	59/60 (98%)	0.52	2 (3%) 45 44	53, 58, 70, 76	0
26	14	69/71 (97%)	0.35	5 (7%) 15 14	54, 70, 80, 85	0
26	24	69/71 (97%)	1.44	20 (28%) 0 0	72, 78, 82, 84	0
27	15	59/60 (98%)	0.47	1 (1%) 70 68	22, 32, 45, 54	0
27	25	59/60 (98%)	0.29	0 100 100	33, 48, 60, 66	0
28	16	53/54 (98%)	0.18	0 100 100	33, 42, 52, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.23	1 (1%) 66 64	47, 56, 63, 67	0
29	17	48/49 (97%)	0.61	2 (4%) 36 35	21, 28, 52, 61	0
29	27	48/49 (97%)	0.50	4 (8%) 11 10	34, 39, 60, 66	0
30	18	64/65 (98%)	0.33	0 100 100	27, 34, 40, 54	0
30	28	64/65 (98%)	0.76	1 (1%) 72 70	40, 51, 58, 63	0
31	19	37/37 (100%)	0.47	0 100 100	30, 39, 51, 58	0
31	29	37/37 (100%)	0.79	2 (5%) 25 24	51, 60, 71, 71	0
32	1a	1488/1521 (97%)	-0.03	23 (1%) 73 72	35, 64, 82, 95	0
32	2a	1492/1521 (98%)	0.14	48 (3%) 47 46	44, 69, 84, 95	0
33	1b	231/256 (90%)	0.41	17 (7%) 14 13	60, 70, 77, 82	0
33	2b	231/256 (90%)	1.09	46 (19%) 1 0	66, 75, 80, 84	0
34	1c	206/239 (86%)	0.67	15 (7%) 15 13	56, 67, 75, 80	0
34	2c	206/239 (86%)	1.23	40 (19%) 1 0	65, 75, 79, 81	0
35	1d	208/209 (99%)	0.56	15 (7%) 15 14	54, 65, 73, 79	0
35	2d	208/209 (99%)	0.79	17 (8%) 11 10	56, 66, 73, 75	0
36	1e	148/162 (91%)	0.49	5 (3%) 45 44	43, 61, 68, 74	0
36	2e	148/162 (91%)	0.50	9 (6%) 21 20	58, 66, 73, 81	0
37	1f	100/101 (99%)	0.03	0 100 100	50, 59, 68, 70	0
37	2f	100/101 (99%)	0.08	0 100 100	56, 64, 72, 77	0
38	1g	155/156 (99%)	0.20	4 (2%) 56 54	53, 65, 71, 77	0
38	2g	155/156 (99%)	1.06	33 (21%) 0 0	66, 73, 78, 80	0
39	1h	137/138 (99%)	0.50	5 (3%) 42 42	52, 62, 67, 72	0
39	2h	137/138 (99%)	0.83	15 (10%) 5 5	61, 68, 73, 75	0
40	1i	127/128 (99%)	0.85	13 (10%) 6 6	56, 69, 75, 77	0
40	2i	126/128 (98%)	2.81	81 (64%) 0 0	68, 76, 80, 83	0
41	1j	97/105 (92%)	0.83	8 (8%) 11 10	57, 71, 76, 78	0
41	2j	96/105 (91%)	2.04	42 (43%) 0 0	68, 76, 81, 84	0
42	1k	114/129 (88%)	0.28	1 (0%) 84 82	42, 59, 68, 71	0
42	2k	114/129 (88%)	0.64	8 (7%) 16 15	56, 67, 73, 76	0
43	1l	121/132 (91%)	0.42	2 (1%) 70 68	48, 57, 65, 70	0
43	2l	121/132 (91%)	0.38	5 (4%) 37 36	53, 61, 68, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	116/126 (92%)	0.24	4 (3%) 45 44	56, 67, 73, 77	0
44	2m	114/126 (90%)	1.13	23 (20%) 1 0	69, 74, 79, 80	0
45	1n	60/61 (98%)	1.11	9 (15%) 2 1	58, 64, 72, 74	0
45	2n	60/61 (98%)	2.62	38 (63%) 0 0	66, 74, 79, 84	0
46	1o	88/89 (98%)	0.34	0 100 100	43, 60, 70, 73	0
46	2o	88/89 (98%)	0.39	1 (1%) 80 79	58, 67, 72, 76	0
47	1p	82/88 (93%)	0.88	9 (10%) 5 5	55, 66, 73, 82	0
47	2p	82/88 (93%)	0.39	1 (1%) 79 77	57, 64, 69, 74	0
48	1q	99/105 (94%)	0.55	5 (5%) 28 26	49, 62, 71, 73	0
48	2q	99/105 (94%)	0.81	11 (11%) 5 4	54, 65, 71, 74	0
49	1r	68/88 (77%)	0.21	1 (1%) 73 72	52, 59, 71, 73	0
49	2r	68/88 (77%)	0.79	6 (8%) 10 9	61, 67, 74, 77	0
50	1s	83/93 (89%)	0.22	0 100 100	59, 69, 74, 77	0
50	2s	83/93 (89%)	1.32	21 (25%) 0 0	63, 75, 80, 81	0
51	1t	96/106 (90%)	0.79	9 (9%) 8 7	59, 65, 73, 76	0
51	2t	98/106 (92%)	0.52	2 (2%) 65 63	54, 64, 72, 74	0
52	1u	23/27 (85%)	1.27	5 (21%) 0 0	61, 66, 69, 71	0
52	2u	23/27 (85%)	2.37	15 (65%) 0 0	71, 74, 76, 79	0
53	1y	97/113 (85%)	0.74	8 (8%) 11 10	49, 60, 70, 77	0
53	2y	96/113 (84%)	3.82	81 (84%) 0 0	69, 78, 84, 85	0
54	1w	4/5 (80%)	0.21	0 100 100	28, 31, 44, 61	0
54	2w	4/5 (80%)	0.03	0 100 100	39, 46, 55, 70	0
55	1x	3/4 (75%)	0.51	0 100 100	29, 29, 34, 51	0
55	2x	3/4 (75%)	-0.21	0 100 100	43, 43, 45, 60	0
56	1v	3/3 (100%)	0.62	0 100 100	23, 23, 29, 38	0
56	2v	3/3 (100%)	1.37	1 (33%) 0 0	46, 46, 51, 57	0
All	All	20798/21492 (96%)	0.40	1066 (5%) 28 26	18, 59, 79, 95	0

All (1066) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
53	2y	40	ILE	11.4
53	2y	88	LEU	10.2

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Mol	Chain	Res	Type	RSRZ
40	2i	76	ALA	8.9
53	2y	77	LEU	8.2
53	2y	48	PHE	7.9
53	2y	10	MET	7.8
40	2i	63	ILE	7.7
53	2y	12	ILE	7.5
1	1A	1087	G	7.2
1	2A	2153	G	7.1
53	2y	51	ASP	6.9
53	2y	63	ALA	6.9
34	2c	159	GLY	6.9
44	2m	116	THR	6.8
53	2y	5	ILE	6.7
21	2Z	192	ALA	6.7
53	2y	50	ALA	6.6
53	2y	42	SER	6.6
32	2a	1030(A)	G	6.6
21	2Z	191	VAL	6.4
53	2y	41	LEU	6.3
1	2A	2174	C	6.3
1	1A	1076	C	6.3
1	2A	2140	C	6.3
45	2n	13	THR	6.2
1	1A	2132	U	6.2
1	1A	1075	C	6.2
53	2y	70	MET	6.1
32	2a	1036	G	6.1
40	2i	36	TYR	6.0
41	2j	96	ILE	6.0
32	2a	1030(B)	C	6.0
32	1a	1030(B)	C	5.9
41	2j	34	VAL	5.9
40	1i	126	SER	5.8
53	2y	52	ALA	5.8
1	1A	1090	U	5.7
26	24	51	ASP	5.7
1	2A	2142	C	5.7
53	2y	39	ILE	5.7
1	2A	2132	U	5.7
40	2i	109	VAL	5.6
53	2y	74	ILE	5.6
1	1A	1089	G	5.6

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Mol	Chain	Res	Type	RSRZ
38	2g	7	ALA	5.6
26	24	52	THR	5.6
53	2y	64	SER	5.6
45	2n	35	ARG	5.6
44	2m	5	ALA	5.5
34	1c	94	LEU	5.5
1	1A	2804	C	5.5
40	2i	42	ARG	5.5
1	2A	2133	G	5.5
34	2c	124	ILE	5.5
41	2j	67	THR	5.4
45	2n	34	TYR	5.4
1	1A	2805	G	5.4
44	2m	6	GLY	5.4
40	2i	67	GLY	5.4
26	24	49	PHE	5.4
45	2n	10	ALA	5.4
1	2A	2136	C	5.4
38	2g	80	VAL	5.4
53	2y	80	LYS	5.3
1	2A	2125	G	5.3
22	10	7	LEU	5.3
52	2u	16	GLY	5.3
53	2y	8	LYS	5.2
53	2y	62	VAL	5.2
1	1A	2141	G	5.2
34	1c	80	GLY	5.2
40	2i	75	ASP	5.2
32	1a	1036	G	5.2
1	2A	2146	C	5.2
40	2i	14	VAL	5.2
53	2y	49	VAL	5.2
22	20	3	HIS	5.1
53	2y	79	ASN	5.1
1	2A	2793	G	5.1
26	24	50	VAL	5.1
7	2H	93	GLY	5.1
1	1A	2803	C	5.0
40	2i	61	ALA	5.0
45	2n	2	ALA	5.0
53	2y	78	ILE	5.0
40	2i	69	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
52	2u	14	TRP	5.0
41	2j	48	THR	5.0
34	2c	152	ILE	5.0
40	2i	125	TYR	5.0
1	2A	2138	C	5.0
1	2A	2124	G	4.9
1	2A	2154	G	4.9
1	2A	2162	G	4.9
1	1A	2794	C	4.9
40	2i	5	TYR	4.9
32	2a	1286	A	4.9
40	2i	90	PRO	4.9
40	2i	44	VAL	4.9
40	2i	18	PHE	4.9
1	1A	2793	G	4.8
53	2y	11	GLU	4.8
1	2A	2169	A	4.8
40	2i	71	SER	4.8
53	2y	58	ASN	4.7
53	2y	9	GLN	4.7
53	2y	35	ILE	4.7
41	2j	90	LEU	4.7
40	2i	62	TYR	4.7
32	2a	1001(A)	G	4.7
34	2c	33	LEU	4.7
53	2y	38	HIS	4.6
41	2j	72	VAL	4.6
40	2i	102	LEU	4.6
53	2y	71	TYR	4.6
34	2c	157	ILE	4.6
40	2i	40	LEU	4.6
45	2n	12	ARG	4.6
53	2y	19	HIS	4.6
1	2A	2147	G	4.6
40	2i	17	VAL	4.5
40	2i	92	TYR	4.5
1	1A	1074	G	4.5
1	2A	2173	A	4.5
32	2a	1257	U	4.5
53	2y	13	THR	4.5
1	2A	2145	C	4.5
53	2y	85	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
40	2i	72	GLY	4.5
43	2l	19	ARG	4.5
1	1A	1176	G	4.4
26	24	40	HIS	4.4
40	2i	88	TYR	4.4
40	2i	8	GLY	4.4
1	2A	1067	A	4.4
1	2A	2141	G	4.4
34	2c	145	GLY	4.4
41	2j	40	LEU	4.4
41	2j	29	ARG	4.4
38	1g	156	TRP	4.4
38	2g	155	ARG	4.4
1	2A	2801(A)	A	4.4
32	1a	1492	A	4.3
35	2d	21	LEU	4.3
53	2y	3	MET	4.3
1	2A	2803	C	4.3
53	2y	4	ASN	4.3
32	2a	1031	G	4.3
53	2y	37	PRO	4.3
53	2y	46	GLN	4.3
1	1A	1067	A	4.3
40	2i	66	ARG	4.3
38	2g	41	ARG	4.3
32	1a	1030	C	4.3
1	2A	2139	C	4.3
53	2y	15	ALA	4.3
1	1A	1091	G	4.3
32	2a	1033	G	4.3
53	2y	21	ALA	4.3
1	1A	1066	U	4.2
35	2d	146	ILE	4.2
22	10	5	LYS	4.2
1	1A	2147	G	4.2
1	2A	2802	G	4.2
51	1t	13	LEU	4.2
40	2i	21	PRO	4.2
6	2G	57	ALA	4.2
7	2H	101	ARG	4.2
45	2n	42	ILE	4.2
45	2n	6	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
41	2j	89	ASP	4.1
32	1a	1031	G	4.1
45	1n	51	GLY	4.1
1	1A	1068	G	4.1
53	2y	6	THR	4.1
45	2n	18	VAL	4.1
32	1a	1257	U	4.1
22	20	4	LYS	4.1
1	1A	1063	G	4.1
1	1A	1064	C	4.1
1	2A	2108	C	4.1
33	2b	81	VAL	4.1
43	2l	18	VAL	4.1
52	2u	6	ARG	4.1
1	1A	1065	U	4.0
1	2A	2123	G	4.0
32	1a	1028	C	4.0
52	1u	2	GLY	4.0
50	2s	41	VAL	4.0
40	2i	47	LEU	4.0
45	2n	39	LEU	4.0
26	24	56	VAL	4.0
1	1A	2792	G	4.0
53	2y	53	THR	4.0
40	2i	33	PHE	4.0
1	2A	2106	G	4.0
1	1A	888	C	3.9
1	2A	2107	C	3.9
32	2a	1030	C	3.9
32	1a	1001	A	3.9
32	2a	1030(C)	G	3.9
35	2d	48	ALA	3.9
33	1b	128	GLU	3.9
38	2g	154	TYR	3.9
26	24	64	GLY	3.9
45	2n	29	ARG	3.9
19	2X	68	ARG	3.9
40	2i	115	GLY	3.9
6	2G	39	ILE	3.9
40	2i	10	ARG	3.9
41	2j	46	ARG	3.9
53	1y	98	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	2A	2126	A	3.9
40	2i	108	VAL	3.9
53	2y	60	VAL	3.9
53	2y	65	GLY	3.9
32	2a	1029	C	3.9
22	10	4	LYS	3.9
32	1a	1030(D)	A	3.9
1	2A	2127	G	3.9
1	2A	2159	G	3.9
1	1A	2144	U	3.9
40	2i	26	VAL	3.9
6	2G	157	ILE	3.8
35	2d	70	ILE	3.8
45	2n	7	ILE	3.8
1	2A	2144	U	3.8
45	2n	14	PRO	3.8
1	2A	2131	G	3.8
1	2A	2168	G	3.8
45	2n	25	VAL	3.8
1	1A	1509	C	3.8
21	2Z	125	LEU	3.8
40	2i	68	GLY	3.8
48	1q	27	PHE	3.8
26	24	57	GLU	3.8
35	1d	167	GLY	3.8
40	2i	28	VAL	3.8
32	1a	1030(A)	G	3.8
48	2q	98	LEU	3.8
41	2j	38	ILE	3.8
47	1p	19	ILE	3.8
40	2i	73	GLN	3.8
40	2i	50	LEU	3.8
33	2b	124	SER	3.8
53	2y	94	ALA	3.8
33	2b	118	LEU	3.8
41	2j	19	SER	3.8
36	2e	12	LEU	3.7
35	1d	2	GLY	3.7
53	2y	61	LEU	3.7
1	2A	2152	G	3.7
1	2A	2894	G	3.7
39	2h	124	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
40	2i	70	LYS	3.7
40	2i	114	TYR	3.7
1	1A	1092	C	3.7
1	2A	2104	G	3.7
35	2d	149	ALA	3.7
41	2j	68	HIS	3.7
1	1A	2146	C	3.7
1	2A	1075	C	3.7
32	2a	1001	A	3.7
53	2y	18	GLN	3.7
1	1A	2140	C	3.7
40	2i	64	THR	3.7
6	1G	146	TYR	3.7
8	2I	74	ASN	3.7
20	2Y	106	LEU	3.7
1	2A	1509	C	3.7
1	1A	1078	U	3.6
22	20	7	LEU	3.6
52	2u	13	ILE	3.6
33	2b	136	VAL	3.6
50	2s	9	VAL	3.6
1	2A	2120	G	3.6
1	2A	2805	G	3.6
1	2A	888	C	3.6
51	1t	18	GLN	3.6
33	2b	123	ALA	3.6
34	2c	65	ALA	3.6
1	2A	2110	G	3.6
6	2G	58	GLN	3.6
44	2m	64	TRP	3.6
41	2j	27	ALA	3.6
40	2i	24	GLY	3.6
32	1a	1026	G	3.6
6	2G	146	TYR	3.6
7	2H	102	ALA	3.6
38	2g	25	ALA	3.6
42	1k	25	TYR	3.6
6	2G	29	TRP	3.6
53	2y	84	GLN	3.6
53	2y	87	LYS	3.6
1	1A	2143	C	3.6
34	1c	41	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
38	1g	80	VAL	3.6
33	2b	227	GLY	3.5
20	2Y	1	MET	3.5
41	2j	44	VAL	3.5
20	2Y	75	ILE	3.5
1	2A	1046	A	3.5
1	2A	2170	A	3.5
32	2a	1027	C	3.5
6	2G	140	ILE	3.5
40	2i	127	LYS	3.5
1	2A	229	A	3.5
53	2y	14	PRO	3.5
33	2b	70	PHE	3.5
41	2j	47	PHE	3.5
31	29	16	VAL	3.5
52	2u	23	PRO	3.5
1	1A	2142	C	3.5
44	2m	87	TYR	3.5
38	2g	42	ILE	3.5
47	1p	59	TRP	3.5
22	10	6	GLY	3.5
53	1y	95	ARG	3.5
40	2i	41	VAL	3.5
1	2A	2176	A	3.4
38	2g	101	LEU	3.4
23	11	2	SER	3.4
26	14	49	PHE	3.4
1	2A	2118	U	3.4
1	2A	2804	C	3.4
45	1n	2	ALA	3.4
40	2i	57	GLY	3.4
19	2X	92	LEU	3.4
26	24	44	THR	3.4
22	20	5	LYS	3.4
45	2n	44	LEU	3.4
40	2i	91	ASP	3.4
40	2i	59	PHE	3.4
41	2j	75	ILE	3.4
33	2b	120	ALA	3.4
1	1A	1072	C	3.4
1	1A	1080	C	3.4
40	2i	65	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
42	2k	75	TYR	3.4
38	2g	9	VAL	3.3
39	2h	131	GLY	3.3
53	2y	75	ASN	3.3
1	1A	2113	U	3.3
38	2g	83	ALA	3.3
1	1A	2116	G	3.3
1	2A	2165	G	3.3
1	2A	2191	G	3.3
32	1a	1001(A)	G	3.3
44	2m	43	THR	3.3
6	2G	159	VAL	3.3
35	1d	178	VAL	3.3
34	2c	32	LEU	3.3
21	2Z	187	ALA	3.3
40	2i	86	VAL	3.3
33	1b	118	LEU	3.3
50	2s	75	ALA	3.3
53	2y	89	GLN	3.3
40	2i	105	ASP	3.3
32	1a	1030(C)	G	3.3
42	2k	109	VAL	3.3
40	2i	25	LYS	3.3
53	2y	45	PRO	3.3
8	2I	86	THR	3.3
45	2n	49	HIS	3.3
1	1A	2107	C	3.3
35	1d	179	GLU	3.3
34	1c	63	ASN	3.2
1	1A	1077	A	3.2
32	2a	1531	A	3.2
50	2s	60	VAL	3.2
40	2i	74	ILE	3.2
41	2j	25	GLU	3.2
51	2t	11	SER	3.2
33	2b	51	LEU	3.2
34	2c	196	LEU	3.2
41	2j	16	LEU	3.2
21	1Z	192	ALA	3.2
45	1n	61	TRP	3.2
6	2G	77	ILE	3.2
1	1A	2152	G	3.2

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Mol	Chain	Res	Type	RSRZ
34	2c	177	THR	3.2
41	2j	26	ALA	3.2
38	2g	81	GLY	3.2
41	2j	37	PRO	3.2
33	2b	165	VAL	3.2
40	1i	28	VAL	3.2
1	1A	1103	A	3.2
41	2j	23	ILE	3.2
39	2h	122	ARG	3.2
52	2u	12	LYS	3.2
1	2A	2151	G	3.2
1	2A	2179	C	3.2
35	1d	157	LEU	3.2
44	2m	102	ARG	3.2
33	2b	232	PRO	3.2
53	2y	17	ARG	3.2
26	24	63	TYR	3.1
41	1j	20	ALA	3.1
1	1A	2145	C	3.1
1	2A	1076	C	3.1
50	2s	10	PHE	3.1
7	2H	21	PRO	3.1
34	2c	164	ARG	3.1
40	1i	109	VAL	3.1
34	2c	160	ALA	3.1
40	2i	7	THR	3.1
41	2j	100	THR	3.1
19	2X	69	TYR	3.1
52	2u	15	ARG	3.1
50	2s	28	LYS	3.1
45	2n	21	TYR	3.1
52	2u	11	GLY	3.1
1	1A	1175	U	3.1
1	1A	2153	G	3.1
1	2A	2157	G	3.1
33	2b	218	ALA	3.1
44	2m	75	ALA	3.1
53	2y	32	THR	3.1
22	20	76	GLY	3.1
41	2j	74	ILE	3.1
53	2y	67	HIS	3.1
40	2i	19	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
7	1H	2	SER	3.1
45	2n	37	PHE	3.1
50	2s	62	ILE	3.1
34	2c	206	GLU	3.1
45	2n	31	ARG	3.1
34	1c	194	GLY	3.1
1	1A	2155	G	3.1
40	2i	4	TYR	3.1
53	2y	23	ARG	3.1
1	2A	2896	C	3.1
26	24	54	GLY	3.1
1	2A	2792	G	3.0
32	1a	1033	G	3.0
50	2s	35	SER	3.0
6	2G	149	VAL	3.0
40	1i	26	VAL	3.0
47	1p	2	VAL	3.0
41	1j	73	ASP	3.0
1	2A	2148	G	3.0
32	2a	1034	G	3.0
51	1t	67	ALA	3.0
32	1a	1029	C	3.0
6	2G	112	PRO	3.0
41	2j	41	PRO	3.0
33	2b	223	ILE	3.0
50	2s	53	ASN	3.0
45	2n	41	ARG	3.0
52	2u	5	ASP	3.0
53	1y	42	SER	3.0
33	2b	44	LEU	3.0
33	2b	201	ILE	3.0
40	2i	6	GLY	3.0
6	2G	138	GLN	3.0
38	2g	32	ARG	3.0
40	2i	56	LEU	3.0
53	2y	72	THR	3.0
1	1A	2159	G	3.0
1	2A	2149	G	3.0
26	24	7	PRO	3.0
29	17	1	MET	3.0
45	2n	55	GLY	3.0
1	1A	1081	U	3.0

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Mol	Chain	Res	Type	RSRZ
6	2G	136	ARG	3.0
34	2c	8	ILE	3.0
23	21	2	SER	3.0
1	2A	2164	C	3.0
1	2A	652(B)	A	3.0
35	2d	157	LEU	3.0
38	1g	12	LEU	3.0
40	2i	85	LEU	3.0
41	2j	18	ALA	3.0
45	2n	61	TRP	3.0
1	2A	2109	U	2.9
39	1h	134	ILE	2.9
1	2A	2111	C	2.9
40	2i	103	THR	2.9
42	2k	126	ARG	2.9
40	2i	53	VAL	2.9
47	1p	1	MET	2.9
34	1c	10	PHE	2.9
41	2j	54	PHE	2.9
26	14	46	GLN	2.9
1	1A	2149	G	2.9
40	2i	30	GLY	2.9
32	2a	1035	A	2.9
38	2g	31	MET	2.9
53	2y	59	GLY	2.9
38	2g	16	LEU	2.9
53	1y	97	ALA	2.9
34	1c	193	TYR	2.9
39	2h	58	TYR	2.9
1	2A	2155	G	2.9
41	2j	62	HIS	2.9
33	2b	122	PHE	2.9
40	2i	27	THR	2.9
45	2n	22	THR	2.9
34	2c	23	TYR	2.9
39	1h	103	VAL	2.9
32	2a	1032	G	2.9
33	2b	214	ILE	2.9
40	2i	77	ILE	2.9
53	2y	22	ASP	2.9
6	2G	135	LEU	2.9
29	17	47	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
33	1b	122	PHE	2.9
1	2A	1085	A	2.9
11	2P	79	ARG	2.9
32	1a	1286	A	2.9
47	1p	49	LEU	2.9
20	2Y	42	VAL	2.8
53	2y	69	ASP	2.8
40	2i	93	ARG	2.8
45	2n	40	CYS	2.8
52	2u	9	ARG	2.8
40	2i	37	PHE	2.8
1	2A	2181	G	2.8
32	2a	1026	G	2.8
32	2a	1030(D)	A	2.8
53	2y	16	ILE	2.8
22	10	2	ALA	2.8
34	1c	47	LEU	2.8
48	1q	98	LEU	2.8
53	2y	93	GLU	2.8
1	2A	2135	A	2.8
14	2S	3	ARG	2.8
38	2g	116	ALA	2.8
34	1c	91	LEU	2.8
38	2g	22	LEU	2.8
41	1j	90	LEU	2.8
26	24	66	SER	2.8
14	2S	46	VAL	2.8
53	2y	76	GLU	2.8
53	2y	82	GLU	2.8
1	2A	2143	C	2.8
6	2G	142	PRO	2.8
40	2i	49	PRO	2.8
39	2h	4	ASP	2.8
32	2a	848	C	2.8
34	2c	87	LEU	2.8
34	2c	66	VAL	2.8
1	2A	6	A	2.8
39	2h	45	ILE	2.8
53	2y	92	GLY	2.8
41	2j	45	ARG	2.8
40	2i	123	PRO	2.8
8	2I	3	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
38	2g	156	TRP	2.7
40	1i	114	TYR	2.7
40	2i	113	LYS	2.7
44	1m	115	LYS	2.7
52	2u	2	GLY	2.7
33	1b	214	ILE	2.7
42	2k	87	THR	2.7
7	2H	95	ARG	2.7
34	2c	190	ARG	2.7
1	1A	1102	C	2.7
32	2a	1028	C	2.7
40	1i	63	ILE	2.7
6	2G	152	LEU	2.7
49	2r	87	ARG	2.7
15	1T	38	ASN	2.7
1	1A	2167	U	2.7
1	2A	1083	U	2.7
7	2H	92	ILE	2.7
14	2S	58	LEU	2.7
26	24	67	TYR	2.7
34	2c	184	TYR	2.7
44	2m	70	LEU	2.7
1	2A	2897	U	2.7
33	2b	132	LYS	2.7
40	2i	45	ALA	2.7
35	2d	4	TYR	2.7
49	2r	58	LEU	2.7
33	2b	48	MET	2.7
44	2m	89	GLY	2.7
34	2c	162	GLN	2.7
34	2c	163	ALA	2.7
1	1A	2112	G	2.7
39	2h	2	LEU	2.7
40	2i	81	ILE	2.7
41	2j	8	LEU	2.7
18	1W	111	HIS	2.7
35	1d	138	TYR	2.7
41	2j	87	THR	2.7
39	1h	38	ILE	2.7
45	2n	4	LYS	2.7
32	1a	1034	G	2.7
41	2j	64	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
29	27	47	ARG	2.6
49	2r	24	ALA	2.6
1	2A	645	C	2.6
1	2A	2105	C	2.6
6	2G	43	LEU	2.6
6	2G	173	LEU	2.6
33	2b	61	LEU	2.6
33	2b	149	LEU	2.6
33	2b	187	LEU	2.6
39	2h	36	LEU	2.6
53	2y	81	LEU	2.6
1	1A	1093	G	2.6
1	1A	2115	G	2.6
45	2n	45	ARG	2.6
1	1A	2169	A	2.6
1	1A	2173	A	2.6
1	1A	2801(A)	A	2.6
35	1d	164	ALA	2.6
47	2p	7	ALA	2.6
14	2S	56	LEU	2.6
44	2m	4	ILE	2.6
44	2m	111	LYS	2.6
32	2a	1202	G	2.6
6	2G	61	ALA	2.6
22	20	2	ALA	2.6
41	2j	65	LEU	2.6
36	1e	6	PHE	2.6
44	2m	84	ILE	2.6
33	2b	217	ARG	2.6
53	2y	91	LYS	2.6
1	1A	1079	C	2.6
1	2A	889	C	2.6
14	2S	36	TYR	2.6
14	2S	92	TYR	2.6
38	2g	11	GLN	2.6
53	1y	49	VAL	2.6
33	2b	181	PHE	2.6
34	1c	124	ILE	2.6
6	2G	86	MET	2.6
21	2Z	193	GLU	2.6
53	2y	86	ASN	2.6
26	14	55	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
40	1i	14	VAL	2.6
40	2i	20	ARG	2.6
7	2H	103	LEU	2.6
32	1a	1000	U	2.6
51	1t	72	LEU	2.6
20	2Y	44	ILE	2.6
32	2a	1385	G	2.6
33	1b	135	GLN	2.6
35	2d	175	SER	2.6
38	2g	105	VAL	2.6
53	2y	24	LEU	2.6
32	1a	1532	U	2.6
33	2b	92	TYR	2.6
53	2y	97	ALA	2.5
25	23	59	VAL	2.5
41	2j	49	VAL	2.5
6	2G	80	PHE	2.5
35	1d	3	ARG	2.5
33	2b	66	GLY	2.5
33	2b	97	TRP	2.5
41	1j	59	SER	2.5
32	2a	1287	A	2.5
1	1A	2807	G	2.5
1	2A	2116	G	2.5
6	2G	74	LYS	2.5
32	2a	1156	G	2.5
32	2a	1149	C	2.5
8	2I	35	LEU	2.5
41	2j	33	GLN	2.5
44	2m	90	LEU	2.5
1	1A	1083	U	2.5
26	24	55	ARG	2.5
14	2S	35	ILE	2.5
41	1j	54	PHE	2.5
45	2n	16	PHE	2.5
33	2b	27	LYS	2.5
32	2a	1492	A	2.5
38	2g	24	THR	2.5
1	2A	1091	G	2.5
34	1c	64	VAL	2.5
1	2A	2130	U	2.5
40	2i	117	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
20	1Y	1	MET	2.5
12	2Q	59	ARG	2.5
35	1d	73	ARG	2.5
38	2g	76	ARG	2.5
26	24	27	THR	2.5
47	1p	7	ALA	2.5
47	1p	46	PRO	2.5
53	2y	25	ALA	2.5
6	2G	139	LEU	2.5
33	2b	93	VAL	2.5
50	2s	69	HIS	2.5
1	1A	2154	G	2.5
33	1b	222	ILE	2.5
34	2c	182	ILE	2.5
26	24	68	ARG	2.5
40	1i	46	ALA	2.5
45	2n	30	ALA	2.5
36	2e	123	LEU	2.5
1	1A	2117	A	2.5
34	2c	139	GLN	2.5
44	2m	67	GLU	2.5
45	1n	16	PHE	2.5
50	2s	66	MET	2.5
32	1a	1024	G	2.5
34	2c	189	ALA	2.5
45	1n	59	ALA	2.5
50	2s	79	THR	2.5
52	2u	8	THR	2.5
8	2I	90	GLY	2.5
33	2b	164	VAL	2.5
45	1n	18	VAL	2.5
45	2n	53	LEU	2.5
1	2A	2150	U	2.5
1	1A	2139	C	2.5
18	2W	60	ASN	2.5
32	2a	1002	G	2.5
8	2I	75	LEU	2.4
33	2b	95	GLN	2.4
41	2j	63	PHE	2.4
6	2G	155	MET	2.4
5	2F	166	ALA	2.4
41	2j	32	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
8	2I	18	VAL	2.4
26	24	43	TYR	2.4
34	2c	58	GLU	2.4
