Full wwPDB X-ray Structure Validation Report (i)

Mar 11, 2024 – 04:49 PM EDT

PDB ID	:	7RQD
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with protein Y, A-site deacylated tRNA analog CACCA, P-site MTI-tripeptidyl-tRNA analog ACCA-ITM, and chloramphenicol at 2.50A resolution
Authors	:	Syroegin, E.A.; Flemmich, L.; Klepacki, D.; Vazquez-Laslop, N.; Micura, R.; Polikanov, Y.S.
Deposited on	:	2021-08-06
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

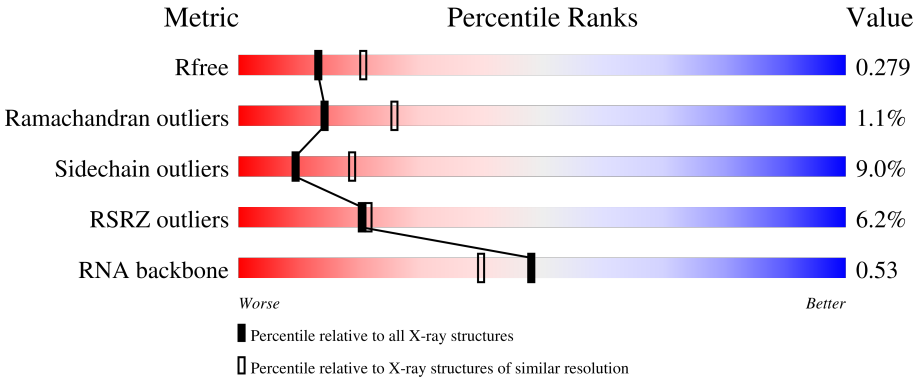
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.50 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	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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% 16%
1	2A	2915	3% 80% 18%
2	1B	121	91% 8%
2	2B	121	86% 13%
3	1D	276	% 95% 5%

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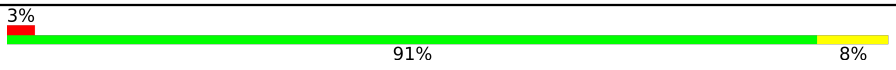
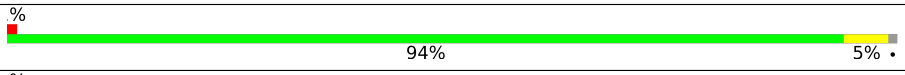
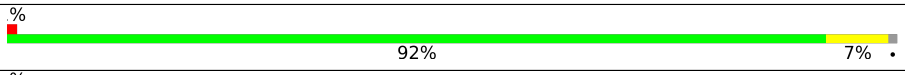
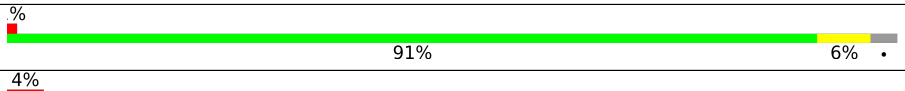
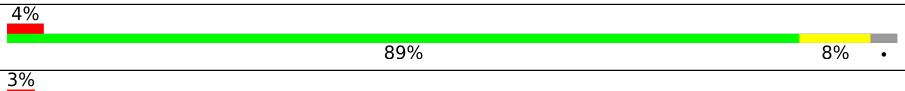
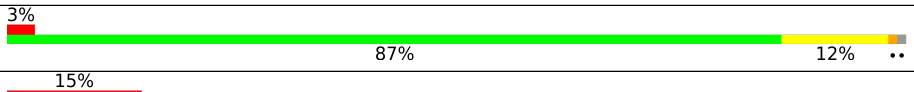
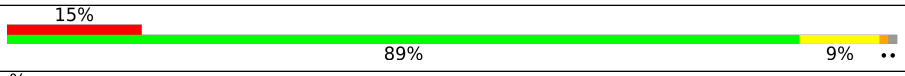
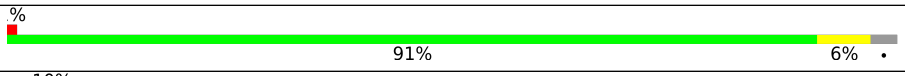
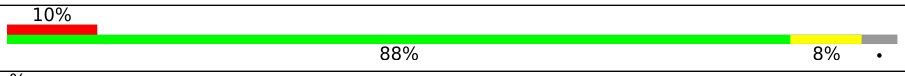
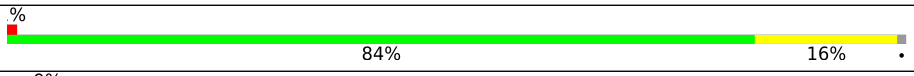
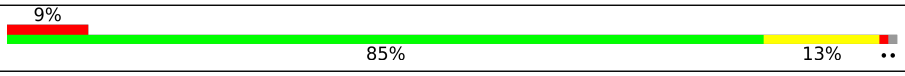
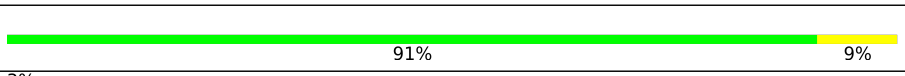
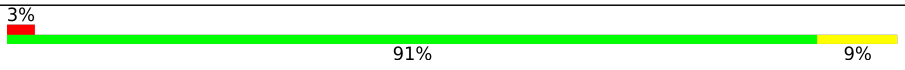
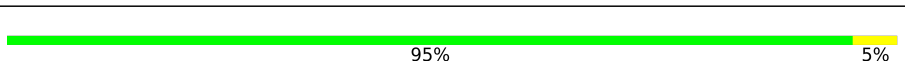
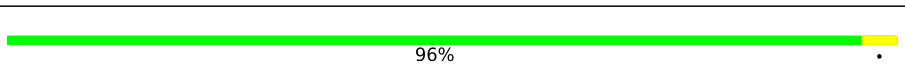
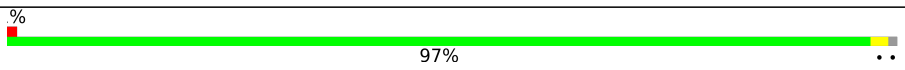
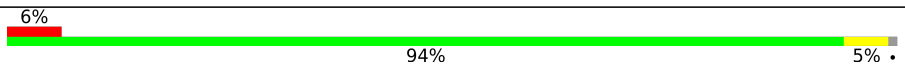
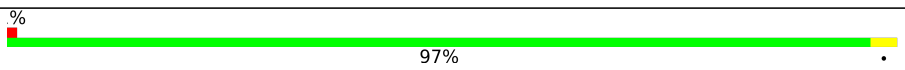
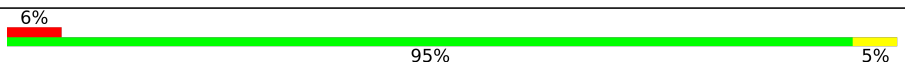
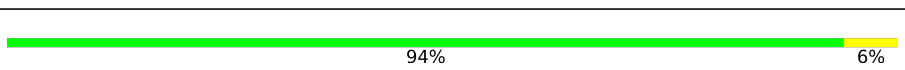
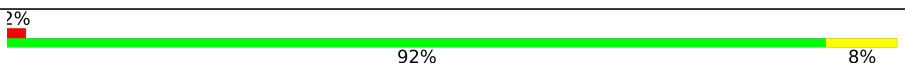
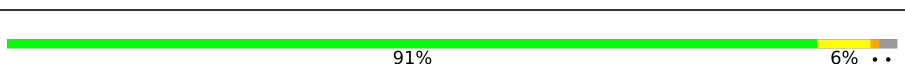
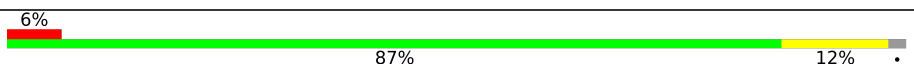
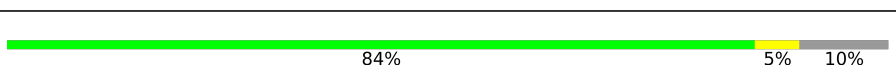
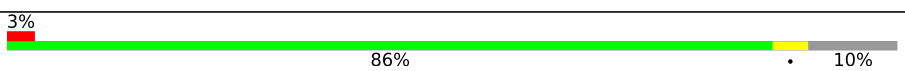
Mol	Chain	Length	Quality of chain
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	
15	2T	146	

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Mol	Chain	Length	Quality of chain
16	1U	118	95%
16	2U	118	5% 92% 7%
17	1V	101	98%
17	2V	101	88% 11%
18	1W	113	94% 5%
18	2W	113	94% 5%
19	1X	96	3% 92% 7%
19	2X	96	7% 97%
20	1Y	110	92% 5%
20	2Y	110	5% 91% 6%
21	1Z	206	90% 8%
21	2Z	206	89% 9%
22	10	85	8% 93% 5%
22	20	85	14% 96%
23	11	98	4% 95%
23	21	98	7% 93% 6%
24	12	72	90% 7%
24	22	72	86% 11%
25	13	60	90% 8%
25	23	60	12% 95%
26	14	71	8% 83% 14%
26	24	71	25% 69% 27%
27	15	60	93% 5%
27	25	60	93% 5%
28	16	54	83% 15%

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Mol	Chain	Length	Quality of chain
28	26	54	4% 87% 11%
29	17	49	4% 90% 8%
29	27	49	4% 84% 14%
30	18	65	2% 89% 9%
30	28	65	11% 86% 12%
31	19	37	97%
31	29	37	5% 95% 5%
32	1a	1521	2% 80% 18%
32	2a	1521	4% 79% 19%
33	1b	256	11% 77% 12% 10%
33	2b	256	17% 78% 11% 10%
34	1c	239	15% 83% 14%
34	2c	239	24% 74% 11% 14%
35	1d	209	11% 89% 10%
35	2d	209	11% 91% 9%
36	1e	162	7% 85% 7% 9%
36	2e	162	9% 85% 6% 9%
37	1f	101	2% 89% 10%
37	2f	101	% 94% 5%
38	1g	156	4% 92% 8%
38	2g	156	18% 90% 9%
39	1h	138	6% 92% 7%
39	2h	138	7% 92% 7%
40	1i	128	30% 87% 12%
40	2i	128	66% 90% 8%

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Mol	Chain	Length	Quality of chain
41	1j	105	16% 81% 11% 8%
41	2j	105	43% 82% 10% 9%
42	1k	129	% 84% 5% 12%
42	2k	129	11% 80% 9% 12%
43	1l	132	5% 86% 7% 8%
43	2l	132	6% 86% 6% 8%
44	1m	126	9% 84% 8% 8%
44	2m	126	14% 75% 15% 10%
45	1n	61	26% 85% 13%
45	2n	61	66% 89% 10%
46	1o	89	3% 92% 7%
46	2o	89	3% 90% 9%
47	1p	88	17% 80% 14% 7%
47	2p	88	8% 84% 9% 7%
48	1q	105	6% 87% 8% 6%
48	2q	105	11% 90% 6%
49	1r	88	% 67% 10% 23%
49	2r	88	2% 70% 7% 23%
50	1s	93	2% 84% 5% 11%
50	2s	93	19% 84% 5% 11%
51	1t	106	9% 82% 8% 9%
51	2t	106	5% 88% 8%
52	1u	27	30% 81% 15%
52	2u	27	44% 85% 15%
53	1y	113	4% 81% 14%

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Mol	Chain	Length	Quality of chain
53	2y	113	73% 75% 9% 15%
54	1w	5	80% 20%
54	2w	5	60% 20% 20%
55	1x	4	50% 75% 25%
55	2x	4	75% 75% 25%
56	1v	3	100% 67% 33%
56	2v	3	100% 67% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1A	3002	-	-	-	X
57	MG	1A	3194	-	-	-	X
57	MG	1A	3697	-	-	-	X
57	MG	1A	3821	-	-	-	X

2 Entry composition (i)

There are 63 unique types of molecules in this entry. The entry contains 297633 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
			23	15	3	4	1			
56	2v	3	Total	C	N	O	S	0	0	0
			23	15	3	4	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1021	Total	Mg	0	0
			1021	1021		
57	1B	31	Total	Mg	0	0
			31	31		
57	1D	18	Total	Mg	0	0
			18	18		
57	1E	9	Total	Mg	0	0
			9	9		
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	5	Total Mg 5 5	0	0
57	1O	1	Total Mg 1 1	0	0
57	1P	4	Total Mg 4 4	0	0
57	1Q	4	Total Mg 4 4	0	0
57	1R	3	Total Mg 3 3	0	0
57	1T	6	Total Mg 6 6	0	0
57	1U	7	Total Mg 7 7	0	0
57	1V	6	Total Mg 6 6	0	0
57	1W	5	Total Mg 5 5	0	0
57	1X	1	Total Mg 1 1	0	0
57	1Y	1	Total Mg 1 1	0	0
57	1Z	1	Total Mg 1 1	0	0
57	10	8	Total Mg 8 8	0	0
57	11	5	Total Mg 5 5	0	0
57	13	3	Total Mg 3 3	0	0
57	15	10	Total Mg 10 10	0	0
57	17	5	Total Mg 5 5	0	0
57	18	2	Total Mg 2 2	0	0
57	19	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1a	270	Total Mg 270 270	0	0
57	1b	1	Total Mg 1 1	0	0
57	1d	5	Total Mg 5 5	0	0
57	1e	1	Total Mg 1 1	0	0
57	1f	2	Total Mg 2 2	0	0
57	1g	3	Total Mg 3 3	0	0
57	1h	2	Total Mg 2 2	0	0
57	1i	2	Total Mg 2 2	0	0
57	1l	2	Total Mg 2 2	0	0
57	1m	2	Total Mg 2 2	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	3	Total Mg 3 3	0	0
57	2A	726	Total Mg 726 726	0	0
57	2B	17	Total Mg 17 17	0	0
57	2D	9	Total Mg 9 9	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
57	2I	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	2	Total Mg 2 2	0	0
57	2Y	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	21	3	Total Mg 3 3	0	0
57	23	1	Total Mg 1 1	0	0
57	25	4	Total Mg 4 4	0	0
57	27	3	Total Mg 3 3	0	0
57	28	3	Total Mg 3 3	0	0
57	29	1	Total Mg 1 1	0	0
57	2a	189	Total Mg 189 189	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0

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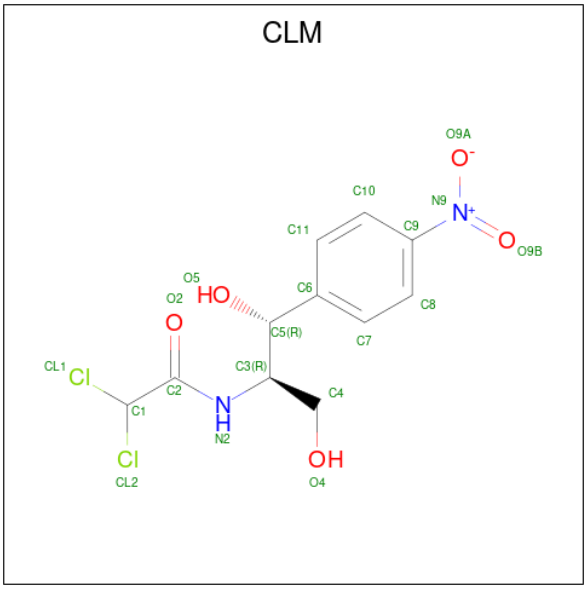
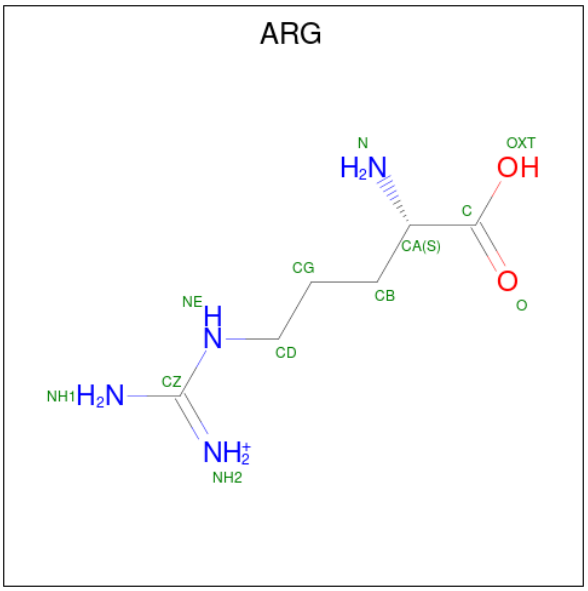
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2l	2	Total Mg 2 2	0	0
57	2n	1	Total Mg 1 1	0	0
57	2p	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2x	1	Total Mg 1 1	0	0

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



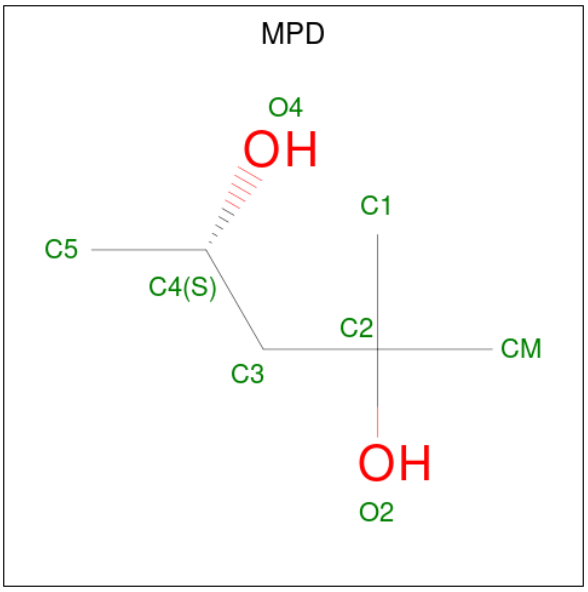
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total C Cl N O 20 11 2 2 5	0	0
58	2A	1	Total C Cl N O 20 11 2 2 5	0	0

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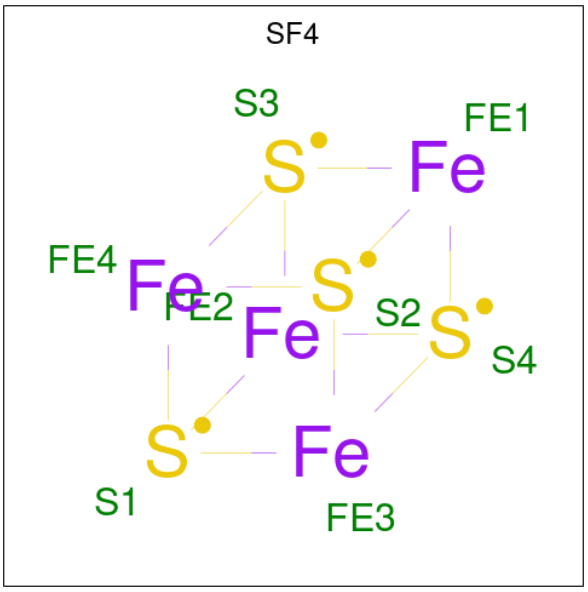
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1T	1	Total C O 8 6 2	0	0
60	18	1	Total C O 8 6 2	0	0
60	1a	1	Total C O 8 6 2	0	0
60	2A	1	Total C O 8 6 2	0	0
60	2B	1	Total C O 8 6 2	0	0

- 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	3946	Total O 3946 3946	0	0
63	1B	90	Total O 90 90	0	0
63	1D	121	Total O 121 121	0	0
63	1E	80	Total O 80 80	0	0
63	1F	59	Total O 59 59	0	0
63	1G	19	Total O 19 19	0	0
63	1H	13	Total O 13 13	0	0
63	1I	5	Total O 5 5	0	0
63	1N	50	Total O 50 50	0	0
63	1O	33	Total O 33 33	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1P	65	Total O 65 65	0	0
63	1Q	35	Total O 35 35	0	0
63	1R	32	Total O 32 32	0	0
63	1S	15	Total O 15 15	0	0
63	1T	28	Total O 28 28	0	0
63	1U	46	Total O 46 46	0	0
63	1V	41	Total O 41 41	0	0
63	1W	30	Total O 30 30	0	0
63	1X	28	Total O 28 28	0	0
63	1Y	21	Total O 21 21	0	0
63	1Z	13	Total O 13 13	0	0
63	10	25	Total O 25 25	0	0
63	11	26	Total O 26 26	0	0
63	12	15	Total O 15 15	0	0
63	13	24	Total O 24 24	0	0
63	14	2	Total O 2 2	0	0
63	15	24	Total O 24 24	0	0
63	16	18	Total O 18 18	0	0
63	17	17	Total O 17 17	0	0
63	18	26	Total O 26 26	0	0
63	19	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1a	412	Total O 412 412	0	0
63	1b	1	Total O 1 1	0	0
63	1c	1	Total O 1 1	0	0
63	1d	7	Total O 7 7	0	0
63	1e	2	Total O 2 2	0	0
63	1f	3	Total O 3 3	0	0
63	1h	1	Total O 1 1	0	0
63	1j	1	Total O 1 1	0	0
63	1l	5	Total O 5 5	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	5	Total O 5 5	0	0
63	1w	5	Total O 5 5	0	0
63	1x	5	Total O 5 5	0	0
63	2A	2126	Total O 2126 2126	0	0
63	2B	46	Total O 46 46	0	0
63	2D	54	Total O 54 54	0	0
63	2E	26	Total O 26 26	0	0
63	2F	24	Total O 24 24	0	0
63	2G	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	2H	3	Total O 3 3	0	0
63	2I	6	Total O 6 6	0	0
63	2N	3	Total O 3 3	0	0
63	2O	22	Total O 22 22	0	0
63	2P	28	Total O 28 28	0	0
63	2Q	19	Total O 19 19	0	0
63	2R	17	Total O 17 17	0	0
63	2S	4	Total O 4 4	0	0
63	2T	11	Total O 11 11	0	0
63	2U	13	Total O 13 13	0	0
63	2V	7	Total O 7 7	0	0
63	2W	19	Total O 19 19	0	0
63	2X	9	Total O 9 9	0	0
63	2Y	4	Total O 4 4	0	0
63	2Z	10	Total O 10 10	0	0
63	20	12	Total O 12 12	0	0
63	21	20	Total O 20 20	0	0
63	22	2	Total O 2 2	0	0
63	23	3	Total O 3 3	0	0
63	24	1	Total O 1 1	0	0
63	25	10	Total O 10 10	0	0

Continued on next page...

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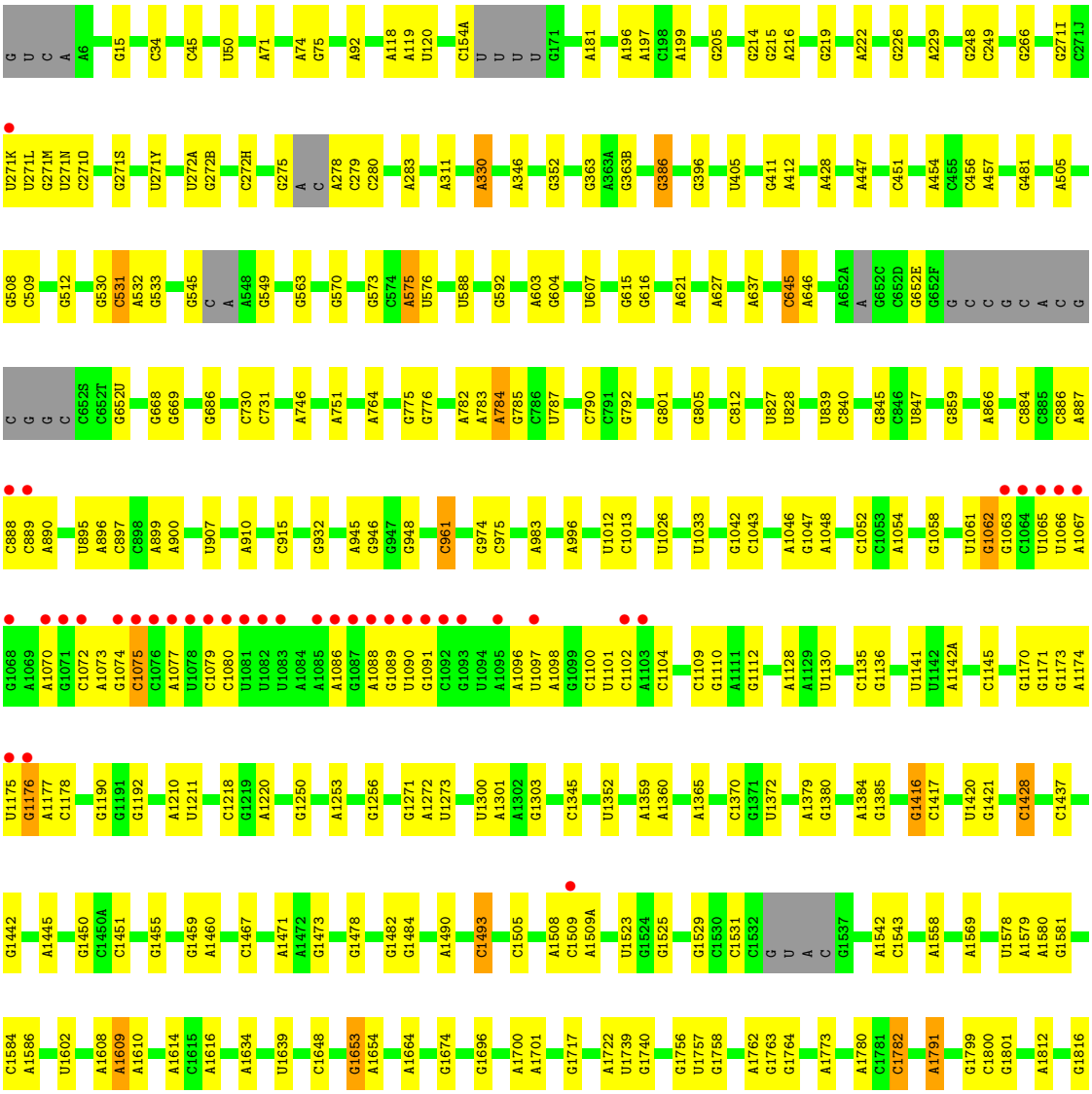
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	26	5	Total O 5 5	0	0
63	27	8	Total O 8 8	0	0
63	28	13	Total O 13 13	0	0
63	29	1	Total O 1 1	0	0
63	2a	294	Total O 294 294	0	0
63	2d	2	Total O 2 2	0	0
63	2e	2	Total O 2 2	0	0
63	2f	2	Total O 2 2	0	0
63	2j	2	Total O 2 2	0	0
63	2l	2	Total O 2 2	0	0
63	2n	1	Total O 1 1	0	0
63	2o	3	Total O 3 3	0	0
63	2p	1	Total O 1 1	0	0
63	2r	3	Total O 3 3	0	0
63	2t	2	Total O 2 2	0	0
63	2y	2	Total O 2 2	0	0
63	2w	2	Total O 2 2	0	0
63	2x	2	Total O 2 2	0	0

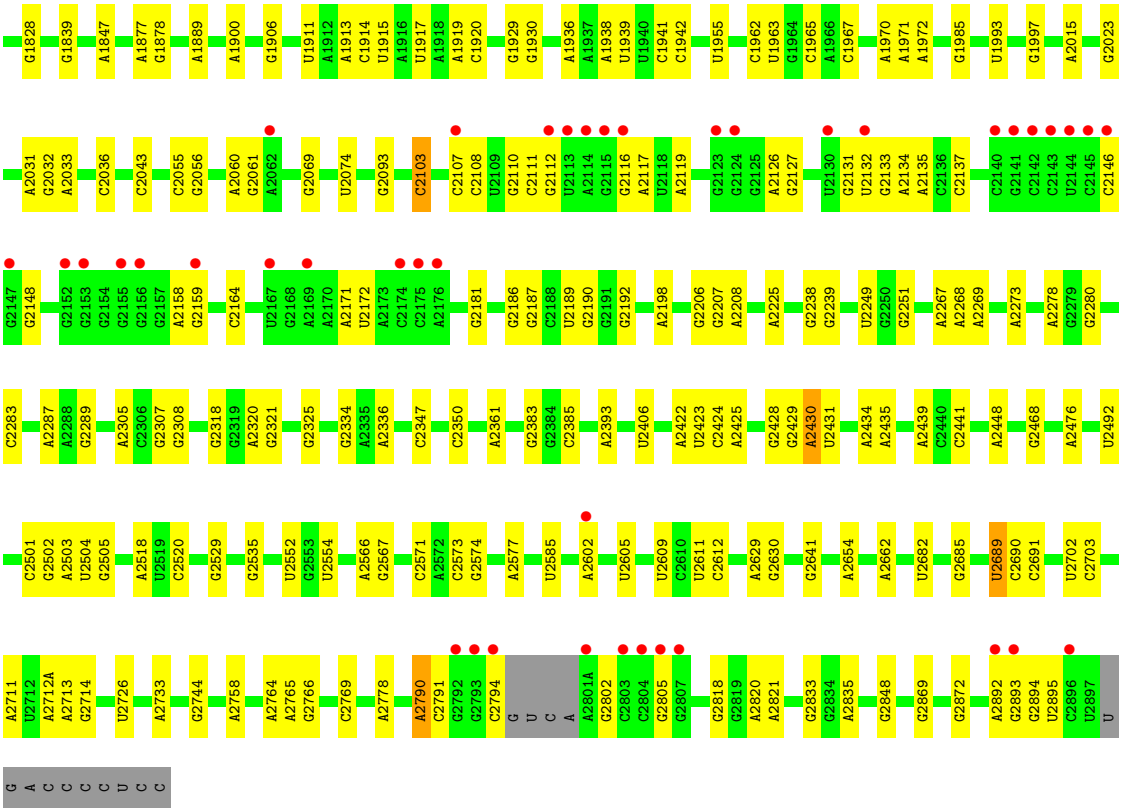
3 Residue-property plots (i)

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

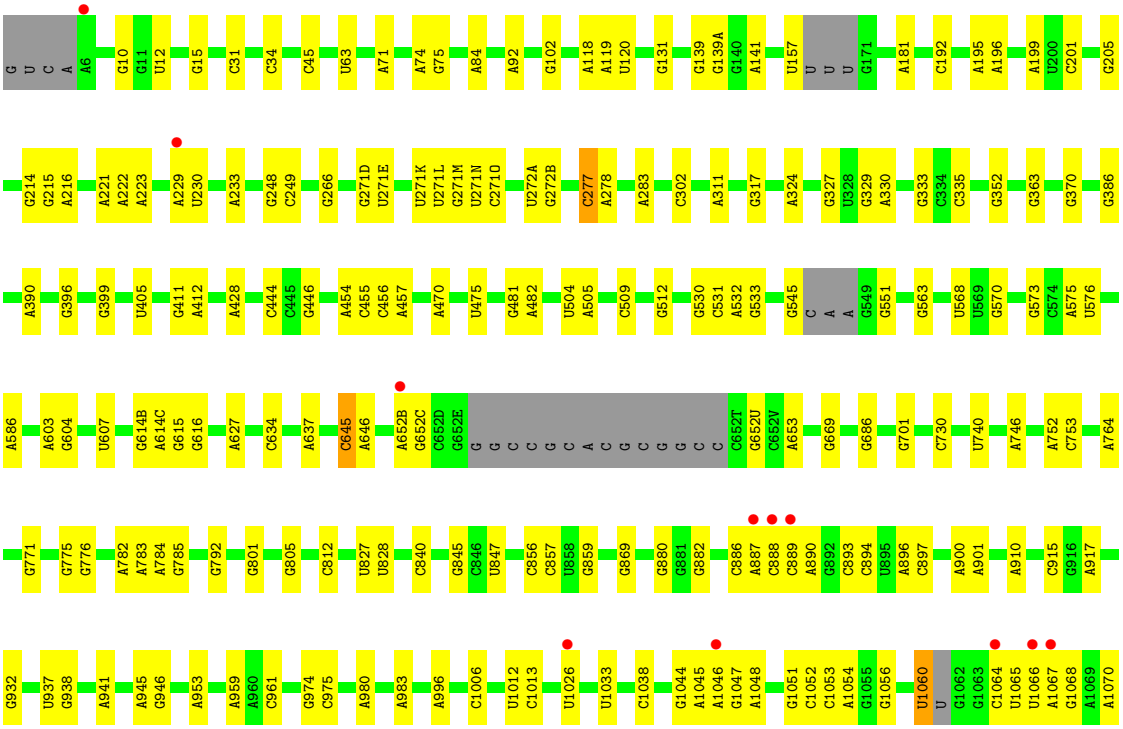
Chain 1A:

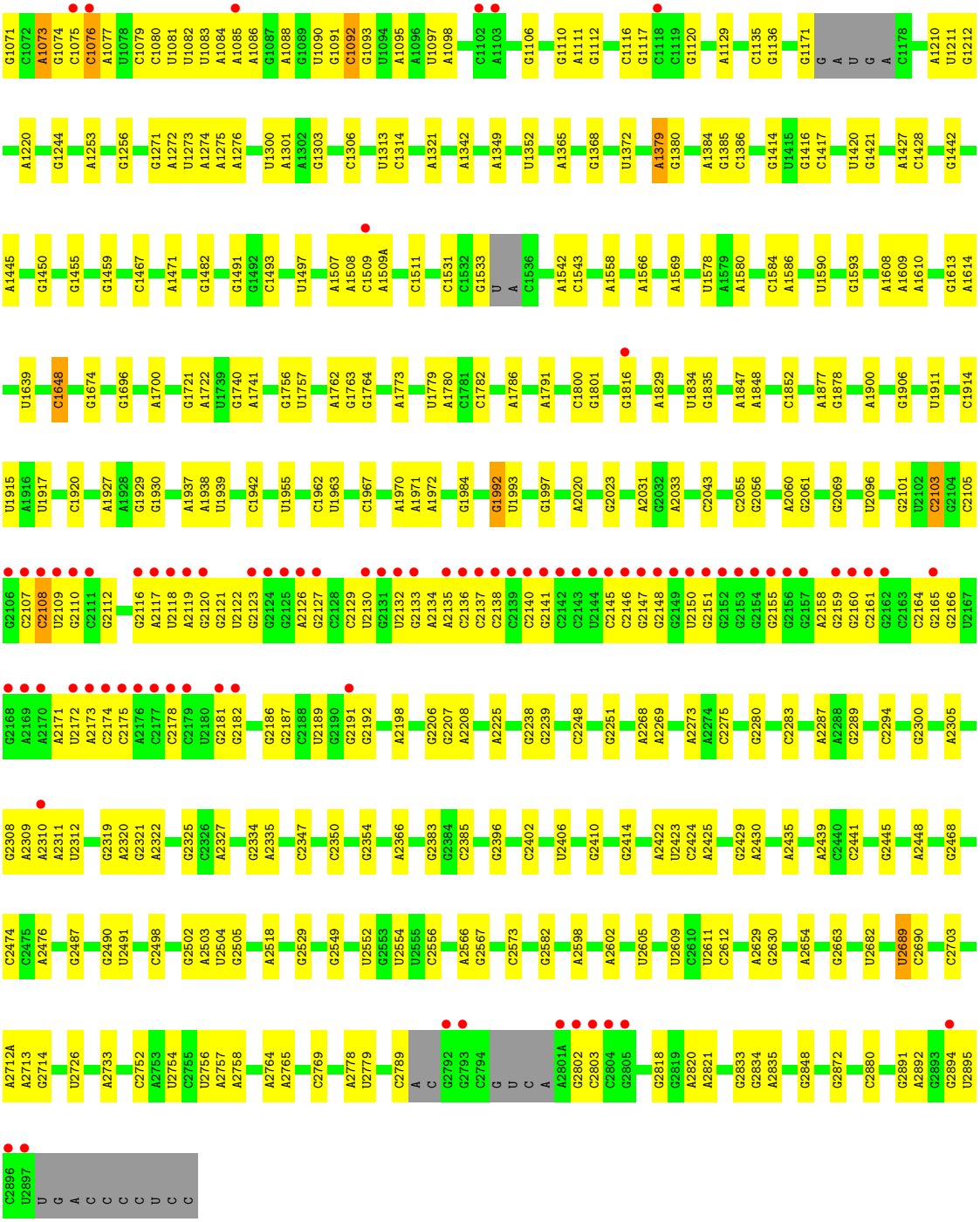




• Molecule 1: 23S Ribosomal RNA

Chain 2A:



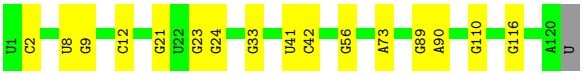


• Molecule 2: 5S Ribosomal RNA

Chain 1B:

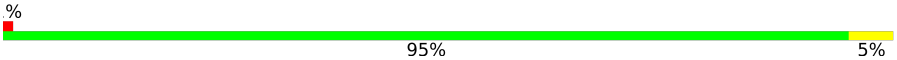
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



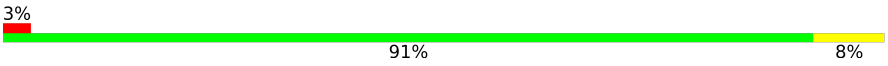
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



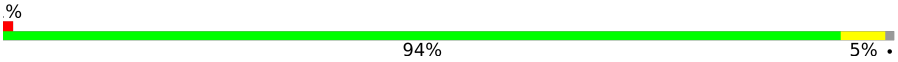
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



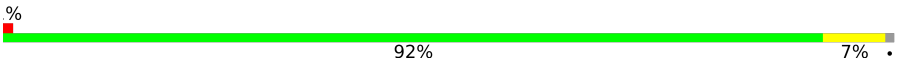
• Molecule 4: 50S ribosomal protein L3

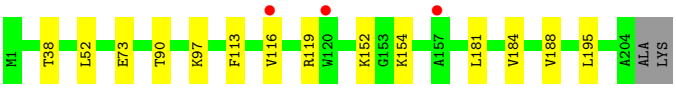
Chain 1E:



• Molecule 4: 50S ribosomal protein L3

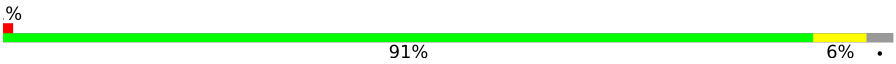
Chain 2E:

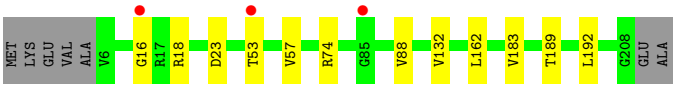




• Molecule 5: 50S ribosomal protein L4

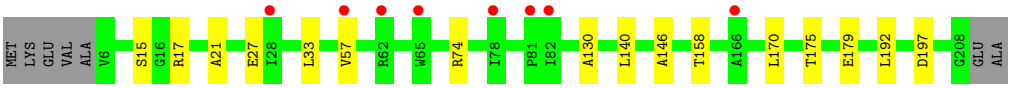
Chain 1F:





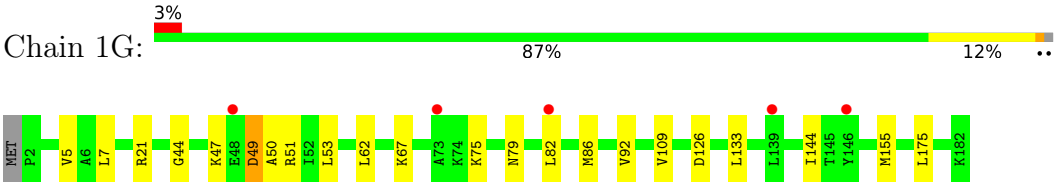
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



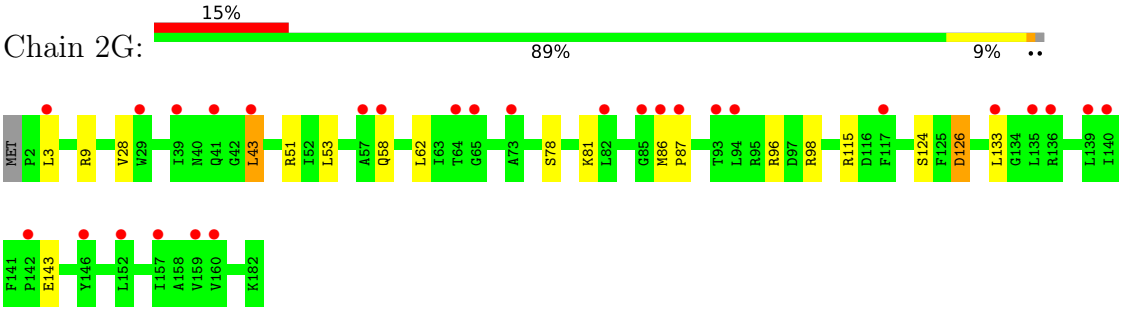
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



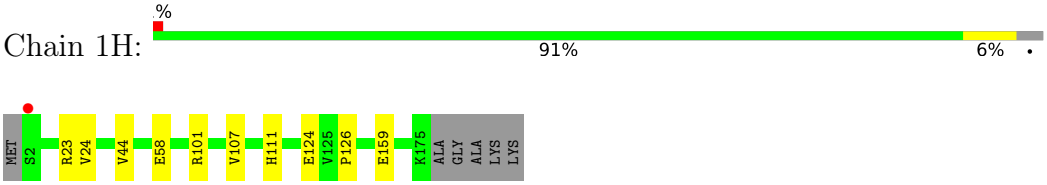
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



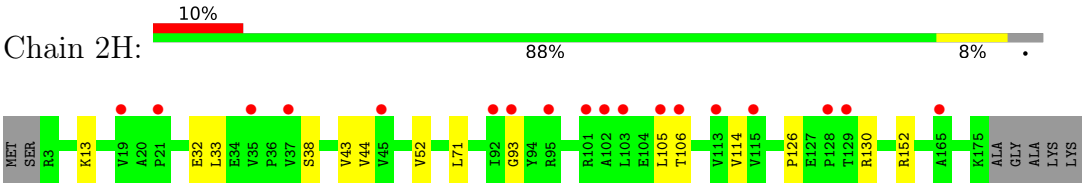
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



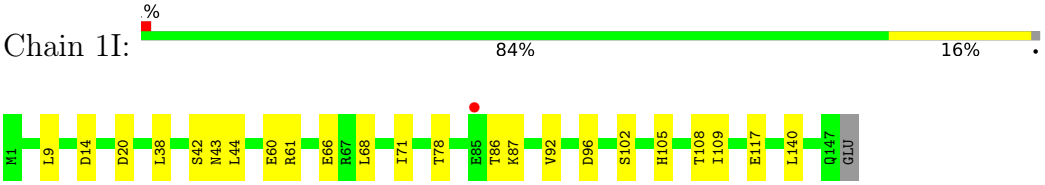
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



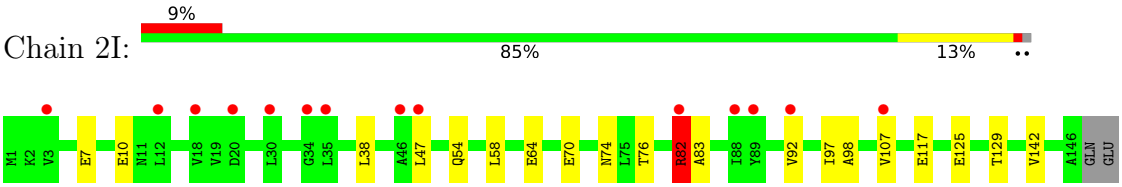
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



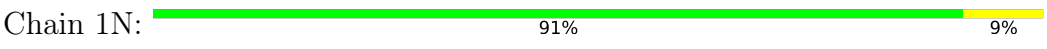
• Molecule 8: 50S ribosomal protein L9

Chain 2I:

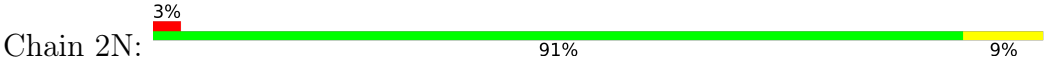


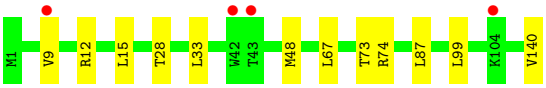
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



• Molecule 9: 50S ribosomal protein L13

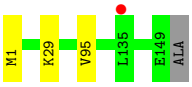




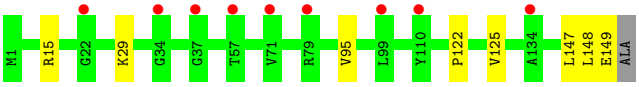
• Molecule 10: 50S ribosomal protein L14

• Molecule 10: 50S ribosomal protein L14

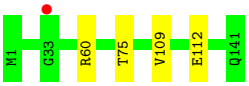
• Molecule 11: 50S ribosomal protein L15



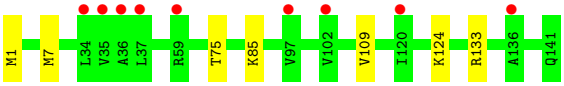
• Molecule 11: 50S ribosomal protein L15



• Molecule 12: 50S ribosomal protein L16

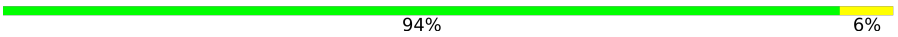


• Molecule 12: 50S ribosomal protein L16



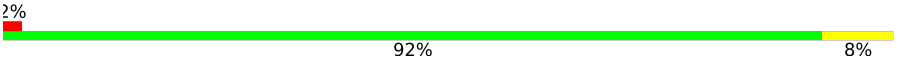
• Molecule 13: 50S ribosomal protein L17

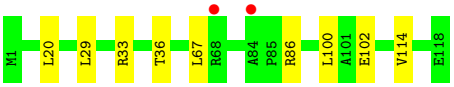
Chain 1R:



• Molecule 13: 50S ribosomal protein L17

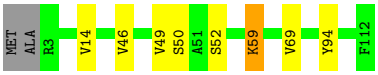
Chain 2R:





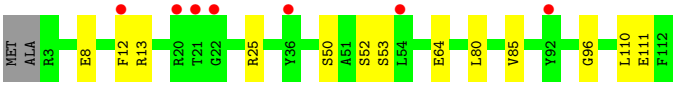
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



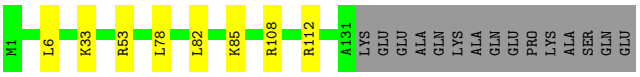
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



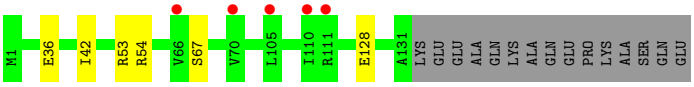
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



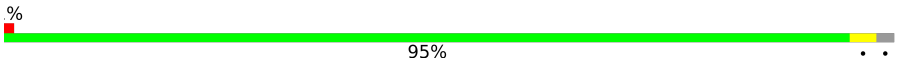
• Molecule 15: 50S ribosomal protein L19

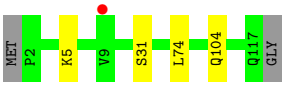
Chain 2T:



• Molecule 16: 50S ribosomal protein L20

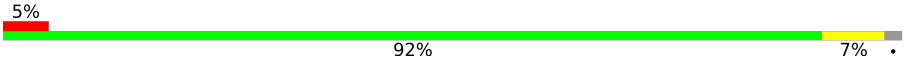
Chain 1U:

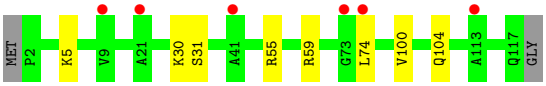




• Molecule 16: 50S ribosomal protein L20

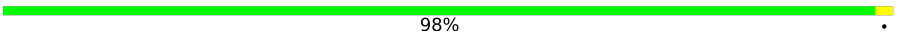
Chain 2U:





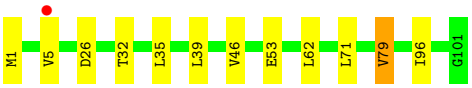
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



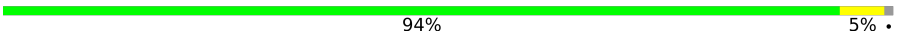
• Molecule 17: 50S ribosomal protein L21

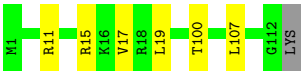
Chain 2V:



• Molecule 18: 50S ribosomal protein L22

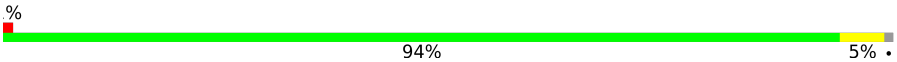
Chain 1W:

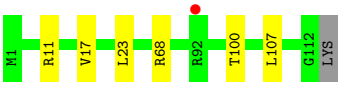




• Molecule 18: 50S ribosomal protein L22

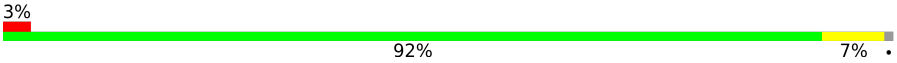
Chain 2W:

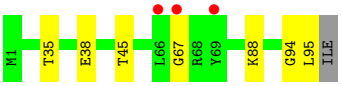




• Molecule 19: 50S ribosomal protein L23

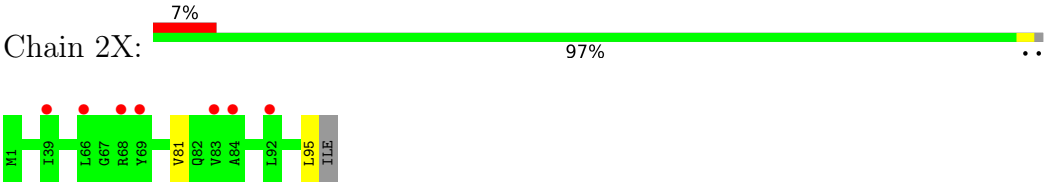
Chain 1X:





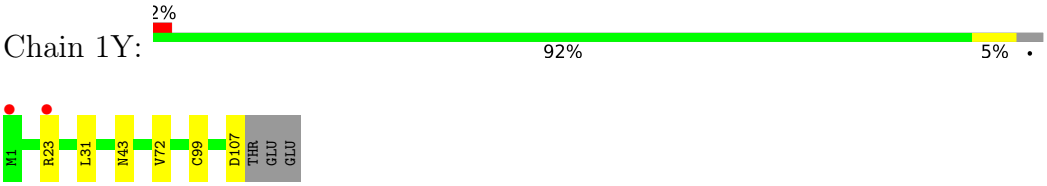
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



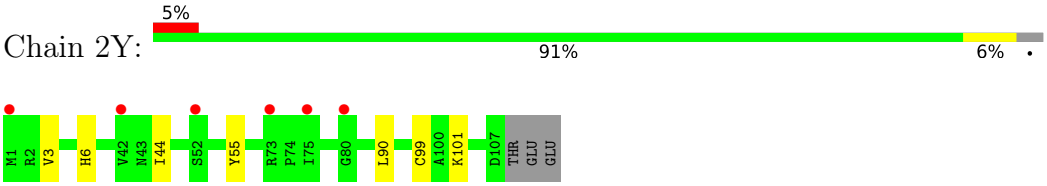
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



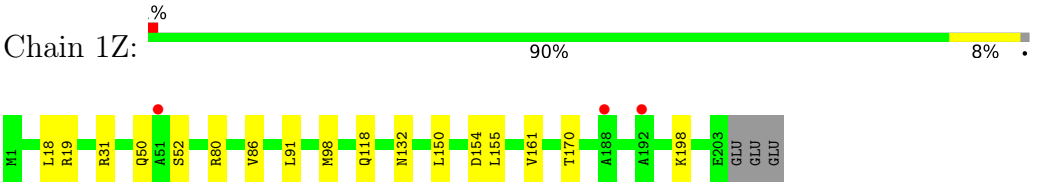
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



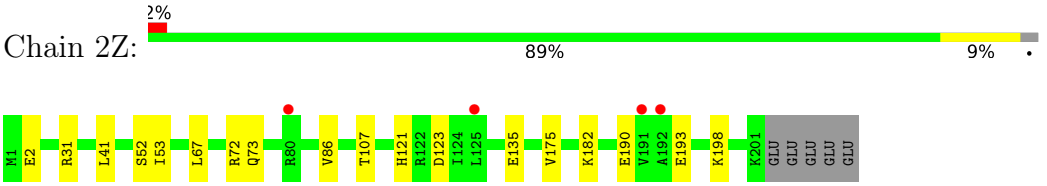
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



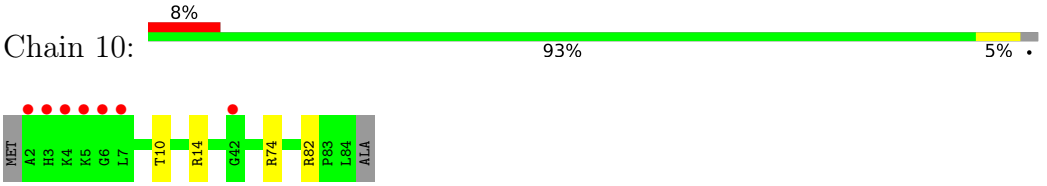
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



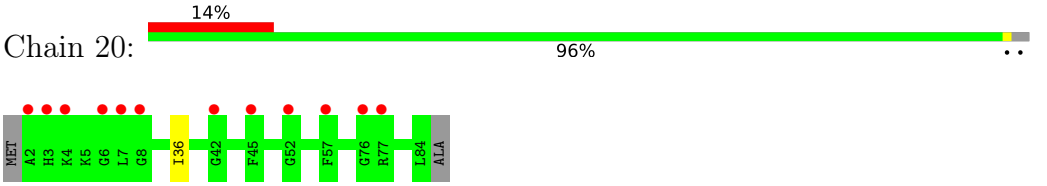
• Molecule 22: 50S ribosomal protein L27

Chain 10:



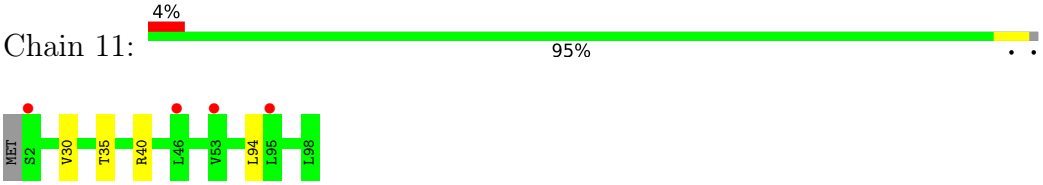
• Molecule 22: 50S ribosomal protein L27

Chain 20:



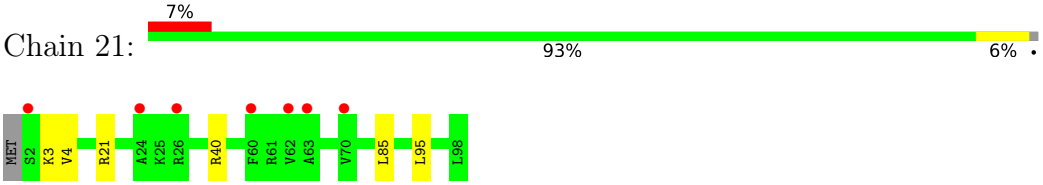
• Molecule 23: 50S ribosomal protein L28

Chain 11:



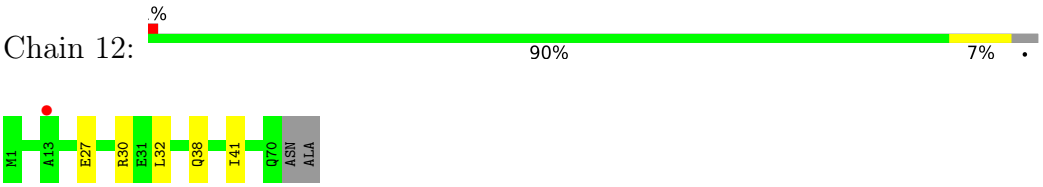
• Molecule 23: 50S ribosomal protein L28

Chain 21:



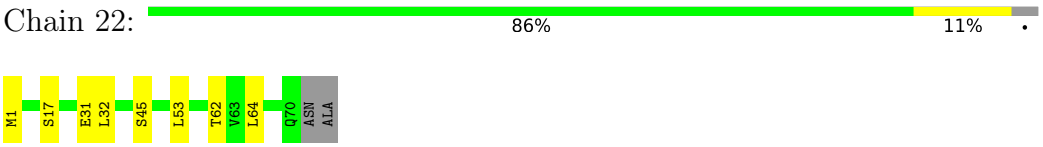
• Molecule 24: 50S ribosomal protein L29

Chain 12:



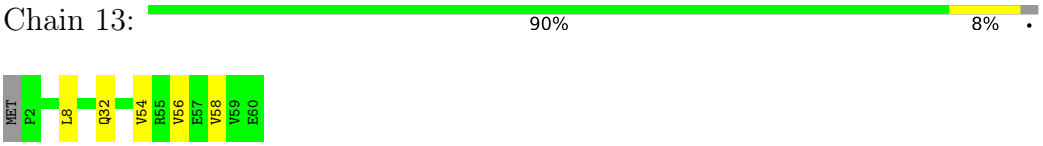
• Molecule 24: 50S ribosomal protein L29

Chain 22:



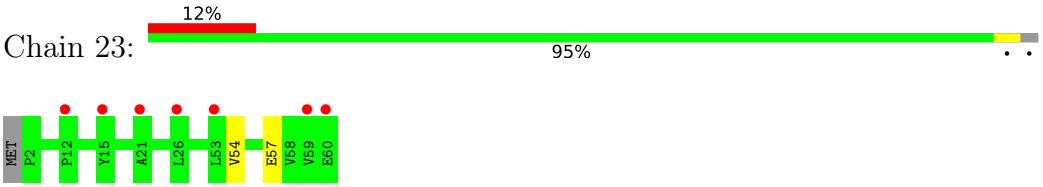
• Molecule 25: 50S ribosomal protein L30

Chain 13:



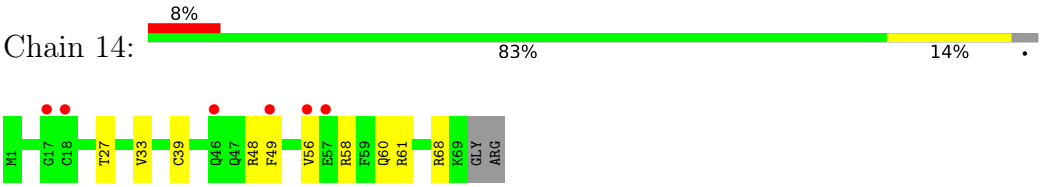
• Molecule 25: 50S ribosomal protein L30

Chain 23:



