Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 06:13 AM EST

PDB ID	:	7RQB
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with protein Y, A-site aminoacyl-tRNA analog ACC-PMN, and P-site MAI-tripeptidyl-tRNA analog ACCA-IAM at 2.45A resolution
Authors	:	Syroegin, E.A.; Flemmich, L.; Klepacki, D.; Vazquez-Laslop, N.; Micura, R.; Polikanov, Y.S.
Deposited on	:	2021-08-06
Resolution	:	2.45 Å(reported)

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

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

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

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

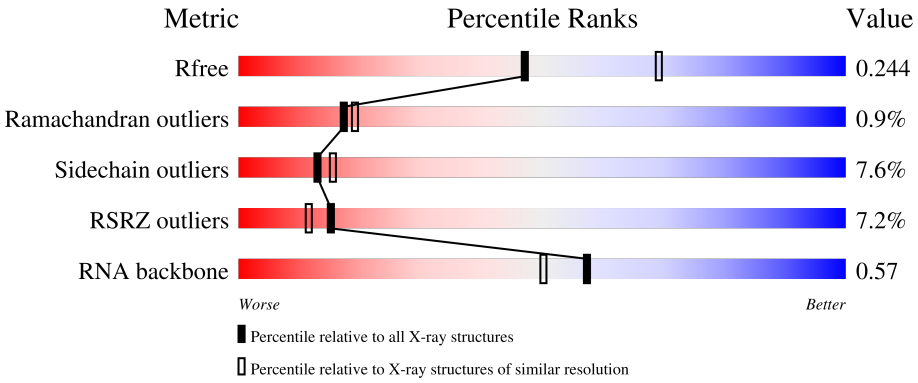
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)
RNA backbone	3102	1001 (2.80-2.12)

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	4% 83% 14%
1	2A	2915	4% 81% 17%
2	1B	121	88% 11%
2	2B	121	87% 12%

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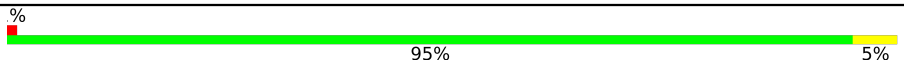
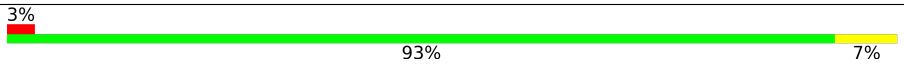
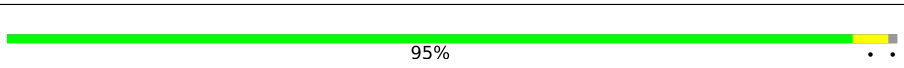
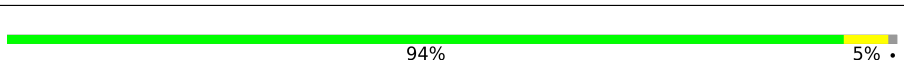
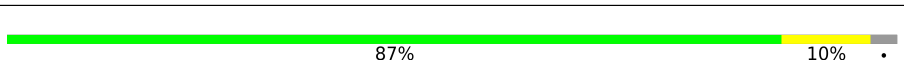
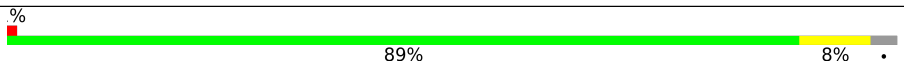
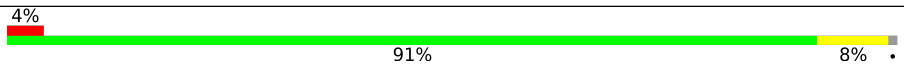
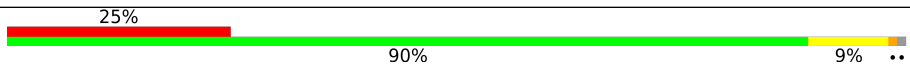
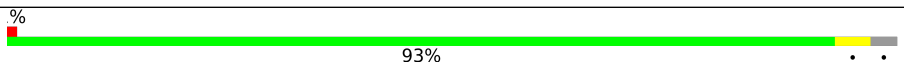
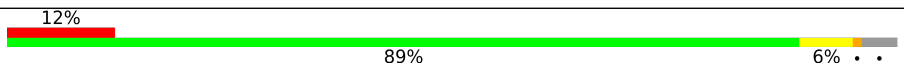
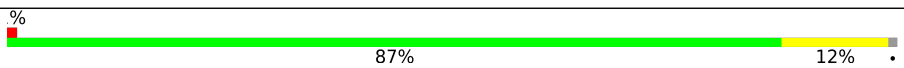
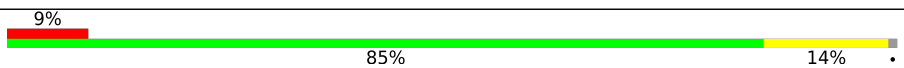
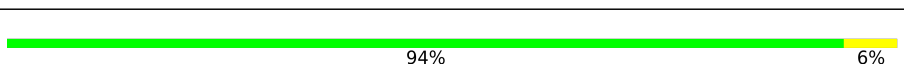
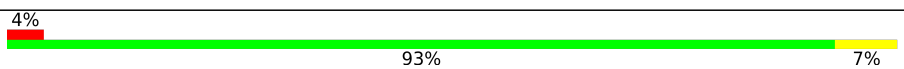
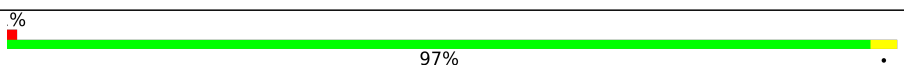
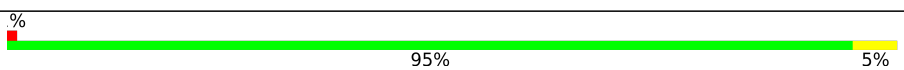
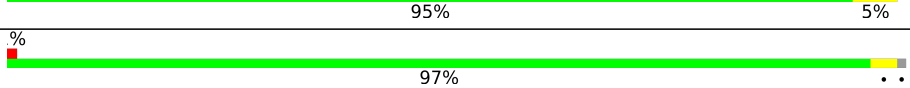
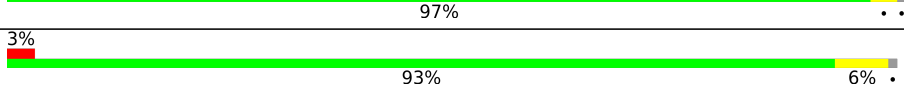
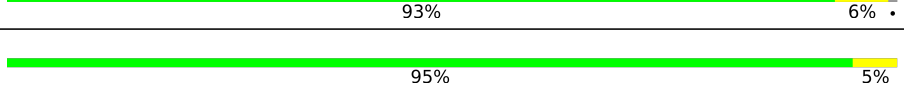
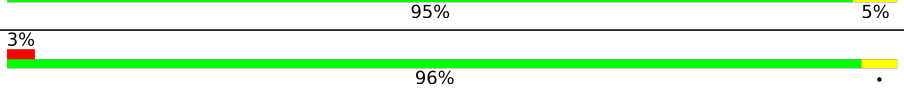
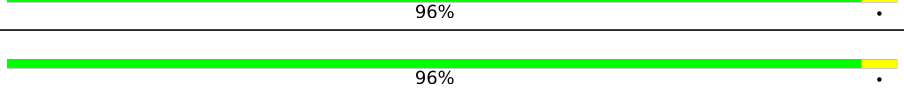
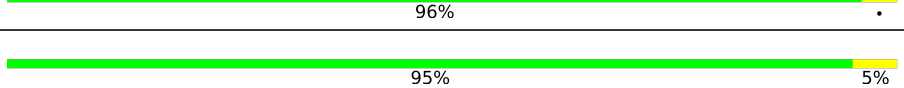
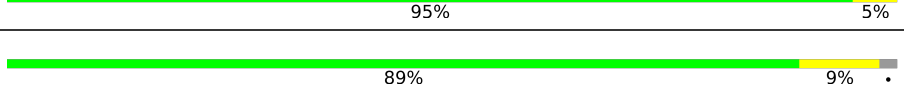
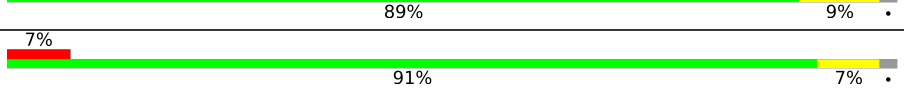
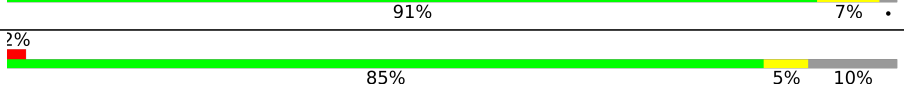
Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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Mol	Chain	Length	Quality of chain
15	2T	146	2% 84% 6% 10%
16	1U	118	93% 5%
16	2U	118	91% 8%
17	1V	101	98%
17	2V	101	% 90% 9%
18	1W	113	2% 94% 5%
18	2W	113	4% 95%
19	1X	96	% 95%
19	2X	96	5% 95%
20	1Y	110	% 92% 5%
20	2Y	110	12% 90% 7%
21	1Z	206	2% 91% 7%
21	2Z	206	10% 91% 6%
22	10	85	93% 5%
22	20	85	8% 94%
23	11	98	3% 93% 6%
23	21	98	5% 91% 7%
24	12	72	% 93%
24	22	72	3% 92% 6%
25	13	60	93% 5%
25	23	60	2% 95%
26	14	71	14% 85% 13%
26	24	71	30% 80% 15%
27	15	60	2% 93% 5%
27	25	60	95%

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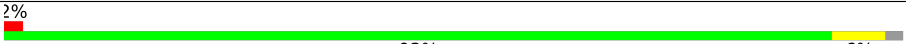
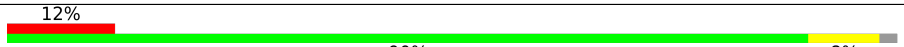
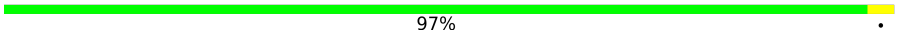
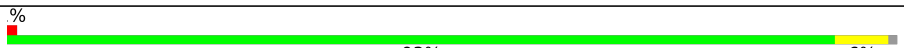
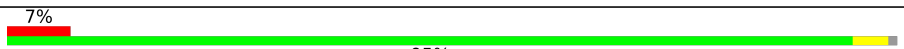
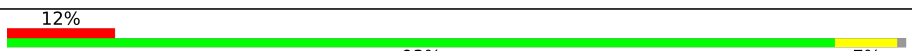
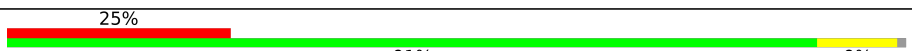
Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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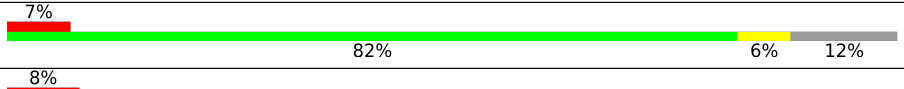
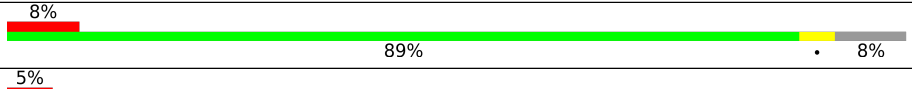
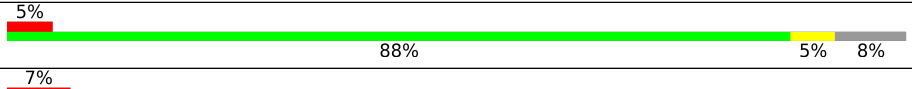
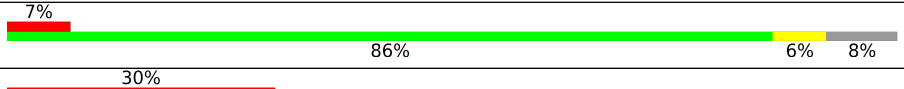
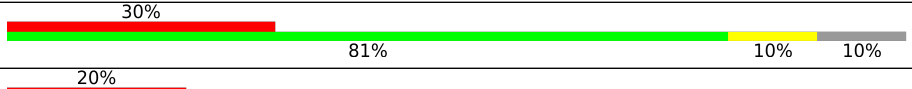
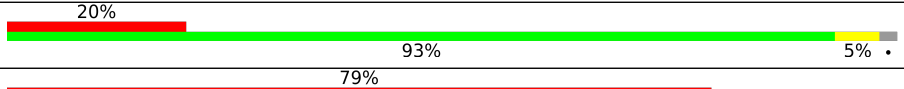
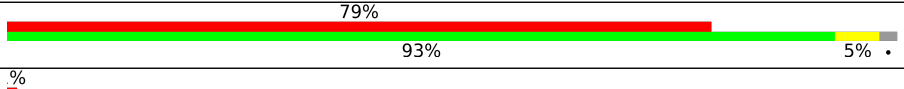
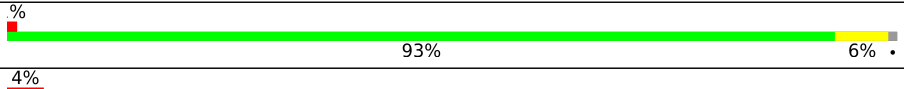
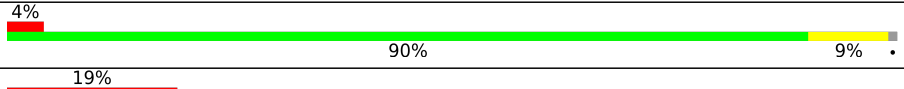
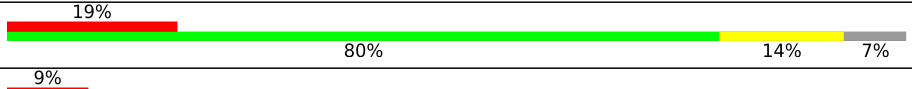
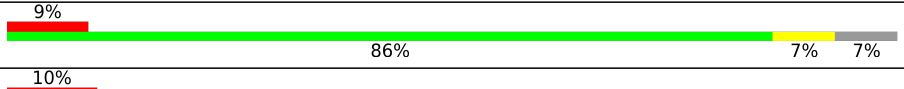
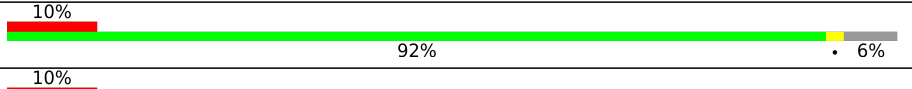
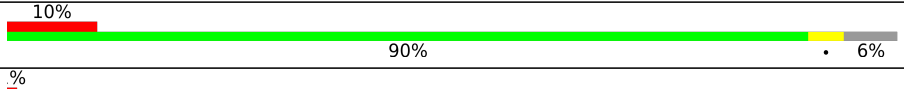
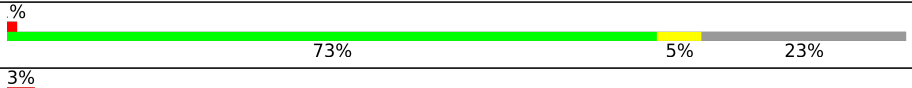
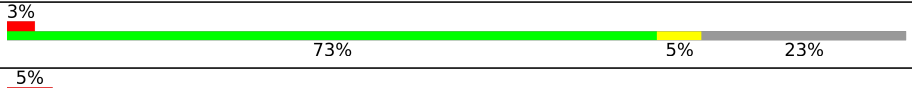
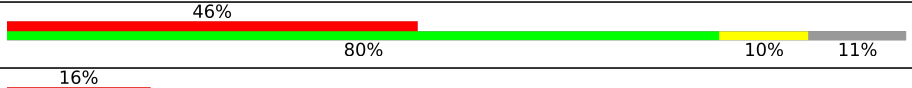
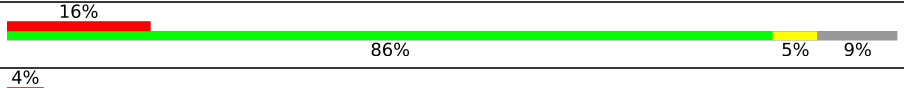
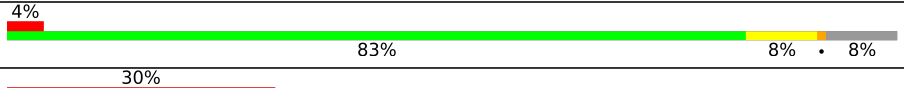
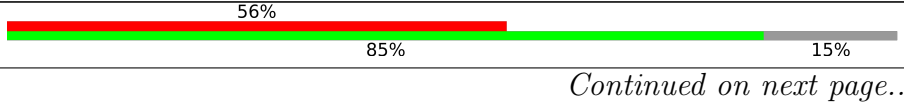
Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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Mol	Chain	Length	Quality of chain
53	1y	113	4% 84% 14%
53	2y	113	68% 80% 5% 15%
54	1w	4	50% 50%
54	2w	4	75% 25%
55	1x	4	75% 25%
55	2x	4	75% 25%
56	1v	3	100%
56	2v	3	33% 100%