35	1d	70	ILE	2.4
48	1q	86	GLU	2.4
17	2V	42	GLY	2.4
41	2j	84	GLN	2.4
45	2n	15	LYS	2.4
46	2o	86	GLY	2.4
1	1A	2174	C	2.4
52	2u	17	THR	2.4
25	23	23	LEU	2.4
45	2n	47	LEU	2.4
47	1p	39	TYR	2.4
12	2Q	65	PHE	2.4
40	2i	83	ARG	2.4
34	2c	155	GLY	2.4
34	2c	158	GLY	2.4
1	2A	1103	A	2.4
33	1b	231	GLU	2.4
23	11	98	LEU	2.4
41	2j	35	SER	2.4
44	1m	56	LEU	2.4
9	1N	9	VAL	2.4
9	2N	46	VAL	2.4
28	26	52	VAL	2.4
33	1b	133	LYS	2.4
33	2b	195	ASP	2.4
35	1d	166	LYS	2.4
42	2k	25	TYR	2.4
14	2S	12	PHE	2.4
14	2S	22	GLY	2.4
26	24	45	GLY	2.4
36	2e	22	GLY	2.4
33	2b	113	HIS	2.4
53	2y	98	ALA	2.4
6	2G	75	LYS	2.4
1	1A	229	A	2.4
32	2a	1363(A)	A	2.4
49	2r	59	SER	2.4
39	1h	102	ARG	2.4
7	2H	43	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
22	20	52	GLY	2.4
35	2d	158	ILE	2.4
12	2Q	104	PHE	2.4
36	2e	45	PHE	2.4
53	1y	48	PHE	2.4
3	2D	2	ALA	2.4
34	1c	168	ALA	2.4
38	2g	108	ALA	2.4
42	2k	13	GLN	2.4
50	2s	5	LEU	2.4
45	2n	33	VAL	2.4
1	2A	2172	U	2.4
33	1b	132	LYS	2.4
34	1c	201	TYR	2.4
35	2d	49	ARG	2.4
36	1e	58	ALA	2.4
40	1i	106	ALA	2.4
40	2i	122	ALA	2.4
53	2y	56	THR	2.4
34	2c	167	TRP	2.4
31	29	11	CYS	2.4
51	1t	75	ASN	2.3
11	2P	76	LYS	2.3
33	1b	29	ALA	2.3
7	2H	108	GLY	2.3
40	2i	29	ASN	2.3
53	1y	41	LEU	2.3
53	2y	34	LEU	2.3
47	1p	48	TRP	2.3
39	2h	61	VAL	2.3
39	2h	95	VAL	2.3
32	2a	1150	U	2.3
52	2u	10	ARG	2.3
33	2b	90	MET	2.3
22	20	45	PHE	2.3
32	2a	1357	A	2.3
38	2g	120	ILE	2.3
50	2s	77	THR	2.3
53	2y	55	ASN	2.3
41	1j	85	LEU	2.3
49	2r	85	LEU	2.3
29	27	46	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
33	2b	229	VAL	2.3
48	2q	93	GLN	2.3
1	2A	2103	C	2.3
1	2A	2137	C	2.3
32	2a	1249	C	2.3
1	1A	2114	A	2.3
32	2a	1111	A	2.3
34	2c	3	ASN	2.3
53	2y	7	SER	2.3
38	2g	34	GLY	2.3
19	2X	66	LEU	2.3
9	2N	104	LYS	2.3
14	2S	57	LYS	2.3
45	1n	14	PRO	2.3
53	2y	20	VAL	2.3
48	2q	90	ILE	2.3
8	2I	26	ALA	2.3
35	1d	23	GLY	2.3
44	2m	42	ALA	2.3
1	1A	1088	A	2.3
1	1A	1095	A	2.3
1	2A	2182	G	2.3
45	2n	57	ARG	2.3
50	2s	52	TYR	2.3
6	2G	106	LEU	2.3
44	2m	15	VAL	2.3
1	2A	1081	U	2.3
33	1b	130	ARG	2.3
34	2c	77	ILE	2.3
40	1i	128	ARG	2.3
34	2c	37	GLN	2.3
1	2A	2161	C	2.3
1	2A	2188	C	2.3
38	1g	85	TYR	2.3
48	2q	23	VAL	2.3
1	2A	1066	U	2.3
52	1u	10	ARG	2.3
22	10	42	GLY	2.3
33	2b	216	SER	2.3
33	2b	55	PHE	2.3
1	2A	1064	C	2.3
1	2A	2175	C	2.3

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Mol	Chain	Res	Type	RSRZ
33	1b	134	GLU	2.3
39	2h	112	LEU	2.3
51	2t	13	LEU	2.3
45	2n	43	CYS	2.3
1	2A	1847	A	2.2
32	1a	1005	A	2.2
32	2a	1041	A	2.2
41	2j	66	ARG	2.2
27	15	60	VAL	2.2
44	2m	95	GLY	2.2
48	2q	10	VAL	2.2
36	2e	20	GLN	2.2
42	2k	29	ILE	2.2
7	2H	159	GLU	2.2
50	2s	63	THR	2.2
6	2G	62	LEU	2.2
34	1c	12	LEU	2.2
38	2g	44	TYR	2.2
44	1m	89	GLY	2.2
45	2n	24	CYS	2.2
53	2y	36	ASN	2.2
1	2A	2119	A	2.2
26	24	19	GLY	2.2
6	2G	49	ASP	2.2
32	2a	1151	A	2.2
50	2s	38	SER	2.2
1	1A	2148	G	2.2
53	2y	44	GLU	2.2
38	2g	40	ALA	2.2
9	2N	73	THR	2.2
50	2s	39	THR	2.2
13	2R	68	ARG	2.2
52	2u	22	ARG	2.2
35	2d	188	LEU	2.2
44	2m	23	TYR	2.2
40	2i	32	ASP	2.2
44	1m	24	GLY	2.2
1	1A	2161	C	2.2
7	2H	35	VAL	2.2
9	2N	140	VAL	2.2
33	2b	133	LYS	2.2
38	2g	144	MET	2.2

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Mol	Chain	Res	Type	RSRZ
48	2q	9	VAL	2.2
53	2y	43	LYS	2.2
33	2b	185	ILE	2.2
36	2e	13	ILE	2.2
38	2g	10	ARG	2.2
43	2l	89	ARG	2.2
44	2m	94	ARG	2.2
48	1q	36	ILE	2.2
14	2S	21	THR	2.2
39	2h	27	PRO	2.2
6	1G	49	ASP	2.2
52	1u	14	TRP	2.2
53	2y	66	LYS	2.2
26	14	66	SER	2.2
32	1a	841	U	2.2
32	2a	841	U	2.2
32	2a	979	C	2.2
32	2a	1362	C	2.2
33	1b	136	VAL	2.2
35	2d	112	VAL	2.2
35	2d	140	VAL	2.2
6	2G	73	ALA	2.2
39	2h	6	ILE	2.2
6	2G	102	PHE	2.2
7	2H	128	PRO	2.2
9	2N	83	LYS	2.2
35	1d	174	LEU	2.2
39	1h	133	LEU	2.2
42	2k	98	LEU	2.2
43	1l	63	GLY	2.2
45	1n	15	LYS	2.2
1	2A	2121	G	2.2
32	2a	1023	G	2.2
22	20	51	VAL	2.2
32	2a	1358	U	2.2
1	2A	1536	C	2.2
32	2a	1114	C	2.2
34	2c	146	ALA	2.2
41	2j	20	ALA	2.2
1	2A	1095	A	2.2
33	2b	215	LEU	2.2
35	2d	162	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
36	1e	110	LEU	2.2
48	2q	91	ARG	2.2
34	2c	4	LYS	2.2
40	2i	31	GLN	2.2
32	2a	1322	C	2.2
33	2b	152	PHE	2.2
33	1b	234	PRO	2.2
33	1b	121	LEU	2.2
34	1c	204	LEU	2.2
36	1e	91	LEU	2.2
44	2m	66	LEU	2.2
50	2s	71	LEU	2.2
26	14	57	GLU	2.2
45	2n	8	GLU	2.2
7	2H	94	TYR	2.1
43	1l	64	TYR	2.1
1	2A	2112	G	2.1
1	2A	2160	G	2.1
1	2A	2893	G	2.1
38	2g	23	VAL	2.1
36	2e	17	ALA	2.1
35	1d	50	ARG	2.1
1	1A	2108	C	2.1
1	1A	2129	C	2.1
32	1a	1037	C	2.1
51	1t	20	LEU	2.1
6	2G	41	GLN	2.1
32	2a	1248	A	2.1
51	1t	73	HIS	2.1
35	2d	26	CYS	2.1
40	2i	60	ASP	2.1
35	1d	170	VAL	2.1
48	1q	23	VAL	2.1
1	1A	171	G	2.1
3	1D	275	LYS	2.1
33	2b	68	ILE	2.1
36	2e	109	ILE	2.1
33	2b	78	GLN	2.1
1	2A	2177	C	2.1
1	1A	2126	A	2.1
34	2c	131	ARG	2.1
40	1i	10	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
6	2G	158	ALA	2.1
7	2H	24	VAL	2.1
40	1i	76	ALA	2.1
40	1i	125	TYR	2.1
48	2q	85	VAL	2.1
51	1t	76	ALA	2.1
34	2c	186	PHE	2.1
40	2i	101	PHE	2.1
7	2H	97	ARG	2.1
32	2a	1356	G	2.1
35	2d	141	ARG	2.1
40	2i	126	SER	2.1
32	2a	1037	C	2.1
51	1t	14	LYS	2.1
35	2d	23	GLY	2.1
1	1A	271(K)	U	2.1
34	2c	193	TYR	2.1
53	2y	73	ALA	2.1
30	28	58	ILE	2.1
38	2g	8	GLU	2.1
38	2g	37	ASN	2.1
1	1A	889	C	2.1
1	1A	1071	G	2.1
1	1A	2106	G	2.1
1	1A	2137	C	2.1
1	1A	2130	U	2.1
6	2G	137	GLU	2.1
21	2Z	58	VAL	2.1
44	2m	60	VAL	2.1
45	2n	20	ALA	2.1
32	2a	1235	U	2.1
41	2j	97	GLU	2.1
49	1r	39	VAL	2.1
11	2P	110	TYR	2.1
33	1b	137	ARG	2.1
41	1j	29	ARG	2.1
33	2b	39	ILE	2.1
1	1A	34	C	2.1
56	2v	1	MET	2.1
1	1A	2124	G	2.1
1	1A	2166	G	2.1
1	2A	2319	G	2.1

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Mol	Chain	Res	Type	RSRZ
32	2a	1155	G	2.1
52	1u	9	ARG	2.1
6	2G	38	VAL	2.1
49	2r	47	THR	2.1
38	2g	85	TYR	2.1
43	2l	7	ILE	2.1
34	2c	128	PHE	2.1
34	2c	89	GLU	2.1
39	2h	135	CYS	2.1
3	2D	276	LYS	2.1
6	2G	51	ARG	2.1
34	2c	199	LYS	2.1
12	2Q	136	ALA	2.0
33	2b	60	ASP	2.0
33	2b	171	ALA	2.0
1	1A	272(A)	U	2.0
41	1j	44	VAL	2.0
1	2A	2166	G	2.0
32	2a	1353	G	2.0
48	2q	51	TYR	2.0
1	1A	2158	A	2.0
7	2H	71	LEU	2.0
40	2i	104	ARG	2.0
45	2n	27	CYS	2.0
4	2E	28	ALA	2.0
1	1A	2138	C	2.0
7	2H	114	VAL	2.0
33	1b	229	VAL	2.0
39	2h	118	VAL	2.0
45	1n	13	THR	2.0
6	2G	63	ILE	2.0
29	27	48	LYS	2.0
38	2g	92	SER	2.0
40	2i	11	LYS	2.0
34	2c	188	LEU	2.0
43	2l	10	LEU	2.0
44	2m	78	ILE	2.0
50	2s	30	LEU	2.0
50	2s	72	GLY	2.0
52	1u	18	TYR	2.0
1	2A	2156	G	2.0
36	1e	95	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
40	2i	15	ALA	2.0
53	1y	94	ALA	2.0
22	10	3	HIS	2.0
3	2D	221	VAL	2.0
6	2G	92	VAL	2.0
23	11	70	VAL	2.0
22	20	77	ARG	2.0
36	2e	14	ARG	2.0
7	2H	89	ILE	2.0
48	2q	59	ILE	2.0
19	1X	69	TYR	2.0
48	2q	71	PHE	2.0
1	2A	2310	A	2.0
29	27	1	MET	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MU	2A	1915	21/22	0.84	0.13	71,79,86,100	0
32	2MG	2a	1207	24/25	0.86	0.22	70,77,81,86	0
32	M2G	2a	966	25/26	0.89	0.20	64,70,83,97	0
1	PSU	2A	1911	20/21	0.89	0.13	66,71,78,83	0
1	5MU	1A	1915	21/22	0.90	0.18	63,71,76,84	0
32	5MC	1a	967	21/22	0.91	0.20	57,63,72,79	0
1	PSU	2A	1917	20/21	0.91	0.17	65,74,85,87	0
32	5MC	2a	1400	21/22	0.91	0.35	62,74,78,82	0
32	5MC	2a	1404	21/22	0.91	0.20	51,61,65,69	0
43	0TD	1l	92	10/11	0.92	0.17	50,56,60,61	0
1	PSU	1A	1917	20/21	0.92	0.16	55,59,65,69	0
43	0TD	2l	92	10/11	0.92	0.13	58,63,69,74	0
32	M2G	1a	966	25/26	0.93	0.20	48,57,63,70	0
32	5MC	2a	967	21/22	0.93	0.19	65,69,75,77	0
32	PSU	2a	516	20/21	0.93	0.14	65,70,72,79	0
32	PSU	1a	516	20/21	0.94	0.15	56,61,65,68	0
32	4OC	2a	1402	22/23	0.94	0.18	52,60,68,70	0
32	2MG	1a	1207	24/25	0.95	0.13	61,67,72,73	0
32	4OC	1a	1402	22/23	0.95	0.18	44,50,59,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	1A	1911	20/21	0.95	0.14	54,60,63,67	0
1	OMC	2A	1920	21/22	0.95	0.16	58,64,68,72	0
32	5MC	1a	1400	21/22	0.96	0.20	49,53,58,60	0
32	5MC	1a	1404	21/22	0.96	0.17	45,48,52,54	0
32	G7M	2a	527	24/25	0.96	0.15	55,60,64,67	0
32	UR3	1a	1498	21/22	0.96	0.18	46,51,54,62	0
32	MA6	2a	1518	24/25	0.96	0.19	54,62,66,67	0
32	MA6	2a	1519	24/25	0.96	0.23	52,59,63,67	0
32	MA6	1a	1519	24/25	0.96	0.18	39,45,50,52	0
1	PSU	2A	2605	20/21	0.97	0.19	31,36,43,43	0
32	G7M	1a	527	24/25	0.97	0.17	41,53,58,60	0
1	5MC	1A	1942	21/22	0.97	0.18	31,40,45,49	0
1	OMG	1A	2251	24/25	0.97	0.20	20,26,31,38	0
32	5MC	1a	1407	21/22	0.97	0.17	42,51,57,59	0
1	OMC	1A	1920	21/22	0.97	0.18	42,53,58,60	0
32	MA6	1a	1518	24/25	0.97	0.19	38,47,50,52	0
1	5MC	2A	1942	21/22	0.97	0.17	47,50,52,62	0
1	5MC	2A	1962	21/22	0.97	0.16	39,45,49,56	0
32	5MC	2a	1407	21/22	0.97	0.13	52,62,64,65	0
32	UR3	2a	1498	21/22	0.97	0.18	55,61,67,72	0
1	OMG	2A	2251	24/25	0.97	0.18	33,40,44,48	0
1	2MA	2A	2503	23/24	0.97	0.20	28,33,38,40	0
1	OMU	2A	2552	21/22	0.97	0.18	33,38,42,43	0
55	8AN	2x	76	22/23	0.97	0.20	39,45,50,54	0
1	PSU	1A	2605	20/21	0.98	0.19	22,27,31,33	0
1	5MC	1A	1962	21/22	0.98	0.20	26,34,38,40	0
1	5MU	1A	1939	21/22	0.98	0.20	23,29,33,36	0
1	5MU	2A	1939	21/22	0.98	0.17	32,38,42,45	0
1	2MA	1A	2503	23/24	0.98	0.21	19,23,25,27	0
55	8AN	1x	76	22/23	0.98	0.20	21,30,34,34	0
1	OMU	1A	2552	21/22	0.98	0.20	22,28,34,35	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	3944	1/1	-0.00	0.31	80,80,80,80	0
57	MG	2A	3718	1/1	0.01	0.17	76,76,76,76	0
57	MG	2A	3677	1/1	0.14	0.10	72,72,72,72	0
57	MG	1A	3747	1/1	0.24	0.20	66,66,66,66	0
57	MG	2A	3663	1/1	0.34	0.13	66,66,66,66	0
57	MG	1A	3897	1/1	0.39	0.12	55,55,55,55	0
57	MG	2A	3645	1/1	0.44	0.15	67,67,67,67	0
57	MG	2A	3643	1/1	0.45	0.21	68,68,68,68	0
57	MG	2A	3664	1/1	0.48	0.12	57,57,57,57	0
57	MG	1a	1628	1/1	0.50	0.25	64,64,64,64	0
57	MG	2A	3504	1/1	0.51	0.09	64,64,64,64	0
57	MG	1A	3638	1/1	0.52	0.27	37,37,37,37	0
57	MG	2T	203	1/1	0.53	0.13	74,74,74,74	0
57	MG	1a	1700	1/1	0.55	0.15	74,74,74,74	0
57	MG	1T	202	1/1	0.56	0.21	67,67,67,67	0
57	MG	1A	3393	1/1	0.56	0.18	32,32,32,32	0
57	MG	1A	3855	1/1	0.56	0.14	56,56,56,56	0
57	MG	2A	3065	1/1	0.56	0.76	63,63,63,63	0
57	MG	2A	3656	1/1	0.57	0.07	68,68,68,68	0
57	MG	1a	1745	1/1	0.57	0.13	70,70,70,70	0
57	MG	1A	3859	1/1	0.58	0.12	46,46,46,46	0
57	MG	1A	3796	1/1	0.58	0.19	61,61,61,61	0
57	MG	2A	3423	1/1	0.58	0.15	61,61,61,61	0
57	MG	1a	1717	1/1	0.58	0.30	73,73,73,73	0
57	MG	1a	1772	1/1	0.59	0.17	69,69,69,69	0
57	MG	1A	3884	1/1	0.59	0.14	44,44,44,44	0
57	MG	2a	3026	1/1	0.59	0.17	75,75,75,75	0
57	MG	2a	3065	1/1	0.59	0.20	74,74,74,74	0
57	MG	2Q	202	1/1	0.60	0.55	56,56,56,56	0
57	MG	1a	1840	1/1	0.60	0.09	58,58,58,58	0
57	MG	2A	3658	1/1	0.60	0.25	75,75,75,75	0
57	MG	2A	3636	1/1	0.60	0.17	70,70,70,70	0
57	MG	1a	1816	1/1	0.61	0.10	64,64,64,64	0
57	MG	2A	3506	1/1	0.61	0.15	69,69,69,69	0
57	MG	1a	1709	1/1	0.61	0.19	65,65,65,65	0
57	MG	1A	3729	1/1	0.62	0.13	58,58,58,58	0
57	MG	2A	3373	1/1	0.62	0.12	69,69,69,69	0
57	MG	2A	3387	1/1	0.62	0.18	51,51,51,51	0
57	MG	2G	203	1/1	0.62	0.12	76,76,76,76	0
57	MG	1A	4011	1/1	0.63	0.21	33,33,33,33	0
57	MG	1A	3916	1/1	0.64	0.15	57,57,57,57	0
57	MG	2A	3682	1/1	0.64	0.11	64,64,64,64	0
57	MG	1B	230	1/1	0.64	0.16	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3377	1/1	0.64	0.12	54,54,54,54	0
57	MG	2A	3594	1/1	0.65	0.20	73,73,73,73	0
57	MG	1A	3836	1/1	0.65	0.11	44,44,44,44	0
57	MG	1A	3620	1/1	0.65	0.08	41,41,41,41	0
57	MG	2A	3545	1/1	0.65	0.12	73,73,73,73	0
57	MG	2a	3011	1/1	0.65	0.17	75,75,75,75	0
57	MG	2A	3586	1/1	0.65	0.31	71,71,71,71	0
57	MG	2A	3686	1/1	0.65	0.18	76,76,76,76	0
57	MG	1A	3624	1/1	0.66	0.19	38,38,38,38	0
57	MG	1a	1622	1/1	0.66	0.18	61,61,61,61	0
57	MG	1A	3881	1/1	0.66	0.08	66,66,66,66	0
57	MG	2A	3611	1/1	0.67	0.10	67,67,67,67	0
57	MG	1a	1650	1/1	0.67	0.13	72,72,72,72	0
57	MG	2A	3188	1/1	0.67	0.21	61,61,61,61	0
57	MG	2a	3121	1/1	0.67	0.17	82,82,82,82	0
57	MG	2a	3153	1/1	0.67	0.20	69,69,69,69	0
57	MG	1a	1698	1/1	0.68	0.19	59,59,59,59	0
57	MG	2A	3476	1/1	0.68	0.16	62,62,62,62	0
57	MG	1N	204	1/1	0.68	0.11	52,52,52,52	0
57	MG	1A	3330	1/1	0.68	0.19	62,62,62,62	0
57	MG	2A	3082	1/1	0.68	0.10	69,69,69,69	0
57	MG	1A	3397	1/1	0.68	0.11	44,44,44,44	0
57	MG	1A	3461	1/1	0.68	0.17	31,31,31,31	0
57	MG	1A	3486	1/1	0.68	0.18	23,23,23,23	0
57	MG	2A	3419	1/1	0.68	0.21	54,54,54,54	0
57	MG	1A	3381	1/1	0.69	0.22	51,51,51,51	0
57	MG	2A	3722	1/1	0.69	0.26	66,66,66,66	0
57	MG	2A	3210	1/1	0.69	0.16	60,60,60,60	0
57	MG	2A	3340	1/1	0.69	0.15	68,68,68,68	0
57	MG	1A	3735	1/1	0.69	0.22	54,54,54,54	0
57	MG	1A	3213	1/1	0.69	0.16	54,54,54,54	0
57	MG	1A	3872	1/1	0.69	0.16	49,49,49,49	0
57	MG	1a	1716	1/1	0.69	0.12	63,63,63,63	0
57	MG	1A	3644	1/1	0.69	0.15	73,73,73,73	0
57	MG	2a	3149	1/1	0.69	0.12	60,60,60,60	0
57	MG	2A	3687	1/1	0.69	0.10	58,58,58,58	0
57	MG	2A	3385	1/1	0.70	0.09	75,75,75,75	0
57	MG	1A	3505	1/1	0.70	0.11	44,44,44,44	0
57	MG	1A	3967	1/1	0.70	0.25	60,60,60,60	0
57	MG	2A	3302	1/1	0.70	0.14	58,58,58,58	0
57	MG	1A	3899	1/1	0.70	0.12	54,54,54,54	0
57	MG	2A	3620	1/1	0.70	0.16	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3677	1/1	0.70	0.10	62,62,62,62	0
57	MG	2j	202	1/1	0.70	0.26	80,80,80,80	0
57	MG	1A	3920	1/1	0.71	0.11	54,54,54,54	0
57	MG	1n	102	1/1	0.71	0.13	55,55,55,55	0
57	MG	1A	3559	1/1	0.71	0.13	59,59,59,59	0
57	MG	1A	3085	1/1	0.71	0.14	66,66,66,66	0
57	MG	2B	214	1/1	0.71	0.13	82,82,82,82	0
57	MG	1A	3211	1/1	0.71	0.27	68,68,68,68	0
57	MG	2A	3195	1/1	0.71	0.15	60,60,60,60	0
57	MG	2A	3650	1/1	0.71	0.27	65,65,65,65	0
57	MG	1a	1757	1/1	0.71	0.16	53,53,53,53	0
57	MG	2a	3025	1/1	0.71	0.14	69,69,69,69	0
57	MG	2A	3234	1/1	0.71	0.29	65,65,65,65	0
57	MG	1A	3625	1/1	0.71	0.15	54,54,54,54	0
57	MG	2A	3550	1/1	0.71	0.25	62,62,62,62	0
57	MG	2a	3134	1/1	0.71	0.13	82,82,82,82	0
57	MG	1A	3420	1/1	0.71	0.14	72,72,72,72	0
57	MG	2A	3678	1/1	0.71	0.10	68,68,68,68	0
57	MG	2A	3588	1/1	0.71	0.20	46,46,46,46	0
57	MG	2a	3024	1/1	0.72	0.19	68,68,68,68	0
57	MG	1A	3808	1/1	0.72	0.12	79,79,79,79	0
57	MG	1a	1679	1/1	0.72	0.11	59,59,59,59	0
57	MG	1E	304	1/1	0.72	0.20	29,29,29,29	0
57	MG	2A	3134	1/1	0.72	0.23	70,70,70,70	0
57	MG	2A	3581	1/1	0.72	0.19	70,70,70,70	0
57	MG	2A	3313	1/1	0.72	0.09	52,52,52,52	0
57	MG	2A	3646	1/1	0.72	0.08	69,69,69,69	0
57	MG	2a	3185	1/1	0.72	0.13	69,69,69,69	0
57	MG	1A	3557	1/1	0.72	0.10	46,46,46,46	0
57	MG	1A	3438	1/1	0.73	0.17	67,67,67,67	0
57	MG	2O	202	1/1	0.73	0.18	80,80,80,80	0
57	MG	1A	3784	1/1	0.73	0.09	42,42,42,42	0
57	MG	2T	201	1/1	0.73	0.15	64,64,64,64	0
57	MG	1A	3924	1/1	0.73	0.12	48,48,48,48	0
57	MG	2A	3593	1/1	0.73	0.05	60,60,60,60	0
57	MG	2a	3022	1/1	0.73	0.12	73,73,73,73	0
57	MG	1A	3456	1/1	0.73	0.20	55,55,55,55	0
57	MG	2A	3600	1/1	0.73	0.23	55,55,55,55	0
57	MG	1A	3432	1/1	0.73	0.22	29,29,29,29	0
57	MG	2a	3035	1/1	0.73	0.23	72,72,72,72	0
57	MG	1a	1601	1/1	0.73	0.17	68,68,68,68	0
57	MG	2a	3078	1/1	0.73	0.07	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3629	1/1	0.73	0.19	40,40,40,40	0
57	MG	2a	3133	1/1	0.73	0.23	64,64,64,64	0
57	MG	2A	3533	1/1	0.73	0.08	67,67,67,67	0
57	MG	2a	3145	1/1	0.73	0.08	57,57,57,57	0
57	MG	2A	3706	1/1	0.73	0.14	56,56,56,56	0
57	MG	2A	3147	1/1	0.73	0.16	59,59,59,59	0
57	MG	2A	3547	1/1	0.73	0.16	60,60,60,60	0
57	MG	1a	1797	1/1	0.73	0.11	77,77,77,77	0
57	MG	2A	3137	1/1	0.74	0.15	51,51,51,51	0
57	MG	1A	3653	1/1	0.74	0.14	58,58,58,58	0
57	MG	1a	1661	1/1	0.74	0.16	64,64,64,64	0
57	MG	2A	3695	1/1	0.74	0.15	41,41,41,41	0
57	MG	2A	3697	1/1	0.74	0.13	58,58,58,58	0
57	MG	2a	3031	1/1	0.74	0.13	55,55,55,55	0
57	MG	1A	3414	1/1	0.74	0.11	72,72,72,72	0
57	MG	1A	3834	1/1	0.74	0.09	41,41,41,41	0
57	MG	2A	3457	1/1	0.74	0.21	78,78,78,78	0
57	MG	2a	3100	1/1	0.74	0.33	60,60,60,60	0
57	MG	2B	211	1/1	0.74	0.21	67,67,67,67	0
57	MG	1a	1699	1/1	0.74	0.26	78,78,78,78	0
57	MG	2A	3662	1/1	0.74	0.10	53,53,53,53	0
57	MG	2A	3263	1/1	0.74	0.26	58,58,58,58	0
57	MG	1A	3652	1/1	0.74	0.14	30,30,30,30	0
57	MG	2A	3089	1/1	0.74	0.21	63,63,63,63	0
57	MG	1a	1782	1/1	0.74	0.47	71,71,71,71	0
57	MG	21	101	1/1	0.74	0.09	69,69,69,69	0
57	MG	1A	3825	1/1	0.75	0.34	35,35,35,35	0
57	MG	2A	3694	1/1	0.75	0.09	67,67,67,67	0
57	MG	2a	3085	1/1	0.75	0.12	60,60,60,60	0
57	MG	1a	1672	1/1	0.75	0.15	53,53,53,53	0
57	MG	1A	3861	1/1	0.75	0.17	49,49,49,49	0
57	MG	1a	1686	1/1	0.75	0.21	67,67,67,67	0
57	MG	1a	1775	1/1	0.75	0.16	67,67,67,67	0
57	MG	1A	3264	1/1	0.75	0.12	69,69,69,69	0
57	MG	1a	1607	1/1	0.75	0.11	67,67,67,67	0
57	MG	1B	229	1/1	0.75	0.18	66,66,66,66	0
57	MG	1A	3522	1/1	0.75	0.12	53,53,53,53	0
57	MG	1A	3273	1/1	0.75	0.11	55,55,55,55	0
57	MG	2A	3246	1/1	0.76	0.24	70,70,70,70	0
57	MG	2A	3490	1/1	0.76	0.10	61,61,61,61	0
57	MG	2A	3128	1/1	0.76	0.15	67,67,67,67	0
57	MG	1A	3792	1/1	0.76	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3517	1/1	0.76	0.34	67,67,67,67	0
57	MG	2A	3701	1/1	0.76	0.08	60,60,60,60	0
57	MG	1a	1823	1/1	0.76	0.21	61,61,61,61	0
57	MG	2a	3069	1/1	0.76	0.18	61,61,61,61	0
57	MG	2A	3322	1/1	0.76	0.08	48,48,48,48	0
57	MG	1Y	202	1/1	0.76	0.07	63,63,63,63	0
57	MG	2a	3091	1/1	0.76	0.14	66,66,66,66	0
57	MG	2a	3096	1/1	0.76	0.12	68,68,68,68	0
57	MG	2A	3151	1/1	0.76	0.28	67,67,67,67	0
57	MG	10	105	1/1	0.76	0.14	39,39,39,39	0
57	MG	1A	3412	1/1	0.76	0.27	51,51,51,51	0
57	MG	2A	3200	1/1	0.76	0.14	73,73,73,73	0
57	MG	2A	3592	1/1	0.76	0.15	58,58,58,58	0
57	MG	2A	3665	1/1	0.76	0.10	56,56,56,56	0
57	MG	1A	3096	1/1	0.76	0.16	33,33,33,33	0
57	MG	1A	3893	1/1	0.76	0.12	56,56,56,56	0
57	MG	2A	3473	1/1	0.76	0.14	59,59,59,59	0
59	ARG	1A	4018	12/12	0.76	0.28	41,65,74,75	0