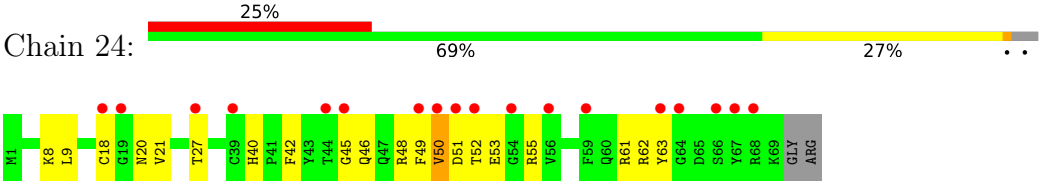
• Molecule 26: 50S ribosomal protein L31

Chain 14:



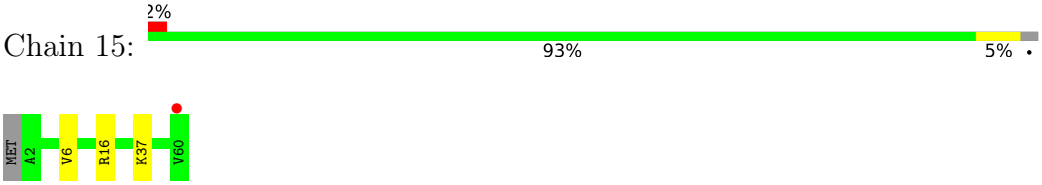
• Molecule 26: 50S ribosomal protein L31

Chain 24:



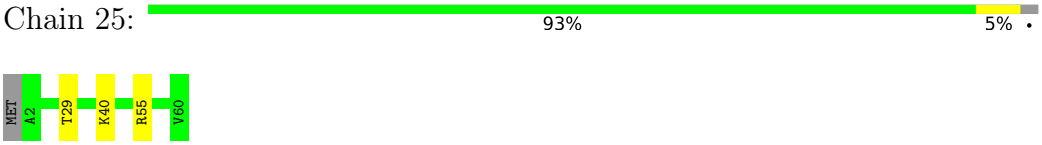
• Molecule 27: 50S ribosomal protein L32

Chain 15:



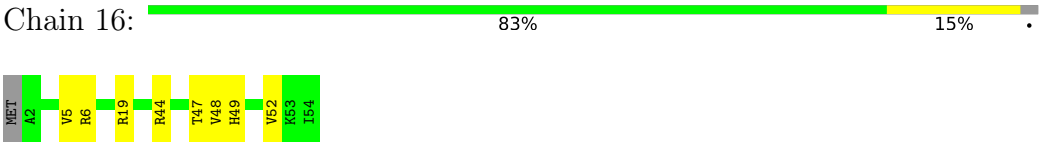
• Molecule 27: 50S ribosomal protein L32

Chain 25:



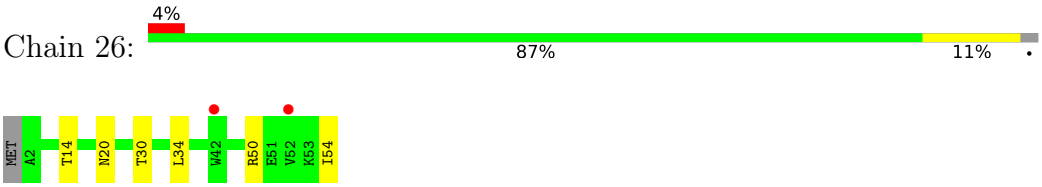
• Molecule 28: 50S ribosomal protein L33

Chain 16:



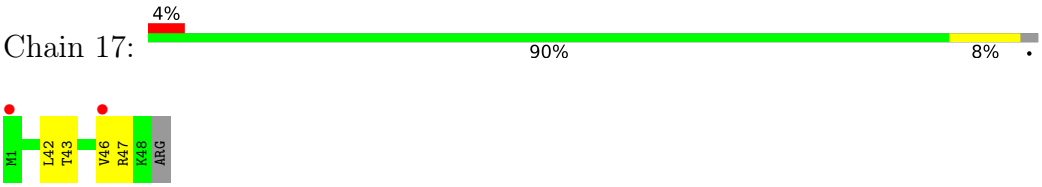
• Molecule 28: 50S ribosomal protein L33

Chain 26:



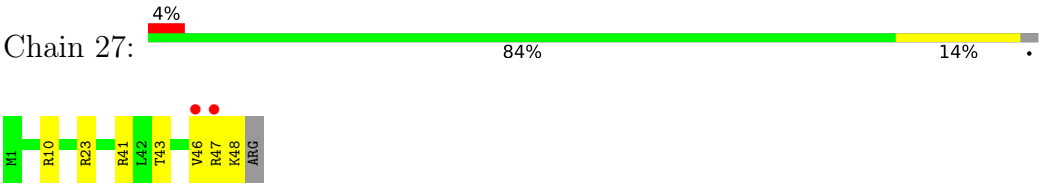
• Molecule 29: 50S ribosomal protein L34

Chain 17:



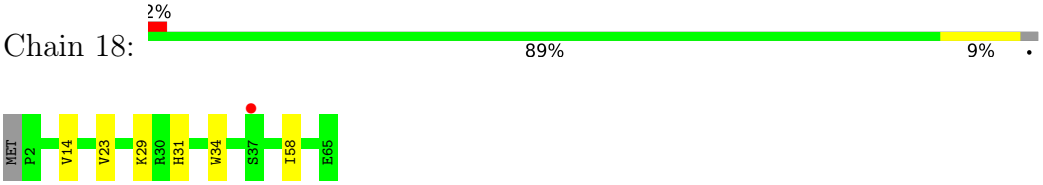
• Molecule 29: 50S ribosomal protein L34

Chain 27:



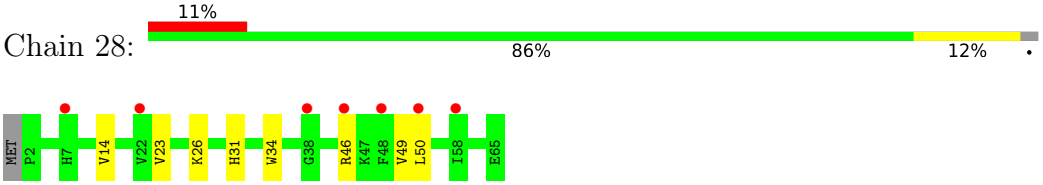
• Molecule 30: 50S ribosomal protein L35

Chain 18:



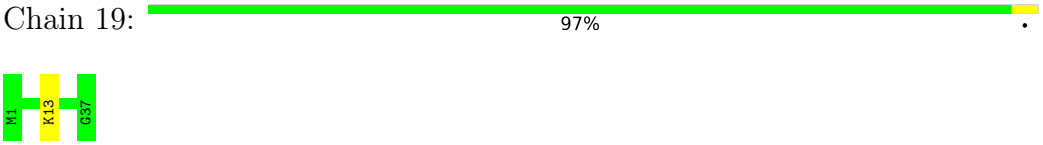
• Molecule 30: 50S ribosomal protein L35

Chain 28:



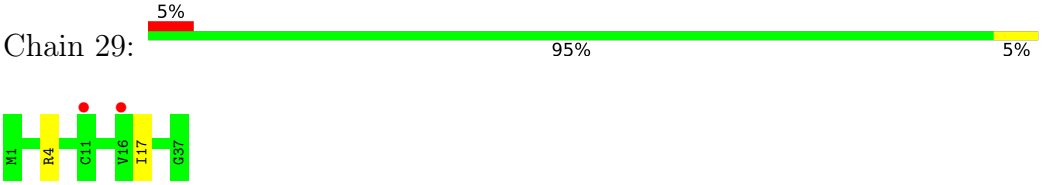
• Molecule 31: 50S ribosomal protein L36

Chain 19:



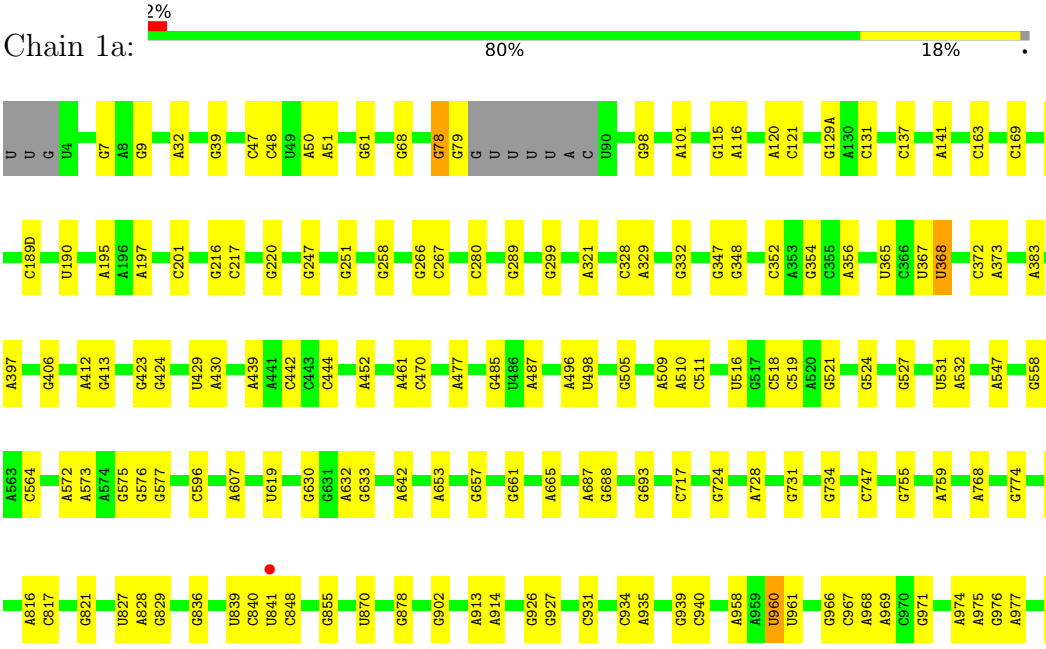
• Molecule 31: 50S ribosomal protein L36

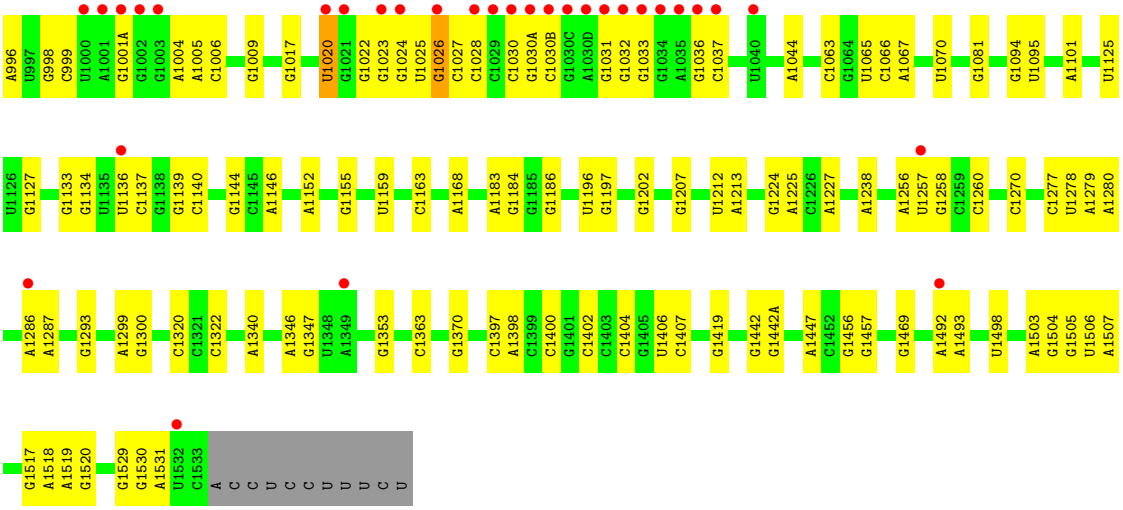
Chain 29:



• Molecule 32: 16S Ribosomal RNA

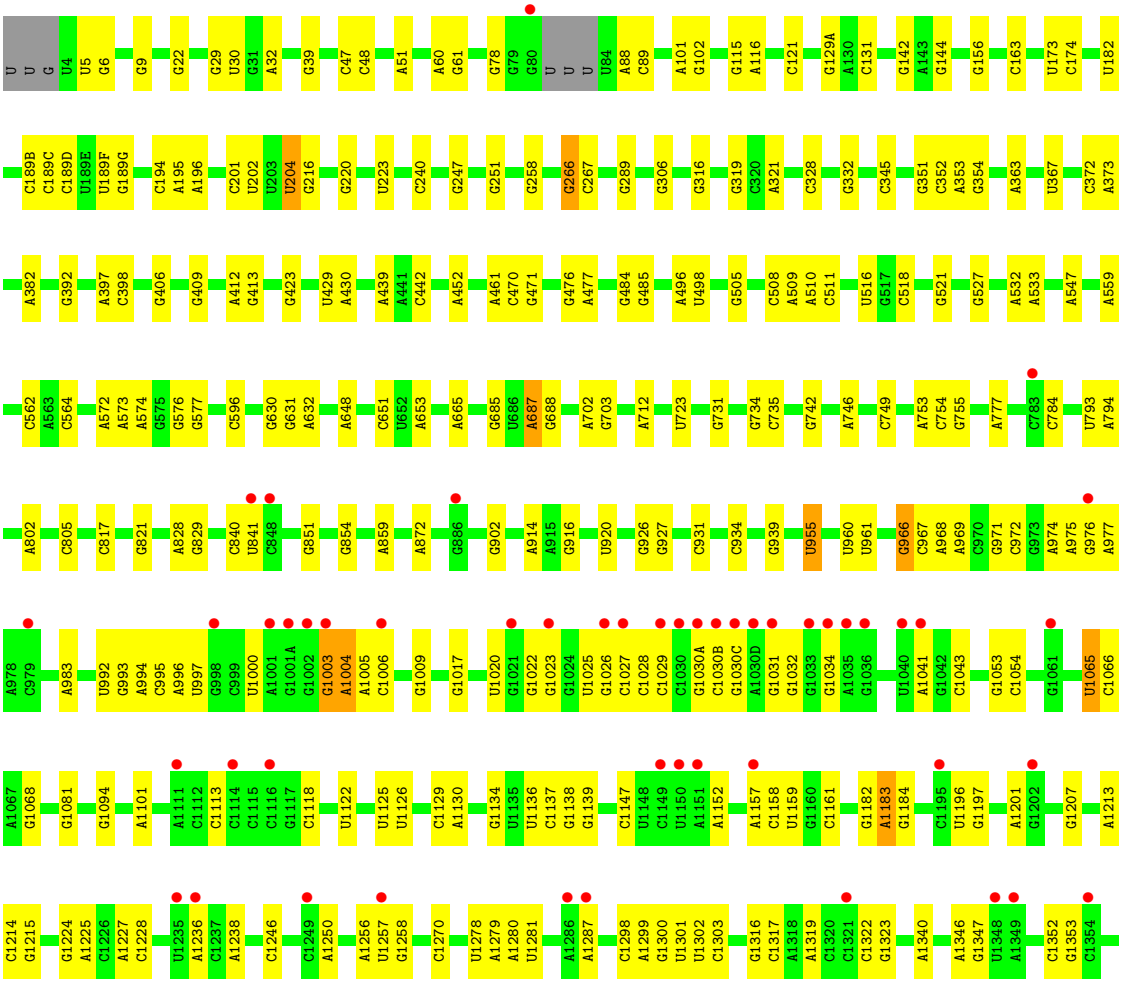
Chain 1a:

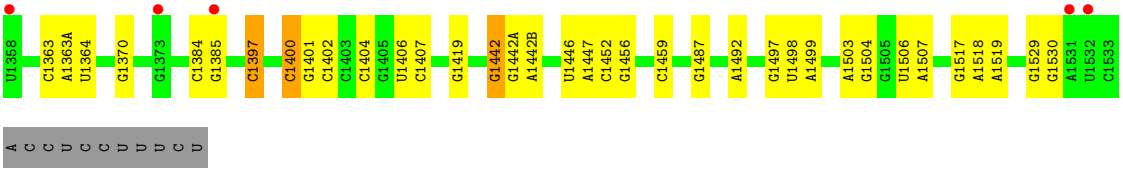




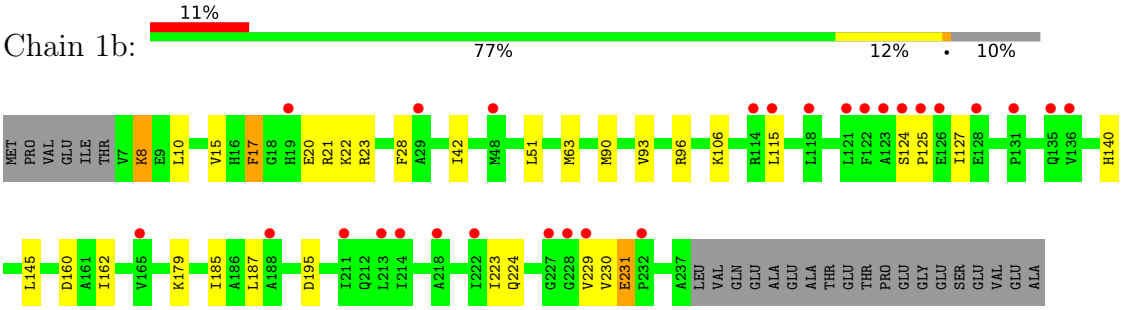
• Molecule 32: 16S Ribosomal RNA

Chain 2a:

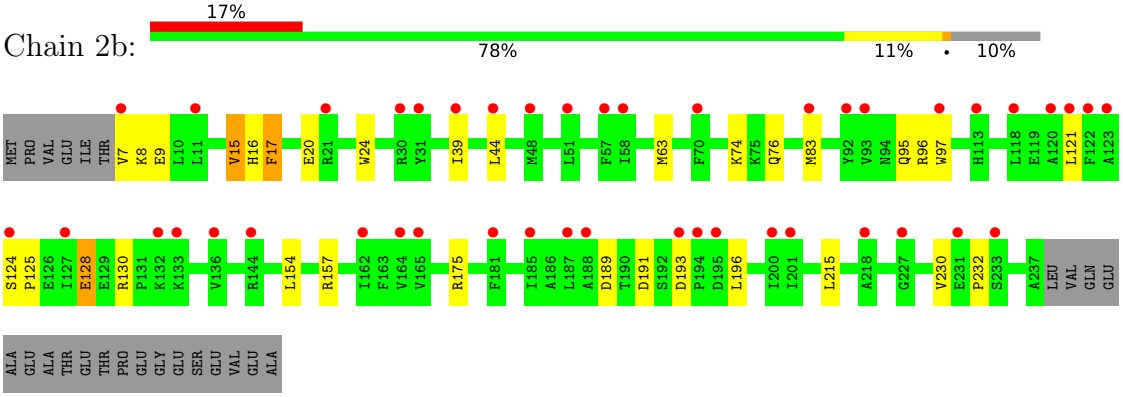




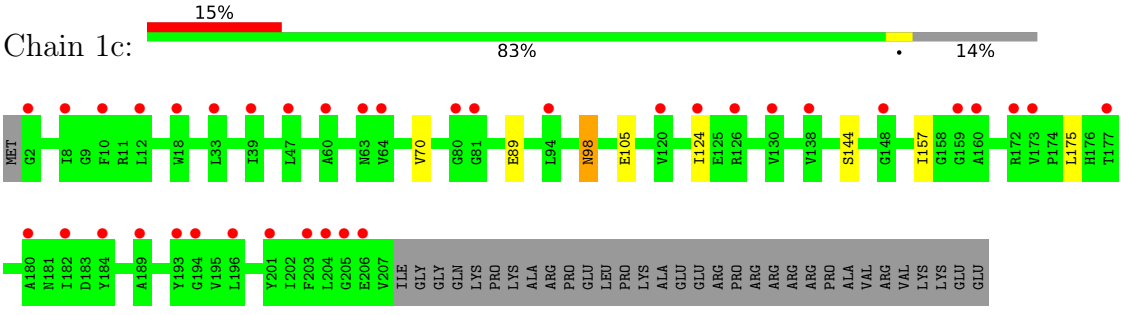
• Molecule 33: 30S ribosomal protein S2



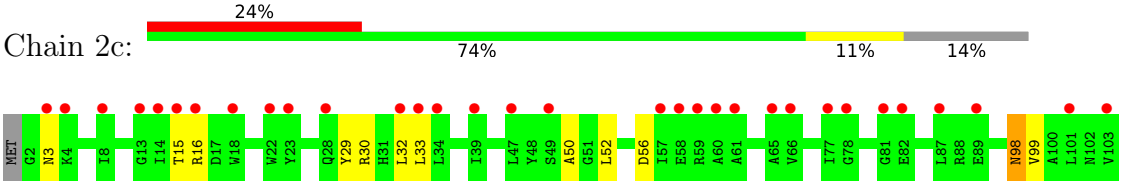
• Molecule 33: 30S ribosomal protein S2

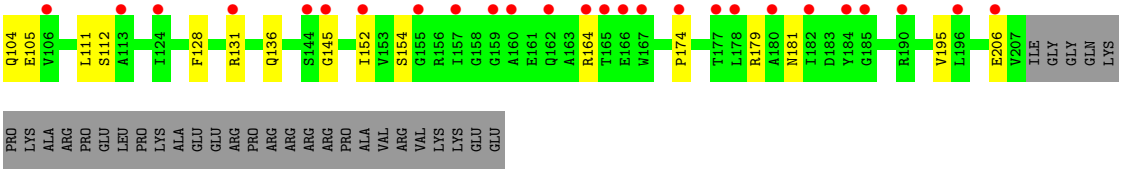


• Molecule 34: 30S ribosomal protein S3

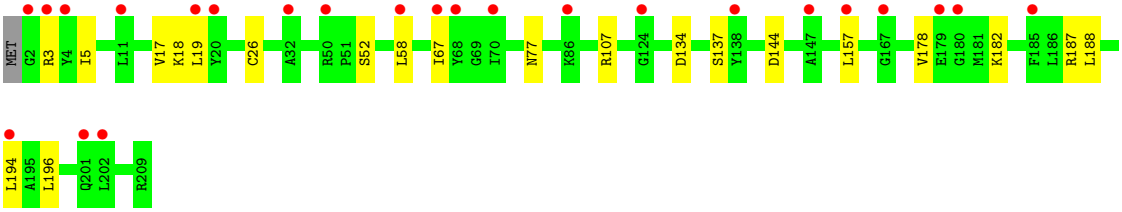


• Molecule 34: 30S ribosomal protein S3

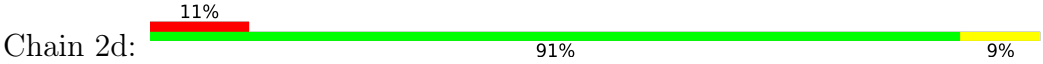


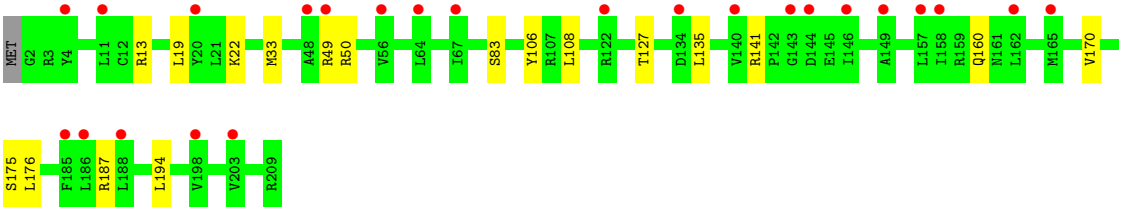


• Molecule 35: 30S ribosomal protein S4

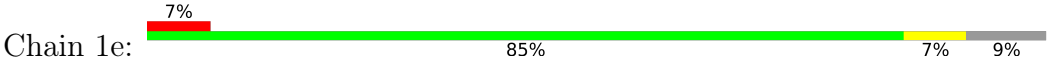


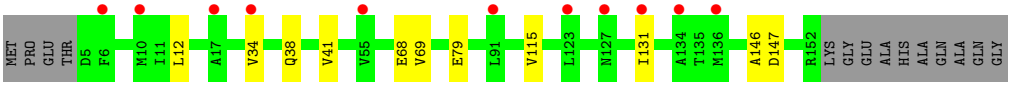
• Molecule 35: 30S ribosomal protein S4



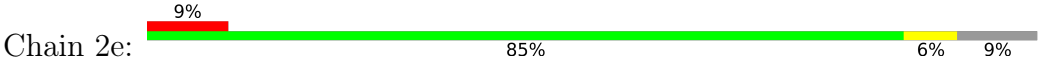


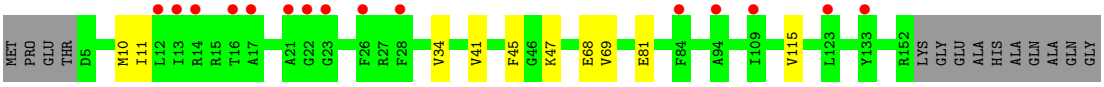
• Molecule 36: 30S ribosomal protein S5



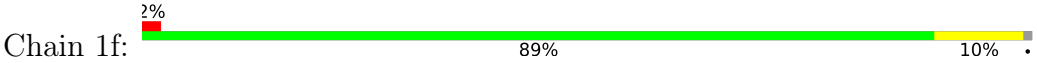


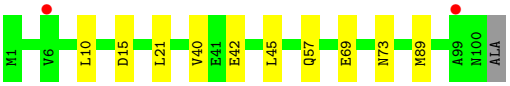
• Molecule 36: 30S ribosomal protein S5





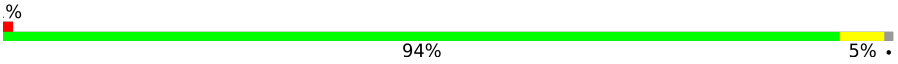
• Molecule 37: 30S ribosomal protein S6

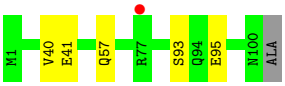




• Molecule 37: 30S ribosomal protein S6

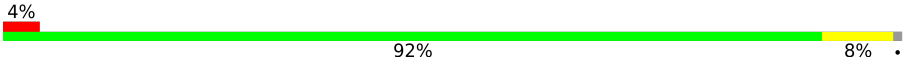
Chain 2f:

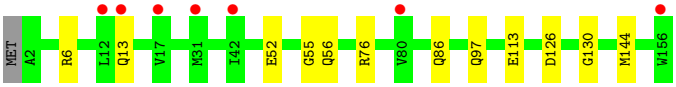




• Molecule 38: 30S ribosomal protein S7

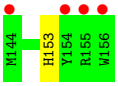
Chain 1g:





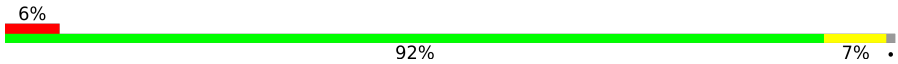
• Molecule 38: 30S ribosomal protein S7

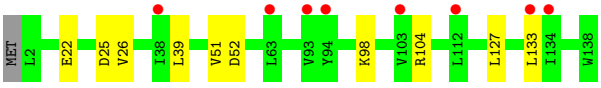
Chain 2g:



• Molecule 39: 30S ribosomal protein S8

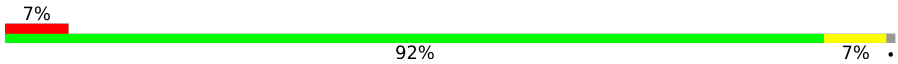
Chain 1h:

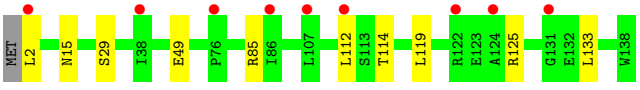




• Molecule 39: 30S ribosomal protein S8

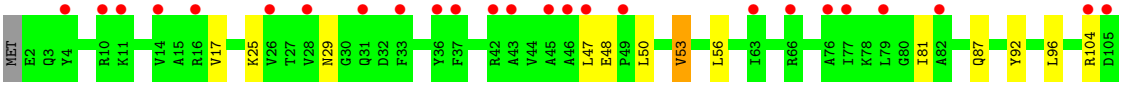
Chain 2h:

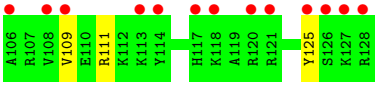




• Molecule 40: 30S ribosomal protein S9

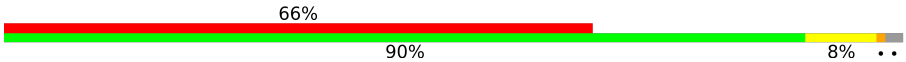
Chain 1i:

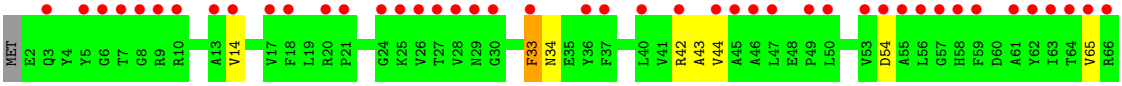


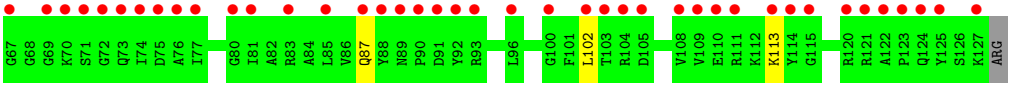


• Molecule 40: 30S ribosomal protein S9

Chain 2i:

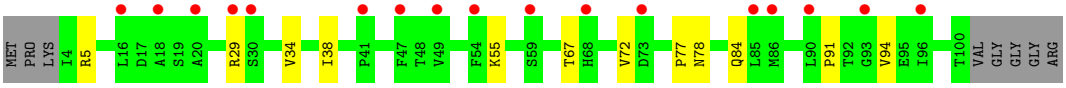






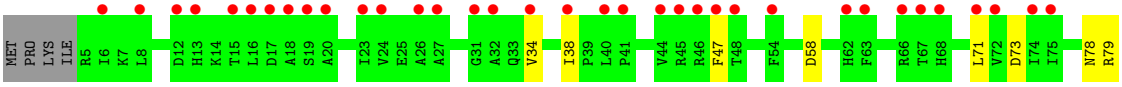
• Molecule 41: 30S ribosomal protein S10

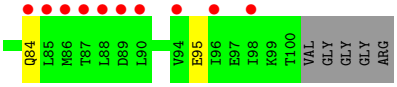
Chain 1j:



• Molecule 41: 30S ribosomal protein S10

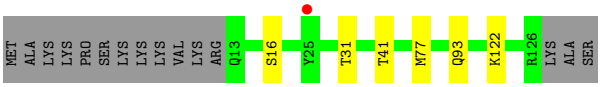
Chain 2j:





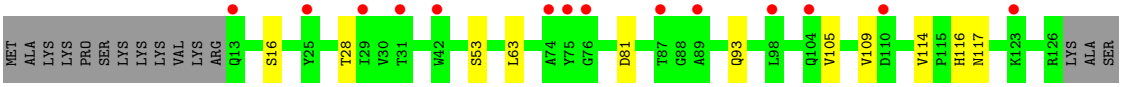
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



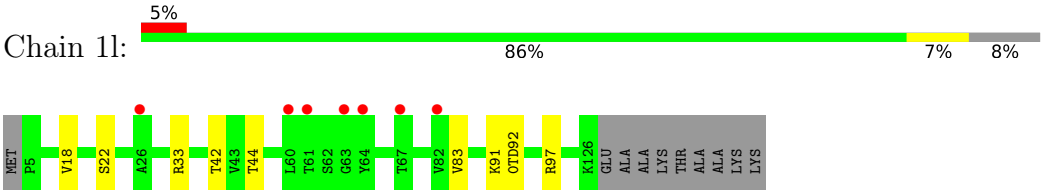
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



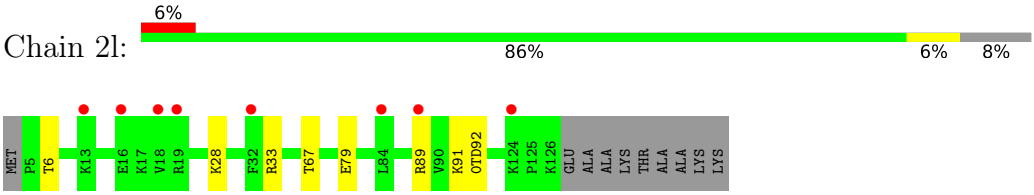
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



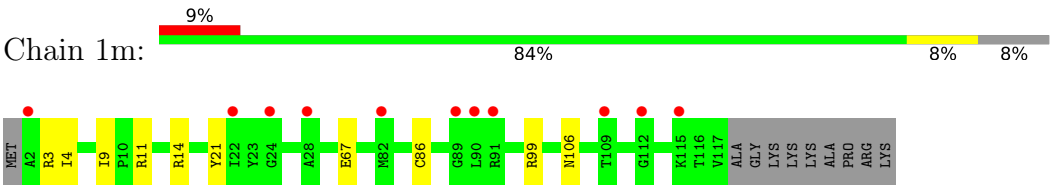
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



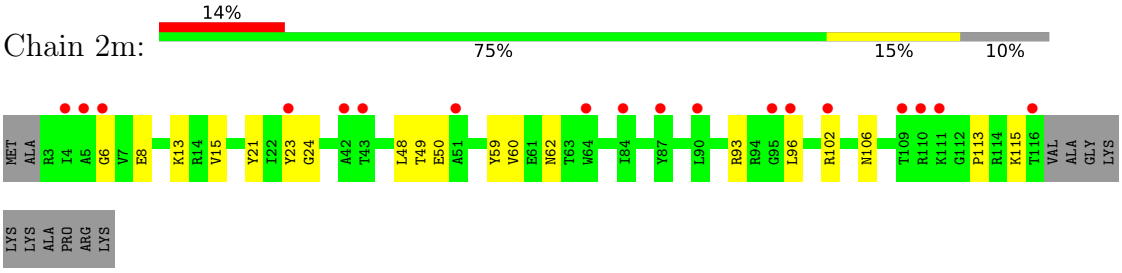
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



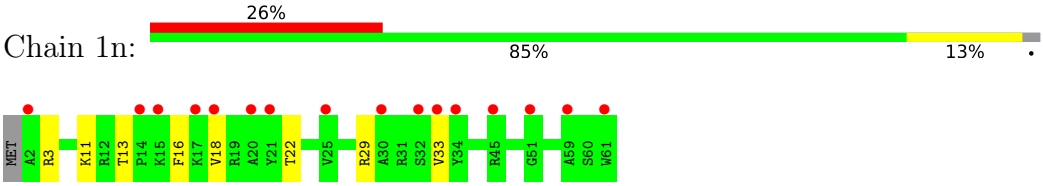
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



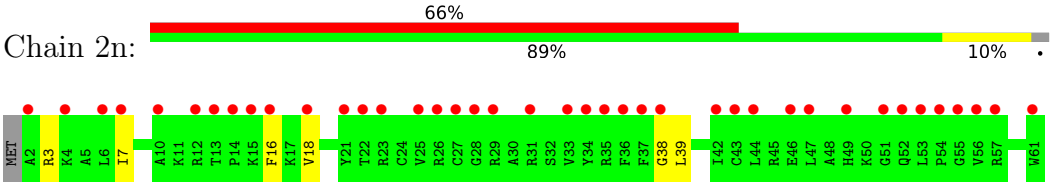
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



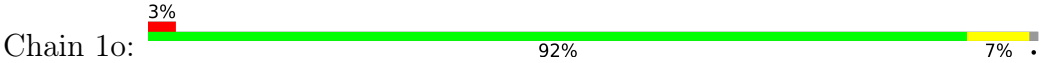
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



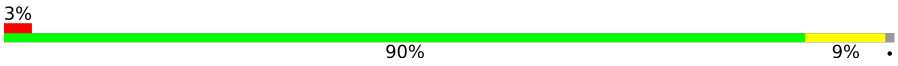
• Molecule 46: 30S ribosomal protein S15

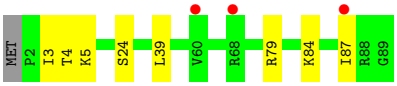
Chain 1o:



• Molecule 46: 30S ribosomal protein S15

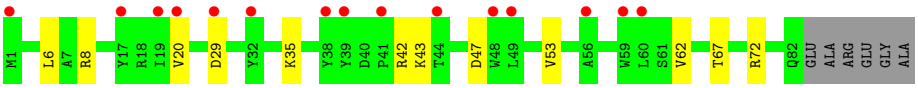
Chain 2o:





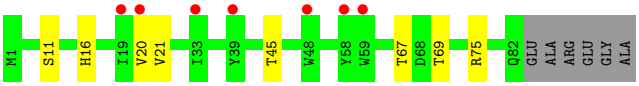
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



• Molecule 47: 30S ribosomal protein S16

Chain 2p:

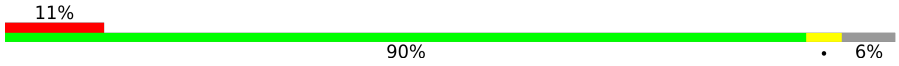


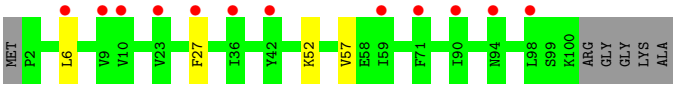
• Molecule 48: 30S ribosomal protein S17

Chain 1q:

• Molecule 48: 30S ribosomal protein S17

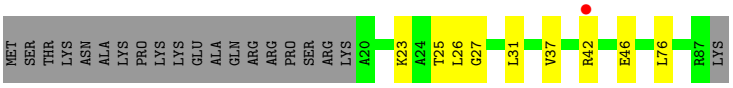
Chain 2q:





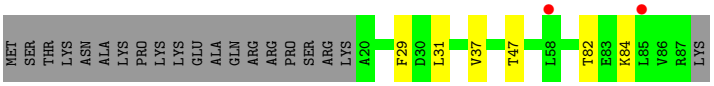
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



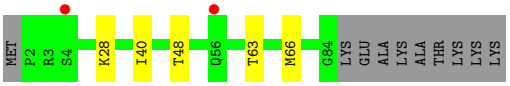
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



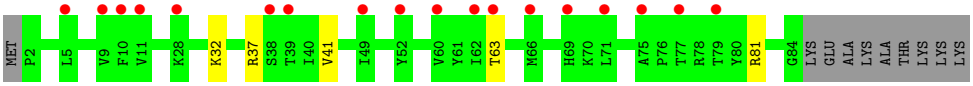
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



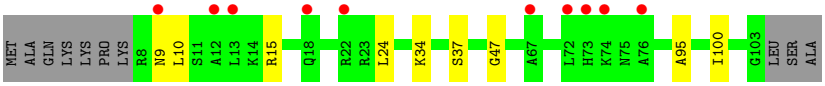
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



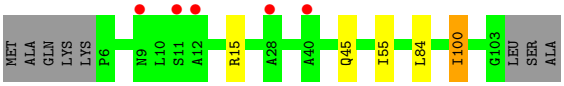
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



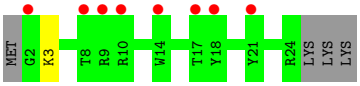
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



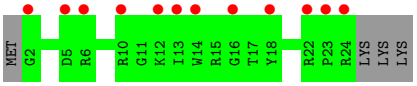
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



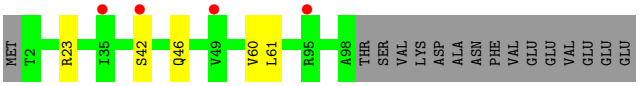
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



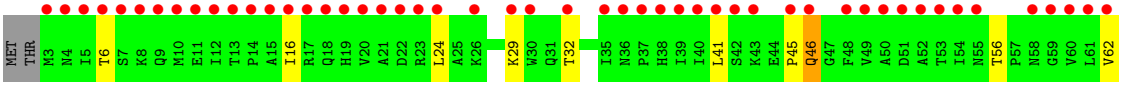
• Molecule 53: Ribosome-associated inhibitor A

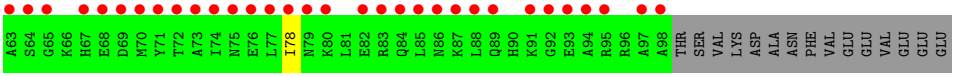
Chain 1y:



• Molecule 53: Ribosome-associated inhibitor A

Chain 2y:





• 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

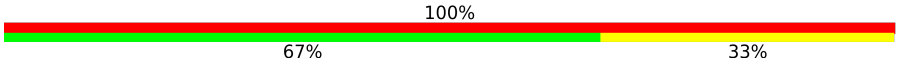
Chain 1x:

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

Chain 2x:

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

Chain 1v:



• 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	209.71Å 449.95Å 621.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.98 – 2.50 310.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (224.98-2.50) 98.5 (310.60-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.229 , 0.280 0.229 , 0.279	Depositor DCC
R_{free} test set	98581 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	297633	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: 8AN, SF4, 2MU, CLM, 2MA, ZN, MG, G7M, 4OC, M2G, 5MU, MPD, OMC, 2MG, PSU, UR3, OMG, MA6, 5MC, 0TD

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	0.52	1/69030 (0.0%)	1.01	77/107750 (0.1%)
1	2A	0.41	0/68902	0.90	51/107548 (0.0%)
2	1B	0.45	0/2876	0.94	1/4486 (0.0%)
2	2B	0.34	0/2878	0.83	0/4490
3	1D	0.36	0/2181	0.57	0/2940
3	2D	0.32	0/2186	0.54	0/2944
4	1E	0.33	0/1592	0.54	0/2149
4	2E	0.31	0/1592	0.52	0/2149
5	1F	0.34	0/1619	0.56	0/2193
5	2F	0.31	0/1615	0.52	0/2188
6	1G	0.31	0/1451	0.50	0/1961
6	2G	0.29	0/1449	0.47	0/1957
7	1H	0.32	0/1356	0.50	0/1834
7	2H	0.29	0/1350	0.49	0/1826
8	1I	0.28	0/1109	0.50	0/1512
8	2I	1.11	3/1091 (0.3%)	0.98	4/1490 (0.3%)
9	1N	0.33	0/1148	0.53	0/1547
9	2N	0.30	0/1144	0.48	0/1543
10	1O	0.35	0/943	0.56	0/1269
10	2O	0.33	0/943	0.55	0/1269
11	1P	0.34	0/1152	0.56	0/1533
11	2P	0.30	0/1152	0.53	0/1533
12	1Q	0.33	0/1143	0.52	0/1527
12	2Q	0.32	0/1143	0.50	0/1527
13	1R	0.33	0/982	0.55	0/1312
13	2R	0.30	0/982	0.50	0/1312
14	1S	0.31	0/887	0.54	0/1180
14	2S	0.31	0/880	0.51	0/1172
15	1T	0.34	0/1105	0.53	0/1477
15	2T	0.31	0/1097	0.48	0/1468
16	1U	0.36	0/977	0.52	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.29	0/977	0.44	0/1301
17	1V	0.35	0/786	0.54	0/1053
17	2V	0.30	0/782	0.54	0/1049
18	1W	0.35	0/897	0.52	0/1205
18	2W	0.31	0/897	0.49	0/1205
19	1X	0.37	0/764	0.56	0/1025
19	2X	0.31	0/764	0.52	0/1025
20	1Y	0.34	0/823	0.55	0/1099
20	2Y	0.32	0/823	0.52	0/1100
21	1Z	0.31	0/1620	0.50	0/2200
21	2Z	0.29	0/1590	0.48	0/2162
22	10	0.36	0/662	0.55	0/881
22	20	0.31	0/659	0.54	0/877
23	11	0.33	0/761	0.52	0/1013
23	21	0.30	0/766	0.50	0/1018
24	12	0.31	0/590	0.49	0/781
24	22	0.29	0/594	0.45	0/785
25	13	0.34	0/474	0.55	0/635
25	23	0.30	0/469	0.49	0/630
26	14	0.30	0/559	0.52	0/754
26	24	0.39	0/549	0.59	0/741
27	15	0.39	0/473	0.62	0/639
27	25	0.28	0/469	0.53	0/635
28	16	0.32	0/460	0.52	0/613
28	26	0.29	0/456	0.49	0/608
29	17	0.37	0/426	0.54	0/561
29	27	0.29	0/426	0.50	0/561
30	18	0.33	0/525	0.55	0/691
30	28	0.30	0/525	0.48	0/691
31	19	0.34	0/310	0.54	0/407
31	29	0.32	0/310	0.55	0/407
32	1a	0.74	6/35795 (0.0%)	0.88	16/55864 (0.0%)
32	2a	0.36	0/35890	0.88	24/56012 (0.0%)
33	1b	0.30	0/1876	0.49	0/2533
33	2b	0.30	0/1860	0.50	0/2518
34	1c	0.29	0/1582	0.49	0/2137
34	2c	0.28	0/1566	0.48	0/2119
35	1d	0.30	0/1695	0.49	0/2274
35	2d	0.29	0/1698	0.47	0/2277
36	1e	0.29	0/1149	0.51	0/1548
36	2e	0.30	0/1149	0.48	0/1548
37	1f	0.30	0/827	0.47	0/1120
37	2f	0.30	0/829	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.28	0/1254	0.43	0/1683
38	2g	0.28	0/1248	0.43	0/1676
39	1h	0.28	0/1118	0.49	0/1506
39	2h	0.28	0/1108	0.48	0/1494
40	1i	0.30	0/1005	0.50	0/1351
40	2i	0.30	0/985	0.53	0/1329
41	1j	0.28	0/732	0.47	0/993
41	2j	0.29	0/723	0.48	0/984
42	1k	0.28	0/849	0.48	0/1150
42	2k	0.28	0/848	0.49	0/1149
43	1l	0.29	0/937	0.49	0/1260
43	2l	0.29	0/937	0.49	0/1260
44	1m	0.28	0/924	0.46	0/1242
44	2m	0.30	0/905	0.48	0/1217
45	1n	0.30	0/501	0.47	0/664
45	2n	0.29	0/501	0.46	0/664
46	1o	0.29	0/739	0.43	0/985
46	2o	0.27	0/739	0.41	0/985
47	1p	0.28	0/697	0.51	0/939
47	2p	0.28	0/693	0.51	0/935
48	1q	0.29	0/836	0.47	0/1117
48	2q	0.28	0/836	0.48	0/1117
49	1r	0.29	0/560	0.49	0/746
49	2r	0.28	0/560	0.46	0/746
50	1s	0.27	0/663	0.47	0/895
50	2s	0.30	0/660	0.51	0/893
51	1t	0.28	0/734	0.43	0/969
51	2t	0.28	0/736	0.41	0/976
52	1u	0.28	0/203	0.46	0/266
52	2u	0.24	0/203	0.48	0/266
53	1y	0.29	0/776	0.47	0/1048
53	2y	0.29	0/761	0.48	0/1030
54	1w	0.50	0/69	0.92	0/106
54	2w	0.41	0/69	0.87	0/106
55	1x	0.59	0/44	1.30	0/67
55	2x	0.65	0/44	1.50	0/67
56	1v	0.35	0/22	0.55	0/28
56	2v	0.29	0/22	0.55	0/28
All	All	0.46	10/310298 (0.0%)	0.84	173/463749 (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
26	24	0	1
33	1b	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	368	U	C2-N3	66.62	1.84	1.37
32	1a	368	U	N3-C4	54.22	1.87	1.38
32	1a	368	U	N1-C2	45.83	1.79	1.38
32	1a	368	U	C4-C5	43.38	1.82	1.43
32	1a	368	U	N1-C6	42.86	1.76	1.38
32	1a	368	U	C5-C6	38.70	1.69	1.34
8	2I	82	ARG	CD-NE	32.04	2.00	1.46
8	2I	82	ARG	NE-CZ	13.15	1.50	1.33
8	2I	82	ARG	CG-CD	7.51	1.70	1.51
1	1A	2790	A	N9-C4	5.17	1.41	1.37

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2I	82	ARG	CD-NE-CZ	22.45	155.03	123.60
8	2I	82	ARG	NE-CZ-NH1	17.37	128.99	120.30
1	1A	1042	G	OP1-P-O3'	-11.28	80.39	105.20
8	2I	82	ARG	CG-CD-NE	11.18	135.28	111.80
1	2A	576	U	O5'-P-OP1	-10.88	95.91	105.70
1	2A	570	G	C5-C6-O6	-9.37	122.98	128.60
1	2A	1092	C	N1-C2-O2	9.32	124.50	118.90
1	1A	1042	G	OP2-P-O3'	-9.04	85.32	105.20
1	1A	570	G	C5-C6-O6	-8.97	123.22	128.60
1	1A	751	A	O5'-P-OP1	-8.78	97.80	105.70
1	1A	512	G	O4'-C1'-N9	8.75	115.20	108.20
1	2A	1092	C	C2-N1-C1'	8.70	128.37	118.80
1	2A	1648	C	O5'-P-OP1	-8.69	97.88	105.70
8	2I	82	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	2A	1092	C	N3-C2-O2	-8.36	116.05	121.90
1	1A	801	G	O5'-P-OP2	-8.32	98.22	105.70
32	2a	955	U	C5-C4-O4	8.32	130.89	125.90
32	2a	1004	A	O4'-C1'-N9	8.23	114.79	108.20
1	2A	1092	C	C6-N1-C2	-8.21	117.02	120.30
1	1A	576	U	O5'-P-OP1	-8.14	98.37	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	558	G	O5'-P-OP1	-8.11	98.40	105.70
1	1A	1372	U	C5-C4-O4	-8.10	121.04	125.90
32	1a	368	U	C2-N3-C4	-7.99	122.21	127.00
1	1A	1653	G	C8-N9-C4	-7.81	103.28	106.40
1	1A	948	G	O5'-P-OP1	-7.80	98.68	105.70
1	1A	1043	C	OP1-P-OP2	7.77	131.25	119.60
1	1A	575	A	O5'-P-OP1	-7.75	98.72	105.70
1	2A	801	G	O5'-P-OP2	-7.68	98.78	105.70
1	1A	570	G	C5-C6-N1	7.47	115.23	111.50
2	1B	57	A	N9-C4-C5	-7.36	102.86	105.80
1	1A	1791	A	O5'-P-OP1	-7.34	99.10	105.70
1	1A	1782	C	O5'-P-OP1	-7.12	99.29	105.70
32	2a	1397	C	C2-N1-C1'	7.11	126.62	118.80
1	2A	570	G	C4-C5-N7	7.10	113.64	110.80
32	1a	299	G	C5-C6-O6	-7.05	124.37	128.60
32	2a	266	G	P-O3'-C3'	7.04	128.15	119.70
1	1A	2074	U	O5'-P-OP1	-7.04	99.36	105.70
1	2A	31	C	O5'-P-OP1	-7.04	99.37	105.70
1	1A	1075	C	N1-C2-O2	7.03	123.12	118.90
1	2A	645	C	C2-N1-C1'	7.03	126.53	118.80
1	1A	570	G	C4-C5-N7	7.02	113.61	110.80
1	1A	784	A	P-O3'-C3'	6.99	128.09	119.70
1	1A	226	G	O4'-C1'-N9	6.94	113.75	108.20
1	1A	570	G	N9-C4-C5	-6.89	102.64	105.40
1	2A	2598	A	O5'-P-OP1	-6.84	99.55	105.70
1	1A	1372	U	N3-C4-O4	6.74	124.11	119.40
1	1A	531	C	O5'-P-OP2	-6.73	99.64	105.70
1	1A	2711	A	O5'-P-OP2	-6.72	99.65	105.70
32	2a	1183	A	P-O3'-C3'	6.68	127.72	119.70
1	1A	1799	G	C5-C6-O6	6.54	132.52	128.60
1	1A	845	G	O4'-C1'-N9	6.51	113.41	108.20
1	1A	1086	A	N1-C6-N6	-6.47	114.72	118.60
32	1a	368	U	C6-N1-C2	6.44	124.86	121.00
1	1A	2249	U	N3-C4-O4	-6.43	114.90	119.40
1	2A	2108	C	C2-N3-C4	6.43	123.12	119.90
1	1A	787	U	O5'-P-OP1	-6.43	99.91	105.70
1	2A	570	G	N1-C6-O6	6.43	123.76	119.90
1	1A	1075	C	C2-N1-C1'	6.39	125.83	118.80
1	2A	568	U	C5-C4-O4	-6.39	122.07	125.90
1	2A	2103	C	C2-N3-C4	6.35	123.08	119.90
1	1A	645	C	C2-N1-C1'	6.33	125.77	118.80
1	1A	1828	G	O5'-P-OP2	-6.31	100.02	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	645	C	N1-C2-O2	6.23	122.64	118.90
1	2A	2122	U	C5-C4-O4	6.17	129.60	125.90
1	2A	2191	G	C5-C6-O6	6.16	132.30	128.60
1	2A	1076	C	OP1-P-O3'	6.15	118.72	105.20
32	2a	754	C	C2-N1-C1'	6.15	125.56	118.80
1	1A	1653	G	N3-C4-C5	-6.10	125.55	128.60
1	1A	751	A	O5'-P-OP2	6.02	117.92	110.70
1	1A	961	C	O5'-P-OP2	-6.02	100.28	105.70
1	2A	570	G	C6-C5-N7	-5.95	126.83	130.40
1	1A	1602	U	N3-C4-O4	-5.92	115.25	119.40
1	1A	2848	G	O4'-C1'-N9	5.92	112.94	108.20
1	1A	1062	G	N3-C2-N2	-5.91	115.76	119.90
1	1A	1192	G	C8-N9-C4	5.89	108.76	106.40
32	2a	754	C	N1-C2-O2	5.87	122.42	118.90
1	2A	645	C	N1-C2-O2	5.85	122.41	118.90
32	1a	1020	U	N1-C2-O2	5.83	126.89	122.80
1	1A	1614	A	O5'-P-OP1	-5.83	100.45	105.70
1	2A	1992	G	P-O3'-C3'	5.83	126.69	119.70
1	2A	570	G	N9-C4-C5	-5.80	103.08	105.40
1	1A	2577	A	O5'-P-OP1	-5.78	100.50	105.70
1	2A	277	C	N1-C2-O2	5.78	122.37	118.90
1	1A	1428	C	C6-N1-C2	5.77	122.61	120.30
1	1A	2036	C	O5'-P-OP1	-5.74	100.54	105.70
1	2A	1779	U	O4'-C1'-N1	5.74	112.79	108.20
1	2A	2248	C	O5'-P-OP2	-5.72	100.55	105.70
32	1a	368	U	O4'-C1'-N1	5.72	112.77	108.20
1	1A	2689	U	P-O3'-C3'	5.71	126.56	119.70
1	1A	1052	C	C2-N1-C1'	5.70	125.07	118.80
1	1A	330	A	C2-N3-C4	-5.68	107.76	110.60
1	1A	2682	U	O5'-P-OP2	-5.68	100.59	105.70
1	1A	1192	G	N7-C8-N9	-5.67	110.27	113.10
32	2a	1065	U	P-O3'-C3'	5.67	126.50	119.70
1	2A	845	G	O4'-C1'-N9	5.67	112.73	108.20
1	1A	2103	C	N1-C2-O2	5.66	122.29	118.90
1	2A	1313	U	C2-N1-C1'	5.64	124.47	117.70
32	2a	997	U	C5-C4-O4	5.62	129.27	125.90
1	2A	1992	G	C8-N9-C4	-5.61	104.16	106.40
32	2a	1003	G	N3-C4-C5	-5.60	125.80	128.60
1	1A	1493	C	N1-C2-O2	5.60	122.26	118.90
32	2a	1183	A	OP1-P-O3'	5.60	117.52	105.20
32	1a	299	G	C4-C5-N7	5.57	113.03	110.80
32	2a	266	G	OP2-P-O3'	5.57	117.45	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	784	A	OP1-P-O3'	5.56	117.44	105.20
1	2A	1060	U	C2-N1-C1'	5.54	124.35	117.70
32	2a	1126	U	N1-C2-O2	5.54	126.68	122.80
32	2a	687	A	P-O3'-C3'	5.54	126.34	119.70
1	1A	784	A	N1-C6-N6	-5.53	115.28	118.60
1	1A	2430	A	C2-N3-C4	5.52	113.36	110.60
1	2A	2103	C	C5-C4-N4	5.51	124.06	120.20
1	2A	570	G	N3-C4-N9	5.48	129.29	126.00
1	2A	1379	A	OP2-P-O3'	5.45	117.20	105.20
1	2A	1092	C	C5-C6-N1	5.43	123.71	121.00
1	1A	330	A	N1-C2-N3	5.41	132.00	129.30
32	2a	1442	G	OP1-P-O3'	5.37	117.02	105.20
1	2A	1992	G	N3-C4-C5	-5.36	125.92	128.60
1	1A	271(Y)	U	O4'-C1'-N1	5.36	112.49	108.20
32	2a	1397	C	C6-N1-C1'	-5.34	114.39	120.80
1	1A	961	C	N1-C2-O2	-5.34	115.70	118.90
1	2A	1614	A	O5'-P-OP1	-5.34	100.90	105.70
32	1a	78	G	C4-N9-C1'	-5.33	119.58	126.50
1	2A	2181	G	C5-C6-O6	5.32	131.79	128.60
1	2A	2181	G	C6-N1-C2	5.32	128.29	125.10
1	1A	1416	G	O4'-C1'-N9	5.30	112.44	108.20
1	1A	961	C	C2-N1-C1'	-5.28	112.99	118.80
32	2a	955	U	C2-N3-C4	5.27	130.16	127.00
1	2A	512	G	O4'-C1'-N9	5.26	112.41	108.20
1	1A	249	C	N1-C2-O2	5.26	122.06	118.90
32	1a	78	G	C8-N9-C1'	5.26	133.84	127.00
1	2A	1073	A	N1-C6-N6	5.24	121.74	118.60
1	1A	783	A	C2-N3-C4	5.24	113.22	110.60
32	2a	754	C	N3-C2-O2	-5.22	118.25	121.90
1	1A	847	U	C2-N1-C1'	5.22	123.96	117.70
1	1A	2492	U	O5'-P-OP1	-5.21	101.01	105.70
1	1A	2685	G	N1-C6-O6	-5.21	116.77	119.90
1	1A	1190	G	C4-C5-N7	-5.20	108.72	110.80
1	1A	1190	G	C5-N7-C8	5.19	106.89	104.30
1	1A	1609	A	C8-N9-C4	5.19	107.87	105.80
1	2A	1092	C	C6-N1-C1'	-5.18	114.59	120.80
32	2a	1009	G	C5-C6-O6	5.18	131.71	128.60
1	1A	588	U	O5'-P-OP2	-5.17	101.05	105.70
1	2A	1076	C	P-O3'-C3'	5.17	125.90	119.70
32	1a	115	G	P-O3'-C3'	5.16	125.89	119.70
32	2a	204	U	C2-N1-C1'	5.16	123.89	117.70
1	1A	1493	C	N3-C2-O2	-5.16	118.29	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	783	A	C2-N3-C4	5.16	113.18	110.60
1	2A	645	C	C6-N1-C1'	-5.15	114.62	120.80
1	2A	1306	C	N1-C2-O2	5.15	121.99	118.90
1	2A	2689	U	P-O3'-C3'	5.15	125.88	119.70
1	2A	1111	A	O4'-C1'-N9	5.14	112.31	108.20
32	1a	365	U	C2-N1-C1'	5.14	123.87	117.70
32	1a	78	G	N3-C4-N9	-5.14	122.92	126.00
32	1a	960	U	N1-C2-O2	5.12	126.39	122.80
1	1A	2571	C	N1-C2-O2	-5.12	115.83	118.90
32	1a	1026	G	N3-C4-C5	-5.11	126.04	128.60
1	2A	1313	U	N3-C2-O2	-5.11	118.62	122.20
1	2A	192	C	O5'-P-OP1	-5.11	101.10	105.70
1	1A	386	G	O4'-C1'-N9	5.11	112.29	108.20
1	1A	2501	C	C2-N1-C1'	-5.10	113.19	118.80
32	2a	115	G	P-O3'-C3'	5.09	125.81	119.70
32	1a	1036	G	C4-N9-C1'	5.09	133.11	126.50
1	2A	894	C	N1-C2-O2	5.08	121.95	118.90
32	2a	1225	A	C6-N1-C2	5.08	121.65	118.60
1	2A	2108	C	C5-C4-N4	5.07	123.75	120.20
1	1A	1176	G	OP1-P-O3'	5.07	116.36	105.20
32	1a	299	G	N9-C4-C5	-5.07	103.37	105.40
32	2a	1225	A	C5-C6-N6	5.06	127.75	123.70
1	1A	1102	C	C2-N1-C1'	5.04	124.34	118.80
32	2a	1126	U	C2-N1-C1'	5.03	123.73	117.70
1	1A	1799	G	N1-C6-O6	-5.02	116.89	119.90
1	1A	645	C	C5-C6-N1	5.01	123.50	121.00
1	1A	2015	A	C8-N9-C4	5.00	107.80	105.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	231	GLU	Peptide
26	24	18	CYS	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100 100
3	2D	273/276 (99%)	255 (93%)	18 (7%)	0	100 100
4	1E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	15 28
4	2E	202/206 (98%)	187 (93%)	14 (7%)	1 (0%)	29 48
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	29 48
5	2F	201/210 (96%)	189 (94%)	9 (4%)	3 (2%)	10 18
6	1G	179/182 (98%)	157 (88%)	17 (10%)	5 (3%)	5 7
6	2G	179/182 (98%)	149 (83%)	24 (13%)	6 (3%)	3 5
7	1H	172/180 (96%)	160 (93%)	10 (6%)	2 (1%)	13 24
7	2H	171/180 (95%)	138 (81%)	31 (18%)	2 (1%)	13 24
8	1I	145/148 (98%)	126 (87%)	16 (11%)	3 (2%)	7 11
8	2I	144/148 (97%)	126 (88%)	13 (9%)	5 (4%)	3 4
9	1N	138/140 (99%)	136 (99%)	2 (1%)	0	100 100
9	2N	138/140 (99%)	126 (91%)	12 (9%)	0	100 100
10	1O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19 35
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100 100
11	1P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	22 39
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22 39
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100 100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100 100
13	1R	116/118 (98%)	112 (97%)	3 (3%)	1 (1%)	17 31
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100 100
14	1S	108/112 (96%)	100 (93%)	6 (6%)	2 (2%)	8 13
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	17 31
15	1T	129/146 (88%)	119 (92%)	10 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	2T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	19 35
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100 100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
17	1V	99/101 (98%)	93 (94%)	6 (6%)	0	100 100
17	2V	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	15 28
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100 100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100 100
19	1X	93/96 (97%)	89 (96%)	2 (2%)	2 (2%)	6 10
19	2X	93/96 (97%)	91 (98%)	2 (2%)	0	100 100
20	1Y	105/110 (96%)	95 (90%)	10 (10%)	0	100 100
20	2Y	105/110 (96%)	96 (91%)	9 (9%)	0	100 100
21	1Z	201/206 (98%)	182 (90%)	18 (9%)	1 (0%)	29 48
21	2Z	199/206 (97%)	172 (86%)	26 (13%)	1 (0%)	29 48
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
22	20	81/85 (95%)	73 (90%)	8 (10%)	0	100 100
23	11	95/98 (97%)	89 (94%)	6 (6%)	0	100 100
23	21	95/98 (97%)	89 (94%)	5 (5%)	1 (1%)	14 26
24	12	68/72 (94%)	68 (100%)	0	0	100 100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100 100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
26	14	67/71 (94%)	47 (70%)	17 (25%)	3 (4%)	2 3
26	24	67/71 (94%)	44 (66%)	14 (21%)	9 (13%)	0 0
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	62 (100%)	0	0	100 100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
33	1b	229/256 (90%)	189 (82%)	30 (13%)	10 (4%)	2 3
33	2b	229/256 (90%)	182 (80%)	37 (16%)	10 (4%)	2 3
34	1c	204/239 (85%)	180 (88%)	23 (11%)	1 (0%)	29 48
34	2c	204/239 (85%)	160 (78%)	37 (18%)	7 (3%)	3 5
35	1d	206/209 (99%)	185 (90%)	21 (10%)	0	100 100
35	2d	206/209 (99%)	184 (89%)	20 (10%)	2 (1%)	15 28
36	1e	146/162 (90%)	136 (93%)	8 (6%)	2 (1%)	11 20
36	2e	146/162 (90%)	134 (92%)	12 (8%)	0	100 100
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
37	2f	98/101 (97%)	90 (92%)	8 (8%)	0	100 100
38	1g	153/156 (98%)	143 (94%)	8 (5%)	2 (1%)	12 21
38	2g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	12 21
39	1h	135/138 (98%)	126 (93%)	9 (7%)	0	100 100
39	2h	135/138 (98%)	124 (92%)	11 (8%)	0	100 100
40	1i	125/128 (98%)	111 (89%)	11 (9%)	3 (2%)	6 9
40	2i	124/128 (97%)	108 (87%)	12 (10%)	4 (3%)	4 5
41	1j	95/105 (90%)	80 (84%)	11 (12%)	4 (4%)	3 3
41	2j	94/105 (90%)	77 (82%)	15 (16%)	2 (2%)	7 11
42	1k	112/129 (87%)	102 (91%)	10 (9%)	0	100 100
42	2k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	17 31
43	1l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	19 35
43	2l	119/132 (90%)	108 (91%)	10 (8%)	1 (1%)	19 35
44	1m	114/126 (90%)	100 (88%)	11 (10%)	3 (3%)	5 8
44	2m	112/126 (89%)	95 (85%)	12 (11%)	5 (4%)	2 3
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100 100
45	2n	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	9 16
46	1o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	13 24
46	2o	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	13 24
47	1p	80/88 (91%)	74 (92%)	6 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	2p	80/88 (91%)	69 (86%)	11 (14%)	0	100 100
48	1q	97/105 (92%)	88 (91%)	9 (9%)	0	100 100
48	2q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	15 28
49	1r	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	10 18
49	2r	66/88 (75%)	60 (91%)	6 (9%)	0	100 100
50	1s	81/93 (87%)	69 (85%)	12 (15%)	0	100 100
50	2s	81/93 (87%)	68 (84%)	13 (16%)	0	100 100
51	1t	94/106 (89%)	83 (88%)	9 (10%)	2 (2%)	7 11
51	2t	96/106 (91%)	82 (85%)	12 (12%)	2 (2%)	7 11
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
52	2u	21/27 (78%)	16 (76%)	5 (24%)	0	100 100
53	1y	95/113 (84%)	93 (98%)	2 (2%)	0	100 100
53	2y	94/113 (83%)	87 (93%)	5 (5%)	2 (2%)	7 11
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%)	10591 (91%)	925 (8%)	127 (1%)	14 26