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	3317	-	-	-	X
57	MG	1A	3576	-	-	-	X
57	MG	1A	3656	-	-	-	X
57	MG	1A	3667	-	-	-	X
57	MG	1A	3698	-	-	-	X
57	MG	1A	3700	-	-	-	X
57	MG	1A	3875	-	-	-	X
57	MG	1a	1657	-	-	-	X
57	MG	1a	1835	-	-	-	X
57	MG	2A	3026	-	-	-	X
57	MG	2A	3148	-	-	-	X
57	MG	2A	3159	-	-	-	X
57	MG	2A	3259	-	-	-	X
57	MG	2A	3267	-	-	-	X
57	MG	2A	3413	-	-	-	X
57	MG	2A	3414	-	-	-	X
57	MG	2A	3542	-	-	-	X
57	MG	2A	3677	-	-	-	X
57	MG	2A	3683	-	-	-	X
57	MG	2E	303	-	-	-	X
57	MG	2a	3004	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 297350 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 Aminoacyl-tRNA Analog.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1v	3	Total	C	N	O	S	0	0	0
			21	14	3	3	1			
56	2v	3	Total	C	N	O	S	0	0	0
			21	14	3	3	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1013	Total	Mg	0	0
			1013	1013		
57	1B	30	Total	Mg	0	0
			30	30		
57	1D	17	Total	Mg	0	0
			17	17		
57	1E	8	Total	Mg	0	0
			8	8		
57	1F	17	Total	Mg	0	0
			17	17		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1G	4	Total Mg 4 4	0	0
57	1H	2	Total Mg 2 2	0	0
57	1N	4	Total Mg 4 4	0	0
57	1O	1	Total Mg 1 1	0	0
57	1P	3	Total Mg 3 3	0	0
57	1Q	5	Total Mg 5 5	0	0
57	1R	7	Total Mg 7 7	0	0
57	1T	7	Total Mg 7 7	0	0
57	1U	5	Total Mg 5 5	0	0
57	1V	7	Total Mg 7 7	0	0
57	1W	3	Total Mg 3 3	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	7	Total Mg 7 7	0	0
57	17	6	Total Mg 6 6	0	0
57	18	3	Total Mg 3 3	0	0
57	19	1	Total Mg 1 1	0	0
57	1a	267	Total Mg 267 267	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1b	1	Total Mg 1 1	0	0
57	1d	5	Total Mg 5 5	0	0
57	1e	5	Total Mg 5 5	0	0
57	1f	2	Total Mg 2 2	0	0
57	1g	2	Total Mg 2 2	0	0
57	1h	2	Total Mg 2 2	0	0
57	1i	1	Total Mg 1 1	0	0
57	1l	2	Total Mg 2 2	0	0
57	1m	1	Total Mg 1 1	0	0
57	1n	3	Total Mg 3 3	0	0
57	1o	3	Total Mg 3 3	0	0
57	1t	2	Total Mg 2 2	0	0
57	1y	2	Total Mg 2 2	0	0
57	1x	2	Total Mg 2 2	0	0
57	2A	731	Total Mg 731 731	0	0
57	2B	19	Total Mg 19 19	0	0
57	2D	10	Total Mg 10 10	0	0
57	2E	6	Total Mg 6 6	0	0
57	2F	5	Total Mg 5 5	0	0
57	2G	2	Total Mg 2 2	0	0
57	2I	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2O	2	Total Mg 2 2	0	0
57	2P	1	Total Mg 1 1	0	0
57	2Q	3	Total Mg 3 3	0	0
57	2R	3	Total Mg 3 3	0	0
57	2T	4	Total Mg 4 4	0	0
57	2U	2	Total Mg 2 2	0	0
57	2V	3	Total Mg 3 3	0	0
57	2W	3	Total Mg 3 3	0	0
57	2X	1	Total Mg 1 1	0	0
57	2Y	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	23	1	Total Mg 1 1	0	0
57	25	2	Total Mg 2 2	0	0
57	27	2	Total Mg 2 2	0	0
57	28	2	Total Mg 2 2	0	0
57	29	1	Total Mg 1 1	0	0
57	2a	183	Total Mg 183 183	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	2	Total Mg 2 2	0	0
57	2j	1	Total Mg 1 1	0	0
57	2k	1	Total Mg 1 1	0	0

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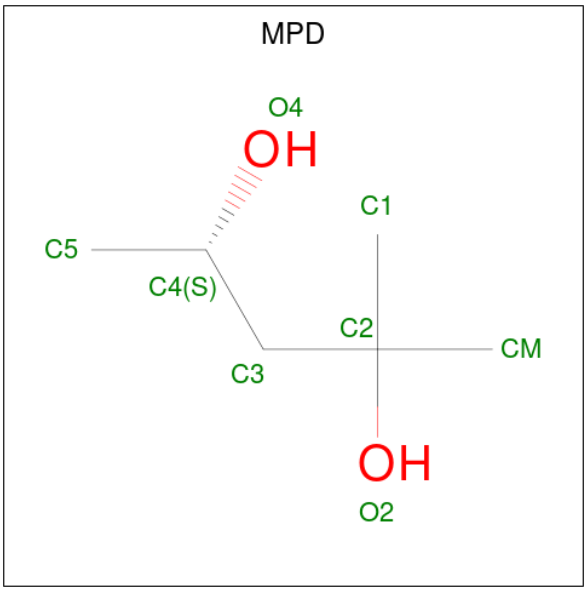
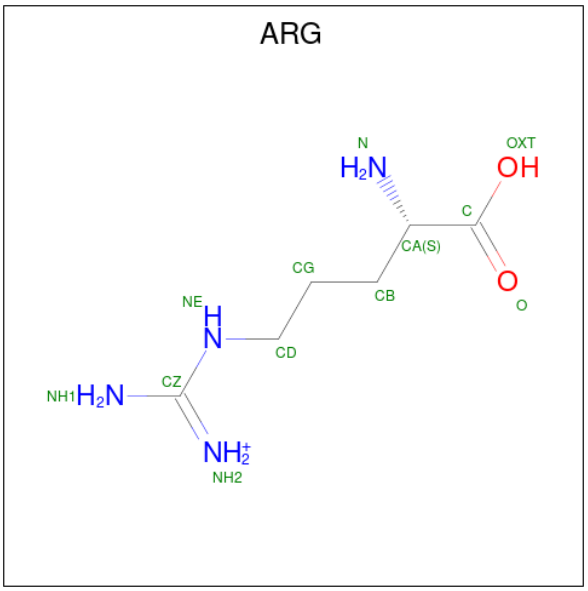
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2p	1	Total Mg 1 1	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2x	2	Total Mg 2 2	0	0

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

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



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	2Y	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0

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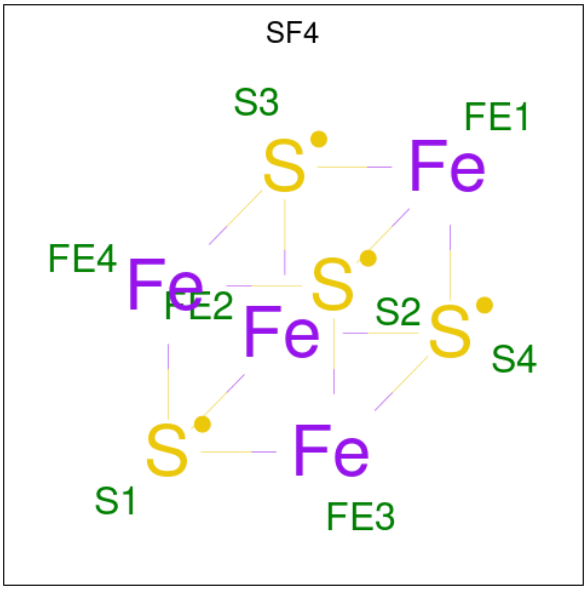
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1A	3935	Total O 3935 3935	0	0
62	1B	80	Total O 80 80	0	0
62	1D	108	Total O 108 108	0	0
62	1E	74	Total O 74 74	0	0
62	1F	60	Total O 60 60	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1G	16	Total O 16 16	0	0
62	1H	15	Total O 15 15	0	0
62	1I	5	Total O 5 5	0	0
62	1N	54	Total O 54 54	0	0
62	1O	21	Total O 21 21	0	0
62	1P	63	Total O 63 63	0	0
62	1Q	39	Total O 39 39	0	0
62	1R	28	Total O 28 28	0	0
62	1S	12	Total O 12 12	0	0
62	1T	32	Total O 32 32	0	0
62	1U	53	Total O 53 53	0	0
62	1V	33	Total O 33 33	0	0
62	1W	24	Total O 24 24	0	0
62	1X	24	Total O 24 24	0	0
62	1Y	15	Total O 15 15	0	0
62	1Z	7	Total O 7 7	0	0
62	10	23	Total O 23 23	0	0
62	11	26	Total O 26 26	0	0
62	12	10	Total O 10 10	0	0
62	13	25	Total O 25 25	0	0
62	14	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	15	18	Total O 18 18	0	0
62	16	18	Total O 18 18	0	0
62	17	17	Total O 17 17	0	0
62	18	25	Total O 25 25	0	0
62	19	5	Total O 5 5	0	0
62	1a	424	Total O 424 424	0	0
62	1b	1	Total O 1 1	0	0
62	1d	8	Total O 8 8	0	0
62	1e	2	Total O 2 2	0	0
62	1f	2	Total O 2 2	0	0
62	1g	1	Total O 1 1	0	0
62	1h	1	Total O 1 1	0	0
62	1l	2	Total O 2 2	0	0
62	1o	4	Total O 4 4	0	0
62	1p	1	Total O 1 1	0	0
62	1t	1	Total O 1 1	0	0
62	1y	2	Total O 2 2	0	0
62	1w	6	Total O 6 6	0	0
62	1x	2	Total O 2 2	0	0
62	2A	2058	Total O 2058 2058	0	0
62	2B	39	Total O 39 39	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2D	51	Total O 51 51	0	0
62	2E	32	Total O 32 32	0	0
62	2F	26	Total O 26 26	0	0
62	2G	7	Total O 7 7	0	0
62	2H	1	Total O 1 1	0	0
62	2I	2	Total O 2 2	0	0
62	2N	5	Total O 5 5	0	0
62	2O	16	Total O 16 16	0	0
62	2P	26	Total O 26 26	0	0
62	2Q	14	Total O 14 14	0	0
62	2R	17	Total O 17 17	0	0
62	2S	3	Total O 3 3	0	0
62	2T	7	Total O 7 7	0	0
62	2U	15	Total O 15 15	0	0
62	2V	3	Total O 3 3	0	0
62	2W	17	Total O 17 17	0	0
62	2X	8	Total O 8 8	0	0
62	2Y	2	Total O 2 2	0	0
62	2Z	6	Total O 6 6	0	0
62	20	8	Total O 8 8	0	0
62	21	15	Total O 15 15	0	0

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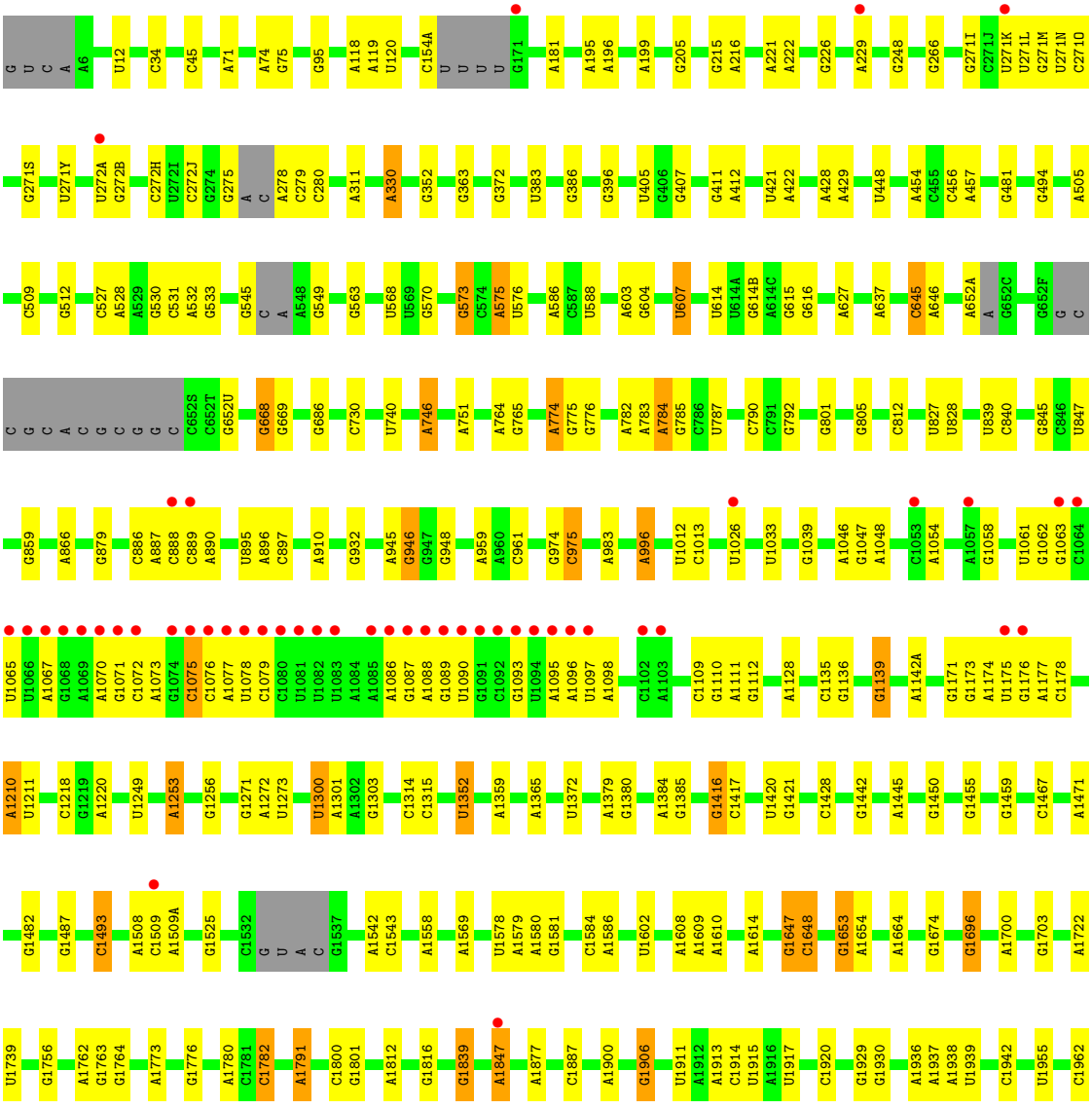
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	23	2	Total O 2 2	0	0
62	25	11	Total O 11 11	0	0
62	26	7	Total O 7 7	0	0
62	27	5	Total O 5 5	0	0
62	28	16	Total O 16 16	0	0
62	2a	243	Total O 243 243	0	0
62	2e	2	Total O 2 2	0	0
62	2l	3	Total O 3 3	0	0
62	2m	1	Total O 1 1	0	0
62	2n	2	Total O 2 2	0	0
62	2o	2	Total O 2 2	0	0
62	2p	1	Total O 1 1	0	0
62	2r	4	Total O 4 4	0	0
62	2t	2	Total O 2 2	0	0
62	2w	4	Total O 4 4	0	0
62	2x	3	Total O 3 3	0	0

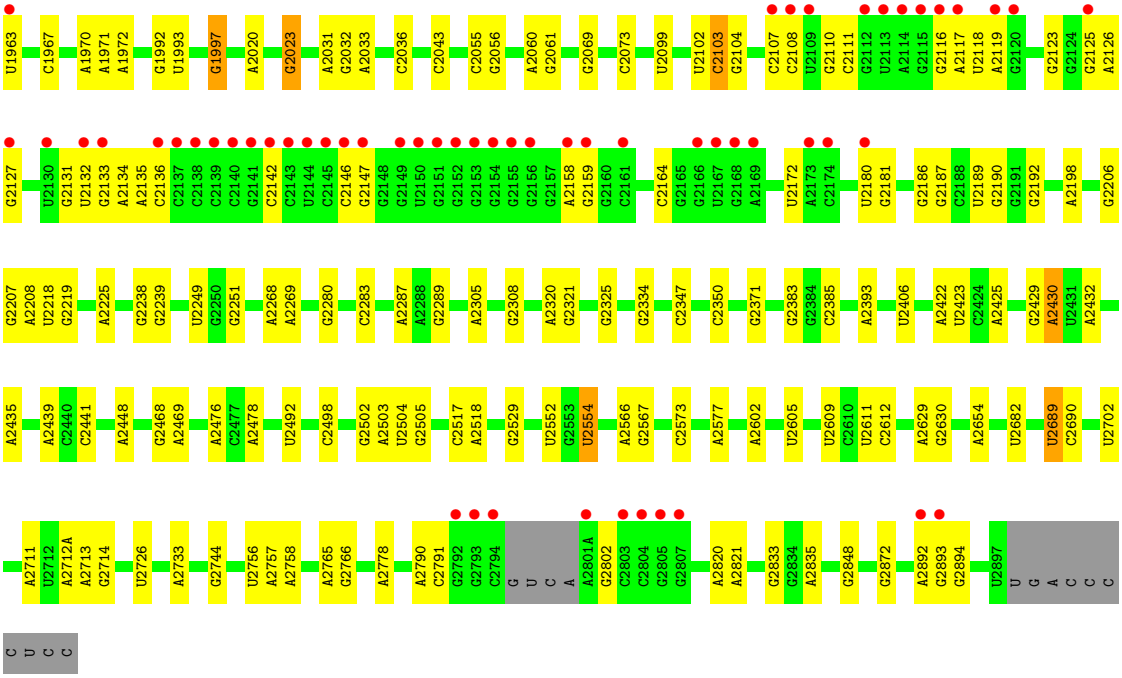
3 Residue-property plots (i)

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

- Molecule 1: 23S Ribosomal RNA

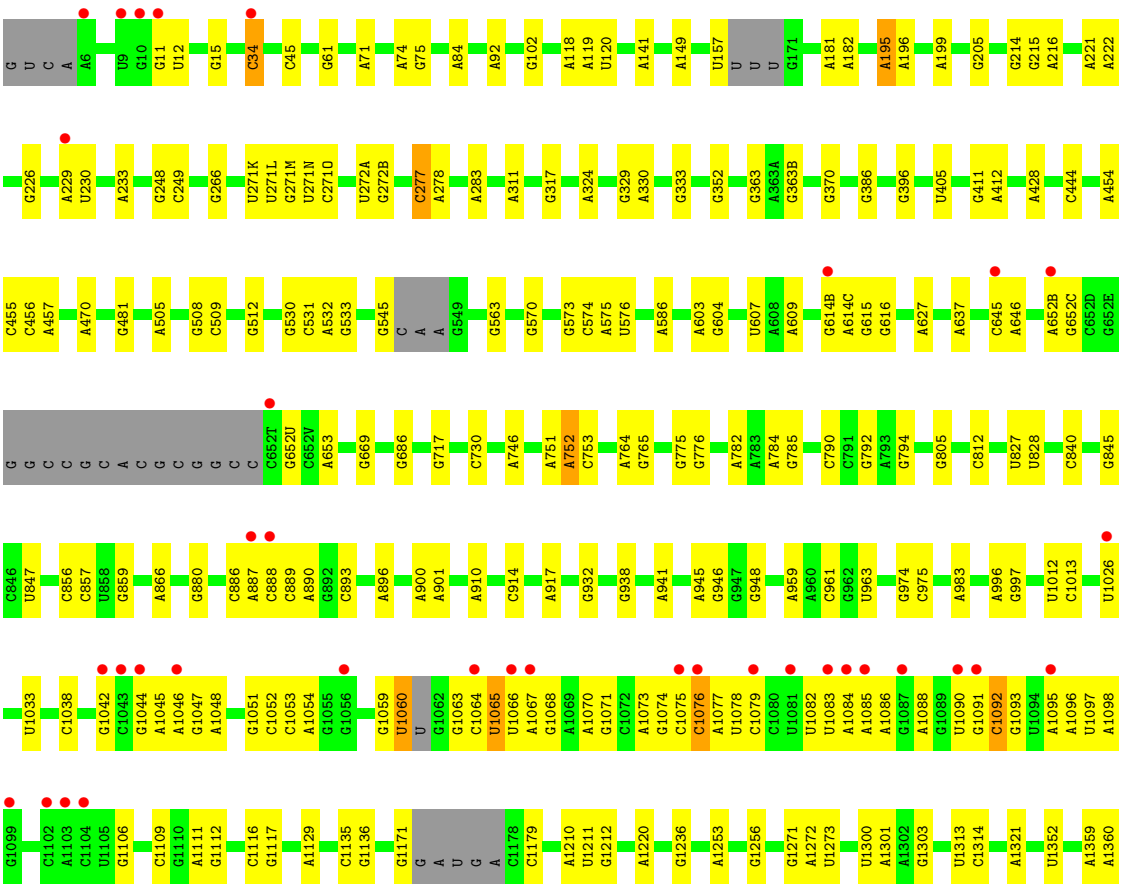
Chain 1A:

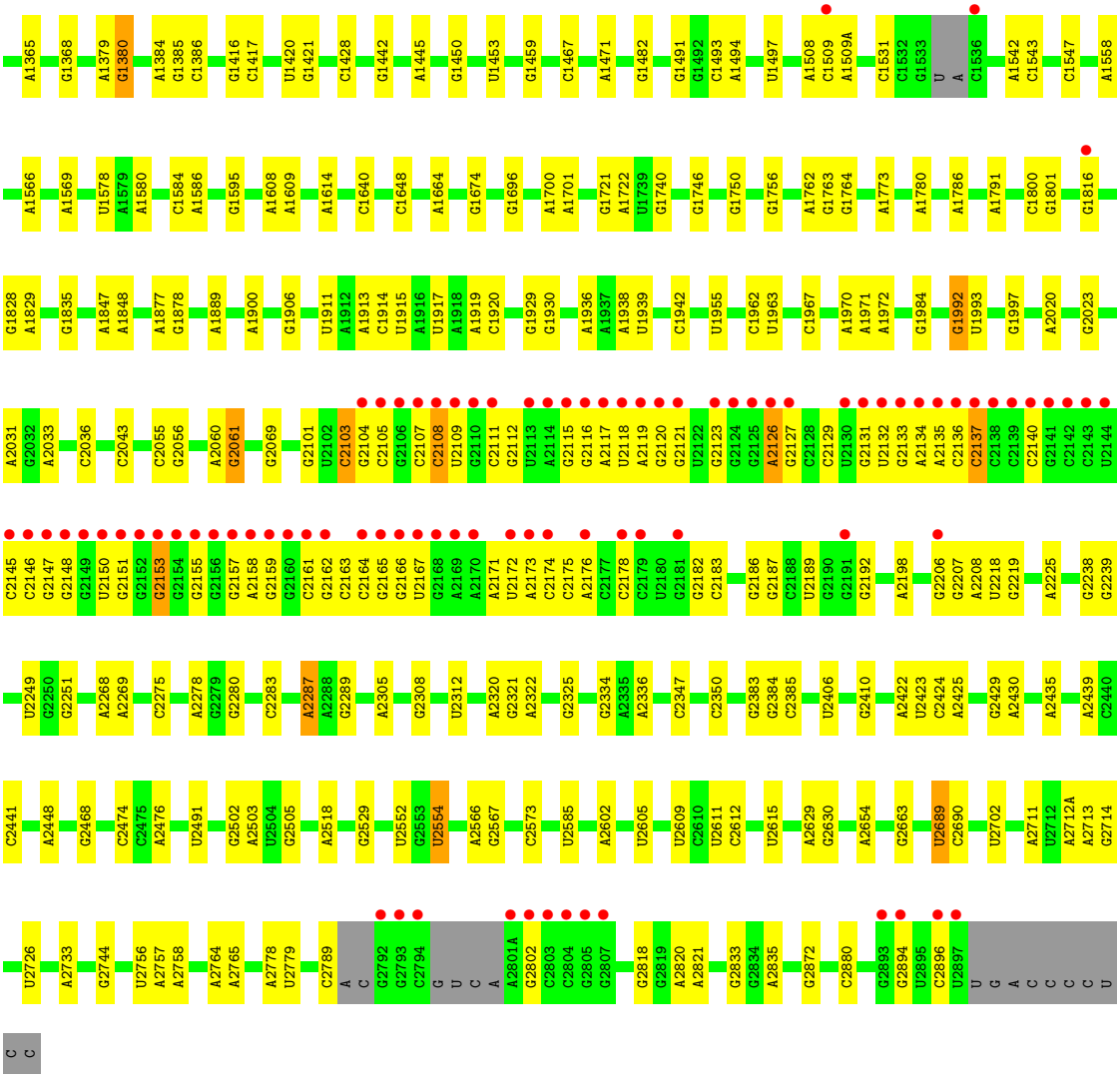




• Molecule 1: 23S Ribosomal RNA

Chain 2A:





• Molecule 2: 5S Ribosomal RNA

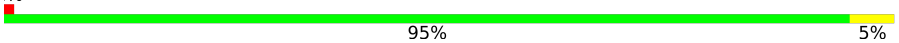
Chain 1B:

• Molecule 2: 5S Ribosomal RNA

Chain 2B:

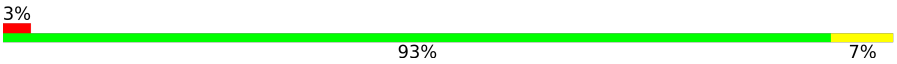
• Molecule 3: 50S ribosomal protein L2

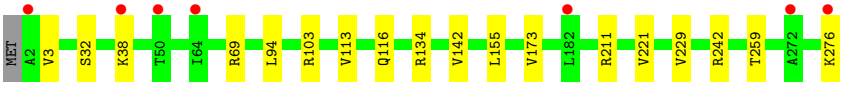
Chain 1D:



• Molecule 3: 50S ribosomal protein L2

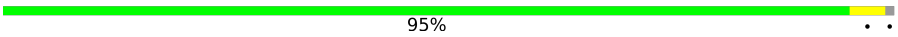
Chain 2D:





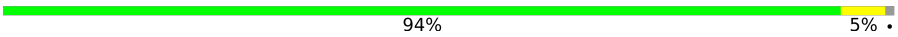
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



• Molecule 4: 50S ribosomal protein L3

Chain 2E:



• Molecule 5: 50S ribosomal protein L4

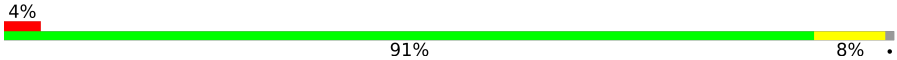
Chain 1F:

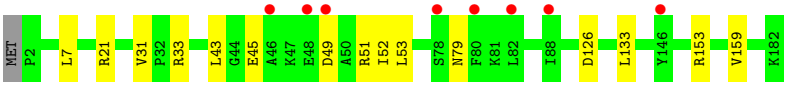
• Molecule 5: 50S ribosomal protein L4

Chain 2F:

• Molecule 6: 50S ribosomal protein L5

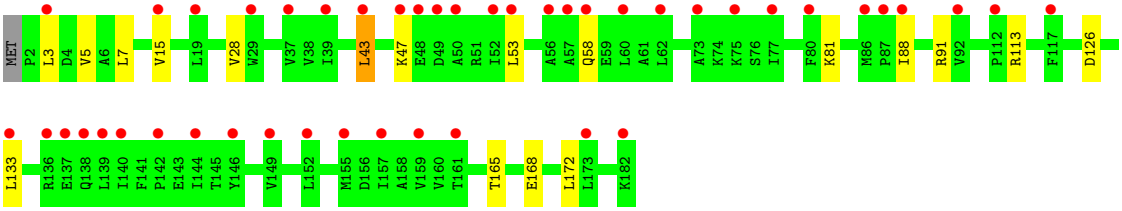
Chain 1G:





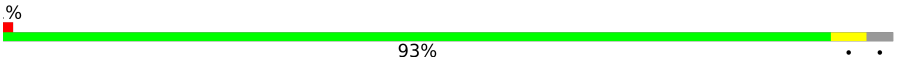
• Molecule 6: 50S ribosomal protein L5

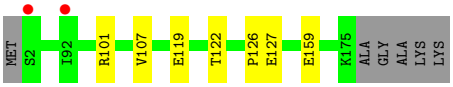
Chain 2G:



• Molecule 7: 50S ribosomal protein L6

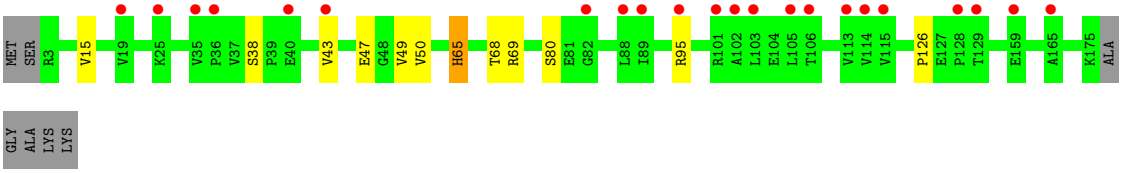
Chain 1H:





• Molecule 7: 50S ribosomal protein L6

Chain 2H:

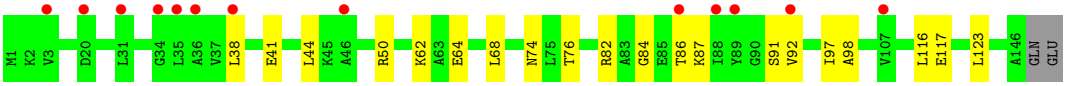


• Molecule 8: 50S ribosomal protein L9

Chain 1I:

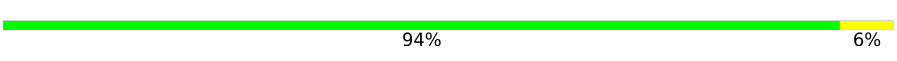
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



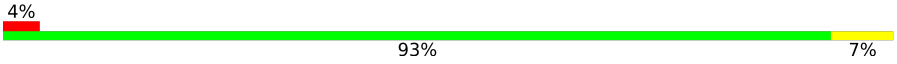
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



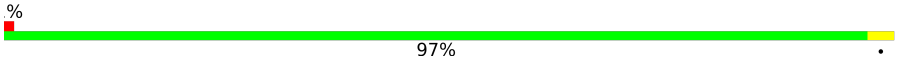
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



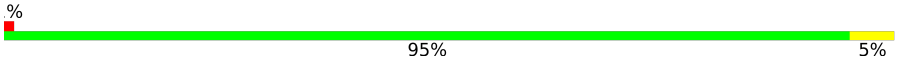
• Molecule 10: 50S ribosomal protein L14

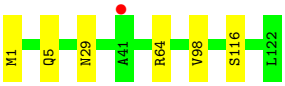
Chain 1O:



• Molecule 10: 50S ribosomal protein L14

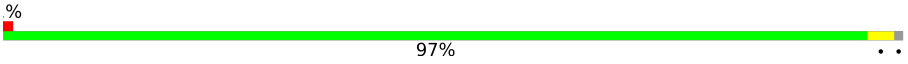
Chain 2O:

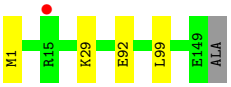




• Molecule 11: 50S ribosomal protein L15

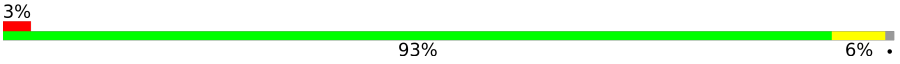
Chain 1P:





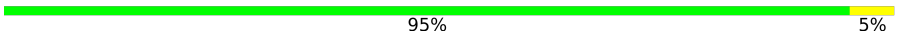
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



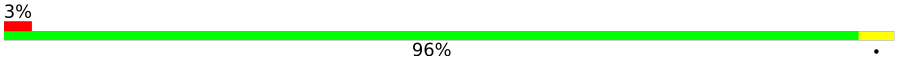
• Molecule 12: 50S ribosomal protein L16

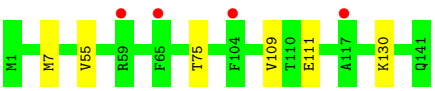
Chain 1Q:



• Molecule 12: 50S ribosomal protein L16

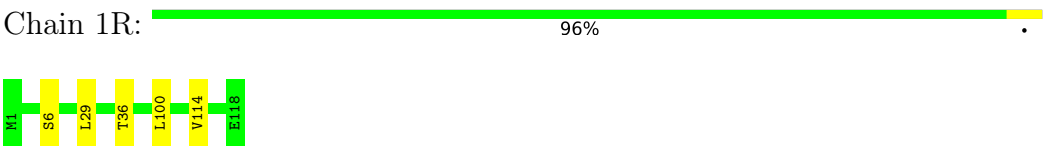
Chain 2Q:





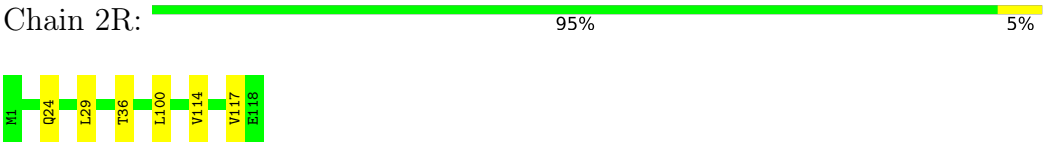
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



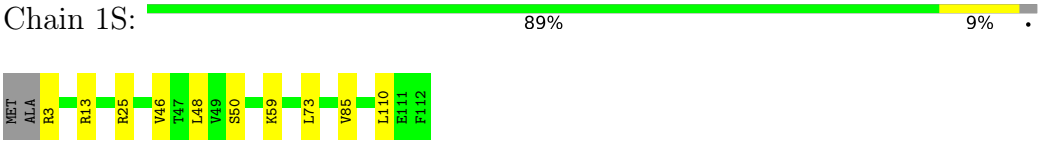
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



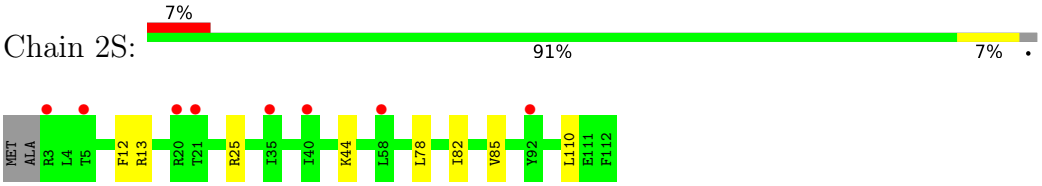
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



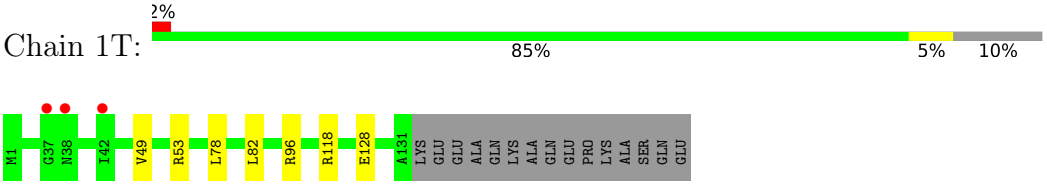
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



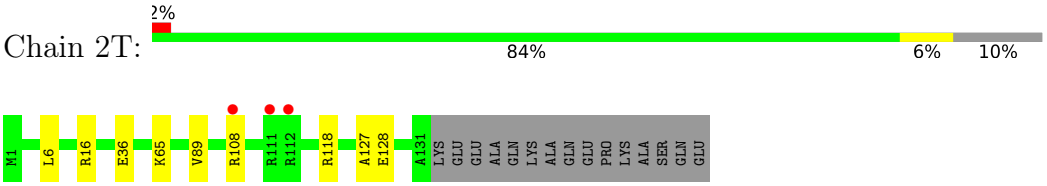
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



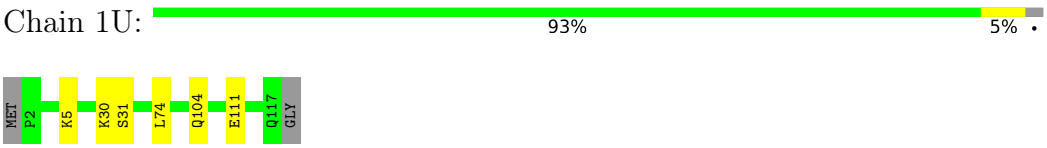
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



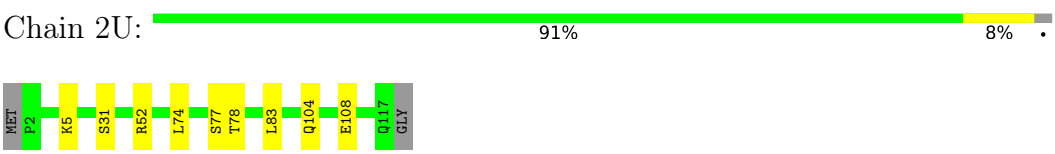
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



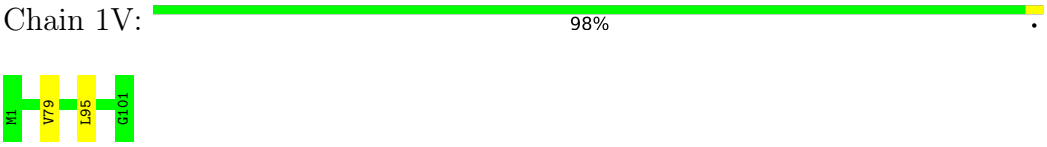
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



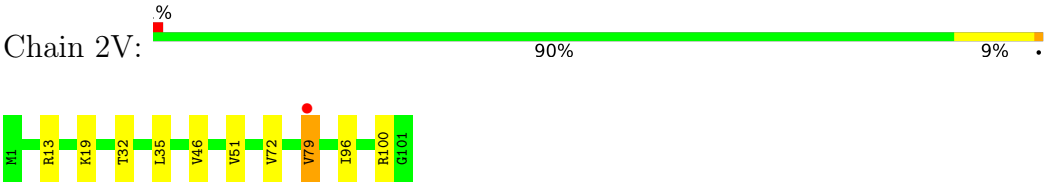
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



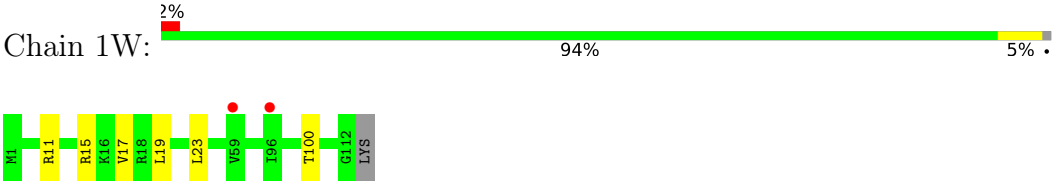
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