57	MG	1a	1853	1/1	0.77	0.07	58,58,58,58	0
57	MG	1d	304	1/1	0.77	0.09	71,71,71,71	0
57	MG	2D	307	1/1	0.77	0.11	35,35,35,35	0
57	MG	2A	3624	1/1	0.77	0.18	40,40,40,40	0
57	MG	1W	203	1/1	0.77	0.39	67,67,67,67	0
57	MG	1t	3102	1/1	0.77	0.13	64,64,64,64	0
57	MG	1A	3147	1/1	0.77	0.28	80,80,80,80	0
57	MG	1A	3768	1/1	0.77	0.22	52,52,52,52	0
57	MG	1a	1731	1/1	0.77	0.09	48,48,48,48	0
57	MG	2A	3254	1/1	0.77	0.09	76,76,76,76	0
57	MG	1a	1733	1/1	0.77	0.20	41,41,41,41	0
57	MG	2A	3657	1/1	0.77	0.10	55,55,55,55	0
57	MG	1a	1821	1/1	0.77	0.14	67,67,67,67	0
57	MG	2a	3169	1/1	0.77	0.09	51,51,51,51	0
57	MG	1B	207	1/1	0.77	0.23	55,55,55,55	0
57	MG	2j	201	1/1	0.77	0.12	66,66,66,66	0
57	MG	1A	3894	1/1	0.77	0.17	50,50,50,50	0
57	MG	2B	207	1/1	0.77	0.11	70,70,70,70	0
61	ZN	24	501	1/1	0.77	0.13	120,120,120,120	0
57	MG	1a	1776	1/1	0.78	0.20	59,59,59,59	0
57	MG	1a	1780	1/1	0.78	0.15	71,71,71,71	0
57	MG	1A	3626	1/1	0.78	0.13	53,53,53,53	0
57	MG	1A	3322	1/1	0.78	0.13	46,46,46,46	0
57	MG	2A	3463	1/1	0.78	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3634	1/1	0.78	0.22	36,36,36,36	0
57	MG	2A	3159	1/1	0.78	0.12	44,44,44,44	0
57	MG	1a	1800	1/1	0.78	0.10	76,76,76,76	0
57	MG	1A	3919	1/1	0.78	0.15	45,45,45,45	0
57	MG	1A	3011	1/1	0.78	0.13	56,56,56,56	0
57	MG	1A	3645	1/1	0.78	0.22	59,59,59,59	0
57	MG	2A	3219	1/1	0.78	0.10	62,62,62,62	0
57	MG	1A	3588	1/1	0.78	0.15	51,51,51,51	0
57	MG	19	102	1/1	0.78	0.14	65,65,65,65	0
57	MG	1A	3954	1/1	0.78	0.10	64,64,64,64	0
57	MG	1A	3431	1/1	0.78	0.16	61,61,61,61	0
57	MG	1A	3993	1/1	0.78	0.19	65,65,65,65	0
57	MG	2A	3064	1/1	0.78	0.22	51,51,51,51	0
57	MG	1A	3797	1/1	0.78	0.09	74,74,74,74	0
57	MG	1A	3342	1/1	0.78	0.12	51,51,51,51	0
57	MG	1A	3709	1/1	0.78	0.29	54,54,54,54	0
57	MG	1A	3238	1/1	0.78	0.18	63,63,63,63	0
57	MG	1A	3144	1/1	0.79	0.20	60,60,60,60	0
57	MG	2A	3167	1/1	0.79	0.40	64,64,64,64	0
57	MG	1A	3682	1/1	0.79	0.16	60,60,60,60	0
57	MG	2A	3047	1/1	0.79	0.16	68,68,68,68	0
57	MG	1A	3169	1/1	0.79	0.14	43,43,43,43	0
57	MG	2A	3445	1/1	0.79	0.16	51,51,51,51	0
57	MG	1A	3943	1/1	0.79	0.17	62,62,62,62	0
57	MG	2a	3037	1/1	0.79	0.14	71,71,71,71	0
57	MG	1A	3617	1/1	0.79	0.40	55,55,55,55	0
57	MG	1A	3419	1/1	0.79	0.18	31,31,31,31	0
57	MG	2A	3114	1/1	0.79	0.10	63,63,63,63	0
57	MG	2A	3625	1/1	0.79	0.09	52,52,52,52	0
57	MG	2a	3086	1/1	0.79	0.13	64,64,64,64	0
57	MG	2A	3703	1/1	0.79	0.10	49,49,49,49	0
57	MG	1a	1743	1/1	0.79	0.11	40,40,40,40	0
57	MG	2A	3501	1/1	0.79	0.18	55,55,55,55	0
57	MG	2A	3502	1/1	0.79	0.06	62,62,62,62	0
57	MG	2A	3728	1/1	0.79	0.25	55,55,55,55	0
57	MG	2A	3642	1/1	0.79	0.17	54,54,54,54	0
57	MG	2a	3142	1/1	0.79	0.07	62,62,62,62	0
57	MG	2a	3144	1/1	0.79	0.13	65,65,65,65	0
57	MG	2A	3131	1/1	0.79	0.10	66,66,66,66	0
57	MG	2A	3287	1/1	0.79	0.20	58,58,58,58	0
57	MG	2a	3151	1/1	0.79	0.09	53,53,53,53	0
57	MG	1A	3554	1/1	0.79	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3748	1/1	0.79	0.24	57,57,57,57	0
57	MG	1A	3464	1/1	0.79	0.18	37,37,37,37	0
57	MG	1A	3664	1/1	0.79	0.19	21,21,21,21	0
57	MG	2A	3345	1/1	0.79	0.17	69,69,69,69	0
57	MG	2A	3577	1/1	0.79	0.13	73,73,73,73	0
57	MG	2A	3580	1/1	0.79	0.09	54,54,54,54	0
57	MG	1d	301	1/1	0.80	0.12	65,65,65,65	0
57	MG	2A	3192	1/1	0.80	0.11	58,58,58,58	0
57	MG	1a	1638	1/1	0.80	0.24	70,70,70,70	0
57	MG	1A	3698	1/1	0.80	0.15	53,53,53,53	0
57	MG	2a	3062	1/1	0.80	0.09	75,75,75,75	0
57	MG	2A	3201	1/1	0.80	0.28	59,59,59,59	0
57	MG	1a	1652	1/1	0.80	0.14	51,51,51,51	0
57	MG	2A	3627	1/1	0.80	0.15	49,49,49,49	0
57	MG	2A	3486	1/1	0.80	0.20	47,47,47,47	0
57	MG	2A	3710	1/1	0.80	0.08	64,64,64,64	0
57	MG	1A	3708	1/1	0.80	1.08	63,63,63,63	0
57	MG	2A	3719	1/1	0.80	0.12	67,67,67,67	0
57	MG	1a	1662	1/1	0.80	0.22	59,59,59,59	0
57	MG	2a	3101	1/1	0.80	0.37	62,62,62,62	0
57	MG	2A	3235	1/1	0.80	0.68	54,54,54,54	0
57	MG	1a	1668	1/1	0.80	0.17	52,52,52,52	0
57	MG	2A	3081	1/1	0.80	0.18	61,61,61,61	0
57	MG	1A	3491	1/1	0.80	0.09	63,63,63,63	0
57	MG	1Y	201	1/1	0.80	0.16	59,59,59,59	0
57	MG	1A	3332	1/1	0.80	0.18	26,26,26,26	0
57	MG	1A	4004	1/1	0.80	0.17	50,50,50,50	0
57	MG	17	104	1/1	0.80	0.71	56,56,56,56	0
57	MG	1A	3095	1/1	0.80	0.23	63,63,63,63	0
57	MG	1a	1817	1/1	0.80	0.11	56,56,56,56	0
57	MG	2A	3348	1/1	0.80	0.16	64,64,64,64	0
57	MG	1A	3870	1/1	0.80	0.13	58,58,58,58	0
57	MG	1A	3416	1/1	0.80	0.16	48,48,48,48	0
57	MG	1A	3823	1/1	0.80	0.19	65,65,65,65	0
57	MG	1A	3692	1/1	0.80	0.14	65,65,65,65	0
57	MG	2A	3732	1/1	0.81	0.17	68,68,68,68	0
57	MG	2A	3039	1/1	0.81	0.17	60,60,60,60	0
57	MG	1A	3616	1/1	0.81	0.40	58,58,58,58	0
57	MG	1B	211	1/1	0.81	0.11	68,68,68,68	0
57	MG	1a	1749	1/1	0.81	0.13	60,60,60,60	0
57	MG	2A	3068	1/1	0.81	0.17	48,48,48,48	0
57	MG	1a	1754	1/1	0.81	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1B	214	1/1	0.81	0.21	43,43,43,43	0
57	MG	1A	3535	1/1	0.81	0.16	58,58,58,58	0
57	MG	2A	3098	1/1	0.81	0.14	57,57,57,57	0
57	MG	20	101	1/1	0.81	0.13	60,60,60,60	0
57	MG	1A	3619	1/1	0.81	0.14	58,58,58,58	0
57	MG	1A	3863	1/1	0.81	0.08	62,62,62,62	0
57	MG	2A	3418	1/1	0.81	0.23	58,58,58,58	0
57	MG	1A	3495	1/1	0.81	0.12	46,46,46,46	0
57	MG	2A	3421	1/1	0.81	0.16	42,42,42,42	0
57	MG	1A	3409	1/1	0.81	0.11	60,60,60,60	0
57	MG	2A	3436	1/1	0.81	0.15	70,70,70,70	0
57	MG	1a	1785	1/1	0.81	0.09	64,64,64,64	0
57	MG	1A	3935	1/1	0.81	0.10	57,57,57,57	0
57	MG	1A	3165	1/1	0.81	0.16	41,41,41,41	0
57	MG	1a	1809	1/1	0.81	0.12	65,65,65,65	0
57	MG	1a	1697	1/1	0.81	0.22	62,62,62,62	0
57	MG	2A	3181	1/1	0.81	0.16	64,64,64,64	0
57	MG	1A	3882	1/1	0.81	0.09	32,32,32,32	0
57	MG	2A	3491	1/1	0.81	0.10	57,57,57,57	0
57	MG	1A	3528	1/1	0.81	0.21	63,63,63,63	0
57	MG	2A	3676	1/1	0.81	0.09	64,64,64,64	0
57	MG	2A	3193	1/1	0.81	0.17	66,66,66,66	0
57	MG	10	106	1/1	0.81	0.12	56,56,56,56	0
57	MG	1a	1832	1/1	0.81	0.40	56,56,56,56	0
57	MG	2a	3127	1/1	0.81	0.09	62,62,62,62	0
57	MG	1A	3960	1/1	0.81	0.29	72,72,72,72	0
57	MG	2A	3520	1/1	0.81	0.19	60,60,60,60	0
57	MG	1A	3885	1/1	0.81	0.14	43,43,43,43	0
57	MG	2A	3540	1/1	0.81	0.08	48,48,48,48	0
57	MG	2A	3213	1/1	0.81	0.13	65,65,65,65	0
57	MG	1b	301	1/1	0.81	0.19	66,66,66,66	0
57	MG	2A	3549	1/1	0.81	0.06	67,67,67,67	0
57	MG	2A	3225	1/1	0.81	0.12	65,65,65,65	0
57	MG	2A	3556	1/1	0.81	0.25	65,65,65,65	0
57	MG	2a	3174	1/1	0.81	0.11	64,64,64,64	0
57	MG	2A	3713	1/1	0.81	0.10	61,61,61,61	0
57	MG	1A	3886	1/1	0.81	0.64	60,60,60,60	0
57	MG	1a	1724	1/1	0.81	0.21	69,69,69,69	0
57	MG	1A	3756	1/1	0.81	0.11	39,39,39,39	0
57	MG	1A	3608	1/1	0.81	0.07	60,60,60,60	0
57	MG	1A	3776	1/1	0.82	0.20	25,25,25,25	0
57	MG	1A	3467	1/1	0.82	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3020	1/1	0.82	0.24	67,67,67,67	0
57	MG	1a	1680	1/1	0.82	0.17	56,56,56,56	0
57	MG	2A	3548	1/1	0.82	0.10	61,61,61,61	0
57	MG	2A	3355	1/1	0.82	0.12	52,52,52,52	0
57	MG	1a	1683	1/1	0.82	0.16	63,63,63,63	0
57	MG	2A	3383	1/1	0.82	0.14	66,66,66,66	0
57	MG	1A	3726	1/1	0.82	0.10	71,71,71,71	0
57	MG	1A	4015	1/1	0.82	0.12	50,50,50,50	0
57	MG	2a	3050	1/1	0.82	0.25	86,86,86,86	0
57	MG	2A	3406	1/1	0.82	0.12	32,32,32,32	0
57	MG	2a	3063	1/1	0.82	0.12	71,71,71,71	0
57	MG	2A	3584	1/1	0.82	0.15	43,43,43,43	0
57	MG	1A	3795	1/1	0.82	0.18	69,69,69,69	0
57	MG	2A	3059	1/1	0.82	0.15	50,50,50,50	0
57	MG	2A	3060	1/1	0.82	0.15	51,51,51,51	0
57	MG	1A	3665	1/1	0.82	0.10	52,52,52,52	0
57	MG	2A	3435	1/1	0.82	0.17	35,35,35,35	0
57	MG	1A	3452	1/1	0.82	0.15	25,25,25,25	0
57	MG	1B	222	1/1	0.82	0.15	42,42,42,42	0
57	MG	2A	3449	1/1	0.82	0.17	58,58,58,58	0
57	MG	2a	3109	1/1	0.82	0.07	64,64,64,64	0
57	MG	2A	3216	1/1	0.82	0.09	55,55,55,55	0
57	MG	1A	3931	1/1	0.82	0.07	45,45,45,45	0
57	MG	2A	3727	1/1	0.82	0.20	64,64,64,64	0
57	MG	1A	3737	1/1	0.82	0.10	46,46,46,46	0
57	MG	1a	1643	1/1	0.82	0.13	59,59,59,59	0
57	MG	2B	203	1/1	0.82	0.12	65,65,65,65	0
57	MG	1A	3345	1/1	0.82	0.16	43,43,43,43	0
57	MG	2a	3146	1/1	0.82	0.06	71,71,71,71	0
57	MG	2A	3241	1/1	0.82	0.15	70,70,70,70	0
57	MG	1A	3372	1/1	0.82	0.09	63,63,63,63	0
57	MG	1A	3183	1/1	0.82	0.14	56,56,56,56	0
57	MG	1A	3759	1/1	0.82	0.15	34,34,34,34	0
57	MG	2A	3271	1/1	0.82	0.37	54,54,54,54	0
57	MG	2a	3180	1/1	0.82	0.07	64,64,64,64	0
57	MG	2P	201	1/1	0.82	0.12	57,57,57,57	0
57	MG	1a	1841	1/1	0.82	0.17	61,61,61,61	0
57	MG	1a	1846	1/1	0.82	0.20	73,73,73,73	0
57	MG	2A	3144	1/1	0.82	0.21	51,51,51,51	0
61	ZN	14	501	1/1	0.82	0.05	108,108,108,108	0
57	MG	1A	3659	1/1	0.82	0.11	47,47,47,47	0
57	MG	1A	3038	1/1	0.83	0.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3421	1/1	0.83	0.12	29,29,29,29	0
57	MG	2A	3522	1/1	0.83	0.06	59,59,59,59	0
57	MG	1A	4009	1/1	0.83	0.14	35,35,35,35	0
57	MG	1a	1602	1/1	0.83	0.22	70,70,70,70	0
57	MG	1A	3723	1/1	0.83	0.11	59,59,59,59	0
57	MG	1a	1834	1/1	0.83	0.15	69,69,69,69	0
57	MG	2A	3146	1/1	0.83	0.17	57,57,57,57	0
57	MG	1a	1838	1/1	0.83	0.10	49,49,49,49	0
57	MG	1A	3481	1/1	0.83	0.21	30,30,30,30	0
57	MG	2a	3059	1/1	0.83	0.08	68,68,68,68	0
57	MG	1A	3040	1/1	0.83	0.10	56,56,56,56	0
57	MG	2A	3691	1/1	0.83	0.18	53,53,53,53	0
57	MG	1a	1730	1/1	0.83	0.16	63,63,63,63	0
57	MG	1A	3258	1/1	0.83	0.08	41,41,41,41	0
57	MG	1A	3599	1/1	0.83	0.18	59,59,59,59	0
57	MG	1A	3918	1/1	0.83	0.18	23,23,23,23	0
57	MG	1A	3739	1/1	0.83	0.06	45,45,45,45	0
57	MG	1A	3063	1/1	0.83	0.12	55,55,55,55	0
57	MG	2A	3198	1/1	0.83	0.14	57,57,57,57	0
57	MG	2A	3430	1/1	0.83	0.11	67,67,67,67	0
57	MG	1A	3498	1/1	0.83	0.09	57,57,57,57	0
57	MG	1y	201	1/1	0.83	0.18	57,57,57,57	0
57	MG	2a	3118	1/1	0.83	0.11	63,63,63,63	0
57	MG	1A	3189	1/1	0.83	0.19	49,49,49,49	0
57	MG	2A	3616	1/1	0.83	0.07	64,64,64,64	0
57	MG	1a	1767	1/1	0.83	0.17	63,63,63,63	0
57	MG	2A	3053	1/1	0.83	0.08	60,60,60,60	0
57	MG	1A	3670	1/1	0.83	0.16	57,57,57,57	0
57	MG	2A	3626	1/1	0.83	0.09	45,45,45,45	0
57	MG	2B	209	1/1	0.83	0.20	57,57,57,57	0
57	MG	2A	3472	1/1	0.83	0.13	57,57,57,57	0
57	MG	1A	3517	1/1	0.83	0.10	42,42,42,42	0
57	MG	1A	3311	1/1	0.83	0.28	49,49,49,49	0
57	MG	2G	201	1/1	0.83	0.16	74,74,74,74	0
57	MG	1a	1681	1/1	0.83	0.09	59,59,59,59	0
57	MG	1A	3002	1/1	0.83	0.25	57,57,57,57	0
57	MG	1a	1685	1/1	0.83	0.12	53,53,53,53	0
57	MG	1A	3533	1/1	0.83	0.13	48,48,48,48	0
57	MG	2A	3257	1/1	0.83	0.30	63,63,63,63	0
57	MG	1a	1691	1/1	0.83	0.28	64,64,64,64	0
57	MG	2x	101	1/1	0.83	0.09	57,57,57,57	0
57	MG	1A	3793	1/1	0.83	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3514	1/1	0.83	0.18	61,61,61,61	0
57	MG	2a	3009	1/1	0.83	0.15	66,66,66,66	0
57	MG	1A	3525	1/1	0.84	0.12	42,42,42,42	0
57	MG	2A	3143	1/1	0.84	0.18	63,63,63,63	0
57	MG	2A	3596	1/1	0.84	0.19	50,50,50,50	0
57	MG	2a	3048	1/1	0.84	0.19	69,69,69,69	0
57	MG	1A	3032	1/1	0.84	0.15	53,53,53,53	0
57	MG	2a	3051	1/1	0.84	0.17	72,72,72,72	0
57	MG	2A	3698	1/1	0.84	0.16	62,62,62,62	0
57	MG	1A	3049	1/1	0.84	0.38	44,44,44,44	0
57	MG	1a	1626	1/1	0.84	0.20	65,65,65,65	0
57	MG	2A	3296	1/1	0.84	0.25	67,67,67,67	0
57	MG	1A	3442	1/1	0.84	0.09	50,50,50,50	0
57	MG	1D	301	1/1	0.84	0.09	59,59,59,59	0
57	MG	1y	202	1/1	0.84	0.30	71,71,71,71	0
57	MG	2A	3330	1/1	0.84	0.17	57,57,57,57	0
57	MG	2A	3016	1/1	0.84	0.09	73,73,73,73	0
57	MG	1a	1798	1/1	0.84	0.16	62,62,62,62	0
57	MG	1A	3680	1/1	0.84	0.11	62,62,62,62	0
57	MG	2A	3641	1/1	0.84	0.21	58,58,58,58	0
57	MG	2A	3742	1/1	0.84	0.10	71,71,71,71	0
57	MG	1A	3468	1/1	0.84	0.09	43,43,43,43	0
57	MG	1a	1813	1/1	0.84	0.09	73,73,73,73	0
57	MG	1A	3867	1/1	0.84	0.10	67,67,67,67	0
57	MG	2a	3129	1/1	0.84	0.10	67,67,67,67	0
57	MG	2A	3539	1/1	0.84	0.19	39,39,39,39	0
57	MG	2A	3647	1/1	0.84	0.10	54,54,54,54	0
57	MG	2A	3648	1/1	0.84	0.07	64,64,64,64	0
57	MG	1A	3746	1/1	0.84	0.13	65,65,65,65	0
57	MG	2A	3652	1/1	0.84	0.08	63,63,63,63	0
57	MG	1A	3151	1/1	0.84	0.12	44,44,44,44	0
57	MG	1a	1822	1/1	0.84	0.10	53,53,53,53	0
57	MG	1A	4010	1/1	0.84	0.39	66,66,66,66	0
57	MG	10	101	1/1	0.84	0.24	39,39,39,39	0
57	MG	1A	3027	1/1	0.84	0.21	64,64,64,64	0
57	MG	1A	3921	1/1	0.84	0.23	61,61,61,61	0
57	MG	2A	3228	1/1	0.84	0.10	62,62,62,62	0
57	MG	2A	3666	1/1	0.84	0.09	50,50,50,50	0
57	MG	15	105	1/1	0.84	0.15	48,48,48,48	0
57	MG	1B	204	1/1	0.84	0.19	48,48,48,48	0
57	MG	2A	3240	1/1	0.84	0.33	58,58,58,58	0
57	MG	1A	3656	1/1	0.84	0.24	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MPD	1A	4019	8/8	0.84	0.15	50,54,62,65	0
57	MG	1A	3581	1/1	0.84	0.17	55,55,55,55	0
57	MG	2A	3461	1/1	0.84	0.12	62,62,62,62	0
57	MG	2A	3265	1/1	0.85	0.19	55,55,55,55	0
57	MG	1a	1824	1/1	0.85	0.12	67,67,67,67	0
57	MG	1A	3184	1/1	0.85	0.13	54,54,54,54	0
57	MG	1a	1729	1/1	0.85	0.11	54,54,54,54	0
57	MG	1a	1641	1/1	0.85	0.11	54,54,54,54	0
57	MG	2A	3306	1/1	0.85	0.13	62,62,62,62	0
57	MG	1A	3185	1/1	0.85	0.20	62,62,62,62	0
57	MG	1A	3597	1/1	0.85	0.07	33,33,33,33	0
57	MG	1E	307	1/1	0.85	0.17	54,54,54,54	0
57	MG	1A	3598	1/1	0.85	0.31	63,63,63,63	0
57	MG	2a	3040	1/1	0.85	0.08	64,64,64,64	0
57	MG	1A	3329	1/1	0.85	0.21	37,37,37,37	0
57	MG	2A	3156	1/1	0.85	0.19	69,69,69,69	0
57	MG	1A	3969	1/1	0.85	0.11	47,47,47,47	0
57	MG	2A	3359	1/1	0.85	0.16	38,38,38,38	0
57	MG	2a	3060	1/1	0.85	0.21	81,81,81,81	0
57	MG	2A	3366	1/1	0.85	0.15	58,58,58,58	0
57	MG	2A	3573	1/1	0.85	0.15	59,59,59,59	0
57	MG	2A	3368	1/1	0.85	0.08	48,48,48,48	0
57	MG	1A	3990	1/1	0.85	0.14	53,53,53,53	0
57	MG	2a	3071	1/1	0.85	0.12	59,59,59,59	0
57	MG	2A	3382	1/1	0.85	0.10	43,43,43,43	0
57	MG	1a	1675	1/1	0.85	0.12	80,80,80,80	0
57	MG	1A	3651	1/1	0.85	0.12	65,65,65,65	0
57	MG	1A	3849	1/1	0.85	0.10	53,53,53,53	0
57	MG	2A	3589	1/1	0.85	0.07	47,47,47,47	0
57	MG	1A	3852	1/1	0.85	0.23	58,58,58,58	0
57	MG	1x	101	1/1	0.85	0.12	33,33,33,33	0
57	MG	2A	3001	1/1	0.85	0.24	61,61,61,61	0
57	MG	2A	3595	1/1	0.85	0.07	44,44,44,44	0
57	MG	2A	3199	1/1	0.85	0.18	50,50,50,50	0
57	MG	1a	1778	1/1	0.85	0.17	62,62,62,62	0
57	MG	1A	3531	1/1	0.85	0.09	56,56,56,56	0
57	MG	1A	3769	1/1	0.85	0.12	55,55,55,55	0
57	MG	1A	3378	1/1	0.85	0.14	48,48,48,48	0
57	MG	2A	3746	1/1	0.85	0.11	52,52,52,52	0
57	MG	2a	3143	1/1	0.85	0.10	61,61,61,61	0
57	MG	2A	3056	1/1	0.85	0.22	62,62,62,62	0
57	MG	2A	3446	1/1	0.85	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1B	201	1/1	0.85	0.16	60,60,60,60	0
57	MG	1A	3121	1/1	0.85	0.14	39,39,39,39	0
57	MG	1A	3657	1/1	0.85	0.16	47,47,47,47	0
57	MG	1A	3199	1/1	0.85	0.34	51,51,51,51	0
57	MG	2A	3469	1/1	0.85	0.06	58,58,58,58	0
57	MG	1a	1616	1/1	0.85	0.12	59,59,59,59	0
57	MG	2a	3179	1/1	0.85	0.07	67,67,67,67	0
57	MG	1A	3396	1/1	0.85	0.16	28,28,28,28	0
57	MG	1a	1710	1/1	0.85	0.18	56,56,56,56	0
57	MG	2a	3189	1/1	0.85	0.15	66,66,66,66	0
57	MG	1a	1714	1/1	0.85	0.32	63,63,63,63	0
57	MG	2R	202	1/1	0.85	0.15	55,55,55,55	0
57	MG	1A	3127	1/1	0.85	0.17	49,49,49,49	0
57	MG	2A	3099	1/1	0.85	0.08	53,53,53,53	0
57	MG	1A	3942	1/1	0.85	0.13	43,43,43,43	0
57	MG	2A	3264	1/1	0.85	0.08	62,62,62,62	0
57	MG	2a	3002	1/1	0.85	0.10	73,73,73,73	0
57	MG	2A	3390	1/1	0.86	0.14	48,48,48,48	0
57	MG	2A	3393	1/1	0.86	0.19	62,62,62,62	0
57	MG	1A	3437	1/1	0.86	0.09	59,59,59,59	0
57	MG	2Q	201	1/1	0.86	0.11	56,56,56,56	0
57	MG	1A	3200	1/1	0.86	0.22	65,65,65,65	0
57	MG	1A	3762	1/1	0.86	0.17	62,62,62,62	0
57	MG	1A	3860	1/1	0.86	0.10	41,41,41,41	0
57	MG	1a	1738	1/1	0.86	0.35	62,62,62,62	0
57	MG	2T	204	1/1	0.86	0.19	56,56,56,56	0
57	MG	1a	1639	1/1	0.86	0.18	69,69,69,69	0
57	MG	2A	3434	1/1	0.86	0.10	56,56,56,56	0
57	MG	1A	3923	1/1	0.86	0.08	59,59,59,59	0
57	MG	2a	3006	1/1	0.86	0.16	63,63,63,63	0
57	MG	2a	3007	1/1	0.86	0.15	53,53,53,53	0
57	MG	1a	1748	1/1	0.86	0.05	62,62,62,62	0
57	MG	2a	3010	1/1	0.86	0.20	73,73,73,73	0
57	MG	2A	3635	1/1	0.86	0.19	49,49,49,49	0
57	MG	1A	3560	1/1	0.86	0.22	71,71,71,71	0
57	MG	1A	3204	1/1	0.86	0.18	36,36,36,36	0
57	MG	1B	224	1/1	0.86	0.06	42,42,42,42	0
57	MG	2A	3217	1/1	0.86	0.15	60,60,60,60	0
57	MG	2A	3034	1/1	0.86	0.23	65,65,65,65	0
57	MG	2A	3462	1/1	0.86	0.21	70,70,70,70	0
57	MG	1a	1761	1/1	0.86	0.17	62,62,62,62	0
57	MG	1a	1766	1/1	0.86	0.08	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3232	1/1	0.86	0.19	48,48,48,48	0
57	MG	1B	225	1/1	0.86	0.15	55,55,55,55	0
57	MG	1a	1768	1/1	0.86	0.10	67,67,67,67	0
57	MG	2A	3477	1/1	0.86	0.10	65,65,65,65	0
57	MG	2A	3479	1/1	0.86	0.12	65,65,65,65	0
57	MG	2A	3237	1/1	0.86	0.27	58,58,58,58	0
57	MG	1B	227	1/1	0.86	0.11	59,59,59,59	0
57	MG	1A	3274	1/1	0.86	0.09	54,54,54,54	0
57	MG	2A	3244	1/1	0.86	0.22	46,46,46,46	0
57	MG	1a	1671	1/1	0.86	0.12	62,62,62,62	0
57	MG	1A	3304	1/1	0.86	0.27	70,70,70,70	0
57	MG	1A	3418	1/1	0.86	0.22	27,27,27,27	0
57	MG	1a	1677	1/1	0.86	0.13	51,51,51,51	0
57	MG	1A	3718	1/1	0.86	0.16	66,66,66,66	0
57	MG	1A	3010	1/1	0.86	0.18	51,51,51,51	0
57	MG	1A	3958	1/1	0.86	0.18	49,49,49,49	0
57	MG	2A	3525	1/1	0.86	0.10	62,62,62,62	0
57	MG	1A	3603	1/1	0.86	0.17	37,37,37,37	0
57	MG	2A	3288	1/1	0.86	0.14	66,66,66,66	0
57	MG	2a	3116	1/1	0.86	0.09	49,49,49,49	0
57	MG	1A	3168	1/1	0.86	0.19	47,47,47,47	0
57	MG	2a	3120	1/1	0.86	0.10	69,69,69,69	0
57	MG	1A	3609	1/1	0.86	0.18	50,50,50,50	0
57	MG	2A	3129	1/1	0.86	0.27	41,41,41,41	0
57	MG	1A	3976	1/1	0.86	0.17	53,53,53,53	0
57	MG	2A	3318	1/1	0.86	0.11	66,66,66,66	0
57	MG	2A	3709	1/1	0.86	0.16	57,57,57,57	0
57	MG	1A	3979	1/1	0.86	0.15	33,33,33,33	0
57	MG	2A	3551	1/1	0.86	0.13	68,68,68,68	0
57	MG	1A	3982	1/1	0.86	0.15	74,74,74,74	0