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
8	1I	86	THR
14	1S	59	LYS
19	1X	94	GLY
26	14	61	ARG
33	1b	17	PHE
33	1b	127	ILE
33	1b	231	GLU
43	1l	91	LYS
44	1m	67	GLU
5	2F	130	ALA
26	24	46	GLN
26	24	51	ASP
33	2b	17	PHE
40	2i	43	ALA
40	2i	54	ASP
43	2l	91	LYS

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Mol	Chain	Res	Type
6	1G	44	GLY
7	1H	126	PRO
7	1H	159	GLU
33	1b	125	PRO
34	1c	98	ASN
41	1j	55	LYS
51	1t	47	GLY
6	2G	81	LYS
8	2I	10	GLU
8	2I	97	ILE
8	2I	98	ALA
26	24	45	GLY
26	24	48	ARG
26	24	62	ARG
26	24	63	TYR
33	2b	9	GLU
34	2c	50	ALA
34	2c	145	GLY
35	2d	22	LYS
38	2g	6	ARG
42	2k	105	VAL
53	2y	45	PRO
4	1E	52	LEU
6	1G	51	ARG
8	1I	71	ILE
14	1S	94	TYR
26	14	39	CYS
33	1b	8	LYS
33	1b	21	ARG
33	1b	63	MET
36	1e	38	GLN
38	1g	55	GLY
41	1j	77	PRO
6	2G	124	SER
7	2H	126	PRO
8	2I	83	ALA
26	24	55	ARG
33	2b	20	GLU
33	2b	95	GLN
34	2c	29	TYR
41	2j	78	ASN
41	2j	79	ARG

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Mol	Chain	Res	Type
44	2m	21	TYR
44	2m	23	TYR
6	1G	49	ASP
8	1I	105	HIS
21	1Z	52	SER
26	14	48	ARG
33	1b	20	GLU
33	1b	124	SER
38	1g	130	GLY
40	1i	48	GLU
41	1j	78	ASN
51	1t	95	ALA
5	2F	21	ALA
6	2G	96	ARG
8	2I	117	GLU
14	2S	96	GLY
15	2T	128	GLU
17	2V	79	VAL
23	21	3	LYS
33	2b	121	LEU
33	2b	124	SER
33	2b	128	GLU
34	2c	104	GLN
35	2d	176	LEU
40	2i	33	PHE
40	2i	44	VAL
44	2m	6	GLY
46	2o	79	ARG
53	2y	46	GLN
4	1E	28	ALA
36	1e	146	ALA
40	1i	109	VAL
4	2E	52	LEU
5	2F	146	ALA
6	2G	43	LEU
6	2G	126	ASP
11	2P	122	PRO
21	2Z	52	SER
26	24	49	PHE
34	2c	98	ASN
45	2n	38	GLY
51	2t	45	GLN

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Mol	Chain	Res	Type
6	1G	50	ALA
10	1O	29	ASN
11	1P	29	LYS
13	1R	71	GLN
33	1b	22	LYS
40	1i	53	VAL
41	1j	91	PRO
44	1m	21	TYR
44	1m	106	ASN
34	2c	174	PRO
48	2q	27	PHE
19	1X	67	GLY
46	1o	23	GLY
7	2H	93	GLY
33	2b	125	PRO
38	2g	55	GLY
51	2t	100	ILE
49	1r	27	GLY
5	1F	16	GLY
6	2G	87	PRO
26	24	50	VAL
44	2m	24	GLY
44	2m	113	PRO
33	2b	15	VAL
33	2b	232	PRO
34	2c	99	VAL

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%)	200 (94%)	14 (6%)	17 33
3	2D	215/218 (99%)	192 (89%)	23 (11%)	6 13
4	1E	164/166 (99%)	155 (94%)	9 (6%)	21 41
4	2E	164/166 (99%)	151 (92%)	13 (8%)	12 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	1F	160/166 (96%)	149 (93%)	11 (7%)	15 30
5	2F	159/166 (96%)	146 (92%)	13 (8%)	11 22
6	1G	144/156 (92%)	126 (88%)	18 (12%)	4 8
6	2G	142/156 (91%)	127 (89%)	15 (11%)	6 13
7	1H	144/148 (97%)	136 (94%)	8 (6%)	21 40
7	2H	143/148 (97%)	130 (91%)	13 (9%)	9 18
8	1I	111/124 (90%)	91 (82%)	20 (18%)	1 3
8	2I	108/124 (87%)	93 (86%)	15 (14%)	3 6
9	1N	119/119 (100%)	106 (89%)	13 (11%)	6 12
9	2N	118/119 (99%)	106 (90%)	12 (10%)	7 14
10	1O	100/100 (100%)	95 (95%)	5 (5%)	24 46
10	2O	100/100 (100%)	95 (95%)	5 (5%)	24 46
11	1P	115/116 (99%)	113 (98%)	2 (2%)	60 82
11	2P	115/116 (99%)	108 (94%)	7 (6%)	18 36
12	1Q	111/111 (100%)	107 (96%)	4 (4%)	35 61
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	18 34
13	1R	101/101 (100%)	95 (94%)	6 (6%)	19 37
13	2R	101/101 (100%)	92 (91%)	9 (9%)	9 19
14	1S	87/88 (99%)	80 (92%)	7 (8%)	12 23
14	2S	85/88 (97%)	73 (86%)	12 (14%)	3 6
15	1T	115/127 (91%)	107 (93%)	8 (7%)	15 29
15	2T	113/127 (89%)	108 (96%)	5 (4%)	28 52
16	1U	93/94 (99%)	89 (96%)	4 (4%)	29 53
16	2U	93/94 (99%)	85 (91%)	8 (9%)	10 20
17	1V	81/82 (99%)	79 (98%)	2 (2%)	47 73
17	2V	80/82 (98%)	68 (85%)	12 (15%)	3 5
18	1W	90/92 (98%)	84 (93%)	6 (7%)	16 31
18	2W	90/92 (98%)	84 (93%)	6 (7%)	16 31
19	1X	77/78 (99%)	72 (94%)	5 (6%)	17 33
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46 72
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	15 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	2Y	86/91 (94%)	79 (92%)	7 (8%)	11 23
21	1Z	169/179 (94%)	153 (90%)	16 (10%)	8 17
21	2Z	165/179 (92%)	148 (90%)	17 (10%)	7 14
22	10	65/67 (97%)	61 (94%)	4 (6%)	18 35
22	20	64/67 (96%)	63 (98%)	1 (2%)	62 84
23	11	79/83 (95%)	75 (95%)	4 (5%)	24 45
23	21	81/83 (98%)	76 (94%)	5 (6%)	18 35
24	12	65/67 (97%)	60 (92%)	5 (8%)	13 25
24	22	66/67 (98%)	58 (88%)	8 (12%)	5 9
25	13	51/52 (98%)	46 (90%)	5 (10%)	8 15
25	23	50/52 (96%)	48 (96%)	2 (4%)	31 56
26	14	58/63 (92%)	51 (88%)	7 (12%)	5 9
26	24	54/63 (86%)	43 (80%)	11 (20%)	1 2
27	15	51/52 (98%)	48 (94%)	3 (6%)	19 37
27	25	50/52 (96%)	47 (94%)	3 (6%)	19 37
28	16	51/52 (98%)	43 (84%)	8 (16%)	2 4
28	26	50/52 (96%)	44 (88%)	6 (12%)	5 9
29	17	41/42 (98%)	37 (90%)	4 (10%)	8 15
29	27	41/42 (98%)	34 (83%)	7 (17%)	2 3
30	18	54/55 (98%)	48 (89%)	6 (11%)	6 11
30	28	54/55 (98%)	46 (85%)	8 (15%)	3 5
31	19	34/34 (100%)	33 (97%)	1 (3%)	42 69
31	29	34/34 (100%)	32 (94%)	2 (6%)	19 37
33	1b	191/220 (87%)	166 (87%)	25 (13%)	4 7
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4 7
34	1c	144/188 (77%)	136 (94%)	8 (6%)	21 40
34	2c	140/188 (74%)	118 (84%)	22 (16%)	2 4
35	1d	171/181 (94%)	150 (88%)	21 (12%)	4 9
35	2d	172/181 (95%)	156 (91%)	16 (9%)	9 17
36	1e	114/123 (93%)	105 (92%)	9 (8%)	12 24
36	2e	114/123 (93%)	104 (91%)	10 (9%)	10 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	1f	85/90 (94%)	75 (88%)	10 (12%)	5 10
37	2f	85/90 (94%)	80 (94%)	5 (6%)	19 37
38	1g	120/127 (94%)	110 (92%)	10 (8%)	11 22
38	2g	119/127 (94%)	105 (88%)	14 (12%)	5 10
39	1h	116/119 (98%)	106 (91%)	10 (9%)	10 20
39	2h	114/119 (96%)	104 (91%)	10 (9%)	10 19
40	1i	91/99 (92%)	77 (85%)	14 (15%)	2 5
40	2i	88/99 (89%)	80 (91%)	8 (9%)	9 18
41	1j	68/92 (74%)	60 (88%)	8 (12%)	5 10
41	2j	68/92 (74%)	60 (88%)	8 (12%)	5 10
42	1k	83/99 (84%)	77 (93%)	6 (7%)	14 28
42	2k	83/99 (84%)	73 (88%)	10 (12%)	5 9
43	1l	96/108 (89%)	89 (93%)	7 (7%)	14 27
43	2l	96/108 (89%)	90 (94%)	6 (6%)	18 34
44	1m	90/101 (89%)	83 (92%)	7 (8%)	12 24
44	2m	87/101 (86%)	73 (84%)	14 (16%)	2 4
45	1n	49/50 (98%)	41 (84%)	8 (16%)	2 4
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7 14
46	1o	78/80 (98%)	73 (94%)	5 (6%)	17 33
46	2o	78/80 (98%)	71 (91%)	7 (9%)	9 19
47	1p	69/74 (93%)	57 (83%)	12 (17%)	2 3
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5 10
48	1q	94/97 (97%)	86 (92%)	8 (8%)	10 21
48	2q	94/97 (97%)	91 (97%)	3 (3%)	39 65
49	1r	59/77 (77%)	51 (86%)	8 (14%)	3 7
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7 14
50	1s	68/80 (85%)	63 (93%)	5 (7%)	13 27
50	2s	67/80 (84%)	62 (92%)	5 (8%)	13 26
51	1t	71/82 (87%)	64 (90%)	7 (10%)	8 15
51	2t	70/82 (85%)	66 (94%)	4 (6%)	20 39
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	2u	18/22 (82%)	18 (100%)	0	100 100
53	1y	82/98 (84%)	77 (94%)	5 (6%)	18 36
53	2y	79/98 (81%)	69 (87%)	10 (13%)	4 8
56	1v	3/3 (100%)	2 (67%)	1 (33%)	0 0
56	2v	3/3 (100%)	2 (67%)	1 (33%)	0 0
All	All	9537/10266 (93%)	8680 (91%)	857 (9%)	9 19

All (857) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	39	LYS
3	1D	94	LEU
3	1D	111	LEU
3	1D	112	GLN
3	1D	141	VAL
3	1D	171	ASP
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	7	VAL
4	1E	9	VAL
4	1E	87	GLU
4	1E	113	PHE
4	1E	116	VAL
4	1E	119	ARG
4	1E	181	LEU
4	1E	184	VAL
4	1E	202	LYS
5	1F	18	ARG
5	1F	23	ASP
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	132	VAL

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Mol	Chain	Res	Type
5	1F	162	LEU
5	1F	183	VAL
5	1F	189	THR
5	1F	192	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	21	ARG
6	1G	49	ASP
6	1G	53	LEU
6	1G	62	LEU
6	1G	67	LYS
6	1G	75	LYS
6	1G	79	ASN
6	1G	82	LEU
6	1G	86	MET
6	1G	92	VAL
6	1G	109	VAL
6	1G	126	ASP
6	1G	133	LEU
6	1G	144	ILE
6	1G	155	MET
6	1G	175	LEU
7	1H	23	ARG
7	1H	24	VAL
7	1H	44	VAL
7	1H	58	GLU
7	1H	101	ARG
7	1H	107	VAL
7	1H	111	HIS
7	1H	124	GLU
8	1I	9	LEU
8	1I	14	ASP
8	1I	20	ASP
8	1I	38	LEU
8	1I	42	SER
8	1I	43	ASN
8	1I	44	LEU
8	1I	60	GLU
8	1I	61	ARG
8	1I	66	GLU
8	1I	68	LEU
8	1I	78	THR

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Mol	Chain	Res	Type
8	1I	87	LYS
8	1I	92	VAL
8	1I	96	ASP
8	1I	102	SER
8	1I	108	THR
8	1I	109	ILE
8	1I	117	GLU
8	1I	140	LEU
9	1N	1	MET
9	1N	5	VAL
9	1N	8	GLN
9	1N	14	VAL
9	1N	34	LEU
9	1N	48	MET
9	1N	62	VAL
9	1N	67	LEU
9	1N	73	THR
9	1N	87	LEU
9	1N	89	LYS
9	1N	99	LEU
9	1N	133	GLN
10	1O	9	GLU
10	1O	28	SER
10	1O	69	ILE
10	1O	96	THR
10	1O	113	LYS
11	1P	1	MET
11	1P	95	VAL
12	1Q	60	ARG
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	112	GLU
13	1R	14	SER
13	1R	29	LEU
13	1R	36	THR
13	1R	56	LYS
13	1R	67	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	46	VAL
14	1S	49	VAL
14	1S	50	SER

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Mol	Chain	Res	Type
14	1S	52	SER
14	1S	59	LYS
14	1S	69	VAL
15	1T	6	LEU
15	1T	33	LYS
15	1T	53	ARG
15	1T	78	LEU
15	1T	82	LEU
15	1T	85	LYS
15	1T	108	ARG
15	1T	112	ARG
16	1U	5	LYS
16	1U	31	SER
16	1U	74	LEU
16	1U	104	GLN
17	1V	72	VAL
17	1V	79	VAL
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	100	THR
18	1W	107	LEU
19	1X	35	THR
19	1X	38	GLU
19	1X	45	THR
19	1X	88	LYS
19	1X	95	LEU
20	1Y	23	ARG
20	1Y	31	LEU
20	1Y	43	ASN
20	1Y	72	VAL
20	1Y	99	CYS
20	1Y	107	ASP
21	1Z	18	LEU
21	1Z	19	ARG
21	1Z	31	ARG
21	1Z	50	GLN
21	1Z	80	ARG
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	98	MET

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Mol	Chain	Res	Type
21	1Z	118	GLN
21	1Z	132	ASN
21	1Z	150	LEU
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	161	VAL
21	1Z	170	THR
21	1Z	198	LYS
22	10	10	THR
22	10	14	ARG
22	10	74	ARG
22	10	82	ARG
23	11	30	VAL
23	11	35	THR
23	11	40	ARG
23	11	94	LEU
24	12	27	GLU
24	12	30	ARG
24	12	32	LEU
24	12	38	GLN
24	12	41	ILE
25	13	8	LEU
25	13	32	GLN
25	13	54	VAL
25	13	56	VAL
25	13	58	VAL
26	14	27	THR
26	14	33	VAL
26	14	49	PHE
26	14	56	VAL
26	14	58	ARG
26	14	60	GLN
26	14	68	ARG
27	15	6	VAL
27	15	16	ARG
27	15	37	LYS
28	16	5	VAL
28	16	6	ARG
28	16	19	ARG
28	16	44	ARG
28	16	47	THR
28	16	48	VAL

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Mol	Chain	Res	Type
28	16	49	HIS
28	16	52	VAL
29	17	42	LEU
29	17	43	THR
29	17	46	VAL
29	17	47	ARG
30	18	14	VAL
30	18	23	VAL
30	18	29	LYS
30	18	31	HIS
30	18	34	TRP
30	18	58	ILE
31	19	13	LYS
33	1b	8	LYS
33	1b	10	LEU
33	1b	15	VAL
33	1b	17	PHE
33	1b	23	ARG
33	1b	28	PHE
33	1b	42	ILE
33	1b	51	LEU
33	1b	90	MET
33	1b	93	VAL
33	1b	96	ARG
33	1b	106	LYS
33	1b	115	LEU
33	1b	140	HIS
33	1b	145	LEU
33	1b	160	ASP
33	1b	162	ILE
33	1b	179	LYS
33	1b	185	ILE
33	1b	187	LEU
33	1b	195	ASP
33	1b	223	ILE
33	1b	224	GLN
33	1b	229	VAL
33	1b	230	VAL
34	1c	70	VAL
34	1c	89	GLU
34	1c	98	ASN
34	1c	105	GLU

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Mol	Chain	Res	Type
34	1c	124	ILE
34	1c	144	SER
34	1c	157	ILE
34	1c	175	LEU
35	1d	3	ARG
35	1d	5	ILE
35	1d	17	VAL
35	1d	18	LYS
35	1d	19	LEU
35	1d	26	CYS
35	1d	52	SER
35	1d	58	LEU
35	1d	67	ILE
35	1d	77	ASN
35	1d	107	ARG
35	1d	134	ASP
35	1d	137	SER
35	1d	144	ASP
35	1d	157	LEU
35	1d	178	VAL
35	1d	182	LYS
35	1d	187	ARG
35	1d	188	LEU
35	1d	194	LEU
35	1d	196	LEU
36	1e	12	LEU
36	1e	34	VAL
36	1e	41	VAL
36	1e	68	GLU
36	1e	69	VAL
36	1e	79	GLU
36	1e	115	VAL
36	1e	131	ILE
36	1e	147	ASP
37	1f	10	LEU
37	1f	15	ASP
37	1f	21	LEU
37	1f	40	VAL
37	1f	42	GLU
37	1f	45	LEU
37	1f	57	GLN
37	1f	69	GLU

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Mol	Chain	Res	Type
37	1f	73	ASN
37	1f	89	MET
38	1g	6	ARG
38	1g	13	GLN
38	1g	52	GLU
38	1g	56	GLN
38	1g	76	ARG
38	1g	86	GLN
38	1g	97	GLN
38	1g	113	GLU
38	1g	126	ASP
38	1g	144	MET
39	1h	22	GLU
39	1h	25	ASP
39	1h	26	VAL
39	1h	39	LEU
39	1h	51	VAL
39	1h	52	ASP
39	1h	98	LYS
39	1h	104	ARG
39	1h	127	LEU
39	1h	133	LEU
40	1i	17	VAL
40	1i	25	LYS
40	1i	29	ASN
40	1i	47	LEU
40	1i	50	LEU
40	1i	53	VAL
40	1i	56	LEU
40	1i	81	ILE
40	1i	87	GLN
40	1i	92	TYR
40	1i	96	LEU
40	1i	104	ARG
40	1i	111	ARG
40	1i	125	TYR
41	1j	5	ARG
41	1j	29	ARG
41	1j	34	VAL
41	1j	38	ILE
41	1j	67	THR
41	1j	72	VAL

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Mol	Chain	Res	Type
41	1j	84	GLN
41	1j	94	VAL
42	1k	16	SER
42	1k	31	THR
42	1k	41	THR
42	1k	77	MET
42	1k	93	GLN
42	1k	122	LYS
43	1l	18	VAL
43	1l	22	SER
43	1l	33	ARG
43	1l	42	THR
43	1l	44	THR
43	1l	83	VAL
43	1l	97	ARG
44	1m	3	ARG
44	1m	4	ILE
44	1m	9	ILE
44	1m	11	ARG
44	1m	14	ARG
44	1m	86	CYS
44	1m	99	ARG
45	1n	3	ARG
45	1n	11	LYS
45	1n	13	THR
45	1n	16	PHE
45	1n	18	VAL
45	1n	22	THR
45	1n	29	ARG
45	1n	33	VAL
46	1o	3	ILE
46	1o	25	THR
46	1o	39	LEU
46	1o	76	GLU
46	1o	84	LYS
47	1p	6	LEU
47	1p	8	ARG
47	1p	20	VAL
47	1p	29	ASP
47	1p	35	LYS
47	1p	42	ARG
47	1p	43	LYS

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Mol	Chain	Res	Type
47	1p	47	ASP
47	1p	53	VAL
47	1p	62	VAL
47	1p	67	THR
47	1p	72	ARG
48	1q	6	LEU
48	1q	9	VAL
48	1q	35	VAL
48	1q	45	HIS
48	1q	52	LYS
48	1q	61	GLU
48	1q	85	VAL
48	1q	93	GLN
49	1r	23	LYS
49	1r	25	THR
49	1r	26	LEU
49	1r	31	LEU
49	1r	37	VAL
49	1r	42	ARG
49	1r	46	GLU
49	1r	76	LEU
50	1s	28	LYS
50	1s	40	ILE
50	1s	48	THR
50	1s	63	THR
50	1s	66	MET
51	1t	9	ASN
51	1t	10	LEU
51	1t	15	ARG
51	1t	24	LEU
51	1t	34	LYS
51	1t	37	SER
51	1t	100	ILE
52	1u	3	LYS
53	1y	23	ARG
53	1y	42	SER
53	1y	46	GLN
53	1y	60	VAL
53	1y	61	LEU
56	1v	2	THR
3	2D	3	VAL
3	2D	18	VAL

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Mol	Chain	Res	Type
3	2D	27	THR
3	2D	38	LYS
3	2D	61	LEU
3	2D	71	ASP
3	2D	75	ILE
3	2D	94	LEU
3	2D	103	ARG
3	2D	113	VAL
3	2D	134	ARG
3	2D	141	VAL
3	2D	155	LEU
3	2D	173	VAL
3	2D	183	ARG
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	260	ARG
3	2D	274	ARG
3	2D	276	LYS
4	2E	38	THR
4	2E	73	GLU
4	2E	90	THR
4	2E	97	LYS
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	152	LYS
4	2E	154	LYS
4	2E	181	LEU
4	2E	184	VAL
4	2E	188	VAL
4	2E	195	LEU
5	2F	15	SER
5	2F	17	ARG
5	2F	27	GLU
5	2F	33	LEU
5	2F	57	VAL
5	2F	74	ARG
5	2F	140	LEU
5	2F	158	THR

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Mol	Chain	Res	Type
5	2F	170	LEU
5	2F	175	THR
5	2F	179	GLU
5	2F	192	LEU
5	2F	197	ASP
6	2G	3	LEU
6	2G	9	ARG
6	2G	28	VAL
6	2G	43	LEU
6	2G	51	ARG
6	2G	53	LEU
6	2G	58	GLN
6	2G	62	LEU
6	2G	78	SER
6	2G	86	MET
6	2G	98	ARG
6	2G	115	ARG
6	2G	126	ASP
6	2G	133	LEU
6	2G	143	GLU
7	2H	13	LYS
7	2H	32	GLU
7	2H	33	LEU
7	2H	38	SER
7	2H	43	VAL
7	2H	44	VAL
7	2H	52	VAL
7	2H	71	LEU
7	2H	105	LEU
7	2H	106	THR
7	2H	114	VAL
7	2H	130	ARG
7	2H	152	ARG
8	2I	7	GLU
8	2I	38	LEU
8	2I	47	LEU
8	2I	54	GLN
8	2I	58	LEU
8	2I	64	GLU
8	2I	70	GLU
8	2I	74	ASN
8	2I	76	THR

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Mol	Chain	Res	Type
8	2I	82	ARG
8	2I	92	VAL
8	2I	107	VAL
8	2I	125	GLU
8	2I	129	THR
8	2I	142	VAL
9	2N	9	VAL
9	2N	12	ARG
9	2N	15	LEU
9	2N	28	THR
9	2N	33	LEU
9	2N	48	MET
9	2N	67	LEU
9	2N	73	THR
9	2N	74	ARG
9	2N	87	LEU
9	2N	99	LEU
9	2N	140	VAL
10	2O	35	VAL
10	2O	69	ILE
10	2O	70	LYS
10	2O	78	ARG
10	2O	88	ASN
11	2P	15	ARG
11	2P	29	LYS
11	2P	95	VAL
11	2P	125	VAL
11	2P	147	LEU
11	2P	148	LEU
11	2P	149	GLU
12	2Q	1	MET
12	2Q	7	MET
12	2Q	75	THR
12	2Q	85	LYS
12	2Q	109	VAL
12	2Q	124	LYS
12	2Q	133	ARG
13	2R	20	LEU
13	2R	29	LEU
13	2R	33	ARG
13	2R	36	THR
13	2R	67	LEU

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Mol	Chain	Res	Type
13	2R	86	ARG
13	2R	100	LEU
13	2R	102	GLU
13	2R	114	VAL
14	2S	8	GLU
14	2S	12	PHE
14	2S	13	ARG
14	2S	25	ARG
14	2S	50	SER
14	2S	52	SER
14	2S	53	SER
14	2S	64	GLU
14	2S	80	LEU
14	2S	85	VAL
14	2S	110	LEU
14	2S	111	GLU
15	2T	36	GLU
15	2T	42	ILE
15	2T	53	ARG
15	2T	54	ARG
15	2T	67	SER
16	2U	5	LYS
16	2U	30	LYS
16	2U	31	SER
16	2U	55	ARG
16	2U	59	ARG
16	2U	74	LEU
16	2U	100	VAL
16	2U	104	GLN
17	2V	1	MET
17	2V	5	VAL
17	2V	26	ASP
17	2V	32	THR
17	2V	35	LEU
17	2V	39	LEU
17	2V	46	VAL
17	2V	53	GLU
17	2V	62	LEU
17	2V	71	LEU
17	2V	79	VAL
17	2V	96	ILE
18	2W	11	ARG

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Mol	Chain	Res	Type
18	2W	17	VAL
18	2W	23	LEU
18	2W	68	ARG
18	2W	100	THR
18	2W	107	LEU
19	2X	81	VAL
19	2X	95	LEU
20	2Y	3	VAL
20	2Y	6	HIS
20	2Y	44	ILE
20	2Y	55	TYR
20	2Y	90	LEU
20	2Y	99	CYS
20	2Y	101	LYS
21	2Z	2	GLU
21	2Z	31	ARG
21	2Z	41	LEU
21	2Z	53	ILE
21	2Z	67	LEU
21	2Z	72	ARG
21	2Z	73	GLN
21	2Z	86	VAL
21	2Z	107	THR
21	2Z	121	HIS
21	2Z	123	ASP
21	2Z	135	GLU
21	2Z	175	VAL
21	2Z	182	LYS
21	2Z	190	GLU
21	2Z	193	GLU
21	2Z	198	LYS
22	20	36	ILE
23	21	4	VAL
23	21	21	ARG
23	21	40	ARG
23	21	85	LEU
23	21	95	LEU
24	22	1	MET
24	22	17	SER
24	22	31	GLU
24	22	32	LEU
24	22	45	SER

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Mol	Chain	Res	Type
24	22	53	LEU
24	22	62	THR
24	22	64	LEU
25	23	54	VAL
25	23	57	GLU
26	24	8	LYS
26	24	9	LEU
26	24	20	ASN
26	24	21	VAL
26	24	27	THR
26	24	40	HIS
26	24	42	PHE
26	24	50	VAL
26	24	52	THR
26	24	53	GLU
26	24	61	ARG
27	25	29	THR
27	25	40	LYS
27	25	55	ARG
28	26	14	THR
28	26	20	ASN
28	26	30	THR
28	26	34	LEU
28	26	50	ARG
28	26	54	ILE
29	27	10	ARG
29	27	23	ARG
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
29	27	47	ARG
29	27	48	LYS
30	28	14	VAL
30	28	23	VAL
30	28	26	LYS
30	28	31	HIS
30	28	34	TRP
30	28	46	ARG
30	28	49	VAL
30	28	50	LEU
31	29	4	ARG
31	29	17	ILE

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Mol	Chain	Res	Type
33	2b	7	VAL
33	2b	8	LYS
33	2b	15	VAL
33	2b	16	HIS
33	2b	17	PHE
33	2b	24	TRP
33	2b	39	ILE
33	2b	44	LEU
33	2b	63	MET
33	2b	74	LYS
33	2b	76	GLN
33	2b	83	MET
33	2b	96	ARG
33	2b	97	TRP
33	2b	128	GLU
33	2b	130	ARG
33	2b	154	LEU
33	2b	157	ARG
33	2b	175	ARG
33	2b	189	ASP
33	2b	191	ASP
33	2b	193	ASP
33	2b	196	LEU
33	2b	215	LEU
33	2b	230	VAL
34	2c	3	ASN
34	2c	15	THR
34	2c	16	ARG
34	2c	30	ARG
34	2c	32	LEU
34	2c	33	LEU
34	2c	52	LEU
34	2c	56	ASP
34	2c	98	ASN
34	2c	105	GLU
34	2c	111	LEU
34	2c	112	SER
34	2c	128	PHE
34	2c	131	ARG
34	2c	136	GLN
34	2c	152	ILE
34	2c	154	SER

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Mol	Chain	Res	Type
34	2c	164	ARG
34	2c	179	ARG
34	2c	181	ASN
34	2c	195	VAL
34	2c	206	GLU
35	2d	13	ARG
35	2d	19	LEU
35	2d	33	MET
35	2d	49	ARG
35	2d	50	ARG
35	2d	83	SER
35	2d	106	TYR
35	2d	108	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	141	ARG
35	2d	160	GLN
35	2d	170	VAL
35	2d	175	SER
35	2d	187	ARG
35	2d	194	LEU
36	2e	10	MET
36	2e	11	ILE
36	2e	34	VAL
36	2e	41	VAL
36	2e	45	PHE
36	2e	47	LYS
36	2e	68	GLU
36	2e	69	VAL
36	2e	81	GLU
36	2e	115	VAL
37	2f	40	VAL
37	2f	41	GLU
37	2f	57	GLN
37	2f	93	SER
37	2f	95	GLU
38	2g	6	ARG
38	2g	9	VAL
38	2g	15	ASP
38	2g	16	LEU
38	2g	21	VAL
38	2g	33	ASP

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Mol	Chain	Res	Type
38	2g	47	CYS
38	2g	51	GLN
38	2g	75	VAL
38	2g	92	SER
38	2g	104	LEU
38	2g	115	ARG
38	2g	126	ASP
38	2g	153	HIS
39	2h	2	LEU
39	2h	15	ASN
39	2h	29	SER
39	2h	49	GLU
39	2h	85	ARG
39	2h	112	LEU
39	2h	114	THR
39	2h	119	LEU
39	2h	125	ARG
39	2h	133	LEU
40	2i	14	VAL
40	2i	33	PHE
40	2i	34	ASN
40	2i	42	ARG
40	2i	65	VAL
40	2i	87	GLN
40	2i	102	LEU
40	2i	113	LYS
41	2j	34	VAL
41	2j	38	ILE
41	2j	47	PHE
41	2j	58	ASP
41	2j	71	LEU
41	2j	73	ASP
41	2j	84	GLN
41	2j	95	GLU
42	2k	16	SER
42	2k	28	THR
42	2k	53	SER
42	2k	63	LEU
42	2k	81	ASP
42	2k	93	GLN
42	2k	109	VAL
42	2k	114	VAL

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Mol	Chain	Res	Type
42	2k	116	HIS
42	2k	117	ASN
43	2l	6	THR
43	2l	28	LYS
43	2l	33	ARG
43	2l	67	THR
43	2l	79	GLU
43	2l	89	ARG
44	2m	8	GLU
44	2m	13	LYS
44	2m	15	VAL
44	2m	48	LEU
44	2m	49	THR
44	2m	50	GLU
44	2m	59	TYR
44	2m	60	VAL
44	2m	62	ASN
44	2m	93	ARG
44	2m	96	LEU
44	2m	102	ARG
44	2m	106	ASN
44	2m	115	LYS
45	2n	3	ARG
45	2n	7	ILE
45	2n	16	PHE
45	2n	18	VAL
45	2n	39	LEU
46	2o	3	ILE
46	2o	4	THR
46	2o	5	LYS
46	2o	24	SER
46	2o	39	LEU
46	2o	84	LYS
46	2o	87	ILE
47	2p	11	SER
47	2p	16	HIS
47	2p	20	VAL
47	2p	21	VAL
47	2p	45	THR
47	2p	67	THR
47	2p	69	THR
47	2p	75	ARG

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Mol	Chain	Res	Type
48	2q	6	LEU
48	2q	52	LYS
48	2q	57	VAL
49	2r	29	PHE
49	2r	31	LEU
49	2r	37	VAL
49	2r	47	THR
49	2r	82	THR
49	2r	84	LYS
50	2s	32	LYS
50	2s	37	ARG
50	2s	41	VAL
50	2s	63	THR
50	2s	81	ARG
51	2t	15	ARG
51	2t	55	ILE
51	2t	84	LEU
51	2t	100	ILE
53	2y	6	THR
53	2y	16	ILE
53	2y	24	LEU
53	2y	29	LYS
53	2y	32	THR
53	2y	41	LEU
53	2y	46	GLN
53	2y	56	THR
53	2y	62	VAL
53	2y	78	ILE
56	2v	2	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) 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
7	1H	139	GLN
8	1I	43	ASN
9	1N	8	GLN
9	1N	69	GLN
9	1N	94	HIS

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Mol	Chain	Res	Type
9	1N	133	GLN
10	1O	3	GLN
10	1O	88	ASN
11	1P	84	ASN
14	1S	84	GLN
15	1T	58	ASN
15	1T	123	GLN
16	1U	117	GLN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	50	GLN
23	11	56	GLN
25	13	32	GLN
26	14	20	ASN
33	1b	212	GLN
34	1c	6	HIS
34	1c	102	ASN
34	1c	104	GLN
34	1c	110	ASN
35	1d	77	ASN
35	1d	129	ASN
36	1e	78	HIS
37	1f	57	GLN
37	1f	84	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	37	ASN
38	1g	64	GLN
38	1g	86	GLN
38	1g	96	GLN
40	1i	3	GLN
40	1i	31	GLN
40	1i	73	GLN
40	1i	87	GLN
40	1i	124	GLN
41	1j	13	HIS
41	1j	56	HIS
41	1j	84	GLN
42	1k	93	GLN
42	1k	117	ASN
43	1l	99	HIS

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Mol	Chain	Res	Type
44	1m	106	ASN
46	1o	13	GLN
47	1p	16	HIS
48	1q	16	GLN
50	1s	69	HIS
50	1s	83	HIS
51	1t	42	GLN
51	1t	90	GLN
53	1y	38	HIS
53	1y	89	GLN
3	2D	87	ASN
3	2D	143	HIS
3	2D	253	GLN
4	2E	48	GLN
6	2G	58	GLN
6	2G	79	ASN
6	2G	130	ASN
7	2H	143	GLN
8	2I	43	ASN
8	2I	105	HIS
8	2I	133	HIS
12	2Q	123	HIS
15	2T	38	ASN
15	2T	58	ASN
15	2T	123	GLN
16	2U	104	GLN
17	2V	64	HIS
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
21	2Z	73	GLN
24	22	9	GLN
26	24	60	GLN
28	26	20	ASN
30	28	35	GLN
33	2b	19	HIS
33	2b	212	GLN
33	2b	224	GLN
34	2c	176	HIS
34	2c	181	ASN
35	2d	42	GLN
35	2d	77	ASN

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Mol	Chain	Res	Type
35	2d	116	GLN
35	2d	123	HIS
35	2d	160	GLN
35	2d	161	ASN
35	2d	201	GLN
36	2e	141	GLN
37	2f	100	ASN
38	2g	13	GLN
38	2g	28	ASN
38	2g	56	GLN
38	2g	64	GLN
39	2h	15	ASN
40	2i	58	HIS
41	2j	62	HIS
41	2j	84	GLN
42	2k	62	GLN
42	2k	116	HIS
42	2k	117	ASN
43	2l	99	HIS
44	2m	62	ASN
44	2m	77	ASN
44	2m	92	HIS
44	2m	106	ASN
46	2o	9	GLN
46	2o	13	GLN
46	2o	37	ASN
50	2s	14	HIS
50	2s	23	ASN
51	2t	90	GLN
53	2y	46	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	427 (14%)	28 (0%)
1	2A	2856/2915 (97%)	497 (17%)	35 (1%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	119/121 (98%)	16 (13%)	0
32	1a	1494/1521 (98%)	264 (17%)	0
32	2a	1498/1521 (98%)	290 (19%)	0
54	1w	3/5 (60%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	2w	3/5 (60%)	1 (33%)	0
55	1x	1/4 (25%)	0	0
55	2x	1/4 (25%)	0	0
All	All	8957/9132 (98%)	1504 (16%)	63 (0%)

All (1504) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	50	U
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	92	A
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	197	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	219	G
1	1A	222	A
1	1A	229	A
1	1A	248	G
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	275	G

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Mol	Chain	Res	Type
1	1A	279	C
1	1A	280	C
1	1A	283	A
1	1A	311	A
1	1A	330	A
1	1A	346	A
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	447	A
1	1A	451	C
1	1A	454	A
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	615	G
1	1A	616	G
1	1A	621	A
1	1A	627	A
1	1A	637	A

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Mol	Chain	Res	Type
1	1A	645	C
1	1A	646	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	731	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	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	896	A
1	1A	897	C
1	1A	899	A
1	1A	900	A
1	1A	907	U
1	1A	910	A
1	1A	915	C
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A

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Mol	Chain	Res	Type
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1026	U
1	1A	1033	U
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1058	G
1	1A	1061	U
1	1A	1062	G
1	1A	1063	G
1	1A	1065	U
1	1A	1066	U
1	1A	1067	A
1	1A	1070	A
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	1080	C
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1096	A
1	1A	1097	U
1	1A	1098	A
1	1A	1100	C
1	1A	1101	U
1	1A	1104	C
1	1A	1109	C
1	1A	1110	G
1	1A	1112	G
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1141	U

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Mol	Chain	Res	Type
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1210	A
1	1A	1211	U
1	1A	1218	C
1	1A	1220	A
1	1A	1250	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1345	C
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	1437	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

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Mol	Chain	Res	Type
1	1A	1467	C
1	1A	1471	A
1	1A	1473	G
1	1A	1478	G
1	1A	1482	G
1	1A	1484	G
1	1A	1490	A
1	1A	1493	C
1	1A	1505	C
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1523	U
1	1A	1525	G
1	1A	1529	G
1	1A	1531	C
1	1A	1542	A
1	1A	1543	C
1	1A	1558	A
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1616	A
1	1A	1634	A
1	1A	1639	U
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	1717	G
1	1A	1722	A
1	1A	1739	U

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Mol	Chain	Res	Type
1	1A	1740	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
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A
1	1A	1816	G
1	1A	1839	G
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1914	C
1	1A	1919	A
1	1A	1929	G
1	1A	1930	G
1	1A	1936	A
1	1A	1938	A
1	1A	1941	C
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1985	G
1	1A	1993	U
1	1A	1997	G
1	1A	2023	G
1	1A	2031	A

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Mol	Chain	Res	Type
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2093	G
1	1A	2103	C
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	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	2146	C
1	1A	2148	G
1	1A	2158	A
1	1A	2159	G
1	1A	2164	C
1	1A	2171	A
1	1A	2172	U
1	1A	2181	G
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

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Mol	Chain	Res	Type
1	1A	2208	A
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2267	A
1	1A	2268	A
1	1A	2269	A
1	1A	2273	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	2321	G
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2393	A
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2424	C
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2434	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A

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Mol	Chain	Res	Type
1	1A	2468	G
1	1A	2476	A
1	1A	2502	G
1	1A	2504	U
1	1A	2505	G
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2585	U
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2641	G
1	1A	2654	A
1	1A	2662	A
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2744	G
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2769	C
1	1A	2778	A
1	1A	2790	A

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Mol	Chain	Res	Type
1	1A	2791	C
1	1A	2794	C
1	1A	2802	G
1	1A	2805	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2869	G
1	1A	2872	G
1	1A	2892	A
1	1A	2893	G
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	3	C
2	1B	13	A
2	1B	45	A
2	1B	56	G
2	1B	66	A
2	1B	73	A
2	1B	106	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	68	G
32	1a	78	G
32	1a	79	G
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	129(A)	G

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Mol	Chain	Res	Type
32	1a	131	C
32	1a	137	C
32	1a	141	A
32	1a	163	C
32	1a	169	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	190	U
32	1a	195	A
32	1a	197	A
32	1a	201	C
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	266	G
32	1a	267	C
32	1a	280	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	347	G
32	1a	348	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	383	A
32	1a	392	G
32	1a	393	A
32	1a	397	A
32	1a	406	G
32	1a	412	A
32	1a	413	G

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Mol	Chain	Res	Type
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	442	C
32	1a	444	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	477	A
32	1a	485	G
32	1a	487	A
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	519	C
32	1a	521	G
32	1a	524	G
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	564	C
32	1a	572	A
32	1a	573	A
32	1a	575	G
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	619	U
32	1a	630	G
32	1a	632	A
32	1a	633	G
32	1a	642	A

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Mol	Chain	Res	Type
32	1a	653	A
32	1a	657	G
32	1a	661	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	717	C
32	1a	724	G
32	1a	728	A
32	1a	731	G
32	1a	734	G
32	1a	747	C
32	1a	755	G
32	1a	759	A
32	1a	768	A
32	1a	774	G
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	827	U
32	1a	828	A
32	1a	829	G
32	1a	836	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	855	G
32	1a	870	U
32	1a	878	G
32	1a	902	G
32	1a	913	A
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	931	C
32	1a	934	C
32	1a	935	A

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Mol	Chain	Res	Type
32	1a	939	G
32	1a	940	C
32	1a	958	A
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	991	U
32	1a	992	U
32	1a	993	G
32	1a	996	A
32	1a	998	G
32	1a	999	C
32	1a	1001(A)	G
32	1a	1004	A
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1017	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1031	G
32	1a	1032	G
32	1a	1033	G
32	1a	1037	C
32	1a	1044	A
32	1a	1063	C
32	1a	1065	U

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Mol	Chain	Res	Type
32	1a	1066	C
32	1a	1067	A
32	1a	1070	U
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1125	U
32	1a	1127	G
32	1a	1133	G
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1144	G
32	1a	1146	A
32	1a	1152	A
32	1a	1155	G
32	1a	1159	U
32	1a	1163	C
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1186	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1224	G
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	1260	C
32	1a	1270	C
32	1a	1277	C
32	1a	1278	U
32	1a	1279	A

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Mol	Chain	Res	Type
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	1320	C
32	1a	1322	C
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1397	C
32	1a	1398	A
32	1a	1406	U
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	1469	G
32	1a	1492	A
32	1a	1493	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	10	G
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	45	C
1	2A	63	U

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Mol	Chain	Res	Type
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	139	G
1	2A	139(A)	G
1	2A	141	A
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	201	C
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	223	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	271(D)	G
1	2A	271(E)	U
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	302	C

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Mol	Chain	Res	Type
1	2A	311	A
1	2A	317	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	335	C
1	2A	352	G
1	2A	363	G
1	2A	370	G
1	2A	386	G
1	2A	390	A
1	2A	396	G
1	2A	399	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	444	C
1	2A	446	G
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	470	A
1	2A	475	U
1	2A	481	G
1	2A	482	A
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	551	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A

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Mol	Chain	Res	Type
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	701	G
1	2A	730	C
1	2A	740	U
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	828	U
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	869	G
1	2A	880	G
1	2A	882	G
1	2A	886	C
1	2A	887	A

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Mol	Chain	Res	Type
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	896	A
1	2A	897	C
1	2A	901	A
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	937	U
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1044	G
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1052	C
1	2A	1054	A
1	2A	1056	G
1	2A	1060	U
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U

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Mol	Chain	Res	Type
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	1080	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	1088	A
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1095	A
1	2A	1097	U
1	2A	1098	A
1	2A	1106	G
1	2A	1110	G
1	2A	1112	G
1	2A	1116	C
1	2A	1117	G
1	2A	1120	G
1	2A	1129	A
1	2A	1135	C
1	2A	1136	G
1	2A	1171	G
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G

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Mol	Chain	Res	Type
1	2A	1272	A
1	2A	1273	U
1	2A	1274	A
1	2A	1276	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1321	A
1	2A	1342	A
1	2A	1349	A
1	2A	1352	U
1	2A	1365	A
1	2A	1368	G
1	2A	1372	U
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1414	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	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	1511	C
1	2A	1531	C
1	2A	1533	G

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Mol	Chain	Res	Type
1	2A	1542	A
1	2A	1543	C
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	1593	G
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1613	G
1	2A	1639	U
1	2A	1648	C
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	1756	G
1	2A	1757	U
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A
1	2A	1834	U
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A

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Mol	Chain	Res	Type
1	2A	1852	C
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2096	U
1	2A	2101	G
1	2A	2103	C
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2110	G
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U

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Mol	Chain	Res	Type
1	2A	2119	A
1	2A	2120	G
1	2A	2121	G
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2141	G
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	2158	A
1	2A	2159	G
1	2A	2160	G
1	2A	2161	C
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2175	C
1	2A	2178	C
1	2A	2182	G
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A

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Mol	Chain	Res	Type
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2273	A
1	2A	2275	C
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2294	C
1	2A	2300	G
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
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	2327	A
1	2A	2334	G
1	2A	2335	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	2396	G
1	2A	2402	C
1	2A	2406	U
1	2A	2410	G
1	2A	2414	G
1	2A	2422	A

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Mol	Chain	Res	Type
1	2A	2423	U
1	2A	2424	C
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	2468	G
1	2A	2474	C
1	2A	2476	A
1	2A	2487	G
1	2A	2490	G
1	2A	2491	U
1	2A	2498	C
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2518	A
1	2A	2529	G
1	2A	2549	G
1	2A	2554	U
1	2A	2556	C
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2582	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
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	2703	C
1	2A	2712(A)	A

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Mol	Chain	Res	Type
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2752	C
1	2A	2754	U
1	2A	2757	A
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2769	C
1	2A	2778	A
1	2A	2779	U
1	2A	2789	C
1	2A	2802	G
1	2A	2803	C
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2834	G
1	2A	2835	A
1	2A	2848	G
1	2A	2872	G
1	2A	2880	C
1	2A	2891	G
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
2	2B	2	C
2	2B	8	U
2	2B	9	G
2	2B	12	C
2	2B	21	G
2	2B	23	G
2	2B	24	G
2	2B	33	G
2	2B	41	U
2	2B	42	C
2	2B	56	G
2	2B	73	A
2	2B	89	G

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Mol	Chain	Res	Type
2	2B	90	A
2	2B	110	G
2	2B	116	G
32	2a	5	U
32	2a	6	G
32	2a	9	G
32	2a	22	G
32	2a	29	G
32	2a	30	U
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	60	A
32	2a	61	G
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	129(A)	G
32	2a	131	C
32	2a	142	G
32	2a	144	G
32	2a	156	G
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(B)	C
32	2a	189(C)	C
32	2a	189(D)	C
32	2a	189(F)	U
32	2a	189(G)	G
32	2a	194	C
32	2a	195	A
32	2a	196	A
32	2a	201	C
32	2a	202	U

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Mol	Chain	Res	Type
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	289	G
32	2a	306	G
32	2a	316	G
32	2a	319	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	363	A
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	382	A
32	2a	392	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	409	G
32	2a	412	A
32	2a	413	G
32	2a	423	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C

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Mol	Chain	Res	Type
32	2a	471	G
32	2a	476	G
32	2a	477	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	508	C
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	562	C
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	631	G
32	2a	632	A
32	2a	648	A
32	2a	651	C
32	2a	653	A
32	2a	665	A
32	2a	685	G
32	2a	687	A
32	2a	688	G
32	2a	702	A
32	2a	703	G
32	2a	712	A
32	2a	723	U
32	2a	731	G
32	2a	734	G

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Mol	Chain	Res	Type
32	2a	735	C
32	2a	742	G
32	2a	746	A
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	777	A
32	2a	784	C
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
32	2a	829	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	854	G
32	2a	859	A
32	2a	872	A
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	920	U
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	939	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	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G

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Mol	Chain	Res	Type
32	2a	977	A
32	2a	983	A
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	996	A
32	2a	1000	U
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1017	G
32	2a	1020	U
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	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	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	1094	G
32	2a	1101	A
32	2a	1113	C
32	2a	1118	C
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C

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Mol	Chain	Res	Type
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	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1161	C
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1213	A
32	2a	1214	C
32	2a	1215	G
32	2a	1224	G
32	2a	1227	A
32	2a	1228	C
32	2a	1236	A
32	2a	1238	A
32	2a	1246	C
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1287	A
32	2a	1298	C
32	2a	1299	A
32	2a	1300	G
32	2a	1301	U
32	2a	1302	U

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Mol	Chain	Res	Type
32	2a	1303	C
32	2a	1316	G
32	2a	1317	C
32	2a	1319	A
32	2a	1322	C
32	2a	1323	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1352	C
32	2a	1353	G
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1364	U
32	2a	1370	G
32	2a	1384	C
32	2a	1385	G
32	2a	1397	C
32	2a	1400	5MC
32	2a	1401	G
32	2a	1406	U
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	1452	C
32	2a	1456	G
32	2a	1459	C
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 (63) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	214	G
1	1A	266	G
1	1A	278	A
1	1A	746	A
1	1A	764	A
1	1A	784	A
1	1A	839	U
1	1A	840	C
1	1A	888	C
1	1A	895	U
1	1A	974	G
1	1A	1047	G
1	1A	1089	G
1	1A	1142(A)	A
1	1A	1145	C
1	1A	1175	U
1	1A	1210	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	2430	A
1	1A	2689	U
1	1A	2893	G
1	2A	195	A
1	2A	196	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	746	A
1	2A	752	A
1	2A	764	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	900	A
1	2A	1047	G

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Mol	Chain	Res	Type
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	1275	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2321	G
1	2A	2406	U
1	2A	2422	A
1	2A	2689	U
1	2A	2756	U