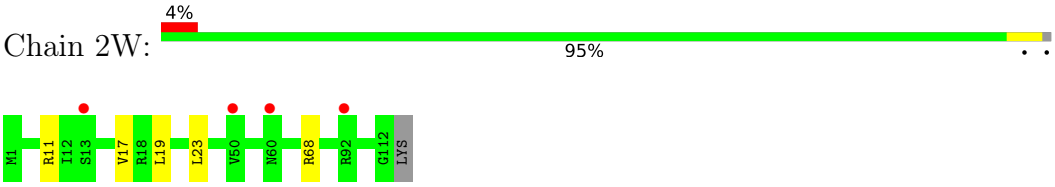
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



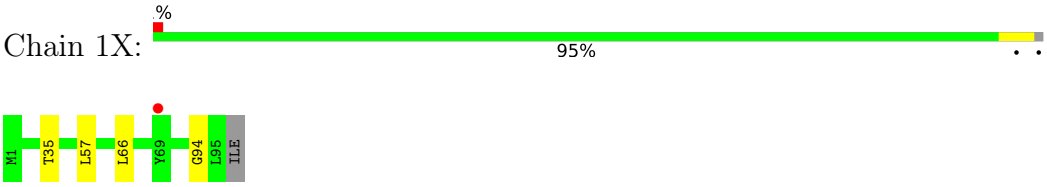
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



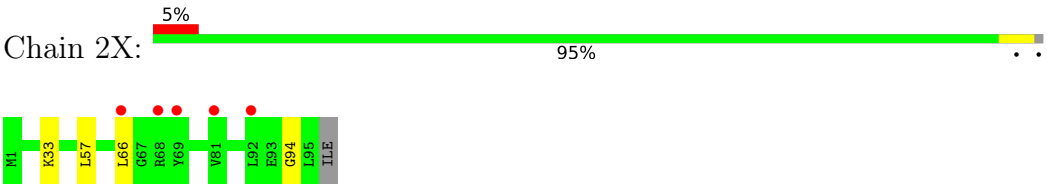
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



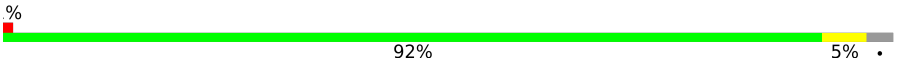
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



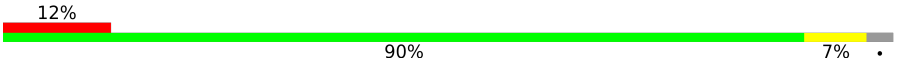
• Molecule 20: 50S ribosomal protein L24

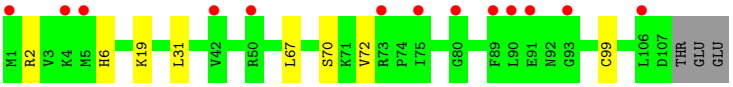
Chain 1Y:



• Molecule 20: 50S ribosomal protein L24

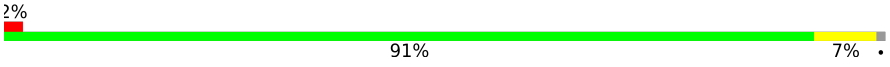
Chain 2Y:





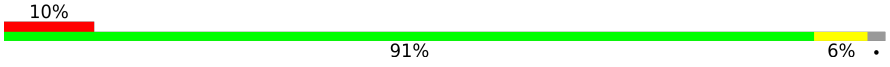
• Molecule 21: 50S ribosomal protein L25

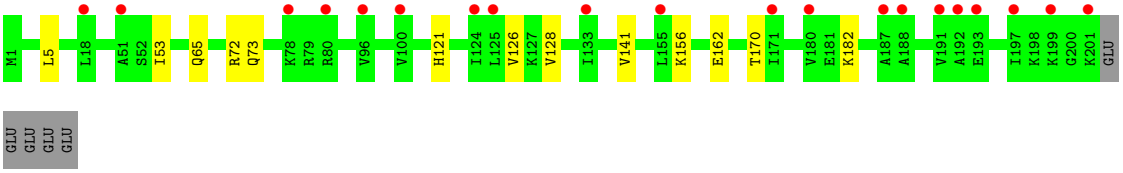
Chain 1Z:



• Molecule 21: 50S ribosomal protein L25

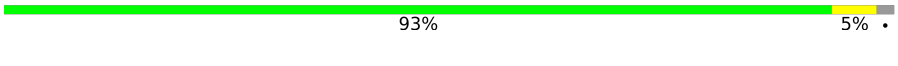
Chain 2Z:





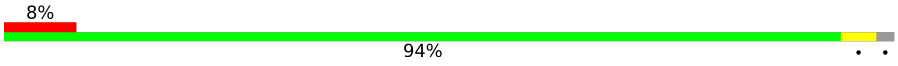
• Molecule 22: 50S ribosomal protein L27

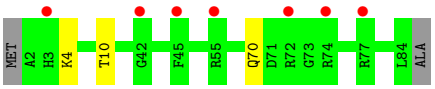
Chain 10:



• Molecule 22: 50S ribosomal protein L27

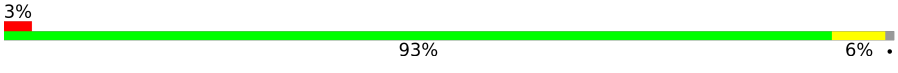
Chain 20:

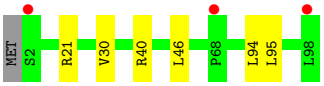




• Molecule 23: 50S ribosomal protein L28

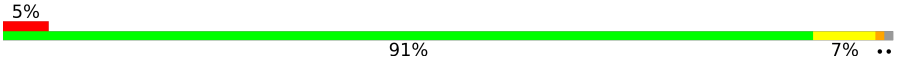
Chain 11:

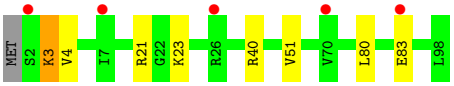




• Molecule 23: 50S ribosomal protein L28

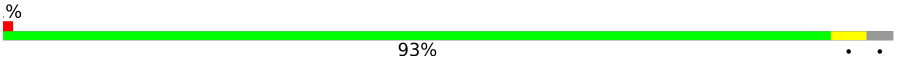
Chain 21:

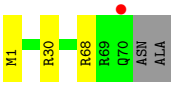




• Molecule 24: 50S ribosomal protein L29

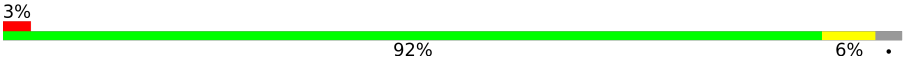
Chain 12:

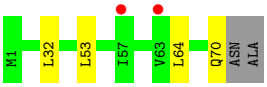




• Molecule 24: 50S ribosomal protein L29

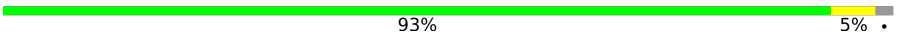
Chain 22:





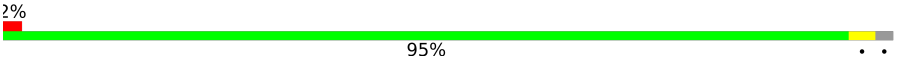
• Molecule 25: 50S ribosomal protein L30

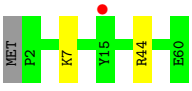
Chain 13:



• Molecule 25: 50S ribosomal protein L30

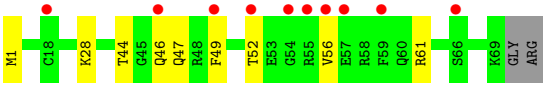
Chain 23:





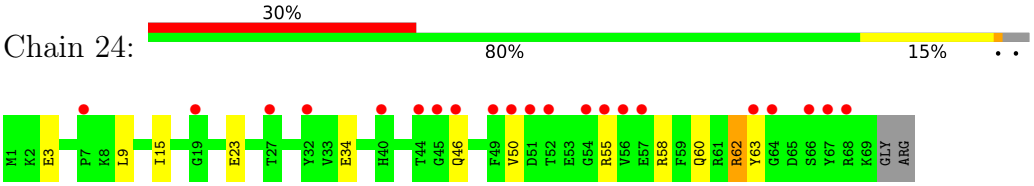
• Molecule 26: 50S ribosomal protein L31

Chain 14:



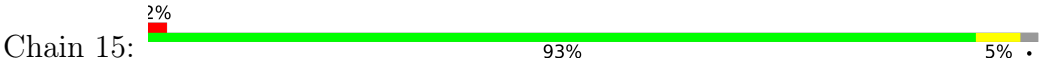
• Molecule 26: 50S ribosomal protein L31

Chain 24:



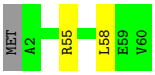
• Molecule 27: 50S ribosomal protein L32

Chain 15:



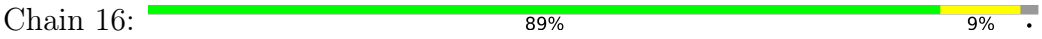
• Molecule 27: 50S ribosomal protein L32

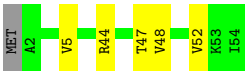
Chain 25:



• Molecule 28: 50S ribosomal protein L33

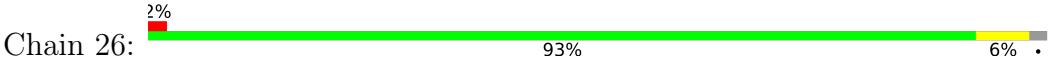
Chain 16:

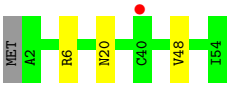




• Molecule 28: 50S ribosomal protein L33

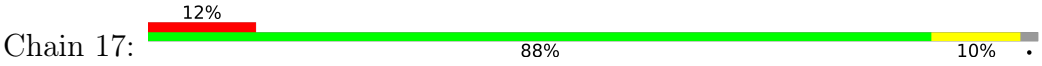
Chain 26:

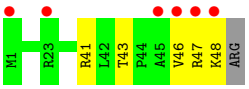




• Molecule 29: 50S ribosomal protein L34

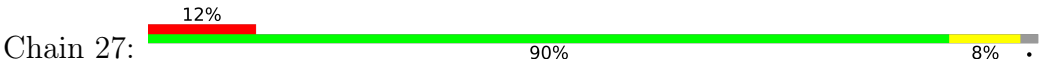
Chain 17:

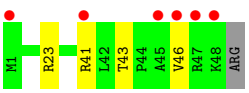




• Molecule 29: 50S ribosomal protein L34

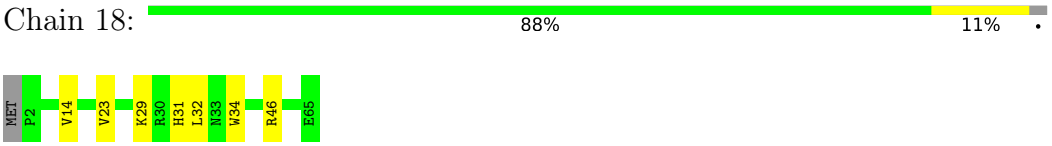
Chain 27:





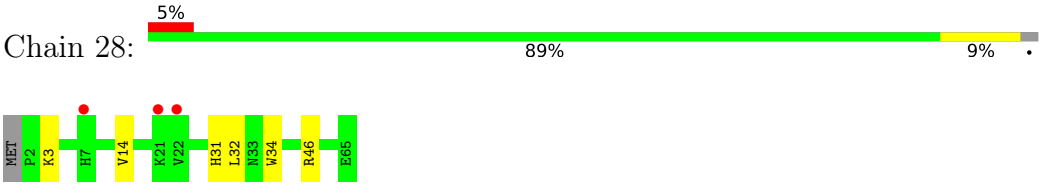
• Molecule 30: 50S ribosomal protein L35

Chain 18:



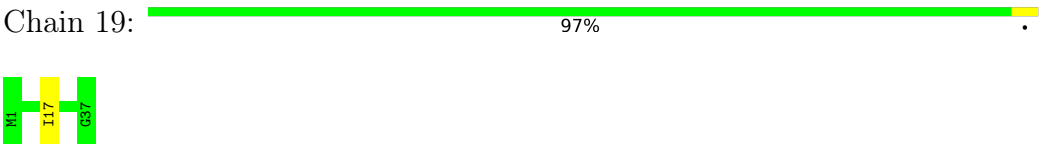
• Molecule 30: 50S ribosomal protein L35

Chain 28:



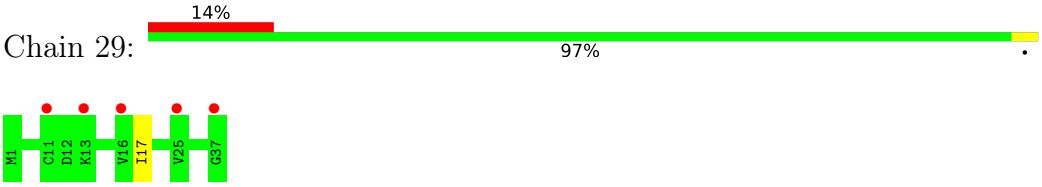
• Molecule 31: 50S ribosomal protein L36

Chain 19:



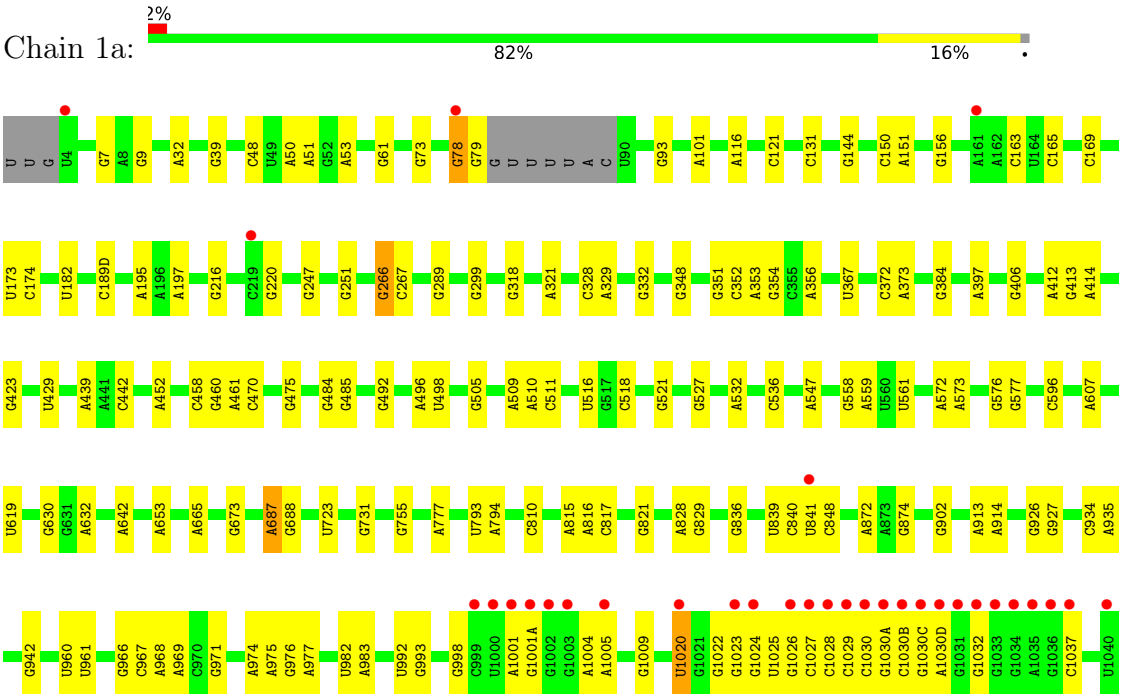
• Molecule 31: 50S ribosomal protein L36

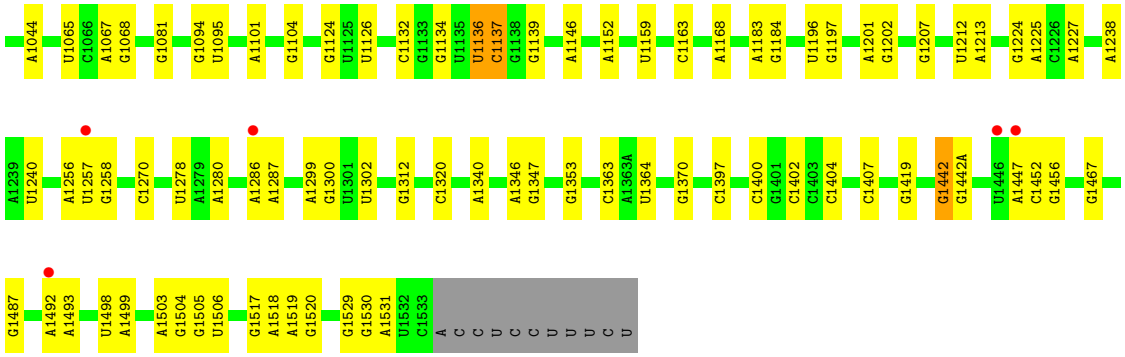
Chain 29:



• Molecule 32: 16S Ribosomal RNA

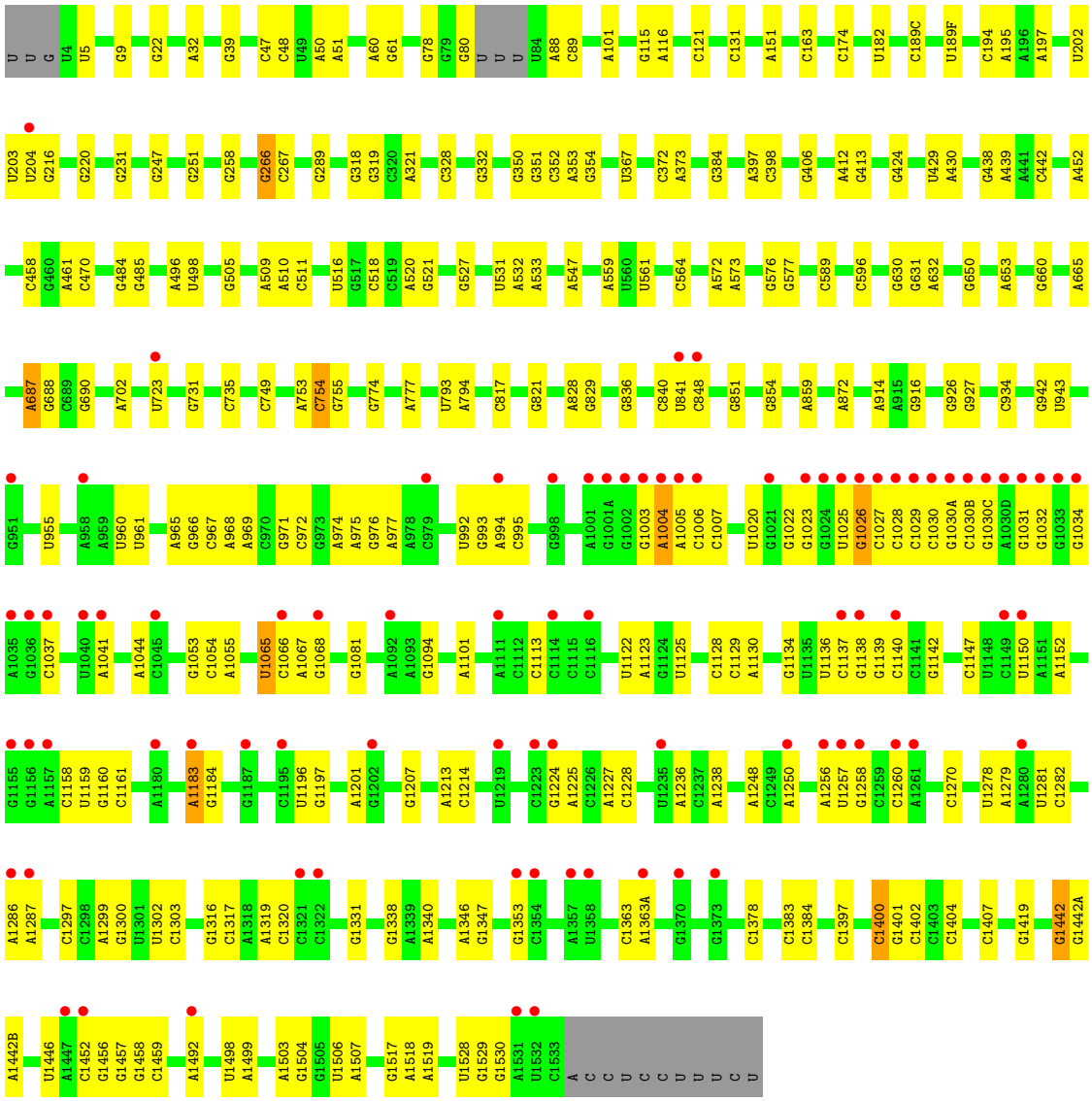
Chain 1a:





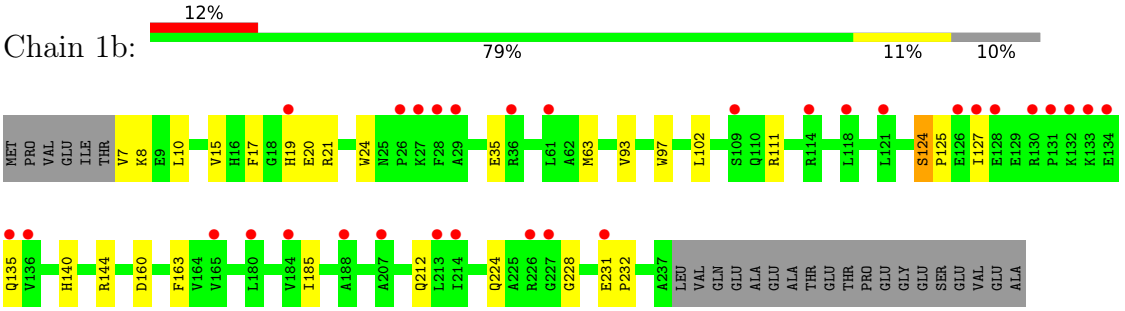
• Molecule 32: 16S Ribosomal RNA

Chain 2a:



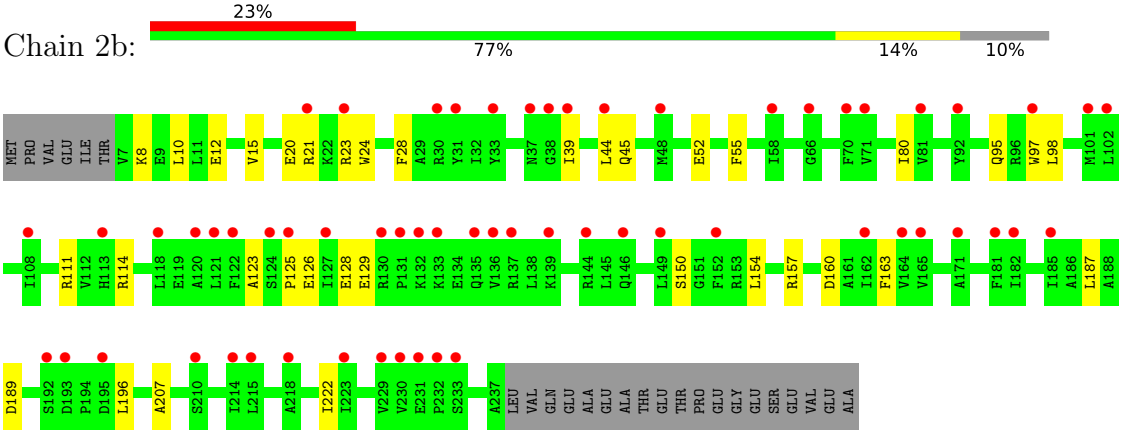
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



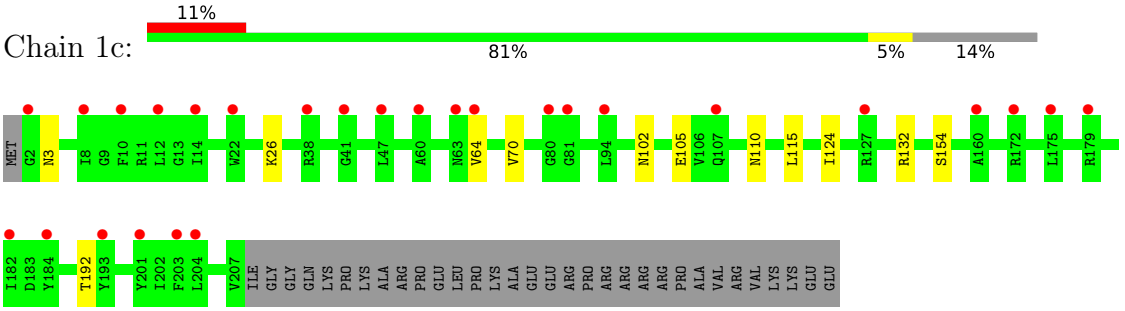
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



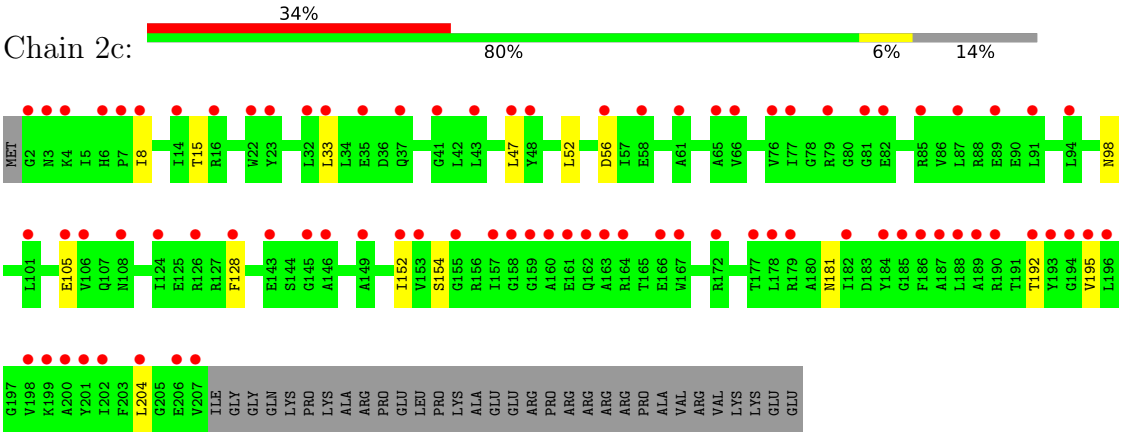
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



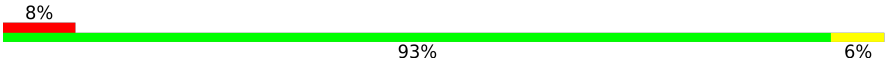
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



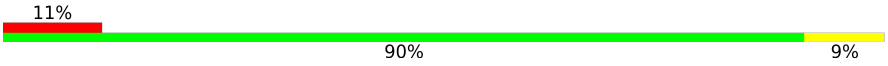
• Molecule 35: 30S ribosomal protein S4

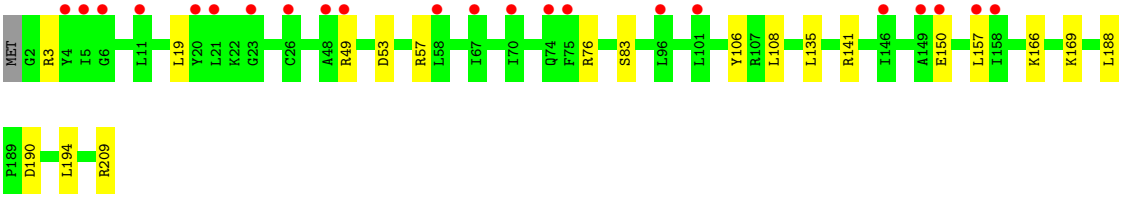
Chain 1d:



• Molecule 35: 30S ribosomal protein S4

Chain 2d:



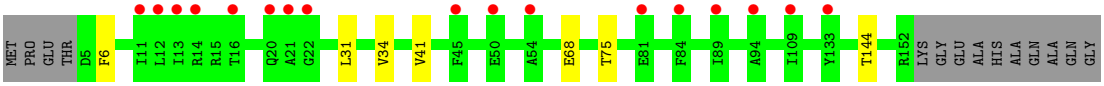


• Molecule 36: 30S ribosomal protein S5

Chain 1e:

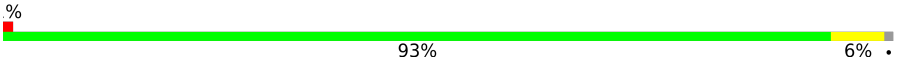
• Molecule 36: 30S ribosomal protein S5

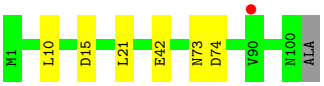
Chain 2e:



• Molecule 37: 30S ribosomal protein S6

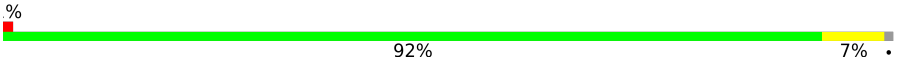
Chain 1f:

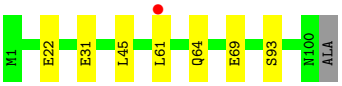




• Molecule 37: 30S ribosomal protein S6

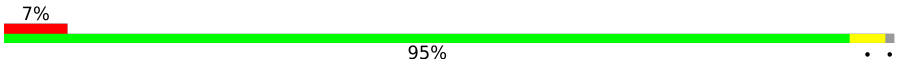
Chain 2f:

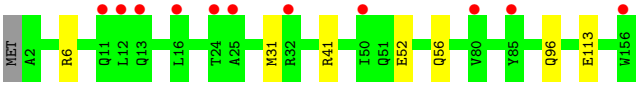




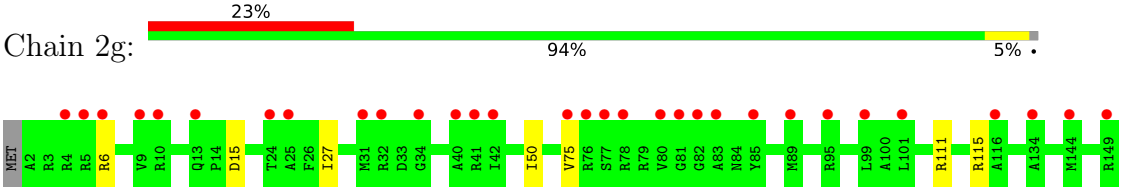
• Molecule 38: 30S ribosomal protein S7

Chain 1g:

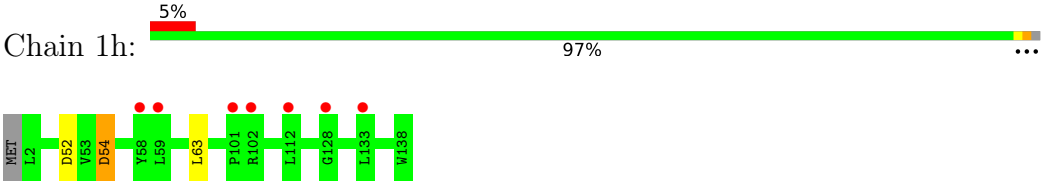




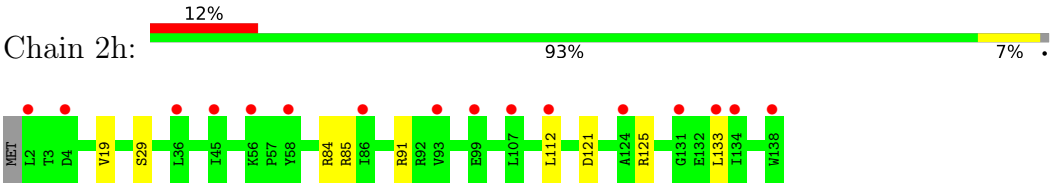
• Molecule 38: 30S ribosomal protein S7



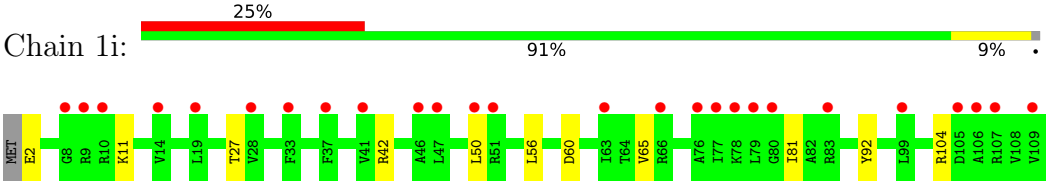
• Molecule 39: 30S ribosomal protein S8



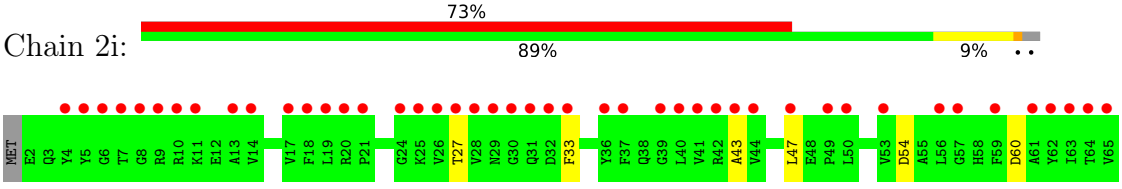
• Molecule 39: 30S ribosomal protein S8

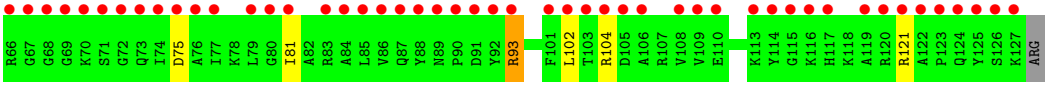


• Molecule 40: 30S ribosomal protein S9

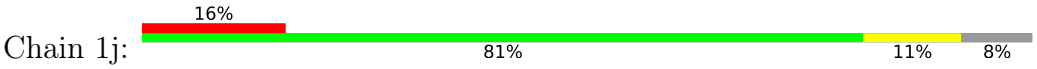


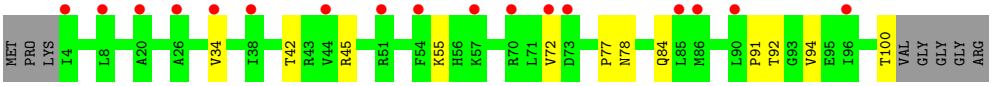
• Molecule 40: 30S ribosomal protein S9



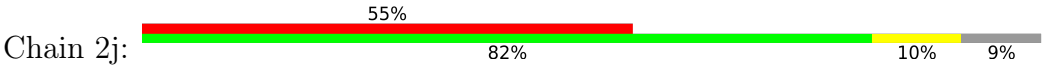


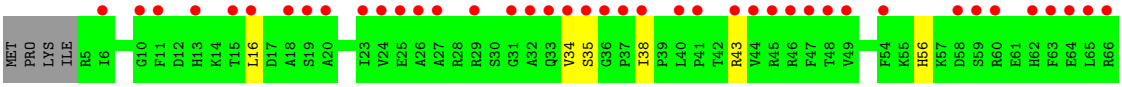
• Molecule 41: 30S ribosomal protein S10

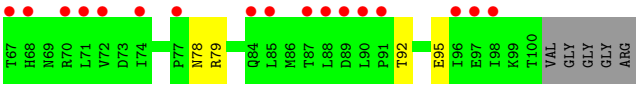




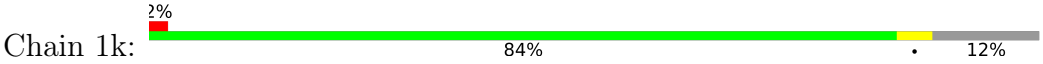
• Molecule 41: 30S ribosomal protein S10

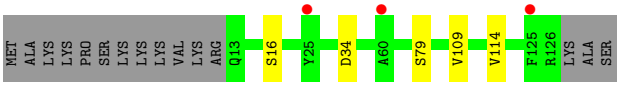




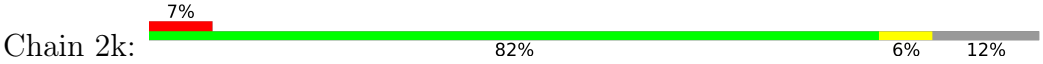


• Molecule 42: 30S ribosomal protein S11

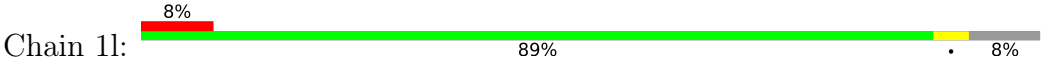


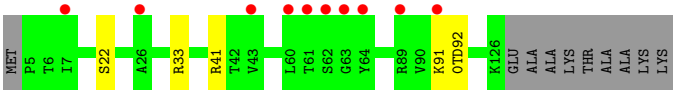


• Molecule 42: 30S ribosomal protein S11

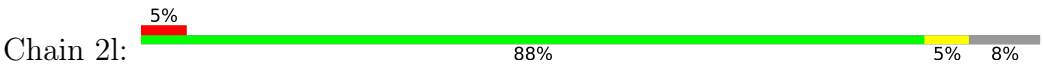


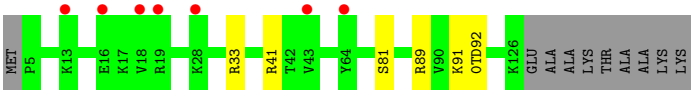
• Molecule 43: 30S ribosomal protein S12