57	MG	1A	3988	1/1	0.86	0.24	55,55,55,55	0
57	MG	2A	3574	1/1	0.86	0.11	52,52,52,52	0
57	MG	2A	3725	1/1	0.86	0.13	52,52,52,52	0
57	MG	1A	3989	1/1	0.86	0.30	49,49,49,49	0
57	MG	1A	3008	1/1	0.86	0.14	36,36,36,36	0
57	MG	1A	3239	1/1	0.86	0.30	60,60,60,60	0
57	MG	1A	3896	1/1	0.86	0.10	43,43,43,43	0
57	MG	2A	3585	1/1	0.86	0.21	49,49,49,49	0
57	MG	2B	201	1/1	0.86	0.12	71,71,71,71	0
57	MG	2A	3153	1/1	0.86	0.14	47,47,47,47	0
57	MG	2B	206	1/1	0.86	0.12	61,61,61,61	0
57	MG	1a	1715	1/1	0.86	0.20	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3035	1/1	0.86	0.22	50,50,50,50	0
57	MG	1A	3487	1/1	0.86	0.14	54,54,54,54	0
57	MG	2A	3174	1/1	0.86	0.10	59,59,59,59	0
57	MG	2B	215	1/1	0.86	0.15	66,66,66,66	0
57	MG	1A	3672	1/1	0.86	0.25	51,51,51,51	0
57	MG	2A	3184	1/1	0.86	0.12	52,52,52,52	0
57	MG	1E	305	1/1	0.87	0.06	39,39,39,39	0
57	MG	1a	1654	1/1	0.87	0.17	56,56,56,56	0
57	MG	2A	3653	1/1	0.87	0.10	52,52,52,52	0
57	MG	2a	3008	1/1	0.87	0.19	53,53,53,53	0
57	MG	1a	1660	1/1	0.87	0.19	62,62,62,62	0
57	MG	1A	3507	1/1	0.87	0.21	61,61,61,61	0
57	MG	1A	3714	1/1	0.87	0.09	30,30,30,30	0
57	MG	1A	3511	1/1	0.87	0.18	20,20,20,20	0
57	MG	1A	3537	1/1	0.87	0.23	60,60,60,60	0
57	MG	1A	3515	1/1	0.87	0.11	59,59,59,59	0
57	MG	1a	1674	1/1	0.87	0.12	55,55,55,55	0
57	MG	1a	1755	1/1	0.87	0.18	61,61,61,61	0
57	MG	2A	3350	1/1	0.87	0.18	43,43,43,43	0
57	MG	1e	201	1/1	0.87	0.23	60,60,60,60	0
57	MG	1e	202	1/1	0.87	0.11	65,65,65,65	0
57	MG	1g	201	1/1	0.87	0.17	47,47,47,47	0
57	MG	2a	3047	1/1	0.87	0.14	60,60,60,60	0
57	MG	1g	202	1/1	0.87	0.12	61,61,61,61	0
57	MG	1A	3350	1/1	0.87	0.09	53,53,53,53	0
57	MG	2A	3688	1/1	0.87	0.11	50,50,50,50	0
57	MG	2A	3374	1/1	0.87	0.11	33,33,33,33	0
57	MG	2A	3693	1/1	0.87	0.08	64,64,64,64	0
57	MG	1A	3676	1/1	0.87	0.11	61,61,61,61	0
57	MG	10	102	1/1	0.87	0.25	36,36,36,36	0
57	MG	1A	3648	1/1	0.87	0.16	36,36,36,36	0
57	MG	2A	3572	1/1	0.87	0.35	61,61,61,61	0
57	MG	1A	3928	1/1	0.87	0.14	56,56,56,56	0
57	MG	2a	3073	1/1	0.87	0.24	71,71,71,71	0
57	MG	15	101	1/1	0.87	0.26	43,43,43,43	0
57	MG	2A	3704	1/1	0.87	0.13	34,34,34,34	0
57	MG	1A	3521	1/1	0.87	0.19	37,37,37,37	0
57	MG	2A	3397	1/1	0.87	0.21	66,66,66,66	0
57	MG	2A	3017	1/1	0.87	0.11	56,56,56,56	0
57	MG	2A	3414	1/1	0.87	0.16	34,34,34,34	0
57	MG	2A	3717	1/1	0.87	0.35	44,44,44,44	0
57	MG	2a	3107	1/1	0.87	0.18	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	3032	1/1	0.87	0.52	59,59,59,59	0
57	MG	1A	3056	1/1	0.87	0.15	48,48,48,48	0
57	MG	1A	3941	1/1	0.87	0.19	45,45,45,45	0
57	MG	1A	3817	1/1	0.87	0.11	62,62,62,62	0
57	MG	1A	3373	1/1	0.87	0.16	52,52,52,52	0
57	MG	1a	1784	1/1	0.87	0.09	60,60,60,60	0
57	MG	2A	3230	1/1	0.87	0.16	43,43,43,43	0
57	MG	1A	3014	1/1	0.87	0.13	49,49,49,49	0
57	MG	1a	1789	1/1	0.87	0.06	70,70,70,70	0
57	MG	1A	3952	1/1	0.87	0.33	58,58,58,58	0
57	MG	2A	3447	1/1	0.87	0.09	54,54,54,54	0
57	MG	2A	3613	1/1	0.87	0.09	65,65,65,65	0
57	MG	1a	1704	1/1	0.87	0.19	62,62,62,62	0
57	MG	1A	3829	1/1	0.87	0.13	38,38,38,38	0
57	MG	2A	3622	1/1	0.87	0.14	52,52,52,52	0
57	MG	1a	1802	1/1	0.87	0.12	57,57,57,57	0
57	MG	1A	3887	1/1	0.87	0.13	53,53,53,53	0
57	MG	2a	3161	1/1	0.87	0.21	66,66,66,66	0
57	MG	2a	3162	1/1	0.87	0.11	59,59,59,59	0
57	MG	1a	1713	1/1	0.87	0.30	54,54,54,54	0
57	MG	2A	3464	1/1	0.87	0.14	61,61,61,61	0
57	MG	2A	3466	1/1	0.87	0.17	67,67,67,67	0
57	MG	2A	3467	1/1	0.87	0.18	45,45,45,45	0
57	MG	2A	3091	1/1	0.87	0.16	63,63,63,63	0
57	MG	1A	3831	1/1	0.87	0.15	48,48,48,48	0
57	MG	1A	3701	1/1	0.87	0.20	42,42,42,42	0
57	MG	1A	3968	1/1	0.87	0.12	52,52,52,52	0
57	MG	1A	3707	1/1	0.87	0.10	44,44,44,44	0
57	MG	2A	3478	1/1	0.87	0.13	53,53,53,53	0
57	MG	1A	3246	1/1	0.87	0.17	34,34,34,34	0
60	MPD	2A	3748	8/8	0.87	0.25	56,60,66,66	0
57	MG	1A	3978	1/1	0.87	0.18	35,35,35,35	0
61	ZN	2Y	202	1/1	0.87	0.09	88,88,88,88	0
57	MG	1a	1831	1/1	0.87	0.09	57,57,57,57	0
57	MG	1a	1851	1/1	0.88	0.10	55,55,55,55	0
57	MG	1A	3472	1/1	0.88	0.17	60,60,60,60	0
57	MG	2P	202	1/1	0.88	0.10	73,73,73,73	0
57	MG	1B	205	1/1	0.88	0.12	47,47,47,47	0
57	MG	2A	3619	1/1	0.88	0.12	42,42,42,42	0
57	MG	1A	3289	1/1	0.88	0.15	52,52,52,52	0
57	MG	1B	210	1/1	0.88	0.19	53,53,53,53	0
57	MG	2A	3623	1/1	0.88	0.09	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3202	1/1	0.88	0.34	59,59,59,59	0
57	MG	1A	3346	1/1	0.88	0.17	50,50,50,50	0
57	MG	1f	202	1/1	0.88	0.15	49,49,49,49	0
57	MG	28	3800	1/1	0.88	0.10	55,55,55,55	0
57	MG	28	3801	1/1	0.88	0.17	48,48,48,48	0
57	MG	1a	1647	1/1	0.88	0.15	54,54,54,54	0
57	MG	1A	3402	1/1	0.88	0.20	21,21,21,21	0
57	MG	2A	3630	1/1	0.88	0.11	61,61,61,61	0
57	MG	2A	3632	1/1	0.88	0.15	57,57,57,57	0
57	MG	1m	201	1/1	0.88	0.09	72,72,72,72	0
57	MG	1A	3494	1/1	0.88	0.12	32,32,32,32	0
57	MG	1A	3106	1/1	0.88	0.18	42,42,42,42	0
57	MG	2a	3019	1/1	0.88	0.13	57,57,57,57	0
57	MG	2A	3460	1/1	0.88	0.14	77,77,77,77	0
57	MG	1A	3703	1/1	0.88	0.42	64,64,64,64	0
57	MG	1A	3706	1/1	0.88	0.25	44,44,44,44	0
57	MG	1A	3883	1/1	0.88	0.09	47,47,47,47	0
57	MG	1a	1664	1/1	0.88	0.20	55,55,55,55	0
57	MG	2a	3030	1/1	0.88	0.12	58,58,58,58	0
57	MG	2A	3003	1/1	0.88	0.19	52,52,52,52	0
57	MG	1a	1666	1/1	0.88	0.08	64,64,64,64	0
57	MG	1A	3205	1/1	0.88	0.18	52,52,52,52	0
57	MG	2A	3031	1/1	0.88	0.16	55,55,55,55	0
57	MG	2a	3044	1/1	0.88	0.07	71,71,71,71	0
57	MG	1A	3564	1/1	0.88	0.09	49,49,49,49	0
57	MG	1A	3577	1/1	0.88	0.15	22,22,22,22	0
57	MG	1A	3447	1/1	0.88	0.12	64,64,64,64	0
57	MG	2A	3243	1/1	0.88	0.12	52,52,52,52	0
57	MG	2A	3661	1/1	0.88	0.14	58,58,58,58	0
57	MG	1a	1779	1/1	0.88	0.12	56,56,56,56	0
57	MG	2A	3050	1/1	0.88	0.14	59,59,59,59	0
57	MG	1F	315	1/1	0.88	0.16	33,33,33,33	0
57	MG	2a	3064	1/1	0.88	0.22	66,66,66,66	0
57	MG	1A	3972	1/1	0.88	0.11	46,46,46,46	0
57	MG	1P	205	1/1	0.88	0.12	67,67,67,67	0
57	MG	1T	201	1/1	0.88	0.18	67,67,67,67	0
57	MG	1A	3328	1/1	0.88	0.22	47,47,47,47	0
57	MG	2a	3077	1/1	0.88	0.07	74,74,74,74	0
57	MG	1a	1791	1/1	0.88	0.10	61,61,61,61	0
57	MG	2a	3080	1/1	0.88	0.15	61,61,61,61	0
57	MG	2a	3084	1/1	0.88	0.11	75,75,75,75	0
57	MG	2A	3508	1/1	0.88	0.22	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1794	1/1	0.88	0.11	59,59,59,59	0
57	MG	2a	3087	1/1	0.88	0.17	59,59,59,59	0
57	MG	1V	205	1/1	0.88	0.09	57,57,57,57	0
57	MG	2A	3292	1/1	0.88	0.14	45,45,45,45	0
57	MG	2A	3293	1/1	0.88	0.26	52,52,52,52	0
57	MG	1A	3591	1/1	0.88	0.10	63,63,63,63	0
57	MG	1A	3454	1/1	0.88	0.12	51,51,51,51	0
57	MG	2A	3536	1/1	0.88	0.08	52,52,52,52	0
57	MG	2a	3112	1/1	0.88	0.17	74,74,74,74	0
57	MG	2a	3113	1/1	0.88	0.13	73,73,73,73	0
57	MG	1A	3415	1/1	0.88	0.15	32,32,32,32	0
57	MG	2A	3311	1/1	0.88	0.14	51,51,51,51	0
57	MG	2A	3092	1/1	0.88	0.12	64,64,64,64	0
57	MG	2A	3546	1/1	0.88	0.09	79,79,79,79	0
57	MG	1a	1806	1/1	0.88	0.15	70,70,70,70	0
57	MG	1A	3983	1/1	0.88	0.09	55,55,55,55	0
57	MG	2a	3132	1/1	0.88	0.12	59,59,59,59	0
57	MG	1a	1810	1/1	0.88	0.14	54,54,54,54	0
57	MG	2A	3116	1/1	0.88	0.12	72,72,72,72	0
57	MG	1A	3458	1/1	0.88	0.16	51,51,51,51	0
57	MG	2A	3552	1/1	0.88	0.14	58,58,58,58	0
57	MG	1A	3904	1/1	0.88	0.19	28,28,28,28	0
57	MG	1A	3832	1/1	0.88	0.16	49,49,49,49	0
57	MG	2A	3720	1/1	0.88	0.09	65,65,65,65	0
57	MG	1A	3917	1/1	0.88	0.05	51,51,51,51	0
57	MG	1a	1706	1/1	0.88	0.13	56,56,56,56	0
57	MG	2A	3140	1/1	0.88	0.11	61,61,61,61	0
57	MG	1A	3663	1/1	0.88	0.12	41,41,41,41	0
57	MG	2A	3730	1/1	0.88	0.24	59,59,59,59	0
57	MG	1A	4005	1/1	0.88	0.20	56,56,56,56	0
57	MG	2A	3737	1/1	0.88	0.09	67,67,67,67	0
57	MG	1a	1828	1/1	0.88	0.20	75,75,75,75	0
57	MG	1A	3196	1/1	0.88	0.21	48,48,48,48	0
57	MG	1A	3846	1/1	0.88	0.10	41,41,41,41	0
57	MG	1A	3123	1/1	0.88	0.28	59,59,59,59	0
57	MG	1A	4014	1/1	0.88	0.11	61,61,61,61	0
57	MG	1A	3155	1/1	0.88	0.17	46,46,46,46	0
57	MG	2A	3164	1/1	0.88	0.15	60,60,60,60	0
57	MG	1a	1618	1/1	0.88	0.17	56,56,56,56	0
57	MG	2A	3169	1/1	0.88	0.34	69,69,69,69	0
57	MG	1A	3391	1/1	0.88	0.14	43,43,43,43	0
57	MG	2A	3598	1/1	0.88	0.25	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3599	1/1	0.88	0.08	43,43,43,43	0
57	MG	2A	3415	1/1	0.88	0.16	37,37,37,37	0
57	MG	1a	1756	1/1	0.89	0.13	48,48,48,48	0
57	MG	2A	3597	1/1	0.89	0.17	39,39,39,39	0
57	MG	1A	3728	1/1	0.89	0.19	43,43,43,43	0
57	MG	2A	3409	1/1	0.89	0.12	48,48,48,48	0
57	MG	1A	3892	1/1	0.89	0.15	42,42,42,42	0
57	MG	2A	3607	1/1	0.89	0.12	48,48,48,48	0
57	MG	2A	3197	1/1	0.89	0.29	49,49,49,49	0
57	MG	2A	3416	1/1	0.89	0.12	50,50,50,50	0
57	MG	1A	3641	1/1	0.89	0.22	33,33,33,33	0
57	MG	1a	1658	1/1	0.89	0.12	60,60,60,60	0
57	MG	1A	3031	1/1	0.89	0.10	50,50,50,50	0
57	MG	1a	1769	1/1	0.89	0.06	69,69,69,69	0
57	MG	2A	3209	1/1	0.89	0.10	63,63,63,63	0
57	MG	2A	3433	1/1	0.89	0.16	55,55,55,55	0
57	MG	1A	3826	1/1	0.89	0.19	25,25,25,25	0
57	MG	1A	3475	1/1	0.89	0.20	20,20,20,20	0
57	MG	1a	1663	1/1	0.89	0.28	53,53,53,53	0
57	MG	2A	3024	1/1	0.89	0.13	62,62,62,62	0
57	MG	1H	202	1/1	0.89	0.20	41,41,41,41	0
57	MG	1A	3681	1/1	0.89	0.21	68,68,68,68	0
57	MG	2A	3226	1/1	0.89	0.17	46,46,46,46	0
57	MG	2A	3451	1/1	0.89	0.35	46,46,46,46	0
57	MG	2A	3452	1/1	0.89	0.15	61,61,61,61	0
57	MG	2A	3639	1/1	0.89	0.04	78,78,78,78	0
57	MG	2A	3453	1/1	0.89	0.27	51,51,51,51	0
57	MG	2A	3454	1/1	0.89	0.10	79,79,79,79	0
57	MG	2A	3227	1/1	0.89	0.12	65,65,65,65	0
57	MG	1A	3742	1/1	0.89	0.13	49,49,49,49	0
57	MG	1A	3913	1/1	0.89	0.06	41,41,41,41	0
57	MG	1A	3646	1/1	0.89	0.21	34,34,34,34	0
57	MG	1U	201	1/1	0.89	0.34	47,47,47,47	0
57	MG	1a	1787	1/1	0.89	0.15	61,61,61,61	0
57	MG	2a	3049	1/1	0.89	0.15	65,65,65,65	0
57	MG	1V	204	1/1	0.89	0.17	47,47,47,47	0
57	MG	2A	3239	1/1	0.89	0.12	59,59,59,59	0
57	MG	1A	3690	1/1	0.89	0.11	55,55,55,55	0
57	MG	1W	202	1/1	0.89	0.18	41,41,41,41	0
57	MG	2A	3063	1/1	0.89	0.16	47,47,47,47	0
57	MG	1A	3842	1/1	0.89	0.12	54,54,54,54	0
57	MG	1A	3558	1/1	0.89	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3750	1/1	0.89	0.24	28,28,28,28	0
57	MG	2A	3255	1/1	0.89	0.19	39,39,39,39	0
57	MG	2a	3070	1/1	0.89	0.17	60,60,60,60	0
57	MG	1A	4007	1/1	0.89	0.15	59,59,59,59	0
57	MG	1A	3695	1/1	0.89	0.07	54,54,54,54	0
57	MG	1a	1688	1/1	0.89	0.10	59,59,59,59	0
57	MG	2A	3494	1/1	0.89	0.09	68,68,68,68	0
57	MG	2A	3495	1/1	0.89	0.10	67,67,67,67	0
57	MG	2a	3081	1/1	0.89	0.30	56,56,56,56	0
57	MG	2A	3499	1/1	0.89	0.14	58,58,58,58	0
57	MG	1A	3449	1/1	0.89	0.10	38,38,38,38	0
57	MG	1A	3303	1/1	0.89	0.36	66,66,66,66	0
57	MG	2A	3281	1/1	0.89	0.16	41,41,41,41	0
57	MG	10	107	1/1	0.89	0.09	50,50,50,50	0
57	MG	1A	3271	1/1	0.89	0.18	34,34,34,34	0
57	MG	2a	3097	1/1	0.89	0.15	71,71,71,71	0
57	MG	2a	3099	1/1	0.89	0.28	51,51,51,51	0
57	MG	2A	3512	1/1	0.89	0.18	25,25,25,25	0
57	MG	1A	3704	1/1	0.89	0.13	34,34,34,34	0
57	MG	15	107	1/1	0.89	0.13	66,66,66,66	0
57	MG	2A	3519	1/1	0.89	0.10	38,38,38,38	0
57	MG	2A	3295	1/1	0.89	0.18	59,59,59,59	0
57	MG	2A	3521	1/1	0.89	0.21	62,62,62,62	0
57	MG	2A	3119	1/1	0.89	0.12	55,55,55,55	0
57	MG	2a	3117	1/1	0.89	0.09	55,55,55,55	0
57	MG	2A	3299	1/1	0.89	0.29	61,61,61,61	0
57	MG	2A	3123	1/1	0.89	0.09	83,83,83,83	0
57	MG	1A	3934	1/1	0.89	0.31	53,53,53,53	0
57	MG	1A	3384	1/1	0.89	0.29	53,53,53,53	0
57	MG	1A	3390	1/1	0.89	0.16	40,40,40,40	0
57	MG	2A	3541	1/1	0.89	0.35	58,58,58,58	0
57	MG	1A	3435	1/1	0.89	0.11	66,66,66,66	0
57	MG	2A	3319	1/1	0.89	0.16	34,34,34,34	0
57	MG	2a	3141	1/1	0.89	0.12	63,63,63,63	0
57	MG	1A	3364	1/1	0.89	0.11	53,53,53,53	0
57	MG	2A	3327	1/1	0.89	0.10	58,58,58,58	0
57	MG	1A	3217	1/1	0.89	0.16	54,54,54,54	0
57	MG	1A	3630	1/1	0.89	0.16	29,29,29,29	0
57	MG	1a	1619	1/1	0.89	0.16	57,57,57,57	0
57	MG	2a	3147	1/1	0.89	0.20	77,77,77,77	0
57	MG	2A	3347	1/1	0.89	0.19	35,35,35,35	0
57	MG	1B	218	1/1	0.89	0.10	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3739	1/1	0.89	0.08	68,68,68,68	0
57	MG	2a	3154	1/1	0.89	0.08	65,65,65,65	0
57	MG	1a	1624	1/1	0.89	0.23	58,58,58,58	0
57	MG	1B	219	1/1	0.89	0.14	44,44,44,44	0
57	MG	2a	3165	1/1	0.89	0.08	60,60,60,60	0
57	MG	2a	3167	1/1	0.89	0.08	64,64,64,64	0
57	MG	1a	1627	1/1	0.89	0.12	67,67,67,67	0
57	MG	2a	3173	1/1	0.89	0.05	64,64,64,64	0
57	MG	2A	3362	1/1	0.89	0.10	46,46,46,46	0
57	MG	2a	3176	1/1	0.89	0.08	73,73,73,73	0
57	MG	1a	1863	1/1	0.89	0.12	63,63,63,63	0
57	MG	1B	220	1/1	0.89	0.18	30,30,30,30	0
57	MG	2a	3184	1/1	0.89	0.24	72,72,72,72	0
57	MG	2B	208	1/1	0.89	0.16	57,57,57,57	0
57	MG	1a	1631	1/1	0.89	0.10	63,63,63,63	0
57	MG	1a	1635	1/1	0.89	0.21	56,56,56,56	0
57	MG	1A	3637	1/1	0.89	0.17	37,37,37,37	0
57	MG	2r	101	1/1	0.89	0.22	74,74,74,74	0
57	MG	1A	3798	1/1	0.89	0.08	42,42,42,42	0
57	MG	2A	3384	1/1	0.89	0.11	41,41,41,41	0
57	MG	1A	3800	1/1	0.89	0.13	46,46,46,46	0
57	MG	2G	202	1/1	0.89	0.16	66,66,66,66	0
60	MPD	2B	220	8/8	0.89	0.17	59,60,67,75	0
57	MG	1A	3963	1/1	0.89	0.14	51,51,51,51	0
57	MG	2A	3186	1/1	0.89	0.18	61,61,61,61	0
57	MG	1A	3088	1/1	0.89	0.12	53,53,53,53	0
57	MG	1A	3684	1/1	0.90	0.08	71,71,71,71	0
57	MG	1a	1702	1/1	0.90	0.14	63,63,63,63	0
57	MG	2A	3391	1/1	0.90	0.20	69,69,69,69	0
57	MG	1A	3686	1/1	0.90	0.08	33,33,33,33	0
57	MG	1a	1842	1/1	0.90	0.28	74,74,74,74	0
57	MG	2A	3400	1/1	0.90	0.24	63,63,63,63	0
57	MG	1A	3161	1/1	0.90	0.22	46,46,46,46	0
57	MG	1A	3691	1/1	0.90	0.14	65,65,65,65	0
57	MG	1A	3228	1/1	0.90	0.13	39,39,39,39	0
57	MG	2A	3191	1/1	0.90	0.19	44,44,44,44	0
57	MG	1A	3636	1/1	0.90	0.15	46,46,46,46	0
57	MG	1A	3354	1/1	0.90	0.15	57,57,57,57	0
57	MG	2A	3604	1/1	0.90	0.17	55,55,55,55	0
57	MG	2A	3194	1/1	0.90	0.17	64,64,64,64	0
57	MG	1A	3268	1/1	0.90	0.24	45,45,45,45	0
57	MG	2A	3422	1/1	0.90	0.20	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3316	1/1	0.90	0.22	45,45,45,45	0
57	MG	2A	3425	1/1	0.90	0.12	45,45,45,45	0
57	MG	1A	3571	1/1	0.90	0.09	65,65,65,65	0
57	MG	2a	3014	1/1	0.90	0.18	69,69,69,69	0
57	MG	2a	3015	1/1	0.90	0.23	51,51,51,51	0
57	MG	2A	3621	1/1	0.90	0.09	53,53,53,53	0
57	MG	1a	1603	1/1	0.90	0.27	64,64,64,64	0
57	MG	1A	3500	1/1	0.90	0.13	53,53,53,53	0
57	MG	1A	3269	1/1	0.90	0.25	56,56,56,56	0
57	MG	1A	3903	1/1	0.90	0.23	25,25,25,25	0
57	MG	2A	3442	1/1	0.90	0.10	38,38,38,38	0
57	MG	2a	3027	1/1	0.90	0.11	67,67,67,67	0
57	MG	1A	3801	1/1	0.90	0.10	48,48,48,48	0
57	MG	2A	3211	1/1	0.90	0.13	42,42,42,42	0
57	MG	1a	1734	1/1	0.90	0.09	66,66,66,66	0
57	MG	2A	3448	1/1	0.90	0.07	53,53,53,53	0
57	MG	1A	3323	1/1	0.90	0.37	79,79,79,79	0
57	MG	1A	3813	1/1	0.90	0.09	46,46,46,46	0
57	MG	1B	206	1/1	0.90	0.16	47,47,47,47	0
57	MG	2A	3222	1/1	0.90	0.10	56,56,56,56	0
57	MG	2A	3640	1/1	0.90	0.08	54,54,54,54	0
57	MG	1A	3136	1/1	0.90	0.17	46,46,46,46	0
57	MG	2A	3456	1/1	0.90	0.34	68,68,68,68	0
57	MG	1A	3710	1/1	0.90	0.09	49,49,49,49	0
57	MG	2A	3644	1/1	0.90	0.10	53,53,53,53	0
57	MG	1a	1629	1/1	0.90	0.15	47,47,47,47	0
57	MG	2A	3014	1/1	0.90	0.08	59,59,59,59	0
57	MG	1A	3712	1/1	0.90	0.19	69,69,69,69	0
57	MG	1a	1632	1/1	0.90	0.13	42,42,42,42	0
57	MG	2a	3068	1/1	0.90	0.12	67,67,67,67	0
57	MG	1a	1633	1/1	0.90	0.18	48,48,48,48	0
57	MG	1A	3596	1/1	0.90	0.11	34,34,34,34	0
57	MG	1a	1762	1/1	0.90	0.10	52,52,52,52	0
57	MG	1A	3715	1/1	0.90	0.08	38,38,38,38	0
57	MG	1A	3460	1/1	0.90	0.18	16,16,16,16	0
57	MG	1A	3719	1/1	0.90	0.26	33,33,33,33	0
57	MG	2A	3474	1/1	0.90	0.14	61,61,61,61	0
57	MG	2A	3475	1/1	0.90	0.05	53,53,53,53	0
57	MG	1A	3833	1/1	0.90	0.14	40,40,40,40	0
57	MG	1A	3930	1/1	0.90	0.12	35,35,35,35	0
57	MG	2A	3055	1/1	0.90	0.21	63,63,63,63	0
57	MG	1A	3721	1/1	0.90	0.12	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3670	1/1	0.90	0.16	37,37,37,37	0
57	MG	1A	3932	1/1	0.90	0.13	50,50,50,50	0
57	MG	1A	3272	1/1	0.90	0.14	53,53,53,53	0
57	MG	1A	3840	1/1	0.90	0.11	41,41,41,41	0
57	MG	1a	1659	1/1	0.90	0.17	54,54,54,54	0
57	MG	1A	3139	1/1	0.90	0.15	37,37,37,37	0
57	MG	2A	3067	1/1	0.90	0.14	57,57,57,57	0
57	MG	2A	3279	1/1	0.90	0.21	50,50,50,50	0
57	MG	2A	3280	1/1	0.90	0.22	49,49,49,49	0
57	MG	1A	3602	1/1	0.90	0.12	44,44,44,44	0
57	MG	1A	3387	1/1	0.90	0.18	24,24,24,24	0
57	MG	1A	3077	1/1	0.90	0.18	62,62,62,62	0
57	MG	1E	308	1/1	0.90	0.10	36,36,36,36	0
57	MG	1a	1790	1/1	0.90	0.13	67,67,67,67	0
57	MG	1A	3469	1/1	0.90	0.16	42,42,42,42	0
57	MG	2a	3122	1/1	0.90	0.10	75,75,75,75	0
57	MG	2A	3518	1/1	0.90	0.22	44,44,44,44	0
57	MG	1A	3953	1/1	0.90	0.05	56,56,56,56	0
57	MG	1a	1796	1/1	0.90	0.16	58,58,58,58	0
57	MG	2A	3708	1/1	0.90	0.15	51,51,51,51	0
57	MG	2A	3100	1/1	0.90	0.14	60,60,60,60	0
57	MG	2a	3138	1/1	0.90	0.21	52,52,52,52	0
57	MG	2A	3112	1/1	0.90	0.24	47,47,47,47	0
57	MG	2A	3113	1/1	0.90	0.17	46,46,46,46	0
57	MG	2A	3716	1/1	0.90	0.17	69,69,69,69	0
57	MG	2A	3526	1/1	0.90	0.11	47,47,47,47	0
57	MG	2A	3530	1/1	0.90	0.15	69,69,69,69	0
57	MG	1a	1670	1/1	0.90	0.17	53,53,53,53	0
57	MG	2A	3534	1/1	0.90	0.09	60,60,60,60	0
57	MG	1A	3614	1/1	0.90	0.12	48,48,48,48	0
57	MG	1O	201	1/1	0.90	0.11	54,54,54,54	0
57	MG	2a	3152	1/1	0.90	0.07	56,56,56,56	0
57	MG	2A	3122	1/1	0.90	0.23	50,50,50,50	0
57	MG	1A	3336	1/1	0.90	0.14	32,32,32,32	0
57	MG	2a	3156	1/1	0.90	0.05	53,53,53,53	0
57	MG	2a	3157	1/1	0.90	0.12	50,50,50,50	0
57	MG	1A	3673	1/1	0.90	0.13	36,36,36,36	0
57	MG	1A	3862	1/1	0.90	0.13	48,48,48,48	0
57	MG	1T	206	1/1	0.90	0.11	70,70,70,70	0
57	MG	2a	3166	1/1	0.90	0.10	69,69,69,69	0
57	MG	2A	3738	1/1	0.90	0.13	64,64,64,64	0
57	MG	1A	3252	1/1	0.90	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3740	1/1	0.90	0.12	71,71,71,71	0