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

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	PSU	2a	516	57,32	18,21,22	1.38	3 (16%)	22,30,33	1.96	5 (22%)
1	5MU	1A	1939	1	19,22,23	1.39	5 (26%)	28,32,35	1.99	6 (21%)
1	5MU	2A	1939	57,1	19,22,23	1.38	5 (26%)	28,32,35	2.06	6 (21%)
43	0TD	2l	92	43	7,9,10	4.49	1 (14%)	6,11,13	7.31	3 (50%)
32	MA6	2a	1518	32	19,26,27	0.79	0	18,38,41	1.44	2 (11%)
32	M2G	1a	966	32	20,27,28	1.40	3 (15%)	22,40,43	1.01	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	2MU	1A	2552	57,1	19,22,24	1.29	3 (15%)	26,31,36	1.75	6 (23%)
32	G7M	1a	527	57,32	20,26,27	1.18	2 (10%)	17,39,42	0.59	0
43	0TD	1l	92	43	7,9,10	4.86	1 (14%)	6,11,13	4.44	3 (50%)
32	5MC	2a	1400	32	18,22,23	0.95	2 (11%)	26,32,35	1.26	3 (11%)
32	MA6	1a	1518	32	19,26,27	0.80	0	18,38,41	1.34	2 (11%)
32	UR3	2a	1498	32	19,22,23	1.01	2 (10%)	26,32,35	1.43	2 (7%)
1	PSU	1A	1917	1	18,21,22	1.33	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	22,30,33	1.85	4 (18%)
32	UR3	1a	1498	32	19,22,23	0.98	1 (5%)	26,32,35	1.45	1 (3%)
32	5MC	1a	1404	32	18,22,23	0.94	1 (5%)	26,32,35	1.17	4 (15%)
1	PSU	2A	1911	1	18,21,22	1.40	3 (16%)	22,30,33	1.84	4 (18%)
32	MA6	2a	1519	32	19,26,27	0.83	0	18,38,41	1.62	2 (11%)
55	8AN	1x	76	57,55,56	19,24,25	1.19	3 (15%)	13,35,38	1.79	1 (7%)
1	OMG	2A	2251	57,55,12,1	18,26,27	0.92	1 (5%)	19,38,41	1.17	4 (21%)
1	5MU	1A	1915	1	19,22,23	1.41	5 (26%)	28,32,35	2.28	9 (32%)
1	5MC	1A	1942	57,1	18,22,23	0.98	2 (11%)	26,32,35	1.08	2 (7%)
1	2MA	1A	2503	57,1	17,25,26	1.04	2 (11%)	17,37,40	0.98	2 (11%)
32	2MG	1a	1207	32	18,26,27	0.92	1 (5%)	16,38,41	1.20	3 (18%)
1	5MC	2A	1942	1	18,22,23	0.98	2 (11%)	26,32,35	1.19	2 (7%)
1	2MA	2A	2503	57,1	17,25,26	0.97	0	17,37,40	1.11	2 (11%)
1	PSU	1A	2605	1	18,21,22	1.48	4 (22%)	22,30,33	1.97	5 (22%)
32	4OC	2a	1402	32	20,23,24	0.78	0	26,32,35	1.03	1 (3%)
1	OMG	1A	2251	55,1	18,26,27	1.03	1 (5%)	19,38,41	1.12	2 (10%)
32	PSU	1a	516	57,32	18,21,22	1.37	2 (11%)	22,30,33	1.76	4 (18%)
1	5MU	2A	1915	1	19,22,23	1.47	4 (21%)	28,32,35	2.09	8 (28%)
1	PSU	2A	1917	1	18,21,22	1.32	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	2A	2605	1	18,21,22	1.35	3 (16%)	22,30,33	1.83	4 (18%)
1	5MC	1A	1962	57,1	18,22,23	0.96	2 (11%)	26,32,35	1.11	1 (3%)
32	2MG	2a	1207	32	18,26,27	0.89	1 (5%)	16,38,41	1.06	1 (6%)
1	5MC	2A	1962	1	18,22,23	0.98	2 (11%)	26,32,35	1.22	3 (11%)
32	5MC	2a	967	32	18,22,23	0.98	2 (11%)	26,32,35	1.04	2 (7%)
32	5MC	2a	1404	32	18,22,23	0.96	2 (11%)	26,32,35	1.16	3 (11%)
1	OMC	1A	1920	1	19,22,23	0.89	0	26,31,34	1.18	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.75	0	26,32,35	0.96	1 (3%)
32	G7M	2a	527	32	20,26,27	1.20	2 (10%)	17,39,42	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	5MC	1a	1407	32	18,22,23	1.06	1 (5%)	26,32,35	1.14	2 (7%)
32	5MC	1a	967	32	18,22,23	0.96	2 (11%)	26,32,35	1.04	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.83	0	26,31,34	0.95	1 (3%)
32	5MC	2a	1407	32	18,22,23	0.98	2 (11%)	26,32,35	1.18	3 (11%)
32	5MC	1a	1400	32	18,22,23	1.02	2 (11%)	26,32,35	1.18	2 (7%)
1	2MU	2A	2552	57,1	19,22,24	1.17	2 (10%)	26,31,36	1.73	5 (19%)
32	MA6	1a	1519	32	19,26,27	0.82	0	18,38,41	1.50	2 (11%)
32	M2G	2a	966	57,32	20,27,28	1.53	3 (15%)	22,40,43	0.85	1 (4%)
55	8AN	2x	76	57,55,56	19,24,25	1.21	3 (15%)	13,35,38	1.77	2 (15%)

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	PSU	2a	516	57,32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	2MU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
32	G7M	1a	527	57,32	-	1/3/25/26	0/3/3/3
43	0TD	1l	92	43	-	4/7/12/14	-
32	5MC	2a	1400	32	-	4/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	2/7/29/30	0/3/3/3
55	8AN	1x	76	57,55,56	-	1/3/25/26	0/3/3/3
1	OMG	2A	2251	57,55,12,1	-	0/5/27/28	0/3/3/3
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	5MC	1A	1942	57,1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	2/3/25/26	0/3/3/3

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

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.48	1.69	1.82
43	2l	92	0TD	CB-SB	-11.58	1.70	1.82
32	2a	966	M2G	C2-N3	4.98	1.36	1.30
32	1a	966	M2G	C2-N3	4.38	1.36	1.30
32	1a	527	G7M	C5-C4	3.65	1.46	1.39
1	1A	2605	PSU	C4-N3	-3.64	1.32	1.38
1	2A	1911	PSU	C6-C5	3.51	1.39	1.35
32	1a	516	PSU	C6-C5	3.48	1.39	1.35
32	2a	527	G7M	C5-C4	3.46	1.46	1.39
32	1a	1407	5MC	C6-C5	3.33	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1911	PSU	C6-C5	3.25	1.39	1.35
1	2A	1915	5MU	C6-C5	3.15	1.39	1.34
1	1A	1917	PSU	C6-C5	3.15	1.39	1.35
32	2a	966	M2G	C2-N2	3.06	1.41	1.35
32	2a	516	PSU	C6-C5	3.02	1.38	1.35
1	1A	1942	5MC	C6-C5	3.01	1.39	1.34
32	2a	1407	5MC	C6-C5	3.00	1.39	1.34
1	2A	2605	PSU	C6-C5	2.99	1.38	1.35
1	1A	1939	5MU	C6-C5	2.98	1.39	1.34
32	2a	967	5MC	C6-C5	2.94	1.39	1.34
1	1A	1915	5MU	C2-N1	2.89	1.43	1.38
1	2A	1939	5MU	C6-C5	2.89	1.39	1.34
1	2A	1917	PSU	C6-C5	2.85	1.38	1.35
1	2A	1915	5MU	C2-N1	2.84	1.43	1.38
55	2x	76	8AN	C5-C4	-2.83	1.33	1.40
32	1a	1404	5MC	C6-C5	2.82	1.39	1.34
32	1a	966	M2G	C2-N2	2.82	1.40	1.35
1	2A	1911	PSU	C4-N3	-2.80	1.33	1.38
1	2A	1942	5MC	C6-C5	2.78	1.39	1.34
1	2A	1962	5MC	C6-C5	2.78	1.39	1.34
1	1A	1911	PSU	C4-N3	-2.76	1.33	1.38
55	1x	76	8AN	C5-C4	-2.75	1.33	1.40
32	1a	1400	5MC	C6-N1	-2.75	1.33	1.38
32	2a	1404	5MC	C6-C5	2.74	1.39	1.34
32	1a	1400	5MC	C6-C5	2.69	1.39	1.34
32	1a	967	5MC	C6-C5	2.67	1.39	1.34
1	1A	2605	PSU	C2-N3	-2.66	1.32	1.37
32	2a	516	PSU	C4-N3	-2.63	1.33	1.38
1	1A	2552	2MU	C4-N3	-2.63	1.33	1.38
55	2x	76	8AN	C6-C5	-2.58	1.33	1.43
1	2A	1939	5MU	C4-N3	-2.58	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.57	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.57	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.56	1.33	1.38
1	1A	1962	5MC	C6-C5	2.55	1.38	1.34
32	2a	1400	5MC	C6-C5	2.52	1.38	1.34
1	1A	1915	5MU	C6-C5	2.52	1.38	1.34
1	1A	1915	5MU	C4-N3	-2.52	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.49	1.34	1.38
1	2A	1915	5MU	C4-C5	2.49	1.48	1.44
1	1A	2251	OMG	C6-N1	-2.48	1.34	1.37
32	2a	1400	5MC	C6-N1	-2.46	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C4-C5	2.43	1.48	1.44
1	2A	2251	OMG	C6-N1	-2.42	1.34	1.37
1	1A	1939	5MU	C4-N3	-2.41	1.34	1.38
1	1A	2552	2MU	C2-N1	2.41	1.42	1.38
55	1x	76	8AN	C6-C5	-2.40	1.34	1.43
32	2a	1207	2MG	C6-N1	-2.39	1.34	1.37
1	2A	1939	5MU	C4-C5	2.39	1.48	1.44
32	1a	516	PSU	C4-N3	-2.37	1.34	1.38
32	2a	527	G7M	C6-N1	-2.37	1.34	1.37
1	2A	1917	PSU	C4-N3	-2.35	1.34	1.38
1	1A	2605	PSU	C6-C5	2.35	1.38	1.35
32	1a	1207	2MG	C6-N1	-2.34	1.34	1.37
1	2A	1962	5MC	C6-N1	-2.33	1.34	1.38
1	1A	2503	2MA	C2-N3	2.32	1.36	1.31
32	2a	966	M2G	C6-N1	-2.30	1.34	1.37
1	2A	2552	2MU	C4-N3	-2.25	1.34	1.38
1	1A	2552	2MU	C5-C4	2.23	1.48	1.43
32	2a	1404	5MC	C6-N1	-2.22	1.34	1.38
1	2A	2552	2MU	C5-C4	2.20	1.48	1.43
1	2A	1939	5MU	C2-N1	2.19	1.42	1.38
1	1A	1915	5MU	C4-C5	2.18	1.48	1.44
32	1a	966	M2G	C6-N1	-2.18	1.34	1.37
1	2A	1942	5MC	C6-N1	-2.17	1.34	1.38
55	1x	76	8AN	C5-N7	-2.15	1.31	1.39
1	2A	2605	PSU	C2-N3	-2.15	1.33	1.37
32	2a	1498	UR3	C2-N1	2.13	1.41	1.38
32	1a	527	G7M	C6-N1	-2.12	1.34	1.37
1	1A	2605	PSU	C2-N1	-2.11	1.33	1.36
1	1A	1942	5MC	C6-N1	-2.11	1.34	1.38
1	1A	1939	5MU	C2-N1	2.10	1.41	1.38
32	2a	1498	UR3	C6-C5	2.10	1.39	1.35
1	2A	1911	PSU	C2-N3	-2.09	1.33	1.37
32	1a	967	5MC	C6-N1	-2.07	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.07	1.34	1.38
32	2a	967	5MC	C6-N1	-2.06	1.34	1.38
55	2x	76	8AN	C5-N7	-2.06	1.32	1.39
32	1a	1498	UR3	C6-C5	2.06	1.39	1.35
1	1A	2503	2MA	C6-N1	-2.04	1.33	1.38
1	1A	1939	5MU	C6-N1	-2.03	1.34	1.38
32	2a	516	PSU	O4'-C1'	-2.02	1.41	1.43
1	2A	1939	5MU	C6-N1	-2.02	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.01	1.34	1.38

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	17.37	133.86	102.44
43	1l	92	0TD	CSB-SB-CB	10.13	120.76	102.44
32	2a	516	PSU	N1-C2-N3	6.20	122.15	115.13
1	1A	2605	PSU	N1-C2-N3	6.17	122.12	115.13
32	1a	1498	UR3	C4-N3-C2	-6.02	118.90	124.56
1	1A	1911	PSU	N1-C2-N3	5.84	121.75	115.13
55	1x	76	8AN	N3-C2-N1	-5.79	119.63	128.68
1	2A	1917	PSU	N1-C2-N3	5.77	121.66	115.13
1	2A	1911	PSU	N1-C2-N3	5.72	121.61	115.13
32	2a	1498	UR3	C4-N3-C2	-5.63	119.26	124.56
1	1A	1917	PSU	N1-C2-N3	5.57	121.44	115.13
55	2x	76	8AN	N3-C2-N1	-5.54	120.02	128.68
1	2A	2605	PSU	N1-C2-N3	5.44	121.30	115.13
32	1a	516	PSU	N1-C2-N3	5.38	121.23	115.13
1	2A	2552	2MU	N3-C2-N1	5.12	121.69	114.89
1	2A	1939	5MU	N3-C2-N1	5.10	121.66	114.89
1	2A	1915	5MU	N3-C2-N1	5.10	121.66	114.89
1	2A	1939	5MU	C4-N3-C2	-5.08	120.77	127.35
1	1A	1939	5MU	C4-N3-C2	-4.84	121.08	127.35
32	2a	1519	MA6	N3-C2-N1	-4.82	121.14	128.68
32	2a	1518	MA6	N3-C2-N1	-4.76	121.24	128.68
1	1A	2552	2MU	N3-C2-N1	4.76	121.20	114.89
32	1a	1518	MA6	N3-C2-N1	-4.72	121.30	128.68
1	2A	1915	5MU	C4-N3-C2	-4.72	121.25	127.35
32	1a	1519	MA6	N3-C2-N1	-4.70	121.33	128.68
1	1A	1915	5MU	C4-N3-C2	-4.63	121.35	127.35
1	1A	1915	5MU	C1'-N1-C2	4.63	125.96	117.57
1	1A	1915	5MU	C5-C4-N3	4.58	119.22	115.31
1	1A	1939	5MU	C5-C4-N3	4.52	119.17	115.31
1	1A	1939	5MU	N3-C2-N1	4.44	120.79	114.89
1	1A	1915	5MU	N3-C2-N1	4.42	120.76	114.89
1	2A	1939	5MU	C5-C4-N3	4.39	119.06	115.31
1	1A	2605	PSU	C4-N3-C2	-4.26	120.20	126.34
1	1A	1915	5MU	C1'-N1-C6	-4.18	114.17	121.12
1	2A	1917	PSU	O2-C2-N1	-4.15	118.22	122.79
1	1A	1915	5MU	O4-C4-C5	-4.14	120.10	124.90
32	1a	1400	5MC	C5-C6-N1	-4.03	119.19	123.34
1	2A	1942	5MC	C5-C6-N1	-4.02	119.20	123.34
1	2A	2552	2MU	C4-N3-C2	-3.99	121.32	126.58
1	2A	1915	5MU	C5-C4-N3	3.97	118.70	115.31
1	1A	2552	2MU	C4-N3-C2	-3.96	121.35	126.58
32	2a	516	PSU	C4-N3-C2	-3.95	120.65	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2605	PSU	C4-N3-C2	-3.90	120.72	126.34
1	2A	1939	5MU	O4-C4-C5	-3.88	120.40	124.90
1	1A	1911	PSU	C4-N3-C2	-3.88	120.75	126.34
1	1A	1917	PSU	C4-N3-C2	-3.83	120.82	126.34
1	1A	1962	5MC	C5-C6-N1	-3.81	119.42	123.34
1	2A	1911	PSU	C4-N3-C2	-3.79	120.88	126.34
1	1A	1939	5MU	C5-C6-N1	-3.76	119.47	123.34
1	1A	1939	5MU	O4-C4-C5	-3.74	120.56	124.90
1	2A	2552	2MU	O2-C2-N1	-3.69	117.88	122.79
1	2A	1917	PSU	C4-N3-C2	-3.63	121.11	126.34
1	1A	2552	2MU	C2'-C1'-N1	-3.61	107.20	114.22
32	1a	516	PSU	C4-N3-C2	-3.60	121.16	126.34
32	2a	1400	5MC	C5-C6-N1	-3.58	119.66	123.34
32	2a	1519	MA6	C4-C5-N7	-3.55	105.70	109.40
1	1A	1942	5MC	C5-C6-N1	-3.54	119.69	123.34
32	2a	967	5MC	C5-C6-N1	-3.51	119.73	123.34
32	2a	1404	5MC	C5-C6-N1	-3.48	119.76	123.34
1	1A	1917	PSU	O2-C2-N1	-3.47	118.97	122.79
1	2A	1915	5MU	O4-C4-C5	-3.43	120.92	124.90
32	2a	516	PSU	O2-C2-N1	-3.42	119.03	122.79
1	2A	1915	5MU	C1'-N1-C2	3.41	123.74	117.57
32	1a	1519	MA6	C4-C5-N7	-3.31	105.95	109.40
1	2A	1939	5MU	C5-C6-N1	-3.30	119.95	123.34
1	2A	1962	5MC	C5-C6-N1	-3.29	119.95	123.34
1	1A	1911	PSU	O2-C2-N1	-3.21	119.26	122.79
43	2l	92	0TD	OD2-CG-CB	3.21	120.08	113.15
32	2a	1407	5MC	C5-C6-N1	-3.20	120.04	123.34
32	1a	1407	5MC	C5-C6-N1	-3.13	120.12	123.34
32	1a	967	5MC	C5-C6-N1	-3.06	120.19	123.34
32	1a	1404	5MC	C5-C6-N1	-3.02	120.23	123.34
1	1A	1920	OMC	O2-C2-N3	-3.01	117.44	122.33
43	1l	92	0TD	OD2-CG-CB	3.00	119.64	113.15
1	2A	2605	PSU	O2-C2-N1	-2.99	119.50	122.79
32	2a	1518	MA6	C4-C5-N7	-2.97	106.31	109.40
32	2a	1407	5MC	C5-C4-N3	-2.84	118.61	121.67
1	2A	1915	5MU	C5-C6-N1	-2.84	120.42	123.34
32	1a	1404	5MC	C5-C4-N3	-2.81	118.65	121.67
32	2a	1404	5MC	C5-C4-N3	-2.76	118.69	121.67
1	1A	2251	OMG	C8-N7-C5	2.73	108.19	102.99
1	2A	2503	2MA	C8-N7-C5	2.70	108.13	102.99
32	1a	1407	5MC	C5-C4-N3	-2.68	118.78	121.67
32	1a	516	PSU	O2-C2-N1	-2.65	119.87	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2605	PSU	O2-C2-N1	-2.63	119.89	122.79
1	2A	2552	2MU	O4-C4-C5	-2.62	120.55	125.16
1	2A	1915	5MU	C1'-N1-C6	-2.59	116.81	121.12
32	1a	1402	4OC	C6-C5-C4	2.59	120.13	116.96
1	2A	1911	PSU	O2-C2-N1	-2.58	119.95	122.79
55	2x	76	8AN	O4'-C1'-C2'	-2.58	103.16	106.93
1	1A	1920	OMC	C1'-N1-C2	2.57	124.16	118.42
32	1a	1207	2MG	C8-N7-C5	2.53	107.82	102.99
32	1a	967	5MC	C5-C4-N3	-2.52	118.95	121.67
32	1a	1400	5MC	C5-C4-N3	-2.50	118.98	121.67
43	2l	92	0TD	OD1-CG-CB	-2.48	117.25	122.44
1	1A	1939	5MU	O2-C2-N1	-2.47	119.50	122.79
1	1A	2503	2MA	C5-C6-N1	2.46	118.27	114.02
1	2A	2503	2MA	C5-C6-N1	2.46	118.27	114.02
1	1A	2605	PSU	C5-C6-N1	-2.46	118.42	122.11
1	2A	2251	OMG	C8-N7-C5	2.45	107.66	102.99
32	2a	516	PSU	O4'-C1'-C2'	2.44	108.58	105.14
1	2A	2251	OMG	C5-C6-N1	2.43	118.24	113.95
1	1A	2552	2MU	O4-C4-C5	-2.43	120.89	125.16
32	1a	1404	5MC	O2-C2-N3	-2.42	118.39	122.33
1	2A	1962	5MC	C5-C4-N3	-2.40	119.08	121.67
1	1A	1915	5MU	C5-C6-N1	-2.37	120.89	123.34
1	1A	1915	5MU	O2-C2-N3	-2.37	117.09	121.50
32	2a	1407	5MC	O2-C2-N3	-2.37	118.48	122.33
1	1A	2552	2MU	C5-C4-N3	2.32	118.31	114.84
32	2a	1400	5MC	C1'-N1-C6	-2.31	117.28	121.12
1	2A	1915	5MU	O2-C2-N3	-2.31	117.21	121.50
32	1a	1518	MA6	C4-C5-N7	-2.30	107.00	109.40
1	1A	1915	5MU	C5M-C5-C4	2.30	121.30	118.77
32	2a	1207	2MG	C8-N7-C5	2.30	107.37	102.99
32	1a	966	M2G	C8-N7-C5	2.28	107.33	102.99
32	1a	966	M2G	C5-C6-N1	2.28	117.97	113.95
32	2a	967	5MC	C5-C4-N3	-2.27	119.22	121.67
32	1a	1207	2MG	CM2-N2-C2	-2.26	118.88	123.86
1	2A	1939	5MU	O2-C2-N1	-2.25	119.80	122.79
1	1A	2503	2MA	C8-N7-C5	2.25	107.27	102.99
1	2A	2552	2MU	C2'-C1'-N1	-2.24	109.88	114.22
32	2a	1400	5MC	C5-C4-N3	-2.24	119.26	121.67
32	2a	966	M2G	C8-N7-C5	2.23	107.25	102.99
32	2a	1402	4OC	C6-C5-C4	2.23	119.69	116.96
32	1a	1404	5MC	CM5-C5-C6	-2.21	119.90	122.85
1	1A	1942	5MC	C5-C4-N3	-2.21	119.29	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1942	5MC	C5-C4-N3	-2.16	119.35	121.67
32	1a	1207	2MG	C5-C6-N1	2.15	117.76	113.95
32	2a	516	PSU	C5-C6-N1	-2.14	118.90	122.11
1	2A	1962	5MC	C1'-N1-C6	-2.13	117.58	121.12
1	2A	2251	OMG	C2-N1-C6	-2.12	121.19	125.10
1	2A	1920	OMC	O2-C2-N3	-2.12	118.88	122.33
1	1A	2251	OMG	C5-C6-N1	2.12	117.69	113.95
32	2a	1404	5MC	O2-C2-N3	-2.11	118.91	122.33
1	2A	2251	OMG	O6-C6-C5	-2.10	120.27	124.37
1	2A	1911	PSU	C6-C5-C4	-2.10	116.73	118.20
32	2a	1498	UR3	C1'-N1-C2	2.08	120.50	116.99
1	2A	2605	PSU	C5-C6-N1	-2.06	119.01	122.11
1	1A	2552	2MU	O2-C2-N1	-2.06	120.05	122.79
32	1a	516	PSU	O4'-C1'-C2'	2.06	108.05	105.14
1	1A	1911	PSU	O4'-C1'-C2'	2.04	108.03	105.14
1	1A	2605	PSU	O2-C2-N3	-2.03	117.99	121.82
43	1l	92	0TD	OD1-CG-CB	-2.00	118.24	122.44

There are no chirality outliers.

All (38) 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	O-C-CA-CB
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	CG-CB-SB-CSB
43	2l	92	0TD	SB-CB-CG-OD2
32	2a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
55	1x	76	8AN	C4'-C5'-O5'-P
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
55	2x	76	8AN	C4'-C5'-O5'-P
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	SB-CB-CG-OD1
32	1a	527	G7M	C3'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C6
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
1	1A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	1920	OMC	C3'-C2'-O2'-CM2
1	2A	1920	OMC	C3'-C2'-O2'-CM2
1	1A	1962	5MC	C2'-C1'-N1-C6
1	1A	1962	5MC	O4'-C1'-N1-C6
43	1l	92	0TD	CA-CB-SB-CSB
32	2a	527	G7M	C4'-C5'-O5'-P
32	2a	1400	5MC	C2'-C1'-N1-C6
32	2a	527	G7M	O4'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2
43	1l	92	0TD	SB-CB-CG-OD1
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C1'-N1-C6

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 2510 ligands modelled in this entry, 2498 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	$\#\|Z\| > 2$
60	MPD	1A	4024	-	7,7,7	0.27	0	9,10,10	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
58	CLM	2A	3727	-	19,20,20	0.95	1 (5%)	23,27,27	0.92	1 (4%)
60	MPD	1T	207	-	7,7,7	0.26	0	9,10,10	0.17	0
60	MPD	2B	218	-	7,7,7	0.31	0	9,10,10	0.33	0
60	MPD	18	103	-	7,7,7	0.27	0	9,10,10	0.22	0
60	MPD	1a	3271	-	7,7,7	0.37	0	9,10,10	0.58	0
58	CLM	1A	4022	-	19,20,20	1.06	1 (5%)	23,27,27	1.21	3 (13%)
59	ARG	1B	232	57	10,11,11	0.76	1 (10%)	11,13,13	1.11	2 (18%)
59	ARG	1A	4023	-	10,11,11	0.74	1 (10%)	11,13,13	1.06	1 (9%)
60	MPD	2A	3728	-	7,7,7	0.24	0	9,10,10	0.19	0
62	SF4	1d	306	35	0,12,12	-	-	-		
62	SF4	2d	501	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	MPD	1A	4024	-	-	1/5/5/5	-
58	CLM	2A	3727	-	-	0/20/22/22	0/1/1/1
60	MPD	1T	207	-	-	0/5/5/5	-
60	MPD	2B	218	-	-	2/5/5/5	-
60	MPD	18	103	-	-	1/5/5/5	-
60	MPD	1a	3271	-	-	3/5/5/5	-
58	CLM	1A	4022	-	-	4/20/22/22	0/1/1/1
59	ARG	1B	232	57	-	3/11/11/11	-
59	ARG	1A	4023	-	-	1/11/11/11	-
60	MPD	2A	3728	-	-	2/5/5/5	-
62	SF4	1d	306	35	-	-	0/6/5/5
62	SF4	2d	501	35	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4022	CLM	C6-C5	-2.38	1.48	1.51
59	1B	232	ARG	OXT-C	-2.29	1.23	1.30
58	2A	3727	CLM	C6-C5	-2.24	1.48	1.51
59	1A	4023	ARG	OXT-C	-2.09	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	1A	4022	CLM	C10-C9-N9	2.93	121.58	119.38
59	1A	4023	ARG	OXT-C-O	-2.82	117.69	124.09
59	1B	232	ARG	OXT-C-O	-2.62	118.14	124.09
59	1B	232	ARG	OXT-C-CA	2.30	121.22	113.38
58	2A	3727	CLM	C8-C9-N9	2.29	121.10	119.38
58	1A	4022	CLM	O5-C5-C6	-2.19	106.42	111.19
58	1A	4022	CLM	C3-N2-C2	-2.18	119.22	123.07

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1A	4022	CLM	C5-C3-N2-C2
59	1B	232	ARG	O-C-CA-N
59	1A	4023	ARG	CA-CB-CG-CD
58	1A	4022	CLM	C5-C3-C4-O4
58	1A	4022	CLM	N2-C3-C4-O4
58	1A	4022	CLM	CL2-C1-C2-N2
59	1B	232	ARG	OXT-C-CA-N
59	1B	232	ARG	CA-CB-CG-CD
60	1a	3271	MPD	O2-C2-C3-C4
60	18	103	MPD	C2-C3-C4-C5
60	2B	218	MPD	C2-C3-C4-C5
60	2A	3728	MPD	O2-C2-C3-C4
60	1A	4024	MPD	C2-C3-C4-C5
60	1a	3271	MPD	C2-C3-C4-C5
60	2A	3728	MPD	C2-C3-C4-C5
60	1a	3271	MPD	C2-C3-C4-O4
60	2B	218	MPD	C2-C3-C4-O4

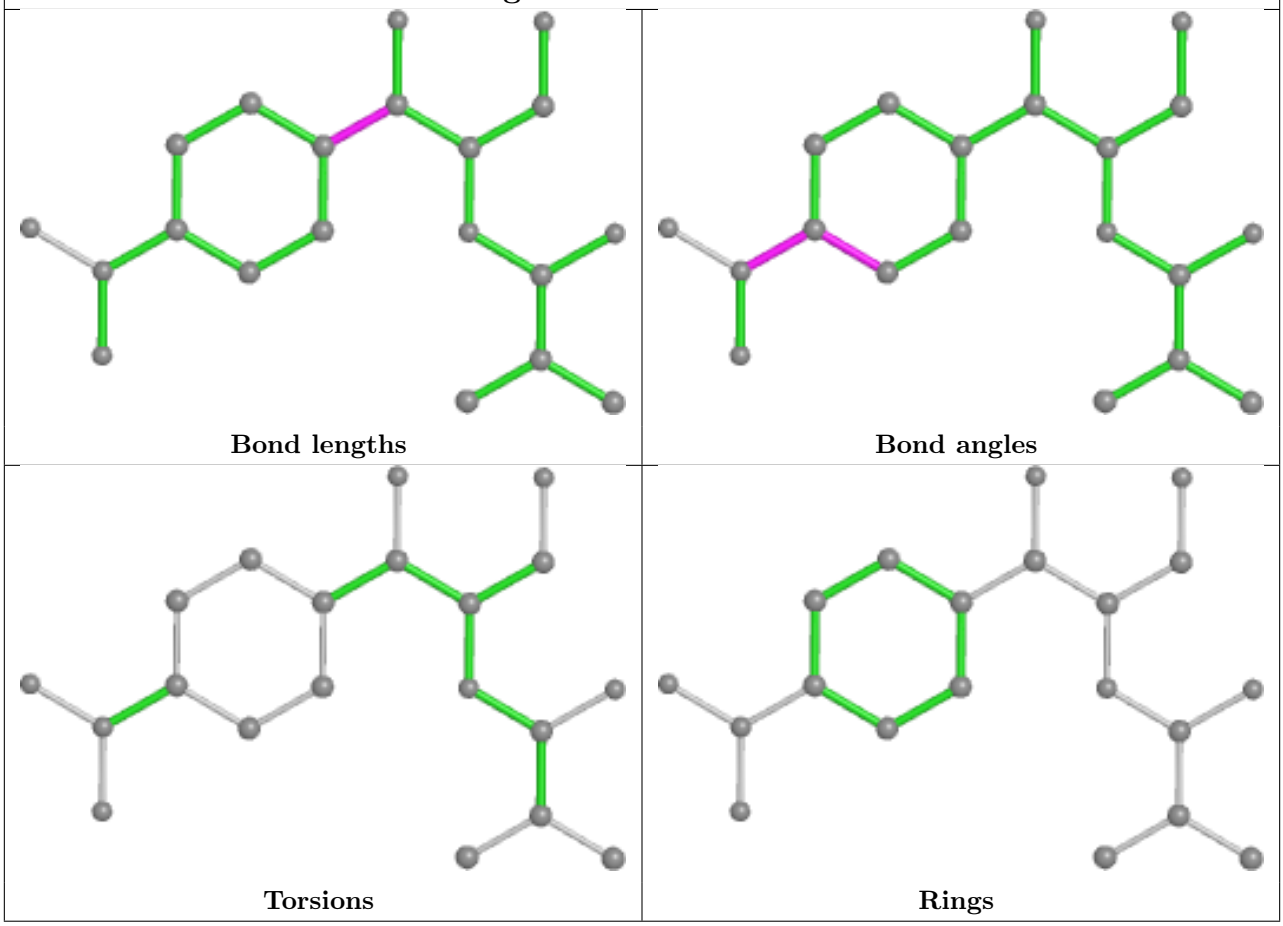
There are no ring outliers.

No monomer is involved in short contacts.

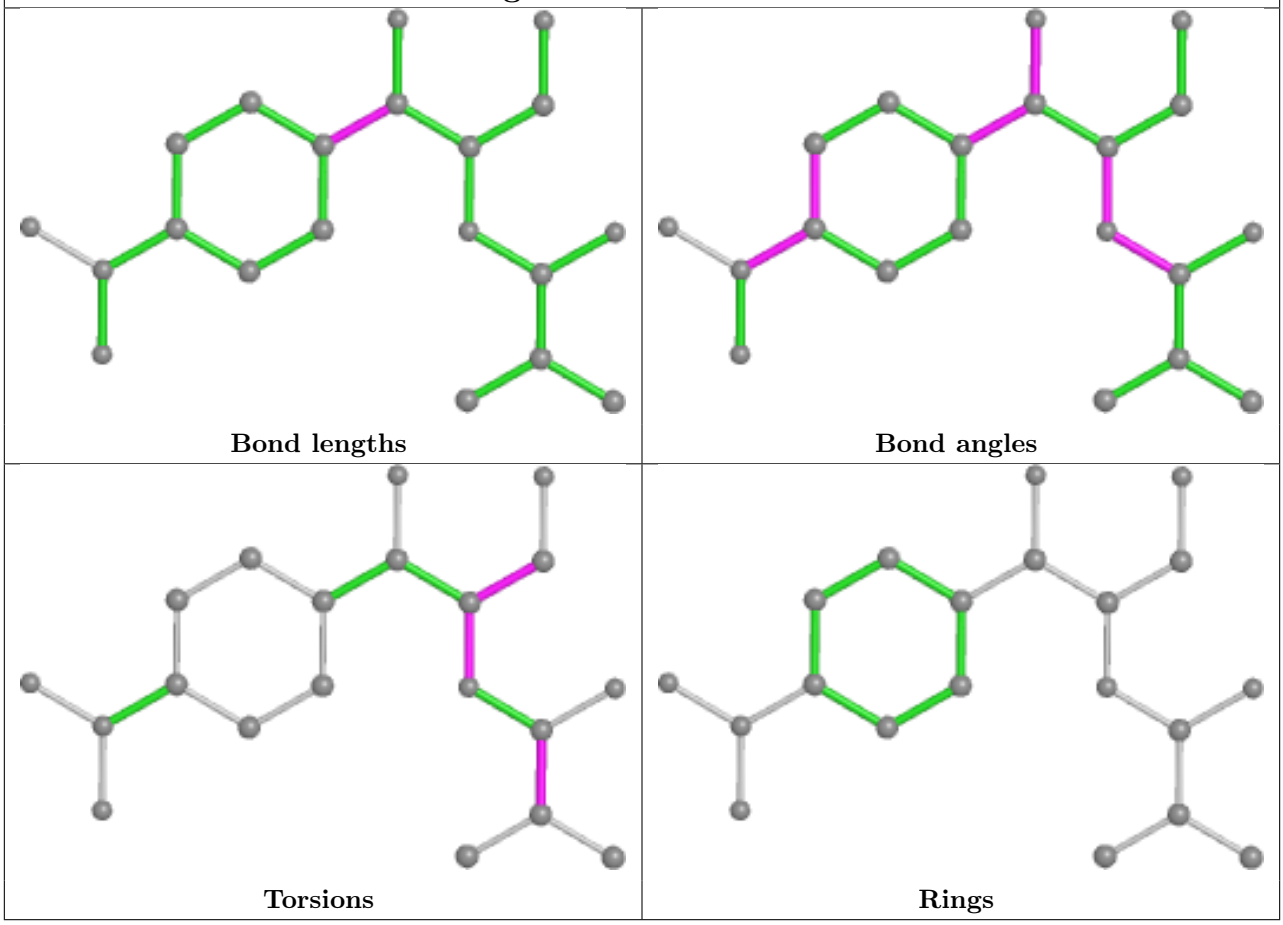
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 3727



Ligand CLM 1A 4022



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%)	0.57	79 (2%) 53 56	15, 32, 79, 90	0
1	2A	2856/2915 (97%)	0.42	92 (3%) 47 51	27, 48, 81, 90	0
2	1B	120/121 (99%)	0.26	0 100 100	24, 43, 54, 68	0
2	2B	120/121 (99%)	0.18	0 100 100	49, 64, 71, 75	0
3	1D	275/276 (99%)	0.70	4 (1%) 73 75	18, 33, 44, 58	0
3	2D	275/276 (99%)	0.73	7 (2%) 57 61	27, 43, 54, 67	0
4	1E	204/206 (99%)	0.68	2 (0%) 82 84	16, 36, 52, 64	0
4	2E	204/206 (99%)	0.65	3 (1%) 73 75	25, 48, 62, 68	0
5	1F	203/210 (96%)	0.62	3 (1%) 73 75	14, 36, 58, 74	0
5	2F	203/210 (96%)	0.59	8 (3%) 39 42	28, 55, 65, 73	0
6	1G	181/182 (99%)	0.40	5 (2%) 53 56	40, 56, 66, 72	0
6	2G	181/182 (99%)	1.07	28 (15%) 2 1	58, 68, 74, 77	0
7	1H	174/180 (96%)	0.43	1 (0%) 89 90	30, 45, 55, 58	0
7	2H	173/180 (96%)	0.74	18 (10%) 6 6	58, 66, 72, 76	0
8	1I	147/148 (99%)	0.30	1 (0%) 87 89	37, 61, 70, 76	0
8	2I	146/148 (98%)	0.61	14 (9%) 8 7	46, 64, 72, 76	0
9	1N	140/140 (100%)	0.61	0 100 100	22, 32, 48, 65	0
9	2N	140/140 (100%)	0.60	4 (2%) 51 55	39, 52, 62, 70	0
10	1O	122/122 (100%)	0.56	0 100 100	23, 35, 50, 57	0
10	2O	122/122 (100%)	0.53	0 100 100	38, 47, 59, 64	0
11	1P	149/150 (99%)	0.57	1 (0%) 87 89	15, 40, 58, 63	0
11	2P	149/150 (99%)	0.75	9 (6%) 21 22	31, 55, 67, 72	0
12	1Q	141/141 (100%)	0.62	1 (0%) 87 89	22, 34, 45, 51	0
12	2Q	141/141 (100%)	0.67	9 (6%) 19 20	37, 52, 61, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.60	0 100 100	21, 30, 43, 50	0
13	2R	118/118 (100%)	0.57	2 (1%) 70 72	33, 44, 52, 58	0
14	1S	110/112 (98%)	0.42	0 100 100	32, 43, 54, 58	0
14	2S	110/112 (98%)	0.60	7 (6%) 19 20	52, 59, 63, 68	0
15	1T	131/146 (89%)	0.51	0 100 100	28, 38, 57, 70	0
15	2T	131/146 (89%)	0.50	5 (3%) 40 43	39, 50, 63, 68	0
16	1U	116/118 (98%)	0.73	1 (0%) 84 86	17, 26, 40, 51	0
16	2U	116/118 (98%)	0.82	6 (5%) 27 29	33, 48, 61, 68	0
17	1V	101/101 (100%)	0.55	0 100 100	16, 35, 49, 54	0
17	2V	101/101 (100%)	0.51	1 (0%) 82 84	38, 57, 63, 67	0
18	1W	112/113 (99%)	0.69	0 100 100	18, 26, 45, 62	0
18	2W	112/113 (99%)	0.60	1 (0%) 84 86	32, 42, 57, 76	0
19	1X	95/96 (98%)	0.67	3 (3%) 47 51	22, 33, 52, 63	0
19	2X	95/96 (98%)	0.88	7 (7%) 14 15	38, 52, 64, 69	0
20	1Y	107/110 (97%)	0.55	2 (1%) 66 69	32, 42, 55, 63	0
20	2Y	107/110 (97%)	0.71	6 (5%) 24 25	45, 57, 66, 72	0
21	1Z	203/206 (98%)	0.38	3 (1%) 73 75	32, 49, 61, 71	0
21	2Z	201/206 (97%)	0.46	4 (1%) 65 68	50, 62, 69, 77	0
22	10	83/85 (97%)	0.88	7 (8%) 11 11	23, 32, 58, 68	0
22	20	83/85 (97%)	1.22	12 (14%) 2 2	40, 51, 62, 69	0
23	11	97/98 (98%)	0.75	4 (4%) 37 40	24, 39, 59, 61	0
23	21	97/98 (98%)	0.70	7 (7%) 15 16	35, 48, 63, 68	0
24	12	70/72 (97%)	0.52	1 (1%) 75 77	30, 43, 51, 62	0
24	22	70/72 (97%)	0.43	0 100 100	46, 58, 62, 65	0
25	13	59/60 (98%)	0.59	0 100 100	22, 31, 49, 56	0
25	23	59/60 (98%)	0.96	7 (11%) 4 4	41, 49, 63, 72	0
26	14	69/71 (97%)	0.65	6 (8%) 10 10	50, 68, 75, 79	0
26	24	69/71 (97%)	1.38	18 (26%) 0 0	67, 73, 79, 81	0
27	15	59/60 (98%)	0.79	1 (1%) 70 72	17, 28, 44, 55	0
27	25	59/60 (98%)	0.55	0 100 100	27, 42, 55, 65	0
28	16	53/54 (98%)	0.36	0 100 100	27, 36, 49, 51	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.55	2 (3%) 40 43	44, 51, 59, 63	0
29	17	48/49 (97%)	0.83	2 (4%) 36 39	16, 23, 48, 51	0
29	27	48/49 (97%)	0.81	2 (4%) 36 39	29, 36, 51, 62	0
30	18	64/65 (98%)	0.71	1 (1%) 72 74	22, 29, 36, 50	0
30	28	64/65 (98%)	1.03	7 (10%) 5 5	36, 45, 50, 59	0
31	19	37/37 (100%)	0.72	0 100 100	26, 35, 50, 53	0
31	29	37/37 (100%)	1.01	2 (5%) 25 27	46, 54, 64, 66	0
32	1a	1488/1521 (97%)	0.34	32 (2%) 62 65	33, 60, 78, 90	0
32	2a	1492/1521 (98%)	0.41	55 (3%) 41 45	41, 65, 80, 90	0
33	1b	231/256 (90%)	0.75	27 (11%) 4 4	56, 66, 73, 79	0
33	2b	231/256 (90%)	1.05	44 (19%) 1 1	59, 69, 75, 80	0
34	1c	206/239 (86%)	1.10	37 (17%) 1 1	52, 63, 71, 74	0
34	2c	206/239 (86%)	1.36	58 (28%) 0 0	57, 69, 74, 80	0
35	1d	208/209 (99%)	0.92	24 (11%) 4 4	48, 61, 69, 73	0
35	2d	208/209 (99%)	0.96	24 (11%) 4 4	49, 61, 67, 70	0
36	1e	148/162 (91%)	0.69	11 (7%) 14 15	42, 57, 64, 69	0
36	2e	148/162 (91%)	0.89	15 (10%) 7 6	51, 61, 69, 74	0
37	1f	100/101 (99%)	0.46	2 (2%) 65 68	46, 58, 65, 67	0
37	2f	100/101 (99%)	0.37	1 (1%) 82 84	48, 60, 65, 67	0
38	1g	155/156 (99%)	0.50	7 (4%) 33 36	52, 62, 67, 72	0
38	2g	155/156 (99%)	1.01	28 (18%) 1 1	59, 67, 71, 75	0
39	1h	137/138 (99%)	0.70	8 (5%) 23 24	47, 59, 64, 67	0
39	2h	137/138 (99%)	0.78	9 (6%) 18 19	54, 61, 66, 68	0
40	1i	127/128 (99%)	1.47	38 (29%) 0 0	56, 66, 72, 74	0
40	2i	126/128 (98%)	2.62	85 (67%) 0 0	61, 70, 75, 79	0
41	1j	97/105 (92%)	1.20	17 (17%) 1 1	55, 66, 73, 78	0
41	2j	96/105 (91%)	1.90	45 (46%) 0 0	61, 70, 75, 77	0
42	1k	114/129 (88%)	0.49	1 (0%) 84 86	40, 55, 64, 67	0
42	2k	114/129 (88%)	0.98	14 (12%) 4 3	49, 61, 68, 71	0
43	1l	121/132 (91%)	0.80	7 (5%) 23 24	45, 53, 60, 63	0
43	2l	121/132 (91%)	0.65	8 (6%) 18 19	44, 56, 63, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	116/126 (92%)	0.75	11 (9%) 8 8	54, 65, 70, 77	0
44	2m	114/126 (90%)	1.10	18 (15%) 2 1	61, 69, 73, 76	0
45	1n	60/61 (98%)	1.52	16 (26%) 0 0	54, 61, 66, 71	0
45	2n	60/61 (98%)	2.51	40 (66%) 0 0	60, 68, 73, 79	0
46	1o	88/89 (98%)	0.58	3 (3%) 45 48	38, 55, 66, 72	0
46	2o	88/89 (98%)	0.72	3 (3%) 45 48	51, 61, 67, 74	0
47	1p	82/88 (93%)	1.10	15 (18%) 1 1	50, 61, 67, 74	0
47	2p	82/88 (93%)	0.86	7 (8%) 10 10	54, 60, 66, 70	0
48	1q	99/105 (94%)	0.76	6 (6%) 21 22	45, 58, 64, 69	0
48	2q	99/105 (94%)	0.88	12 (12%) 4 4	47, 59, 66, 70	0
49	1r	68/88 (77%)	0.40	1 (1%) 73 75	48, 57, 66, 73	0
49	2r	68/88 (77%)	0.69	2 (2%) 51 55	52, 61, 69, 74	0
50	1s	83/93 (89%)	0.51	2 (2%) 59 62	56, 65, 70, 76	0
50	2s	83/93 (89%)	1.30	18 (21%) 0 0	59, 70, 74, 78	0
51	1t	96/106 (90%)	0.90	10 (10%) 6 6	53, 61, 68, 70	0
51	2t	98/106 (92%)	0.75	5 (5%) 28 29	50, 60, 66, 71	0
52	1u	23/27 (85%)	1.72	8 (34%) 0 0	59, 62, 66, 69	0
52	2u	23/27 (85%)	2.09	12 (52%) 0 0	62, 68, 70, 71	0
53	1y	97/113 (85%)	0.79	4 (4%) 37 40	47, 56, 67, 71	0
53	2y	96/113 (84%)	3.69	82 (85%) 0 0	66, 74, 80, 82	0
54	1w	4/5 (80%)	0.34	0 100 100	45, 49, 56, 71	0
54	2w	4/5 (80%)	0.60	0 100 100	50, 58, 65, 72	0
55	1x	3/4 (75%)	3.43	2 (66%) 0 0	61, 61, 67, 73	0
55	2x	3/4 (75%)	4.93	3 (100%) 0 0	65, 65, 69, 77	0
56	1v	3/3 (100%)	7.19	3 (100%) 0 0	50, 50, 59, 61	0
56	2v	3/3 (100%)	7.31	3 (100%) 0 0	58, 58, 66, 67	0
All	All	20798/21492 (96%)	0.65	1299 (6%) 20 21	14, 54, 74, 90	0

All (1299) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
56	1v	1	MET	10.4
21	2Z	192	ALA	8.9

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Mol	Chain	Res	Type	RSRZ
53	2y	88	LEU	8.6
56	2v	2	THR	8.5
55	2x	73	A	8.5
56	2v	1	MET	8.5
53	2y	40	ILE	8.3
53	2y	41	LEU	8.3
53	2y	50	ALA	8.1
34	2c	157	ILE	7.7
1	1A	1087	G	7.6
53	2y	12	ILE	7.3
53	2y	78	ILE	7.3
45	2n	2	ALA	7.0
53	2y	48	PHE	6.7
1	2A	2153	G	6.5
22	10	7	LEU	6.4
32	2a	1030(A)	G	6.3
53	2y	10	MET	6.2
1	1A	1076	C	6.0
45	2n	13	THR	5.9
41	2j	67	THR	5.9
56	1v	2	THR	5.8
53	2y	51	ASP	5.8
1	2A	2142	C	5.8
53	2y	52	ALA	5.7
53	2y	64	SER	5.7
1	2A	2139	C	5.7
53	2y	42	SER	5.7
40	2i	76	ALA	5.6
53	2y	39	ILE	5.6
32	2a	1030(B)	C	5.6
1	2A	2125	G	5.6
40	2i	75	ASP	5.5
55	1x	75	C	5.5
53	2y	77	LEU	5.5
40	2i	36	TYR	5.5
1	2A	2132	U	5.5
32	1a	1030(B)	C	5.5
1	2A	2138	C	5.4
22	10	2	ALA	5.4
40	2i	42	ARG	5.4
40	2i	63	ILE	5.4
1	1A	1091	G	5.4

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Mol	Chain	Res	Type	RSRZ
40	2i	108	VAL	5.4
53	2y	74	ILE	5.3
56	1v	3	ILE	5.3
1	1A	1090	U	5.3
53	2y	71	TYR	5.3
53	2y	79	ASN	5.3
40	2i	18	PHE	5.3
41	2j	34	VAL	5.3
1	2A	2140	C	5.3
1	2A	2147	G	5.2
53	2y	49	VAL	5.2
19	2X	92	LEU	5.2
45	1n	51	GLY	5.2
40	1i	14	VAL	5.1
53	2y	70	MET	5.1
53	2y	38	HIS	5.1
22	20	3	HIS	5.1
34	2c	177	THR	5.0
34	2c	152	ILE	5.0
56	2v	3	ILE	5.0
40	2i	72	GLY	5.0
53	2y	63	ALA	4.9
44	2m	116	THR	4.9
1	2A	2124	G	4.9
1	1A	2141	G	4.9
40	2i	8	GLY	4.9
40	2i	103	THR	4.9
40	2i	102	LEU	4.8
32	1a	1257	U	4.8
20	2Y	1	MET	4.8
45	2n	25	VAL	4.8
1	1A	1068	G	4.8
1	2A	2802	G	4.8
44	1m	2	ALA	4.8
53	2y	5	ILE	4.8
32	1a	1001	A	4.8
53	2y	62	VAL	4.7
53	2y	73	ALA	4.7
40	2i	69	GLY	4.7
1	1A	1089	G	4.7
32	2a	1257	U	4.7
53	2y	9	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
21	2Z	191	VAL	4.7
1	2A	2141	G	4.7
53	2y	11	GLU	4.7
41	2j	26	ALA	4.7
34	2c	8	ILE	4.7
34	2c	124	ILE	4.7
45	2n	12	ARG	4.6
22	20	2	ALA	4.6
32	2a	1001	A	4.6
23	11	2	SER	4.6
40	2i	30	GLY	4.6
32	2a	1036	G	4.6
6	2G	87	PRO	4.6
40	2i	109	VAL	4.6
33	2b	39	ILE	4.6
40	1i	63	ILE	4.6
1	1A	1072	C	4.5
1	1A	1092	C	4.5
41	2j	27	ALA	4.5
26	24	51	ASP	4.5
1	2A	2146	C	4.5
32	1a	1030	C	4.5
36	2e	12	LEU	4.5
53	2y	67	HIS	4.5
53	2y	87	LYS	4.5
53	2y	69	ASP	4.4
53	2y	53	THR	4.4
39	2h	2	LEU	4.4
1	1A	1064	C	4.4
1	1A	1063	G	4.4
53	2y	65	GLY	4.3
32	1a	1029	C	4.3
40	2i	26	VAL	4.3
53	2y	92	GLY	4.3
45	2n	44	LEU	4.3
26	24	52	THR	4.3
45	2n	61	TRP	4.3
1	1A	2132	U	4.3
53	2y	84	GLN	4.3
33	1b	118	LEU	4.3
45	1n	34	TYR	4.3
36	2e	109	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
41	2j	96	ILE	4.3
40	2i	21	PRO	4.3
38	2g	154	TYR	4.3
1	2A	2106	G	4.3
1	2A	2793	G	4.3
26	24	45	GLY	4.2
40	2i	62	TYR	4.2
55	1x	74	C	4.2
6	2G	135	LEU	4.2
31	29	16	VAL	4.2
41	2j	72	VAL	4.2
40	1i	106	ALA	4.2
40	2i	61	ALA	4.2
35	1d	2	GLY	4.2
41	1j	29	ARG	4.2
1	2A	2174	C	4.2
53	2y	37	PRO	4.2
40	2i	66	ARG	4.2
53	2y	58	ASN	4.2
1	2A	2173	A	4.2
26	24	49	PHE	4.2
53	2y	4	ASN	4.2
40	2i	115	GLY	4.2
53	2y	8	LYS	4.2
40	2i	5	TYR	4.1
36	2e	13	ILE	4.1
1	1A	2792	G	4.1
32	1a	1001(A)	G	4.1
34	2c	159	GLY	4.1
52	2u	2	GLY	4.1
7	2H	93	GLY	4.1
34	1c	148	GLY	4.1
1	2A	2136	C	4.1
22	10	6	GLY	4.1
1	1A	2805	G	4.1
1	2A	2152	G	4.1
1	1A	1080	C	4.1
23	21	2	SER	4.1
41	2j	6	ILE	4.0
32	2a	1033	G	4.0
1	1A	1065	U	4.0
53	2y	7	SER	4.0

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Mol	Chain	Res	Type	RSRZ
34	1c	194	GLY	4.0
53	2y	19	HIS	4.0
53	2y	82	GLU	4.0
50	2s	66	MET	4.0
1	2A	2107	C	4.0
44	2m	6	GLY	4.0
33	2b	136	VAL	4.0
1	1A	1074	G	4.0
32	2a	1286	A	4.0
50	1s	4	SER	4.0
40	2i	56	LEU	4.0
1	1A	2116	G	4.0
29	27	47	ARG	4.0
22	20	7	LEU	3.9
40	1i	37	PHE	3.9
22	20	76	GLY	3.9
52	2u	16	GLY	3.9
41	2j	23	ILE	3.9
1	1A	2794	C	3.9
53	2y	18	GLN	3.9
53	2y	35	ILE	3.9
34	2c	164	ARG	3.9
45	2n	10	ALA	3.9
1	2A	2169	A	3.9
41	2j	48	THR	3.9
1	1A	1083	U	3.9
43	2l	18	VAL	3.9
39	1h	134	ILE	3.9
1	1A	2793	G	3.9
6	2G	73	ALA	3.9
44	1m	24	GLY	3.9
53	2y	21	ALA	3.9
33	1b	214	ILE	3.8
7	2H	101	ARG	3.8
11	2P	79	ARG	3.8
1	2A	1509	C	3.8
1	2A	2896	C	3.8
1	1A	1067	A	3.8
38	1g	156	TRP	3.8
1	1A	1176	G	3.8
1	2A	2159	G	3.8
53	2y	61	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
34	2c	155	GLY	3.8
34	1c	204	LEU	3.8
7	2H	102	ALA	3.8
34	1c	80	GLY	3.8
51	1t	18	GLN	3.8
8	2I	46	ALA	3.8
40	2i	74	ILE	3.8
35	2d	146	ILE	3.8
52	2u	13	ILE	3.8
32	2a	1031	G	3.8
42	2k	75	TYR	3.7
1	1A	2804	C	3.7
32	1a	1031	G	3.7
1	2A	1085	A	3.7
40	2i	67	GLY	3.7
7	2H	165	ALA	3.7
47	1p	48	TRP	3.7
35	1d	3	ARG	3.7
1	2A	2131	G	3.7
1	2A	2151	G	3.7
32	1a	1030(D)	A	3.7
40	2i	92	TYR	3.7
1	1A	1509	C	3.7
32	1a	1030(A)	G	3.7
40	2i	88	TYR	3.7
40	1i	28	VAL	3.7
45	2n	56	VAL	3.7
1	1A	1075	C	3.7
32	2a	1029	C	3.7
50	2s	10	PHE	3.6
35	1d	179	GLU	3.6
1	1A	1093	G	3.6
1	2A	2123	G	3.6
32	1a	1030(C)	G	3.6
22	10	5	LYS	3.6
40	2i	28	VAL	3.6
26	24	18	CYS	3.6
34	2c	33	LEU	3.6
41	2j	62	HIS	3.6
33	2b	218	ALA	3.6
22	20	4	LYS	3.6
40	2i	111	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
53	2y	94	ALA	3.6
1	2A	2110	G	3.6
53	2y	24	LEU	3.6
1	2A	2803	C	3.6
34	1c	63	ASN	3.6
34	2c	23	TYR	3.6
44	2m	5	ALA	3.6
52	1u	18	TYR	3.6
53	2y	46	GLN	3.6
43	2l	19	ARG	3.5
48	2q	71	PHE	3.5
1	1A	1103	A	3.5
32	2a	1030(D)	A	3.5
53	2y	13	THR	3.5
1	2A	2191	G	3.5
1	2A	2805	G	3.5
26	24	56	VAL	3.5
40	2i	114	TYR	3.5
52	2u	6	ARG	3.5
26	14	49	PHE	3.5
53	2y	45	PRO	3.5
47	1p	19	ILE	3.5
1	2A	2801(A)	A	3.5
38	1g	12	LEU	3.5
38	2g	5	ARG	3.5
23	21	70	VAL	3.5
32	2a	1026	G	3.5
33	2b	44	LEU	3.5
33	2b	118	LEU	3.5
40	1i	109	VAL	3.5
25	23	15	TYR	3.5
40	2i	50	LEU	3.5
20	2Y	42	VAL	3.5
1	2A	2133	G	3.5
7	1H	2	SER	3.5
34	2c	66	VAL	3.5
38	1g	80	VAL	3.5
6	2G	157	ILE	3.5
26	14	18	CYS	3.5
40	2i	40	LEU	3.5
48	1q	98	LEU	3.5
38	2g	82	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
53	2y	80	LYS	3.5
6	1G	146	TYR	3.4
8	2I	89	TYR	3.4
1	2A	2804	C	3.4
55	2x	74	C	3.4
34	1c	94	LEU	3.4
40	2i	7	THR	3.4
32	1a	1286	A	3.4
42	2k	25	TYR	3.4
53	2y	15	ALA	3.4
32	1a	1036	G	3.4
40	2i	125	TYR	3.4
1	1A	1082	U	3.4
1	1A	1175	U	3.4
36	2e	16	THR	3.4
45	1n	14	PRO	3.4
40	1i	10	ARG	3.4
48	2q	98	LEU	3.4
33	1b	29	ALA	3.4
41	2j	44	VAL	3.4
45	2n	18	VAL	3.4
48	2q	9	VAL	3.4
50	2s	69	HIS	3.4
52	2u	14	TRP	3.4
40	2i	47	LEU	3.4
35	1d	32	ALA	3.4
44	2m	102	ARG	3.4
50	2s	79	THR	3.4
34	1c	130	VAL	3.4
6	2G	152	LEU	3.4
41	2j	16	LEU	3.4
42	2k	74	ALA	3.4
1	2A	2162	G	3.4
53	1y	49	VAL	3.4
40	2i	6	GLY	3.3
40	2i	14	VAL	3.3
41	1j	49	VAL	3.3
32	2a	1030(C)	G	3.3
1	1A	1066	U	3.3
40	1i	46	ALA	3.3
45	2n	55	GLY	3.3
1	1A	888	C	3.3