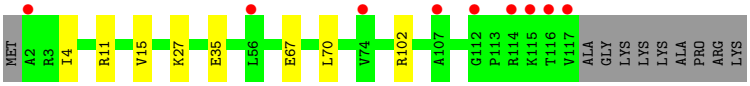
• Molecule 43: 30S ribosomal protein S12





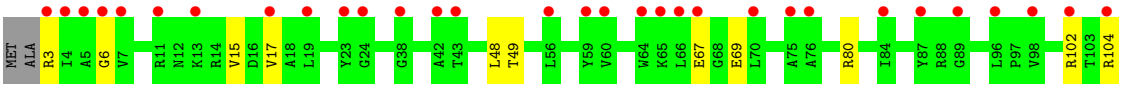
• Molecule 44: 30S ribosomal protein S13

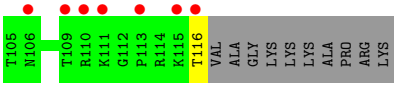
Chain 1m:



• Molecule 44: 30S ribosomal protein S13

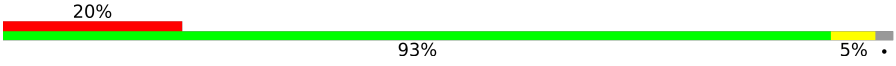
Chain 2m:

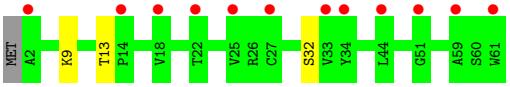




• Molecule 45: 30S ribosomal protein S14 type Z

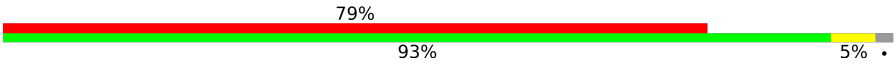
Chain 1n:

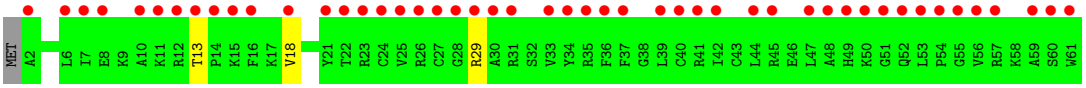




• Molecule 45: 30S ribosomal protein S14 type Z

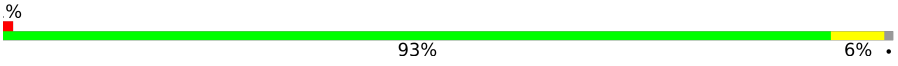
Chain 2n:

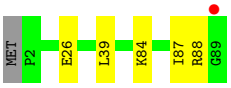




• Molecule 46: 30S ribosomal protein S15

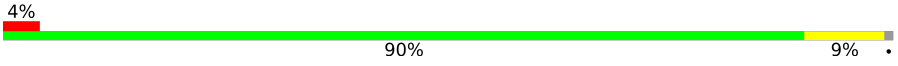
Chain 1o:

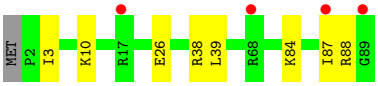




• Molecule 46: 30S ribosomal protein S15

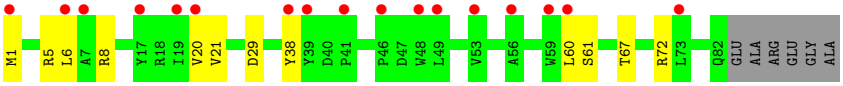
Chain 2o:





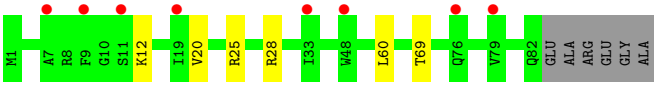
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



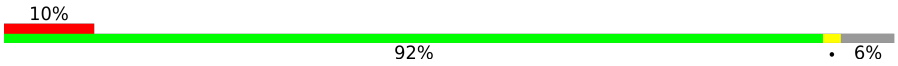
• Molecule 47: 30S ribosomal protein S16

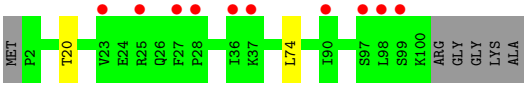
Chain 2p:



• Molecule 48: 30S ribosomal protein S17

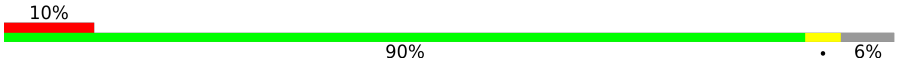
Chain 1q:

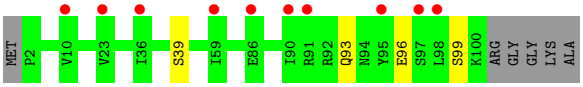




• Molecule 48: 30S ribosomal protein S17

Chain 2q:



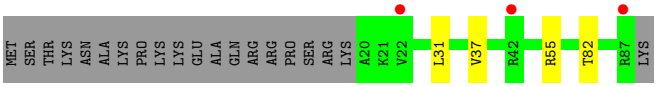


• Molecule 49: 30S ribosomal protein S18

Chain 1r:

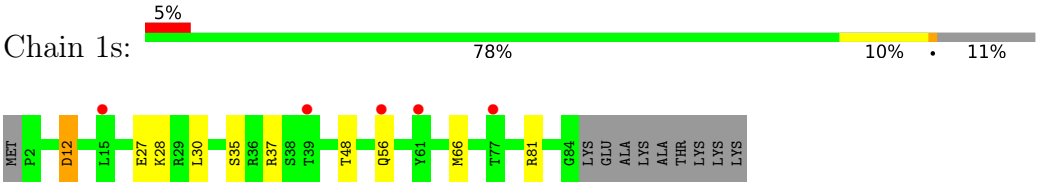
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



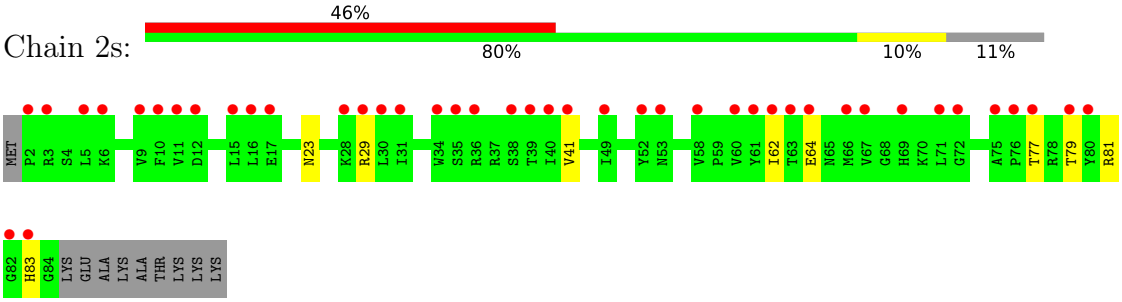
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



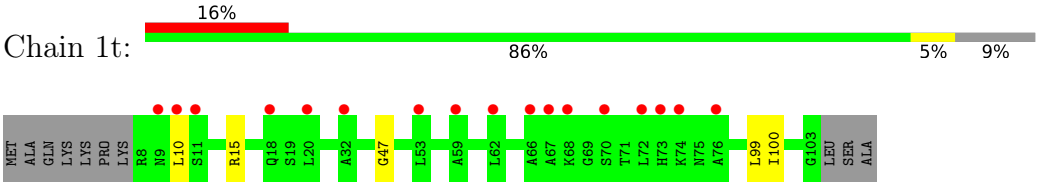
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



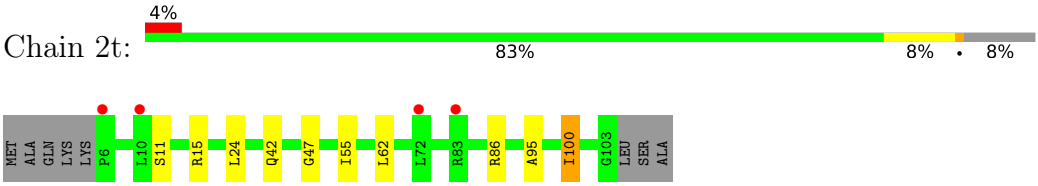
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



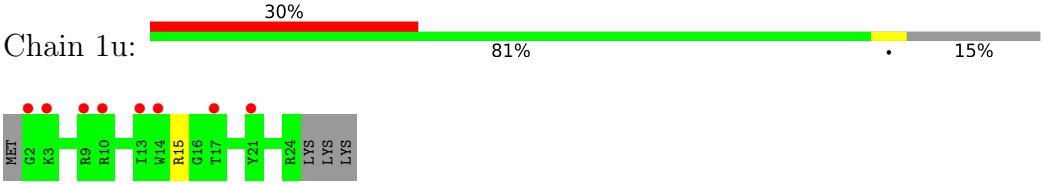
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



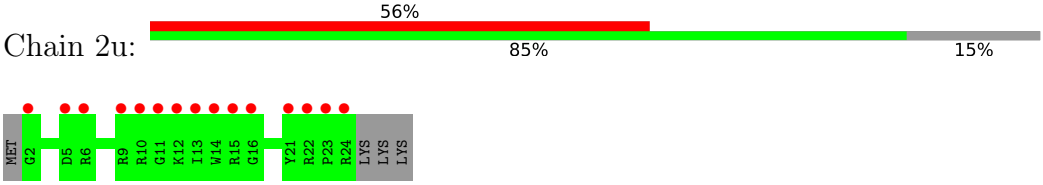
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



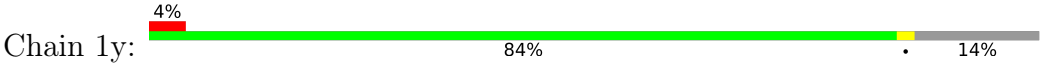
• Molecule 52: 30S ribosomal protein Thx

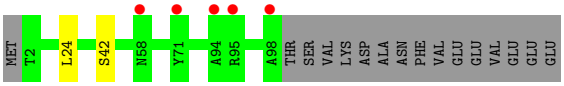
Chain 2u:



• Molecule 53: Ribosome-associated inhibitor A

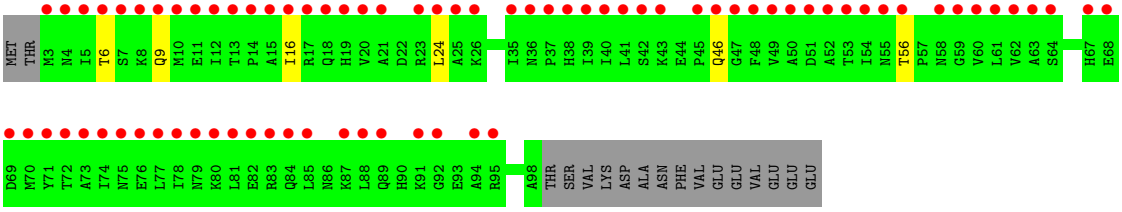
Chain 1y:





• Molecule 53: Ribosome-associated inhibitor A

Chain 2y:



• Molecule 54: A-site Aminoacyl-tRNA Analog

Chain 1w:

• Molecule 54: A-site Aminoacyl-tRNA Analog

Chain 2w:

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

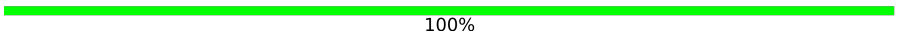
Chain 1x:

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

Chain 2x:

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

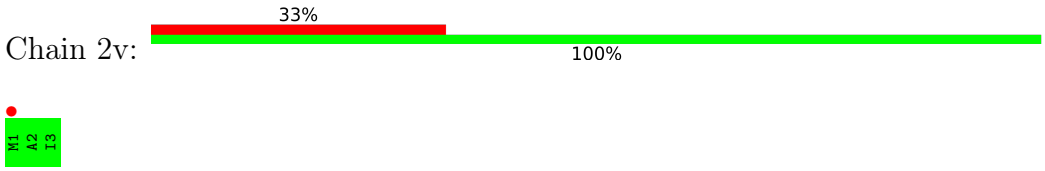
Chain 1v:



There are no outlier residues recorded for this chain.

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

Chain 2v:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.61Å 448.45Å 618.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	187.31 – 2.45 309.23 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (187.31-2.45) 99.9 (309.23-2.45)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.205 , 0.244 0.205 , 0.244	Depositor DCC
R_{free} test set	105390 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	51.3	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	297350	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, G7M, PPU, SF4, OMU, 4OC, MG, 0TD, 2MA, MA6, UR3, 8AN, ZN, M2G, OMG, OMC, 5MC, MPD, 5MU, 2MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.50	1/69031 (0.0%)	0.97	98/107754 (0.1%)
1	2A	0.40	0/68903	0.87	51/107552 (0.0%)
2	1B	0.41	0/2876	0.87	1/4486 (0.0%)
2	2B	0.34	0/2878	0.79	0/4490
3	1D	0.36	0/2181	0.60	0/2940
3	2D	0.32	0/2186	0.53	0/2944
4	1E	0.32	0/1592	0.54	0/2149
4	2E	0.30	0/1592	0.51	0/2149
5	1F	0.34	0/1619	0.55	0/2193
5	2F	0.30	0/1615	0.52	0/2188
6	1G	0.29	0/1451	0.48	0/1961
6	2G	0.31	0/1449	0.46	0/1957
7	1H	0.31	0/1356	0.50	0/1834
7	2H	0.29	0/1350	0.48	0/1826
8	1I	0.28	0/1109	0.49	0/1512
8	2I	0.28	0/1091	0.50	0/1490
9	1N	0.33	0/1148	0.53	0/1547
9	2N	0.28	0/1144	0.46	0/1543
10	1O	0.35	0/943	0.56	0/1269
10	2O	0.31	0/943	0.53	0/1269
11	1P	0.33	0/1152	0.57	0/1533
11	2P	0.31	0/1152	0.54	0/1533
12	1Q	0.37	0/1143	0.54	1/1527 (0.1%)
12	2Q	0.30	0/1143	0.47	0/1527
13	1R	0.33	0/982	0.53	0/1312
13	2R	0.28	0/982	0.50	0/1312
14	1S	0.31	0/887	0.52	0/1180
14	2S	0.30	0/880	0.49	0/1172
15	1T	0.33	0/1105	0.54	0/1477
15	2T	0.30	0/1097	0.48	0/1468
16	1U	0.36	0/977	0.54	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.29	0/977	0.46	0/1301
17	1V	0.34	0/786	0.57	0/1053
17	2V	0.30	0/782	0.53	0/1049
18	1W	0.35	0/897	0.52	0/1205
18	2W	0.31	0/897	0.48	0/1205
19	1X	0.37	0/764	0.54	0/1025
19	2X	0.30	0/764	0.50	0/1025
20	1Y	0.34	0/823	0.56	0/1099
20	2Y	0.30	0/823	0.53	0/1100
21	1Z	0.31	0/1620	0.50	0/2200
21	2Z	0.29	0/1590	0.47	0/2162
22	10	0.34	0/662	0.55	0/881
22	20	0.31	0/659	0.50	0/877
23	11	0.33	0/761	0.53	0/1013
23	21	0.32	0/766	0.52	0/1018
24	12	0.30	0/590	0.49	0/781
24	22	0.29	0/594	0.44	0/785
25	13	0.33	0/474	0.53	0/635
25	23	0.28	0/469	0.47	0/630
26	14	0.31	0/559	0.55	0/754
26	24	0.34	0/549	0.56	0/741
27	15	0.33	0/473	0.60	0/639
27	25	0.29	0/469	0.54	1/635 (0.2%)
28	16	0.33	0/460	0.54	0/613
28	26	0.29	0/456	0.50	0/608
29	17	0.32	0/426	0.56	0/561
29	27	0.27	0/426	0.51	0/561
30	18	0.33	0/525	0.58	0/691
30	28	0.30	0/525	0.51	0/691
31	19	0.35	0/310	0.53	0/407
31	29	0.29	0/310	0.50	0/407
32	1a	0.36	0/35795	0.86	20/55864 (0.0%)
32	2a	0.35	0/35890	0.85	27/56012 (0.0%)
33	1b	0.31	0/1876	0.47	0/2533
33	2b	0.31	0/1860	0.51	1/2518 (0.0%)
34	1c	0.29	0/1582	0.46	0/2137
34	2c	0.30	0/1566	0.47	0/2119
35	1d	0.29	0/1695	0.50	0/2274
35	2d	0.28	0/1698	0.46	0/2277
36	1e	0.29	0/1149	0.51	0/1548
36	2e	0.29	0/1149	0.48	0/1548
37	1f	0.29	0/827	0.47	0/1120
37	2f	0.28	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.28	0/1254	0.42	0/1683
38	2g	0.28	0/1248	0.42	0/1676
39	1h	0.28	0/1118	0.48	0/1506
39	2h	0.28	0/1108	0.47	0/1494
40	1i	0.29	0/1005	0.47	0/1351
40	2i	0.30	0/985	0.47	0/1329
41	1j	0.28	0/732	0.49	0/993
41	2j	0.29	0/723	0.49	0/984
42	1k	0.28	0/849	0.49	0/1150
42	2k	0.29	0/848	0.54	0/1149
43	1l	0.29	0/937	0.51	0/1260
43	2l	0.29	0/937	0.50	0/1260
44	1m	0.27	0/924	0.48	0/1242
44	2m	0.29	0/905	0.49	0/1217
45	1n	0.31	0/501	0.46	0/664
45	2n	0.29	0/501	0.45	0/664
46	1o	0.29	0/739	0.45	0/985
46	2o	0.27	0/739	0.42	0/985
47	1p	0.29	0/697	0.51	0/939
47	2p	0.28	0/693	0.50	0/935
48	1q	0.28	0/836	0.46	0/1117
48	2q	0.29	0/836	0.46	0/1117
49	1r	0.28	0/560	0.48	0/746
49	2r	0.29	0/560	0.47	0/746
50	1s	0.28	0/663	0.47	0/895
50	2s	0.29	0/660	0.49	0/893
51	1t	0.28	0/734	0.43	0/969
51	2t	0.27	0/736	0.42	0/976
52	1u	0.28	0/203	0.47	0/266
52	2u	0.25	0/203	0.47	0/266
53	1y	0.27	0/776	0.48	0/1048
53	2y	0.28	0/761	0.45	0/1030
54	1w	0.60	0/44	0.93	0/67
54	2w	0.40	0/44	1.07	0/67
55	1x	0.56	0/44	1.06	0/67
55	2x	0.46	0/44	1.17	0/67
56	1v	0.23	0/20	0.55	0/25
56	2v	0.27	0/20	0.49	0/25
All	All	0.39	1/310246 (0.0%)	0.81	200/463673 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	330	A	N9-C4	-6.61	1.33	1.37