57	MG	2A	3136	1/1	0.90	0.14	58,58,58,58	0
57	MG	2a	3175	1/1	0.90	0.10	71,71,71,71	0
57	MG	1A	3477	1/1	0.90	0.22	21,21,21,21	0
57	MG	1A	3869	1/1	0.90	0.13	38,38,38,38	0
57	MG	1W	201	1/1	0.90	0.26	42,42,42,42	0
57	MG	1A	3436	1/1	0.90	0.12	48,48,48,48	0
57	MG	2A	3567	1/1	0.90	0.12	56,56,56,56	0
57	MG	2A	3569	1/1	0.90	0.06	58,58,58,58	0
57	MG	1a	1687	1/1	0.90	0.13	54,54,54,54	0
57	MG	1A	3975	1/1	0.90	0.13	42,42,42,42	0
57	MG	1A	3552	1/1	0.90	0.13	37,37,37,37	0
57	MG	1a	1830	1/1	0.90	0.08	62,62,62,62	0
57	MG	2B	218	1/1	0.90	0.14	74,74,74,74	0
57	MG	2A	3579	1/1	0.90	0.08	61,61,61,61	0
57	MG	2D	308	1/1	0.90	0.21	54,54,54,54	0
57	MG	1A	3875	1/1	0.90	0.16	51,51,51,51	0
57	MG	1A	3879	1/1	0.90	0.16	44,44,44,44	0
57	MG	2A	3162	1/1	0.90	0.27	50,50,50,50	0
57	MG	1A	3298	1/1	0.90	0.13	48,48,48,48	0
57	MG	1a	1605	1/1	0.91	0.12	52,52,52,52	0
57	MG	1A	3526	1/1	0.91	0.14	22,22,22,22	0
57	MG	1a	1614	1/1	0.91	0.11	65,65,65,65	0
57	MG	1A	3315	1/1	0.91	0.27	36,36,36,36	0
57	MG	2A	3073	1/1	0.91	0.16	32,32,32,32	0
57	MG	1A	3529	1/1	0.91	0.18	37,37,37,37	0
57	MG	1a	1815	1/1	0.91	0.07	54,54,54,54	0
57	MG	1A	3154	1/1	0.91	0.14	38,38,38,38	0
57	MG	1A	3255	1/1	0.91	0.13	43,43,43,43	0
57	MG	1A	3039	1/1	0.91	0.20	37,37,37,37	0
57	MG	2A	3247	1/1	0.91	0.16	59,59,59,59	0
57	MG	1A	3970	1/1	0.91	0.15	22,22,22,22	0
57	MG	1A	3012	1/1	0.91	0.11	35,35,35,35	0
57	MG	1D	321	1/1	0.91	0.26	51,51,51,51	0
57	MG	2A	3101	1/1	0.91	0.15	51,51,51,51	0
57	MG	2A	3108	1/1	0.91	0.10	52,52,52,52	0
57	MG	2A	3470	1/1	0.91	0.13	50,50,50,50	0
57	MG	1A	3973	1/1	0.91	0.14	52,52,52,52	0
57	MG	1A	3479	1/1	0.91	0.21	27,27,27,27	0
57	MG	2A	3273	1/1	0.91	0.10	57,57,57,57	0
57	MG	2A	3278	1/1	0.91	0.31	50,50,50,50	0
57	MG	1A	3738	1/1	0.91	0.19	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3115	1/1	0.91	0.15	60,60,60,60	0
57	MG	2a	3041	1/1	0.91	0.18	65,65,65,65	0
57	MG	1A	3977	1/1	0.91	0.08	48,48,48,48	0
57	MG	1F	305	1/1	0.91	0.19	35,35,35,35	0
57	MG	2A	3480	1/1	0.91	0.08	62,62,62,62	0
57	MG	1A	3082	1/1	0.91	0.44	35,35,35,35	0
57	MG	1A	3129	1/1	0.91	0.12	41,41,41,41	0
57	MG	1A	3683	1/1	0.91	0.10	69,69,69,69	0
57	MG	1A	3030	1/1	0.91	0.10	34,34,34,34	0
57	MG	1a	1742	1/1	0.91	0.12	61,61,61,61	0
57	MG	2A	3498	1/1	0.91	0.11	54,54,54,54	0
57	MG	2A	3132	1/1	0.91	0.54	65,65,65,65	0
57	MG	1A	3987	1/1	0.91	0.20	39,39,39,39	0
57	MG	1a	1648	1/1	0.91	0.11	68,68,68,68	0
57	MG	2A	3503	1/1	0.91	0.14	31,31,31,31	0
57	MG	2A	3668	1/1	0.91	0.10	54,54,54,54	0
57	MG	2A	3307	1/1	0.91	0.39	55,55,55,55	0
57	MG	2A	3674	1/1	0.91	0.05	75,75,75,75	0
57	MG	2a	3072	1/1	0.91	0.06	71,71,71,71	0
57	MG	1a	1856	1/1	0.91	0.11	68,68,68,68	0
57	MG	1a	1857	1/1	0.91	0.14	65,65,65,65	0
57	MG	2A	3511	1/1	0.91	0.06	61,61,61,61	0
57	MG	2A	3141	1/1	0.91	0.08	49,49,49,49	0
57	MG	1a	1858	1/1	0.91	0.09	67,67,67,67	0
57	MG	1A	3629	1/1	0.91	0.13	43,43,43,43	0
57	MG	2A	3145	1/1	0.91	0.13	62,62,62,62	0
57	MG	1a	1865	1/1	0.91	0.12	60,60,60,60	0
57	MG	2A	3339	1/1	0.91	0.11	49,49,49,49	0
57	MG	2a	3089	1/1	0.91	0.11	63,63,63,63	0
57	MG	1a	1866	1/1	0.91	0.20	70,70,70,70	0
57	MG	2a	3092	1/1	0.91	0.13	69,69,69,69	0
57	MG	2A	3148	1/1	0.91	0.15	36,36,36,36	0
57	MG	2A	3696	1/1	0.91	0.11	37,37,37,37	0
57	MG	1A	3440	1/1	0.91	0.20	54,54,54,54	0
57	MG	1A	3174	1/1	0.91	0.12	50,50,50,50	0
57	MG	2A	3155	1/1	0.91	0.14	44,44,44,44	0
57	MG	1d	303	1/1	0.91	0.30	55,55,55,55	0
57	MG	2A	3356	1/1	0.91	0.18	38,38,38,38	0
57	MG	2a	3110	1/1	0.91	0.08	77,77,77,77	0
57	MG	1A	3444	1/1	0.91	0.14	26,26,26,26	0
57	MG	1A	3858	1/1	0.91	0.08	53,53,53,53	0
57	MG	1A	3216	1/1	0.91	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3050	1/1	0.91	0.35	43,43,43,43	0
57	MG	1A	3643	1/1	0.91	0.15	64,64,64,64	0
57	MG	1A	3775	1/1	0.91	0.11	37,37,37,37	0
57	MG	2A	3177	1/1	0.91	0.10	56,56,56,56	0
57	MG	2A	3179	1/1	0.91	0.29	57,57,57,57	0
57	MG	1h	202	1/1	0.91	0.15	63,63,63,63	0
57	MG	1A	3285	1/1	0.91	0.11	63,63,63,63	0
57	MG	2a	3130	1/1	0.91	0.14	61,61,61,61	0
57	MG	1A	4013	1/1	0.91	0.19	40,40,40,40	0
57	MG	2A	3723	1/1	0.91	0.26	51,51,51,51	0
57	MG	1A	3227	1/1	0.91	0.14	38,38,38,38	0
57	MG	2A	3553	1/1	0.91	0.12	76,76,76,76	0
57	MG	1A	3589	1/1	0.91	0.18	44,44,44,44	0
57	MG	2A	3557	1/1	0.91	0.12	62,62,62,62	0
57	MG	2A	3559	1/1	0.91	0.05	54,54,54,54	0
57	MG	2A	3733	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3413	1/1	0.91	0.14	28,28,28,28	0
57	MG	2A	3395	1/1	0.91	0.10	62,62,62,62	0
57	MG	1A	3937	1/1	0.91	0.17	65,65,65,65	0
57	MG	1A	3938	1/1	0.91	0.08	61,61,61,61	0
57	MG	2a	3150	1/1	0.91	0.06	55,55,55,55	0
57	MG	2A	3404	1/1	0.91	0.10	76,76,76,76	0
57	MG	2A	3002	1/1	0.91	0.12	50,50,50,50	0
57	MG	2A	3408	1/1	0.91	0.14	61,61,61,61	0
57	MG	10	108	1/1	0.91	0.16	54,54,54,54	0
57	MG	1A	3595	1/1	0.91	0.10	67,67,67,67	0
57	MG	1a	1781	1/1	0.91	0.12	71,71,71,71	0
57	MG	1A	3052	1/1	0.91	0.34	30,30,30,30	0
57	MG	1A	3358	1/1	0.91	0.16	20,20,20,20	0
57	MG	2A	3027	1/1	0.91	0.31	60,60,60,60	0
57	MG	2B	213	1/1	0.91	0.18	70,70,70,70	0
57	MG	1A	3016	1/1	0.91	0.19	36,36,36,36	0
57	MG	2A	3591	1/1	0.91	0.06	50,50,50,50	0
57	MG	2a	3170	1/1	0.91	0.17	54,54,54,54	0
57	MG	2B	217	1/1	0.91	0.17	57,57,57,57	0
57	MG	18	101	1/1	0.91	0.68	57,57,57,57	0
57	MG	2D	303	1/1	0.91	0.17	52,52,52,52	0
57	MG	19	101	1/1	0.91	0.16	58,58,58,58	0
57	MG	1B	212	1/1	0.91	0.09	51,51,51,51	0
57	MG	2A	3428	1/1	0.91	0.11	41,41,41,41	0
57	MG	2a	3183	1/1	0.91	0.15	75,75,75,75	0
57	MG	2A	3429	1/1	0.91	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	19	103	1/1	0.91	0.10	54,54,54,54	0
57	MG	1A	3150	1/1	0.91	0.14	40,40,40,40	0
57	MG	1a	1690	1/1	0.91	0.10	70,70,70,70	0
57	MG	1A	3600	1/1	0.91	0.23	31,31,31,31	0
57	MG	1a	1693	1/1	0.91	0.15	73,73,73,73	0
57	MG	2A	3606	1/1	0.91	0.13	50,50,50,50	0
57	MG	2Q	203	1/1	0.91	0.10	57,57,57,57	0
57	MG	1a	1799	1/1	0.91	0.12	65,65,65,65	0
60	MPD	1T	208	8/8	0.91	0.15	59,64,68,69	0
60	MPD	1a	1867	8/8	0.91	0.19	52,59,62,64	0
57	MG	2A	3610	1/1	0.91	0.09	67,67,67,67	0
57	MG	2A	3444	1/1	0.91	0.13	46,46,46,46	0
57	MG	1A	3058	1/1	0.91	0.19	46,46,46,46	0
57	MG	1a	1801	1/1	0.91	0.10	55,55,55,55	0
57	MG	2A	3231	1/1	0.91	0.15	54,54,54,54	0
57	MG	25	103	1/1	0.92	0.25	55,55,55,55	0
57	MG	1A	3915	1/1	0.92	0.14	35,35,35,35	0
57	MG	1a	1751	1/1	0.92	0.06	82,82,82,82	0
57	MG	1A	3786	1/1	0.92	0.12	45,45,45,45	0
57	MG	11	101	1/1	0.92	0.17	39,39,39,39	0
57	MG	2A	3631	1/1	0.92	0.26	51,51,51,51	0
57	MG	1a	1855	1/1	0.92	0.09	58,58,58,58	0
57	MG	13	102	1/1	0.92	0.14	59,59,59,59	0
57	MG	1A	3974	1/1	0.92	0.10	50,50,50,50	0
57	MG	15	104	1/1	0.92	0.17	26,26,26,26	0
57	MG	2A	3637	1/1	0.92	0.18	59,59,59,59	0
57	MG	2A	3286	1/1	0.92	0.22	53,53,53,53	0
57	MG	2a	3017	1/1	0.92	0.07	58,58,58,58	0
57	MG	1A	3389	1/1	0.92	0.12	28,28,28,28	0
57	MG	1a	1763	1/1	0.92	0.18	71,71,71,71	0
57	MG	1A	3570	1/1	0.92	0.17	33,33,33,33	0
57	MG	1A	3725	1/1	0.92	0.12	39,39,39,39	0
57	MG	1A	3685	1/1	0.92	0.19	20,20,20,20	0
57	MG	1B	228	1/1	0.92	0.09	70,70,70,70	0
57	MG	2A	3298	1/1	0.92	0.24	56,56,56,56	0
57	MG	2a	3029	1/1	0.92	0.17	62,62,62,62	0
57	MG	1a	1770	1/1	0.92	0.12	59,59,59,59	0
57	MG	2A	3300	1/1	0.92	0.17	51,51,51,51	0
57	MG	1A	3251	1/1	0.92	0.16	58,58,58,58	0
57	MG	2A	3304	1/1	0.92	0.22	58,58,58,58	0
57	MG	2A	3305	1/1	0.92	0.30	63,63,63,63	0
57	MG	1A	3434	1/1	0.92	0.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3497	1/1	0.92	0.08	68,68,68,68	0
57	MG	2a	3045	1/1	0.92	0.10	64,64,64,64	0
57	MG	2a	3046	1/1	0.92	0.20	55,55,55,55	0
57	MG	1A	3133	1/1	0.92	0.13	51,51,51,51	0
57	MG	1A	3985	1/1	0.92	0.52	48,48,48,48	0
57	MG	1A	3926	1/1	0.92	0.22	57,57,57,57	0
57	MG	2A	3317	1/1	0.92	0.12	64,64,64,64	0
57	MG	1A	3349	1/1	0.92	0.22	25,25,25,25	0
57	MG	2a	3053	1/1	0.92	0.13	55,55,55,55	0
57	MG	2a	3055	1/1	0.92	0.20	59,59,59,59	0
57	MG	1i	201	1/1	0.92	0.17	54,54,54,54	0
57	MG	2A	3149	1/1	0.92	0.21	46,46,46,46	0
57	MG	2A	3667	1/1	0.92	0.13	47,47,47,47	0
57	MG	1A	3805	1/1	0.92	0.14	44,44,44,44	0
57	MG	1A	3045	1/1	0.92	0.23	55,55,55,55	0
57	MG	1A	3536	1/1	0.92	0.11	56,56,56,56	0
57	MG	2a	3066	1/1	0.92	0.10	68,68,68,68	0
57	MG	1F	306	1/1	0.92	0.19	35,35,35,35	0
57	MG	1A	3594	1/1	0.92	0.13	48,48,48,48	0
57	MG	1A	3880	1/1	0.92	0.19	25,25,25,25	0
57	MG	1N	201	1/1	0.92	0.10	36,36,36,36	0
57	MG	2A	3684	1/1	0.92	0.14	40,40,40,40	0
57	MG	1N	202	1/1	0.92	0.14	36,36,36,36	0
57	MG	1a	1792	1/1	0.92	0.14	65,65,65,65	0
57	MG	2A	3005	1/1	0.92	0.40	63,63,63,63	0
57	MG	2A	3689	1/1	0.92	0.10	73,73,73,73	0
57	MG	2A	3175	1/1	0.92	0.31	49,49,49,49	0
57	MG	2A	3360	1/1	0.92	0.16	55,55,55,55	0
57	MG	1N	203	1/1	0.92	0.17	48,48,48,48	0
57	MG	2A	3365	1/1	0.92	0.18	30,30,30,30	0
57	MG	1a	1795	1/1	0.92	0.17	68,68,68,68	0
57	MG	1a	1701	1/1	0.92	0.17	59,59,59,59	0
57	MG	2a	3090	1/1	0.92	0.18	68,68,68,68	0
57	MG	2A	3369	1/1	0.92	0.19	38,38,38,38	0
57	MG	2A	3700	1/1	0.92	0.08	54,54,54,54	0
57	MG	2a	3093	1/1	0.92	0.29	52,52,52,52	0
57	MG	1A	3820	1/1	0.92	0.18	36,36,36,36	0
57	MG	2A	3025	1/1	0.92	0.12	52,52,52,52	0
57	MG	2A	3544	1/1	0.92	0.08	67,67,67,67	0
57	MG	2A	3380	1/1	0.92	0.13	73,73,73,73	0
57	MG	2A	3707	1/1	0.92	0.10	51,51,51,51	0
57	MG	2a	3105	1/1	0.92	0.07	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3381	1/1	0.92	0.15	44,44,44,44	0
57	MG	1a	1703	1/1	0.92	0.22	62,62,62,62	0
57	MG	1A	3513	1/1	0.92	0.22	20,20,20,20	0
57	MG	1P	202	1/1	0.92	0.27	48,48,48,48	0
57	MG	1a	1708	1/1	0.92	0.27	45,45,45,45	0
57	MG	2A	3037	1/1	0.92	0.17	66,66,66,66	0
57	MG	1A	3547	1/1	0.92	0.14	44,44,44,44	0
57	MG	2A	3046	1/1	0.92	0.12	60,60,60,60	0
57	MG	2A	3554	1/1	0.92	0.07	51,51,51,51	0
57	MG	1a	1803	1/1	0.92	0.07	54,54,54,54	0
57	MG	2A	3048	1/1	0.92	0.07	62,62,62,62	0
57	MG	2a	3123	1/1	0.92	0.11	64,64,64,64	0
57	MG	2A	3724	1/1	0.92	0.13	38,38,38,38	0
57	MG	2A	3049	1/1	0.92	0.10	55,55,55,55	0
57	MG	1A	3240	1/1	0.92	0.22	53,53,53,53	0
57	MG	2A	3403	1/1	0.92	0.13	62,62,62,62	0
57	MG	2A	3202	1/1	0.92	0.26	64,64,64,64	0
57	MG	2A	3204	1/1	0.92	0.14	52,52,52,52	0
57	MG	2A	3206	1/1	0.92	0.11	46,46,46,46	0
57	MG	1a	1808	1/1	0.92	0.10	59,59,59,59	0
57	MG	2A	3578	1/1	0.92	0.11	52,52,52,52	0
57	MG	2A	3413	1/1	0.92	0.14	53,53,53,53	0
57	MG	1A	3668	1/1	0.92	0.09	50,50,50,50	0
57	MG	1A	3633	1/1	0.92	0.13	45,45,45,45	0
57	MG	2A	3058	1/1	0.92	0.15	38,38,38,38	0
57	MG	1a	1812	1/1	0.92	0.22	56,56,56,56	0
57	MG	2a	3148	1/1	0.92	0.07	62,62,62,62	0
57	MG	1A	3302	1/1	0.92	0.10	61,61,61,61	0
57	MG	2B	204	1/1	0.92	0.12	70,70,70,70	0
57	MG	2B	205	1/1	0.92	0.14	68,68,68,68	0
57	MG	2A	3587	1/1	0.92	0.15	43,43,43,43	0
57	MG	2A	3218	1/1	0.92	0.25	47,47,47,47	0
57	MG	1A	3519	1/1	0.92	0.12	52,52,52,52	0
57	MG	2A	3221	1/1	0.92	0.19	54,54,54,54	0
57	MG	1a	1642	1/1	0.92	0.17	63,63,63,63	0
57	MG	1B	203	1/1	0.92	0.13	59,59,59,59	0
57	MG	1a	1727	1/1	0.92	0.25	57,57,57,57	0
57	MG	2a	3163	1/1	0.92	0.07	64,64,64,64	0
57	MG	1a	1644	1/1	0.92	0.22	56,56,56,56	0
57	MG	1A	3462	1/1	0.92	0.28	63,63,63,63	0
57	MG	2A	3075	1/1	0.92	0.06	63,63,63,63	0
57	MG	2B	219	1/1	0.92	0.16	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3078	1/1	0.92	0.32	55,55,55,55	0
57	MG	1A	3404	1/1	0.92	0.14	25,25,25,25	0
57	MG	1A	3771	1/1	0.92	0.12	37,37,37,37	0
57	MG	2E	305	1/1	0.92	0.10	63,63,63,63	0
57	MG	2F	302	1/1	0.92	0.15	40,40,40,40	0
57	MG	2A	3083	1/1	0.92	0.16	61,61,61,61	0
57	MG	1A	3774	1/1	0.92	0.15	43,43,43,43	0
57	MG	2a	3181	1/1	0.92	0.09	77,77,77,77	0
57	MG	1A	3844	1/1	0.92	0.11	42,42,42,42	0
57	MG	2I	201	1/1	0.92	0.12	65,65,65,65	0
57	MG	2N	201	1/1	0.92	0.14	70,70,70,70	0
57	MG	1A	3642	1/1	0.92	0.16	34,34,34,34	0
57	MG	2A	3097	1/1	0.92	0.19	47,47,47,47	0
57	MG	1a	1833	1/1	0.92	0.10	59,59,59,59	0
57	MG	2A	3450	1/1	0.92	0.11	61,61,61,61	0
57	MG	2A	3618	1/1	0.92	0.24	48,48,48,48	0
57	MG	1A	3053	1/1	0.92	0.22	30,30,30,30	0
59	ARG	1B	231	12/12	0.92	0.21	29,39,47,50	0
57	MG	1A	3605	1/1	0.92	0.15	46,46,46,46	0
57	MG	1a	1839	1/1	0.92	0.06	72,72,72,72	0
60	MPD	18	104	8/8	0.92	0.21	30,35,42,46	0
57	MG	2A	3103	1/1	0.92	0.15	51,51,51,51	0
57	MG	2A	3104	1/1	0.92	0.17	53,53,53,53	0
57	MG	2X	101	1/1	0.92	0.10	47,47,47,47	0
57	MG	2Y	201	1/1	0.92	0.26	61,61,61,61	0
57	MG	1a	1746	1/1	0.92	0.11	61,61,61,61	0
57	MG	1B	216	1/1	0.92	0.20	48,48,48,48	0
57	MG	1A	3615	1/1	0.93	0.21	34,34,34,34	0
57	MG	1A	3191	1/1	0.93	0.10	59,59,59,59	0
57	MG	1f	201	1/1	0.93	0.29	74,74,74,74	0
57	MG	2A	3388	1/1	0.93	0.10	43,43,43,43	0
57	MG	1A	3478	1/1	0.93	0.15	28,28,28,28	0
57	MG	2A	3183	1/1	0.93	0.13	41,41,41,41	0
57	MG	1A	3160	1/1	0.93	0.28	62,62,62,62	0
57	MG	2A	3394	1/1	0.93	0.16	39,39,39,39	0
57	MG	1A	3029	1/1	0.93	0.16	35,35,35,35	0
57	MG	1A	3898	1/1	0.93	0.18	64,64,64,64	0
57	MG	1A	3788	1/1	0.93	0.28	57,57,57,57	0
57	MG	20	102	1/1	0.93	0.10	69,69,69,69	0
57	MG	2A	3602	1/1	0.93	0.09	46,46,46,46	0
57	MG	1A	3789	1/1	0.93	0.11	25,25,25,25	0
57	MG	1n	101	1/1	0.93	0.25	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1606	1/1	0.93	0.13	48,48,48,48	0
57	MG	2A	3608	1/1	0.93	0.12	34,34,34,34	0
57	MG	1A	3553	1/1	0.93	0.07	49,49,49,49	0
57	MG	2A	3196	1/1	0.93	0.25	71,71,71,71	0
57	MG	1a	1608	1/1	0.93	0.12	58,58,58,58	0
57	MG	2A	3615	1/1	0.93	0.13	32,32,32,32	0
57	MG	1a	1613	1/1	0.93	0.15	49,49,49,49	0
57	MG	2A	3617	1/1	0.93	0.12	40,40,40,40	0
57	MG	1A	3912	1/1	0.93	0.17	18,18,18,18	0
57	MG	1A	3333	1/1	0.93	0.18	45,45,45,45	0
57	MG	1A	3015	1/1	0.93	0.12	37,37,37,37	0
57	MG	2a	3018	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	3693	1/1	0.93	0.16	37,37,37,37	0
57	MG	1A	3694	1/1	0.93	0.13	54,54,54,54	0
57	MG	2A	3205	1/1	0.93	0.16	46,46,46,46	0
57	MG	1A	3627	1/1	0.93	0.12	26,26,26,26	0
57	MG	1A	3490	1/1	0.93	0.13	31,31,31,31	0
57	MG	1A	3392	1/1	0.93	0.20	30,30,30,30	0
57	MG	1A	3493	1/1	0.93	0.14	22,22,22,22	0
57	MG	2A	3212	1/1	0.93	0.08	57,57,57,57	0
57	MG	1A	3340	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3214	1/1	0.93	0.30	61,61,61,61	0
57	MG	1A	3811	1/1	0.93	0.14	29,29,29,29	0
57	MG	1A	3565	1/1	0.93	0.13	56,56,56,56	0
57	MG	2a	3038	1/1	0.93	0.14	63,63,63,63	0
57	MG	2A	3438	1/1	0.93	0.14	64,64,64,64	0
57	MG	1A	3294	1/1	0.93	0.25	42,42,42,42	0
57	MG	1A	3120	1/1	0.93	0.14	35,35,35,35	0
57	MG	1a	1636	1/1	0.93	0.10	38,38,38,38	0
57	MG	1A	3576	1/1	0.93	0.09	50,50,50,50	0
57	MG	1a	1774	1/1	0.93	0.19	69,69,69,69	0
57	MG	1A	3033	1/1	0.93	0.13	34,34,34,34	0
57	MG	1A	3502	1/1	0.93	0.08	62,62,62,62	0
57	MG	1A	3583	1/1	0.93	0.20	45,45,45,45	0
57	MG	2A	3229	1/1	0.93	0.11	47,47,47,47	0
57	MG	2a	3052	1/1	0.93	0.22	59,59,59,59	0
57	MG	1D	318	1/1	0.93	0.17	53,53,53,53	0
57	MG	1A	3584	1/1	0.93	0.12	51,51,51,51	0
57	MG	1a	1645	1/1	0.93	0.19	54,54,54,54	0
57	MG	1A	3348	1/1	0.93	0.17	50,50,50,50	0
57	MG	1A	3068	1/1	0.93	0.37	30,30,30,30	0
57	MG	1E	306	1/1	0.93	0.21	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3411	1/1	0.93	0.08	35,35,35,35	0
57	MG	1a	1653	1/1	0.93	0.11	36,36,36,36	0
57	MG	1A	3722	1/1	0.93	0.13	24,24,24,24	0
57	MG	2A	3242	1/1	0.93	0.23	62,62,62,62	0
57	MG	2A	3465	1/1	0.93	0.14	37,37,37,37	0
57	MG	1a	1657	1/1	0.93	0.15	57,57,57,57	0
57	MG	1A	3180	1/1	0.93	0.18	49,49,49,49	0
57	MG	1A	3654	1/1	0.93	0.20	38,38,38,38	0
57	MG	2A	3072	1/1	0.93	0.16	51,51,51,51	0
57	MG	2a	3076	1/1	0.93	0.09	54,54,54,54	0
57	MG	2A	3253	1/1	0.93	0.44	57,57,57,57	0
57	MG	1F	311	1/1	0.93	0.14	38,38,38,38	0
57	MG	2A	3669	1/1	0.93	0.16	36,36,36,36	0
57	MG	1F	314	1/1	0.93	0.41	42,42,42,42	0
57	MG	2A	3256	1/1	0.93	0.17	53,53,53,53	0
57	MG	1A	3306	1/1	0.93	0.35	32,32,32,32	0
57	MG	2A	3258	1/1	0.93	0.20	45,45,45,45	0
57	MG	2A	3260	1/1	0.93	0.16	57,57,57,57	0
57	MG	1A	3459	1/1	0.93	0.17	45,45,45,45	0
57	MG	1A	3848	1/1	0.93	0.12	27,27,27,27	0
57	MG	1A	3260	1/1	0.93	0.30	33,33,33,33	0
57	MG	1A	3962	1/1	0.93	0.14	44,44,44,44	0
57	MG	1a	1669	1/1	0.93	0.11	61,61,61,61	0
57	MG	2a	3095	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3851	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3732	1/1	0.93	0.12	20,20,20,20	0
57	MG	1A	3661	1/1	0.93	0.09	46,46,46,46	0
57	MG	1P	204	1/1	0.93	0.10	39,39,39,39	0
57	MG	1A	3361	1/1	0.93	0.14	46,46,46,46	0
57	MG	2a	3103	1/1	0.93	0.15	54,54,54,54	0
57	MG	1Q	204	1/1	0.93	0.09	35,35,35,35	0
57	MG	2a	3106	1/1	0.93	0.05	64,64,64,64	0
57	MG	1R	205	1/1	0.93	0.26	44,44,44,44	0
57	MG	2A	3290	1/1	0.93	0.13	44,44,44,44	0
57	MG	2A	3699	1/1	0.93	0.40	46,46,46,46	0
57	MG	1a	1814	1/1	0.93	0.09	58,58,58,58	0
57	MG	1A	3182	1/1	0.93	0.13	39,39,39,39	0
57	MG	2A	3702	1/1	0.93	0.13	51,51,51,51	0
57	MG	2A	3507	1/1	0.93	0.10	66,66,66,66	0
57	MG	1A	3089	1/1	0.93	0.14	32,32,32,32	0
57	MG	1A	3094	1/1	0.93	0.26	44,44,44,44	0
57	MG	1a	1818	1/1	0.93	0.06	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3743	1/1	0.93	0.17	38,38,38,38	0
57	MG	1U	203	1/1	0.93	0.20	60,60,60,60	0
57	MG	2a	3125	1/1	0.93	0.06	73,73,73,73	0
57	MG	2A	3301	1/1	0.93	0.26	53,53,53,53	0
57	MG	2A	3711	1/1	0.93	0.12	46,46,46,46	0
57	MG	1U	206	1/1	0.93	0.20	36,36,36,36	0
57	MG	2a	3131	1/1	0.93	0.05	63,63,63,63	0
57	MG	2A	3715	1/1	0.93	0.17	59,59,59,59	0
57	MG	1A	3669	1/1	0.93	0.09	50,50,50,50	0
57	MG	1a	1827	1/1	0.93	0.14	59,59,59,59	0
57	MG	2a	3137	1/1	0.93	0.11	65,65,65,65	0