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Mol	Chain	Res	Type	RSRZ
32	1a	1028	C	3.3
40	2i	49	PRO	3.3
48	1q	27	PHE	3.3
53	2y	85	LEU	3.3
53	2y	72	THR	3.3
53	2y	3	MET	3.3
45	1n	33	VAL	3.3
1	2A	2897	U	3.3
50	2s	75	ALA	3.3
19	2X	68	ARG	3.3
38	2g	80	VAL	3.3
1	2A	1046	A	3.3
32	2a	1249	C	3.3
40	2i	122	ALA	3.3
26	24	50	VAL	3.3
40	1i	26	VAL	3.3
41	1j	90	LEU	3.3
1	2A	229	A	3.3
32	2a	1531	A	3.3
26	24	63	TYR	3.3
1	2A	2154	G	3.2
6	2G	43	LEU	3.2
42	2k	89	ALA	3.2
45	2n	51	GLY	3.2
51	1t	67	ALA	3.2
40	2i	105	ASP	3.2
53	2y	83	ARG	3.2
43	1l	64	TYR	3.2
45	2n	21	TYR	3.2
48	2q	23	VAL	3.2
16	2U	73	GLY	3.2
34	1c	2	GLY	3.2
40	2i	127	LYS	3.2
6	2G	86	MET	3.2
40	2i	90	PRO	3.2
45	2n	53	LEU	3.2
45	1n	30	ALA	3.2
35	2d	158	ILE	3.2
41	2j	47	PHE	3.2
1	1A	2115	G	3.2
32	2a	1030	C	3.2
35	1d	180	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
40	2i	91	ASP	3.2
40	2i	85	LEU	3.2
41	2j	19	SER	3.2
38	2g	34	GLY	3.2
1	1A	2140	C	3.2
7	2H	113	VAL	3.2
1	1A	1081	U	3.2
45	2n	36	PHE	3.2
32	1a	1026	G	3.2
7	2H	105	LEU	3.2
33	1b	121	LEU	3.2
35	2d	149	ALA	3.2
47	2p	19	ILE	3.2
41	1j	86	MET	3.2
33	2b	164	VAL	3.2
42	1k	25	TYR	3.1
1	1A	2107	C	3.1
1	2A	2126	A	3.1
40	2i	73	GLN	3.1
53	2y	17	ARG	3.1
26	24	44	THR	3.1
53	2y	20	VAL	3.1
34	2c	160	ALA	3.1
38	2g	83	ALA	3.1
1	2A	2137	C	3.1
35	1d	70	ILE	3.1
41	2j	31	GLY	3.1
44	1m	115	LYS	3.1
34	1c	18	TRP	3.1
33	1b	165	VAL	3.1
34	2c	60	ALA	3.1
35	2d	144	ASP	3.1
45	1n	59	ALA	3.1
14	2S	22	GLY	3.1
34	1c	81	GLY	3.1
53	2y	16	ILE	3.1
33	2b	165	VAL	3.1
41	2j	87	THR	3.1
51	1t	13	LEU	3.1
44	1m	112	GLY	3.1
30	28	58	ILE	3.1
3	2D	2	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
19	2X	84	ALA	3.1
34	2c	3	ASN	3.1
45	2n	22	THR	3.1
53	2y	60	VAL	3.1
1	1A	1079	C	3.1
1	2A	1076	C	3.1
33	1b	128	GLU	3.1
25	23	26	LEU	3.1
44	2m	43	THR	3.1
45	2n	47	LEU	3.1
32	2a	1001(A)	G	3.1
32	2a	1373	G	3.1
1	1A	2113	U	3.1
32	1a	1000	U	3.1
52	1u	9	ARG	3.1
11	2P	34	GLY	3.1
45	2n	28	GLY	3.1
14	2S	21	THR	3.1
40	2i	64	THR	3.1
47	2p	20	VAL	3.1
1	1A	2144	U	3.0
32	1a	1033	G	3.0
33	2b	93	VAL	3.0
40	2i	65	VAL	3.0
46	2o	68	ARG	3.0
38	2g	156	TRP	3.0
1	2A	2168	G	3.0
26	24	66	SER	3.0
41	2j	68	HIS	3.0
40	2i	45	ALA	3.0
6	2G	39	ILE	3.0
40	2i	81	ILE	3.0
26	24	64	GLY	3.0
51	2t	9	ASN	3.0
53	2y	75	ASN	3.0
53	1y	95	ARG	3.0
33	1b	188	ALA	3.0
34	2c	87	LEU	3.0
34	2c	165	THR	3.0
40	1i	76	ALA	3.0
53	2y	76	GLU	3.0
1	2A	2118	U	3.0

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Mol	Chain	Res	Type	RSRZ
6	2G	65	GLY	3.0
50	2s	62	ILE	3.0
35	1d	11	LEU	3.0
38	2g	22	LEU	3.0
43	1l	61	THR	3.0
1	2A	2120	G	3.0
29	17	46	VAL	3.0
1	2A	2108	C	3.0
33	2b	31	TYR	3.0
33	2b	124	SER	3.0
53	2y	93	GLU	3.0
14	2S	54	LEU	3.0
49	2r	58	LEU	3.0
52	1u	14	TRP	3.0
7	2H	19	VAL	3.0
36	2e	22	GLY	3.0
38	2g	155	ARG	3.0
40	1i	128	ARG	3.0
26	24	39	CYS	3.0
40	2i	59	PHE	3.0
52	2u	12	LYS	3.0
6	2G	94	LEU	3.0
51	1t	72	LEU	3.0
33	2b	30	ARG	3.0
36	2e	28	PHE	2.9
1	2A	888	C	2.9
1	2A	2177	C	2.9
1	2A	2178	C	2.9
6	2G	85	GLY	2.9
34	1c	159	GLY	2.9
40	2i	57	GLY	2.9
33	2b	7	VAL	2.9
53	2y	43	LYS	2.9
36	2e	84	PHE	2.9
48	2q	27	PHE	2.9
3	2D	37	LEU	2.9
7	2H	21	PRO	2.9
42	2k	31	THR	2.9
27	15	60	VAL	2.9
29	17	1	MET	2.9
42	2k	13	GLN	2.9
45	2n	35	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
34	2c	180	ALA	2.9
34	1c	201	TYR	2.9
35	2d	20	TYR	2.9
40	2i	10	ARG	2.9
1	2A	2176	A	2.9
6	1G	48	GLU	2.9
33	2b	233	SER	2.9
35	1d	138	TYR	2.9
53	2y	89	GLN	2.9
38	1g	17	VAL	2.9
1	2A	2109	U	2.9
6	2G	117	PHE	2.9
6	2G	82	LEU	2.9
34	1c	196	LEU	2.9
19	2X	69	TYR	2.9
55	2x	75	C	2.9
23	21	62	VAL	2.9
32	2a	1202	G	2.9
41	2j	63	PHE	2.9
1	1A	2801(A)	A	2.9
1	2A	652(B)	A	2.9
3	2D	215	LEU	2.9
36	1e	134	ALA	2.9
50	2s	63	THR	2.9
1	2A	2179	C	2.8
8	2I	107	VAL	2.8
34	1c	138	VAL	2.8
22	20	45	PHE	2.8
25	23	21	ALA	2.8
34	1c	180	ALA	2.8
33	1b	213	LEU	2.8
33	2b	187	LEU	2.8
40	1i	117	HIS	2.8
44	2m	64	TRP	2.8
22	20	42	GLY	2.8
33	1b	122	PHE	2.8
41	1j	20	ALA	2.8
1	1A	2893	G	2.8
1	1A	2142	C	2.8
6	2G	140	ILE	2.8
32	2a	1114	C	2.8
40	1i	49	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
39	1h	133	LEU	2.8
45	2n	6	LEU	2.8
40	2i	71	SER	2.8
1	2A	2181	G	2.8
8	1I	85	GLU	2.8
50	2s	52	TYR	2.8
34	1c	203	PHE	2.8
36	1e	131	ILE	2.8
4	1E	28	ALA	2.8
34	2c	61	ALA	2.8
38	2g	40	ALA	2.8
38	2g	41	ARG	2.8
40	2i	13	ALA	2.8
41	2j	15	THR	2.8
8	2I	47	LEU	2.8
44	2m	90	LEU	2.8
8	2I	92	VAL	2.8
45	1n	61	TRP	2.8
22	10	3	HIS	2.8
35	1d	4	TYR	2.8
40	1i	104	ARG	2.8
43	2l	89	ARG	2.8
1	2A	2150	U	2.8
34	1c	39	ILE	2.8
41	2j	75	ILE	2.8
33	2b	120	ALA	2.8
50	1s	56	GLN	2.8
1	2A	2145	C	2.8
3	2D	38	LYS	2.8
12	2Q	59	ARG	2.8
7	2H	45	VAL	2.8
1	1A	1097	U	2.8
11	2P	37	GLY	2.8
1	2A	2148	G	2.8
1	2A	2160	G	2.8
30	28	50	LEU	2.8
35	2d	64	LEU	2.8
39	2h	112	LEU	2.8
32	2a	1116	C	2.8
48	1q	79	SER	2.8
51	2t	11	SER	2.8
15	2T	111	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
40	2i	121	ARG	2.8
33	1b	19	HIS	2.8
26	14	46	GLN	2.7
36	2e	23	GLY	2.7
44	2m	87	TYR	2.7
5	2F	166	ALA	2.7
35	2d	67	ILE	2.7
11	2P	99	LEU	2.7
40	1i	66	ARG	2.7
32	2a	1321	C	2.7
17	2V	5	VAL	2.7
50	2s	60	VAL	2.7
1	1A	2167	U	2.7
11	2P	110	TYR	2.7
23	21	26	ARG	2.7
35	2d	162	LEU	2.7
26	14	57	GLU	2.7
34	2c	162	GLN	2.7
45	2n	52	GLN	2.7
1	2A	2161	C	2.7
20	1Y	1	MET	2.7
7	2H	115	VAL	2.7
11	2P	134	ALA	2.7
40	2i	27	THR	2.7
1	1A	1077	A	2.7
33	2b	132	LYS	2.7
51	1t	73	HIS	2.7
40	2i	123	PRO	2.7
8	2I	34	GLY	2.7
32	1a	1024	G	2.7
36	2e	26	PHE	2.7
45	2n	16	PHE	2.7
33	2b	113	HIS	2.7
22	20	8	GLY	2.7
51	1t	76	ALA	2.7
1	1A	2147	G	2.7
6	1G	82	LEU	2.7
33	2b	185	ILE	2.7
33	2b	200	ILE	2.7
36	2e	133	TYR	2.7
44	2m	23	TYR	2.7
20	1Y	23	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
53	2y	68	GLU	2.7
45	2n	14	PRO	2.7
33	2b	231	GLU	2.7
34	2c	178	LEU	2.7
43	2l	32	PHE	2.7
40	1i	125	TYR	2.7
52	1u	2	GLY	2.7
41	1j	73	ASP	2.7
47	1p	59	TRP	2.7
1	1A	2602	A	2.6
1	2A	2170	A	2.6
33	1b	126	GLU	2.6
45	1n	18	VAL	2.6
50	2s	9	VAL	2.6
35	1d	50	ARG	2.6
36	2e	21	ALA	2.6
52	1u	17	THR	2.6
45	2n	29	ARG	2.6
1	1A	2176	A	2.6
32	2a	1035	A	2.6
47	1p	44	THR	2.6
32	2a	1348	U	2.6
36	1e	127	ASN	2.6
34	2c	39	ILE	2.6
40	1i	77	ILE	2.6
34	2c	58	GLU	2.6
40	1i	114	TYR	2.6
16	2U	41	ALA	2.6
40	2i	29	ASN	2.6
43	1l	26	ALA	2.6
50	2s	11	VAL	2.6
1	2A	6	A	2.6
36	1e	91	LEU	2.6
40	2i	110	GLU	2.6
7	2H	92	ILE	2.6
42	2k	110	ASP	2.6
26	24	68	ARG	2.6
40	2i	20	ARG	2.6
1	1A	2803	C	2.6
6	2G	146	TYR	2.6
34	1c	205	GLY	2.6
53	2y	98	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
6	2G	3	LEU	2.6
33	2b	195	ASP	2.6
33	2b	201	ILE	2.6
41	2j	41	PRO	2.6
41	2j	46	ARG	2.6
1	2A	1067	A	2.6
1	1A	1102	C	2.6
40	1i	118	LYS	2.6
16	1U	9	VAL	2.6
21	1Z	188	ALA	2.6
25	23	59	VAL	2.6
41	2j	94	VAL	2.6
44	2m	51	ALA	2.6
35	2d	157	LEU	2.6
48	2q	90	ILE	2.6
1	1A	2152	G	2.6
26	24	67	TYR	2.6
32	2a	1006	C	2.6
33	2b	227	GLY	2.6
45	2n	34	TYR	2.6
33	1b	218	ALA	2.6
33	2b	123	ALA	2.6
33	1b	136	VAL	2.6
35	2d	203	VAL	2.6
20	2Y	75	ILE	2.6
40	1i	127	LYS	2.6
5	1F	16	GLY	2.6
8	2I	20	ASP	2.6
45	2n	26	ARG	2.6
47	2p	39	TYR	2.6
1	1A	2146	C	2.6
1	2A	1075	C	2.6
31	29	11	CYS	2.5
34	2c	65	ALA	2.5
38	2g	8	GLU	2.6
45	2n	46	GLU	2.6
6	2G	159	VAL	2.5
19	2X	83	VAL	2.5
38	2g	24	THR	2.5
39	1h	93	VAL	2.5
52	1u	8	THR	2.5
39	2h	107	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
32	1a	841	U	2.5
41	2j	98	ILE	2.5
33	2b	21	ARG	2.5
35	2d	49	ARG	2.5
51	1t	22	ARG	2.5
34	2c	89	GLU	2.5
1	2A	2157	G	2.5
32	2a	998	G	2.5
33	2b	92	TYR	2.5
13	2R	84	ALA	2.5
32	2a	979	C	2.5
34	1c	47	LEU	2.5
35	1d	202	LEU	2.5
38	1g	13	GLN	2.5
40	2i	3	GLN	2.5
40	2i	83	ARG	2.5
30	28	48	PHE	2.5
41	2j	13	HIS	2.5
1	1A	2114	A	2.5
36	2e	17	ALA	2.5
38	2g	85	TYR	2.5
45	2n	57	ARG	2.5
1	2A	2111	C	2.5
34	1c	206	GLU	2.5
1	1A	1078	U	2.5
1	2A	1066	U	2.5
35	1d	124	GLY	2.5
9	2N	104	LYS	2.5
40	2i	37	PHE	2.5
41	2j	38	ILE	2.5
48	1q	36	ILE	2.5
45	2n	43	CYS	2.5
41	1j	30	SER	2.5
38	2g	13	GLN	2.5
47	2p	48	TRP	2.5
26	24	27	THR	2.5
34	2c	113	ALA	2.5
53	2y	6	THR	2.5
7	2H	103	LEU	2.5
21	2Z	125	LEU	2.5
22	10	42	GLY	2.5
1	2A	1064	C	2.5

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Mol	Chain	Res	Type	RSRZ
32	2a	1532	U	2.5
46	1o	89	GLY	2.5
33	2b	70	PHE	2.5
34	2c	14	ILE	2.5
34	2c	16	ARG	2.5
40	2i	120	ARG	2.5
33	1b	131	PRO	2.5
45	2n	54	PRO	2.5
30	28	22	VAL	2.5
35	2d	11	LEU	2.5
40	2i	17	VAL	2.5
41	1j	68	HIS	2.5
32	2a	1287	A	2.5
1	1A	2174	C	2.5
33	2b	57	PHE	2.5
34	1c	8	ILE	2.5
34	1c	10	PHE	2.5
41	2j	54	PHE	2.5
38	2g	31	MET	2.5
1	1A	2155	G	2.5
32	1a	1032	G	2.5
33	2b	188	ALA	2.5
33	2b	193	ASP	2.5
37	1f	99	ALA	2.5
41	1j	41	PRO	2.5
34	2c	81	GLY	2.5
40	2i	24	GLY	2.5
53	2y	55	ASN	2.5
8	2I	30	LEU	2.5
15	2T	66	VAL	2.5
45	1n	21	TYR	2.5
39	2h	122	ARG	2.5
1	2A	2135	A	2.5
34	1c	182	ILE	2.5
41	2j	89	ASP	2.5
40	1i	82	ALA	2.5
41	2j	20	ALA	2.5
52	2u	23	PRO	2.5
1	2A	2792	G	2.5
26	24	54	GLY	2.5
32	1a	1003	G	2.5
44	2m	95	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
30	28	7	HIS	2.4
34	2c	196	LEU	2.4
38	2g	101	LEU	2.4
22	10	4	LYS	2.4
45	2n	31	ARG	2.4
28	26	42	TRP	2.4
34	2c	18	TRP	2.4
53	1y	42	SER	2.4
1	1A	2062	A	2.4
22	20	6	GLY	2.4
41	1j	93	GLY	2.4
43	1l	63	GLY	2.4
44	2m	42	ALA	2.4
40	2i	113	LYS	2.4
50	2s	39	THR	2.4
40	2i	96	LEU	2.4
12	2Q	97	VAL	2.4
39	1h	103	VAL	2.4
33	2b	97	TRP	2.4
20	2Y	73	ARG	2.4
33	1b	114	ARG	2.4
33	1b	227	GLY	2.4
35	2d	122	ARG	2.4
34	1c	177	THR	2.4
41	2j	24	VAL	2.4
1	2A	2116	G	2.4
34	1c	184	TYR	2.4
47	1p	38	TYR	2.4
38	2g	120	ILE	2.4
41	1j	96	ILE	2.4
47	1p	1	MET	2.4
26	14	17	GLY	2.4
21	1Z	51	ALA	2.4
38	2g	7	ALA	2.4
45	1n	2	ALA	2.4
45	1n	20	ALA	2.4
51	2t	40	ALA	2.4
1	2A	1103	A	2.4
33	2b	51	LEU	2.4
40	2i	53	VAL	2.4
38	2g	79	ARG	2.4
40	2i	104	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
53	2y	23	ARG	2.4
53	1y	35	ILE	2.4
1	1A	2807	G	2.4
34	2c	174	PRO	2.4
53	2y	30	TRP	2.4
39	2h	124	ALA	2.4
1	1A	2143	C	2.4
1	2A	2310	A	2.4
30	28	46	ARG	2.4
32	1a	1035	A	2.4
33	2b	121	LEU	2.4
34	1c	12	LEU	2.4
34	2c	34	LEU	2.4
13	2R	68	ARG	2.4
34	1c	172	ARG	2.4
8	2I	3	VAL	2.4
26	14	56	VAL	2.4
32	2a	1358	U	2.4
34	2c	145	GLY	2.4
35	1d	167	GLY	2.4
40	2i	100	GLY	2.4
53	2y	36	ASN	2.4
33	2b	48	MET	2.4
33	2b	58	ILE	2.4
7	2H	128	PRO	2.4
3	1D	275	LYS	2.4
45	1n	17	LYS	2.4
16	2U	113	ALA	2.4
38	2g	25	ALA	2.4
40	1i	43	ALA	2.4
53	2y	97	ALA	2.4
1	2A	2127	G	2.4
1	2A	2182	G	2.4
40	1i	126	SER	2.4
32	2a	1349	A	2.4
34	2c	106	VAL	2.4
33	2b	194	PRO	2.4
34	2c	182	ILE	2.4
40	1i	36	TYR	2.4
40	2i	33	PHE	2.4
41	1j	47	PHE	2.4
33	1b	123	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
34	2c	59	ARG	2.4
40	1i	105	ASP	2.4
47	1p	29	ASP	2.4
36	1e	17	ALA	2.4
6	2G	58	GLN	2.4
42	2k	104	GLN	2.4
47	2p	59	TRP	2.4
6	2G	139	LEU	2.4
35	2d	188	LEU	2.4
50	2s	5	LEU	2.4
1	2A	2894	G	2.3
42	2k	123	LYS	2.3
32	2a	1149	C	2.3
45	2n	49	HIS	2.3
5	2F	62	ARG	2.3
45	2n	42	ILE	2.3
53	2y	54	ILE	2.3
16	2U	21	ALA	2.3
48	1q	99	SER	2.3
45	2n	4	LYS	2.3
41	1j	16	LEU	2.3
43	1l	60	LEU	2.3
47	1p	49	LEU	2.3
6	2G	29	TRP	2.3
34	2c	22	TRP	2.3
1	2A	1816	G	2.3
47	1p	20	VAL	2.3
48	2q	10	VAL	2.3
40	2i	54	ASP	2.3
45	2n	23	ARG	2.3
49	1r	42	ARG	2.3
52	2u	5	ASP	2.3
1	1A	889	C	2.3
1	1A	2175	C	2.3
8	2I	88	ILE	2.3
44	2m	84	ILE	2.3
6	2G	57	ALA	2.3
23	21	24	ALA	2.3
36	2e	94	ALA	2.3
3	2D	50	THR	2.3
7	2H	106	THR	2.3
53	2y	32	THR	2.3

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Mol	Chain	Res	Type	RSRZ
34	2c	185	GLY	2.3
45	2n	38	GLY	2.3
15	2T	105	LEU	2.3
34	1c	33	LEU	2.3
34	2c	32	LEU	2.3
35	1d	194	LEU	2.3
40	1i	47	LEU	2.3
34	2c	190	ARG	2.3
33	1b	135	GLN	2.3
1	2A	2144	U	2.3
32	2a	1235	U	2.3
1	1A	2159	G	2.3
35	1d	67	ILE	2.3
1	1A	2896	C	2.3
33	2b	122	PHE	2.3
34	1c	189	ALA	2.3
34	2c	15	THR	2.3
45	1n	32	SER	2.3
50	2s	38	SER	2.3
39	2h	131	GLY	2.3
11	1P	135	LEU	2.3
38	2g	10	ARG	2.3
41	2j	40	LEU	2.3
44	2m	96	LEU	2.3
50	2s	71	LEU	2.3
44	2m	111	LYS	2.3
6	2G	142	PRO	2.3
47	2p	33	ILE	2.3
8	2I	82	ARG	2.3
11	2P	22	GLY	2.3
32	2a	1354	C	2.3
40	1i	42	ARG	2.3
40	2i	93	ARG	2.3
51	2t	12	ALA	2.3
32	1a	1492	A	2.3
41	2j	85	LEU	2.3
41	2j	90	LEU	2.3
4	2E	116	VAL	2.3
32	2a	1150	U	2.3
34	2c	167	TRP	2.3
36	2e	14	ARG	2.3
44	2m	110	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
45	2n	7	ILE	2.3
48	2q	94	ASN	2.3
12	2Q	136	ALA	2.3
1	2A	1118	C	2.3
1	2A	2156	G	2.3
32	2a	1021	G	2.3
32	2a	1385	G	2.3
7	2H	95	ARG	2.3
28	26	52	VAL	2.3
34	1c	173	VAL	2.3
34	2c	103	VAL	2.3
40	2i	44	VAL	2.3
32	1a	1020	U	2.3
53	2y	26	LYS	2.3
53	2y	86	ASN	2.3
39	1h	38	ILE	2.3
39	2h	86	ILE	2.3
48	2q	36	ILE	2.3
35	1d	147	ALA	2.3
45	2n	37	PHE	2.3
35	1d	157	LEU	2.3
36	1e	123	LEU	2.3
41	2j	8	LEU	2.3
1	2A	2117	A	2.2
34	2c	4	LYS	2.2
43	2l	13	LYS	2.2
52	1u	10	ARG	2.2
52	2u	22	ARG	2.2
1	1A	2153	G	2.2
5	2F	57	VAL	2.2
32	2a	1040	U	2.2
41	2j	12	ASP	2.2
19	2X	39	ILE	2.2
21	1Z	192	ALA	2.2
33	1b	211	ILE	2.2
38	1g	42	ILE	2.2
35	1d	185	PHE	2.2
34	2c	206	GLU	2.2
43	1l	67	THR	2.2
6	2G	136	ARG	2.2
14	2S	20	ARG	2.2
19	2X	66	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
35	1d	86	LYS	2.2
37	2f	77	ARG	2.2
40	2i	9	ARG	2.2
52	1u	21	TYR	2.2
52	2u	24	ARG	2.2
1	2A	889	C	2.2
1	1A	1085	A	2.2
1	1A	1088	A	2.2
32	1a	1349	A	2.2
46	2o	60	VAL	2.2
1	1A	2130	U	2.2
1	1A	2112	G	2.2
32	1a	1034	G	2.2
32	2a	1034	G	2.2
12	2Q	36	ALA	2.2
35	2d	48	ALA	2.2
40	2i	46	ALA	2.2
46	1o	87	ILE	2.2
22	20	57	PHE	2.2
8	2I	12	LEU	2.2
9	2N	42	TRP	2.2
44	1m	90	LEU	2.2
14	2S	92	TYR	2.2
34	1c	193	TYR	2.2
47	1p	41	PRO	2.2
51	1t	9	ASN	2.2
35	2d	143	GLY	2.2
1	2A	2143	C	2.2
9	2N	9	VAL	2.2
15	2T	70	VAL	2.2
41	1j	59	SER	2.2
41	2j	86	MET	2.2
43	2l	124	LYS	2.2
45	2n	33	VAL	2.2
1	1A	2892	A	2.2
53	2y	91	LYS	2.2
45	1n	45	ARG	2.2
50	2s	77	THR	2.2
32	1a	1002	G	2.2
33	1b	115	LEU	2.2
42	2k	98	LEU	2.2
34	2c	82	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
20	2Y	80	GLY	2.2
34	2c	78	GLY	2.2
35	1d	20	TYR	2.2
35	2d	4	TYR	2.2
36	1e	34	VAL	2.2
32	2a	1236	A	2.2
34	1c	60	ALA	2.2
44	1m	22	ILE	2.2
41	1j	54	PHE	2.2
40	1i	113	LYS	2.2
41	2j	71	LEU	2.2
1	1A	1071	G	2.2
32	2a	886	G	2.2
32	2a	1061	G	2.2
22	20	77	ARG	2.2
38	2g	32	ARG	2.2
12	2Q	35	VAL	2.2
29	27	46	VAL	2.2
38	2g	144	MET	2.2
32	2a	848	C	2.2
34	2c	28	GLN	2.2
50	2s	28	LYS	2.2
1	1A	1095	A	2.2
32	2a	1111	A	2.2
12	2Q	34	LEU	2.2
38	2g	16	LEU	2.2
40	1i	79	LEU	2.2
40	1i	121	ARG	2.2
44	1m	91	ARG	2.2
53	2y	95	ARG	2.2
14	2S	36	TYR	2.2
52	2u	18	TYR	2.2
1	1A	271(K)	U	2.2
35	2d	56	VAL	2.2
3	2D	272	ALA	2.2
24	12	13	ALA	2.2
41	2j	32	ALA	2.2
1	2A	1102	C	2.2
41	2j	17	ASP	2.2
41	2j	74	ILE	2.2
34	2c	131	ARG	2.2
39	2h	76	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
53	2y	14	PRO	2.2
1	1A	1086	A	2.2
8	2I	35	LEU	2.2
16	2U	74	LEU	2.2
32	2a	1151	A	2.2
25	23	60	GLU	2.2
45	2n	27	CYS	2.2
19	1X	69	TYR	2.1
40	1i	4	TYR	2.1
44	1m	82	MET	2.1
47	2p	58	TYR	2.1
32	1a	1023	G	2.1
32	2a	841	U	2.1
34	1c	120	VAL	2.1
38	2g	9	VAL	2.1
43	1l	82	VAL	2.1
6	1G	73	ALA	2.1
41	1j	18	ALA	2.1
5	1F	53	THR	2.1
52	2u	10	ARG	2.1
34	1c	124	ILE	2.1
40	2i	77	ILE	2.1
53	2y	59	GLY	2.1
3	2D	155	LEU	2.1
41	1j	85	LEU	2.1
48	2q	6	LEU	2.1
1	1A	1070	A	2.1
1	2A	887	A	2.1
30	18	37	SER	2.1
21	2Z	80	ARG	2.1
39	1h	94	TYR	2.1
3	1D	199	ALA	2.1
32	1a	1136	U	2.1
33	1b	229	VAL	2.1
40	1i	120	ARG	2.1
4	1E	163	GLU	2.1
38	2g	116	ALA	2.1
40	2i	55	ALA	2.1
42	2k	42	TRP	2.1
47	1p	56	ALA	2.1
32	2a	80	G	2.1
33	2b	127	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
40	2i	25	LYS	2.1
42	2k	29	ILE	2.1
44	2m	4	ILE	2.1
6	2G	133	LEU	2.1
12	2Q	37	LEU	2.1
34	2c	47	LEU	2.1
39	1h	63	LEU	2.1
47	1p	60	LEU	2.1
49	2r	85	LEU	2.1
20	2Y	52	SER	2.1
34	1c	126	ARG	2.1
34	2c	13	GLY	2.1
7	2H	35	VAL	2.1
11	2P	71	VAL	2.1
40	2i	70	LYS	2.1
51	1t	74	LYS	2.1
32	1a	1532	U	2.1
5	2F	65	TRP	2.1
35	1d	201	GLN	2.1
40	2i	124	GLN	2.1
40	1i	33	PHE	2.1
19	1X	66	LEU	2.1
1	1A	2124	G	2.1
1	2A	2149	G	2.1
1	2A	2155	G	2.1
18	2W	92	ARG	2.1
32	2a	1002	G	2.1
32	1a	1037	C	2.1
32	2a	783	C	2.1
19	1X	67	GLY	2.1
1	1A	2169	A	2.1
36	1e	10	MET	2.1
36	1e	136	MET	2.1
1	2A	1026	U	2.1
36	1e	55	VAL	2.1
40	1i	45	ALA	2.1
41	2j	18	ALA	2.1
44	1m	109	THR	2.1
47	1p	32	TYR	2.1
47	1p	39	TYR	2.1
51	2t	28	ALA	2.1
11	2P	57	THR	2.1