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	512	G	O4'-C1'-N9	10.72	116.78	108.20
1	1A	570	G	C5-C6-O6	-10.04	122.58	128.60
1	1A	330	A	C2-N3-C4	-9.66	105.77	110.60
1	1A	1352	U	O5'-P-OP1	-9.60	97.06	105.70
32	1a	299	G	C5-C6-O6	-9.37	122.98	128.60
1	1A	2430	A	O5'-P-OP2	-9.23	97.39	105.70
1	1A	1075	C	N1-C2-O2	9.21	124.43	118.90
1	1A	1139	G	O5'-P-OP2	-9.00	97.60	105.70
1	1A	330	A	N1-C2-N3	8.82	133.71	129.30
1	1A	1653	G	C8-N9-C4	-8.77	102.89	106.40
1	2A	1614	A	O5'-P-OP1	-8.70	97.87	105.70
1	1A	948	G	O5'-P-OP1	-8.49	98.06	105.70
1	2A	1092	C	N1-C2-O2	8.48	123.99	118.90
1	1A	588	U	O5'-P-OP2	-8.02	98.48	105.70
1	1A	1372	U	C5-C4-O4	-7.98	121.11	125.90
32	1a	558	G	O5'-P-OP1	-7.97	98.53	105.70
1	1A	1372	U	N3-C4-O4	7.92	124.94	119.40
1	1A	575	A	O5'-P-OP1	-7.85	98.64	105.70
1	1A	1086	A	N1-C6-N6	-7.69	113.99	118.60
1	1A	1602	U	N3-C4-O4	-7.63	114.06	119.40
1	1A	1997	G	O5'-P-OP2	-7.54	98.91	105.70
1	2A	1092	C	C2-N1-C1'	7.42	126.96	118.80
1	2A	576	U	O5'-P-OP1	-7.41	99.03	105.70
1	2A	277	C	N1-C2-O2	7.40	123.34	118.90
1	1A	2023	G	O5'-P-OP1	-7.28	99.14	105.70
1	1A	570	G	C5-C6-N1	7.20	115.10	111.50
32	2a	1004	A	O4'-C1'-N9	7.17	113.94	108.20
32	2a	266	G	P-O3'-C3'	7.15	128.28	119.70
1	1A	2554	U	O5'-P-OP1	-7.12	99.29	105.70
1	1A	751	A	O5'-P-OP1	-7.09	99.32	105.70
1	1A	946	G	O5'-P-OP1	-7.01	99.39	105.70
1	1A	226	G	O4'-C1'-N9	6.96	113.77	108.20
1	2A	512	G	O4'-C1'-N9	6.92	113.73	108.20
1	2A	751	A	O5'-P-OP1	-6.91	99.48	105.70
1	1A	2848	G	O4'-C1'-N9	6.90	113.72	108.20
1	1A	527	C	N1-C2-O2	-6.85	114.79	118.90
1	2A	963	U	O5'-P-OP2	-6.83	99.55	105.70
32	1a	1137	C	C6-N1-C2	-6.80	117.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	955	U	C5-C4-O4	6.79	129.97	125.90
1	1A	1300	U	P-O3'-C3'	6.78	127.84	119.70
32	2a	1003	G	N3-C4-C5	-6.78	125.21	128.60
1	2A	2036	C	O5'-P-OP1	-6.72	99.65	105.70
1	1A	2023	G	O5'-P-OP2	6.70	118.74	110.70
1	2A	2689	U	N3-C2-O2	-6.69	117.52	122.20
1	1A	2249	U	N3-C4-O4	-6.66	114.74	119.40
1	2A	1092	C	C6-N1-C2	-6.63	117.65	120.30
1	1A	801	G	O5'-P-OP2	-6.56	99.80	105.70
1	1A	1791	A	O5'-P-OP1	-6.51	99.84	105.70
1	1A	1936	A	O4'-C1'-N9	6.51	113.41	108.20
1	2A	1092	C	N3-C2-O2	-6.50	117.35	121.90
1	1A	570	G	N9-C4-C5	-6.49	102.80	105.40
1	2A	214	G	O4'-C1'-N9	6.41	113.33	108.20
1	1A	2036	C	O5'-P-OP1	-6.40	99.94	105.70
1	2A	1076	C	OP1-P-O3'	6.34	119.14	105.20
1	1A	787	U	O5'-P-OP1	-6.32	100.01	105.70
1	1A	1075	C	C2-N3-C4	6.32	123.06	119.90
1	1A	2103	C	N1-C2-O2	6.31	122.69	118.90
1	2A	2137	C	C5-C4-N4	6.28	124.60	120.20
32	2a	955	U	C2-N3-C4	6.24	130.75	127.00
1	1A	645	C	C2-N1-C1'	6.17	125.59	118.80
32	2a	754	C	C2-N1-C1'	6.17	125.59	118.80
1	1A	576	U	O5'-P-OP1	-6.16	100.15	105.70
1	1A	2711	A	O5'-P-OP2	-6.16	100.16	105.70
1	1A	746	A	O4'-C1'-N9	6.14	113.11	108.20
32	2a	1225	A	C6-N1-C2	6.12	122.27	118.60
32	1a	1020	U	N1-C2-O2	6.10	127.07	122.80
1	1A	2577	A	O5'-P-OP1	-6.09	100.21	105.70
1	1A	1315	C	O5'-P-OP2	-6.09	100.22	105.70
1	1A	372	G	O4'-C1'-N9	6.08	113.06	108.20
1	1A	1075	C	N3-C2-O2	-6.07	117.65	121.90
1	1A	845	G	O4'-C1'-N9	6.06	113.05	108.20
1	1A	570	G	C8-N9-C4	5.95	108.78	106.40
1	2A	2103	C	C2-N3-C4	5.93	122.86	119.90
1	2A	2153	G	C5-C6-O6	-5.91	125.06	128.60
32	1a	1137	C	C5-C6-N1	5.90	123.95	121.00
1	1A	975	C	O5'-P-OP1	-5.89	100.40	105.70
1	1A	614	U	N3-C2-O2	-5.87	118.09	122.20
1	1A	1648	C	O5'-P-OP1	-5.87	100.42	105.70
1	1A	1210	A	P-O3'-C3'	5.86	126.74	119.70
1	1A	1696	G	O5'-P-OP2	-5.86	100.43	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	115	G	P-O3'-C3'	5.85	126.72	119.70
32	2a	1225	A	C5-C6-N6	5.83	128.36	123.70
1	1A	573	G	C5-C6-O6	-5.83	125.10	128.60
32	2a	1158	C	C2-N1-C1'	5.82	125.20	118.80
1	1A	570	G	C4-C5-N7	5.82	113.13	110.80
1	2A	845	G	O4'-C1'-N9	5.81	112.85	108.20
1	2A	1313	U	C2-N1-C1'	5.81	124.67	117.70
1	2A	2249	U	N3-C4-O4	-5.80	115.34	119.40
1	2A	277	C	N3-C2-O2	-5.79	117.85	121.90
1	2A	2689	U	P-O3'-C3'	5.79	126.64	119.70
1	1A	607	U	O5'-P-OP1	-5.76	100.51	105.70
1	1A	1647	G	O4'-C1'-N9	-5.75	103.60	108.20
1	2A	2153	G	N1-C6-O6	5.74	123.35	119.90
1	1A	568	U	N3-C4-C5	5.72	118.03	114.60
32	1a	1067	A	P-O3'-C3'	5.71	126.56	119.70
1	2A	1065	U	P-O3'-C3'	5.70	126.54	119.70
1	1A	12	U	C2-N1-C1'	5.70	124.54	117.70
32	1a	299	G	C4-C5-N7	5.69	113.08	110.80
1	1A	1782	C	O5'-P-OP1	-5.68	100.59	105.70
1	2A	948	G	O5'-P-OP1	-5.67	100.60	105.70
1	1A	195	A	C5-N7-C8	5.67	106.73	103.90
1	2A	2137	C	N3-C4-N4	-5.63	114.06	118.00
1	1A	1416	G	O4'-C1'-N9	5.59	112.67	108.20
1	1A	1653	G	N3-C4-C5	-5.59	125.81	128.60
1	1A	1220	A	O5'-P-OP2	-5.57	100.69	105.70
1	2A	752	A	P-O3'-C3'	5.57	126.38	119.70
32	2a	687	A	P-O3'-C3'	5.56	126.37	119.70
33	2b	129	GLU	C-N-CA	5.56	135.59	121.70
32	2a	1003	G	N3-C4-N9	5.55	129.33	126.00
1	2A	847	U	C2-N1-C1'	5.54	124.34	117.70
32	2a	1158	C	N1-C2-O2	5.52	122.21	118.90
1	1A	12	U	N3-C2-O2	-5.51	118.34	122.20
32	2a	1183	A	P-O3'-C3'	5.51	126.31	119.70
1	1A	271(Y)	U	O4'-C1'-N1	5.50	112.60	108.20
32	1a	299	G	N1-C6-O6	5.50	123.20	119.90
1	2A	574	C	N1-C2-O2	-5.48	115.61	118.90
1	2A	2554	U	O5'-P-OP1	-5.47	100.78	105.70
1	2A	2126	A	P-O3'-C3'	5.43	126.22	119.70
32	1a	1136	U	N1-C2-O2	5.42	126.60	122.80
1	1A	1839	G	O5'-P-OP2	-5.42	100.83	105.70
1	1A	512	G	C5-N7-C8	5.40	107.00	104.30
1	2A	1092	C	C5-C6-N1	5.40	123.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1150	U	C5-C4-O4	5.39	129.14	125.90
1	2A	746	A	O4'-C1'-N9	5.38	112.50	108.20
1	2A	214	G	C4-N9-C1'	-5.38	119.51	126.50
1	1A	2492	U	O5'-P-OP1	-5.37	100.86	105.70
1	1A	996	A	O5'-P-OP1	-5.37	100.87	105.70
32	1a	73	G	C5-C6-O6	5.37	131.82	128.60
32	1a	687	A	P-O3'-C3'	5.37	126.14	119.70
1	2A	1936	A	O4'-C1'-N9	5.37	112.49	108.20
1	1A	2032	G	C5-N7-C8	5.34	106.97	104.30
1	1A	740	U	O5'-P-OP2	-5.34	100.90	105.70
1	2A	2103	C	C5-C4-N4	5.33	123.93	120.20
1	1A	2371	G	C5-C6-N1	5.32	114.16	111.50
1	1A	847	U	C2-N1-C1'	5.31	124.07	117.70
32	2a	1158	C	C6-N1-C2	-5.31	118.18	120.30
32	1a	299	G	N9-C4-C5	-5.31	103.28	105.40
1	2A	1992	G	P-O3'-C3'	5.30	126.06	119.70
1	1A	383	U	O4'-C1'-N1	5.30	112.44	108.20
1	2A	794	G	O5'-P-OP2	-5.28	100.95	105.70
32	1a	78	G	O4'-C1'-N9	5.28	112.42	108.20
1	1A	570	G	N3-C4-N9	5.27	129.16	126.00
1	1A	2682	U	O5'-P-OP2	-5.26	100.97	105.70
32	2a	1065	U	P-O3'-C3'	5.25	126.00	119.70
1	1A	774	A	C8-N9-C4	-5.24	103.70	105.80
1	2A	2689	U	N1-C2-O2	5.24	126.47	122.80
32	2a	60	A	P-O3'-C3'	5.22	125.97	119.70
1	2A	570	G	C5-C6-O6	-5.22	125.47	128.60
32	1a	266	G	N3-C4-C5	-5.22	125.99	128.60
1	1A	1249	U	O5'-P-OP1	-5.21	101.01	105.70
1	1A	195	A	P-O3'-C3'	5.21	125.95	119.70
1	1A	668	G	OP2-P-O3'	5.21	116.67	105.20
1	2A	2108	C	C2-N3-C4	5.21	122.50	119.90
32	1a	913	A	P-O3'-C3'	5.20	125.94	119.70
1	1A	2689	U	P-O3'-C3'	5.20	125.94	119.70
32	2a	1067	A	P-O3'-C3'	5.20	125.94	119.70
1	1A	1614	A	O5'-P-OP1	-5.20	101.02	105.70
2	1B	41	U	C5-C6-N1	-5.20	120.10	122.70
1	2A	195	A	P-O3'-C3'	5.19	125.93	119.70
1	1A	12	U	N1-C2-O2	5.19	126.44	122.80
32	2a	266	G	OP2-P-O3'	5.19	116.62	105.20
1	2A	34	C	C6-N1-C2	-5.19	118.22	120.30
1	2A	2711	A	O5'-P-OP1	-5.19	101.03	105.70
1	1A	1653	G	N9-C4-C5	5.18	107.47	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1123	A	C5-C6-N6	5.16	127.83	123.70
1	2A	2153	G	C6-C5-N7	-5.16	127.30	130.40
32	1a	872	A	O4'-C1'-N9	5.16	112.33	108.20
32	1a	78	G	C8-N9-C1'	5.15	133.70	127.00
32	2a	1442	G	N3-C4-C5	-5.15	126.03	128.60
1	1A	784	A	OP1-P-O3'	5.13	116.49	105.20
32	1a	266	G	P-O3'-C3'	5.13	125.86	119.70
32	2a	754	C	N1-C2-O2	5.13	121.98	118.90
1	1A	1776	G	O5'-P-OP2	-5.12	101.09	105.70
1	1A	2517	C	O4'-C1'-N1	5.12	112.30	108.20
1	1A	1493	C	C2-N1-C1'	5.11	124.42	118.80
32	1a	1442	G	P-O3'-C3'	5.11	125.84	119.70
1	1A	783	A	C2-N3-C4	5.11	113.16	110.60
1	1A	1602	U	N3-C4-C5	5.10	117.66	114.60
1	1A	2103	C	C2-N3-C4	5.10	122.45	119.90
1	1A	330	A	C5-N7-C8	-5.10	101.35	103.90
1	2A	2061	G	O5'-P-OP2	-5.10	101.11	105.70
1	1A	1847	A	O4'-C1'-N9	5.06	112.25	108.20
32	2a	1331	G	O4'-C1'-N9	5.06	112.25	108.20
1	1A	1493	C	N1-C2-O2	5.06	121.94	118.90
1	1A	2073	C	OP2-P-O3'	5.05	116.31	105.20
1	2A	1060	U	C2-N1-C1'	5.05	123.76	117.70
1	1A	1314	C	C2-N1-C1'	5.05	124.35	118.80
32	2a	1026	G	C4-N9-C1'	5.05	133.06	126.50
32	1a	1201	A	P-O3'-C3'	5.04	125.75	119.70
27	25	58	LEU	CA-CB-CG	5.04	126.90	115.30
32	2a	1378	C	C2-N1-C1'	5.04	124.34	118.80
1	2A	1380	G	O5'-P-OP2	-5.04	101.17	105.70
1	2A	214	G	C8-N9-C1'	5.04	133.55	127.00
1	1A	645	C	C5-C6-N1	5.03	123.51	121.00
12	1Q	82	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	2A	226	G	O4'-C1'-N9	5.02	112.22	108.20
1	1A	1253	A	C5-N7-C8	5.02	106.41	103.90
1	2A	2287	A	O4'-C1'-N9	5.02	112.21	108.20
1	1A	1906	G	O5'-P-OP1	-5.01	101.19	105.70
32	2a	1123	A	C6-N1-C2	5.01	121.61	118.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	260 (95%)	13 (5%)	0	100 100
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100 100
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	29 34
4	2E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29 34
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	29 34
5	2F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	29 34
6	1G	179/182 (98%)	159 (89%)	18 (10%)	2 (1%)	14 14
6	2G	179/182 (98%)	157 (88%)	19 (11%)	3 (2%)	9 7
7	1H	172/180 (96%)	162 (94%)	8 (5%)	2 (1%)	13 12
7	2H	171/180 (95%)	148 (86%)	21 (12%)	2 (1%)	13 12
8	1I	145/148 (98%)	130 (90%)	14 (10%)	1 (1%)	22 25
8	2I	144/148 (97%)	128 (89%)	13 (9%)	3 (2%)	7 5
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100 100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100 100
10	1O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19 22
10	2O	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	9 7
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22 25
11	2P	147/150 (98%)	139 (95%)	6 (4%)	2 (1%)	11 9
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100 100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100 100
13	1R	116/118 (98%)	114 (98%)	2 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100 100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100 100
14	2S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	17 19
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100 100
15	2T	129/146 (88%)	121 (94%)	6 (5%)	2 (2%)	9 8
16	1U	114/118 (97%)	114 (100%)	0	0	100 100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100 100
17	1V	99/101 (98%)	96 (97%)	3 (3%)	0	100 100
17	2V	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	7 5
18	1W	110/113 (97%)	110 (100%)	0	0	100 100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
19	1X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	14 14
19	2X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	14 14
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100 100
20	2Y	105/110 (96%)	95 (90%)	10 (10%)	0	100 100
21	1Z	201/206 (98%)	187 (93%)	12 (6%)	2 (1%)	15 16
21	2Z	199/206 (97%)	186 (94%)	11 (6%)	2 (1%)	15 16
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100 100
22	20	81/85 (95%)	78 (96%)	2 (2%)	1 (1%)	13 12
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100 100
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14 14
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
26	14	67/71 (94%)	47 (70%)	16 (24%)	4 (6%)	1 0
26	24	67/71 (94%)	47 (70%)	18 (27%)	2 (3%)	4 1
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
27	25	57/60 (95%)	55 (96%)	2 (4%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	17	46/49 (94%)	45 (98%)	0	1 (2%)	6 4
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100 100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100 100
30	28	62/65 (95%)	62 (100%)	0	0	100 100
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
33	1b	229/256 (90%)	191 (83%)	28 (12%)	10 (4%)	2 1
33	2b	229/256 (90%)	199 (87%)	21 (9%)	9 (4%)	3 1
34	1c	204/239 (85%)	191 (94%)	12 (6%)	1 (0%)	29 34
34	2c	204/239 (85%)	179 (88%)	24 (12%)	1 (0%)	29 34
35	1d	206/209 (99%)	196 (95%)	10 (5%)	0	100 100
35	2d	206/209 (99%)	200 (97%)	6 (3%)	0	100 100
36	1e	146/162 (90%)	141 (97%)	4 (3%)	1 (1%)	22 25
36	2e	146/162 (90%)	141 (97%)	5 (3%)	0	100 100
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100 100
38	1g	153/156 (98%)	146 (95%)	7 (5%)	0	100 100
38	2g	153/156 (98%)	144 (94%)	9 (6%)	0	100 100
39	1h	135/138 (98%)	127 (94%)	7 (5%)	1 (1%)	22 25
39	2h	135/138 (98%)	126 (93%)	9 (7%)	0	100 100
40	1i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	19 22
40	2i	124/128 (97%)	106 (86%)	15 (12%)	3 (2%)	6 3
41	1j	95/105 (90%)	82 (86%)	9 (10%)	4 (4%)	3 1
41	2j	94/105 (90%)	81 (86%)	9 (10%)	4 (4%)	2 1
42	1k	112/129 (87%)	104 (93%)	8 (7%)	0	100 100
42	2k	112/129 (87%)	106 (95%)	3 (3%)	3 (3%)	5 2
43	1l	119/132 (90%)	113 (95%)	5 (4%)	1 (1%)	19 22
43	2l	119/132 (90%)	111 (93%)	7 (6%)	1 (1%)	19 22
44	1m	114/126 (90%)	104 (91%)	9 (8%)	1 (1%)	17 19
44	2m	112/126 (89%)	96 (86%)	13 (12%)	3 (3%)	5 2
45	1n	58/61 (95%)	57 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100 100
46	1o	86/89 (97%)	82 (95%)	2 (2%)	2 (2%)	6 4
46	2o	86/89 (97%)	81 (94%)	3 (4%)	2 (2%)	6 4
47	1p	80/88 (91%)	73 (91%)	7 (9%)	0	100 100
47	2p	80/88 (91%)	75 (94%)	5 (6%)	0	100 100
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100 100
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100 100
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100 100
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100 100
50	1s	81/93 (87%)	76 (94%)	3 (4%)	2 (2%)	5 3
50	2s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	13 12
51	1t	94/106 (89%)	88 (94%)	3 (3%)	3 (3%)	4 1
51	2t	96/106 (91%)	89 (93%)	4 (4%)	3 (3%)	4 1
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
53	1y	95/113 (84%)	92 (97%)	3 (3%)	0	100 100
53	2y	94/113 (83%)	88 (94%)	6 (6%)	0	100 100
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%)	10886 (94%)	657 (6%)	100 (1%)	17 19