57	MG	2A	3125	1/1	0.93	0.12	36,36,36,36	0
57	MG	1A	3074	1/1	0.93	0.12	41,41,41,41	0
57	MG	2A	3308	1/1	0.93	0.18	65,65,65,65	0
57	MG	2A	3529	1/1	0.93	0.08	51,51,51,51	0
57	MG	2A	3309	1/1	0.93	0.27	58,58,58,58	0
57	MG	1A	3671	1/1	0.93	0.14	43,43,43,43	0
57	MG	1A	3325	1/1	0.93	0.16	30,30,30,30	0
57	MG	2A	3535	1/1	0.93	0.07	69,69,69,69	0
57	MG	1A	3753	1/1	0.93	0.09	39,39,39,39	0
57	MG	1X	101	1/1	0.93	0.22	33,33,33,33	0
57	MG	2A	3135	1/1	0.93	0.12	54,54,54,54	0
57	MG	2A	3320	1/1	0.93	0.14	50,50,50,50	0
57	MG	2A	3734	1/1	0.93	0.07	63,63,63,63	0
57	MG	1A	3874	1/1	0.93	0.20	31,31,31,31	0
57	MG	1A	3755	1/1	0.93	0.13	44,44,44,44	0
57	MG	2A	3328	1/1	0.93	0.18	42,42,42,42	0
57	MG	2A	3139	1/1	0.93	0.13	63,63,63,63	0
57	MG	2a	3160	1/1	0.93	0.28	68,68,68,68	0
57	MG	2A	3334	1/1	0.93	0.12	41,41,41,41	0
57	MG	2A	3744	1/1	0.93	0.14	69,69,69,69	0
57	MG	2A	3745	1/1	0.93	0.23	59,59,59,59	0
57	MG	1A	3878	1/1	0.93	0.14	59,59,59,59	0
57	MG	1A	3606	1/1	0.93	0.21	37,37,37,37	0
57	MG	1A	3758	1/1	0.93	0.12	54,54,54,54	0
57	MG	1A	3675	1/1	0.93	0.20	38,38,38,38	0
57	MG	1a	1845	1/1	0.93	0.08	62,62,62,62	0
57	MG	1a	1705	1/1	0.93	0.15	57,57,57,57	0
57	MG	1A	3607	1/1	0.93	0.18	31,31,31,31	0
57	MG	1A	3991	1/1	0.93	0.12	35,35,35,35	0
57	MG	2A	3357	1/1	0.93	0.12	48,48,48,48	0
57	MG	2A	3560	1/1	0.93	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3564	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3765	1/1	0.93	0.15	56,56,56,56	0
57	MG	2a	3182	1/1	0.93	0.17	73,73,73,73	0
57	MG	1A	4002	1/1	0.93	0.11	24,24,24,24	0
57	MG	1a	1712	1/1	0.93	0.34	55,55,55,55	0
57	MG	2A	3364	1/1	0.93	0.17	34,34,34,34	0
57	MG	2A	3154	1/1	0.93	0.13	56,56,56,56	0
57	MG	2e	201	1/1	0.93	0.26	68,68,68,68	0
57	MG	2f	201	1/1	0.93	0.17	60,60,60,60	0
57	MG	2A	3575	1/1	0.93	0.09	35,35,35,35	0
57	MG	2D	304	1/1	0.93	0.30	51,51,51,51	0
57	MG	2D	306	1/1	0.93	0.35	44,44,44,44	0
57	MG	1A	3767	1/1	0.93	0.11	33,33,33,33	0
58	CLM	2A	3747	20/20	0.93	0.22	33,38,53,58	0
57	MG	1A	3471	1/1	0.93	0.08	39,39,39,39	0
57	MG	2E	303	1/1	0.93	0.24	45,45,45,45	0
57	MG	1A	4006	1/1	0.93	0.15	32,32,32,32	0
57	MG	2A	3372	1/1	0.93	0.19	50,50,50,50	0
57	MG	1A	3426	1/1	0.93	0.20	22,22,22,22	0
57	MG	2A	3583	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	3156	1/1	0.93	0.12	25,25,25,25	0
57	MG	2A	3165	1/1	0.93	0.12	58,58,58,58	0
57	MG	1a	1719	1/1	0.93	0.18	57,57,57,57	0
57	MG	1a	1721	1/1	0.93	0.20	65,65,65,65	0
57	MG	1a	1723	1/1	0.93	0.19	64,64,64,64	0
57	MG	2E	306	1/1	0.94	0.07	42,42,42,42	0
57	MG	2A	3565	1/1	0.94	0.12	47,47,47,47	0
57	MG	1A	3021	1/1	0.94	0.10	39,39,39,39	0
57	MG	2A	3568	1/1	0.94	0.11	57,57,57,57	0
57	MG	2A	3351	1/1	0.94	0.20	49,49,49,49	0
57	MG	1A	3407	1/1	0.94	0.11	45,45,45,45	0
57	MG	1A	3190	1/1	0.94	0.14	43,43,43,43	0
57	MG	1A	3463	1/1	0.94	0.11	54,54,54,54	0
57	MG	1Z	301	1/1	0.94	0.14	60,60,60,60	0
57	MG	1A	3410	1/1	0.94	0.16	19,19,19,19	0
57	MG	1A	3534	1/1	0.94	0.13	48,48,48,48	0
57	MG	2A	3363	1/1	0.94	0.21	39,39,39,39	0
57	MG	1A	3618	1/1	0.94	0.17	26,26,26,26	0
57	MG	1a	1848	1/1	0.94	0.14	35,35,35,35	0
57	MG	1A	4003	1/1	0.94	0.10	48,48,48,48	0
57	MG	2A	3367	1/1	0.94	0.15	33,33,33,33	0
57	MG	1a	1852	1/1	0.94	0.07	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2U	201	1/1	0.94	0.11	68,68,68,68	0
57	MG	2V	203	1/1	0.94	0.16	62,62,62,62	0
57	MG	1A	3108	1/1	0.94	0.07	58,58,58,58	0
57	MG	2A	3370	1/1	0.94	0.16	33,33,33,33	0
57	MG	1A	3296	1/1	0.94	0.18	38,38,38,38	0
57	MG	2A	3163	1/1	0.94	0.10	62,62,62,62	0
57	MG	1A	3782	1/1	0.94	0.11	38,38,38,38	0
57	MG	25	101	1/1	0.94	0.65	52,52,52,52	0
57	MG	1A	3622	1/1	0.94	0.23	26,26,26,26	0
57	MG	1A	3623	1/1	0.94	0.19	29,29,29,29	0
57	MG	1a	1862	1/1	0.94	0.17	60,60,60,60	0
57	MG	2a	3001	1/1	0.94	0.19	40,40,40,40	0
57	MG	1A	3787	1/1	0.94	0.11	21,21,21,21	0
57	MG	2a	3003	1/1	0.94	0.14	64,64,64,64	0
57	MG	2a	3004	1/1	0.94	0.07	61,61,61,61	0
57	MG	2a	3005	1/1	0.94	0.25	62,62,62,62	0
57	MG	1A	3192	1/1	0.94	0.11	59,59,59,59	0
57	MG	1A	4012	1/1	0.94	0.23	42,42,42,42	0
57	MG	1A	3539	1/1	0.94	0.16	51,51,51,51	0
57	MG	2A	3180	1/1	0.94	0.11	47,47,47,47	0
57	MG	17	105	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3601	1/1	0.94	0.11	58,58,58,58	0
57	MG	2a	3012	1/1	0.94	0.22	67,67,67,67	0
57	MG	1A	3791	1/1	0.94	0.15	29,29,29,29	0
57	MG	1A	3299	1/1	0.94	0.20	31,31,31,31	0
57	MG	2A	3605	1/1	0.94	0.17	44,44,44,44	0
57	MG	1a	1722	1/1	0.94	0.19	47,47,47,47	0
57	MG	1A	4016	1/1	0.94	0.11	42,42,42,42	0
57	MG	2A	3396	1/1	0.94	0.17	49,49,49,49	0
57	MG	2a	3021	1/1	0.94	0.11	53,53,53,53	0
57	MG	1A	3551	1/1	0.94	0.10	33,33,33,33	0
57	MG	2A	3398	1/1	0.94	0.15	32,32,32,32	0
57	MG	1A	3794	1/1	0.94	0.12	58,58,58,58	0
57	MG	2A	3401	1/1	0.94	0.12	56,56,56,56	0
57	MG	1A	3628	1/1	0.94	0.10	53,53,53,53	0
57	MG	1A	3901	1/1	0.94	0.15	33,33,33,33	0
57	MG	1h	201	1/1	0.94	0.22	49,49,49,49	0
57	MG	1A	3301	1/1	0.94	0.19	51,51,51,51	0
57	MG	1A	3355	1/1	0.94	0.14	31,31,31,31	0
57	MG	1A	3906	1/1	0.94	0.17	27,27,27,27	0
57	MG	1A	3356	1/1	0.94	0.15	22,22,22,22	0
57	MG	2a	3039	1/1	0.94	0.08	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1739	1/1	0.94	0.09	58,58,58,58	0
57	MG	1t	3101	1/1	0.94	0.12	50,50,50,50	0
57	MG	2a	3042	1/1	0.94	0.13	68,68,68,68	0
57	MG	2A	3417	1/1	0.94	0.14	50,50,50,50	0
57	MG	1a	1611	1/1	0.94	0.15	66,66,66,66	0
57	MG	1A	3635	1/1	0.94	0.12	45,45,45,45	0
57	MG	2A	3420	1/1	0.94	0.17	40,40,40,40	0
57	MG	1A	3070	1/1	0.94	0.14	37,37,37,37	0
57	MG	1A	3197	1/1	0.94	0.10	53,53,53,53	0
57	MG	1a	1747	1/1	0.94	0.11	64,64,64,64	0
57	MG	1a	1617	1/1	0.94	0.14	55,55,55,55	0
57	MG	2A	3427	1/1	0.94	0.13	68,68,68,68	0
57	MG	1A	3167	1/1	0.94	0.21	45,45,45,45	0
57	MG	1A	3640	1/1	0.94	0.12	29,29,29,29	0
57	MG	2a	3056	1/1	0.94	0.11	58,58,58,58	0
57	MG	2A	3008	1/1	0.94	0.15	37,37,37,37	0
57	MG	2A	3009	1/1	0.94	0.16	34,34,34,34	0
57	MG	1a	1753	1/1	0.94	0.09	53,53,53,53	0
57	MG	1A	3812	1/1	0.94	0.18	45,45,45,45	0
57	MG	1A	3482	1/1	0.94	0.15	44,44,44,44	0
57	MG	2A	3020	1/1	0.94	0.22	39,39,39,39	0
57	MG	2A	3441	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3220	1/1	0.94	0.18	46,46,46,46	0
57	MG	2A	3443	1/1	0.94	0.07	48,48,48,48	0
57	MG	2A	3023	1/1	0.94	0.23	58,58,58,58	0
57	MG	1a	1625	1/1	0.94	0.13	44,44,44,44	0
57	MG	1A	3563	1/1	0.94	0.16	60,60,60,60	0
57	MG	1A	3425	1/1	0.94	0.31	41,41,41,41	0
57	MG	1A	3821	1/1	0.94	0.14	36,36,36,36	0
57	MG	1A	3822	1/1	0.94	0.23	29,29,29,29	0
57	MG	1a	1764	1/1	0.94	0.11	49,49,49,49	0
57	MG	2a	3079	1/1	0.94	0.16	47,47,47,47	0
57	MG	1a	1765	1/1	0.94	0.14	52,52,52,52	0
57	MG	1a	1630	1/1	0.94	0.17	41,41,41,41	0
57	MG	2a	3083	1/1	0.94	0.31	60,60,60,60	0
57	MG	1A	3086	1/1	0.94	0.12	35,35,35,35	0
57	MG	1A	3488	1/1	0.94	0.14	25,25,25,25	0
57	MG	1A	3081	1/1	0.94	0.14	46,46,46,46	0
57	MG	1D	303	1/1	0.94	0.28	35,35,35,35	0
57	MG	1A	3125	1/1	0.94	0.20	51,51,51,51	0
57	MG	1D	319	1/1	0.94	0.07	61,61,61,61	0
57	MG	1A	3176	1/1	0.94	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3380	1/1	0.94	0.11	47,47,47,47	0
57	MG	1a	1777	1/1	0.94	0.14	55,55,55,55	0
57	MG	2a	3094	1/1	0.94	0.14	55,55,55,55	0
57	MG	1A	3317	1/1	0.94	0.17	34,34,34,34	0
57	MG	1A	3497	1/1	0.94	0.20	26,26,26,26	0
57	MG	1A	3939	1/1	0.94	0.12	42,42,42,42	0
57	MG	2A	3248	1/1	0.94	0.48	52,52,52,52	0
57	MG	1A	3207	1/1	0.94	0.26	37,37,37,37	0
57	MG	1A	3386	1/1	0.94	0.16	32,32,32,32	0
57	MG	1A	3841	1/1	0.94	0.20	55,55,55,55	0
57	MG	1A	3126	1/1	0.94	0.14	66,66,66,66	0
57	MG	1a	1651	1/1	0.94	0.15	39,39,39,39	0
57	MG	2A	3690	1/1	0.94	0.05	65,65,65,65	0
57	MG	1F	312	1/1	0.94	0.11	49,49,49,49	0
57	MG	2A	3692	1/1	0.94	0.12	33,33,33,33	0
57	MG	1A	3951	1/1	0.94	0.17	49,49,49,49	0
57	MG	2A	3261	1/1	0.94	0.14	51,51,51,51	0
57	MG	2a	3115	1/1	0.94	0.20	63,63,63,63	0
57	MG	2A	3262	1/1	0.94	0.16	52,52,52,52	0
57	MG	1A	3504	1/1	0.94	0.14	43,43,43,43	0
57	MG	2A	3481	1/1	0.94	0.07	59,59,59,59	0
57	MG	1a	1656	1/1	0.94	0.16	51,51,51,51	0
57	MG	2A	3487	1/1	0.94	0.10	66,66,66,66	0
57	MG	2A	3488	1/1	0.94	0.08	59,59,59,59	0
57	MG	1a	1793	1/1	0.94	0.12	61,61,61,61	0
57	MG	1G	202	1/1	0.94	0.20	51,51,51,51	0
57	MG	2A	3492	1/1	0.94	0.12	48,48,48,48	0
57	MG	2A	3272	1/1	0.94	0.21	30,30,30,30	0
57	MG	2A	3705	1/1	0.94	0.23	48,48,48,48	0
57	MG	2A	3085	1/1	0.94	0.12	58,58,58,58	0
57	MG	1G	203	1/1	0.94	0.09	51,51,51,51	0
57	MG	2A	3090	1/1	0.94	0.11	38,38,38,38	0
57	MG	1A	3270	1/1	0.94	0.25	44,44,44,44	0
57	MG	2a	3136	1/1	0.94	0.16	61,61,61,61	0
57	MG	2A	3500	1/1	0.94	0.05	68,68,68,68	0
57	MG	1A	3741	1/1	0.94	0.14	48,48,48,48	0
57	MG	2a	3139	1/1	0.94	0.15	56,56,56,56	0
57	MG	2A	3712	1/1	0.94	0.09	51,51,51,51	0
57	MG	2A	3285	1/1	0.94	0.17	55,55,55,55	0
57	MG	2A	3096	1/1	0.94	0.12	76,76,76,76	0
57	MG	1A	3098	1/1	0.94	0.27	37,37,37,37	0
57	MG	1A	3850	1/1	0.94	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3289	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3101	1/1	0.94	0.17	37,37,37,37	0
57	MG	1A	3666	1/1	0.94	0.11	48,48,48,48	0
57	MG	2A	3721	1/1	0.94	0.09	57,57,57,57	0
57	MG	1A	3854	1/1	0.94	0.16	24,24,24,24	0
57	MG	2A	3513	1/1	0.94	0.12	35,35,35,35	0
57	MG	2A	3294	1/1	0.94	0.42	65,65,65,65	0
57	MG	2A	3515	1/1	0.94	0.11	46,46,46,46	0
57	MG	2A	3516	1/1	0.94	0.13	56,56,56,56	0
57	MG	1A	3130	1/1	0.94	0.46	37,37,37,37	0
57	MG	1A	3450	1/1	0.94	0.15	45,45,45,45	0
57	MG	2a	3158	1/1	0.94	0.07	62,62,62,62	0
57	MG	2A	3297	1/1	0.94	0.23	40,40,40,40	0
57	MG	2A	3105	1/1	0.94	0.27	53,53,53,53	0
57	MG	1Q	202	1/1	0.94	0.19	31,31,31,31	0
57	MG	2A	3735	1/1	0.94	0.18	52,52,52,52	0
57	MG	1A	3159	1/1	0.94	0.22	32,32,32,32	0
57	MG	1Q	205	1/1	0.94	0.17	54,54,54,54	0
57	MG	1R	204	1/1	0.94	0.15	48,48,48,48	0
57	MG	1A	3751	1/1	0.94	0.19	26,26,26,26	0
57	MG	2A	3741	1/1	0.94	0.17	56,56,56,56	0
57	MG	1A	3394	1/1	0.94	0.18	18,18,18,18	0
57	MG	2A	3532	1/1	0.94	0.12	62,62,62,62	0
57	MG	1a	1678	1/1	0.94	0.14	55,55,55,55	0
57	MG	2A	3120	1/1	0.94	0.10	72,72,72,72	0
57	MG	2a	3177	1/1	0.94	0.12	54,54,54,54	0
57	MG	1A	3754	1/1	0.94	0.26	57,57,57,57	0
57	MG	1T	205	1/1	0.94	0.20	59,59,59,59	0
57	MG	2A	3310	1/1	0.94	0.13	51,51,51,51	0
57	MG	1A	3275	1/1	0.94	0.13	37,37,37,37	0
57	MG	1A	3864	1/1	0.94	0.21	28,28,28,28	0
57	MG	2A	3315	1/1	0.94	0.14	58,58,58,58	0
57	MG	1A	3865	1/1	0.94	0.10	35,35,35,35	0
57	MG	2a	3188	1/1	0.94	0.14	57,57,57,57	0
57	MG	2A	3130	1/1	0.94	0.15	46,46,46,46	0
57	MG	2a	3190	1/1	0.94	0.07	67,67,67,67	0
57	MG	2B	210	1/1	0.94	0.11	66,66,66,66	0
57	MG	1A	3866	1/1	0.94	0.09	40,40,40,40	0
57	MG	2B	212	1/1	0.94	0.19	64,64,64,64	0
57	MG	1A	3277	1/1	0.94	0.17	27,27,27,27	0
57	MG	2A	3133	1/1	0.94	0.17	43,43,43,43	0
57	MG	1a	1825	1/1	0.94	0.09	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2B	216	1/1	0.94	0.23	77,77,77,77	0
57	MG	1A	3868	1/1	0.94	0.08	40,40,40,40	0
57	MG	1a	1689	1/1	0.94	0.14	64,64,64,64	0
57	MG	2A	3331	1/1	0.94	0.11	66,66,66,66	0
57	MG	1a	1829	1/1	0.94	0.06	71,71,71,71	0
57	MG	1V	206	1/1	0.94	0.20	53,53,53,53	0
57	MG	2D	305	1/1	0.94	0.10	34,34,34,34	0
57	MG	1A	3524	1/1	0.94	0.12	58,58,58,58	0
57	MG	1A	3278	1/1	0.94	0.16	57,57,57,57	0
57	MG	2A	3142	1/1	0.94	0.11	39,39,39,39	0
57	MG	2A	3563	1/1	0.94	0.17	32,32,32,32	0
57	MG	1a	1696	1/1	0.94	0.25	57,57,57,57	0
57	MG	1A	3550	1/1	0.95	0.18	42,42,42,42	0
57	MG	2F	301	1/1	0.95	0.30	41,41,41,41	0
57	MG	1A	3466	1/1	0.95	0.20	63,63,63,63	0
57	MG	2F	303	1/1	0.95	0.19	52,52,52,52	0
57	MG	1A	3071	1/1	0.95	0.12	32,32,32,32	0
57	MG	1A	3740	1/1	0.95	0.19	24,24,24,24	0
57	MG	2A	3312	1/1	0.95	0.12	46,46,46,46	0
57	MG	1A	3398	1/1	0.95	0.12	33,33,33,33	0
57	MG	1A	3090	1/1	0.95	0.15	25,25,25,25	0
57	MG	1A	3164	1/1	0.95	0.13	33,33,33,33	0
57	MG	2A	3555	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3028	1/1	0.95	0.28	28,28,28,28	0
57	MG	1a	1621	1/1	0.95	0.13	58,58,58,58	0
57	MG	1A	3647	1/1	0.95	0.25	65,65,65,65	0
57	MG	1A	3473	1/1	0.95	0.28	39,39,39,39	0
57	MG	1A	3075	1/1	0.95	0.27	29,29,29,29	0
57	MG	1a	1786	1/1	0.95	0.06	61,61,61,61	0
57	MG	1A	3562	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3871	1/1	0.95	0.16	26,26,26,26	0
57	MG	1A	3752	1/1	0.95	0.10	42,42,42,42	0
57	MG	2A	3337	1/1	0.95	0.05	35,35,35,35	0
57	MG	2A	3338	1/1	0.95	0.15	64,64,64,64	0
57	MG	1A	3339	1/1	0.95	0.18	31,31,31,31	0
57	MG	2A	3118	1/1	0.95	0.13	48,48,48,48	0
57	MG	2A	3341	1/1	0.95	0.23	47,47,47,47	0
57	MG	2A	3344	1/1	0.95	0.16	59,59,59,59	0
57	MG	23	101	1/1	0.95	0.36	59,59,59,59	0
57	MG	1A	3020	1/1	0.95	0.24	30,30,30,30	0
57	MG	25	102	1/1	0.95	0.23	45,45,45,45	0
57	MG	2A	3346	1/1	0.95	0.21	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3876	1/1	0.95	0.21	40,40,40,40	0
57	MG	1A	3097	1/1	0.95	0.09	53,53,53,53	0
57	MG	1A	3569	1/1	0.95	0.19	14,14,14,14	0
57	MG	1a	1634	1/1	0.95	0.19	58,58,58,58	0
57	MG	2A	3352	1/1	0.95	0.06	43,43,43,43	0
57	MG	1B	209	1/1	0.95	0.16	38,38,38,38	0
57	MG	1A	3480	1/1	0.95	0.15	24,24,24,24	0
57	MG	1A	3061	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3662	1/1	0.95	0.18	14,14,14,14	0
57	MG	1A	3763	1/1	0.95	0.17	42,42,42,42	0
57	MG	2A	3361	1/1	0.95	0.11	45,45,45,45	0
57	MG	1A	3572	1/1	0.95	0.20	45,45,45,45	0
57	MG	1B	217	1/1	0.95	0.26	61,61,61,61	0
57	MG	1a	1804	1/1	0.95	0.09	67,67,67,67	0
57	MG	1A	3574	1/1	0.95	0.15	33,33,33,33	0
57	MG	1A	3005	1/1	0.95	0.18	26,26,26,26	0
57	MG	2A	3138	1/1	0.95	0.20	24,24,24,24	0
57	MG	1A	3347	1/1	0.95	0.12	38,38,38,38	0
57	MG	1A	3890	1/1	0.95	0.12	34,34,34,34	0
57	MG	1A	3578	1/1	0.95	0.15	45,45,45,45	0
57	MG	1A	3772	1/1	0.95	0.10	41,41,41,41	0
57	MG	1B	226	1/1	0.95	0.17	32,32,32,32	0
57	MG	2a	3023	1/1	0.95	0.13	50,50,50,50	0
57	MG	1A	3773	1/1	0.95	0.16	23,23,23,23	0
57	MG	2A	3378	1/1	0.95	0.12	40,40,40,40	0
57	MG	1A	3895	1/1	0.95	0.12	27,27,27,27	0
57	MG	1a	1655	1/1	0.95	0.10	61,61,61,61	0
57	MG	1A	3105	1/1	0.95	0.14	30,30,30,30	0
57	MG	1A	3582	1/1	0.95	0.43	42,42,42,42	0
57	MG	1A	3281	1/1	0.95	0.16	25,25,25,25	0
57	MG	2a	3034	1/1	0.95	0.17	63,63,63,63	0
57	MG	1A	3777	1/1	0.95	0.20	43,43,43,43	0
57	MG	2A	3386	1/1	0.95	0.17	43,43,43,43	0
57	MG	2A	3152	1/1	0.95	0.15	41,41,41,41	0
57	MG	1D	314	1/1	0.95	0.13	50,50,50,50	0
57	MG	1A	3780	1/1	0.95	0.21	43,43,43,43	0
57	MG	1A	3489	1/1	0.95	0.16	24,24,24,24	0
57	MG	2A	3392	1/1	0.95	0.12	59,59,59,59	0
57	MG	2a	3043	1/1	0.95	0.29	59,59,59,59	0
57	MG	1A	3283	1/1	0.95	0.15	54,54,54,54	0
57	MG	1A	3674	1/1	0.95	0.55	60,60,60,60	0
57	MG	1a	1665	1/1	0.95	0.20	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3909	1/1	0.95	0.20	44,44,44,44	0
57	MG	1a	1667	1/1	0.95	0.15	62,62,62,62	0
57	MG	1A	3284	1/1	0.95	0.27	49,49,49,49	0
57	MG	1A	3590	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3492	1/1	0.95	0.11	27,27,27,27	0
57	MG	2A	3402	1/1	0.95	0.08	50,50,50,50	0
57	MG	2A	3170	1/1	0.95	0.21	62,62,62,62	0
57	MG	2a	3054	1/1	0.95	0.20	62,62,62,62	0
57	MG	1A	3790	1/1	0.95	0.15	53,53,53,53	0
57	MG	2A	3405	1/1	0.95	0.18	58,58,58,58	0
57	MG	1A	3679	1/1	0.95	0.11	55,55,55,55	0
57	MG	1a	1673	1/1	0.95	0.21	44,44,44,44	0
57	MG	2a	3061	1/1	0.95	0.18	61,61,61,61	0
57	MG	2A	3638	1/1	0.95	0.10	50,50,50,50	0
57	MG	1A	3592	1/1	0.95	0.19	49,49,49,49	0
57	MG	1a	1844	1/1	0.95	0.11	57,57,57,57	0
57	MG	1A	3219	1/1	0.95	0.23	46,46,46,46	0
57	MG	1A	3422	1/1	0.95	0.10	61,61,61,61	0
57	MG	1A	3223	1/1	0.95	0.24	33,33,33,33	0
57	MG	1F	316	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3187	1/1	0.95	0.24	56,56,56,56	0
57	MG	1G	201	1/1	0.95	0.07	58,58,58,58	0
57	MG	1A	3357	1/1	0.95	0.17	26,26,26,26	0
57	MG	1A	3226	1/1	0.95	0.14	29,29,29,29	0
57	MG	1G	204	1/1	0.95	0.15	41,41,41,41	0
57	MG	1A	3083	1/1	0.95	0.28	34,34,34,34	0
57	MG	2A	3424	1/1	0.95	0.18	61,61,61,61	0
57	MG	1A	3927	1/1	0.95	0.13	35,35,35,35	0
57	MG	1a	1860	1/1	0.95	0.15	62,62,62,62	0
57	MG	1A	3799	1/1	0.95	0.17	31,31,31,31	0
57	MG	2A	3660	1/1	0.95	0.15	43,43,43,43	0
57	MG	1A	3433	1/1	0.95	0.20	26,26,26,26	0
57	MG	1a	1864	1/1	0.95	0.18	62,62,62,62	0
57	MG	1A	3362	1/1	0.95	0.14	39,39,39,39	0
57	MG	1A	3145	1/1	0.95	0.14	38,38,38,38	0
57	MG	1P	201	1/1	0.95	0.23	31,31,31,31	0
57	MG	2A	3203	1/1	0.95	0.19	67,67,67,67	0
57	MG	2A	3437	1/1	0.95	0.09	43,43,43,43	0
57	MG	1A	3933	1/1	0.95	0.15	58,58,58,58	0
57	MG	2A	3439	1/1	0.95	0.13	42,42,42,42	0
57	MG	2A	3440	1/1	0.95	0.08	66,66,66,66	0
57	MG	1d	302	1/1	0.95	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3675	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3370	1/1	0.95	0.16	24,24,24,24	0
57	MG	2A	3207	1/1	0.95	0.11	53,53,53,53	0
57	MG	1A	3809	1/1	0.95	0.16	23,23,23,23	0
57	MG	1A	3936	1/1	0.95	0.11	41,41,41,41	0
57	MG	1Q	203	1/1	0.95	0.18	46,46,46,46	0
57	MG	1A	3509	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3232	1/1	0.95	0.15	27,27,27,27	0
57	MG	1A	3234	1/1	0.95	0.14	33,33,33,33	0
57	MG	2A	3215	1/1	0.95	0.15	57,57,57,57	0
57	MG	1A	3814	1/1	0.95	0.06	42,42,42,42	0
57	MG	1A	3815	1/1	0.95	0.19	37,37,37,37	0
57	MG	1A	3816	1/1	0.95	0.15	39,39,39,39	0
57	MG	1A	3700	1/1	0.95	0.16	40,40,40,40	0
57	MG	1A	3946	1/1	0.95	0.08	27,27,27,27	0
57	MG	1T	207	1/1	0.95	0.26	60,60,60,60	0
57	MG	2A	3458	1/1	0.95	0.20	51,51,51,51	0
57	MG	2a	3119	1/1	0.95	0.11	59,59,59,59	0
57	MG	1a	1711	1/1	0.95	0.08	59,59,59,59	0