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Mol	Chain	Res	Type	RSRZ
5	2F	78	ILE	2.1
15	2T	110	ILE	2.1
33	2b	162	ILE	2.1
39	2h	38	ILE	2.1
23	11	95	LEU	2.1
23	21	60	PHE	2.1
41	2j	66	ARG	2.1
41	2j	88	LEU	2.1
34	2c	144	SER	2.1
3	1D	47	GLY	2.1
32	2a	1003	G	2.1
42	2k	76	GLY	2.1
33	2b	83	MET	2.1
1	2A	2119	A	2.1
1	2A	2130	U	2.1
6	2G	64	THR	2.1
6	2G	93	THR	2.1
23	11	53	VAL	2.1
32	2a	1157	A	2.1
35	2d	140	VAL	2.1
37	1f	6	VAL	2.1
41	2j	45	ARG	2.1
48	2q	42	TYR	2.1
5	2F	82	ILE	2.1
45	2n	15	LYS	2.1
35	1d	19	LEU	2.1
35	1d	58	LEU	2.1
39	1h	112	LEU	2.1
26	24	19	GLY	2.1
40	2i	80	GLY	2.1
44	1m	89	GLY	2.1
41	2j	84	GLN	2.1
43	2l	16	GLU	2.1
1	2A	2165	G	2.1
23	21	63	ALA	2.1
32	1a	1021	G	2.1
33	2b	144	ARG	2.1
3	1D	10	THR	2.1
5	2F	81	PRO	2.1
34	1c	160	ALA	2.1
44	1m	28	ALA	2.1
45	1n	15	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
8	2I	18	VAL	2.1
9	2N	43	THR	2.1
12	2Q	102	VAL	2.1
34	1c	64	VAL	2.1
40	1i	108	VAL	2.1
32	2a	1041	A	2.1
35	1d	68	TYR	2.1
47	1p	17	TYR	2.1
23	11	46	LEU	2.1
33	1b	124	SER	2.1
36	1e	6	PHE	2.1
5	1F	85	GLY	2.1
22	20	52	GLY	2.1
40	2i	87	GLN	2.1
4	2E	120	TRP	2.1
34	2c	166	GLU	2.1
33	1b	232	PRO	2.0
32	1a	1040	U	2.0
42	2k	87	THR	2.0
12	2Q	120	ILE	2.0
34	2c	77	ILE	2.0
34	2c	184	TYR	2.0
6	1G	139	LEU	2.0
26	24	59	PHE	2.0
30	28	38	GLY	2.0
33	2b	181	PHE	2.0
35	2d	134	ASP	2.0
35	2d	165	MET	2.0
53	2y	22	ASP	2.0
4	2E	157	ALA	2.0
33	1b	125	PRO	2.0
48	1q	28	PRO	2.0
1	1A	2145	C	2.0
6	2G	160	VAL	2.0
7	2H	37	VAL	2.0
7	2H	129	THR	2.0
16	2U	9	VAL	2.0
40	2i	58	HIS	2.0
44	2m	109	THR	2.0
34	2c	49	SER	2.0
12	1Q	33	GLY	2.0
25	23	53	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
33	1b	228	GLY	2.0
34	2c	57	ILE	2.0
38	2g	63	LYS	2.0
40	1i	11	LYS	2.0
36	2e	123	LEU	2.0
46	2o	87	ILE	2.0
48	2q	59	ILE	2.0
50	2s	49	ILE	2.0
1	1A	2156	G	2.0
25	23	12	PRO	2.0
38	1g	31	MET	2.0
6	2G	41	GLN	2.0
46	1o	80	ALA	2.0
51	1t	12	ALA	2.0
53	2y	29	LYS	2.0
1	2A	2172	U	2.0
35	2d	198	VAL	2.0
40	2i	89	ASN	2.0
45	1n	25	VAL	2.0
40	1i	16	ARG	2.0
1	2A	2175	C	2.0
5	2F	28	ILE	2.0
32	2a	1027	C	2.0
32	2a	1195	C	2.0
33	1b	222	ILE	2.0
33	2b	11	LEU	2.0
34	2c	101	LEU	2.0
35	2d	186	LEU	2.0
43	2l	84	LEU	2.0
14	2S	12	PHE	2.0
35	2d	185	PHE	2.0
1	1A	2123	G	2.0
32	2a	976	G	2.0
32	2a	1023	G	2.0
33	2b	133	LYS	2.0
33	1b	48	MET	2.0
40	1i	31	GLN	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	0.80	0.18	63,76,78,90	0
1	PSU	2A	1911	20/21	0.84	0.16	62,67,77,78	0
1	PSU	2A	1917	20/21	0.88	0.18	63,70,85,92	0
55	8AN	1x	76	22/23	0.88	0.50	42,60,70,72	0
55	8AN	2x	76	22/23	0.88	0.42	49,64,72,84	0
32	M2G	2a	966	25/26	0.89	0.20	57,64,74,84	0
32	2MG	2a	1207	24/25	0.89	0.22	67,73,77,83	0
32	5MC	1a	967	21/22	0.90	0.20	57,62,69,73	0
43	0TD	2l	92	10/11	0.90	0.16	53,60,62,62	0
1	5MU	1A	1915	21/22	0.91	0.17	54,65,69,74	0
32	5MC	2a	1404	21/22	0.92	0.20	51,55,58,60	0
32	5MC	2a	967	21/22	0.92	0.21	60,65,71,72	0
1	PSU	1A	1911	20/21	0.93	0.17	49,57,64,68	0
32	4OC	2a	1402	22/23	0.93	0.21	53,59,65,67	0
32	2MG	1a	1207	24/25	0.93	0.19	54,65,69,72	0
32	MA6	2a	1518	24/25	0.93	0.18	52,58,61,64	0
1	OMC	2A	1920	21/22	0.93	0.18	52,60,66,69	0
43	0TD	1l	92	10/11	0.93	0.17	45,52,57,58	0
1	PSU	1A	1917	20/21	0.93	0.16	54,62,70,72	0
32	M2G	1a	966	25/26	0.94	0.18	46,54,61,62	0
32	PSU	1a	516	20/21	0.94	0.17	54,60,67,78	0
32	PSU	2a	516	20/21	0.94	0.13	63,68,75,76	0
32	5MC	1a	1407	21/22	0.95	0.17	40,50,54,58	0
32	G7M	2a	527	24/25	0.95	0.17	53,57,60,66	0
32	5MC	1a	1404	21/22	0.95	0.18	40,47,50,53	0
32	MA6	2a	1519	24/25	0.95	0.26	46,55,60,63	0
1	2MU	2A	2552	21/23	0.95	0.20	28,37,42,43	0
1	PSU	2A	2605	20/21	0.95	0.24	26,36,43,44	0
32	5MC	2a	1400	21/22	0.95	0.33	51,68,74,76	0
1	OMG	2A	2251	24/25	0.96	0.20	33,37,42,46	0
32	MA6	1a	1518	24/25	0.96	0.22	36,43,49,55	0
32	MA6	1a	1519	24/25	0.96	0.21	40,43,49,50	0
32	5MC	2a	1407	21/22	0.96	0.16	50,59,63,67	0
32	5MC	1a	1400	21/22	0.96	0.20	42,50,61,61	0
32	4OC	1a	1402	22/23	0.96	0.18	47,49,53,62	0
32	G7M	1a	527	24/25	0.96	0.16	44,51,55,57	0
1	OMC	1A	1920	21/22	0.96	0.20	41,51,58,59	0
32	UR3	1a	1498	21/22	0.96	0.19	38,46,49,62	0
1	5MU	2A	1939	21/22	0.97	0.19	32,38,43,44	0
1	5MC	2A	1942	21/22	0.97	0.18	39,46,52,58	0
32	UR3	2a	1498	21/22	0.97	0.22	52,56,60,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MC	2A	1962	21/22	0.97	0.17	32,41,47,52	0
1	PSU	1A	2605	20/21	0.97	0.20	18,26,29,29	0
1	2MA	2A	2503	23/24	0.97	0.20	23,29,34,35	0
1	5MC	1A	1942	21/22	0.97	0.18	28,33,38,42	0
1	5MC	1A	1962	21/22	0.97	0.20	26,30,35,38	0
1	5MU	1A	1939	21/22	0.98	0.20	19,24,27,28	0
1	OMG	1A	2251	24/25	0.98	0.20	15,21,32,36	0
1	2MA	1A	2503	23/24	0.98	0.22	14,19,22,23	0
1	2MU	1A	2552	21/23	0.98	0.21	20,28,33,34	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	3940	1/1	-0.07	0.30	74,74,74,74	0
57	MG	1A	4009	1/1	0.29	0.14	54,54,54,54	0
57	MG	2a	3008	1/1	0.36	0.16	63,63,63,63	0
57	MG	2O	202	1/1	0.40	0.38	73,73,73,73	0
57	MG	2A	3549	1/1	0.40	0.12	70,70,70,70	0
57	MG	2A	3646	1/1	0.42	0.19	67,67,67,67	0
57	MG	1A	3560	1/1	0.43	0.13	52,52,52,52	0
57	MG	1A	3712	1/1	0.46	0.13	60,60,60,60	0
57	MG	2A	3168	1/1	0.46	0.22	58,58,58,58	0
57	MG	2a	3023	1/1	0.46	0.23	59,59,59,59	0
57	MG	1B	219	1/1	0.52	0.13	46,46,46,46	0
57	MG	2A	3607	1/1	0.52	0.11	42,42,42,42	0
57	MG	1A	3977	1/1	0.52	0.18	34,34,34,34	0
57	MG	2A	3564	1/1	0.55	0.15	67,67,67,67	0
57	MG	1d	305	1/1	0.56	0.12	75,75,75,75	0
57	MG	1A	3939	1/1	0.57	0.18	58,58,58,58	0
57	MG	1A	3194	1/1	0.59	0.55	54,54,54,54	0
57	MG	1A	3002	1/1	0.60	0.60	57,57,57,57	0
57	MG	1A	3663	1/1	0.61	0.23	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3143	1/1	0.61	0.08	62,62,62,62	0
57	MG	2A	3159	1/1	0.62	0.17	63,63,63,63	0
57	MG	2A	3624	1/1	0.62	0.21	70,70,70,70	0
57	MG	1A	3924	1/1	0.62	0.15	57,57,57,57	0
57	MG	2E	301	1/1	0.62	0.22	39,39,39,39	0
57	MG	1A	3915	1/1	0.63	0.13	47,47,47,47	0
57	MG	2a	3177	1/1	0.63	0.06	64,64,64,64	0
57	MG	2A	3121	1/1	0.64	0.14	73,73,73,73	0
57	MG	1A	3705	1/1	0.65	0.14	64,64,64,64	0
57	MG	1D	315	1/1	0.65	0.25	68,68,68,68	0
57	MG	1a	3248	1/1	0.65	0.11	45,45,45,45	0
57	MG	2a	3086	1/1	0.65	0.13	60,60,60,60	0
57	MG	2A	3477	1/1	0.65	0.18	51,51,51,51	0
57	MG	1A	3830	1/1	0.65	0.07	41,41,41,41	0
57	MG	1a	3228	1/1	0.66	0.19	72,72,72,72	0
57	MG	2a	3057	1/1	0.66	0.12	68,68,68,68	0
57	MG	2A	3064	1/1	0.66	0.17	51,51,51,51	0
57	MG	2A	3194	1/1	0.66	0.16	59,59,59,59	0
57	MG	2a	3145	1/1	0.66	0.12	52,52,52,52	0
57	MG	1A	3504	1/1	0.66	0.14	50,50,50,50	0
57	MG	1N	205	1/1	0.67	0.10	46,46,46,46	0
57	MG	1A	4012	1/1	0.67	0.15	40,40,40,40	0
57	MG	1A	3753	1/1	0.67	0.15	45,45,45,45	0
57	MG	1A	3533	1/1	0.67	0.22	48,48,48,48	0
57	MG	2a	3182	1/1	0.67	0.16	82,82,82,82	0
57	MG	1a	3077	1/1	0.68	0.23	65,65,65,65	0
57	MG	1A	3380	1/1	0.68	0.16	43,43,43,43	0
57	MG	2A	3499	1/1	0.68	0.19	49,49,49,49	0
57	MG	1A	3990	1/1	0.69	0.20	82,82,82,82	0
57	MG	2A	3631	1/1	0.69	0.10	58,58,58,58	0
57	MG	1A	3926	1/1	0.69	0.08	35,35,35,35	0
57	MG	2B	216	1/1	0.69	0.12	68,68,68,68	0
57	MG	1a	3239	1/1	0.69	0.18	74,74,74,74	0
57	MG	1A	3311	1/1	0.69	0.30	62,62,62,62	0
57	MG	10	106	1/1	0.69	0.13	50,50,50,50	0
57	MG	1A	3302	1/1	0.70	0.23	58,58,58,58	0
57	MG	2B	204	1/1	0.70	0.09	69,69,69,69	0
57	MG	2A	3235	1/1	0.70	0.15	62,62,62,62	0
57	MG	2A	3253	1/1	0.70	0.13	54,54,54,54	0
57	MG	2G	203	1/1	0.70	0.13	65,65,65,65	0
57	MG	2A	3257	1/1	0.70	0.18	52,52,52,52	0
57	MG	2A	3275	1/1	0.70	0.14	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	1Y	201	1/1	0.70	0.12	41,41,41,41	0
57	MG	1B	211	1/1	0.70	0.20	62,62,62,62	0
57	MG	1n	101	1/1	0.70	0.28	64,64,64,64	0
57	MG	2a	3133	1/1	0.70	0.15	72,72,72,72	0
57	MG	1A	3677	1/1	0.70	0.10	64,64,64,64	0
57	MG	1a	3092	1/1	0.70	0.33	68,68,68,68	0
57	MG	1a	3184	1/1	0.70	0.12	56,56,56,56	0
57	MG	1A	3697	1/1	0.70	0.68	59,59,59,59	0
57	MG	1A	3852	1/1	0.71	0.13	52,52,52,52	0
57	MG	1A	3437	1/1	0.71	0.24	64,64,64,64	0
57	MG	2A	3025	1/1	0.71	0.15	48,48,48,48	0
57	MG	1a	3255	1/1	0.71	0.16	61,61,61,61	0
57	MG	2A	3116	1/1	0.71	0.10	51,51,51,51	0
59	ARG	1A	4023	12/12	0.71	0.26	43,60,64,64	0
57	MG	1A	3783	1/1	0.72	0.29	59,59,59,59	0
57	MG	1A	3889	1/1	0.72	0.13	52,52,52,52	0
57	MG	2A	3679	1/1	0.72	0.14	58,58,58,58	0
57	MG	1a	3185	1/1	0.72	0.09	58,58,58,58	0
57	MG	2A	3178	1/1	0.72	0.20	48,48,48,48	0
57	MG	1a	3058	1/1	0.72	0.17	61,61,61,61	0
57	MG	2A	3207	1/1	0.72	0.17	64,64,64,64	0
57	MG	1a	3076	1/1	0.72	0.27	56,56,56,56	0
57	MG	1A	3078	1/1	0.72	0.25	54,54,54,54	0
57	MG	1A	3918	1/1	0.73	0.13	38,38,38,38	0
57	MG	2A	3691	1/1	0.73	0.10	57,57,57,57	0
57	MG	2A	3246	1/1	0.73	0.25	55,55,55,55	0
57	MG	2A	3023	1/1	0.73	0.16	56,56,56,56	0
57	MG	1a	3114	1/1	0.73	0.13	68,68,68,68	0
57	MG	1A	3984	1/1	0.73	0.38	38,38,38,38	0
57	MG	2A	3350	1/1	0.73	0.14	28,28,28,28	0
57	MG	2T	204	1/1	0.73	0.14	60,60,60,60	0
57	MG	1P	203	1/1	0.73	0.24	42,42,42,42	0
57	MG	1a	3197	1/1	0.73	0.17	49,49,49,49	0
57	MG	2a	3034	1/1	0.73	0.12	70,70,70,70	0
57	MG	1A	3195	1/1	0.73	0.14	45,45,45,45	0
57	MG	2a	3069	1/1	0.73	0.11	62,62,62,62	0
57	MG	1A	3868	1/1	0.73	0.16	41,41,41,41	0
57	MG	2A	3592	1/1	0.73	0.14	40,40,40,40	0
57	MG	1A	3821	1/1	0.73	0.62	36,36,36,36	0
57	MG	2A	3191	1/1	0.73	0.18	65,65,65,65	0
57	MG	2a	3173	1/1	0.73	0.07	64,64,64,64	0
57	MG	1A	3568	1/1	0.73	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3975	1/1	0.73	0.09	56,56,56,56	0
57	MG	2A	3657	1/1	0.73	0.07	58,58,58,58	0
61	ZN	24	501	1/1	0.73	0.15	127,127,127,127	0
57	MG	2A	3320	1/1	0.74	0.18	53,53,53,53	0
57	MG	1A	3620	1/1	0.74	0.18	34,34,34,34	0
57	MG	2A	3408	1/1	0.74	0.20	63,63,63,63	0
57	MG	2A	3433	1/1	0.74	0.12	76,76,76,76	0
57	MG	2A	3436	1/1	0.74	0.14	65,65,65,65	0
57	MG	1A	3646	1/1	0.74	0.12	59,59,59,59	0
57	MG	2B	207	1/1	0.74	0.14	59,59,59,59	0
57	MG	1A	3907	1/1	0.74	0.22	56,56,56,56	0
57	MG	1A	3215	1/1	0.74	0.15	46,46,46,46	0
57	MG	1a	3085	1/1	0.74	0.18	57,57,57,57	0
57	MG	1A	3467	1/1	0.74	0.15	41,41,41,41	0
57	MG	1A	3057	1/1	0.74	0.20	44,44,44,44	0
57	MG	1A	3594	1/1	0.74	0.25	66,66,66,66	0
57	MG	2a	3039	1/1	0.75	0.13	59,59,59,59	0
57	MG	2A	3031	1/1	0.75	0.20	63,63,63,63	0
57	MG	2a	3058	1/1	0.75	0.24	63,63,63,63	0
57	MG	2A	3240	1/1	0.75	0.17	66,66,66,66	0
57	MG	1a	3148	1/1	0.75	0.17	35,35,35,35	0
57	MG	2A	3189	1/1	0.75	0.33	59,59,59,59	0
57	MG	2A	3456	1/1	0.75	0.15	53,53,53,53	0
57	MG	2A	3636	1/1	0.75	0.13	52,52,52,52	0
57	MG	2A	3003	1/1	0.75	0.17	58,58,58,58	0
57	MG	2A	3492	1/1	0.75	0.10	47,47,47,47	0
57	MG	2a	3019	1/1	0.75	0.13	64,64,64,64	0
57	MG	1A	3742	1/1	0.75	0.14	74,74,74,74	0
61	ZN	14	501	1/1	0.75	0.07	104,104,104,104	0
57	MG	1A	3181	1/1	0.75	0.15	49,49,49,49	0
57	MG	2A	3577	1/1	0.76	0.09	52,52,52,52	0
57	MG	1A	3791	1/1	0.76	0.12	70,70,70,70	0
57	MG	2a	3065	1/1	0.76	0.09	69,69,69,69	0
57	MG	2A	3439	1/1	0.76	0.16	53,53,53,53	0
57	MG	1a	3261	1/1	0.76	0.16	60,60,60,60	0
57	MG	2A	3474	1/1	0.76	0.15	61,61,61,61	0
57	MG	1A	3087	1/1	0.76	0.14	48,48,48,48	0
57	MG	2A	3334	1/1	0.76	0.08	37,37,37,37	0
57	MG	2a	3010	1/1	0.76	0.20	61,61,61,61	0
57	MG	2A	3057	1/1	0.76	0.18	56,56,56,56	0
57	MG	2A	3528	1/1	0.76	0.19	64,64,64,64	0
57	MG	1a	3029	1/1	0.76	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3037	1/1	0.76	0.16	67,67,67,67	0
57	MG	1A	3460	1/1	0.76	0.12	36,36,36,36	0
57	MG	1A	3197	1/1	0.77	0.27	53,53,53,53	0
57	MG	2A	3515	1/1	0.77	0.11	67,67,67,67	0
57	MG	1A	3948	1/1	0.77	0.15	53,53,53,53	0
57	MG	2A	3532	1/1	0.77	0.10	53,53,53,53	0
57	MG	1A	3880	1/1	0.77	0.11	35,35,35,35	0
57	MG	10	105	1/1	0.77	0.07	43,43,43,43	0
57	MG	2A	3568	1/1	0.77	0.15	37,37,37,37	0
57	MG	1A	3586	1/1	0.77	0.14	51,51,51,51	0
57	MG	1A	3893	1/1	0.77	0.16	47,47,47,47	0
57	MG	2A	3341	1/1	0.77	0.13	42,42,42,42	0
57	MG	1a	3241	1/1	0.77	0.11	49,49,49,49	0
57	MG	2A	3398	1/1	0.77	0.18	56,56,56,56	0
57	MG	1A	3514	1/1	0.77	0.13	53,53,53,53	0
57	MG	2a	3079	1/1	0.77	0.19	60,60,60,60	0
57	MG	1a	3073	1/1	0.77	0.17	53,53,53,53	0
57	MG	1A	3595	1/1	0.77	0.20	54,54,54,54	0
57	MG	1A	3829	1/1	0.77	0.16	41,41,41,41	0
57	MG	2A	3455	1/1	0.77	0.09	46,46,46,46	0
57	MG	1A	3209	1/1	0.77	0.32	67,67,67,67	0
57	MG	1A	3842	1/1	0.77	0.13	41,41,41,41	0
57	MG	2B	214	1/1	0.77	0.16	51,51,51,51	0
57	MG	1A	3189	1/1	0.77	0.20	51,51,51,51	0
57	MG	2A	3484	1/1	0.77	0.14	57,57,57,57	0
57	MG	2A	3024	1/1	0.77	0.15	58,58,58,58	0
57	MG	1A	3912	1/1	0.78	0.09	53,53,53,53	0
57	MG	2A	3659	1/1	0.78	0.14	65,65,65,65	0
57	MG	1a	3142	1/1	0.78	0.34	62,62,62,62	0
57	MG	2A	3415	1/1	0.78	0.11	33,33,33,33	0
57	MG	1A	3866	1/1	0.78	0.08	65,65,65,65	0
57	MG	2A	3540	1/1	0.78	0.11	55,55,55,55	0
57	MG	1a	3044	1/1	0.78	0.18	50,50,50,50	0
57	MG	1A	3353	1/1	0.78	0.11	30,30,30,30	0
57	MG	2A	3454	1/1	0.78	0.31	72,72,72,72	0
57	MG	1N	204	1/1	0.78	0.13	50,50,50,50	0
57	MG	2A	3578	1/1	0.78	0.06	40,40,40,40	0
57	MG	2a	3166	1/1	0.78	0.10	62,62,62,62	0
57	MG	2A	3299	1/1	0.78	0.13	33,33,33,33	0
57	MG	1A	3834	1/1	0.78	0.08	34,34,34,34	0
57	MG	1A	3584	1/1	0.78	0.16	35,35,35,35	0
57	MG	1A	3848	1/1	0.78	0.22	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	3486	1/1	0.78	0.10	54,54,54,54	0
61	ZN	2Y	202	1/1	0.78	0.12	81,81,81,81	0
57	MG	1A	3472	1/1	0.78	0.19	43,43,43,43	0
57	MG	1A	3386	1/1	0.79	0.16	20,20,20,20	0
57	MG	2A	3196	1/1	0.79	0.26	55,55,55,55	0
57	MG	1a	3100	1/1	0.79	0.14	61,61,61,61	0
57	MG	2A	3208	1/1	0.79	0.17	56,56,56,56	0
57	MG	2A	3212	1/1	0.79	0.12	61,61,61,61	0
57	MG	2A	3497	1/1	0.79	0.15	40,40,40,40	0
57	MG	1a	3262	1/1	0.79	0.14	61,61,61,61	0
57	MG	2A	3507	1/1	0.79	0.15	59,59,59,59	0
57	MG	1d	301	1/1	0.79	0.10	57,57,57,57	0
57	MG	1a	3105	1/1	0.79	0.30	64,64,64,64	0
57	MG	1A	3395	1/1	0.79	0.18	34,34,34,34	0
57	MG	1a	3116	1/1	0.79	0.15	51,51,51,51	0
57	MG	1a	3034	1/1	0.79	0.19	47,47,47,47	0
57	MG	1a	3147	1/1	0.79	0.14	54,54,54,54	0
57	MG	1a	3038	1/1	0.79	0.18	56,56,56,56	0
57	MG	2a	3063	1/1	0.79	0.24	63,63,63,63	0
57	MG	2A	3572	1/1	0.79	0.16	42,42,42,42	0
57	MG	1a	3161	1/1	0.79	0.15	41,41,41,41	0
57	MG	1a	3182	1/1	0.79	0.14	77,77,77,77	0
57	MG	1A	3978	1/1	0.79	0.17	36,36,36,36	0
57	MG	2a	3124	1/1	0.79	0.21	64,64,64,64	0
57	MG	2A	3380	1/1	0.79	0.18	49,49,49,49	0
57	MG	2A	3079	1/1	0.79	0.16	50,50,50,50	0
57	MG	1a	3045	1/1	0.79	0.16	60,60,60,60	0
57	MG	1A	3413	1/1	0.79	0.14	62,62,62,62	0
57	MG	1A	3598	1/1	0.79	0.12	40,40,40,40	0
57	MG	1A	3492	1/1	0.79	0.12	34,34,34,34	0
57	MG	1A	3376	1/1	0.79	0.17	48,48,48,48	0
57	MG	1a	3245	1/1	0.79	0.08	52,52,52,52	0
57	MG	1A	4013	1/1	0.79	0.29	57,57,57,57	0
57	MG	2A	3192	1/1	0.79	0.15	39,39,39,39	0
57	MG	2A	3473	1/1	0.79	0.08	58,58,58,58	0
57	MG	1O	201	1/1	0.80	0.10	41,41,41,41	0
57	MG	1A	3779	1/1	0.80	0.09	39,39,39,39	0
57	MG	1A	3916	1/1	0.80	0.15	52,52,52,52	0
57	MG	2a	3024	1/1	0.80	0.17	58,58,58,58	0
57	MG	1a	3227	1/1	0.80	0.24	62,62,62,62	0
57	MG	1A	3671	1/1	0.80	0.14	53,53,53,53	0
57	MG	1a	3233	1/1	0.80	0.23	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	3050	1/1	0.80	0.19	56,56,56,56	0
57	MG	1a	3094	1/1	0.80	0.19	57,57,57,57	0
57	MG	1A	3286	1/1	0.80	0.16	63,63,63,63	0
57	MG	1A	3187	1/1	0.80	0.21	47,47,47,47	0
57	MG	2A	3286	1/1	0.80	0.20	61,61,61,61	0
57	MG	1A	3200	1/1	0.80	0.32	52,52,52,52	0
57	MG	1a	3252	1/1	0.80	0.15	46,46,46,46	0
57	MG	2a	3081	1/1	0.80	0.22	52,52,52,52	0
57	MG	1A	3283	1/1	0.80	0.19	66,66,66,66	0
57	MG	2a	3093	1/1	0.80	0.12	45,45,45,45	0
57	MG	1A	3833	1/1	0.80	0.22	40,40,40,40	0
57	MG	2A	3708	1/1	0.80	0.13	62,62,62,62	0
57	MG	2A	3717	1/1	0.80	0.15	61,61,61,61	0
57	MG	1A	3969	1/1	0.80	0.14	30,30,30,30	0
57	MG	1A	3521	1/1	0.80	0.12	46,46,46,46	0
57	MG	1a	3065	1/1	0.80	0.25	61,61,61,61	0
57	MG	2A	3400	1/1	0.80	0.14	41,41,41,41	0
57	MG	1A	3593	1/1	0.80	0.07	30,30,30,30	0
57	MG	2f	201	1/1	0.80	0.14	50,50,50,50	0
57	MG	1y	203	1/1	0.80	0.26	59,59,59,59	0
57	MG	2A	3555	1/1	0.80	0.08	65,65,65,65	0
57	MG	2A	3559	1/1	0.80	0.12	62,62,62,62	0
57	MG	2A	3429	1/1	0.80	0.13	47,47,47,47	0
57	MG	1a	3179	1/1	0.81	0.16	55,55,55,55	0
57	MG	2F	302	1/1	0.81	0.17	33,33,33,33	0
57	MG	2A	3266	1/1	0.81	0.12	54,54,54,54	0
57	MG	2A	3273	1/1	0.81	0.26	51,51,51,51	0
57	MG	2A	3509	1/1	0.81	0.19	55,55,55,55	0
57	MG	1a	3181	1/1	0.81	0.14	51,51,51,51	0
57	MG	1A	3178	1/1	0.81	0.16	52,52,52,52	0
57	MG	1A	3202	1/1	0.81	0.16	38,38,38,38	0
57	MG	1A	3979	1/1	0.81	0.09	53,53,53,53	0
57	MG	1A	3785	1/1	0.81	0.20	59,59,59,59	0
57	MG	1a	3201	1/1	0.81	0.10	59,59,59,59	0
57	MG	1a	3210	1/1	0.81	0.22	59,59,59,59	0
57	MG	1a	3212	1/1	0.81	0.07	64,64,64,64	0
57	MG	2A	3385	1/1	0.81	0.18	71,71,71,71	0
57	MG	2A	3397	1/1	0.81	0.10	50,50,50,50	0
57	MG	1a	3222	1/1	0.81	0.10	75,75,75,75	0
57	MG	2a	3062	1/1	0.81	0.17	56,56,56,56	0
57	MG	1A	3933	1/1	0.81	0.13	50,50,50,50	0
57	MG	1A	3617	1/1	0.81	0.19	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3318	1/1	0.81	0.22	47,47,47,47	0
57	MG	2A	3609	1/1	0.81	0.27	51,51,51,51	0
57	MG	2A	3426	1/1	0.81	0.16	57,57,57,57	0
57	MG	1a	3236	1/1	0.81	0.28	46,46,46,46	0
57	MG	1a	3099	1/1	0.81	0.10	60,60,60,60	0
57	MG	1A	3849	1/1	0.81	0.08	50,50,50,50	0
57	MG	1a	3018	1/1	0.81	0.21	56,56,56,56	0
57	MG	1B	203	1/1	0.81	0.16	56,56,56,56	0
57	MG	2A	3677	1/1	0.81	0.18	33,33,33,33	0
57	MG	1B	207	1/1	0.81	0.21	50,50,50,50	0
57	MG	1A	3827	1/1	0.81	0.13	45,45,45,45	0
57	MG	2A	3704	1/1	0.81	0.15	42,42,42,42	0
57	MG	1a	3144	1/1	0.81	0.15	78,78,78,78	0
57	MG	1A	3692	1/1	0.81	0.16	50,50,50,50	0
57	MG	1B	222	1/1	0.81	0.17	42,42,42,42	0
57	MG	1a	3155	1/1	0.81	0.08	73,73,73,73	0
57	MG	1B	231	1/1	0.81	0.16	60,60,60,60	0
57	MG	1y	202	1/1	0.81	0.11	61,61,61,61	0
57	MG	2B	209	1/1	0.82	0.15	70,70,70,70	0
57	MG	2B	212	1/1	0.82	0.14	53,53,53,53	0
57	MG	2A	3495	1/1	0.82	0.18	55,55,55,55	0
57	MG	2A	3094	1/1	0.82	0.11	61,61,61,61	0
57	MG	2A	3097	1/1	0.82	0.21	48,48,48,48	0
57	MG	2A	3113	1/1	0.82	0.17	49,49,49,49	0
57	MG	1a	3087	1/1	0.82	0.23	57,57,57,57	0
57	MG	2A	3117	1/1	0.82	0.28	47,47,47,47	0
57	MG	2A	3328	1/1	0.82	0.15	59,59,59,59	0
57	MG	2a	3007	1/1	0.82	0.19	53,53,53,53	0
57	MG	11	104	1/1	0.82	0.17	47,47,47,47	0
57	MG	2A	3336	1/1	0.82	0.14	44,44,44,44	0
57	MG	2A	3143	1/1	0.82	0.20	42,42,42,42	0
57	MG	1A	3478	1/1	0.82	0.16	26,26,26,26	0
57	MG	2A	3360	1/1	0.82	0.15	77,77,77,77	0
57	MG	1A	3919	1/1	0.82	0.14	46,46,46,46	0
57	MG	2A	3169	1/1	0.82	0.34	49,49,49,49	0
57	MG	1B	227	1/1	0.82	0.11	58,58,58,58	0
57	MG	1A	3708	1/1	0.82	0.15	34,34,34,34	0
57	MG	1A	3611	1/1	0.82	0.38	34,34,34,34	0
57	MG	2A	3585	1/1	0.82	0.07	38,38,38,38	0
57	MG	2A	3589	1/1	0.82	0.17	41,41,41,41	0
57	MG	1A	3010	1/1	0.82	0.16	57,57,57,57	0
57	MG	2A	3604	1/1	0.82	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	3118	1/1	0.82	0.15	55,55,55,55	0
57	MG	1a	3132	1/1	0.82	0.19	50,50,50,50	0
57	MG	1A	3895	1/1	0.82	0.08	44,44,44,44	0
57	MG	2A	3629	1/1	0.82	0.10	54,54,54,54	0
57	MG	1A	3747	1/1	0.82	0.12	41,41,41,41	0
57	MG	1a	3229	1/1	0.82	0.11	63,63,63,63	0
57	MG	2A	3214	1/1	0.82	0.27	51,51,51,51	0
57	MG	2A	3647	1/1	0.82	0.08	40,40,40,40	0
57	MG	2A	3233	1/1	0.82	0.21	47,47,47,47	0
57	MG	1A	3571	1/1	0.82	0.21	49,49,49,49	0
57	MG	2A	3236	1/1	0.82	0.25	38,38,38,38	0
57	MG	2A	3459	1/1	0.82	0.12	53,53,53,53	0
57	MG	1A	3857	1/1	0.82	0.10	41,41,41,41	0
57	MG	2A	3046	1/1	0.82	0.10	53,53,53,53	0
57	MG	1A	3971	1/1	0.82	0.13	37,37,37,37	0
57	MG	1A	3343	1/1	0.82	0.15	54,54,54,54	0
57	MG	1a	3166	1/1	0.82	0.08	48,48,48,48	0
57	MG	2A	3271	1/1	0.82	0.17	44,44,44,44	0
57	MG	1A	3751	1/1	0.83	0.07	37,37,37,37	0
57	MG	1A	3061	1/1	0.83	0.21	36,36,36,36	0
57	MG	1a	3124	1/1	0.83	0.16	53,53,53,53	0
57	MG	2A	3127	1/1	0.83	0.32	41,41,41,41	0
57	MG	2A	3133	1/1	0.83	0.23	58,58,58,58	0
57	MG	1A	3528	1/1	0.83	0.18	44,44,44,44	0
57	MG	1a	3141	1/1	0.83	0.09	59,59,59,59	0
57	MG	2A	3353	1/1	0.83	0.12	54,54,54,54	0
57	MG	2a	3005	1/1	0.83	0.15	64,64,64,64	0
57	MG	1B	224	1/1	0.83	0.09	38,38,38,38	0
57	MG	1A	3909	1/1	0.83	0.06	40,40,40,40	0
57	MG	1A	3911	1/1	0.83	0.10	52,52,52,52	0
57	MG	1a	3063	1/1	0.83	0.19	69,69,69,69	0
57	MG	1a	3150	1/1	0.83	0.14	59,59,59,59	0
57	MG	1a	3265	1/1	0.83	0.23	56,56,56,56	0
57	MG	2a	3029	1/1	0.83	0.18	57,57,57,57	0
57	MG	1A	3780	1/1	0.83	0.09	43,43,43,43	0
57	MG	2A	3413	1/1	0.83	0.16	55,55,55,55	0
57	MG	2A	3602	1/1	0.83	0.15	36,36,36,36	0
57	MG	1G	204	1/1	0.83	0.16	49,49,49,49	0
57	MG	1a	3074	1/1	0.83	0.25	54,54,54,54	0
57	MG	1y	201	1/1	0.83	0.25	67,67,67,67	0
57	MG	2A	3611	1/1	0.83	0.13	33,33,33,33	0
57	MG	2A	3613	1/1	0.83	0.16	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3458	1/1	0.83	0.16	38,38,38,38	0
57	MG	1A	3621	1/1	0.83	0.11	40,40,40,40	0
57	MG	2a	3076	1/1	0.83	0.13	54,54,54,54	0
57	MG	2A	3218	1/1	0.83	0.19	71,71,71,71	0
57	MG	2A	3634	1/1	0.83	0.15	48,48,48,48	0
57	MG	1a	3078	1/1	0.83	0.16	70,70,70,70	0
57	MG	2a	3087	1/1	0.83	0.18	69,69,69,69	0
57	MG	1A	3082	1/1	0.83	0.14	34,34,34,34	0
57	MG	2a	3112	1/1	0.83	0.12	65,65,65,65	0
57	MG	1A	3659	1/1	0.83	0.14	36,36,36,36	0
57	MG	1a	3194	1/1	0.83	0.14	65,65,65,65	0
57	MG	1A	3923	1/1	0.83	0.30	50,50,50,50	0
57	MG	2A	3675	1/1	0.83	0.09	43,43,43,43	0
57	MG	2A	3249	1/1	0.83	0.28	49,49,49,49	0
57	MG	1A	3732	1/1	0.83	0.10	48,48,48,48	0
57	MG	1a	3095	1/1	0.83	0.12	52,52,52,52	0
57	MG	2A	3264	1/1	0.83	0.17	54,54,54,54	0
57	MG	2a	3185	1/1	0.83	0.12	63,63,63,63	0
57	MG	1A	3465	1/1	0.83	0.17	37,37,37,37	0
57	MG	1A	3881	1/1	0.83	0.17	38,38,38,38	0
57	MG	1A	3245	1/1	0.83	0.33	48,48,48,48	0
57	MG	1a	3110	1/1	0.83	0.13	56,56,56,56	0
57	MG	1a	3024	1/1	0.83	0.17	51,51,51,51	0
57	MG	1a	3040	1/1	0.84	0.18	58,58,58,58	0
57	MG	2A	3705	1/1	0.84	0.14	55,55,55,55	0
57	MG	2A	3237	1/1	0.84	0.15	52,52,52,52	0
57	MG	2A	3037	1/1	0.84	0.15	39,39,39,39	0
57	MG	2A	3718	1/1	0.84	0.19	63,63,63,63	0
57	MG	2A	3726	1/1	0.84	0.09	43,43,43,43	0
57	MG	1A	3685	1/1	0.84	0.13	51,51,51,51	0
57	MG	1A	3553	1/1	0.84	0.19	49,49,49,49	0
57	MG	1a	3126	1/1	0.84	0.17	65,65,65,65	0
57	MG	2A	3254	1/1	0.84	0.22	58,58,58,58	0
57	MG	1A	3284	1/1	0.84	0.14	64,64,64,64	0
57	MG	1A	3643	1/1	0.84	0.17	52,52,52,52	0
57	MG	1a	3237	1/1	0.84	0.11	53,53,53,53	0
57	MG	2A	3101	1/1	0.84	0.16	41,41,41,41	0
57	MG	2A	3104	1/1	0.84	0.23	54,54,54,54	0
57	MG	1E	303	1/1	0.84	0.18	22,22,22,22	0
57	MG	2T	201	1/1	0.84	0.18	51,51,51,51	0
57	MG	2A	3514	1/1	0.84	0.09	58,58,58,58	0
57	MG	2U	201	1/1	0.84	0.12	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	2A	3114	1/1	0.84	0.13	53,53,53,53	0
57	MG	2A	3292	1/1	0.84	0.28	59,59,59,59	0
57	MG	2A	3293	1/1	0.84	0.14	46,46,46,46	0
57	MG	2A	3298	1/1	0.84	0.10	71,71,71,71	0
57	MG	2a	3013	1/1	0.84	0.20	56,56,56,56	0
57	MG	2a	3017	1/1	0.84	0.10	46,46,46,46	0
57	MG	1A	3858	1/1	0.84	0.18	43,43,43,43	0
57	MG	2A	3312	1/1	0.84	0.11	59,59,59,59	0
57	MG	1A	3093	1/1	0.84	0.20	56,56,56,56	0
57	MG	2a	3025	1/1	0.84	0.12	57,57,57,57	0
57	MG	1A	3650	1/1	0.84	0.17	42,42,42,42	0
57	MG	1A	3035	1/1	0.84	0.21	32,32,32,32	0
57	MG	2A	3569	1/1	0.84	0.14	33,33,33,33	0
57	MG	1A	3996	1/1	0.84	0.11	83,83,83,83	0
57	MG	1A	3741	1/1	0.84	0.14	47,47,47,47	0
57	MG	1A	4011	1/1	0.84	0.44	64,64,64,64	0
57	MG	2A	3582	1/1	0.84	0.12	42,42,42,42	0
57	MG	1A	3883	1/1	0.84	0.14	57,57,57,57	0
57	MG	2A	3354	1/1	0.84	0.12	27,27,27,27	0
57	MG	1a	3270	1/1	0.84	0.16	46,46,46,46	0
57	MG	2A	3594	1/1	0.84	0.13	54,54,54,54	0
57	MG	2a	3071	1/1	0.84	0.23	58,58,58,58	0
57	MG	2A	3364	1/1	0.84	0.08	36,36,36,36	0
57	MG	1a	3093	1/1	0.84	0.29	57,57,57,57	0
57	MG	2A	3182	1/1	0.84	0.15	56,56,56,56	0
57	MG	1A	3602	1/1	0.84	0.17	24,24,24,24	0
57	MG	1i	201	1/1	0.84	0.23	60,60,60,60	0
57	MG	1a	3016	1/1	0.84	0.12	54,54,54,54	0
57	MG	2A	3616	1/1	0.84	0.09	55,55,55,55	0
57	MG	2a	3119	1/1	0.84	0.14	60,60,60,60	0
57	MG	1o	102	1/1	0.84	0.17	53,53,53,53	0
57	MG	2a	3129	1/1	0.84	0.07	67,67,67,67	0
57	MG	1A	3936	1/1	0.84	0.18	36,36,36,36	0
57	MG	1A	3190	1/1	0.84	0.20	52,52,52,52	0
57	MG	2A	3633	1/1	0.84	0.08	70,70,70,70	0
57	MG	2A	3424	1/1	0.84	0.15	44,44,44,44	0
57	MG	1A	3676	1/1	0.84	0.11	57,57,57,57	0
57	MG	2A	3210	1/1	0.84	0.19	64,64,64,64	0
57	MG	2A	3002	1/1	0.84	0.12	38,38,38,38	0
57	MG	2A	3434	1/1	0.84	0.16	44,44,44,44	0
57	MG	1A	3060	1/1	0.84	0.16	47,47,47,47	0
57	MG	1a	3203	1/1	0.84	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MPD	1A	4024	8/8	0.84	0.18	46,51,56,64	0
57	MG	2A	3445	1/1	0.84	0.12	49,49,49,49	0
57	MG	1a	3111	1/1	0.84	0.26	60,60,60,60	0
57	MG	1A	3957	1/1	0.84	0.33	67,67,67,67	0
57	MG	1A	3992	1/1	0.85	0.09	48,48,48,48	0
57	MG	1a	3107	1/1	0.85	0.24	55,55,55,55	0
57	MG	2A	3496	1/1	0.85	0.17	65,65,65,65	0
57	MG	1a	3010	1/1	0.85	0.30	63,63,63,63	0
57	MG	2A	3112	1/1	0.85	0.10	52,52,52,52	0
57	MG	1a	3014	1/1	0.85	0.16	61,61,61,61	0
57	MG	2E	306	1/1	0.85	0.10	40,40,40,40	0
57	MG	1A	3913	1/1	0.85	0.17	27,27,27,27	0
57	MG	1A	3535	1/1	0.85	0.11	71,71,71,71	0
57	MG	2O	201	1/1	0.85	0.19	47,47,47,47	0
57	MG	2A	3297	1/1	0.85	0.11	51,51,51,51	0
57	MG	1A	3549	1/1	0.85	0.13	30,30,30,30	0
57	MG	2A	3530	1/1	0.85	0.13	55,55,55,55	0
57	MG	1a	3028	1/1	0.85	0.29	55,55,55,55	0
57	MG	2A	3126	1/1	0.85	0.20	57,57,57,57	0
57	MG	2A	3315	1/1	0.85	0.10	38,38,38,38	0
57	MG	1A	3550	1/1	0.85	0.15	58,58,58,58	0
57	MG	2A	3324	1/1	0.85	0.16	58,58,58,58	0
57	MG	1A	3632	1/1	0.85	0.18	40,40,40,40	0
57	MG	1A	3034	1/1	0.85	0.18	47,47,47,47	0
57	MG	2A	3156	1/1	0.85	0.22	46,46,46,46	0
57	MG	2a	3022	1/1	0.85	0.15	46,46,46,46	0
57	MG	1B	206	1/1	0.85	0.16	36,36,36,36	0
57	MG	1A	3468	1/1	0.85	0.09	27,27,27,27	0
57	MG	1A	3096	1/1	0.85	0.34	43,43,43,43	0
57	MG	1a	3049	1/1	0.85	0.20	63,63,63,63	0
57	MG	1A	3327	1/1	0.85	0.26	24,24,24,24	0
57	MG	2A	3185	1/1	0.85	0.26	44,44,44,44	0
57	MG	1a	3061	1/1	0.85	0.09	63,63,63,63	0
57	MG	1A	3760	1/1	0.85	0.17	52,52,52,52	0
57	MG	2a	3051	1/1	0.85	0.21	59,59,59,59	0
57	MG	1A	3489	1/1	0.85	0.09	53,53,53,53	0
57	MG	1A	3157	1/1	0.85	0.27	54,54,54,54	0
57	MG	1A	3672	1/1	0.85	0.10	52,52,52,52	0
57	MG	2A	3199	1/1	0.85	0.14	55,55,55,55	0
57	MG	1A	3494	1/1	0.85	0.09	45,45,45,45	0
57	MG	2a	3067	1/1	0.85	0.23	57,57,57,57	0
57	MG	1A	3349	1/1	0.85	0.10	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	3423	1/1	0.85	0.40	58,58,58,58	0
57	MG	2A	3618	1/1	0.85	0.23	57,57,57,57	0
57	MG	1G	202	1/1	0.85	0.11	56,56,56,56	0
57	MG	2A	3005	1/1	0.85	0.51	58,58,58,58	0
57	MG	1a	3191	1/1	0.85	0.14	59,59,59,59	0
57	MG	2A	3430	1/1	0.85	0.54	48,48,48,48	0
57	MG	1A	3891	1/1	0.85	0.18	24,24,24,24	0
57	MG	2A	3223	1/1	0.85	0.20	57,57,57,57	0
57	MG	2A	3225	1/1	0.85	0.12	44,44,44,44	0
57	MG	1A	3794	1/1	0.85	0.24	39,39,39,39	0
57	MG	1a	3090	1/1	0.85	0.28	54,54,54,54	0
57	MG	2A	3450	1/1	0.85	0.09	48,48,48,48	0
57	MG	2A	3032	1/1	0.85	0.21	51,51,51,51	0
57	MG	2A	3035	1/1	0.85	0.27	51,51,51,51	0
57	MG	1A	3446	1/1	0.85	0.14	58,58,58,58	0
57	MG	1A	3166	1/1	0.85	0.14	39,39,39,39	0
57	MG	2A	3703	1/1	0.85	0.31	42,42,42,42	0
57	MG	2A	3470	1/1	0.85	0.10	60,60,60,60	0
57	MG	1A	3828	1/1	0.85	0.20	34,34,34,34	0
57	MG	1A	3361	1/1	0.85	0.16	27,27,27,27	0
57	MG	2l	201	1/1	0.85	0.16	60,60,60,60	0
57	MG	2A	3712	1/1	0.85	0.13	41,41,41,41	0
57	MG	1A	3988	1/1	0.85	0.25	41,41,41,41	0
57	MG	2A	3483	1/1	0.85	0.14	59,59,59,59	0
57	MG	1A	3221	1/1	0.85	0.24	32,32,32,32	0
57	MG	2A	3096	1/1	0.85	0.12	44,44,44,44	0
57	MG	2A	3416	1/1	0.86	0.11	49,49,49,49	0
57	MG	1A	3865	1/1	0.86	0.10	32,32,32,32	0
57	MG	1A	3211	1/1	0.86	0.13	45,45,45,45	0
57	MG	2W	202	1/1	0.86	0.11	53,53,53,53	0
57	MG	21	101	1/1	0.86	0.27	53,53,53,53	0
57	MG	1B	209	1/1	0.86	0.14	45,45,45,45	0
57	MG	2A	3428	1/1	0.86	0.16	52,52,52,52	0
57	MG	1A	3388	1/1	0.86	0.13	23,23,23,23	0
57	MG	1B	216	1/1	0.86	0.23	43,43,43,43	0
57	MG	1B	218	1/1	0.86	0.12	64,64,64,64	0
57	MG	1A	3673	1/1	0.86	0.27	36,36,36,36	0
57	MG	1A	3392	1/1	0.86	0.17	27,27,27,27	0
57	MG	1a	3052	1/1	0.86	0.17	50,50,50,50	0
57	MG	2A	3440	1/1	0.86	0.22	60,60,60,60	0
57	MG	1A	3949	1/1	0.86	0.08	59,59,59,59	0
57	MG	1A	3950	1/1	0.86	0.09	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3095	1/1	0.86	0.18	43,43,43,43	0
57	MG	2a	3031	1/1	0.86	0.12	71,71,71,71	0
57	MG	1D	312	1/1	0.86	0.31	46,46,46,46	0
57	MG	2A	3285	1/1	0.86	0.23	54,54,54,54	0
57	MG	1A	3787	1/1	0.86	0.16	49,49,49,49	0
57	MG	1d	304	1/1	0.86	0.07	55,55,55,55	0
57	MG	2A	3149	1/1	0.86	0.20	44,44,44,44	0
57	MG	2A	3640	1/1	0.86	0.09	47,47,47,47	0
57	MG	1A	3397	1/1	0.86	0.17	29,29,29,29	0
57	MG	2a	3060	1/1	0.86	0.12	66,66,66,66	0
57	MG	1A	3406	1/1	0.86	0.16	48,48,48,48	0
57	MG	1A	3408	1/1	0.86	0.25	71,71,71,71	0
57	MG	1A	3046	1/1	0.86	0.20	44,44,44,44	0
57	MG	2A	3664	1/1	0.86	0.07	58,58,58,58	0
57	MG	2a	3068	1/1	0.86	0.39	60,60,60,60	0
57	MG	1A	3706	1/1	0.86	0.25	52,52,52,52	0
57	MG	1A	3641	1/1	0.86	0.21	46,46,46,46	0
57	MG	2A	3493	1/1	0.86	0.19	46,46,46,46	0
57	MG	1a	3189	1/1	0.86	0.11	58,58,58,58	0
57	MG	1A	3987	1/1	0.86	0.24	47,47,47,47	0
57	MG	1A	3120	1/1	0.86	0.20	38,38,38,38	0
57	MG	1A	3251	1/1	0.86	0.17	39,39,39,39	0
57	MG	2A	3339	1/1	0.86	0.12	35,35,35,35	0
57	MG	2a	3110	1/1	0.86	0.23	63,63,63,63	0
57	MG	1a	3199	1/1	0.86	0.09	69,69,69,69	0
57	MG	1A	3648	1/1	0.86	0.15	31,31,31,31	0
57	MG	1A	3509	1/1	0.86	0.16	28,28,28,28	0
57	MG	1a	3005	1/1	0.86	0.12	58,58,58,58	0
57	MG	2a	3132	1/1	0.86	0.25	58,58,58,58	0
57	MG	1A	3743	1/1	0.86	0.21	51,51,51,51	0
57	MG	1a	3220	1/1	0.86	0.07	57,57,57,57	0
57	MG	2B	208	1/1	0.86	0.21	57,57,57,57	0
57	MG	2a	3150	1/1	0.86	0.11	45,45,45,45	0
57	MG	2a	3162	1/1	0.86	0.07	49,49,49,49	0
57	MG	2A	3539	1/1	0.86	0.26	56,56,56,56	0
57	MG	2A	3373	1/1	0.86	0.11	44,44,44,44	0
57	MG	1A	3655	1/1	0.86	0.11	40,40,40,40	0
57	MG	2a	3181	1/1	0.86	0.20	62,62,62,62	0
57	MG	1a	3225	1/1	0.86	0.16	60,60,60,60	0
57	MG	1A	3455	1/1	0.86	0.15	41,41,41,41	0
57	MG	2A	3058	1/1	0.86	0.14	51,51,51,51	0
57	MG	2A	3224	1/1	0.86	0.40	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	2G	201	1/1	0.86	0.17	63,63,63,63	0
57	MG	2G	202	1/1	0.86	0.13	70,70,70,70	0
57	MG	1A	3752	1/1	0.86	0.15	27,27,27,27	0
57	MG	1A	3022	1/1	0.86	0.15	43,43,43,43	0
57	MG	2A	3080	1/1	0.86	0.15	78,78,78,78	0
57	MG	1A	3972	1/1	0.87	0.13	45,45,45,45	0
57	MG	1A	3973	1/1	0.87	0.09	49,49,49,49	0
57	MG	2A	3387	1/1	0.87	0.12	32,32,32,32	0
57	MG	1A	3203	1/1	0.87	0.25	46,46,46,46	0
57	MG	1A	3838	1/1	0.87	0.19	53,53,53,53	0
57	MG	1A	3080	1/1	0.87	0.30	37,37,37,37	0
57	MG	2A	3407	1/1	0.87	0.20	56,56,56,56	0
57	MG	2A	3256	1/1	0.87	0.17	53,53,53,53	0
57	MG	1A	3554	1/1	0.87	0.08	32,32,32,32	0
57	MG	2A	3152	1/1	0.87	0.17	53,53,53,53	0
57	MG	2A	3019	1/1	0.87	0.54	41,41,41,41	0
57	MG	1a	3053	1/1	0.87	0.21	57,57,57,57	0
57	MG	1A	3981	1/1	0.87	0.14	60,60,60,60	0
57	MG	1A	3122	1/1	0.87	0.24	37,37,37,37	0
57	MG	2A	3027	1/1	0.87	0.20	39,39,39,39	0
57	MG	2a	3066	1/1	0.87	0.11	55,55,55,55	0
57	MG	2A	3719	1/1	0.87	0.17	47,47,47,47	0
57	MG	1A	3616	1/1	0.87	0.14	32,32,32,32	0
57	MG	1A	3856	1/1	0.87	0.31	46,46,46,46	0
57	MG	1A	3355	1/1	0.87	0.17	20,20,20,20	0
57	MG	1A	3715	1/1	0.87	0.10	29,29,29,29	0
57	MG	2A	3576	1/1	0.87	0.12	49,49,49,49	0
57	MG	1A	3859	1/1	0.87	0.12	49,49,49,49	0
57	MG	1A	3724	1/1	0.87	0.12	49,49,49,49	0
57	MG	2A	3581	1/1	0.87	0.31	62,62,62,62	0
57	MG	1A	3929	1/1	0.87	0.36	45,45,45,45	0
57	MG	2E	304	1/1	0.87	0.22	37,37,37,37	0
57	MG	2A	3442	1/1	0.87	0.10	60,60,60,60	0
57	MG	2A	3061	1/1	0.87	0.12	43,43,43,43	0
57	MG	2A	3448	1/1	0.87	0.19	43,43,43,43	0
57	MG	1A	3126	1/1	0.87	0.24	34,34,34,34	0
57	MG	2A	3601	1/1	0.87	0.15	32,32,32,32	0
57	MG	1A	3803	1/1	0.87	0.08	73,73,73,73	0
57	MG	1A	3182	1/1	0.87	0.20	49,49,49,49	0
57	MG	1A	3825	1/1	0.87	0.15	32,32,32,32	0
57	MG	2A	3335	1/1	0.87	0.14	32,32,32,32	0
57	MG	1A	3627	1/1	0.87	0.13	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3312	1/1	0.87	0.18	37,37,37,37	0
57	MG	2A	3340	1/1	0.87	0.17	49,49,49,49	0
57	MG	2A	3476	1/1	0.87	0.14	55,55,55,55	0
57	MG	2a	3006	1/1	0.87	0.10	54,54,54,54	0
57	MG	1A	3142	1/1	0.87	0.16	45,45,45,45	0
57	MG	1B	214	1/1	0.87	0.17	32,32,32,32	0
57	MG	2e	201	1/1	0.87	0.21	63,63,63,63	0
57	MG	1A	3684	1/1	0.87	0.14	54,54,54,54	0
57	MG	1g	202	1/1	0.87	0.16	64,64,64,64	0
57	MG	2a	3014	1/1	0.87	0.18	55,55,55,55	0
57	MG	1a	3102	1/1	0.87	0.10	61,61,61,61	0
60	MPD	2B	218	8/8	0.87	0.17	44,53,60,60	0
57	MG	1A	3832	1/1	0.87	0.13	33,33,33,33	0
57	MG	2A	3494	1/1	0.87	0.09	47,47,47,47	0
57	MG	1A	3027	1/1	0.87	0.13	56,56,56,56	0
57	MG	1A	3130	1/1	0.88	0.16	47,47,47,47	0
57	MG	1A	3597	1/1	0.88	0.09	38,38,38,38	0
57	MG	2A	3522	1/1	0.88	0.20	38,38,38,38	0
57	MG	2A	3136	1/1	0.88	0.15	61,61,61,61	0
57	MG	1A	3249	1/1	0.88	0.14	54,54,54,54	0
57	MG	1a	3159	1/1	0.88	0.12	64,64,64,64	0
57	MG	2Q	203	1/1	0.88	0.15	55,55,55,55	0
57	MG	1e	201	1/1	0.88	0.14	61,61,61,61	0
57	MG	1E	309	1/1	0.88	0.14	51,51,51,51	0
57	MG	2A	3157	1/1	0.88	0.16	57,57,57,57	0
57	MG	1A	3986	1/1	0.88	0.13	28,28,28,28	0
57	MG	2A	3161	1/1	0.88	0.10	52,52,52,52	0
57	MG	2A	3349	1/1	0.88	0.15	38,38,38,38	0
57	MG	1i	202	1/1	0.88	0.18	55,55,55,55	0
57	MG	1A	3359	1/1	0.88	0.12	43,43,43,43	0
57	MG	1A	3798	1/1	0.88	0.08	46,46,46,46	0
57	MG	1A	3717	1/1	0.88	0.17	45,45,45,45	0
57	MG	2A	3362	1/1	0.88	0.11	37,37,37,37	0
57	MG	1A	3991	1/1	0.88	0.07	42,42,42,42	0
57	MG	2A	3580	1/1	0.88	0.15	36,36,36,36	0
57	MG	2A	3187	1/1	0.88	0.13	52,52,52,52	0
57	MG	1A	3610	1/1	0.88	0.17	32,32,32,32	0
57	MG	1A	3665	1/1	0.88	0.09	47,47,47,47	0
57	MG	1A	3934	1/1	0.88	0.16	22,22,22,22	0
57	MG	2A	3393	1/1	0.88	0.17	51,51,51,51	0
57	MG	1a	3192	1/1	0.88	0.19	56,56,56,56	0
57	MG	2A	3012	1/1	0.88	0.18	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	2A	3198	1/1	0.88	0.18	41,41,41,41	0
57	MG	2a	3036	1/1	0.88	0.21	62,62,62,62	0
57	MG	1A	3870	1/1	0.88	0.18	30,30,30,30	0
57	MG	10	108	1/1	0.88	0.17	51,51,51,51	0
57	MG	2a	3043	1/1	0.88	0.12	64,64,64,64	0
57	MG	2a	3047	1/1	0.88	0.25	51,51,51,51	0
57	MG	1A	3250	1/1	0.88	0.13	50,50,50,50	0
57	MG	2A	3209	1/1	0.88	0.16	49,49,49,49	0
57	MG	15	108	1/1	0.88	0.15	34,34,34,34	0
57	MG	17	104	1/1	0.88	0.15	33,33,33,33	0
57	MG	2A	3617	1/1	0.88	0.18	37,37,37,37	0
57	MG	1a	3001	1/1	0.88	0.16	52,52,52,52	0
57	MG	2A	3622	1/1	0.88	0.23	57,57,57,57	0
57	MG	2A	3216	1/1	0.88	0.21	63,63,63,63	0
57	MG	1A	3050	1/1	0.88	0.45	37,37,37,37	0
57	MG	2A	3222	1/1	0.88	0.12	40,40,40,40	0
57	MG	1A	4020	1/1	0.88	0.46	48,48,48,48	0
57	MG	2A	3036	1/1	0.88	0.12	59,59,59,59	0
57	MG	1a	3221	1/1	0.88	0.21	62,62,62,62	0
57	MG	2a	3073	1/1	0.88	0.16	58,58,58,58	0
57	MG	1A	3499	1/1	0.88	0.10	51,51,51,51	0
57	MG	2A	3052	1/1	0.88	0.26	62,62,62,62	0
57	MG	2A	3053	1/1	0.88	0.22	58,58,58,58	0
57	MG	1A	3258	1/1	0.88	0.29	35,35,35,35	0
57	MG	1A	3272	1/1	0.88	0.17	41,41,41,41	0
57	MG	2A	3663	1/1	0.88	0.14	61,61,61,61	0
57	MG	2a	3106	1/1	0.88	0.27	52,52,52,52	0
57	MG	1a	3019	1/1	0.88	0.19	53,53,53,53	0
57	MG	2A	3670	1/1	0.88	0.11	49,49,49,49	0
57	MG	1A	3682	1/1	0.88	0.06	43,43,43,43	0
57	MG	2A	3072	1/1	0.88	0.18	44,44,44,44	0
57	MG	1a	3232	1/1	0.88	0.16	53,53,53,53	0
57	MG	2A	3255	1/1	0.88	0.20	54,54,54,54	0
57	MG	1A	3965	1/1	0.88	0.14	34,34,34,34	0
57	MG	2a	3137	1/1	0.88	0.19	45,45,45,45	0
57	MG	2a	3142	1/1	0.88	0.07	60,60,60,60	0
57	MG	2A	3087	1/1	0.88	0.17	53,53,53,53	0
57	MG	2A	3089	1/1	0.88	0.17	58,58,58,58	0
57	MG	1A	3968	1/1	0.88	0.15	21,21,21,21	0
57	MG	2a	3151	1/1	0.88	0.07	63,63,63,63	0
57	MG	2a	3158	1/1	0.88	0.20	57,57,57,57	0
57	MG	2a	3159	1/1	0.88	0.09	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	3119	1/1	0.88	0.28	55,55,55,55	0
57	MG	2A	3716	1/1	0.88	0.07	45,45,45,45	0
57	MG	2a	3168	1/1	0.88	0.09	45,45,45,45	0
57	MG	1a	3123	1/1	0.88	0.13	45,45,45,45	0
57	MG	2A	3480	1/1	0.88	0.13	45,45,45,45	0
57	MG	2a	3180	1/1	0.88	0.18	63,63,63,63	0
57	MG	1A	3053	1/1	0.88	0.88	31,31,31,31	0
57	MG	2A	3280	1/1	0.88	0.28	53,53,53,53	0
57	MG	2A	3282	1/1	0.88	0.25	45,45,45,45	0
57	MG	2a	3187	1/1	0.88	0.12	57,57,57,57	0
57	MG	1A	3345	1/1	0.88	0.08	48,48,48,48	0
57	MG	1a	3131	1/1	0.88	0.11	43,43,43,43	0
57	MG	2A	3289	1/1	0.88	0.20	45,45,45,45	0
57	MG	1A	3590	1/1	0.88	0.18	40,40,40,40	0
57	MG	1A	3843	1/1	0.88	0.12	44,44,44,44	0
57	MG	1A	3846	1/1	0.88	0.10	43,43,43,43	0
57	MG	1A	3012	1/1	0.88	0.16	32,32,32,32	0
57	MG	1A	3350	1/1	0.88	0.10	20,20,20,20	0
57	MG	1a	3268	1/1	0.88	0.13	47,47,47,47	0
57	MG	2A	3330	1/1	0.89	0.14	39,39,39,39	0
57	MG	2A	3153	1/1	0.89	0.17	37,37,37,37	0
57	MG	1a	3033	1/1	0.89	0.24	60,60,60,60	0
57	MG	1A	3059	1/1	0.89	0.22	35,35,35,35	0
57	MG	2A	3554	1/1	0.89	0.11	43,43,43,43	0
57	MG	1A	3379	1/1	0.89	0.11	44,44,44,44	0
57	MG	2A	3557	1/1	0.89	0.11	54,54,54,54	0
57	MG	21	102	1/1	0.89	0.22	48,48,48,48	0
57	MG	28	103	1/1	0.89	0.16	52,52,52,52	0
57	MG	2A	3160	1/1	0.89	0.10	52,52,52,52	0
57	MG	1A	3433	1/1	0.89	0.11	40,40,40,40	0
57	MG	2A	3167	1/1	0.89	0.33	46,46,46,46	0
57	MG	1A	3789	1/1	0.89	0.11	55,55,55,55	0
57	MG	1A	3876	1/1	0.89	0.15	24,24,24,24	0
57	MG	1a	3048	1/1	0.89	0.18	52,52,52,52	0
57	MG	1A	3966	1/1	0.89	0.23	41,41,41,41	0
57	MG	1a	3163	1/1	0.89	0.12	69,69,69,69	0
57	MG	1a	3165	1/1	0.89	0.10	53,53,53,53	0
57	MG	2A	3371	1/1	0.89	0.20	63,63,63,63	0
57	MG	1A	3483	1/1	0.89	0.17	22,22,22,22	0
57	MG	1a	3173	1/1	0.89	0.14	44,44,44,44	0
57	MG	2A	3587	1/1	0.89	0.08	42,42,42,42	0
57	MG	2A	3384	1/1	0.89	0.14	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	2a	3030	1/1	0.89	0.10	42,42,42,42	0
57	MG	1a	3174	1/1	0.89	0.24	75,75,75,75	0
57	MG	1A	3004	1/1	0.89	0.29	40,40,40,40	0
57	MG	1B	229	1/1	0.89	0.10	46,46,46,46	0
57	MG	2A	3011	1/1	0.89	0.12	27,27,27,27	0
57	MG	1A	3795	1/1	0.89	0.09	44,44,44,44	0
57	MG	1A	3566	1/1	0.89	0.17	15,15,15,15	0
57	MG	2A	3404	1/1	0.89	0.08	52,52,52,52	0
57	MG	1A	3639	1/1	0.89	0.22	51,51,51,51	0
57	MG	1a	3186	1/1	0.89	0.11	53,53,53,53	0
57	MG	2a	3053	1/1	0.89	0.17	58,58,58,58	0
57	MG	1a	3188	1/1	0.89	0.16	68,68,68,68	0
57	MG	1a	3070	1/1	0.89	0.15	41,41,41,41	0
57	MG	2A	3213	1/1	0.89	0.20	49,49,49,49	0
57	MG	1A	3224	1/1	0.89	0.18	29,29,29,29	0
57	MG	1E	307	1/1	0.89	0.20	44,44,44,44	0
57	MG	1a	3075	1/1	0.89	0.18	40,40,40,40	0
57	MG	1A	3450	1/1	0.89	0.22	20,20,20,20	0
57	MG	1A	3574	1/1	0.89	0.15	26,26,26,26	0
57	MG	2A	3042	1/1	0.89	0.24	66,66,66,66	0
57	MG	1A	3454	1/1	0.89	0.10	36,36,36,36	0
57	MG	1A	3585	1/1	0.89	0.20	42,42,42,42	0
57	MG	1a	3204	1/1	0.89	0.09	47,47,47,47	0
57	MG	1a	3208	1/1	0.89	0.09	48,48,48,48	0
57	MG	2A	3653	1/1	0.89	0.16	27,27,27,27	0
57	MG	1A	3982	1/1	0.89	0.09	44,44,44,44	0
57	MG	1A	3502	1/1	0.89	0.15	35,35,35,35	0
57	MG	1A	3227	1/1	0.89	0.37	47,47,47,47	0
57	MG	1A	3275	1/1	0.89	0.17	26,26,26,26	0
57	MG	2A	3252	1/1	0.89	0.14	46,46,46,46	0
57	MG	2A	3452	1/1	0.89	0.17	44,44,44,44	0
57	MG	2A	3075	1/1	0.89	0.32	48,48,48,48	0
57	MG	2a	3116	1/1	0.89	0.07	47,47,47,47	0
57	MG	1A	3158	1/1	0.89	0.21	52,52,52,52	0
57	MG	1A	3989	1/1	0.89	0.12	30,30,30,30	0
57	MG	2A	3699	1/1	0.89	0.12	67,67,67,67	0
57	MG	2a	3130	1/1	0.89	0.15	64,64,64,64	0
57	MG	2A	3081	1/1	0.89	0.15	51,51,51,51	0
57	MG	1A	3516	1/1	0.89	0.13	52,52,52,52	0
57	MG	1A	3519	1/1	0.89	0.11	51,51,51,51	0
57	MG	2a	3138	1/1	0.89	0.15	54,54,54,54	0
57	MG	1A	3921	1/1	0.89	0.26	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	3268	1/1	0.89	0.21	49,49,49,49	0
57	MG	2A	3715	1/1	0.89	0.17	60,60,60,60	0
57	MG	2A	3095	1/1	0.89	0.15	48,48,48,48	0
57	MG	1a	3230	1/1	0.89	0.19	52,52,52,52	0
57	MG	1A	3995	1/1	0.89	0.40	61,61,61,61	0
57	MG	2A	3277	1/1	0.89	0.23	33,33,33,33	0
57	MG	1A	3464	1/1	0.89	0.14	54,54,54,54	0
57	MG	2A	3490	1/1	0.89	0.08	55,55,55,55	0
57	MG	2a	3167	1/1	0.89	0.32	73,73,73,73	0
57	MG	2B	206	1/1	0.89	0.15	54,54,54,54	0
57	MG	1a	3109	1/1	0.89	0.21	46,46,46,46	0
57	MG	2a	3176	1/1	0.89	0.09	55,55,55,55	0
57	MG	1a	3003	1/1	0.89	0.12	45,45,45,45	0
57	MG	1A	3755	1/1	0.89	0.13	22,22,22,22	0
57	MG	1A	3214	1/1	0.89	0.15	49,49,49,49	0
57	MG	1a	3012	1/1	0.89	0.17	52,52,52,52	0
57	MG	1A	3766	1/1	0.89	0.10	30,30,30,30	0
57	MG	2D	303	1/1	0.89	0.19	44,44,44,44	0
57	MG	1a	3251	1/1	0.89	0.24	64,64,64,64	0
57	MG	1A	3775	1/1	0.89	0.13	43,43,43,43	0
57	MG	1A	3777	1/1	0.89	0.14	41,41,41,41	0
57	MG	1A	3466	1/1	0.89	0.14	37,37,37,37	0
57	MG	1a	3021	1/1	0.89	0.10	44,44,44,44	0
57	MG	1A	3371	1/1	0.89	0.14	44,44,44,44	0
57	MG	1A	3781	1/1	0.89	0.10	46,46,46,46	0
57	MG	2I	201	1/1	0.89	0.15	47,47,47,47	0
57	MG	1A	3944	1/1	0.89	0.13	21,21,21,21	0
57	MG	2A	3518	1/1	0.90	0.09	58,58,58,58	0
57	MG	2A	3520	1/1	0.90	0.44	52,52,52,52	0
57	MG	1A	3951	1/1	0.90	0.14	36,36,36,36	0
57	MG	2A	3523	1/1	0.90	0.08	47,47,47,47	0
57	MG	1A	3543	1/1	0.90	0.22	45,45,45,45	0
57	MG	1a	3054	1/1	0.90	0.10	62,62,62,62	0
57	MG	1a	3056	1/1	0.90	0.20	51,51,51,51	0
57	MG	2A	3535	1/1	0.90	0.12	47,47,47,47	0
57	MG	1A	3049	1/1	0.90	0.18	28,28,28,28	0
57	MG	1A	3867	1/1	0.90	0.15	23,23,23,23	0
57	MG	1A	3403	1/1	0.90	0.13	14,14,14,14	0
57	MG	2A	3551	1/1	0.90	0.07	46,46,46,46	0
57	MG	1A	3618	1/1	0.90	0.16	20,20,20,20	0
57	MG	1A	3790	1/1	0.90	0.15	44,44,44,44	0
57	MG	20	101	1/1	0.90	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3348	1/1	0.90	0.09	43,43,43,43	0
57	MG	1A	3141	1/1	0.90	0.16	47,47,47,47	0
57	MG	28	102	1/1	0.90	0.23	45,45,45,45	0
57	MG	2A	3193	1/1	0.90	0.12	56,56,56,56	0
57	MG	2A	3565	1/1	0.90	0.30	56,56,56,56	0
57	MG	2A	3026	1/1	0.90	0.15	24,24,24,24	0
57	MG	1A	3974	1/1	0.90	0.12	49,49,49,49	0
57	MG	1A	3882	1/1	0.90	0.18	52,52,52,52	0
57	MG	1A	3622	1/1	0.90	0.19	35,35,35,35	0
57	MG	2A	3365	1/1	0.90	0.17	56,56,56,56	0
57	MG	2A	3204	1/1	0.90	0.22	43,43,43,43	0
57	MG	2a	3015	1/1	0.90	0.23	52,52,52,52	0
57	MG	1A	3011	1/1	0.90	0.09	42,42,42,42	0
57	MG	1A	3802	1/1	0.90	0.20	36,36,36,36	0
57	MG	1a	3086	1/1	0.90	0.15	50,50,50,50	0
57	MG	2A	3038	1/1	0.90	0.26	46,46,46,46	0
57	MG	2A	3211	1/1	0.90	0.18	37,37,37,37	0
57	MG	2A	3391	1/1	0.90	0.15	57,57,57,57	0
57	MG	1A	3631	1/1	0.90	0.12	30,30,30,30	0
57	MG	1T	201	1/1	0.90	0.15	40,40,40,40	0
57	MG	2A	3595	1/1	0.90	0.06	61,61,61,61	0
57	MG	2A	3600	1/1	0.90	0.09	59,59,59,59	0
57	MG	1A	3232	1/1	0.90	0.20	30,30,30,30	0
57	MG	2A	3399	1/1	0.90	0.61	66,66,66,66	0
57	MG	1A	3899	1/1	0.90	0.22	21,21,21,21	0
57	MG	2a	3041	1/1	0.90	0.16	65,65,65,65	0
57	MG	1A	3901	1/1	0.90	0.05	49,49,49,49	0
57	MG	2A	3219	1/1	0.90	0.14	39,39,39,39	0
57	MG	1A	3822	1/1	0.90	0.17	25,25,25,25	0
57	MG	1A	3716	1/1	0.90	0.16	21,21,21,21	0
57	MG	13	102	1/1	0.90	0.19	51,51,51,51	0
57	MG	2a	3054	1/1	0.90	0.19	53,53,53,53	0
57	MG	2A	3066	1/1	0.90	0.22	34,34,34,34	0
57	MG	2A	3418	1/1	0.90	0.13	51,51,51,51	0
57	MG	15	107	1/1	0.90	0.21	24,24,24,24	0
57	MG	2A	3623	1/1	0.90	0.19	49,49,49,49	0
57	MG	1A	3826	1/1	0.90	0.17	42,42,42,42	0
57	MG	2A	3627	1/1	0.90	0.12	58,58,58,58	0
57	MG	1A	3240	1/1	0.90	0.26	43,43,43,43	0
57	MG	19	102	1/1	0.90	0.09	44,44,44,44	0
57	MG	2A	3632	1/1	0.90	0.12	59,59,59,59	0
57	MG	2A	3239	1/1	0.90	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	1A	3123	1/1	0.90	0.08	64,64,64,64	0
57	MG	1A	3642	1/1	0.90	0.23	35,35,35,35	0
57	MG	2A	3637	1/1	0.90	0.13	39,39,39,39	0
57	MG	2A	3639	1/1	0.90	0.11	55,55,55,55	0
57	MG	2a	3080	1/1	0.90	0.13	47,47,47,47	0
57	MG	2A	3248	1/1	0.90	0.17	50,50,50,50	0
57	MG	1A	3993	1/1	0.90	0.24	54,54,54,54	0
57	MG	1a	3115	1/1	0.90	0.30	49,49,49,49	0
57	MG	2a	3089	1/1	0.90	0.13	54,54,54,54	0
57	MG	1a	3006	1/1	0.90	0.13	59,59,59,59	0
57	MG	1A	3500	1/1	0.90	0.16	38,38,38,38	0
57	MG	2a	3108	1/1	0.90	0.15	50,50,50,50	0
57	MG	1A	3644	1/1	0.90	0.25	40,40,40,40	0
57	MG	2A	3661	1/1	0.90	0.14	50,50,50,50	0
57	MG	2A	3446	1/1	0.90	0.17	46,46,46,46	0
57	MG	1A	3580	1/1	0.90	0.15	37,37,37,37	0
57	MG	2a	3121	1/1	0.90	0.12	54,54,54,54	0
57	MG	2a	3122	1/1	0.90	0.08	69,69,69,69	0
57	MG	2A	3669	1/1	0.90	0.19	58,58,58,58	0
57	MG	1A	3124	1/1	0.90	0.24	46,46,46,46	0
57	MG	2A	3673	1/1	0.90	0.07	45,45,45,45	0
57	MG	2A	3262	1/1	0.90	0.59	47,47,47,47	0
57	MG	2A	3110	1/1	0.90	0.16	45,45,45,45	0
57	MG	1A	3452	1/1	0.90	0.29	60,60,60,60	0
57	MG	2A	3689	1/1	0.90	0.13	62,62,62,62	0
57	MG	2a	3139	1/1	0.90	0.16	60,60,60,60	0
57	MG	2A	3690	1/1	0.90	0.14	50,50,50,50	0
57	MG	1A	3164	1/1	0.90	0.18	30,30,30,30	0
57	MG	2A	3697	1/1	0.90	0.19	73,73,73,73	0
57	MG	1a	3260	1/1	0.90	0.06	62,62,62,62	0
57	MG	2A	3115	1/1	0.90	0.26	52,52,52,52	0
57	MG	1A	3114	1/1	0.90	0.23	28,28,28,28	0
57	MG	1a	3139	1/1	0.90	0.14	62,62,62,62	0
57	MG	2A	3278	1/1	0.90	0.17	57,57,57,57	0
57	MG	1A	3661	1/1	0.90	0.12	35,35,35,35	0
57	MG	1A	3323	1/1	0.90	0.16	26,26,26,26	0
57	MG	1A	3325	1/1	0.90	0.12	46,46,46,46	0
57	MG	1A	3171	1/1	0.90	0.16	42,42,42,42	0
57	MG	1A	3855	1/1	0.90	0.09	51,51,51,51	0
57	MG	1A	3522	1/1	0.90	0.10	29,29,29,29	0
57	MG	1B	215	1/1	0.90	0.13	41,41,41,41	0
57	MG	1a	3041	1/1	0.90	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	3329	1/1	0.90	0.14	28,28,28,28	0
57	MG	1A	3270	1/1	0.90	0.16	51,51,51,51	0
57	MG	2A	3311	1/1	0.90	0.07	53,53,53,53	0
57	MG	1A	3344	1/1	0.90	0.13	53,53,53,53	0
57	MG	2A	3313	1/1	0.90	0.10	42,42,42,42	0
57	MG	2A	3314	1/1	0.90	0.09	34,34,34,34	0
57	MG	2B	215	1/1	0.90	0.15	61,61,61,61	0
57	MG	1A	3863	1/1	0.90	0.17	51,51,51,51	0
57	MG	2A	3316	1/1	0.90	0.11	34,34,34,34	0
57	MG	2D	306	1/1	0.90	0.41	41,41,41,41	0
57	MG	2D	308	1/1	0.90	0.16	34,34,34,34	0
57	MG	1a	3171	1/1	0.90	0.15	58,58,58,58	0
57	MG	1A	3285	1/1	0.91	0.21	29,29,29,29	0
57	MG	1l	201	1/1	0.91	0.17	56,56,56,56	0
57	MG	2A	3172	1/1	0.91	0.18	34,34,34,34	0
57	MG	1m	202	1/1	0.91	0.14	58,58,58,58	0
57	MG	1A	3346	1/1	0.91	0.18	43,43,43,43	0
57	MG	2A	3183	1/1	0.91	0.16	48,48,48,48	0
57	MG	1n	102	1/1	0.91	0.10	52,52,52,52	0
57	MG	1A	4000	1/1	0.91	0.21	42,42,42,42	0
57	MG	1A	4008	1/1	0.91	0.41	39,39,39,39	0
57	MG	1A	3479	1/1	0.91	0.19	18,18,18,18	0
57	MG	1A	3570	1/1	0.91	0.17	39,39,39,39	0
57	MG	27	101	1/1	0.91	0.16	49,49,49,49	0
57	MG	2A	3575	1/1	0.91	0.17	52,52,52,52	0
57	MG	1A	3077	1/1	0.91	0.20	25,25,25,25	0
57	MG	1A	3297	1/1	0.91	0.36	30,30,30,30	0
57	MG	1A	4016	1/1	0.91	0.25	54,54,54,54	0
57	MG	2A	3381	1/1	0.91	0.13	47,47,47,47	0
57	MG	2A	3383	1/1	0.91	0.23	56,56,56,56	0
57	MG	1A	3051	1/1	0.91	0.16	31,31,31,31	0
57	MG	1A	3840	1/1	0.91	0.12	44,44,44,44	0
57	MG	2A	3200	1/1	0.91	0.16	57,57,57,57	0
57	MG	2A	3202	1/1	0.91	0.19	62,62,62,62	0
57	MG	2A	3016	1/1	0.91	0.16	63,63,63,63	0
57	MG	1A	3581	1/1	0.91	0.08	33,33,33,33	0
57	MG	1A	3415	1/1	0.91	0.12	40,40,40,40	0
57	MG	1A	3065	1/1	0.91	0.11	45,45,45,45	0
57	MG	1A	3847	1/1	0.91	0.23	41,41,41,41	0
57	MG	1A	3435	1/1	0.91	0.14	47,47,47,47	0
57	MG	1A	3660	1/1	0.91	0.22	18,18,18,18	0
57	MG	1A	3071	1/1	0.91	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3608	1/1	0.91	0.11	32,32,32,32	0
57	MG	2A	3410	1/1	0.91	0.13	33,33,33,33	0
57	MG	1A	3765	1/1	0.91	0.14	25,25,25,25	0
57	MG	1A	3662	1/1	0.91	0.26	28,28,28,28	0
57	MG	1A	3445	1/1	0.91	0.14	46,46,46,46	0
57	MG	1A	3945	1/1	0.91	0.12	47,47,47,47	0
57	MG	1a	3187	1/1	0.91	0.16	68,68,68,68	0
57	MG	2a	3045	1/1	0.91	0.16	54,54,54,54	0
57	MG	2A	3040	1/1	0.91	0.21	33,33,33,33	0
57	MG	2a	3048	1/1	0.91	0.14	58,58,58,58	0
57	MG	1A	3262	1/1	0.91	0.09	68,68,68,68	0
57	MG	1A	3778	1/1	0.91	0.13	35,35,35,35	0
57	MG	1A	3862	1/1	0.91	0.20	44,44,44,44	0
57	MG	1A	3448	1/1	0.91	0.10	39,39,39,39	0
57	MG	2A	3431	1/1	0.91	0.12	45,45,45,45	0
57	MG	1A	3321	1/1	0.91	0.18	48,48,48,48	0
57	MG	1A	3518	1/1	0.91	0.34	35,35,35,35	0
57	MG	1E	305	1/1	0.91	0.07	40,40,40,40	0
57	MG	1A	3363	1/1	0.91	0.13	42,42,42,42	0
57	MG	1E	308	1/1	0.91	0.14	29,29,29,29	0
57	MG	2A	3070	1/1	0.91	0.17	46,46,46,46	0
57	MG	1A	3229	1/1	0.91	0.53	31,31,31,31	0
57	MG	1F	315	1/1	0.91	0.15	43,43,43,43	0
57	MG	1a	3081	1/1	0.91	0.16	54,54,54,54	0
57	MG	2a	3070	1/1	0.91	0.14	55,55,55,55	0
57	MG	1a	3082	1/1	0.91	0.18	56,56,56,56	0
57	MG	2A	3654	1/1	0.91	0.10	29,29,29,29	0
57	MG	2A	3451	1/1	0.91	0.16	56,56,56,56	0
57	MG	1F	318	1/1	0.91	0.17	41,41,41,41	0
57	MG	1A	3681	1/1	0.91	0.19	32,32,32,32	0
57	MG	1A	3970	1/1	0.91	0.13	39,39,39,39	0
57	MG	2a	3083	1/1	0.91	0.32	54,54,54,54	0
57	MG	2A	3261	1/1	0.91	0.15	20,20,20,20	0
57	MG	2A	3668	1/1	0.91	0.31	68,68,68,68	0
57	MG	1a	3089	1/1	0.91	0.13	43,43,43,43	0
57	MG	2A	3463	1/1	0.91	0.16	58,58,58,58	0
57	MG	2a	3095	1/1	0.91	0.11	67,67,67,67	0
57	MG	2a	3101	1/1	0.91	0.23	57,57,57,57	0
57	MG	2a	3103	1/1	0.91	0.30	61,61,61,61	0
57	MG	2A	3672	1/1	0.91	0.07	60,60,60,60	0
57	MG	2a	3107	1/1	0.91	0.10	60,60,60,60	0
57	MG	1A	3874	1/1	0.91	0.18	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	3373	1/1	0.91	0.16	41,41,41,41	0
57	MG	1A	3878	1/1	0.91	0.13	25,25,25,25	0
57	MG	1A	3683	1/1	0.91	0.12	29,29,29,29	0
57	MG	2A	3681	1/1	0.91	0.09	55,55,55,55	0
57	MG	2a	3120	1/1	0.91	0.16	44,44,44,44	0
57	MG	1A	3615	1/1	0.91	0.14	50,50,50,50	0
57	MG	2A	3478	1/1	0.91	0.16	47,47,47,47	0
57	MG	2a	3123	1/1	0.91	0.13	42,42,42,42	0
57	MG	2A	3479	1/1	0.91	0.09	66,66,66,66	0
57	MG	2A	3108	1/1	0.91	0.19	56,56,56,56	0
57	MG	1a	3096	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3976	1/1	0.91	0.10	48,48,48,48	0
57	MG	10	101	1/1	0.91	0.16	36,36,36,36	0
57	MG	1A	3105	1/1	0.91	0.15	51,51,51,51	0
57	MG	2A	3491	1/1	0.91	0.26	44,44,44,44	0
57	MG	2A	3711	1/1	0.91	0.13	38,38,38,38	0
57	MG	1a	3104	1/1	0.91	0.25	61,61,61,61	0
57	MG	1A	3689	1/1	0.91	0.07	40,40,40,40	0
57	MG	10	107	1/1	0.91	0.10	42,42,42,42	0
57	MG	2a	3148	1/1	0.91	0.07	39,39,39,39	0
57	MG	2A	3119	1/1	0.91	0.18	38,38,38,38	0
57	MG	1A	3886	1/1	0.91	0.11	30,30,30,30	0
57	MG	1A	3888	1/1	0.91	0.19	34,34,34,34	0
57	MG	2A	3724	1/1	0.91	0.10	50,50,50,50	0
57	MG	2a	3160	1/1	0.91	0.18	52,52,52,52	0
57	MG	1A	3326	1/1	0.91	0.24	39,39,39,39	0
57	MG	1a	3112	1/1	0.91	0.18	53,53,53,53	0
57	MG	1A	3462	1/1	0.91	0.10	46,46,46,46	0
57	MG	1A	3892	1/1	0.91	0.07	37,37,37,37	0
57	MG	2a	3169	1/1	0.91	0.15	52,52,52,52	0
57	MG	2A	3146	1/1	0.91	0.25	45,45,45,45	0
57	MG	17	103	1/1	0.91	0.20	31,31,31,31	0
57	MG	1A	3703	1/1	0.91	0.13	44,44,44,44	0
57	MG	1A	3273	1/1	0.91	0.11	32,32,32,32	0
57	MG	1A	3328	1/1	0.91	0.13	54,54,54,54	0
57	MG	1A	3236	1/1	0.91	0.36	47,47,47,47	0
57	MG	2A	3529	1/1	0.91	0.14	70,70,70,70	0
57	MG	2A	3158	1/1	0.91	0.20	44,44,44,44	0
57	MG	1A	3902	1/1	0.91	0.18	18,18,18,18	0
57	MG	1A	3085	1/1	0.91	0.16	38,38,38,38	0
57	MG	1A	3118	1/1	0.91	0.15	24,24,24,24	0
57	MG	1a	3136	1/1	0.91	0.17	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	3542	1/1	0.91	0.09	40,40,40,40	0
60	MPD	1T	207	8/8	0.91	0.16	56,60,62,64	0
60	MPD	2A	3728	8/8	0.91	0.20	50,53,58,58	0
57	MG	2F	303	1/1	0.91	0.19	43,43,43,43	0
57	MG	2A	3543	1/1	0.91	0.12	33,33,33,33	0
57	MG	2A	3544	1/1	0.91	0.12	36,36,36,36	0
57	MG	2A	3546	1/1	0.91	0.16	25,25,25,25	0
57	MG	2E	305	1/1	0.92	0.18	43,43,43,43	0
57	MG	2A	3099	1/1	0.92	0.20	47,47,47,47	0
57	MG	1A	3188	1/1	0.92	0.14	41,41,41,41	0
57	MG	1A	3905	1/1	0.92	0.10	37,37,37,37	0
57	MG	1A	3634	1/1	0.92	0.29	26,26,26,26	0
57	MG	1A	3637	1/1	0.92	0.20	40,40,40,40	0
57	MG	1A	3396	1/1	0.92	0.11	28,28,28,28	0
57	MG	1a	3098	1/1	0.92	0.09	57,57,57,57	0
57	MG	1A	3729	1/1	0.92	0.14	42,42,42,42	0
57	MG	1A	3557	1/1	0.92	0.07	58,58,58,58	0
57	MG	2P	201	1/1	0.92	0.10	49,49,49,49	0
57	MG	1A	3737	1/1	0.92	0.24	39,39,39,39	0
57	MG	1A	3165	1/1	0.92	0.16	43,43,43,43	0
57	MG	1a	3240	1/1	0.92	0.20	56,56,56,56	0
57	MG	1A	3400	1/1	0.92	0.17	11,11,11,11	0
57	MG	2V	202	1/1	0.92	0.31	49,49,49,49	0
57	MG	2W	201	1/1	0.92	0.34	51,51,51,51	0
57	MG	1a	3243	1/1	0.92	0.10	53,53,53,53	0
57	MG	2A	3545	1/1	0.92	0.10	38,38,38,38	0
57	MG	1A	3296	1/1	0.92	0.12	42,42,42,42	0
57	MG	2A	3548	1/1	0.92	0.14	35,35,35,35	0
57	MG	2A	3130	1/1	0.92	0.18	38,38,38,38	0
57	MG	2A	3131	1/1	0.92	0.22	52,52,52,52	0
57	MG	1a	3246	1/1	0.92	0.09	55,55,55,55	0
57	MG	2a	3003	1/1	0.92	0.12	52,52,52,52	0
57	MG	1A	3476	1/1	0.92	0.12	24,24,24,24	0
57	MG	2A	3140	1/1	0.92	0.22	60,60,60,60	0
57	MG	1A	3008	1/1	0.92	0.15	25,25,25,25	0
57	MG	2A	3144	1/1	0.92	0.09	40,40,40,40	0
57	MG	1A	3193	1/1	0.92	0.25	36,36,36,36	0
57	MG	2A	3148	1/1	0.92	0.37	57,57,57,57	0
57	MG	2A	3343	1/1	0.92	0.13	27,27,27,27	0
57	MG	1A	3579	1/1	0.92	0.17	37,37,37,37	0
57	MG	1A	3754	1/1	0.92	0.16	26,26,26,26	0
57	MG	2a	3018	1/1	0.92	0.17	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	1A	4014	1/1	0.92	0.15	27,27,27,27	0
57	MG	2a	3020	1/1	0.92	0.22	58,58,58,58	0
57	MG	1a	3007	1/1	0.92	0.23	56,56,56,56	0
57	MG	1a	3264	1/1	0.92	0.32	72,72,72,72	0
57	MG	1A	3931	1/1	0.92	0.10	41,41,41,41	0
57	MG	1A	3412	1/1	0.92	0.16	15,15,15,15	0
57	MG	2a	3026	1/1	0.92	0.19	64,64,64,64	0
57	MG	1a	3122	1/1	0.92	0.11	56,56,56,56	0
57	MG	2A	3368	1/1	0.92	0.10	34,34,34,34	0
57	MG	1B	202	1/1	0.92	0.19	44,44,44,44	0
57	MG	1d	303	1/1	0.92	0.18	45,45,45,45	0
57	MG	2A	3591	1/1	0.92	0.13	38,38,38,38	0
57	MG	2A	3377	1/1	0.92	0.15	70,70,70,70	0
57	MG	1A	3759	1/1	0.92	0.14	33,33,33,33	0
57	MG	1A	3485	1/1	0.92	0.20	39,39,39,39	0
57	MG	2A	3171	1/1	0.92	0.10	48,48,48,48	0
57	MG	1a	3127	1/1	0.92	0.19	52,52,52,52	0
57	MG	2a	3046	1/1	0.92	0.12	59,59,59,59	0
57	MG	2A	3174	1/1	0.92	0.12	44,44,44,44	0
57	MG	2A	3603	1/1	0.92	0.10	37,37,37,37	0
57	MG	1a	3128	1/1	0.92	0.11	52,52,52,52	0
57	MG	2A	3388	1/1	0.92	0.15	49,49,49,49	0
57	MG	1A	3486	1/1	0.92	0.14	20,20,20,20	0
57	MG	1A	3306	1/1	0.92	0.15	35,35,35,35	0
57	MG	2a	3056	1/1	0.92	0.17	49,49,49,49	0
57	MG	1a	3134	1/1	0.92	0.08	38,38,38,38	0
57	MG	1A	3942	1/1	0.92	0.11	25,25,25,25	0
57	MG	1a	3027	1/1	0.92	0.13	55,55,55,55	0
57	MG	1A	3254	1/1	0.92	0.13	41,41,41,41	0
57	MG	1A	3664	1/1	0.92	0.14	49,49,49,49	0
57	MG	2a	3064	1/1	0.92	0.14	47,47,47,47	0
57	MG	2A	3619	1/1	0.92	0.17	44,44,44,44	0
57	MG	2A	3621	1/1	0.92	0.17	28,28,28,28	0
57	MG	2A	3406	1/1	0.92	0.14	43,43,43,43	0
57	MG	1A	3864	1/1	0.92	0.15	38,38,38,38	0
57	MG	1A	3143	1/1	0.92	0.17	30,30,30,30	0
57	MG	2A	3626	1/1	0.92	0.06	67,67,67,67	0
57	MG	1A	3434	1/1	0.92	0.14	52,52,52,52	0
57	MG	2A	3411	1/1	0.92	0.17	44,44,44,44	0
57	MG	1A	3313	1/1	0.92	0.12	30,30,30,30	0
57	MG	1a	3152	1/1	0.92	0.12	45,45,45,45	0
57	MG	1a	3153	1/1	0.92	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3062	1/1	0.92	0.14	35,35,35,35	0
57	MG	1A	3959	1/1	0.92	0.20	42,42,42,42	0
57	MG	2a	3084	1/1	0.92	0.35	51,51,51,51	0
57	MG	1A	3439	1/1	0.92	0.14	46,46,46,46	0
57	MG	1a	3047	1/1	0.92	0.16	44,44,44,44	0
57	MG	1A	3443	1/1	0.92	0.14	21,21,21,21	0
57	MG	1A	3319	1/1	0.92	0.13	37,37,37,37	0
57	MG	1a	3170	1/1	0.92	0.10	49,49,49,49	0
57	MG	2a	3099	1/1	0.92	0.35	46,46,46,46	0
57	MG	1A	3604	1/1	0.92	0.12	55,55,55,55	0
57	MG	1D	316	1/1	0.92	0.15	49,49,49,49	0
57	MG	1A	3267	1/1	0.92	0.24	58,58,58,58	0
57	MG	2A	3658	1/1	0.92	0.08	42,42,42,42	0
57	MG	1a	3175	1/1	0.92	0.13	43,43,43,43	0
57	MG	2A	3660	1/1	0.92	0.08	58,58,58,58	0
57	MG	2A	3033	1/1	0.92	0.18	58,58,58,58	0
57	MG	1A	3110	1/1	0.92	0.17	25,25,25,25	0
57	MG	2A	3441	1/1	0.92	0.07	61,61,61,61	0
57	MG	2A	3220	1/1	0.92	0.16	57,57,57,57	0
57	MG	1a	3057	1/1	0.92	0.14	55,55,55,55	0
57	MG	1A	3271	1/1	0.92	0.18	62,62,62,62	0
57	MG	2A	3671	1/1	0.92	0.14	65,65,65,65	0
57	MG	1A	3451	1/1	0.92	0.17	19,19,19,19	0
57	MG	2a	3125	1/1	0.92	0.11	49,49,49,49	0
57	MG	2a	3126	1/1	0.92	0.13	64,64,64,64	0
57	MG	2a	3127	1/1	0.92	0.09	53,53,53,53	0
57	MG	1A	3377	1/1	0.92	0.19	49,49,49,49	0
57	MG	2A	3229	1/1	0.92	0.13	27,27,27,27	0
57	MG	1A	3162	1/1	0.92	0.16	37,37,37,37	0
57	MG	2A	3453	1/1	0.92	0.15	49,49,49,49	0
57	MG	1a	3067	1/1	0.92	0.10	64,64,64,64	0
57	MG	1a	3069	1/1	0.92	0.26	54,54,54,54	0
57	MG	1F	317	1/1	0.92	0.14	52,52,52,52	0
57	MG	2A	3054	1/1	0.92	0.16	66,66,66,66	0
57	MG	2A	3056	1/1	0.92	0.20	29,29,29,29	0
57	MG	1A	3700	1/1	0.92	0.18	40,40,40,40	0
57	MG	2A	3701	1/1	0.92	0.07	55,55,55,55	0
57	MG	1A	3814	1/1	0.92	0.21	22,22,22,22	0
57	MG	1a	3193	1/1	0.92	0.11	47,47,47,47	0
57	MG	2a	3152	1/1	0.92	0.13	55,55,55,55	0
57	MG	2A	3251	1/1	0.92	0.23	47,47,47,47	0
57	MG	1G	203	1/1	0.92	0.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3710	1/1	0.92	0.13	44,44,44,44	0
57	MG	1A	3186	1/1	0.92	0.12	41,41,41,41	0
57	MG	1a	3198	1/1	0.92	0.18	65,65,65,65	0
57	MG	1A	3235	1/1	0.92	0.13	60,60,60,60	0
57	MG	1a	3200	1/1	0.92	0.17	54,54,54,54	0
57	MG	1A	3079	1/1	0.92	0.28	35,35,35,35	0
57	MG	1A	3390	1/1	0.92	0.15	38,38,38,38	0
57	MG	2A	3487	1/1	0.92	0.19	48,48,48,48	0
57	MG	1A	3983	1/1	0.92	0.11	16,16,16,16	0
57	MG	2A	3084	1/1	0.92	0.13	35,35,35,35	0
57	MG	2A	3086	1/1	0.92	0.15	44,44,44,44	0
57	MG	1a	3084	1/1	0.92	0.20	46,46,46,46	0
57	MG	2a	3184	1/1	0.92	0.23	59,59,59,59	0
57	MG	2A	3088	1/1	0.92	0.17	40,40,40,40	0
57	MG	1A	3204	1/1	0.92	0.31	38,38,38,38	0
57	MG	2A	3274	1/1	0.92	0.22	57,57,57,57	0
57	MG	1T	205	1/1	0.92	0.17	50,50,50,50	0
57	MG	2A	3498	1/1	0.92	0.11	36,36,36,36	0
57	MG	1V	205	1/1	0.92	0.12	41,41,41,41	0
57	MG	2A	3502	1/1	0.92	0.11	57,57,57,57	0
57	MG	2A	3505	1/1	0.92	0.07	38,38,38,38	0
60	MPD	1a	3271	8/8	0.92	0.25	49,51,53,60	0
57	MG	1W	201	1/1	0.92	0.26	45,45,45,45	0
57	MG	2A	3279	1/1	0.92	0.31	61,61,61,61	0
57	MG	2D	309	1/1	0.92	0.12	61,61,61,61	0
57	MG	1W	205	1/1	0.92	0.15	48,48,48,48	0
57	MG	2A	3098	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3723	1/1	0.93	0.20	39,39,39,39	0
57	MG	2A	3694	1/1	0.93	0.11	44,44,44,44	0
57	MG	2A	3695	1/1	0.93	0.41	53,53,53,53	0
57	MG	1A	3168	1/1	0.93	0.20	43,43,43,43	0
57	MG	2A	3163	1/1	0.93	0.19	35,35,35,35	0
57	MG	2A	3700	1/1	0.93	0.24	46,46,46,46	0
57	MG	2A	3417	1/1	0.93	0.10	38,38,38,38	0
57	MG	1a	3256	1/1	0.93	0.25	55,55,55,55	0
57	MG	2A	3419	1/1	0.93	0.10	28,28,28,28	0
57	MG	1a	3258	1/1	0.93	0.11	44,44,44,44	0
57	MG	1A	3619	1/1	0.93	0.21	20,20,20,20	0
57	MG	1A	3125	1/1	0.93	0.17	29,29,29,29	0
57	MG	1a	3097	1/1	0.93	0.97	81,81,81,81	0
57	MG	1R	203	1/1	0.93	0.23	39,39,39,39	0
57	MG	2A	3714	1/1	0.93	0.14	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3860	1/1	0.93	0.16	30,30,30,30	0
57	MG	1a	3266	1/1	0.93	0.10	67,67,67,67	0
57	MG	1T	202	1/1	0.93	0.08	43,43,43,43	0
57	MG	1T	204	1/1	0.93	0.17	52,52,52,52	0
57	MG	1A	3173	1/1	0.93	0.10	48,48,48,48	0
57	MG	2A	3437	1/1	0.93	0.23	51,51,51,51	0
57	MG	1U	207	1/1	0.93	0.11	37,37,37,37	0
57	MG	2B	203	1/1	0.93	0.22	54,54,54,54	0
57	MG	1a	3106	1/1	0.93	0.11	62,62,62,62	0
57	MG	1A	3526	1/1	0.93	0.21	26,26,26,26	0
57	MG	1A	3383	1/1	0.93	0.11	39,39,39,39	0
57	MG	1f	201	1/1	0.93	0.31	55,55,55,55	0
57	MG	1g	201	1/1	0.93	0.26	49,49,49,49	0
57	MG	1A	3529	1/1	0.93	0.09	41,41,41,41	0
57	MG	1X	101	1/1	0.93	0.13	32,32,32,32	0
57	MG	1A	3038	1/1	0.93	0.24	32,32,32,32	0
57	MG	1Z	301	1/1	0.93	0.12	51,51,51,51	0
57	MG	2B	217	1/1	0.93	0.16	53,53,53,53	0
57	MG	1l	202	1/1	0.93	0.17	64,64,64,64	0
57	MG	2D	305	1/1	0.93	0.21	30,30,30,30	0
57	MG	1A	3749	1/1	0.93	0.15	40,40,40,40	0
57	MG	2D	307	1/1	0.93	0.17	53,53,53,53	0
57	MG	10	103	1/1	0.93	0.15	37,37,37,37	0
57	MG	10	104	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	3179	1/1	0.93	0.17	36,36,36,36	0
57	MG	2A	3460	1/1	0.93	0.13	55,55,55,55	0
57	MG	1A	3540	1/1	0.93	0.18	41,41,41,41	0
57	MG	2A	3465	1/1	0.93	0.16	50,50,50,50	0
57	MG	2A	3466	1/1	0.93	0.15	40,40,40,40	0
57	MG	1A	3389	1/1	0.93	0.16	22,22,22,22	0
57	MG	1A	3103	1/1	0.93	0.34	34,34,34,34	0
57	MG	11	102	1/1	0.93	0.29	42,42,42,42	0
57	MG	2A	3215	1/1	0.93	0.08	52,52,52,52	0
57	MG	1A	3391	1/1	0.93	0.13	26,26,26,26	0
57	MG	1A	3135	1/1	0.93	0.22	35,35,35,35	0
57	MG	2A	3009	1/1	0.93	0.18	34,34,34,34	0
57	MG	15	101	1/1	0.93	0.17	29,29,29,29	0
57	MG	2P	202	1/1	0.93	0.12	56,56,56,56	0
57	MG	1A	3185	1/1	0.93	0.31	33,33,33,33	0
57	MG	2R	202	1/1	0.93	0.27	47,47,47,47	0
57	MG	1A	3219	1/1	0.93	0.17	43,43,43,43	0
57	MG	2A	3017	1/1	0.93	0.12	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3064	1/1	0.93	0.07	46,46,46,46	0
57	MG	2V	201	1/1	0.93	0.22	53,53,53,53	0
57	MG	2A	3488	1/1	0.93	0.12	34,34,34,34	0
57	MG	2V	203	1/1	0.93	0.20	53,53,53,53	0
57	MG	1A	3564	1/1	0.93	0.08	50,50,50,50	0
57	MG	2A	3231	1/1	0.93	0.57	45,45,45,45	0
57	MG	2Y	201	1/1	0.93	0.29	56,56,56,56	0
57	MG	2A	3232	1/1	0.93	0.20	51,51,51,51	0
57	MG	18	101	1/1	0.93	0.17	32,32,32,32	0
57	MG	2A	3234	1/1	0.93	0.20	40,40,40,40	0
57	MG	25	101	1/1	0.93	0.40	46,46,46,46	0
57	MG	1A	3652	1/1	0.93	0.14	46,46,46,46	0
57	MG	27	102	1/1	0.93	0.29	37,37,37,37	0
57	MG	28	101	1/1	0.93	0.16	46,46,46,46	0
57	MG	1A	3109	1/1	0.93	0.14	31,31,31,31	0
57	MG	1a	3146	1/1	0.93	0.19	29,29,29,29	0
57	MG	1a	3002	1/1	0.93	0.18	49,49,49,49	0
57	MG	1A	3015	1/1	0.93	0.14	29,29,29,29	0
57	MG	2A	3244	1/1	0.93	0.54	37,37,37,37	0
57	MG	2A	3504	1/1	0.93	0.14	39,39,39,39	0
57	MG	1A	3081	1/1	0.93	0.20	24,24,24,24	0
57	MG	2a	3009	1/1	0.93	0.18	54,54,54,54	0
57	MG	2A	3506	1/1	0.93	0.10	41,41,41,41	0
57	MG	1A	3473	1/1	0.93	0.17	17,17,17,17	0
57	MG	2A	3508	1/1	0.93	0.10	43,43,43,43	0
57	MG	1A	3572	1/1	0.93	0.15	45,45,45,45	0
57	MG	2a	3016	1/1	0.93	0.13	50,50,50,50	0
57	MG	1a	3154	1/1	0.93	0.14	47,47,47,47	0
57	MG	1A	4007	1/1	0.93	0.10	37,37,37,37	0
57	MG	2A	3516	1/1	0.93	0.08	61,61,61,61	0
57	MG	1A	3291	1/1	0.93	0.11	51,51,51,51	0
57	MG	1A	3577	1/1	0.93	0.17	43,43,43,43	0
57	MG	2A	3043	1/1	0.93	0.12	39,39,39,39	0
57	MG	1A	3788	1/1	0.93	0.17	42,42,42,42	0
57	MG	2A	3527	1/1	0.93	0.08	55,55,55,55	0
57	MG	2A	3047	1/1	0.93	0.07	52,52,52,52	0
57	MG	2a	3028	1/1	0.93	0.35	59,59,59,59	0
57	MG	2A	3049	1/1	0.93	0.14	54,54,54,54	0
57	MG	1a	3164	1/1	0.93	0.26	55,55,55,55	0
57	MG	1A	3410	1/1	0.93	0.10	35,35,35,35	0
57	MG	2A	3533	1/1	0.93	0.25	59,59,59,59	0
57	MG	2A	3534	1/1	0.93	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3066	1/1	0.93	0.14	32,32,32,32	0
57	MG	2A	3538	1/1	0.93	0.10	46,46,46,46	0
57	MG	1A	3481	1/1	0.93	0.14	23,23,23,23	0
57	MG	2a	3042	1/1	0.93	0.25	48,48,48,48	0
57	MG	2A	3270	1/1	0.93	0.14	36,36,36,36	0
57	MG	1a	3023	1/1	0.93	0.17	42,42,42,42	0
57	MG	1a	3172	1/1	0.93	0.07	65,65,65,65	0
57	MG	1A	3191	1/1	0.93	0.20	53,53,53,53	0
57	MG	1A	3069	1/1	0.93	0.37	27,27,27,27	0
57	MG	2a	3049	1/1	0.93	0.26	61,61,61,61	0
57	MG	2A	3276	1/1	0.93	0.31	50,50,50,50	0
57	MG	1B	201	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3067	1/1	0.93	0.14	40,40,40,40	0
57	MG	2A	3550	1/1	0.93	0.12	51,51,51,51	0
57	MG	1a	3178	1/1	0.93	0.10	51,51,51,51	0
57	MG	2A	3553	1/1	0.93	0.11	39,39,39,39	0
57	MG	1A	3419	1/1	0.93	0.15	64,64,64,64	0
57	MG	1a	3030	1/1	0.93	0.18	38,38,38,38	0
57	MG	2A	3283	1/1	0.93	0.28	53,53,53,53	0
57	MG	2A	3077	1/1	0.93	0.27	43,43,43,43	0
57	MG	2A	3563	1/1	0.93	0.14	51,51,51,51	0
57	MG	1A	3914	1/1	0.93	0.06	34,34,34,34	0
57	MG	2A	3287	1/1	0.93	0.28	63,63,63,63	0
57	MG	2A	3567	1/1	0.93	0.12	49,49,49,49	0
57	MG	1A	3680	1/1	0.93	0.10	37,37,37,37	0
57	MG	1a	3036	1/1	0.93	0.15	58,58,58,58	0
57	MG	2A	3570	1/1	0.93	0.07	51,51,51,51	0
57	MG	2A	3083	1/1	0.93	0.17	56,56,56,56	0
57	MG	2A	3296	1/1	0.93	0.10	30,30,30,30	0
57	MG	1A	3587	1/1	0.93	0.09	47,47,47,47	0
57	MG	1A	3917	1/1	0.93	0.10	57,57,57,57	0
57	MG	1A	3420	1/1	0.93	0.14	23,23,23,23	0
57	MG	2A	3302	1/1	0.93	0.11	43,43,43,43	0
57	MG	2A	3307	1/1	0.93	0.19	41,41,41,41	0
57	MG	2A	3308	1/1	0.93	0.15	68,68,68,68	0
57	MG	2A	3583	1/1	0.93	0.10	50,50,50,50	0
57	MG	2A	3310	1/1	0.93	0.14	35,35,35,35	0
57	MG	1B	213	1/1	0.93	0.19	33,33,33,33	0
57	MG	1a	3190	1/1	0.93	0.07	68,68,68,68	0
57	MG	2A	3093	1/1	0.93	0.28	63,63,63,63	0
57	MG	2a	3096	1/1	0.93	0.19	55,55,55,55	0
57	MG	1A	3591	1/1	0.93	0.14	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	3431	1/1	0.93	0.15	22,22,22,22	0
57	MG	1A	3305	1/1	0.93	0.34	25,25,25,25	0
57	MG	2a	3104	1/1	0.93	0.35	48,48,48,48	0
57	MG	2A	3597	1/1	0.93	0.15	53,53,53,53	0
57	MG	1B	217	1/1	0.93	0.13	50,50,50,50	0
57	MG	1a	3050	1/1	0.93	0.14	36,36,36,36	0
57	MG	1A	3688	1/1	0.93	0.20	41,41,41,41	0
57	MG	2A	3329	1/1	0.93	0.14	47,47,47,47	0
57	MG	2A	3100	1/1	0.93	0.14	40,40,40,40	0
57	MG	2a	3117	1/1	0.93	0.11	56,56,56,56	0
57	MG	2a	3118	1/1	0.93	0.09	54,54,54,54	0
57	MG	1A	3030	1/1	0.93	0.12	31,31,31,31	0
57	MG	1A	3927	1/1	0.93	0.15	52,52,52,52	0
57	MG	1A	3690	1/1	0.93	0.27	39,39,39,39	0
57	MG	2A	3337	1/1	0.93	0.16	40,40,40,40	0
57	MG	2A	3109	1/1	0.93	0.21	42,42,42,42	0
57	MG	2A	3615	1/1	0.93	0.19	26,26,26,26	0
57	MG	1B	226	1/1	0.93	0.10	35,35,35,35	0
57	MG	2A	3111	1/1	0.93	0.13	42,42,42,42	0
57	MG	1A	3074	1/1	0.93	0.14	33,33,33,33	0
57	MG	2A	3344	1/1	0.93	0.14	37,37,37,37	0
57	MG	2A	3345	1/1	0.93	0.15	31,31,31,31	0
57	MG	1a	3060	1/1	0.93	0.25	51,51,51,51	0
57	MG	1A	3694	1/1	0.93	0.23	29,29,29,29	0
57	MG	2A	3351	1/1	0.93	0.17	40,40,40,40	0
57	MG	1A	3831	1/1	0.93	0.14	25,25,25,25	0
57	MG	1a	3213	1/1	0.93	0.09	68,68,68,68	0
57	MG	2a	3140	1/1	0.93	0.15	54,54,54,54	0
57	MG	1a	3216	1/1	0.93	0.21	67,67,67,67	0
57	MG	2A	3361	1/1	0.93	0.19	35,35,35,35	0
57	MG	2a	3144	1/1	0.93	0.23	64,64,64,64	0
57	MG	1D	306	1/1	0.93	0.12	45,45,45,45	0
57	MG	1A	3436	1/1	0.93	0.09	44,44,44,44	0
57	MG	2A	3123	1/1	0.93	0.15	33,33,33,33	0
57	MG	1A	3599	1/1	0.93	0.18	39,39,39,39	0
57	MG	1A	3702	1/1	0.93	0.69	50,50,50,50	0
57	MG	2a	3157	1/1	0.93	0.15	54,54,54,54	0
57	MG	1A	3196	1/1	0.93	0.15	40,40,40,40	0
57	MG	1E	304	1/1	0.93	0.08	33,33,33,33	0
57	MG	2A	3132	1/1	0.93	0.15	54,54,54,54	0
57	MG	1A	3372	1/1	0.93	0.18	40,40,40,40	0
57	MG	2A	3649	1/1	0.93	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3650	1/1	0.93	0.14	36,36,36,36	0
57	MG	2A	3134	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	3510	1/1	0.93	0.18	14,14,14,14	0
57	MG	2A	3137	1/1	0.93	0.20	55,55,55,55	0
57	MG	2A	3386	1/1	0.93	0.20	56,56,56,56	0
57	MG	2A	3138	1/1	0.93	0.23	46,46,46,46	0
57	MG	1A	3513	1/1	0.93	0.15	10,10,10,10	0
57	MG	1A	3612	1/1	0.93	0.12	48,48,48,48	0
57	MG	1a	3080	1/1	0.93	0.13	55,55,55,55	0
57	MG	2A	3396	1/1	0.93	0.14	29,29,29,29	0
57	MG	1F	304	1/1	0.93	0.21	27,27,27,27	0
57	MG	2A	3147	1/1	0.93	0.15	43,43,43,43	0
57	MG	1F	305	1/1	0.93	0.11	28,28,28,28	0
57	MG	1F	309	1/1	0.93	0.26	44,44,44,44	0
57	MG	1A	3442	1/1	0.93	0.18	56,56,56,56	0
57	MG	2t	201	1/1	0.93	0.15	40,40,40,40	0
57	MG	2x	101	1/1	0.93	0.14	62,62,62,62	0
58	CLM	2A	3727	20/20	0.93	0.27	33,38,57,59	0
57	MG	2A	3405	1/1	0.93	0.12	55,55,55,55	0
57	MG	1A	3054	1/1	0.93	0.27	25,25,25,25	0
57	MG	1A	3199	1/1	0.93	0.18	32,32,32,32	0
57	MG	1A	3718	1/1	0.93	0.12	30,30,30,30	0
57	MG	1A	3853	1/1	0.93	0.11	31,31,31,31	0
57	MG	2A	3683	1/1	0.93	0.13	37,37,37,37	0
57	MG	2A	3688	1/1	0.93	0.10	49,49,49,49	0
57	MG	1A	3720	1/1	0.93	0.09	62,62,62,62	0
57	MG	2A	3412	1/1	0.93	0.09	30,30,30,30	0
57	MG	2A	3468	1/1	0.94	0.09	44,44,44,44	0
57	MG	1A	3094	1/1	0.94	0.19	23,23,23,23	0
57	MG	2A	3472	1/1	0.94	0.13	59,59,59,59	0
57	MG	2A	3230	1/1	0.94	0.14	43,43,43,43	0
57	MG	1A	3032	1/1	0.94	0.17	45,45,45,45	0
57	MG	1A	3292	1/1	0.94	0.08	37,37,37,37	0
57	MG	15	109	1/1	0.94	0.14	46,46,46,46	0
57	MG	1A	3575	1/1	0.94	0.18	20,20,20,20	0
57	MG	1A	3180	1/1	0.94	0.13	32,32,32,32	0
57	MG	17	105	1/1	0.94	0.24	39,39,39,39	0
57	MG	1A	3997	1/1	0.94	0.22	27,27,27,27	0
57	MG	19	101	1/1	0.94	0.22	41,41,41,41	0
57	MG	2D	304	1/1	0.94	0.17	44,44,44,44	0
57	MG	1a	3149	1/1	0.94	0.11	51,51,51,51	0
57	MG	1A	3999	1/1	0.94	0.15	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	3493	1/1	0.94	0.14	39,39,39,39	0
57	MG	1A	4001	1/1	0.94	0.25	30,30,30,30	0
57	MG	1A	3334	1/1	0.94	0.18	28,28,28,28	0
57	MG	1A	3890	1/1	0.94	0.11	34,34,34,34	0
57	MG	1a	3158	1/1	0.94	0.07	41,41,41,41	0
57	MG	2A	3045	1/1	0.94	0.20	55,55,55,55	0
57	MG	1A	3338	1/1	0.94	0.07	51,51,51,51	0
57	MG	1a	3160	1/1	0.94	0.13	56,56,56,56	0
57	MG	1A	4010	1/1	0.94	0.32	39,39,39,39	0
57	MG	1a	3162	1/1	0.94	0.13	55,55,55,55	0
57	MG	2A	3259	1/1	0.94	0.17	43,43,43,43	0
57	MG	2A	3260	1/1	0.94	0.19	48,48,48,48	0
57	MG	2A	3503	1/1	0.94	0.10	41,41,41,41	0
57	MG	2N	201	1/1	0.94	0.10	59,59,59,59	0
57	MG	1A	3669	1/1	0.94	0.66	45,45,45,45	0
57	MG	1a	3011	1/1	0.94	0.18	26,26,26,26	0
57	MG	1A	3441	1/1	0.94	0.16	25,25,25,25	0
57	MG	2A	3265	1/1	0.94	0.65	45,45,45,45	0
57	MG	2Q	202	1/1	0.94	0.25	52,52,52,52	0
57	MG	1A	3341	1/1	0.94	0.16	32,32,32,32	0
57	MG	1a	3167	1/1	0.94	0.18	62,62,62,62	0
57	MG	2A	3269	1/1	0.94	0.18	43,43,43,43	0
57	MG	1a	3015	1/1	0.94	0.09	59,59,59,59	0
57	MG	2A	3063	1/1	0.94	0.42	43,43,43,43	0
57	MG	1A	3896	1/1	0.94	0.15	36,36,36,36	0
57	MG	2A	3065	1/1	0.94	0.13	45,45,45,45	0
57	MG	2A	3521	1/1	0.94	0.12	49,49,49,49	0
57	MG	1A	3897	1/1	0.94	0.14	22,22,22,22	0
57	MG	1A	4017	1/1	0.94	0.14	38,38,38,38	0
57	MG	2A	3525	1/1	0.94	0.12	27,27,27,27	0
57	MG	1A	4018	1/1	0.94	0.21	50,50,50,50	0
57	MG	1a	3022	1/1	0.94	0.10	55,55,55,55	0
57	MG	2A	3074	1/1	0.94	0.25	39,39,39,39	0
57	MG	1A	3234	1/1	0.94	0.12	25,25,25,25	0
57	MG	25	102	1/1	0.94	0.34	41,41,41,41	0
57	MG	25	103	1/1	0.94	0.11	48,48,48,48	0
57	MG	2A	3076	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	3507	1/1	0.94	0.14	17,17,17,17	0
57	MG	27	103	1/1	0.94	0.28	38,38,38,38	0
57	MG	2A	3078	1/1	0.94	0.11	43,43,43,43	0
57	MG	1a	3025	1/1	0.94	0.16	45,45,45,45	0
57	MG	2A	3536	1/1	0.94	0.11	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	29	101	1/1	0.94	0.18	53,53,53,53	0
57	MG	1A	3589	1/1	0.94	0.17	16,16,16,16	0
57	MG	1A	3300	1/1	0.94	0.20	43,43,43,43	0
57	MG	1B	204	1/1	0.94	0.33	42,42,42,42	0
57	MG	1A	3269	1/1	0.94	0.16	23,23,23,23	0
57	MG	2A	3295	1/1	0.94	0.13	53,53,53,53	0
57	MG	1a	3032	1/1	0.94	0.13	43,43,43,43	0
57	MG	1A	3511	1/1	0.94	0.14	36,36,36,36	0
57	MG	2a	3011	1/1	0.94	0.23	49,49,49,49	0
57	MG	1A	3303	1/1	0.94	0.14	76,76,76,76	0
57	MG	2A	3547	1/1	0.94	0.07	44,44,44,44	0
57	MG	1a	3035	1/1	0.94	0.12	38,38,38,38	0
57	MG	1A	3449	1/1	0.94	0.14	41,41,41,41	0
57	MG	2A	3304	1/1	0.94	0.13	37,37,37,37	0
57	MG	1A	3799	1/1	0.94	0.15	47,47,47,47	0
57	MG	2A	3552	1/1	0.94	0.05	48,48,48,48	0
57	MG	1A	3801	1/1	0.94	0.13	40,40,40,40	0
57	MG	1A	3596	1/1	0.94	0.10	27,27,27,27	0
57	MG	1a	3042	1/1	0.94	0.12	54,54,54,54	0
57	MG	1A	3686	1/1	0.94	0.12	54,54,54,54	0
57	MG	2A	3558	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3809	1/1	0.94	0.08	30,30,30,30	0
57	MG	1a	3046	1/1	0.94	0.23	34,34,34,34	0
57	MG	1A	3813	1/1	0.94	0.12	45,45,45,45	0
57	MG	2A	3103	1/1	0.94	0.21	47,47,47,47	0
57	MG	1A	3394	1/1	0.94	0.22	18,18,18,18	0
57	MG	2A	3321	1/1	0.94	0.17	54,54,54,54	0
57	MG	1B	220	1/1	0.94	0.19	22,22,22,22	0
57	MG	1a	3205	1/1	0.94	0.07	59,59,59,59	0
57	MG	1A	3815	1/1	0.94	0.14	28,28,28,28	0
57	MG	1B	223	1/1	0.94	0.07	37,37,37,37	0
57	MG	2A	3332	1/1	0.94	0.15	47,47,47,47	0
57	MG	1a	3211	1/1	0.94	0.17	69,69,69,69	0
57	MG	2a	3044	1/1	0.94	0.06	61,61,61,61	0
57	MG	1A	3819	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3138	1/1	0.94	0.13	35,35,35,35	0
57	MG	1A	3925	1/1	0.94	0.10	27,27,27,27	0
57	MG	1a	3217	1/1	0.94	0.17	54,54,54,54	0
57	MG	1B	228	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3090	1/1	0.94	0.13	32,32,32,32	0
57	MG	1A	3824	1/1	0.94	0.06	41,41,41,41	0
57	MG	1A	3600	1/1	0.94	0.12	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	3930	1/1	0.94	0.12	48,48,48,48	0
57	MG	1a	3064	1/1	0.94	0.31	57,57,57,57	0
57	MG	2A	3129	1/1	0.94	0.13	57,57,57,57	0
57	MG	1A	3184	1/1	0.94	0.14	24,24,24,24	0
57	MG	2a	3059	1/1	0.94	0.18	53,53,53,53	0
57	MG	1A	3932	1/1	0.94	0.14	50,50,50,50	0
57	MG	2a	3061	1/1	0.94	0.10	69,69,69,69	0
57	MG	2A	3598	1/1	0.94	0.07	36,36,36,36	0
57	MG	1a	3231	1/1	0.94	0.11	42,42,42,42	0
57	MG	2A	3355	1/1	0.94	0.08	34,34,34,34	0
57	MG	2A	3359	1/1	0.94	0.08	37,37,37,37	0
57	MG	1A	3351	1/1	0.94	0.11	30,30,30,30	0
57	MG	1A	3525	1/1	0.94	0.12	56,56,56,56	0
57	MG	2A	3605	1/1	0.94	0.14	42,42,42,42	0
57	MG	2A	3606	1/1	0.94	0.07	49,49,49,49	0
57	MG	1a	3235	1/1	0.94	0.11	64,64,64,64	0
57	MG	1a	3071	1/1	0.94	0.16	56,56,56,56	0
57	MG	1A	3244	1/1	0.94	0.29	28,28,28,28	0
57	MG	2A	3367	1/1	0.94	0.14	40,40,40,40	0
57	MG	2a	3078	1/1	0.94	0.11	66,66,66,66	0
57	MG	1A	3112	1/1	0.94	0.13	28,28,28,28	0
57	MG	2A	3141	1/1	0.94	0.24	43,43,43,43	0
57	MG	2A	3142	1/1	0.94	0.09	42,42,42,42	0
57	MG	2a	3082	1/1	0.94	0.25	46,46,46,46	0
57	MG	1A	3317	1/1	0.94	0.20	44,44,44,44	0
57	MG	1A	3531	1/1	0.94	0.26	43,43,43,43	0
57	MG	1A	3463	1/1	0.94	0.10	46,46,46,46	0
57	MG	2A	3382	1/1	0.94	0.11	61,61,61,61	0
57	MG	1A	3710	1/1	0.94	0.22	21,21,21,21	0
57	MG	2a	3090	1/1	0.94	0.25	50,50,50,50	0
57	MG	1F	307	1/1	0.94	0.18	19,19,19,19	0
57	MG	2a	3094	1/1	0.94	0.25	60,60,60,60	0
57	MG	1A	3946	1/1	0.94	0.15	39,39,39,39	0
57	MG	1a	3249	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3947	1/1	0.94	0.21	46,46,46,46	0
57	MG	1A	3534	1/1	0.94	0.07	49,49,49,49	0
57	MG	1A	3360	1/1	0.94	0.10	45,45,45,45	0
57	MG	2A	3392	1/1	0.94	0.15	38,38,38,38	0
57	MG	1G	201	1/1	0.94	0.09	63,63,63,63	0
57	MG	2A	3395	1/1	0.94	0.12	27,27,27,27	0
57	MG	1A	3841	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3411	1/1	0.94	0.29	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3952	1/1	0.94	0.14	54,54,54,54	0
57	MG	1A	3953	1/1	0.94	0.18	48,48,48,48	0
57	MG	1A	3276	1/1	0.94	0.11	56,56,56,56	0
57	MG	1A	3544	1/1	0.94	0.15	33,33,33,33	0
57	MG	1A	3623	1/1	0.94	0.16	14,14,14,14	0
57	MG	1Q	204	1/1	0.94	0.19	33,33,33,33	0
57	MG	1A	3626	1/1	0.94	0.13	30,30,30,30	0
57	MG	1A	3545	1/1	0.94	0.23	46,46,46,46	0
57	MG	2A	3175	1/1	0.94	0.16	58,58,58,58	0
57	MG	2A	3177	1/1	0.94	0.15	33,33,33,33	0
57	MG	1d	302	1/1	0.94	0.08	61,61,61,61	0
57	MG	1A	3279	1/1	0.94	0.19	21,21,21,21	0
57	MG	1A	3730	1/1	0.94	0.18	47,47,47,47	0
57	MG	1a	3101	1/1	0.94	0.27	58,58,58,58	0
57	MG	2A	3186	1/1	0.94	0.16	60,60,60,60	0
57	MG	2A	3665	1/1	0.94	0.11	52,52,52,52	0
57	MG	1A	3854	1/1	0.94	0.17	30,30,30,30	0
57	MG	2a	3135	1/1	0.94	0.14	58,58,58,58	0
57	MG	1U	205	1/1	0.94	0.12	34,34,34,34	0
57	MG	2A	3190	1/1	0.94	0.22	49,49,49,49	0
57	MG	1f	202	1/1	0.94	0.13	45,45,45,45	0
57	MG	1A	3366	1/1	0.94	0.18	50,50,50,50	0
57	MG	1V	204	1/1	0.94	0.28	46,46,46,46	0
57	MG	1h	202	1/1	0.94	0.14	69,69,69,69	0
57	MG	1A	3734	1/1	0.94	0.11	44,44,44,44	0
57	MG	1A	3551	1/1	0.94	0.14	42,42,42,42	0
57	MG	2A	3680	1/1	0.94	0.22	39,39,39,39	0
57	MG	2a	3149	1/1	0.94	0.10	45,45,45,45	0
57	MG	2A	3432	1/1	0.94	0.28	44,44,44,44	0
57	MG	2A	3682	1/1	0.94	0.17	37,37,37,37	0
57	MG	1W	204	1/1	0.94	0.22	39,39,39,39	0
57	MG	2A	3687	1/1	0.94	0.19	47,47,47,47	0
57	MG	1A	3470	1/1	0.94	0.15	41,41,41,41	0
57	MG	1A	3102	1/1	0.94	0.20	25,25,25,25	0
57	MG	2A	3203	1/1	0.94	0.08	40,40,40,40	0
57	MG	1A	3640	1/1	0.94	0.21	59,59,59,59	0
57	MG	2A	3693	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3745	1/1	0.94	0.21	25,25,25,25	0
57	MG	1A	3555	1/1	0.94	0.15	43,43,43,43	0
57	MG	2A	3696	1/1	0.94	0.34	65,65,65,65	0
57	MG	1t	202	1/1	0.94	0.18	48,48,48,48	0
57	MG	2A	3698	1/1	0.94	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3148	1/1	0.94	0.15	48,48,48,48	0
57	MG	1A	3421	1/1	0.94	0.16	50,50,50,50	0
57	MG	1a	3121	1/1	0.94	0.22	58,58,58,58	0
57	MG	2A	3702	1/1	0.94	0.12	61,61,61,61	0
57	MG	2A	3001	1/1	0.94	0.23	49,49,49,49	0
57	MG	1A	3422	1/1	0.94	0.23	19,19,19,19	0
57	MG	2a	3186	1/1	0.94	0.10	52,52,52,52	0
57	MG	1A	3423	1/1	0.94	0.19	27,27,27,27	0
57	MG	2A	3706	1/1	0.94	0.10	33,33,33,33	0
57	MG	2A	3707	1/1	0.94	0.13	35,35,35,35	0
57	MG	2j	201	1/1	0.94	0.17	68,68,68,68	0
57	MG	1A	3430	1/1	0.94	0.17	44,44,44,44	0
57	MG	2A	3217	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3569	1/1	0.94	0.19	39,39,39,39	0
57	MG	1A	3756	1/1	0.94	0.13	48,48,48,48	0
57	MG	2A	3713	1/1	0.94	0.13	40,40,40,40	0
57	MG	2A	3458	1/1	0.94	0.16	48,48,48,48	0
57	MG	1A	3758	1/1	0.94	0.21	43,43,43,43	0
60	MPD	18	103	8/8	0.94	0.20	25,28,37,43	0
57	MG	2A	3013	1/1	0.94	0.14	19,19,19,19	0
57	MG	2A	3461	1/1	0.94	0.11	53,53,53,53	0
57	MG	2A	3462	1/1	0.94	0.10	48,48,48,48	0
57	MG	2A	3014	1/1	0.94	0.35	51,51,51,51	0
57	MG	11	105	1/1	0.94	0.12	39,39,39,39	0
57	MG	1A	3040	1/1	0.94	0.18	47,47,47,47	0
57	MG	2A	3102	1/1	0.95	0.23	40,40,40,40	0
57	MG	2A	3290	1/1	0.95	0.21	47,47,47,47	0
57	MG	2A	3291	1/1	0.95	0.29	33,33,33,33	0
57	MG	1A	3567	1/1	0.95	0.20	32,32,32,32	0
57	MG	2E	308	1/1	0.95	0.15	24,24,24,24	0
57	MG	1A	3304	1/1	0.95	0.37	39,39,39,39	0
57	MG	2A	3105	1/1	0.95	0.16	46,46,46,46	0
57	MG	1A	3418	1/1	0.95	0.20	19,19,19,19	0
57	MG	1A	3879	1/1	0.95	0.12	31,31,31,31	0
57	MG	1U	206	1/1	0.95	0.19	29,29,29,29	0
57	MG	1A	3356	1/1	0.95	0.18	17,17,17,17	0
57	MG	1A	3484	1/1	0.95	0.17	19,19,19,19	0
57	MG	1A	3140	1/1	0.95	0.13	21,21,21,21	0
57	MG	1A	3259	1/1	0.95	0.15	32,32,32,32	0
57	MG	2A	3531	1/1	0.95	0.08	53,53,53,53	0
57	MG	1W	202	1/1	0.95	0.19	30,30,30,30	0
57	MG	1A	3487	1/1	0.95	0.15	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3007	1/1	0.95	0.25	24,24,24,24	0
57	MG	1A	3490	1/1	0.95	0.12	23,23,23,23	0
57	MG	1a	3244	1/1	0.95	0.12	56,56,56,56	0
57	MG	2T	202	1/1	0.95	0.17	61,61,61,61	0
57	MG	1A	3994	1/1	0.95	0.16	42,42,42,42	0
57	MG	1A	3491	1/1	0.95	0.12	22,22,22,22	0
57	MG	1a	3247	1/1	0.95	0.07	45,45,45,45	0
57	MG	2A	3541	1/1	0.95	0.11	48,48,48,48	0
57	MG	2A	3318	1/1	0.95	0.06	28,28,28,28	0
57	MG	2A	3128	1/1	0.95	0.19	37,37,37,37	0
57	MG	1A	3075	1/1	0.95	0.13	32,32,32,32	0
57	MG	10	102	1/1	0.95	0.19	31,31,31,31	0
57	MG	2A	3325	1/1	0.95	0.19	55,55,55,55	0
57	MG	20	102	1/1	0.95	0.24	59,59,59,59	0
57	MG	1A	3583	1/1	0.95	0.10	29,29,29,29	0
57	MG	1A	3425	1/1	0.95	0.18	21,21,21,21	0
57	MG	21	103	1/1	0.95	0.07	54,54,54,54	0
57	MG	1A	3894	1/1	0.95	0.13	45,45,45,45	0
57	MG	2A	3331	1/1	0.95	0.17	43,43,43,43	0
57	MG	1A	3678	1/1	0.95	0.19	52,52,52,52	0
57	MG	1A	4003	1/1	0.95	0.10	27,27,27,27	0
57	MG	1a	3259	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3428	1/1	0.95	0.14	16,16,16,16	0
57	MG	1A	3792	1/1	0.95	0.07	34,34,34,34	0
57	MG	1A	3498	1/1	0.95	0.09	38,38,38,38	0
57	MG	1A	3900	1/1	0.95	0.18	26,26,26,26	0
57	MG	1A	3092	1/1	0.95	0.11	36,36,36,36	0
57	MG	2a	3001	1/1	0.95	0.18	46,46,46,46	0
57	MG	2a	3002	1/1	0.95	0.19	57,57,57,57	0
57	MG	1a	3113	1/1	0.95	0.34	45,45,45,45	0
57	MG	2a	3004	1/1	0.95	0.20	46,46,46,46	0
57	MG	1A	3797	1/1	0.95	0.15	41,41,41,41	0
57	MG	1a	3269	1/1	0.95	0.29	48,48,48,48	0
57	MG	2A	3348	1/1	0.95	0.08	45,45,45,45	0
57	MG	1A	3588	1/1	0.95	0.17	46,46,46,46	0
57	MG	1b	301	1/1	0.95	0.24	52,52,52,52	0
57	MG	1A	3367	1/1	0.95	0.30	23,23,23,23	0
57	MG	1A	3800	1/1	0.95	0.11	35,35,35,35	0
57	MG	2A	3154	1/1	0.95	0.19	45,45,45,45	0
57	MG	17	101	1/1	0.95	0.17	23,23,23,23	0
57	MG	2A	3356	1/1	0.95	0.17	32,32,32,32	0
57	MG	2A	3358	1/1	0.95	0.14	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	1A	3368	1/1	0.95	0.10	22,22,22,22	0
57	MG	1A	3315	1/1	0.95	0.12	24,24,24,24	0
57	MG	1A	3316	1/1	0.95	0.36	34,34,34,34	0
57	MG	1A	3052	1/1	0.95	0.21	33,33,33,33	0
57	MG	2A	3363	1/1	0.95	0.06	50,50,50,50	0
57	MG	1a	3125	1/1	0.95	0.20	55,55,55,55	0
57	MG	1A	3811	1/1	0.95	0.12	42,42,42,42	0
57	MG	2A	3164	1/1	0.95	0.19	53,53,53,53	0
57	MG	1A	3812	1/1	0.95	0.12	37,37,37,37	0
57	MG	1g	203	1/1	0.95	0.14	55,55,55,55	0
57	MG	1A	3149	1/1	0.95	0.27	35,35,35,35	0
57	MG	2A	3374	1/1	0.95	0.15	38,38,38,38	0
57	MG	2A	3375	1/1	0.95	0.12	57,57,57,57	0
57	MG	2a	3033	1/1	0.95	0.22	48,48,48,48	0
57	MG	2A	3170	1/1	0.95	0.16	37,37,37,37	0
57	MG	1a	3130	1/1	0.95	0.13	47,47,47,47	0
57	MG	1B	205	1/1	0.95	0.10	37,37,37,37	0
57	MG	1A	3150	1/1	0.95	0.68	38,38,38,38	0
57	MG	2a	3040	1/1	0.95	0.18	56,56,56,56	0
57	MG	1A	3151	1/1	0.95	0.12	24,24,24,24	0
57	MG	2A	3176	1/1	0.95	0.16	43,43,43,43	0
57	MG	1A	3154	1/1	0.95	0.24	19,19,19,19	0
57	MG	1B	210	1/1	0.95	0.22	46,46,46,46	0
57	MG	1a	3008	1/1	0.95	0.27	46,46,46,46	0
57	MG	1a	3009	1/1	0.95	0.17	51,51,51,51	0
57	MG	2A	3184	1/1	0.95	0.10	51,51,51,51	0
57	MG	2A	3612	1/1	0.95	0.20	31,31,31,31	0
57	MG	1A	3922	1/1	0.95	0.14	30,30,30,30	0
57	MG	1a	3145	1/1	0.95	0.13	55,55,55,55	0
57	MG	2A	3394	1/1	0.95	0.12	45,45,45,45	0
57	MG	1A	3699	1/1	0.95	0.15	44,44,44,44	0
57	MG	2A	3188	1/1	0.95	0.20	48,48,48,48	0
57	MG	1A	3381	1/1	0.95	0.11	45,45,45,45	0
57	MG	1A	3823	1/1	0.95	0.17	15,15,15,15	0
57	MG	1A	3324	1/1	0.95	0.16	34,34,34,34	0
57	MG	1A	3384	1/1	0.95	0.19	33,33,33,33	0
57	MG	2A	3401	1/1	0.95	0.14	30,30,30,30	0
57	MG	2A	3402	1/1	0.95	0.14	40,40,40,40	0
57	MG	1a	3151	1/1	0.95	0.21	61,61,61,61	0
57	MG	2A	3006	1/1	0.95	0.13	54,54,54,54	0
57	MG	2A	3008	1/1	0.95	0.13	36,36,36,36	0
57	MG	2A	3197	1/1	0.95	0.20	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	3014	1/1	0.95	0.16	46,46,46,46	0
57	MG	1A	3605	1/1	0.95	0.17	43,43,43,43	0
57	MG	1A	3009	1/1	0.95	0.19	23,23,23,23	0
57	MG	1A	3524	1/1	0.95	0.23	21,21,21,21	0
57	MG	1a	3157	1/1	0.95	0.09	49,49,49,49	0
57	MG	2A	3015	1/1	0.95	0.16	31,31,31,31	0
57	MG	2A	3642	1/1	0.95	0.33	46,46,46,46	0
57	MG	2a	3075	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3645	1/1	0.95	0.12	38,38,38,38	0
57	MG	2A	3205	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3711	1/1	0.95	0.19	28,28,28,28	0
57	MG	1A	3281	1/1	0.95	0.17	48,48,48,48	0
57	MG	1B	225	1/1	0.95	0.15	47,47,47,47	0
57	MG	2A	3651	1/1	0.95	0.14	40,40,40,40	0
57	MG	1A	3282	1/1	0.95	0.31	40,40,40,40	0
57	MG	1A	3016	1/1	0.95	0.16	28,28,28,28	0
57	MG	2a	3085	1/1	0.95	0.07	67,67,67,67	0
57	MG	1A	3453	1/1	0.95	0.10	50,50,50,50	0
57	MG	2A	3427	1/1	0.95	0.11	34,34,34,34	0
57	MG	1A	3331	1/1	0.95	0.28	33,33,33,33	0
57	MG	1A	3033	1/1	0.95	0.27	30,30,30,30	0
57	MG	2a	3091	1/1	0.95	0.14	53,53,53,53	0
57	MG	1D	301	1/1	0.95	0.13	38,38,38,38	0
57	MG	1A	3020	1/1	0.95	0.37	33,33,33,33	0
57	MG	1a	3168	1/1	0.95	0.11	41,41,41,41	0
57	MG	1D	308	1/1	0.95	0.39	44,44,44,44	0
57	MG	2A	3666	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3459	1/1	0.95	0.18	17,17,17,17	0
57	MG	2a	3102	1/1	0.95	0.28	52,52,52,52	0
57	MG	1a	3037	1/1	0.95	0.18	59,59,59,59	0
57	MG	2A	3221	1/1	0.95	0.14	55,55,55,55	0
57	MG	2a	3105	1/1	0.95	0.36	51,51,51,51	0
57	MG	1A	3727	1/1	0.95	0.15	16,16,16,16	0
57	MG	1a	3039	1/1	0.95	0.12	58,58,58,58	0
57	MG	1A	3844	1/1	0.95	0.13	25,25,25,25	0
57	MG	2A	3674	1/1	0.95	0.19	36,36,36,36	0
57	MG	1a	3176	1/1	0.95	0.09	63,63,63,63	0
57	MG	2a	3113	1/1	0.95	0.15	50,50,50,50	0
57	MG	2A	3676	1/1	0.95	0.12	37,37,37,37	0
57	MG	2A	3226	1/1	0.95	0.25	52,52,52,52	0
57	MG	1D	317	1/1	0.95	0.14	38,38,38,38	0
57	MG	1A	3239	1/1	0.95	0.27	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	3542	1/1	0.95	0.09	31,31,31,31	0
57	MG	1A	3461	1/1	0.95	0.18	55,55,55,55	0
57	MG	1a	3183	1/1	0.95	0.13	37,37,37,37	0
57	MG	2A	3684	1/1	0.95	0.20	35,35,35,35	0
57	MG	1A	3084	1/1	0.95	0.32	34,34,34,34	0
57	MG	1A	3106	1/1	0.95	0.18	28,28,28,28	0
57	MG	2A	3055	1/1	0.95	0.24	49,49,49,49	0
57	MG	1A	3955	1/1	0.95	0.13	42,42,42,42	0
57	MG	2a	3128	1/1	0.95	0.14	53,53,53,53	0
57	MG	1F	301	1/1	0.95	0.12	21,21,21,21	0
57	MG	1A	3547	1/1	0.95	0.20	33,33,33,33	0
57	MG	1A	3958	1/1	0.95	0.11	37,37,37,37	0
57	MG	2A	3062	1/1	0.95	0.36	40,40,40,40	0
57	MG	2A	3247	1/1	0.95	0.19	28,28,28,28	0
57	MG	1A	3169	1/1	0.95	0.24	21,21,21,21	0
57	MG	2A	3464	1/1	0.95	0.18	43,43,43,43	0
57	MG	1A	3635	1/1	0.95	0.11	28,28,28,28	0
57	MG	2A	3250	1/1	0.95	0.12	33,33,33,33	0
57	MG	1a	3055	1/1	0.95	0.17	36,36,36,36	0
57	MG	1F	313	1/1	0.95	0.59	37,37,37,37	0
57	MG	1F	314	1/1	0.95	0.14	33,33,33,33	0
57	MG	2A	3068	1/1	0.95	0.16	47,47,47,47	0
57	MG	1A	3134	1/1	0.95	0.13	32,32,32,32	0
57	MG	2A	3475	1/1	0.95	0.15	48,48,48,48	0
57	MG	1a	3059	1/1	0.95	0.17	50,50,50,50	0
57	MG	2A	3073	1/1	0.95	0.13	56,56,56,56	0
57	MG	1A	3407	1/1	0.95	0.11	28,28,28,28	0
57	MG	2a	3153	1/1	0.95	0.08	61,61,61,61	0
57	MG	1A	3748	1/1	0.95	0.14	48,48,48,48	0
57	MG	1A	3299	1/1	0.95	0.26	27,27,27,27	0
57	MG	1a	3202	1/1	0.95	0.06	57,57,57,57	0
57	MG	1A	3409	1/1	0.95	0.13	18,18,18,18	0
57	MG	2A	3485	1/1	0.95	0.10	54,54,54,54	0
57	MG	2a	3163	1/1	0.95	0.08	48,48,48,48	0
57	MG	2a	3164	1/1	0.95	0.17	61,61,61,61	0
57	MG	1A	3108	1/1	0.95	0.16	33,33,33,33	0
57	MG	1A	3556	1/1	0.95	0.13	47,47,47,47	0
57	MG	2A	3267	1/1	0.95	0.39	48,48,48,48	0
57	MG	1a	3206	1/1	0.95	0.09	51,51,51,51	0
57	MG	2a	3172	1/1	0.95	0.06	50,50,50,50	0
57	MG	2A	3720	1/1	0.95	0.21	52,52,52,52	0
57	MG	2A	3722	1/1	0.95	0.20	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	3723	1/1	0.95	0.11	58,58,58,58	0
57	MG	2a	3179	1/1	0.95	0.18	56,56,56,56	0
57	MG	1N	203	1/1	0.95	0.13	45,45,45,45	0
57	MG	2A	3725	1/1	0.95	0.11	64,64,64,64	0
57	MG	1A	3301	1/1	0.95	0.15	53,53,53,53	0
57	MG	2B	201	1/1	0.95	0.09	59,59,59,59	0
57	MG	2A	3085	1/1	0.95	0.29	40,40,40,40	0
57	MG	1A	3175	1/1	0.95	0.14	19,19,19,19	0
57	MG	1a	3072	1/1	0.95	0.24	46,46,46,46	0
57	MG	1A	3561	1/1	0.95	0.13	31,31,31,31	0
57	MG	1a	3214	1/1	0.95	0.09	59,59,59,59	0
57	MG	1P	201	1/1	0.95	0.24	28,28,28,28	0
57	MG	2B	210	1/1	0.95	0.27	52,52,52,52	0
57	MG	1A	3757	1/1	0.95	0.10	56,56,56,56	0
57	MG	2B	213	1/1	0.95	0.13	54,54,54,54	0
57	MG	2A	3500	1/1	0.95	0.19	53,53,53,53	0
57	MG	1a	3218	1/1	0.95	0.12	60,60,60,60	0
57	MG	1a	3219	1/1	0.95	0.07	56,56,56,56	0
57	MG	1A	3072	1/1	0.95	0.16	24,24,24,24	0
57	MG	1R	202	1/1	0.95	0.17	37,37,37,37	0
57	MG	1A	3414	1/1	0.95	0.18	26,26,26,26	0
57	MG	1a	3079	1/1	0.95	0.60	53,53,53,53	0
57	MG	1A	3871	1/1	0.95	0.19	34,34,34,34	0
57	MG	2A	3288	1/1	0.95	0.11	37,37,37,37	0
57	MG	2A	3510	1/1	0.95	0.35	54,54,54,54	0
57	MG	2A	3511	1/1	0.95	0.08	61,61,61,61	0
61	ZN	2n	102	1/1	0.95	0.10	73,73,73,73	0
57	MG	2A	3059	1/1	0.96	0.11	41,41,41,41	0
57	MG	2A	3263	1/1	0.96	0.20	20,20,20,20	0
57	MG	2A	3060	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	4002	1/1	0.96	0.21	42,42,42,42	0
57	MG	1A	3606	1/1	0.96	0.19	24,24,24,24	0
57	MG	1A	4006	1/1	0.96	0.13	38,38,38,38	0
57	MG	1A	3607	1/1	0.96	0.20	24,24,24,24	0
57	MG	1A	3515	1/1	0.96	0.07	38,38,38,38	0
57	MG	1A	3736	1/1	0.96	0.15	35,35,35,35	0
57	MG	1A	3100	1/1	0.96	0.28	27,27,27,27	0
57	MG	1A	3206	1/1	0.96	0.22	28,28,28,28	0
57	MG	1A	3613	1/1	0.96	0.35	48,48,48,48	0
57	MG	1A	3877	1/1	0.96	0.14	38,38,38,38	0
57	MG	1a	3013	1/1	0.96	0.13	49,49,49,49	0
57	MG	2F	304	1/1	0.96	0.25	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	1A	3083	1/1	0.96	0.44	29,29,29,29	0
57	MG	1A	3520	1/1	0.96	0.22	20,20,20,20	0
57	MG	1A	3444	1/1	0.96	0.26	26,26,26,26	0
57	MG	1A	3253	1/1	0.96	0.17	47,47,47,47	0
57	MG	2A	3517	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	4019	1/1	0.96	0.14	43,43,43,43	0
57	MG	2A	3519	1/1	0.96	0.17	48,48,48,48	0
57	MG	1a	3020	1/1	0.96	0.19	43,43,43,43	0
57	MG	1A	3210	1/1	0.96	0.23	26,26,26,26	0
57	MG	1A	3750	1/1	0.96	0.14	33,33,33,33	0
57	MG	1A	3378	1/1	0.96	0.14	26,26,26,26	0
57	MG	1A	3314	1/1	0.96	0.11	32,32,32,32	0
57	MG	1A	3527	1/1	0.96	0.13	17,17,17,17	0
57	MG	1a	3026	1/1	0.96	0.22	53,53,53,53	0
57	MG	1A	3255	1/1	0.96	0.15	66,66,66,66	0
57	MG	1A	3624	1/1	0.96	0.16	39,39,39,39	0
57	MG	1A	3257	1/1	0.96	0.17	35,35,35,35	0
57	MG	2A	3090	1/1	0.96	0.30	48,48,48,48	0
57	MG	2A	3091	1/1	0.96	0.15	44,44,44,44	0
57	MG	1B	208	1/1	0.96	0.27	48,48,48,48	0
57	MG	1A	3530	1/1	0.96	0.25	24,24,24,24	0
57	MG	1A	3628	1/1	0.96	0.14	16,16,16,16	0
57	MG	2A	3537	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3039	1/1	0.96	0.22	29,29,29,29	0
57	MG	1B	212	1/1	0.96	0.06	45,45,45,45	0
57	MG	1A	3017	1/1	0.96	0.21	33,33,33,33	0
57	MG	1A	3762	1/1	0.96	0.10	30,30,30,30	0
57	MG	23	101	1/1	0.96	0.28	42,42,42,42	0
57	MG	1A	3763	1/1	0.96	0.11	46,46,46,46	0
57	MG	1A	3764	1/1	0.96	0.17	46,46,46,46	0
57	MG	1A	3127	1/1	0.96	0.41	42,42,42,42	0
57	MG	1A	3320	1/1	0.96	0.17	22,22,22,22	0
57	MG	1A	3767	1/1	0.96	0.12	31,31,31,31	0
57	MG	1a	3043	1/1	0.96	0.12	41,41,41,41	0
57	MG	2A	3106	1/1	0.96	0.17	31,31,31,31	0
57	MG	1A	3770	1/1	0.96	0.11	28,28,28,28	0
57	MG	2A	3319	1/1	0.96	0.15	49,49,49,49	0
57	MG	1A	3771	1/1	0.96	0.21	12,12,12,12	0
57	MG	1a	3215	1/1	0.96	0.13	44,44,44,44	0
57	MG	2A	3322	1/1	0.96	0.18	45,45,45,45	0
57	MG	1A	3772	1/1	0.96	0.17	37,37,37,37	0
57	MG	1A	3539	1/1	0.96	0.16	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3556	1/1	0.96	0.17	34,34,34,34	0
57	MG	2A	3326	1/1	0.96	0.17	42,42,42,42	0
57	MG	1A	3776	1/1	0.96	0.19	33,33,33,33	0
57	MG	1A	3457	1/1	0.96	0.27	40,40,40,40	0
57	MG	2A	3562	1/1	0.96	0.08	42,42,42,42	0
57	MG	1A	3541	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3263	1/1	0.96	0.28	37,37,37,37	0
57	MG	1A	3266	1/1	0.96	0.13	39,39,39,39	0
57	MG	1a	3224	1/1	0.96	0.12	68,68,68,68	0
57	MG	1A	3217	1/1	0.96	0.12	43,43,43,43	0
57	MG	1a	3226	1/1	0.96	0.14	49,49,49,49	0
57	MG	2A	3124	1/1	0.96	0.17	33,33,33,33	0
57	MG	2A	3338	1/1	0.96	0.18	35,35,35,35	0
57	MG	2A	3573	1/1	0.96	0.13	43,43,43,43	0
57	MG	1A	3268	1/1	0.96	0.09	37,37,37,37	0
57	MG	1A	3920	1/1	0.96	0.09	41,41,41,41	0
57	MG	1D	307	1/1	0.96	0.17	31,31,31,31	0
57	MG	1A	3218	1/1	0.96	0.13	22,22,22,22	0
57	MG	2A	3579	1/1	0.96	0.13	41,41,41,41	0
57	MG	1A	3647	1/1	0.96	0.12	58,58,58,58	0
57	MG	1A	3129	1/1	0.96	0.24	32,32,32,32	0
57	MG	2A	3346	1/1	0.96	0.21	42,42,42,42	0
57	MG	1A	3649	1/1	0.96	0.18	48,48,48,48	0
57	MG	2A	3584	1/1	0.96	0.21	47,47,47,47	0
57	MG	1A	3042	1/1	0.96	0.20	16,16,16,16	0
57	MG	2A	3586	1/1	0.96	0.18	48,48,48,48	0
57	MG	1A	3651	1/1	0.96	0.19	34,34,34,34	0
57	MG	1A	3223	1/1	0.96	0.23	27,27,27,27	0
57	MG	1a	3066	1/1	0.96	0.12	45,45,45,45	0
57	MG	1A	3928	1/1	0.96	0.07	36,36,36,36	0
57	MG	1a	3068	1/1	0.96	0.12	53,53,53,53	0
57	MG	1A	3132	1/1	0.96	0.18	23,23,23,23	0
57	MG	2A	3357	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	3402	1/1	0.96	0.14	11,11,11,11	0
57	MG	1A	3225	1/1	0.96	0.20	31,31,31,31	0
57	MG	1A	3469	1/1	0.96	0.07	33,33,33,33	0
57	MG	2A	3145	1/1	0.96	0.25	29,29,29,29	0
57	MG	1A	3405	1/1	0.96	0.14	40,40,40,40	0
57	MG	1A	3558	1/1	0.96	0.14	31,31,31,31	0
57	MG	1A	3935	1/1	0.96	0.11	42,42,42,42	0
57	MG	1a	3250	1/1	0.96	0.17	42,42,42,42	0
57	MG	2a	3052	1/1	0.96	0.19	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	3151	1/1	0.96	0.13	41,41,41,41	0
57	MG	1F	308	1/1	0.96	0.19	26,26,26,26	0
57	MG	2A	3370	1/1	0.96	0.15	44,44,44,44	0
57	MG	2A	3610	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3471	1/1	0.96	0.19	37,37,37,37	0
57	MG	2A	3372	1/1	0.96	0.23	43,43,43,43	0
57	MG	1F	311	1/1	0.96	0.29	35,35,35,35	0
57	MG	2A	3155	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3937	1/1	0.96	0.18	29,29,29,29	0
57	MG	2A	3376	1/1	0.96	0.24	49,49,49,49	0
57	MG	1A	3337	1/1	0.96	0.20	26,26,26,26	0
57	MG	1A	3562	1/1	0.96	0.18	56,56,56,56	0
57	MG	1F	316	1/1	0.96	0.25	35,35,35,35	0
57	MG	1a	3083	1/1	0.96	0.21	52,52,52,52	0
57	MG	1A	3806	1/1	0.96	0.15	22,22,22,22	0
57	MG	2A	3162	1/1	0.96	0.15	32,32,32,32	0
57	MG	1A	3943	1/1	0.96	0.24	18,18,18,18	0
57	MG	1A	3808	1/1	0.96	0.10	32,32,32,32	0
57	MG	2A	3628	1/1	0.96	0.13	47,47,47,47	0
57	MG	2A	3165	1/1	0.96	0.07	67,67,67,67	0
57	MG	2A	3166	1/1	0.96	0.10	59,59,59,59	0
57	MG	2a	3077	1/1	0.96	0.15	54,54,54,54	0
57	MG	2A	3389	1/1	0.96	0.17	53,53,53,53	0
57	MG	1A	3563	1/1	0.96	0.17	34,34,34,34	0
57	MG	1a	3088	1/1	0.96	0.18	46,46,46,46	0
57	MG	1A	3810	1/1	0.96	0.13	24,24,24,24	0
57	MG	1A	3226	1/1	0.96	0.14	38,38,38,38	0
57	MG	1H	201	1/1	0.96	0.17	42,42,42,42	0
57	MG	1H	202	1/1	0.96	0.13	40,40,40,40	0
57	MG	2A	3641	1/1	0.96	0.10	60,60,60,60	0
57	MG	1A	3474	1/1	0.96	0.16	31,31,31,31	0
57	MG	2A	3644	1/1	0.96	0.20	50,50,50,50	0
57	MG	2a	3088	1/1	0.96	0.18	50,50,50,50	0
57	MG	1A	3340	1/1	0.96	0.12	41,41,41,41	0
57	MG	1A	3477	1/1	0.96	0.15	22,22,22,22	0
57	MG	1A	3088	1/1	0.96	0.12	25,25,25,25	0
57	MG	2A	3648	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3342	1/1	0.96	0.16	25,25,25,25	0
57	MG	2A	3181	1/1	0.96	0.20	45,45,45,45	0
57	MG	2A	3403	1/1	0.96	0.20	41,41,41,41	0
57	MG	2a	3097	1/1	0.96	0.21	51,51,51,51	0
57	MG	2a	3098	1/1	0.96	0.31	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	3652	1/1	0.96	0.18	31,31,31,31	0
57	MG	1P	202	1/1	0.96	0.19	26,26,26,26	0
57	MG	1A	3480	1/1	0.96	0.13	35,35,35,35	0
57	MG	2A	3656	1/1	0.96	0.15	24,24,24,24	0
57	MG	1P	204	1/1	0.96	0.10	59,59,59,59	0
57	MG	1Q	201	1/1	0.96	0.24	27,27,27,27	0
57	MG	1Q	202	1/1	0.96	0.16	33,33,33,33	0
57	MG	1h	201	1/1	0.96	0.23	42,42,42,42	0
57	MG	1A	3954	1/1	0.96	0.12	49,49,49,49	0
57	MG	2a	3109	1/1	0.96	0.24	50,50,50,50	0
57	MG	2A	3662	1/1	0.96	0.10	37,37,37,37	0
57	MG	1A	3228	1/1	0.96	0.32	24,24,24,24	0
57	MG	1A	3956	1/1	0.96	0.10	32,32,32,32	0
57	MG	1A	3573	1/1	0.96	0.20	21,21,21,21	0
57	MG	1A	3482	1/1	0.96	0.17	27,27,27,27	0
57	MG	2A	3667	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3089	1/1	0.96	0.19	21,21,21,21	0
57	MG	1A	3961	1/1	0.96	0.14	40,40,40,40	0
57	MG	1T	206	1/1	0.96	0.15	47,47,47,47	0
57	MG	1n	103	1/1	0.96	0.15	60,60,60,60	0
57	MG	1o	101	1/1	0.96	0.16	49,49,49,49	0
57	MG	2A	3425	1/1	0.96	0.14	41,41,41,41	0
57	MG	1A	3576	1/1	0.96	0.22	32,32,32,32	0
57	MG	1t	201	1/1	0.96	0.18	48,48,48,48	0
57	MG	2A	3201	1/1	0.96	0.31	45,45,45,45	0
57	MG	1A	3231	1/1	0.96	0.27	35,35,35,35	0
57	MG	1A	3967	1/1	0.96	0.11	19,19,19,19	0
57	MG	1V	203	1/1	0.96	0.13	31,31,31,31	0
57	MG	1A	3136	1/1	0.96	0.22	36,36,36,36	0
57	MG	2A	3206	1/1	0.96	0.14	39,39,39,39	0
57	MG	1a	3120	1/1	0.96	0.28	50,50,50,50	0
57	MG	2a	3136	1/1	0.96	0.07	43,43,43,43	0
57	MG	2A	3435	1/1	0.96	0.15	42,42,42,42	0
57	MG	1A	3043	1/1	0.96	0.19	23,23,23,23	0
57	MG	1A	3691	1/1	0.96	0.18	54,54,54,54	0
57	MG	2A	3004	1/1	0.96	0.14	39,39,39,39	0
57	MG	1A	3417	1/1	0.96	0.23	14,14,14,14	0
57	MG	1A	3111	1/1	0.96	0.32	36,36,36,36	0
57	MG	1A	3695	1/1	0.96	0.10	35,35,35,35	0
57	MG	2A	3443	1/1	0.96	0.22	48,48,48,48	0
57	MG	2a	3147	1/1	0.96	0.22	67,67,67,67	0
57	MG	1A	3287	1/1	0.96	0.15	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3698	1/1	0.96	0.10	21,21,21,21	0
57	MG	1A	3021	1/1	0.96	0.20	30,30,30,30	0
57	MG	2A	3449	1/1	0.96	0.08	44,44,44,44	0
57	MG	1A	3237	1/1	0.96	0.27	47,47,47,47	0
57	MG	1A	3294	1/1	0.96	0.20	36,36,36,36	0
57	MG	2a	3154	1/1	0.96	0.16	32,32,32,32	0
57	MG	1A	3238	1/1	0.96	0.35	29,29,29,29	0
57	MG	1A	3980	1/1	0.96	0.15	32,32,32,32	0
57	MG	1a	3135	1/1	0.96	0.13	29,29,29,29	0
57	MG	2A	3018	1/1	0.96	0.28	34,34,34,34	0
57	MG	1A	3047	1/1	0.96	0.18	18,18,18,18	0
57	MG	1A	3426	1/1	0.96	0.19	23,23,23,23	0
57	MG	1a	3140	1/1	0.96	0.16	49,49,49,49	0
57	MG	2a	3165	1/1	0.96	0.10	58,58,58,58	0
57	MG	1A	3068	1/1	0.96	0.18	38,38,38,38	0
57	MG	2A	3709	1/1	0.96	0.21	42,42,42,42	0
57	MG	1A	3501	1/1	0.96	0.15	36,36,36,36	0
57	MG	11	101	1/1	0.96	0.38	42,42,42,42	0
57	MG	2a	3171	1/1	0.96	0.10	47,47,47,47	0
57	MG	2A	3028	1/1	0.96	0.08	28,28,28,28	0
57	MG	1A	3985	1/1	0.96	0.26	35,35,35,35	0
57	MG	2a	3175	1/1	0.96	0.11	42,42,42,42	0
57	MG	1A	3241	1/1	0.96	0.15	26,26,26,26	0
57	MG	1A	3362	1/1	0.96	0.13	10,10,10,10	0
57	MG	2A	3467	1/1	0.96	0.30	60,60,60,60	0
57	MG	2A	3034	1/1	0.96	0.15	45,45,45,45	0
57	MG	13	101	1/1	0.96	0.15	28,28,28,28	0
57	MG	1A	3713	1/1	0.96	0.28	29,29,29,29	0
57	MG	1A	3714	1/1	0.96	0.15	36,36,36,36	0
57	MG	15	102	1/1	0.96	0.14	27,27,27,27	0
57	MG	2A	3243	1/1	0.96	0.43	49,49,49,49	0
57	MG	15	106	1/1	0.96	0.15	30,30,30,30	0
57	MG	2a	3189	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3245	1/1	0.96	0.30	43,43,43,43	0
57	MG	1A	3505	1/1	0.96	0.13	44,44,44,44	0
57	MG	1A	3058	1/1	0.96	0.18	21,21,21,21	0
57	MG	2B	202	1/1	0.96	0.07	69,69,69,69	0
57	MG	2l	202	1/1	0.96	0.16	52,52,52,52	0
57	MG	2p	101	1/1	0.96	0.14	49,49,49,49	0
57	MG	2A	3044	1/1	0.96	0.15	44,44,44,44	0
57	MG	1A	3029	1/1	0.96	0.20	36,36,36,36	0
58	CLM	1A	4022	20/20	0.96	0.24	18,30,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3246	1/1	0.96	0.22	24,24,24,24	0
57	MG	17	102	1/1	0.96	0.21	26,26,26,26	0
57	MG	1A	3248	1/1	0.96	0.18	43,43,43,43	0
57	MG	2A	3051	1/1	0.96	0.15	34,34,34,34	0
57	MG	1A	3722	1/1	0.96	0.14	35,35,35,35	0
57	MG	1A	3861	1/1	0.96	0.07	32,32,32,32	0
57	MG	1A	3512	1/1	0.96	0.15	42,42,42,42	0
57	MG	18	102	1/1	0.96	0.18	32,32,32,32	0
57	MG	1A	3603	1/1	0.96	0.26	20,20,20,20	0
57	MG	1A	3369	1/1	0.96	0.13	23,23,23,23	0
57	MG	1A	3370	1/1	0.96	0.17	38,38,38,38	0
61	ZN	26	501	1/1	0.96	0.16	56,56,56,56	0
61	ZN	29	102	1/1	0.96	0.13	63,63,63,63	0
57	MG	2D	301	1/1	0.96	0.18	25,25,25,25	0
57	MG	1A	3687	1/1	0.97	0.17	36,36,36,36	0
57	MG	2A	3571	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3006	1/1	0.97	0.15	16,16,16,16	0
57	MG	1A	3523	1/1	0.97	0.14	23,23,23,23	0
57	MG	1A	3332	1/1	0.97	0.19	23,23,23,23	0
57	MG	1A	3393	1/1	0.97	0.18	12,12,12,12	0
57	MG	1A	3333	1/1	0.97	0.19	18,18,18,18	0
57	MG	1A	3601	1/1	0.97	0.13	45,45,45,45	0
57	MG	1A	3804	1/1	0.97	0.15	15,15,15,15	0
57	MG	2A	3378	1/1	0.97	0.17	22,22,22,22	0
57	MG	1B	221	1/1	0.97	0.12	28,28,28,28	0
57	MG	1A	3805	1/1	0.97	0.17	33,33,33,33	0
57	MG	25	104	1/1	0.97	0.15	40,40,40,40	0
57	MG	1A	3198	1/1	0.97	0.15	42,42,42,42	0
57	MG	1A	3696	1/1	0.97	0.48	40,40,40,40	0
57	MG	2A	3022	1/1	0.97	0.50	44,44,44,44	0
57	MG	1A	3336	1/1	0.97	0.17	35,35,35,35	0
57	MG	1A	3005	1/1	0.97	0.15	18,18,18,18	0
57	MG	1A	3167	1/1	0.97	0.08	21,21,21,21	0
57	MG	1A	3041	1/1	0.97	0.29	46,46,46,46	0
57	MG	1A	3701	1/1	0.97	0.09	31,31,31,31	0
57	MG	2A	3593	1/1	0.97	0.12	30,30,30,30	0
57	MG	1A	3532	1/1	0.97	0.12	46,46,46,46	0
57	MG	2A	3029	1/1	0.97	0.20	31,31,31,31	0
57	MG	2A	3596	1/1	0.97	0.22	56,56,56,56	0
57	MG	1A	3288	1/1	0.97	0.18	16,16,16,16	0
57	MG	1D	302	1/1	0.97	0.22	25,25,25,25	0
57	MG	1D	303	1/1	0.97	0.18	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	1D	304	1/1	0.97	0.09	40,40,40,40	0
57	MG	1D	305	1/1	0.97	0.25	28,28,28,28	0
57	MG	1A	3816	1/1	0.97	0.14	29,29,29,29	0
57	MG	2a	3012	1/1	0.97	0.14	45,45,45,45	0
57	MG	1A	3404	1/1	0.97	0.15	16,16,16,16	0
57	MG	1A	3938	1/1	0.97	0.16	32,32,32,32	0
57	MG	1D	311	1/1	0.97	0.21	28,28,28,28	0
57	MG	2A	3041	1/1	0.97	0.11	21,21,21,21	0
57	MG	1a	3031	1/1	0.97	0.11	33,33,33,33	0
57	MG	1A	3820	1/1	0.97	0.13	11,11,11,11	0
57	MG	1A	3290	1/1	0.97	0.17	38,38,38,38	0
57	MG	1a	3180	1/1	0.97	0.17	60,60,60,60	0
57	MG	2a	3021	1/1	0.97	0.11	58,58,58,58	0
57	MG	1A	3537	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3538	1/1	0.97	0.16	17,17,17,17	0
57	MG	2A	3409	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3023	1/1	0.97	0.20	19,19,19,19	0
57	MG	2A	3050	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	3113	1/1	0.97	0.25	31,31,31,31	0
57	MG	1A	3172	1/1	0.97	0.17	26,26,26,26	0
57	MG	2A	3620	1/1	0.97	0.09	61,61,61,61	0
57	MG	2A	3414	1/1	0.97	0.09	49,49,49,49	0
57	MG	2a	3032	1/1	0.97	0.13	55,55,55,55	0
57	MG	1E	306	1/1	0.97	0.16	15,15,15,15	0
57	MG	1A	3207	1/1	0.97	0.44	30,30,30,30	0
57	MG	1A	3036	1/1	0.97	0.10	23,23,23,23	0
57	MG	2A	3625	1/1	0.97	0.14	46,46,46,46	0
57	MG	2a	3038	1/1	0.97	0.09	74,74,74,74	0
57	MG	1A	3298	1/1	0.97	0.16	31,31,31,31	0
57	MG	1A	3174	1/1	0.97	0.32	39,39,39,39	0
57	MG	2A	3420	1/1	0.97	0.14	42,42,42,42	0
57	MG	2A	3227	1/1	0.97	0.26	38,38,38,38	0
57	MG	2A	3630	1/1	0.97	0.15	37,37,37,37	0
57	MG	1F	302	1/1	0.97	0.25	25,25,25,25	0
57	MG	1A	3115	1/1	0.97	0.21	16,16,16,16	0
57	MG	1A	3719	1/1	0.97	0.09	35,35,35,35	0
57	MG	1F	306	1/1	0.97	0.17	23,23,23,23	0
57	MG	1a	3195	1/1	0.97	0.12	52,52,52,52	0
57	MG	1a	3196	1/1	0.97	0.18	40,40,40,40	0
57	MG	2A	3638	1/1	0.97	0.14	29,29,29,29	0
57	MG	1A	3352	1/1	0.97	0.10	53,53,53,53	0
57	MG	1A	3721	1/1	0.97	0.11	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3835	1/1	0.97	0.18	29,29,29,29	0
57	MG	1a	3051	1/1	0.97	0.14	52,52,52,52	0
57	MG	2a	3055	1/1	0.97	0.04	53,53,53,53	0
57	MG	2A	3643	1/1	0.97	0.13	31,31,31,31	0
57	MG	1A	3837	1/1	0.97	0.20	46,46,46,46	0
57	MG	1F	312	1/1	0.97	0.20	24,24,24,24	0
57	MG	1A	3625	1/1	0.97	0.13	45,45,45,45	0
57	MG	1A	3177	1/1	0.97	0.61	35,35,35,35	0
57	MG	1A	3354	1/1	0.97	0.14	15,15,15,15	0
57	MG	1A	3960	1/1	0.97	0.11	46,46,46,46	0
57	MG	1a	3207	1/1	0.97	0.16	63,63,63,63	0
57	MG	1A	3116	1/1	0.97	0.20	26,26,26,26	0
57	MG	1A	3963	1/1	0.97	0.14	25,25,25,25	0
57	MG	1A	3964	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3728	1/1	0.97	0.15	27,27,27,27	0
57	MG	2A	3447	1/1	0.97	0.11	23,23,23,23	0
57	MG	1a	3062	1/1	0.97	0.26	47,47,47,47	0
57	MG	2A	3082	1/1	0.97	0.15	43,43,43,43	0
57	MG	1A	3629	1/1	0.97	0.07	49,49,49,49	0
57	MG	1A	3256	1/1	0.97	0.09	35,35,35,35	0
57	MG	1A	3357	1/1	0.97	0.18	20,20,20,20	0
57	MG	2A	3258	1/1	0.97	0.22	41,41,41,41	0
57	MG	1A	3633	1/1	0.97	0.26	35,35,35,35	0
57	MG	1N	201	1/1	0.97	0.17	31,31,31,31	0
57	MG	1A	3735	1/1	0.97	0.20	15,15,15,15	0
57	MG	2A	3457	1/1	0.97	0.10	50,50,50,50	0
57	MG	1A	3097	1/1	0.97	0.26	21,21,21,21	0
57	MG	1A	3119	1/1	0.97	0.21	45,45,45,45	0
57	MG	1A	3738	1/1	0.97	0.11	32,32,32,32	0
57	MG	2A	3092	1/1	0.97	0.26	41,41,41,41	0
57	MG	1a	3223	1/1	0.97	0.07	56,56,56,56	0
57	MG	1A	3144	1/1	0.97	0.12	64,64,64,64	0
57	MG	1A	3559	1/1	0.97	0.10	37,37,37,37	0
57	MG	1A	3308	1/1	0.97	0.13	30,30,30,30	0
57	MG	1A	3488	1/1	0.97	0.12	26,26,26,26	0
57	MG	1A	3746	1/1	0.97	0.18	14,14,14,14	0
57	MG	1A	3310	1/1	0.97	0.24	30,30,30,30	0
57	MG	2a	3092	1/1	0.97	0.16	47,47,47,47	0
57	MG	2A	3469	1/1	0.97	0.14	24,24,24,24	0
57	MG	1Q	203	1/1	0.97	0.23	31,31,31,31	0
57	MG	1A	3427	1/1	0.97	0.18	22,22,22,22	0
57	MG	1A	3364	1/1	0.97	0.17	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3429	1/1	0.97	0.12	29,29,29,29	0
57	MG	1A	3260	1/1	0.97	0.17	25,25,25,25	0
57	MG	1A	3147	1/1	0.97	0.21	22,22,22,22	0
57	MG	2a	3100	1/1	0.97	0.32	37,37,37,37	0
57	MG	1T	203	1/1	0.97	0.17	39,39,39,39	0
57	MG	2A	3281	1/1	0.97	0.26	41,41,41,41	0
57	MG	1A	3497	1/1	0.97	0.14	40,40,40,40	0
57	MG	1A	3222	1/1	0.97	0.33	33,33,33,33	0
57	MG	2A	3692	1/1	0.97	0.17	36,36,36,36	0
57	MG	2A	3481	1/1	0.97	0.11	50,50,50,50	0
57	MG	1A	3264	1/1	0.97	0.25	29,29,29,29	0
57	MG	1a	3242	1/1	0.97	0.20	52,52,52,52	0
57	MG	1U	201	1/1	0.97	0.21	28,28,28,28	0
57	MG	1U	202	1/1	0.97	0.15	30,30,30,30	0
57	MG	1U	204	1/1	0.97	0.27	24,24,24,24	0
57	MG	1a	3091	1/1	0.97	0.21	39,39,39,39	0
57	MG	2a	3114	1/1	0.97	0.18	45,45,45,45	0
57	MG	1A	3183	1/1	0.97	0.19	63,63,63,63	0
57	MG	1A	3653	1/1	0.97	0.31	42,42,42,42	0
57	MG	1A	3872	1/1	0.97	0.14	29,29,29,29	0
57	MG	2A	3294	1/1	0.97	0.06	56,56,56,56	0
57	MG	2A	3120	1/1	0.97	0.60	47,47,47,47	0
57	MG	1V	202	1/1	0.97	0.28	20,20,20,20	0
57	MG	2A	3122	1/1	0.97	0.13	41,41,41,41	0
57	MG	1A	3099	1/1	0.97	0.22	25,25,25,25	0
57	MG	1A	3656	1/1	0.97	0.18	17,17,17,17	0
57	MG	2A	3125	1/1	0.97	0.20	42,42,42,42	0
57	MG	2A	3303	1/1	0.97	0.16	52,52,52,52	0
57	MG	1A	3657	1/1	0.97	0.10	45,45,45,45	0
57	MG	2A	3306	1/1	0.97	0.12	36,36,36,36	0
57	MG	1V	206	1/1	0.97	0.22	34,34,34,34	0
57	MG	1a	3257	1/1	0.97	0.14	25,25,25,25	0
57	MG	2a	3131	1/1	0.97	0.17	54,54,54,54	0
57	MG	2A	3309	1/1	0.97	0.17	36,36,36,36	0
57	MG	1A	3761	1/1	0.97	0.21	52,52,52,52	0
57	MG	2a	3134	1/1	0.97	0.17	60,60,60,60	0
57	MG	1A	3658	1/1	0.97	0.18	14,14,14,14	0
57	MG	1A	3121	1/1	0.97	0.12	31,31,31,31	0
57	MG	1a	3103	1/1	0.97	0.24	44,44,44,44	0
57	MG	1A	3503	1/1	0.97	0.19	20,20,20,20	0
57	MG	2A	3721	1/1	0.97	0.17	39,39,39,39	0
57	MG	2A	3512	1/1	0.97	0.10	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	3063	1/1	0.97	0.09	31,31,31,31	0
57	MG	2A	3135	1/1	0.97	0.19	23,23,23,23	0
57	MG	1A	3375	1/1	0.97	0.13	29,29,29,29	0
57	MG	1A	3885	1/1	0.97	0.21	29,29,29,29	0
57	MG	2a	3146	1/1	0.97	0.06	56,56,56,56	0
57	MG	1a	3267	1/1	0.97	0.06	52,52,52,52	0
57	MG	2A	3139	1/1	0.97	0.11	33,33,33,33	0
57	MG	1a	3108	1/1	0.97	0.13	37,37,37,37	0
57	MG	2A	3323	1/1	0.97	0.12	34,34,34,34	0
57	MG	2B	205	1/1	0.97	0.15	50,50,50,50	0
57	MG	1A	3578	1/1	0.97	0.41	36,36,36,36	0
57	MG	1A	3887	1/1	0.97	0.08	34,34,34,34	0
57	MG	2A	3524	1/1	0.97	0.19	50,50,50,50	0
57	MG	2a	3155	1/1	0.97	0.11	57,57,57,57	0
57	MG	2a	3156	1/1	0.97	0.14	52,52,52,52	0
57	MG	1A	3769	1/1	0.97	0.12	32,32,32,32	0
57	MG	2A	3327	1/1	0.97	0.17	38,38,38,38	0
57	MG	2B	211	1/1	0.97	0.14	50,50,50,50	0
57	MG	1A	3086	1/1	0.97	0.12	22,22,22,22	0
57	MG	2a	3161	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3508	1/1	0.97	0.21	15,15,15,15	0
57	MG	1A	3666	1/1	0.97	0.23	30,30,30,30	0
57	MG	1A	3773	1/1	0.97	0.18	21,21,21,21	0
57	MG	1A	3668	1/1	0.97	0.09	33,33,33,33	0
57	MG	2A	3333	1/1	0.97	0.11	44,44,44,44	0
57	MG	1a	3117	1/1	0.97	0.24	36,36,36,36	0
57	MG	2A	3150	1/1	0.97	0.19	52,52,52,52	0
57	MG	1A	3153	1/1	0.97	0.15	22,22,22,22	0
57	MG	2a	3170	1/1	0.97	0.11	49,49,49,49	0
57	MG	1A	3582	1/1	0.97	0.15	38,38,38,38	0
57	MG	1A	3076	1/1	0.97	0.22	24,24,24,24	0
57	MG	1A	4015	1/1	0.97	0.10	52,52,52,52	0
57	MG	2a	3174	1/1	0.97	0.10	62,62,62,62	0
57	MG	1A	3322	1/1	0.97	0.18	17,17,17,17	0
57	MG	1A	3674	1/1	0.97	0.13	43,43,43,43	0
57	MG	2A	3342	1/1	0.97	0.10	44,44,44,44	0
57	MG	2a	3178	1/1	0.97	0.07	62,62,62,62	0
57	MG	2E	302	1/1	0.97	0.23	35,35,35,35	0
57	MG	2E	303	1/1	0.97	0.14	36,36,36,36	0
57	MG	1A	3675	1/1	0.97	0.21	46,46,46,46	0
57	MG	1A	3155	1/1	0.97	0.18	38,38,38,38	0
57	MG	2a	3183	1/1	0.97	0.10	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	15	105	1/1	0.97	0.16	25,25,25,25	0
57	MG	1A	3784	1/1	0.97	0.15	48,48,48,48	0
57	MG	2F	301	1/1	0.97	0.39	38,38,38,38	0
57	MG	2A	3347	1/1	0.97	0.13	24,24,24,24	0
57	MG	2a	3188	1/1	0.97	0.16	57,57,57,57	0
57	MG	1A	4021	1/1	0.97	0.11	41,41,41,41	0
57	MG	1A	3104	1/1	0.97	0.23	30,30,30,30	0
57	MG	1A	3906	1/1	0.97	0.22	22,22,22,22	0
57	MG	15	110	1/1	0.97	0.12	57,57,57,57	0
57	MG	1a	3133	1/1	0.97	0.21	61,61,61,61	0
57	MG	1A	3037	1/1	0.97	0.12	32,32,32,32	0
57	MG	2n	101	1/1	0.97	0.17	62,62,62,62	0
57	MG	1A	3277	1/1	0.97	0.11	19,19,19,19	0
57	MG	1A	3910	1/1	0.97	0.18	26,26,26,26	0
57	MG	1a	3138	1/1	0.97	0.11	36,36,36,36	0
57	MG	1A	3160	1/1	0.97	0.15	35,35,35,35	0
57	MG	1A	3517	1/1	0.97	0.15	16,16,16,16	0
57	MG	2Q	201	1/1	0.97	0.15	51,51,51,51	0
59	ARG	1B	232	12/12	0.97	0.21	26,36,46,51	0
57	MG	1A	3387	1/1	0.97	0.12	15,15,15,15	0
57	MG	2A	3560	1/1	0.97	0.08	33,33,33,33	0
57	MG	2R	201	1/1	0.97	0.09	55,55,55,55	0
57	MG	2A	3173	1/1	0.97	0.10	40,40,40,40	0
57	MG	1A	3055	1/1	0.97	0.11	21,21,21,21	0
57	MG	1a	3143	1/1	0.97	0.16	56,56,56,56	0
61	ZN	1Y	202	1/1	0.97	0.17	52,52,52,52	0
57	MG	2T	203	1/1	0.97	0.13	55,55,55,55	0
61	ZN	1n	104	1/1	0.97	0.10	66,66,66,66	0
57	MG	1A	3026	1/1	0.97	0.21	27,27,27,27	0
57	MG	2A	3566	1/1	0.97	0.12	41,41,41,41	0
57	MG	1A	3330	1/1	0.97	0.12	21,21,21,21	0
57	MG	1A	3796	1/1	0.97	0.13	32,32,32,32	0
57	MG	2A	3180	1/1	0.97	0.12	54,54,54,54	0
57	MG	1A	3679	1/1	0.98	0.23	15,15,15,15	0
57	MG	1A	3447	1/1	0.98	0.17	35,35,35,35	0
57	MG	1N	202	1/1	0.98	0.14	26,26,26,26	0
57	MG	1A	3614	1/1	0.98	0.13	26,26,26,26	0
57	MG	1A	3836	1/1	0.98	0.20	36,36,36,36	0
57	MG	1A	3398	1/1	0.98	0.12	14,14,14,14	0
57	MG	1A	3399	1/1	0.98	0.17	17,17,17,17	0
57	MG	1A	3208	1/1	0.98	0.41	27,27,27,27	0
57	MG	2A	3574	1/1	0.98	0.14	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3048	1/1	0.98	0.09	42,42,42,42	0
57	MG	1a	3129	1/1	0.98	0.26	48,48,48,48	0
57	MG	2a	3072	1/1	0.98	0.07	56,56,56,56	0
57	MG	1a	3234	1/1	0.98	0.15	48,48,48,48	0
57	MG	2a	3074	1/1	0.98	0.20	47,47,47,47	0
57	MG	1A	3401	1/1	0.98	0.19	14,14,14,14	0
57	MG	1A	3137	1/1	0.98	0.13	17,17,17,17	0
57	MG	1A	3242	1/1	0.98	0.24	36,36,36,36	0
57	MG	2A	3300	1/1	0.98	0.15	45,45,45,45	0
57	MG	2A	3438	1/1	0.98	0.11	30,30,30,30	0
57	MG	2A	3301	1/1	0.98	0.11	26,26,26,26	0
57	MG	1a	3238	1/1	0.98	0.22	54,54,54,54	0
57	MG	1A	3506	1/1	0.98	0.07	43,43,43,43	0
57	MG	1A	3845	1/1	0.98	0.14	36,36,36,36	0
57	MG	2A	3305	1/1	0.98	0.13	28,28,28,28	0
57	MG	2A	3444	1/1	0.98	0.13	27,27,27,27	0
57	MG	2A	3590	1/1	0.98	0.17	38,38,38,38	0
57	MG	1A	3098	1/1	0.98	0.19	44,44,44,44	0
57	MG	1A	3358	1/1	0.98	0.13	14,14,14,14	0
57	MG	1R	201	1/1	0.98	0.18	26,26,26,26	0
57	MG	1A	3565	1/1	0.98	0.15	29,29,29,29	0
57	MG	1A	3456	1/1	0.98	0.20	49,49,49,49	0
57	MG	2D	302	1/1	0.98	0.60	40,40,40,40	0
57	MG	1A	3850	1/1	0.98	0.22	33,33,33,33	0
57	MG	1A	3851	1/1	0.98	0.17	15,15,15,15	0
57	MG	1A	3280	1/1	0.98	0.18	34,34,34,34	0
57	MG	2A	3599	1/1	0.98	0.10	29,29,29,29	0
57	MG	1A	3159	1/1	0.98	0.18	23,23,23,23	0
57	MG	1A	3139	1/1	0.98	0.12	27,27,27,27	0
57	MG	1A	3941	1/1	0.98	0.19	19,19,19,19	0
57	MG	2A	3317	1/1	0.98	0.15	28,28,28,28	0
57	MG	1A	3247	1/1	0.98	0.15	26,26,26,26	0
57	MG	2A	3069	1/1	0.98	0.58	41,41,41,41	0
57	MG	1a	3253	1/1	0.98	0.14	44,44,44,44	0
57	MG	2A	3071	1/1	0.98	0.15	20,20,20,20	0
57	MG	1a	3254	1/1	0.98	0.18	45,45,45,45	0
57	MG	2E	307	1/1	0.98	0.12	48,48,48,48	0
57	MG	1A	3630	1/1	0.98	0.17	37,37,37,37	0
57	MG	1A	3774	1/1	0.98	0.12	24,24,24,24	0
57	MG	2A	3195	1/1	0.98	0.26	41,41,41,41	0
57	MG	1A	3161	1/1	0.98	0.15	19,19,19,19	0
57	MG	2a	3111	1/1	0.98	0.13	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3216	1/1	0.98	0.22	21,21,21,21	0
57	MG	2A	3614	1/1	0.98	0.07	21,21,21,21	0
57	MG	1A	3028	1/1	0.98	0.22	26,26,26,26	0
57	MG	2a	3115	1/1	0.98	0.13	42,42,42,42	0
57	MG	1A	3070	1/1	0.98	0.21	24,24,24,24	0
57	MG	1A	3101	1/1	0.98	0.23	23,23,23,23	0
57	MG	1A	3704	1/1	0.98	0.14	18,18,18,18	0
57	MG	1a	3263	1/1	0.98	0.12	49,49,49,49	0
57	MG	1a	3156	1/1	0.98	0.14	39,39,39,39	0
57	MG	1A	3636	1/1	0.98	0.17	21,21,21,21	0
57	MG	1A	3018	1/1	0.98	0.17	18,18,18,18	0
57	MG	1A	3707	1/1	0.98	0.10	28,28,28,28	0
57	MG	1A	3638	1/1	0.98	0.28	37,37,37,37	0
57	MG	1A	3709	1/1	0.98	0.07	15,15,15,15	0
57	MG	1A	3416	1/1	0.98	0.17	21,21,21,21	0
57	MG	1A	3019	1/1	0.98	0.19	22,22,22,22	0
57	MG	1A	3192	1/1	0.98	0.38	27,27,27,27	0
57	MG	2A	3482	1/1	0.98	0.12	21,21,21,21	0
57	MG	1A	3293	1/1	0.98	0.23	27,27,27,27	0
57	MG	1A	3875	1/1	0.98	0.18	32,32,32,32	0
57	MG	1A	3145	1/1	0.98	0.08	41,41,41,41	0
57	MG	1A	3962	1/1	0.98	0.17	30,30,30,30	0
57	MG	1a	3169	1/1	0.98	0.12	43,43,43,43	0
57	MG	1A	3295	1/1	0.98	0.16	35,35,35,35	0
57	MG	2A	3489	1/1	0.98	0.10	37,37,37,37	0
57	MG	1B	230	1/1	0.98	0.13	44,44,44,44	0
57	MG	1A	3146	1/1	0.98	0.29	32,32,32,32	0
57	MG	1A	3335	1/1	0.98	0.18	9,9,9,9	0
57	MG	1A	3475	1/1	0.98	0.18	13,13,13,13	0
57	MG	2a	3141	1/1	0.98	0.09	53,53,53,53	0
57	MG	2A	3352	1/1	0.98	0.23	42,42,42,42	0
57	MG	1A	3424	1/1	0.98	0.23	30,30,30,30	0
57	MG	1A	3170	1/1	0.98	0.16	23,23,23,23	0
57	MG	1a	3177	1/1	0.98	0.10	50,50,50,50	0
57	MG	11	103	1/1	0.98	0.15	37,37,37,37	0
57	MG	1A	3128	1/1	0.98	0.24	24,24,24,24	0
57	MG	1A	3884	1/1	0.98	0.23	23,23,23,23	0
57	MG	2A	3228	1/1	0.98	0.32	51,51,51,51	0
57	MG	2A	3107	1/1	0.98	0.14	30,30,30,30	0
57	MG	1A	3261	1/1	0.98	0.13	40,40,40,40	0
57	MG	1A	3339	1/1	0.98	0.21	22,22,22,22	0
57	MG	13	103	1/1	0.98	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	1D	310	1/1	0.98	0.24	41,41,41,41	0
57	MG	1A	3031	1/1	0.98	0.11	25,25,25,25	0
57	MG	2A	3366	1/1	0.98	0.18	33,33,33,33	0
57	MG	15	103	1/1	0.98	0.15	34,34,34,34	0
57	MG	1A	3726	1/1	0.98	0.16	49,49,49,49	0
57	MG	2A	3369	1/1	0.98	0.13	21,21,21,21	0
57	MG	2A	3513	1/1	0.98	0.10	49,49,49,49	0
57	MG	1D	314	1/1	0.98	0.17	33,33,33,33	0
57	MG	2A	3238	1/1	0.98	0.12	50,50,50,50	0
57	MG	1A	3592	1/1	0.98	0.18	33,33,33,33	0
57	MG	1A	3117	1/1	0.98	0.11	26,26,26,26	0
57	MG	2A	3241	1/1	0.98	0.33	51,51,51,51	0
57	MG	2A	3242	1/1	0.98	0.16	50,50,50,50	0
57	MG	2A	3118	1/1	0.98	0.12	47,47,47,47	0
57	MG	1A	3807	1/1	0.98	0.34	47,47,47,47	0
57	MG	1D	318	1/1	0.98	0.08	38,38,38,38	0
57	MG	1A	3536	1/1	0.98	0.10	20,20,20,20	0
57	MG	1A	3385	1/1	0.98	0.14	15,15,15,15	0
57	MG	1A	3731	1/1	0.98	0.15	24,24,24,24	0
57	MG	2A	3526	1/1	0.98	0.12	39,39,39,39	0
57	MG	1A	3056	1/1	0.98	0.13	34,34,34,34	0
57	MG	1A	3733	1/1	0.98	0.20	20,20,20,20	0
57	MG	2A	3007	1/1	0.98	0.14	36,36,36,36	0
57	MG	2A	3678	1/1	0.98	0.16	33,33,33,33	0
57	MG	1A	3265	1/1	0.98	0.26	24,24,24,24	0
57	MG	1A	3133	1/1	0.98	0.16	34,34,34,34	0
57	MG	2A	3010	1/1	0.98	0.17	51,51,51,51	0
57	MG	1A	3233	1/1	0.98	0.40	27,27,27,27	0
57	MG	1A	3152	1/1	0.98	0.23	35,35,35,35	0
57	MG	2a	3027	1/1	0.98	0.10	52,52,52,52	0
57	MG	1A	3817	1/1	0.98	0.12	26,26,26,26	0
57	MG	2A	3685	1/1	0.98	0.27	38,38,38,38	0
57	MG	2A	3686	1/1	0.98	0.08	45,45,45,45	0
57	MG	1A	3903	1/1	0.98	0.11	27,27,27,27	0
57	MG	1A	3347	1/1	0.98	0.20	22,22,22,22	0
57	MG	1a	3004	1/1	0.98	0.13	49,49,49,49	0
57	MG	1A	3739	1/1	0.98	0.25	44,44,44,44	0
57	MG	2a	3035	1/1	0.98	0.14	31,31,31,31	0
57	MG	1A	3440	1/1	0.98	0.13	21,21,21,21	0
57	MG	1A	3908	1/1	0.98	0.17	9,9,9,9	0
57	MG	2A	3020	1/1	0.98	0.31	37,37,37,37	0
57	MG	2A	3021	1/1	0.98	0.11	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	3209	1/1	0.98	0.14	45,45,45,45	0
57	MG	1F	310	1/1	0.98	0.19	27,27,27,27	0
57	MG	1A	3667	1/1	0.98	0.17	36,36,36,36	0
57	MG	1A	3025	1/1	0.98	0.18	27,27,27,27	0
57	MG	1A	3001	1/1	0.98	0.13	31,31,31,31	0
57	MG	1A	3205	1/1	0.98	0.26	33,33,33,33	0
57	MG	2A	3272	1/1	0.98	0.49	53,53,53,53	0
57	MG	1A	3013	1/1	0.98	0.24	21,21,21,21	0
57	MG	1A	3495	1/1	0.98	0.16	21,21,21,21	0
57	MG	2A	3030	1/1	0.98	0.18	22,22,22,22	0
57	MG	1A	3608	1/1	0.98	0.21	26,26,26,26	0
57	MG	1A	3609	1/1	0.98	0.11	22,22,22,22	0
57	MG	1a	3017	1/1	0.98	0.15	51,51,51,51	0
57	MG	1A	3552	1/1	0.98	0.10	33,33,33,33	0
57	MG	1A	3156	1/1	0.98	0.32	29,29,29,29	0
61	ZN	15	111	1/1	0.98	0.18	37,37,37,37	0
61	ZN	19	103	1/1	0.98	0.20	37,37,37,37	0
57	MG	1A	4004	1/1	0.98	0.11	49,49,49,49	0
57	MG	1A	4005	1/1	0.98	0.19	38,38,38,38	0
57	MG	1A	3274	1/1	0.98	0.21	33,33,33,33	0
57	MG	2A	3284	1/1	0.98	0.27	51,51,51,51	0
57	MG	2A	3039	1/1	0.98	0.22	34,34,34,34	0
57	MG	2A	3422	1/1	0.98	0.09	39,39,39,39	0
62	SF4	1d	306	8/8	0.98	0.13	52,62,71,75	0
57	MG	1A	3382	1/1	0.99	0.14	45,45,45,45	0
57	MG	1V	201	1/1	0.99	0.29	24,24,24,24	0
57	MG	1A	3793	1/1	0.99	0.17	23,23,23,23	0
57	MG	1A	3645	1/1	0.99	0.18	28,28,28,28	0
57	MG	1F	303	1/1	0.99	0.26	28,28,28,28	0
57	MG	2A	3421	1/1	0.99	0.09	36,36,36,36	0
57	MG	2A	3179	1/1	0.99	0.17	55,55,55,55	0
57	MG	1A	3003	1/1	0.99	0.15	20,20,20,20	0
57	MG	1A	3839	1/1	0.99	0.17	14,14,14,14	0
57	MG	1A	3289	1/1	0.99	0.18	8,8,8,8	0
57	MG	1A	3438	1/1	0.99	0.12	9,9,9,9	0
57	MG	1W	203	1/1	0.99	0.14	16,16,16,16	0
57	MG	1A	3176	1/1	0.99	0.13	24,24,24,24	0
57	MG	1A	3496	1/1	0.99	0.19	28,28,28,28	0
57	MG	1A	3201	1/1	0.99	0.31	34,34,34,34	0
57	MG	1A	3252	1/1	0.99	0.20	25,25,25,25	0
57	MG	2A	3561	1/1	0.99	0.16	18,18,18,18	0
57	MG	1A	3048	1/1	0.99	0.13	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	3137	1/1	0.99	0.14	61,61,61,61	0
57	MG	1A	3654	1/1	0.99	0.15	25,25,25,25	0
57	MG	1A	3107	1/1	0.99	0.18	23,23,23,23	0
57	MG	1A	3725	1/1	0.99	0.17	19,19,19,19	0
57	MG	2A	3501	1/1	0.99	0.04	49,49,49,49	0
57	MG	2A	3635	1/1	0.99	0.10	54,54,54,54	0
57	MG	1A	3091	1/1	0.99	0.18	12,12,12,12	0
57	MG	1A	3365	1/1	0.99	0.16	18,18,18,18	0
57	MG	1A	3898	1/1	0.99	0.13	14,14,14,14	0
57	MG	1A	3220	1/1	0.99	0.14	30,30,30,30	0
57	MG	1A	3693	1/1	0.99	0.14	30,30,30,30	0
57	MG	2A	3379	1/1	0.99	0.13	28,28,28,28	0
57	MG	1A	3768	1/1	0.99	0.16	20,20,20,20	0
57	MG	1A	3998	1/1	0.99	0.18	12,12,12,12	0
57	MG	1A	3044	1/1	0.99	0.14	14,14,14,14	0
57	MG	1A	3045	1/1	0.99	0.11	14,14,14,14	0
57	MG	1A	3904	1/1	0.99	0.15	11,11,11,11	0
57	MG	1A	3278	1/1	0.99	0.21	30,30,30,30	0
57	MG	1A	3024	1/1	0.99	0.17	15,15,15,15	0
57	MG	1A	3073	1/1	0.99	0.19	30,30,30,30	0
57	MG	1A	3131	1/1	0.99	0.31	23,23,23,23	0
57	MG	1A	3243	1/1	0.99	0.24	35,35,35,35	0
57	MG	2A	3390	1/1	0.99	0.18	29,29,29,29	0
57	MG	1A	3818	1/1	0.99	0.22	19,19,19,19	0
57	MG	15	104	1/1	0.99	0.24	25,25,25,25	0
57	MG	2A	3655	1/1	0.99	0.17	32,32,32,32	0
57	MG	1A	3374	1/1	0.99	0.15	27,27,27,27	0
57	MG	2A	3588	1/1	0.99	0.05	50,50,50,50	0
57	MG	1A	3067	1/1	0.99	0.18	24,24,24,24	0
57	MG	1A	3163	1/1	0.99	0.28	23,23,23,23	0
57	MG	1A	3740	1/1	0.99	0.11	47,47,47,47	0
57	MG	1A	3212	1/1	0.99	0.17	12,12,12,12	0
57	MG	1A	3670	1/1	0.99	0.34	33,33,33,33	0
57	MG	1A	3869	1/1	0.99	0.13	20,20,20,20	0
57	MG	1D	313	1/1	0.99	0.17	18,18,18,18	0
57	MG	1A	3782	1/1	0.99	0.17	15,15,15,15	0
57	MG	1A	3307	1/1	0.99	0.20	8,8,8,8	0
57	MG	1A	3744	1/1	0.99	0.09	16,16,16,16	0
57	MG	1A	3873	1/1	0.99	0.20	23,23,23,23	0
57	MG	1A	3213	1/1	0.99	0.13	15,15,15,15	0
57	MG	1E	301	1/1	0.99	0.28	27,27,27,27	0
57	MG	1E	302	1/1	0.99	0.21	26,26,26,26	0