57	MG	2A	3223	1/1	0.95	0.25	70,70,70,70	0
57	MG	2A	3224	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3947	1/1	0.95	0.13	25,25,25,25	0
57	MG	1U	202	1/1	0.95	0.28	33,33,33,33	0
57	MG	2a	3126	1/1	0.95	0.15	62,62,62,62	0
57	MG	1A	3374	1/1	0.95	0.13	45,45,45,45	0
57	MG	1A	3375	1/1	0.95	0.13	27,27,27,27	0
57	MG	1A	3066	1/1	0.95	0.13	33,33,33,33	0
57	MG	1A	3148	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3112	1/1	0.95	0.30	34,34,34,34	0
57	MG	1a	1720	1/1	0.95	0.13	60,60,60,60	0
57	MG	1A	3523	1/1	0.95	0.20	20,20,20,20	0
57	MG	1A	3828	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	3245	1/1	0.95	0.33	40,40,40,40	0
57	MG	2A	3010	1/1	0.95	0.13	58,58,58,58	0
57	MG	1A	3965	1/1	0.95	0.12	27,27,27,27	0
57	MG	2A	3015	1/1	0.95	0.17	33,33,33,33	0
57	MG	1A	3451	1/1	0.95	0.18	23,23,23,23	0
57	MG	1A	3113	1/1	0.95	0.26	37,37,37,37	0
57	MG	2A	3019	1/1	0.95	0.53	49,49,49,49	0
57	MG	2A	3482	1/1	0.95	0.07	51,51,51,51	0
57	MG	1A	3713	1/1	0.95	0.14	56,56,56,56	0
57	MG	1A	3453	1/1	0.95	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3971	1/1	0.95	0.15	26,26,26,26	0
57	MG	2A	3251	1/1	0.95	0.27	48,48,48,48	0
57	MG	10	104	1/1	0.95	0.09	57,57,57,57	0
57	MG	2A	3026	1/1	0.95	0.10	42,42,42,42	0
57	MG	1a	1735	1/1	0.95	0.07	56,56,56,56	0
57	MG	2A	3726	1/1	0.95	0.12	38,38,38,38	0
57	MG	1a	1736	1/1	0.95	0.11	39,39,39,39	0
57	MG	2a	3155	1/1	0.95	0.17	60,60,60,60	0
57	MG	1A	3835	1/1	0.95	0.18	25,25,25,25	0
57	MG	2A	3729	1/1	0.95	0.13	52,52,52,52	0
57	MG	1A	3114	1/1	0.95	0.20	31,31,31,31	0
57	MG	2A	3036	1/1	0.95	0.11	50,50,50,50	0
57	MG	1A	3115	1/1	0.95	0.12	33,33,33,33	0
57	MG	2A	3038	1/1	0.95	0.15	48,48,48,48	0
57	MG	1A	3194	1/1	0.95	0.09	34,34,34,34	0
57	MG	1a	1744	1/1	0.95	0.07	54,54,54,54	0
57	MG	1A	3720	1/1	0.95	0.20	47,47,47,47	0
57	MG	1A	3843	1/1	0.95	0.18	19,19,19,19	0
57	MG	1A	3319	1/1	0.95	0.16	52,52,52,52	0
57	MG	15	103	1/1	0.95	0.14	30,30,30,30	0
57	MG	2A	3277	1/1	0.95	0.11	29,29,29,29	0
57	MG	2A	3743	1/1	0.95	0.18	62,62,62,62	0
57	MG	2A	3052	1/1	0.95	0.12	41,41,41,41	0
57	MG	1A	3845	1/1	0.95	0.05	55,55,55,55	0
57	MG	1a	1750	1/1	0.95	0.12	49,49,49,49	0
57	MG	1A	3980	1/1	0.95	0.06	65,65,65,65	0
57	MG	2A	3282	1/1	0.95	0.18	68,68,68,68	0
57	MG	15	106	1/1	0.95	0.10	57,57,57,57	0
57	MG	1A	3981	1/1	0.95	0.21	43,43,43,43	0
57	MG	17	103	1/1	0.95	0.12	38,38,38,38	0
57	MG	2A	3061	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3256	1/1	0.95	0.26	67,67,67,67	0
57	MG	1A	3022	1/1	0.95	0.08	38,38,38,38	0
57	MG	2A	3523	1/1	0.95	0.12	63,63,63,63	0
57	MG	1a	1758	1/1	0.95	0.18	59,59,59,59	0
57	MG	1a	1760	1/1	0.95	0.15	60,60,60,60	0
57	MG	1A	3984	1/1	0.95	0.13	24,24,24,24	0
57	MG	2A	3069	1/1	0.95	0.22	57,57,57,57	0
57	MG	1A	3004	1/1	0.95	0.27	45,45,45,45	0
57	MG	1A	3327	1/1	0.95	0.11	56,56,56,56	0
57	MG	1A	3542	1/1	0.95	0.12	37,37,37,37	0
57	MG	1A	3544	1/1	0.95	0.07	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3198	1/1	0.95	0.10	41,41,41,41	0
57	MG	2D	301	1/1	0.95	0.24	38,38,38,38	0
57	MG	2A	3537	1/1	0.95	0.21	53,53,53,53	0
57	MG	2A	3538	1/1	0.95	0.08	48,48,48,48	0
57	MG	1A	3734	1/1	0.95	0.05	50,50,50,50	0
57	MG	1A	3992	1/1	0.95	0.06	47,47,47,47	0
57	MG	2A	3084	1/1	0.95	0.11	46,46,46,46	0
57	MG	1A	3857	1/1	0.95	0.16	34,34,34,34	0
57	MG	1A	3548	1/1	0.95	0.23	34,34,34,34	0
57	MG	2E	304	1/1	0.95	0.14	36,36,36,36	0
57	MG	1a	1771	1/1	0.95	0.13	55,55,55,55	0
57	MG	1A	3365	1/1	0.96	0.16	21,21,21,21	0
57	MG	1A	3910	1/1	0.96	0.23	25,25,25,25	0
57	MG	2A	3527	1/1	0.96	0.11	65,65,65,65	0
57	MG	2A	3528	1/1	0.96	0.08	67,67,67,67	0
57	MG	1B	223	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3367	1/1	0.96	0.15	72,72,72,72	0
57	MG	2A	3088	1/1	0.96	0.12	41,41,41,41	0
57	MG	1a	1788	1/1	0.96	0.08	70,70,70,70	0
57	MG	1A	3368	1/1	0.96	0.18	37,37,37,37	0
57	MG	1A	3914	1/1	0.96	0.11	35,35,35,35	0
57	MG	1A	3688	1/1	0.96	0.10	46,46,46,46	0
57	MG	2A	3093	1/1	0.96	0.20	45,45,45,45	0
57	MG	2E	302	1/1	0.96	0.15	37,37,37,37	0
57	MG	1A	3508	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3305	1/1	0.96	0.40	40,40,40,40	0
57	MG	1A	3371	1/1	0.96	0.19	29,29,29,29	0
57	MG	1A	3601	1/1	0.96	0.18	40,40,40,40	0
57	MG	2A	3542	1/1	0.96	0.14	34,34,34,34	0
57	MG	2A	3543	1/1	0.96	0.16	49,49,49,49	0
57	MG	1A	3259	1/1	0.96	0.16	49,49,49,49	0
57	MG	1D	305	1/1	0.96	0.16	39,39,39,39	0
57	MG	1D	306	1/1	0.96	0.11	52,52,52,52	0
57	MG	1D	307	1/1	0.96	0.14	34,34,34,34	0
57	MG	1D	312	1/1	0.96	0.29	44,44,44,44	0
57	MG	2A	3314	1/1	0.96	0.13	51,51,51,51	0
57	MG	2A	3106	1/1	0.96	0.25	57,57,57,57	0
57	MG	2A	3316	1/1	0.96	0.13	42,42,42,42	0
57	MG	1a	1649	1/1	0.96	0.08	63,63,63,63	0
57	MG	2A	3110	1/1	0.96	0.16	57,57,57,57	0
57	MG	2A	3111	1/1	0.96	0.21	53,53,53,53	0
57	MG	1A	3807	1/1	0.96	0.32	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2R	201	1/1	0.96	0.18	40,40,40,40	0
57	MG	1D	316	1/1	0.96	0.24	49,49,49,49	0
57	MG	1A	3514	1/1	0.96	0.17	34,34,34,34	0
57	MG	2A	3558	1/1	0.96	0.07	61,61,61,61	0
57	MG	1A	3604	1/1	0.96	0.11	56,56,56,56	0
57	MG	1D	320	1/1	0.96	0.20	47,47,47,47	0
57	MG	2V	201	1/1	0.96	0.20	66,66,66,66	0
57	MG	2V	202	1/1	0.96	0.30	49,49,49,49	0
57	MG	2A	3561	1/1	0.96	0.08	44,44,44,44	0
57	MG	2W	202	1/1	0.96	0.22	50,50,50,50	0
57	MG	2A	3562	1/1	0.96	0.10	37,37,37,37	0
57	MG	2A	3117	1/1	0.96	0.27	49,49,49,49	0
57	MG	2A	3333	1/1	0.96	0.10	36,36,36,36	0
57	MG	1A	3218	1/1	0.96	0.20	28,28,28,28	0
57	MG	2A	3566	1/1	0.96	0.08	61,61,61,61	0
57	MG	1E	302	1/1	0.96	0.22	39,39,39,39	0
57	MG	1A	3314	1/1	0.96	0.18	16,16,16,16	0
57	MG	2A	3121	1/1	0.96	0.12	45,45,45,45	0
57	MG	2A	3570	1/1	0.96	0.10	47,47,47,47	0
57	MG	2A	3571	1/1	0.96	0.15	76,76,76,76	0
57	MG	1A	3702	1/1	0.96	0.17	43,43,43,43	0
57	MG	1A	3929	1/1	0.96	0.12	54,54,54,54	0
57	MG	2A	3124	1/1	0.96	0.16	42,42,42,42	0
57	MG	1A	3518	1/1	0.96	0.09	51,51,51,51	0
57	MG	2A	3576	1/1	0.96	0.18	24,24,24,24	0
57	MG	1A	3262	1/1	0.96	0.14	25,25,25,25	0
57	MG	1A	3520	1/1	0.96	0.17	23,23,23,23	0
57	MG	1A	3613	1/1	0.96	0.13	26,26,26,26	0
57	MG	1a	1819	1/1	0.96	0.13	54,54,54,54	0
57	MG	1A	3819	1/1	0.96	0.15	37,37,37,37	0
57	MG	2A	3582	1/1	0.96	0.13	57,57,57,57	0
57	MG	1A	3445	1/1	0.96	0.16	40,40,40,40	0
57	MG	1A	3446	1/1	0.96	0.10	44,44,44,44	0
57	MG	1A	3376	1/1	0.96	0.17	38,38,38,38	0
57	MG	1A	3060	1/1	0.96	0.31	37,37,37,37	0
57	MG	2a	3016	1/1	0.96	0.16	59,59,59,59	0
57	MG	1a	1826	1/1	0.96	0.14	52,52,52,52	0
57	MG	1F	318	1/1	0.96	0.20	46,46,46,46	0
57	MG	1A	3026	1/1	0.96	0.13	30,30,30,30	0
57	MG	1A	3379	1/1	0.96	0.15	39,39,39,39	0
57	MG	1A	3527	1/1	0.96	0.18	20,20,20,20	0
57	MG	1A	3716	1/1	0.96	0.20	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1H	201	1/1	0.96	0.12	53,53,53,53	0
57	MG	1A	3830	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3717	1/1	0.96	0.18	37,37,37,37	0
57	MG	1a	1835	1/1	0.96	0.09	55,55,55,55	0
57	MG	1A	3037	1/1	0.96	0.18	45,45,45,45	0
57	MG	1A	3948	1/1	0.96	0.15	24,24,24,24	0
57	MG	1A	3949	1/1	0.96	0.10	44,44,44,44	0
57	MG	1A	3320	1/1	0.96	0.14	34,34,34,34	0
57	MG	2a	3032	1/1	0.96	0.07	72,72,72,72	0
57	MG	2a	3033	1/1	0.96	0.09	68,68,68,68	0
57	MG	1A	3382	1/1	0.96	0.12	45,45,45,45	0
57	MG	2A	3603	1/1	0.96	0.06	45,45,45,45	0
57	MG	2A	3376	1/1	0.96	0.09	36,36,36,36	0
57	MG	2A	3377	1/1	0.96	0.08	63,63,63,63	0
57	MG	1A	3455	1/1	0.96	0.09	56,56,56,56	0
57	MG	2A	3379	1/1	0.96	0.11	41,41,41,41	0
57	MG	1A	3152	1/1	0.96	0.18	42,42,42,42	0
57	MG	1A	3956	1/1	0.96	0.17	53,53,53,53	0
57	MG	1A	3957	1/1	0.96	0.17	51,51,51,51	0
57	MG	2A	3612	1/1	0.96	0.22	63,63,63,63	0
57	MG	1a	1850	1/1	0.96	0.11	51,51,51,51	0
57	MG	1A	3064	1/1	0.96	0.24	45,45,45,45	0
57	MG	1A	3229	1/1	0.96	0.35	42,42,42,42	0
57	MG	1A	3230	1/1	0.96	0.21	28,28,28,28	0
57	MG	1R	203	1/1	0.96	0.19	32,32,32,32	0
57	MG	1A	3134	1/1	0.96	0.19	26,26,26,26	0
57	MG	2A	3168	1/1	0.96	0.17	45,45,45,45	0
57	MG	1A	3181	1/1	0.96	0.16	38,38,38,38	0
57	MG	1A	3276	1/1	0.96	0.14	40,40,40,40	0
57	MG	2A	3172	1/1	0.96	0.14	64,64,64,64	0
57	MG	2A	3173	1/1	0.96	0.52	74,74,74,74	0
57	MG	1A	3733	1/1	0.96	0.16	35,35,35,35	0
57	MG	1A	3545	1/1	0.96	0.18	47,47,47,47	0
57	MG	1A	3201	1/1	0.96	0.18	40,40,40,40	0
57	MG	2A	3178	1/1	0.96	0.08	52,52,52,52	0
57	MG	1A	3736	1/1	0.96	0.17	37,37,37,37	0
57	MG	1A	3465	1/1	0.96	0.10	49,49,49,49	0
57	MG	1A	3639	1/1	0.96	0.17	34,34,34,34	0
57	MG	2A	3182	1/1	0.96	0.12	45,45,45,45	0
57	MG	1A	3853	1/1	0.96	0.12	28,28,28,28	0
57	MG	1A	3076	1/1	0.96	0.19	29,29,29,29	0
57	MG	2A	3185	1/1	0.96	0.40	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1707	1/1	0.96	0.25	67,67,67,67	0
57	MG	1A	3137	1/1	0.96	0.15	45,45,45,45	0
57	MG	2A	3410	1/1	0.96	0.06	66,66,66,66	0
57	MG	2A	3412	1/1	0.96	0.06	52,52,52,52	0
57	MG	2a	3075	1/1	0.96	0.11	59,59,59,59	0
57	MG	1A	3338	1/1	0.96	0.19	37,37,37,37	0
57	MG	2A	3189	1/1	0.96	0.11	59,59,59,59	0
57	MG	1A	3282	1/1	0.96	0.19	41,41,41,41	0
57	MG	1A	3400	1/1	0.96	0.22	25,25,25,25	0
57	MG	1A	3555	1/1	0.96	0.09	41,41,41,41	0
57	MG	1A	3556	1/1	0.96	0.19	53,53,53,53	0
57	MG	1A	3401	1/1	0.96	0.20	17,17,17,17	0
57	MG	2A	3649	1/1	0.96	0.09	71,71,71,71	0
57	MG	1A	3244	1/1	0.96	0.10	46,46,46,46	0
57	MG	2A	3651	1/1	0.96	0.16	60,60,60,60	0
57	MG	1A	3649	1/1	0.96	0.12	35,35,35,35	0
57	MG	1A	3650	1/1	0.96	0.09	47,47,47,47	0
57	MG	2A	3654	1/1	0.96	0.13	37,37,37,37	0
57	MG	1A	3403	1/1	0.96	0.15	19,19,19,19	0
57	MG	1l	202	1/1	0.96	0.12	67,67,67,67	0
57	MG	1A	3122	1/1	0.96	0.16	55,55,55,55	0
57	MG	2A	3659	1/1	0.96	0.10	45,45,45,45	0
57	MG	10	103	1/1	0.96	0.16	45,45,45,45	0
57	MG	1A	3343	1/1	0.96	0.17	41,41,41,41	0
57	MG	1A	3344	1/1	0.96	0.18	28,28,28,28	0
57	MG	1A	3655	1/1	0.96	0.16	46,46,46,46	0
57	MG	2A	3431	1/1	0.96	0.14	45,45,45,45	0
57	MG	1a	1726	1/1	0.96	0.09	60,60,60,60	0
57	MG	2a	3102	1/1	0.96	0.12	55,55,55,55	0
57	MG	1A	3206	1/1	0.96	0.42	43,43,43,43	0
57	MG	2a	3104	1/1	0.96	0.28	71,71,71,71	0
57	MG	1a	1728	1/1	0.96	0.16	52,52,52,52	0
57	MG	1A	3286	1/1	0.96	0.08	72,72,72,72	0
57	MG	1A	3994	1/1	0.96	0.28	62,62,62,62	0
57	MG	11	103	1/1	0.96	0.13	43,43,43,43	0
57	MG	2A	3671	1/1	0.96	0.10	37,37,37,37	0
57	MG	2a	3111	1/1	0.96	0.12	51,51,51,51	0
57	MG	2A	3004	1/1	0.96	0.17	38,38,38,38	0
57	MG	11	104	1/1	0.96	0.14	48,48,48,48	0
57	MG	2A	3006	1/1	0.96	0.09	48,48,48,48	0
57	MG	11	105	1/1	0.96	0.09	36,36,36,36	0
57	MG	1A	3995	1/1	0.96	0.19	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3679	1/1	0.96	0.11	55,55,55,55	0
57	MG	2A	3681	1/1	0.96	0.11	56,56,56,56	0
57	MG	1A	3997	1/1	0.96	0.12	50,50,50,50	0
57	MG	2A	3683	1/1	0.96	0.11	58,58,58,58	0
57	MG	2A	3012	1/1	0.96	0.19	58,58,58,58	0
57	MG	1A	3998	1/1	0.96	0.07	43,43,43,43	0
57	MG	2a	3124	1/1	0.96	0.11	59,59,59,59	0
57	MG	1A	4000	1/1	0.96	0.08	44,44,44,44	0
57	MG	1a	1740	1/1	0.96	0.15	62,62,62,62	0
57	MG	1A	3567	1/1	0.96	0.09	46,46,46,46	0
57	MG	2a	3128	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3018	1/1	0.96	0.30	36,36,36,36	0
57	MG	1A	3764	1/1	0.96	0.15	27,27,27,27	0
57	MG	1A	3287	1/1	0.96	0.22	31,31,31,31	0
57	MG	2A	3022	1/1	0.96	0.63	49,49,49,49	0
57	MG	17	101	1/1	0.96	0.15	34,34,34,34	0
57	MG	2A	3455	1/1	0.96	0.10	41,41,41,41	0
57	MG	2a	3135	1/1	0.96	0.21	66,66,66,66	0
57	MG	1A	3483	1/1	0.96	0.15	26,26,26,26	0
57	MG	1A	3250	1/1	0.96	0.21	42,42,42,42	0
57	MG	1A	3293	1/1	0.96	0.14	53,53,53,53	0
57	MG	1A	3573	1/1	0.96	0.20	46,46,46,46	0
57	MG	2A	3233	1/1	0.96	0.20	55,55,55,55	0
57	MG	2A	3030	1/1	0.96	0.15	18,18,18,18	0
57	MG	18	102	1/1	0.96	0.18	35,35,35,35	0
57	MG	2A	3236	1/1	0.96	0.10	39,39,39,39	0
57	MG	18	103	1/1	0.96	0.26	39,39,39,39	0
57	MG	1A	3009	1/1	0.96	0.27	30,30,30,30	0
57	MG	1A	3352	1/1	0.96	0.07	18,18,18,18	0
57	MG	1A	3353	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3186	1/1	0.96	0.23	32,32,32,32	0
57	MG	1A	3297	1/1	0.96	0.13	42,42,42,42	0
57	MG	2A	3040	1/1	0.96	0.18	50,50,50,50	0
57	MG	2A	3245	1/1	0.96	0.18	51,51,51,51	0
57	MG	2A	3041	1/1	0.96	0.19	46,46,46,46	0
57	MG	2A	3045	1/1	0.96	0.11	59,59,59,59	0
57	MG	2A	3714	1/1	0.96	0.14	47,47,47,47	0
57	MG	1A	3253	1/1	0.96	0.14	45,45,45,45	0
57	MG	2A	3250	1/1	0.96	0.11	59,59,59,59	0
57	MG	1A	3779	1/1	0.96	0.10	30,30,30,30	0
57	MG	2A	3252	1/1	0.96	0.48	44,44,44,44	0
57	MG	1A	3254	1/1	0.96	0.20	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1B	202	1/1	0.96	0.16	49,49,49,49	0
57	MG	2A	3484	1/1	0.96	0.15	39,39,39,39	0
57	MG	1A	3781	1/1	0.96	0.13	33,33,33,33	0
57	MG	1a	1610	1/1	0.96	0.25	52,52,52,52	0
57	MG	1A	3423	1/1	0.96	0.26	27,27,27,27	0
57	MG	2A	3054	1/1	0.96	0.12	57,57,57,57	0
57	MG	2A	3259	1/1	0.96	0.19	51,51,51,51	0
57	MG	2a	3171	1/1	0.96	0.09	66,66,66,66	0
57	MG	2a	3172	1/1	0.96	0.12	68,68,68,68	0
57	MG	1a	1612	1/1	0.96	0.20	28,28,28,28	0
57	MG	2A	3493	1/1	0.96	0.10	62,62,62,62	0
57	MG	1A	3585	1/1	0.96	0.05	38,38,38,38	0
57	MG	2A	3057	1/1	0.96	0.20	50,50,50,50	0
57	MG	2A	3731	1/1	0.96	0.32	51,51,51,51	0
57	MG	2a	3178	1/1	0.96	0.07	50,50,50,50	0
57	MG	2A	3496	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3587	1/1	0.96	0.12	38,38,38,38	0
57	MG	1a	1615	1/1	0.96	0.09	61,61,61,61	0
57	MG	1A	3163	1/1	0.96	0.18	40,40,40,40	0
57	MG	2A	3268	1/1	0.96	0.17	54,54,54,54	0
57	MG	1B	208	1/1	0.96	0.27	66,66,66,66	0
57	MG	2A	3062	1/1	0.96	0.15	57,57,57,57	0
57	MG	2a	3186	1/1	0.96	0.18	57,57,57,57	0
57	MG	2a	3187	1/1	0.96	0.24	55,55,55,55	0
57	MG	1A	3678	1/1	0.96	0.20	37,37,37,37	0
57	MG	2A	3274	1/1	0.96	0.49	50,50,50,50	0
57	MG	2A	3275	1/1	0.96	0.12	58,58,58,58	0
57	MG	1A	3034	1/1	0.96	0.16	53,53,53,53	0
57	MG	1A	3257	1/1	0.96	0.14	63,63,63,63	0
57	MG	2A	3509	1/1	0.96	0.15	32,32,32,32	0
57	MG	2A	3510	1/1	0.96	0.12	51,51,51,51	0
57	MG	1A	3902	1/1	0.96	0.11	18,18,18,18	0
57	MG	2t	201	1/1	0.96	0.20	40,40,40,40	0
57	MG	2B	202	1/1	0.96	0.13	71,71,71,71	0
57	MG	1A	3501	1/1	0.96	0.12	55,55,55,55	0
57	MG	1B	215	1/1	0.96	0.12	54,54,54,54	0
57	MG	2A	3070	1/1	0.96	0.22	56,56,56,56	0
57	MG	2A	3284	1/1	0.96	0.12	53,53,53,53	0
57	MG	2A	3071	1/1	0.96	0.30	46,46,46,46	0
57	MG	1A	3069	1/1	0.96	0.10	24,24,24,24	0
57	MG	1A	3905	1/1	0.96	0.05	49,49,49,49	0
57	MG	2A	3074	1/1	0.96	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3503	1/1	0.96	0.16	44,44,44,44	0
57	MG	2A	3076	1/1	0.96	0.26	46,46,46,46	0
61	ZN	15	108	1/1	0.96	0.19	43,43,43,43	0
57	MG	1A	3908	1/1	0.96	0.14	19,19,19,19	0
57	MG	1a	1783	1/1	0.96	0.13	45,45,45,45	0
61	ZN	29	501	1/1	0.96	0.12	65,65,65,65	0
57	MG	2A	3171	1/1	0.97	0.16	53,53,53,53	0
57	MG	1A	3561	1/1	0.97	0.18	33,33,33,33	0
57	MG	1l	201	1/1	0.97	0.23	54,54,54,54	0
57	MG	1A	4001	1/1	0.97	0.13	40,40,40,40	0
57	MG	1A	3135	1/1	0.97	0.20	31,31,31,31	0
57	MG	1a	1725	1/1	0.97	0.18	54,54,54,54	0
57	MG	1A	3873	1/1	0.97	0.12	29,29,29,29	0
57	MG	1n	103	1/1	0.97	0.17	62,62,62,62	0
57	MG	1o	101	1/1	0.97	0.13	49,49,49,49	0
57	MG	1o	102	1/1	0.97	0.20	54,54,54,54	0
57	MG	1A	3220	1/1	0.97	0.13	30,30,30,30	0
57	MG	1A	3221	1/1	0.97	0.20	39,39,39,39	0
57	MG	1A	3177	1/1	0.97	0.11	30,30,30,30	0
57	MG	27	101	1/1	0.97	0.18	41,41,41,41	0
57	MG	15	102	1/1	0.97	0.15	27,27,27,27	0
57	MG	1A	3566	1/1	0.97	0.21	47,47,47,47	0
57	MG	1x	102	1/1	0.97	0.10	38,38,38,38	0
57	MG	1a	1732	1/1	0.97	0.14	33,33,33,33	0
57	MG	1A	4008	1/1	0.97	0.17	34,34,34,34	0
57	MG	2A	3190	1/1	0.97	0.09	51,51,51,51	0
57	MG	1A	3766	1/1	0.97	0.08	34,34,34,34	0
57	MG	1A	3484	1/1	0.97	0.19	26,26,26,26	0
57	MG	1A	3568	1/1	0.97	0.15	38,38,38,38	0
57	MG	2A	3609	1/1	0.97	0.12	46,46,46,46	0
57	MG	1A	3485	1/1	0.97	0.20	25,25,25,25	0
57	MG	2A	3007	1/1	0.97	0.14	40,40,40,40	0
57	MG	17	102	1/1	0.97	0.11	31,31,31,31	0
57	MG	1A	3770	1/1	0.97	0.12	25,25,25,25	0
57	MG	2a	3013	1/1	0.97	0.16	50,50,50,50	0
57	MG	1a	1741	1/1	0.97	0.14	36,36,36,36	0
57	MG	2A	3011	1/1	0.97	0.15	36,36,36,36	0
57	MG	1A	3224	1/1	0.97	0.15	33,33,33,33	0
57	MG	1A	3225	1/1	0.97	0.24	37,37,37,37	0
57	MG	1A	3667	1/1	0.97	0.20	24,24,24,24	0
57	MG	1A	3179	1/1	0.97	0.35	38,38,38,38	0
57	MG	1A	3888	1/1	0.97	0.16	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3048	1/1	0.97	0.15	41,41,41,41	0
57	MG	1A	3891	1/1	0.97	0.11	40,40,40,40	0
57	MG	1A	3084	1/1	0.97	0.24	38,38,38,38	0
57	MG	2A	3208	1/1	0.97	0.15	52,52,52,52	0
57	MG	2A	3021	1/1	0.97	0.15	34,34,34,34	0
57	MG	1A	3107	1/1	0.97	0.23	35,35,35,35	0
57	MG	1A	3778	1/1	0.97	0.17	26,26,26,26	0
57	MG	2a	3028	1/1	0.97	0.08	74,74,74,74	0
57	MG	1A	3141	1/1	0.97	0.20	36,36,36,36	0
57	MG	1a	1604	1/1	0.97	0.15	55,55,55,55	0
57	MG	1A	3231	1/1	0.97	0.35	38,38,38,38	0
57	MG	2A	3633	1/1	0.97	0.18	49,49,49,49	0
57	MG	2A	3426	1/1	0.97	0.17	55,55,55,55	0
57	MG	1A	3579	1/1	0.97	0.20	25,25,25,25	0
57	MG	1A	3288	1/1	0.97	0.05	51,51,51,51	0
57	MG	1A	3142	1/1	0.97	0.16	28,28,28,28	0
57	MG	1a	1759	1/1	0.97	0.13	64,64,64,64	0
57	MG	2A	3033	1/1	0.97	0.19	47,47,47,47	0
57	MG	2A	3432	1/1	0.97	0.10	35,35,35,35	0
57	MG	1a	1609	1/1	0.97	0.15	55,55,55,55	0
57	MG	2A	3035	1/1	0.97	0.21	52,52,52,52	0
57	MG	1B	213	1/1	0.97	0.14	36,36,36,36	0
57	MG	1A	3785	1/1	0.97	0.12	44,44,44,44	0
57	MG	1A	3496	1/1	0.97	0.14	53,53,53,53	0
57	MG	1A	3424	1/1	0.97	0.18	42,42,42,42	0
57	MG	1A	3292	1/1	0.97	0.10	34,34,34,34	0
57	MG	1A	3586	1/1	0.97	0.14	56,56,56,56	0
57	MG	2A	3042	1/1	0.97	0.11	25,25,25,25	0
57	MG	2A	3043	1/1	0.97	0.25	68,68,68,68	0
57	MG	1A	3499	1/1	0.97	0.17	39,39,39,39	0
57	MG	1A	3907	1/1	0.97	0.14	26,26,26,26	0
57	MG	1B	221	1/1	0.97	0.12	35,35,35,35	0
57	MG	1A	3057	1/1	0.97	0.18	19,19,19,19	0
57	MG	1a	1620	1/1	0.97	0.12	39,39,39,39	0
57	MG	1A	3427	1/1	0.97	0.19	26,26,26,26	0
57	MG	2a	3057	1/1	0.97	0.09	63,63,63,63	0
57	MG	2A	3051	1/1	0.97	0.11	48,48,48,48	0
57	MG	1A	3428	1/1	0.97	0.20	24,24,24,24	0
57	MG	2A	3238	1/1	0.97	0.40	44,44,44,44	0
57	MG	1A	3911	1/1	0.97	0.31	55,55,55,55	0
57	MG	1A	3430	1/1	0.97	0.21	37,37,37,37	0
57	MG	1A	3359	1/1	0.97	0.12	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3235	1/1	0.97	0.22	34,34,34,34	0
57	MG	1A	3506	1/1	0.97	0.15	22,22,22,22	0
57	MG	1A	3111	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3363	1/1	0.97	0.21	13,13,13,13	0
57	MG	2A	3459	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3187	1/1	0.97	0.14	27,27,27,27	0
57	MG	1A	3041	1/1	0.97	0.41	47,47,47,47	0
57	MG	1A	3802	1/1	0.97	0.17	33,33,33,33	0
57	MG	2a	3074	1/1	0.97	0.21	51,51,51,51	0
57	MG	2A	3673	1/1	0.97	0.15	19,19,19,19	0
57	MG	2A	3249	1/1	0.97	0.27	59,59,59,59	0
57	MG	1A	3803	1/1	0.97	0.12	31,31,31,31	0
57	MG	1D	308	1/1	0.97	0.16	48,48,48,48	0
57	MG	1D	310	1/1	0.97	0.12	41,41,41,41	0
57	MG	2A	3066	1/1	0.97	0.16	50,50,50,50	0
57	MG	1a	1637	1/1	0.97	0.15	73,73,73,73	0
57	MG	1A	3804	1/1	0.97	0.19	51,51,51,51	0
57	MG	2A	3471	1/1	0.97	0.10	61,61,61,61	0
57	MG	1A	3512	1/1	0.97	0.16	28,28,28,28	0
57	MG	1a	1640	1/1	0.97	0.12	68,68,68,68	0
57	MG	1A	3806	1/1	0.97	0.09	50,50,50,50	0
57	MG	2a	3088	1/1	0.97	0.14	55,55,55,55	0
57	MG	1A	3696	1/1	0.97	0.26	43,43,43,43	0
57	MG	1A	3241	1/1	0.97	0.19	33,33,33,33	0
57	MG	1A	3242	1/1	0.97	0.17	35,35,35,35	0
57	MG	1A	3087	1/1	0.97	0.13	37,37,37,37	0
57	MG	1a	1646	1/1	0.97	0.14	41,41,41,41	0
57	MG	2A	3077	1/1	0.97	0.48	66,66,66,66	0
57	MG	1A	3516	1/1	0.97	0.17	19,19,19,19	0
57	MG	2A	3079	1/1	0.97	0.11	49,49,49,49	0
57	MG	2A	3483	1/1	0.97	0.18	53,53,53,53	0
57	MG	2a	3098	1/1	0.97	0.17	54,54,54,54	0
57	MG	2A	3269	1/1	0.97	0.20	27,27,27,27	0
57	MG	1A	3059	1/1	0.97	0.21	37,37,37,37	0
57	MG	1A	3072	1/1	0.97	0.14	37,37,37,37	0
57	MG	1A	3705	1/1	0.97	0.11	55,55,55,55	0
57	MG	2A	3489	1/1	0.97	0.18	28,28,28,28	0
57	MG	1A	3249	1/1	0.97	0.12	42,42,42,42	0
57	MG	1A	3193	1/1	0.97	0.24	60,60,60,60	0
57	MG	2A	3086	1/1	0.97	0.14	39,39,39,39	0
57	MG	2A	3087	1/1	0.97	0.41	47,47,47,47	0
57	MG	1F	302	1/1	0.97	0.14	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3818	1/1	0.97	0.19	23,23,23,23	0
57	MG	1A	3308	1/1	0.97	0.12	38,38,38,38	0
57	MG	1F	307	1/1	0.97	0.18	27,27,27,27	0
57	MG	1F	308	1/1	0.97	0.19	34,34,34,34	0
57	MG	2a	3114	1/1	0.97	0.12	68,68,68,68	0
57	MG	1a	1811	1/1	0.97	0.11	60,60,60,60	0
57	MG	2A	3095	1/1	0.97	0.20	65,65,65,65	0
57	MG	1A	3611	1/1	0.97	0.18	27,27,27,27	0
57	MG	1A	3448	1/1	0.97	0.16	54,54,54,54	0
57	MG	1F	313	1/1	0.97	0.19	32,32,32,32	0
57	MG	1A	3310	1/1	0.97	0.19	35,35,35,35	0
57	MG	2A	3505	1/1	0.97	0.07	61,61,61,61	0
57	MG	2A	3291	1/1	0.97	0.18	51,51,51,51	0
57	MG	1A	3117	1/1	0.97	0.21	30,30,30,30	0
57	MG	1A	3313	1/1	0.97	0.15	34,34,34,34	0
57	MG	2A	3102	1/1	0.97	0.11	39,39,39,39	0
57	MG	1F	317	1/1	0.97	0.40	47,47,47,47	0
57	MG	1A	3042	1/1	0.97	0.20	17,17,17,17	0
57	MG	1A	3827	1/1	0.97	0.14	18,18,18,18	0
57	MG	1A	3091	1/1	0.97	0.13	36,36,36,36	0
57	MG	2A	3107	1/1	0.97	0.17	64,64,64,64	0
57	MG	1A	3013	1/1	0.97	0.15	16,16,16,16	0
57	MG	2A	3109	1/1	0.97	0.15	33,33,33,33	0
57	MG	1A	3157	1/1	0.97	0.13	29,29,29,29	0
57	MG	2A	3303	1/1	0.97	0.21	43,43,43,43	0
57	MG	1A	3621	1/1	0.97	0.22	18,18,18,18	0
57	MG	1A	3530	1/1	0.97	0.16	25,25,25,25	0
57	MG	1A	3383	1/1	0.97	0.13	48,48,48,48	0
57	MG	1A	3955	1/1	0.97	0.06	42,42,42,42	0
57	MG	1A	3532	1/1	0.97	0.12	26,26,26,26	0
57	MG	2A	3524	1/1	0.97	0.17	30,30,30,30	0
57	MG	2A	3736	1/1	0.97	0.21	46,46,46,46	0
57	MG	1A	3457	1/1	0.97	0.11	43,43,43,43	0
57	MG	1A	3046	1/1	0.97	0.17	19,19,19,19	0
57	MG	1A	3837	1/1	0.97	0.15	37,37,37,37	0
57	MG	1A	3961	1/1	0.97	0.11	44,44,44,44	0
57	MG	1P	203	1/1	0.97	0.14	23,23,23,23	0
57	MG	1A	3838	1/1	0.97	0.06	33,33,33,33	0
57	MG	2A	3531	1/1	0.97	0.14	44,44,44,44	0
57	MG	1a	1836	1/1	0.97	0.10	39,39,39,39	0
57	MG	1a	1837	1/1	0.97	0.14	55,55,55,55	0
57	MG	1A	3839	1/1	0.97	0.15	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3124	1/1	0.97	0.15	34,34,34,34	0
57	MG	2A	3126	1/1	0.97	0.12	40,40,40,40	0
57	MG	2A	3127	1/1	0.97	0.15	55,55,55,55	0
57	MG	2A	3321	1/1	0.97	0.14	37,37,37,37	0
57	MG	1A	3966	1/1	0.97	0.09	37,37,37,37	0
57	MG	1A	3727	1/1	0.97	0.09	35,35,35,35	0
57	MG	1A	3321	1/1	0.97	0.20	26,26,26,26	0
57	MG	2A	3329	1/1	0.97	0.21	47,47,47,47	0
57	MG	1a	1843	1/1	0.97	0.17	49,49,49,49	0
57	MG	1A	3054	1/1	0.97	0.14	34,34,34,34	0
57	MG	2a	3164	1/1	0.97	0.15	63,63,63,63	0
57	MG	1A	3162	1/1	0.97	0.16	27,27,27,27	0
57	MG	1A	3631	1/1	0.97	0.20	33,33,33,33	0
57	MG	2A	3335	1/1	0.97	0.11	41,41,41,41	0
57	MG	2A	3336	1/1	0.97	0.09	33,33,33,33	0
57	MG	1a	1847	1/1	0.97	0.19	59,59,59,59	0
57	MG	1A	3540	1/1	0.97	0.12	23,23,23,23	0
57	MG	1a	1694	1/1	0.97	0.28	68,68,68,68	0
57	MG	1a	1695	1/1	0.97	0.12	55,55,55,55	0
57	MG	1A	3847	1/1	0.97	0.10	46,46,46,46	0
57	MG	1A	3541	1/1	0.97	0.12	28,28,28,28	0
57	MG	1a	1854	1/1	0.97	0.10	60,60,60,60	0
57	MG	1A	3079	1/1	0.97	0.18	41,41,41,41	0
57	MG	1A	3543	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	3261	1/1	0.97	0.19	36,36,36,36	0
57	MG	1A	3065	1/1	0.97	0.17	52,52,52,52	0
57	MG	1A	3263	1/1	0.97	0.07	47,47,47,47	0
57	MG	2E	301	1/1	0.97	0.18	38,38,38,38	0
57	MG	1A	3099	1/1	0.97	0.23	28,28,28,28	0
57	MG	2A	3353	1/1	0.97	0.09	52,52,52,52	0
57	MG	1A	3549	1/1	0.97	0.18	44,44,44,44	0
57	MG	1A	3856	1/1	0.97	0.12	35,35,35,35	0
57	MG	1A	3331	1/1	0.97	0.17	23,23,23,23	0
57	MG	2E	307	1/1	0.97	0.15	33,33,33,33	0
57	MG	2A	3358	1/1	0.97	0.14	39,39,39,39	0
57	MG	1A	3744	1/1	0.97	0.19	54,54,54,54	0
57	MG	1A	3745	1/1	0.97	0.14	50,50,50,50	0
57	MG	2F	304	1/1	0.97	0.34	45,45,45,45	0
57	MG	1A	3209	1/1	0.97	0.19	36,36,36,36	0
57	MG	1A	3470	1/1	0.97	0.12	31,31,31,31	0
57	MG	1A	3166	1/1	0.97	0.18	27,27,27,27	0
57	MG	2A	3157	1/1	0.97	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3158	1/1	0.97	0.29	55,55,55,55	0
58	CLM	1A	4017	20/20	0.97	0.18	18,23,33,39	0
57	MG	2O	201	1/1	0.97	0.10	62,62,62,62	0
57	MG	1A	3335	1/1	0.97	0.18	23,23,23,23	0
57	MG	2A	3160	1/1	0.97	0.11	49,49,49,49	0
57	MG	1A	3100	1/1	0.97	0.09	46,46,46,46	0
57	MG	1A	3474	1/1	0.97	0.13	52,52,52,52	0
57	MG	1A	3132	1/1	0.97	0.29	40,40,40,40	0
57	MG	1A	3055	1/1	0.97	0.20	43,43,43,43	0
57	MG	2A	3166	1/1	0.97	0.15	49,49,49,49	0
57	MG	1A	3406	1/1	0.97	0.11	58,58,58,58	0
57	MG	2A	3375	1/1	0.97	0.11	35,35,35,35	0
57	MG	2T	202	1/1	0.97	0.12	60,60,60,60	0
57	MG	1A	3102	1/1	0.97	0.21	29,29,29,29	0
57	MG	1A	3757	1/1	0.97	0.13	37,37,37,37	0
57	MG	1A	3999	1/1	0.97	0.14	63,63,63,63	0
57	MG	1A	3001	1/1	0.98	0.17	29,29,29,29	0
57	MG	1A	3279	1/1	0.98	0.11	23,23,23,23	0
57	MG	1A	3399	1/1	0.98	0.16	18,18,18,18	0
57	MG	1a	1682	1/1	0.98	0.13	42,42,42,42	0
57	MG	1A	3337	1/1	0.98	0.21	13,13,13,13	0
57	MG	2a	3058	1/1	0.98	0.15	45,45,45,45	0
57	MG	1a	1684	1/1	0.98	0.17	44,44,44,44	0
57	MG	1A	3280	1/1	0.98	0.22	33,33,33,33	0
57	MG	1A	3138	1/1	0.98	0.18	42,42,42,42	0
57	MG	2A	3161	1/1	0.98	0.15	46,46,46,46	0
57	MG	1A	3761	1/1	0.98	0.15	47,47,47,47	0
57	MG	1a	1805	1/1	0.98	0.09	59,59,59,59	0
57	MG	1A	3236	1/1	0.98	0.32	27,27,27,27	0
57	MG	1a	1807	1/1	0.98	0.10	45,45,45,45	0
57	MG	2a	3067	1/1	0.98	0.15	69,69,69,69	0
57	MG	1A	3237	1/1	0.98	0.13	28,28,28,28	0
57	MG	1A	3405	1/1	0.98	0.18	24,24,24,24	0
57	MG	1A	3116	1/1	0.98	0.18	31,31,31,31	0
57	MG	1a	1692	1/1	0.98	0.15	55,55,55,55	0
57	MG	1A	3017	1/1	0.98	0.10	31,31,31,31	0
57	MG	2A	3590	1/1	0.98	0.18	31,31,31,31	0
57	MG	2A	3044	1/1	0.98	0.17	44,44,44,44	0
57	MG	13	101	1/1	0.98	0.17	31,31,31,31	0
57	MG	1A	3408	1/1	0.98	0.17	25,25,25,25	0
57	MG	13	103	1/1	0.98	0.12	40,40,40,40	0
57	MG	1A	3610	1/1	0.98	0.24	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3176	1/1	0.98	0.17	42,42,42,42	0
57	MG	1A	3119	1/1	0.98	0.22	29,29,29,29	0
57	MG	1A	3612	1/1	0.98	0.20	32,32,32,32	0
57	MG	2a	3082	1/1	0.98	0.29	61,61,61,61	0
57	MG	1A	3687	1/1	0.98	0.18	32,32,32,32	0
57	MG	1a	1820	1/1	0.98	0.12	57,57,57,57	0
57	MG	1A	3476	1/1	0.98	0.15	41,41,41,41	0
57	MG	1A	3950	1/1	0.98	0.15	35,35,35,35	0
57	MG	1A	3047	1/1	0.98	0.12	43,43,43,43	0
57	MG	1A	3170	1/1	0.98	0.18	34,34,34,34	0
57	MG	1A	3243	1/1	0.98	0.18	28,28,28,28	0
57	MG	1D	304	1/1	0.98	0.10	38,38,38,38	0
57	MG	1A	3546	1/1	0.98	0.12	31,31,31,31	0
57	MG	1A	3291	1/1	0.98	0.20	16,16,16,16	0
57	MG	1A	3203	1/1	0.98	0.26	42,42,42,42	0
57	MG	1A	3351	1/1	0.98	0.15	51,51,51,51	0
57	MG	1A	3697	1/1	0.98	0.13	63,63,63,63	0
57	MG	2A	3323	1/1	0.98	0.21	18,18,18,18	0
57	MG	2A	3324	1/1	0.98	0.14	36,36,36,36	0
57	MG	2A	3614	1/1	0.98	0.11	50,50,50,50	0
57	MG	2A	3325	1/1	0.98	0.12	40,40,40,40	0
57	MG	2A	3326	1/1	0.98	0.08	36,36,36,36	0
57	MG	2D	302	1/1	0.98	0.49	44,44,44,44	0
57	MG	1A	3959	1/1	0.98	0.08	41,41,41,41	0
57	MG	1D	313	1/1	0.98	0.19	29,29,29,29	0
57	MG	1A	3172	1/1	0.98	0.16	23,23,23,23	0
57	MG	1D	315	1/1	0.98	0.16	39,39,39,39	0
57	MG	1A	3699	1/1	0.98	0.18	39,39,39,39	0
57	MG	2A	3332	1/1	0.98	0.13	54,54,54,54	0
57	MG	2a	3108	1/1	0.98	0.28	63,63,63,63	0
57	MG	1A	3783	1/1	0.98	0.15	40,40,40,40	0
57	MG	1a	1718	1/1	0.98	0.29	62,62,62,62	0
57	MG	1A	3173	1/1	0.98	0.13	23,23,23,23	0
57	MG	1A	3964	1/1	0.98	0.10	46,46,46,46	0
57	MG	1A	3295	1/1	0.98	0.20	31,31,31,31	0
57	MG	2A	3628	1/1	0.98	0.10	21,21,21,21	0
57	MG	1E	301	1/1	0.98	0.12	25,25,25,25	0
57	MG	2E	308	1/1	0.98	0.14	54,54,54,54	0
57	MG	1A	3247	1/1	0.98	0.18	40,40,40,40	0
57	MG	2A	3485	1/1	0.98	0.14	48,48,48,48	0
57	MG	1E	303	1/1	0.98	0.17	31,31,31,31	0
57	MG	1A	3248	1/1	0.98	0.12	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3342	1/1	0.98	0.16	42,42,42,42	0
57	MG	1A	3036	1/1	0.98	0.18	24,24,24,24	0
57	MG	1A	3175	1/1	0.98	0.14	28,28,28,28	0
57	MG	2A	3080	1/1	0.98	0.36	54,54,54,54	0
57	MG	1A	3300	1/1	0.98	0.19	30,30,30,30	0
57	MG	1a	1849	1/1	0.98	0.13	55,55,55,55	0
57	MG	2A	3349	1/1	0.98	0.15	47,47,47,47	0
57	MG	1A	3208	1/1	0.98	0.19	33,33,33,33	0
57	MG	1A	3877	1/1	0.98	0.15	25,25,25,25	0
57	MG	1F	303	1/1	0.98	0.21	25,25,25,25	0
57	MG	1A	3146	1/1	0.98	0.17	29,29,29,29	0
57	MG	2A	3354	1/1	0.98	0.18	46,46,46,46	0
57	MG	1A	3210	1/1	0.98	0.37	32,32,32,32	0
57	MG	1A	3632	1/1	0.98	0.16	21,21,21,21	0
57	MG	1A	3711	1/1	0.98	0.14	27,27,27,27	0
57	MG	1F	309	1/1	0.98	0.19	36,36,36,36	0
57	MG	1a	1737	1/1	0.98	0.15	57,57,57,57	0
57	MG	1a	1859	1/1	0.98	0.10	73,73,73,73	0
57	MG	1F	310	1/1	0.98	0.16	31,31,31,31	0
57	MG	1A	3003	1/1	0.98	0.15	21,21,21,21	0
57	MG	1A	3634	1/1	0.98	0.13	37,37,37,37	0
57	MG	1A	3073	1/1	0.98	0.15	37,37,37,37	0
57	MG	2W	201	1/1	0.98	0.28	49,49,49,49	0
57	MG	1A	3214	1/1	0.98	0.16	18,18,18,18	0
57	MG	2W	203	1/1	0.98	0.12	54,54,54,54	0
57	MG	1A	3307	1/1	0.98	0.18	26,26,26,26	0
57	MG	1A	3369	1/1	0.98	0.15	26,26,26,26	0
57	MG	1A	3215	1/1	0.98	0.17	25,25,25,25	0
57	MG	1A	3889	1/1	0.98	0.17	33,33,33,33	0
57	MG	1A	3149	1/1	0.98	0.26	30,30,30,30	0
57	MG	1A	3986	1/1	0.98	0.18	38,38,38,38	0
57	MG	1A	3103	1/1	0.98	0.20	26,26,26,26	0
57	MG	1A	3312	1/1	0.98	0.19	30,30,30,30	0
57	MG	1A	3104	1/1	0.98	0.18	34,34,34,34	0
57	MG	1A	3006	1/1	0.98	0.14	21,21,21,21	0
57	MG	1A	3724	1/1	0.98	0.11	31,31,31,31	0
57	MG	1A	3441	1/1	0.98	0.15	30,30,30,30	0
57	MG	2a	3159	1/1	0.98	0.11	60,60,60,60	0
57	MG	1A	3810	1/1	0.98	0.09	42,42,42,42	0
57	MG	1A	3153	1/1	0.98	0.43	36,36,36,36	0
57	MG	2A	3672	1/1	0.98	0.14	33,33,33,33	0
57	MG	1A	3443	1/1	0.98	0.19	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3996	1/1	0.98	0.18	15,15,15,15	0
57	MG	1A	3900	1/1	0.98	0.10	54,54,54,54	0
57	MG	1A	3575	1/1	0.98	0.17	53,53,53,53	0
57	MG	1A	3062	1/1	0.98	0.16	26,26,26,26	0
57	MG	2a	3168	1/1	0.98	0.13	55,55,55,55	0
57	MG	1A	3730	1/1	0.98	0.20	24,24,24,24	0
57	MG	1A	3731	1/1	0.98	0.15	49,49,49,49	0
57	MG	1A	3222	1/1	0.98	0.15	40,40,40,40	0
57	MG	2A	3389	1/1	0.98	0.21	32,32,32,32	0
57	MG	1A	3510	1/1	0.98	0.20	16,16,16,16	0
57	MG	1A	3265	1/1	0.98	0.18	39,39,39,39	0
57	MG	2A	3685	1/1	0.98	0.11	34,34,34,34	0
57	MG	1A	3266	1/1	0.98	0.12	23,23,23,23	0
57	MG	1A	3267	1/1	0.98	0.21	30,30,30,30	0
57	MG	1A	3007	1/1	0.98	0.22	29,29,29,29	0
57	MG	1A	3023	1/1	0.98	0.21	32,32,32,32	0
57	MG	1A	3824	1/1	0.98	0.15	12,12,12,12	0
57	MG	1a	1773	1/1	0.98	0.15	58,58,58,58	0
57	MG	1T	204	1/1	0.98	0.12	53,53,53,53	0
57	MG	2A	3399	1/1	0.98	0.11	36,36,36,36	0
57	MG	1A	3324	1/1	0.98	0.16	22,22,22,22	0
57	MG	1A	3658	1/1	0.98	0.14	34,34,34,34	0
57	MG	1A	3385	1/1	0.98	0.20	35,35,35,35	0
57	MG	1A	3188	1/1	0.98	0.06	41,41,41,41	0
57	MG	1A	3326	1/1	0.98	0.20	34,34,34,34	0
57	MG	1A	3388	1/1	0.98	0.20	21,21,21,21	0
57	MG	1U	204	1/1	0.98	0.23	33,33,33,33	0
57	MG	2A	3407	1/1	0.98	0.11	49,49,49,49	0
57	MG	1A	3131	1/1	0.98	0.17	25,25,25,25	0
57	MG	1V	203	1/1	0.98	0.11	42,42,42,42	0
57	MG	2A	3266	1/1	0.98	0.24	39,39,39,39	0
57	MG	2A	3411	1/1	0.98	0.11	61,61,61,61	0
57	MG	2a	3036	1/1	0.98	0.12	43,43,43,43	0
57	MG	2A	3267	1/1	0.98	0.10	37,37,37,37	0
57	MG	1A	3109	1/1	0.98	0.21	31,31,31,31	0
57	MG	2A	3013	1/1	0.98	0.14	23,23,23,23	0
57	MG	2A	3270	1/1	0.98	0.32	44,44,44,44	0
57	MG	1A	3092	1/1	0.98	0.16	28,28,28,28	0
57	MG	1A	3922	1/1	0.98	0.07	52,52,52,52	0
57	MG	1V	207	1/1	0.98	0.10	52,52,52,52	0
57	MG	1A	3593	1/1	0.98	0.19	19,19,19,19	0
57	MG	1A	3749	1/1	0.98	0.08	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3925	1/1	0.98	0.10	49,49,49,49	0
57	MG	1A	3024	1/1	0.98	0.18	15,15,15,15	0
61	ZN	1Y	203	1/1	0.98	0.19	56,56,56,56	0
57	MG	1A	3080	1/1	0.98	0.21	26,26,26,26	0
57	MG	1a	1676	1/1	0.98	0.33	46,46,46,46	0
61	ZN	19	104	1/1	0.98	0.20	40,40,40,40	0
61	ZN	1n	104	1/1	0.98	0.13	63,63,63,63	0
57	MG	1A	3025	1/1	0.98	0.17	33,33,33,33	0
57	MG	1A	3195	1/1	0.98	0.11	33,33,33,33	0
61	ZN	25	104	1/1	0.98	0.20	56,56,56,56	0
61	ZN	26	501	1/1	0.98	0.18	57,57,57,57	0
57	MG	2A	3283	1/1	0.98	0.14	37,37,37,37	0
61	ZN	2n	501	1/1	0.98	0.07	86,86,86,86	0
62	SF4	1d	305	8/8	0.98	0.11	59,64,67,72	0
57	MG	1A	3538	1/1	0.99	0.14	27,27,27,27	0
57	MG	1T	203	1/1	0.99	0.15	48,48,48,48	0
57	MG	1F	304	1/1	0.99	0.15	35,35,35,35	0
57	MG	1A	3334	1/1	0.99	0.15	24,24,24,24	0
57	MG	1A	3128	1/1	0.99	0.14	36,36,36,36	0
57	MG	1A	3940	1/1	0.99	0.21	41,41,41,41	0
57	MG	2A	3680	1/1	0.99	0.09	35,35,35,35	0
57	MG	1A	3118	1/1	0.99	0.18	19,19,19,19	0
57	MG	1A	3212	1/1	0.99	0.24	28,28,28,28	0
57	MG	1A	3093	1/1	0.99	0.16	13,13,13,13	0
57	MG	1A	3689	1/1	0.99	0.06	37,37,37,37	0
57	MG	1U	205	1/1	0.99	0.18	26,26,26,26	0
57	MG	2A	3276	1/1	0.99	0.25	40,40,40,40	0
57	MG	1A	3945	1/1	0.99	0.13	21,21,21,21	0
57	MG	1V	201	1/1	0.99	0.22	25,25,25,25	0
57	MG	1V	202	1/1	0.99	0.20	26,26,26,26	0
57	MG	1D	302	1/1	0.99	0.20	33,33,33,33	0
57	MG	1A	3318	1/1	0.99	0.15	36,36,36,36	0
57	MG	1a	1752	1/1	0.99	0.14	37,37,37,37	0
57	MG	1A	3660	1/1	0.99	0.19	20,20,20,20	0
57	MG	1A	3143	1/1	0.99	0.16	22,22,22,22	0
57	MG	1A	3341	1/1	0.99	0.20	22,22,22,22	0
57	MG	1A	3110	1/1	0.99	0.15	21,21,21,21	0
57	MG	2A	3343	1/1	0.99	0.17	21,21,21,21	0
57	MG	1A	3439	1/1	0.99	0.17	12,12,12,12	0
57	MG	1D	309	1/1	0.99	0.14	16,16,16,16	0
57	MG	1A	3366	1/1	0.99	0.14	18,18,18,18	0
57	MG	1D	311	1/1	0.99	0.16	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1861	1/1	0.99	0.20	52,52,52,52	0
57	MG	1A	3051	1/1	0.99	0.10	30,30,30,30	0
57	MG	1A	3760	1/1	0.99	0.15	33,33,33,33	0
57	MG	1A	3233	1/1	0.99	0.14	32,32,32,32	0
57	MG	2A	3468	1/1	0.99	0.14	32,32,32,32	0
57	MG	1A	3580	1/1	0.99	0.25	26,26,26,26	0
57	MG	1A	3171	1/1	0.99	0.14	35,35,35,35	0
57	MG	1D	317	1/1	0.99	0.23	32,32,32,32	0
57	MG	1A	3417	1/1	0.99	0.19	24,24,24,24	0
57	MG	1A	3158	1/1	0.99	0.46	41,41,41,41	0
57	MG	1A	3067	1/1	0.99	0.26	32,32,32,32	0
57	MG	2A	3028	1/1	0.99	0.08	27,27,27,27	0
57	MG	2A	3029	1/1	0.99	0.13	29,29,29,29	0
57	MG	1A	3395	1/1	0.99	0.18	24,24,24,24	0
57	MG	2A	3655	1/1	0.99	0.17	35,35,35,35	0
57	MG	1a	1623	1/1	0.99	0.12	47,47,47,47	0
57	MG	2a	3140	1/1	0.99	0.13	51,51,51,51	0
57	MG	1A	3043	1/1	0.99	0.15	24,24,24,24	0
57	MG	11	102	1/1	0.99	0.11	34,34,34,34	0
57	MG	1A	3044	1/1	0.99	0.13	20,20,20,20	0
57	MG	1Q	201	1/1	0.99	0.15	36,36,36,36	0
57	MG	1A	3290	1/1	0.99	0.20	20,20,20,20	0
57	MG	1A	3309	1/1	0.99	0.19	19,19,19,19	0
57	MG	1A	3019	1/1	0.99	0.25	28,28,28,28	0
57	MG	1A	3018	1/1	0.99	0.18	27,27,27,27	0
61	ZN	16	501	1/1	0.99	0.21	39,39,39,39	0
57	MG	1R	201	1/1	0.99	0.14	32,32,32,32	0
57	MG	2A	3371	1/1	0.99	0.20	34,34,34,34	0
57	MG	2A	3094	1/1	0.99	0.13	48,48,48,48	0
57	MG	1R	202	1/1	0.99	0.15	34,34,34,34	0
57	MG	2A	3150	1/1	0.99	0.16	50,50,50,50	0
57	MG	1A	3178	1/1	0.99	0.17	29,29,29,29	0
57	MG	1A	3078	1/1	0.99	0.26	32,32,32,32	0
57	MG	1F	301	1/1	0.99	0.14	23,23,23,23	0
57	MG	1A	3429	1/1	0.99	0.19	13,13,13,13	0
62	SF4	2d	501	8/8	0.99	0.11	63,75,82,85	0
57	MG	1A	3360	1/1	1.00	0.14	20,20,20,20	0
57	MG	1A	3140	1/1	1.00	0.15	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.