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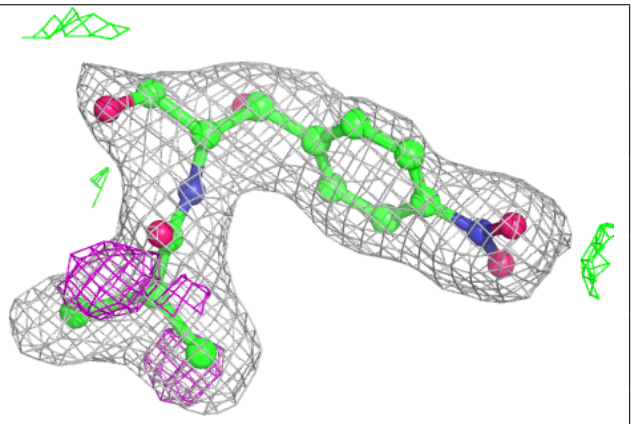
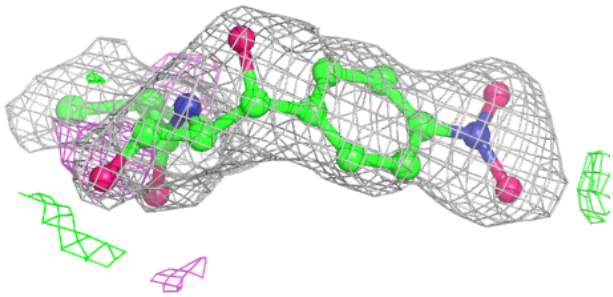
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3471	1/1	0.99	0.11	36,36,36,36	0
61	ZN	16	501	1/1	0.99	0.21	35,35,35,35	0
57	MG	1m	201	1/1	0.99	0.09	60,60,60,60	0
57	MG	1A	3786	1/1	0.99	0.15	27,27,27,27	0
57	MG	1A	3546	1/1	0.99	0.18	54,54,54,54	0
57	MG	1A	3432	1/1	0.99	0.17	27,27,27,27	0
61	ZN	25	105	1/1	0.99	0.21	47,47,47,47	0
57	MG	1U	203	1/1	0.99	0.19	30,30,30,30	0
57	MG	1A	3548	1/1	0.99	0.17	22,22,22,22	0
57	MG	1A	3309	1/1	0.99	0.42	29,29,29,29	0
57	MG	1A	3230	1/1	0.99	0.14	27,27,27,27	0
62	SF4	2d	501	8/8	0.99	0.12	58,67,74,76	0
57	MG	1D	309	1/1	1.00	0.14	13,13,13,13	0

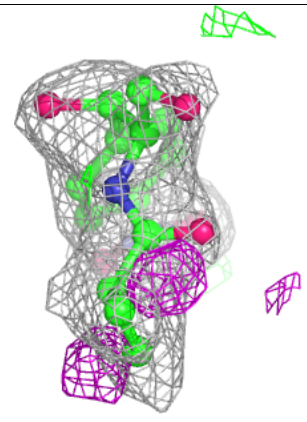
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLM 2A 3727:

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

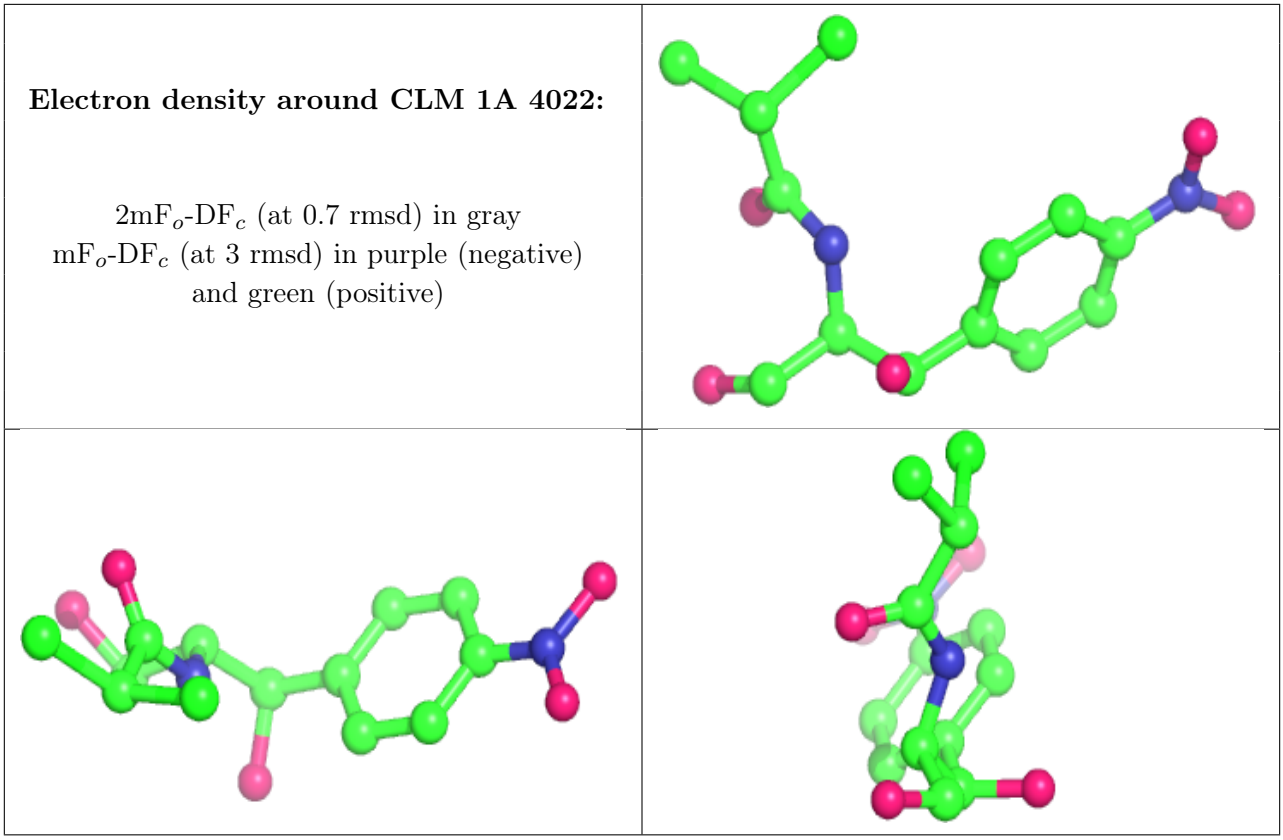






Electron density around CLM 1A 4022:

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



6.5 Other polymers (i)

There are no such residues in this entry.