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	51	ARG
8	1I	86	THR
21	1Z	53	ILE
33	1b	21	ARG
33	1b	127	ILE
41	1j	55	LYS
43	1l	91	LYS
5	2F	130	ALA
6	2G	81	LYS
7	2H	126	PRO

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Mol	Chain	Res	Type
15	2T	128	GLU
26	24	62	ARG
41	2j	56	HIS
41	2j	79	ARG
43	2l	91	LYS
46	2o	88	ARG
19	1X	94	GLY
26	14	47	GLN
26	14	61	ARG
40	1i	11	LYS
44	1m	67	GLU
6	2G	47	LYS
15	2T	127	ALA
17	2V	100	ARG
33	2b	10	LEU
33	2b	21	ARG
33	2b	128	GLU
40	2i	43	ALA
40	2i	54	ASP
50	2s	29	ARG
51	2t	100	ILE
4	1E	52	LEU
6	1G	49	ASP
26	14	44	THR
29	17	47	ARG
33	1b	8	LYS
34	1c	3	ASN
41	1j	77	PRO
46	1o	88	ARG
50	1s	12	ASP
50	1s	27	GLU
51	1t	47	GLY
6	2G	43	LEU
7	2H	65	HIS
8	2I	97	ILE
10	2O	5	GLN
23	21	3	LYS
33	2b	20	GLU
34	2c	98	ASN
44	2m	67	GLU
51	2t	95	ALA
7	1H	126	PRO

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Mol	Chain	Res	Type
10	1O	5	GLN
33	1b	17	PHE
33	1b	20	GLU
41	1j	78	ASN
51	1t	99	LEU
4	2E	52	LEU
8	2I	98	ALA
10	2O	29	ASN
11	2P	29	LYS
11	2P	122	PRO
17	2V	79	VAL
33	2b	95	GLN
33	2b	123	ALA
33	2b	207	ALA
41	2j	35	SER
42	2k	15	ALA
44	2m	6	GLY
44	2m	80	ARG
33	1b	124	SER
39	1h	54	ASP
21	2Z	156	LYS
22	20	4	LYS
26	24	55	ARG
33	2b	125	PRO
33	2b	126	GLU
40	2i	93	ARG
41	2j	78	ASN
42	2k	90	GLY
51	2t	47	GLY
7	1H	159	GLU
11	1P	29	LYS
21	1Z	52	SER
26	14	52	THR
33	1b	231	GLU
46	1o	87	ILE
51	1t	100	ILE
14	2S	82	ILE
33	1b	228	GLY
36	1e	96	PRO
21	2Z	53	ILE
33	1b	232	PRO
42	2k	105	VAL

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Mol	Chain	Res	Type
46	2o	87	ILE
41	1j	91	PRO
8	2I	84	GLY
19	2X	94	GLY
33	1b	125	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	214/218 (98%)	201 (94%)	13 (6%)	18 24
3	2D	215/218 (99%)	197 (92%)	18 (8%)	11 12
4	1E	164/166 (99%)	156 (95%)	8 (5%)	25 32
4	2E	164/166 (99%)	154 (94%)	10 (6%)	18 24
5	1F	160/166 (96%)	141 (88%)	19 (12%)	5 4
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8 9
6	1G	144/156 (92%)	131 (91%)	13 (9%)	9 10
6	2G	142/156 (91%)	126 (89%)	16 (11%)	6 5
7	1H	144/148 (97%)	139 (96%)	5 (4%)	36 47
7	2H	143/148 (97%)	132 (92%)	11 (8%)	13 15
8	1I	111/124 (90%)	94 (85%)	17 (15%)	2 2
8	2I	108/124 (87%)	91 (84%)	17 (16%)	2 1
9	1N	119/119 (100%)	111 (93%)	8 (7%)	16 20
9	2N	118/119 (99%)	108 (92%)	10 (8%)	10 12
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41 52
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31 41
11	1P	115/116 (99%)	112 (97%)	3 (3%)	46 58
11	2P	115/116 (99%)	108 (94%)	7 (6%)	18 24
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	22 28
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	22 28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	1R	101/101 (100%)	96 (95%)	5 (5%)	24 32
13	2R	101/101 (100%)	95 (94%)	6 (6%)	19 25
14	1S	87/88 (99%)	77 (88%)	10 (12%)	5 5
14	2S	85/88 (97%)	78 (92%)	7 (8%)	11 13
15	1T	115/127 (91%)	108 (94%)	7 (6%)	18 24
15	2T	113/127 (89%)	106 (94%)	7 (6%)	18 23
16	1U	93/94 (99%)	87 (94%)	6 (6%)	17 21
16	2U	93/94 (99%)	84 (90%)	9 (10%)	8 8
17	1V	81/82 (99%)	79 (98%)	2 (2%)	47 60
17	2V	80/82 (98%)	71 (89%)	9 (11%)	6 5
18	1W	90/92 (98%)	84 (93%)	6 (7%)	16 20
18	2W	90/92 (98%)	85 (94%)	5 (6%)	21 27
19	1X	77/78 (99%)	74 (96%)	3 (4%)	32 42
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32 42
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	15 18
20	2Y	86/91 (94%)	78 (91%)	8 (9%)	9 9
21	1Z	169/179 (94%)	155 (92%)	14 (8%)	11 12
21	2Z	165/179 (92%)	154 (93%)	11 (7%)	16 20
22	10	65/67 (97%)	61 (94%)	4 (6%)	18 23
22	20	64/67 (96%)	62 (97%)	2 (3%)	40 52
23	11	79/83 (95%)	73 (92%)	6 (8%)	13 15
23	21	81/83 (98%)	73 (90%)	8 (10%)	8 7
24	12	65/67 (97%)	62 (95%)	3 (5%)	27 35
24	22	66/67 (98%)	62 (94%)	4 (6%)	18 24
25	13	51/52 (98%)	48 (94%)	3 (6%)	19 25
25	23	50/52 (96%)	48 (96%)	2 (4%)	31 41
26	14	58/63 (92%)	53 (91%)	5 (9%)	10 11
26	24	54/63 (86%)	43 (80%)	11 (20%)	1 0
27	15	51/52 (98%)	48 (94%)	3 (6%)	19 25
27	25	50/52 (96%)	49 (98%)	1 (2%)	55 67
28	16	51/52 (98%)	46 (90%)	5 (10%)	8 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	26	50/52 (96%)	47 (94%)	3 (6%)	19 24
29	17	41/42 (98%)	37 (90%)	4 (10%)	8 8
29	27	41/42 (98%)	37 (90%)	4 (10%)	8 8
30	18	54/55 (98%)	47 (87%)	7 (13%)	4 3
30	28	54/55 (98%)	48 (89%)	6 (11%)	6 5
31	19	34/34 (100%)	33 (97%)	1 (3%)	42 53
31	29	34/34 (100%)	33 (97%)	1 (3%)	42 53
33	1b	191/220 (87%)	171 (90%)	20 (10%)	7 6
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4 3
34	1c	144/188 (77%)	133 (92%)	11 (8%)	13 15
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7 7
35	1d	171/181 (94%)	158 (92%)	13 (8%)	13 15
35	2d	172/181 (95%)	153 (89%)	19 (11%)	6 5
36	1e	114/123 (93%)	105 (92%)	9 (8%)	12 14
36	2e	114/123 (93%)	107 (94%)	7 (6%)	18 24
37	1f	85/90 (94%)	79 (93%)	6 (7%)	14 17
37	2f	85/90 (94%)	78 (92%)	7 (8%)	11 13
38	1g	120/127 (94%)	113 (94%)	7 (6%)	20 25
38	2g	119/127 (94%)	111 (93%)	8 (7%)	16 20
39	1h	116/119 (98%)	113 (97%)	3 (3%)	46 58
39	2h	114/119 (96%)	105 (92%)	9 (8%)	12 14
40	1i	91/99 (92%)	81 (89%)	10 (11%)	6 5
40	2i	88/99 (89%)	78 (89%)	10 (11%)	5 5
41	1j	68/92 (74%)	60 (88%)	8 (12%)	5 4
41	2j	68/92 (74%)	62 (91%)	6 (9%)	10 11
42	1k	83/99 (84%)	78 (94%)	5 (6%)	19 24
42	2k	83/99 (84%)	78 (94%)	5 (6%)	19 24
43	1l	96/108 (89%)	93 (97%)	3 (3%)	40 52
43	2l	96/108 (89%)	92 (96%)	4 (4%)	30 39
44	1m	90/101 (89%)	83 (92%)	7 (8%)	12 15
44	2m	87/101 (86%)	78 (90%)	9 (10%)	7 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	1n	49/50 (98%)	46 (94%)	3 (6%)	18 24
45	2n	49/50 (98%)	46 (94%)	3 (6%)	18 24
46	1o	78/80 (98%)	75 (96%)	3 (4%)	33 43
46	2o	78/80 (98%)	72 (92%)	6 (8%)	13 15
47	1p	69/74 (93%)	57 (83%)	12 (17%)	2 1
47	2p	68/74 (92%)	62 (91%)	6 (9%)	10 11
48	1q	94/97 (97%)	92 (98%)	2 (2%)	53 66
48	2q	94/97 (97%)	90 (96%)	4 (4%)	29 38
49	1r	59/77 (77%)	55 (93%)	4 (7%)	16 19
49	2r	59/77 (77%)	55 (93%)	4 (7%)	16 19
50	1s	68/80 (85%)	59 (87%)	9 (13%)	4 3
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5 4
51	1t	71/82 (87%)	69 (97%)	2 (3%)	43 56
51	2t	70/82 (85%)	62 (89%)	8 (11%)	5 5
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21 27
52	2u	18/22 (82%)	18 (100%)	0	100 100
53	1y	82/98 (84%)	80 (98%)	2 (2%)	49 61
53	2y	79/98 (81%)	73 (92%)	6 (8%)	13 15
56	1v	2/2 (100%)	2 (100%)	0	100 100
56	2v	2/2 (100%)	2 (100%)	0	100 100
All	All	9535/10264 (93%)	8811 (92%)	724 (8%)	13 15

All (724) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	37	LEU
3	1D	39	LYS
3	1D	71	ASP
3	1D	94	LEU
3	1D	99	ASP
3	1D	111	LEU
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL

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Mol	Chain	Res	Type
3	1D	242	ARG
3	1D	259	THR
3	1D	260	ARG
4	1E	49	LEU
4	1E	75	VAL
4	1E	93	VAL
4	1E	116	VAL
4	1E	119	ARG
4	1E	163	GLU
4	1E	181	LEU
4	1E	184	VAL
5	1F	12	LEU
5	1F	15	SER
5	1F	18	ARG
5	1F	23	ASP
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	95	ARG
5	1F	108	LYS
5	1F	110	LEU
5	1F	125	LEU
5	1F	158	THR
5	1F	161	GLU
5	1F	162	LEU
5	1F	170	LEU
5	1F	192	LEU
5	1F	197	ASP
5	1F	201	VAL
5	1F	203	GLN
6	1G	7	LEU
6	1G	21	ARG
6	1G	31	VAL
6	1G	33	ARG
6	1G	43	LEU
6	1G	45	GLU
6	1G	52	ILE
6	1G	53	LEU
6	1G	79	ASN
6	1G	126	ASP
6	1G	133	LEU
6	1G	153	ARG

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Mol	Chain	Res	Type
6	1G	159	VAL
7	1H	101	ARG
7	1H	107	VAL
7	1H	119	GLU
7	1H	122	THR
7	1H	127	GLU
8	1I	10	GLU
8	1I	12	LEU
8	1I	17	GLN
8	1I	20	ASP
8	1I	40	THR
8	1I	60	GLU
8	1I	64	GLU
8	1I	66	GLU
8	1I	74	ASN
8	1I	78	THR
8	1I	92	VAL
8	1I	101	LEU
8	1I	109	ILE
8	1I	116	LEU
8	1I	117	GLU
8	1I	127	VAL
8	1I	140	LEU
9	1N	12	ARG
9	1N	14	VAL
9	1N	33	LEU
9	1N	48	MET
9	1N	62	VAL
9	1N	73	THR
9	1N	131	GLN
9	1N	133	GLN
10	1O	66	LYS
10	1O	98	VAL
10	1O	113	LYS
11	1P	1	MET
11	1P	92	GLU
11	1P	99	LEU
12	1Q	5	ARG
12	1Q	7	MET
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	130	LYS

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Mol	Chain	Res	Type
12	1Q	133	ARG
13	1R	6	SER
13	1R	29	LEU
13	1R	36	THR
13	1R	100	LEU
13	1R	114	VAL
14	1S	3	ARG
14	1S	13	ARG
14	1S	25	ARG
14	1S	46	VAL
14	1S	48	LEU
14	1S	50	SER
14	1S	59	LYS
14	1S	73	LEU
14	1S	85	VAL
14	1S	110	LEU
15	1T	49	VAL
15	1T	53	ARG
15	1T	78	LEU
15	1T	82	LEU
15	1T	96	ARG
15	1T	118	ARG
15	1T	128	GLU
16	1U	5	LYS
16	1U	30	LYS
16	1U	31	SER
16	1U	74	LEU
16	1U	104	GLN
16	1U	111	GLU
17	1V	79	VAL
17	1V	95	LEU
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	100	THR
19	1X	35	THR
19	1X	57	LEU
19	1X	66	LEU
20	1Y	43	ASN
20	1Y	64	GLU

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Mol	Chain	Res	Type
20	1Y	72	VAL
20	1Y	73	ARG
20	1Y	92	ASN
20	1Y	107	ASP
21	1Z	31	ARG
21	1Z	52	SER
21	1Z	65	GLN
21	1Z	80	ARG
21	1Z	86	VAL
21	1Z	93	ASP
21	1Z	94	GLU
21	1Z	102	LEU
21	1Z	126	VAL
21	1Z	150	LEU
21	1Z	155	LEU
21	1Z	159	PRO
21	1Z	161	VAL
21	1Z	203	GLU
22	10	11	ARG
22	10	59	LEU
22	10	74	ARG
22	10	82	ARG
23	11	21	ARG
23	11	30	VAL
23	11	40	ARG
23	11	46	LEU
23	11	94	LEU
23	11	95	LEU
24	12	1	MET
24	12	30	ARG
24	12	68	ARG
25	13	54	VAL
25	13	56	VAL
25	13	58	VAL
26	14	1	MET
26	14	28	LYS
26	14	46	GLN
26	14	49	PHE
26	14	56	VAL
27	15	6	VAL
27	15	37	LYS
27	15	55	ARG

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Mol	Chain	Res	Type
28	16	5	VAL
28	16	44	ARG
28	16	47	THR
28	16	48	VAL
28	16	52	VAL
29	17	41	ARG
29	17	43	THR
29	17	46	VAL
29	17	48	LYS
30	18	14	VAL
30	18	23	VAL
30	18	29	LYS
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
30	18	46	ARG
31	19	17	ILE
33	1b	7	VAL
33	1b	10	LEU
33	1b	15	VAL
33	1b	19	HIS
33	1b	24	TRP
33	1b	35	GLU
33	1b	63	MET
33	1b	93	VAL
33	1b	97	TRP
33	1b	102	LEU
33	1b	111	ARG
33	1b	124	SER
33	1b	135	GLN
33	1b	140	HIS
33	1b	144	ARG
33	1b	160	ASP
33	1b	163	PHE
33	1b	185	ILE
33	1b	212	GLN
33	1b	224	GLN
34	1c	26	LYS
34	1c	64	VAL
34	1c	70	VAL
34	1c	102	ASN
34	1c	105	GLU

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Mol	Chain	Res	Type
34	1c	110	ASN
34	1c	115	LEU
34	1c	124	ILE
34	1c	132	ARG
34	1c	154	SER
34	1c	192	THR
35	1d	3	ARG
35	1d	8	VAL
35	1d	19	LEU
35	1d	58	LEU
35	1d	85	LYS
35	1d	94	LEU
35	1d	127	THR
35	1d	135	LEU
35	1d	150	GLU
35	1d	168	ARG
35	1d	187	ARG
35	1d	190	ASP
35	1d	194	LEU
36	1e	5	ASP
36	1e	31	LEU
36	1e	41	VAL
36	1e	56	GLN
36	1e	64	ARG
36	1e	68	GLU
36	1e	116	THR
36	1e	144	THR
36	1e	147	ASP
37	1f	10	LEU
37	1f	15	ASP
37	1f	21	LEU
37	1f	42	GLU
37	1f	73	ASN
37	1f	74	ASP
38	1g	6	ARG
38	1g	31	MET
38	1g	41	ARG
38	1g	52	GLU
38	1g	56	GLN
38	1g	96	GLN
38	1g	113	GLU
39	1h	52	ASP

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Mol	Chain	Res	Type
39	1h	54	ASP
39	1h	63	LEU
40	1i	2	GLU
40	1i	27	THR
40	1i	42	ARG
40	1i	50	LEU
40	1i	56	LEU
40	1i	60	ASP
40	1i	65	VAL
40	1i	81	ILE
40	1i	92	TYR
40	1i	104	ARG
41	1j	34	VAL
41	1j	42	THR
41	1j	45	ARG
41	1j	72	VAL
41	1j	84	GLN
41	1j	92	THR
41	1j	94	VAL
41	1j	100	THR
42	1k	16	SER
42	1k	34	ASP
42	1k	79	SER
42	1k	109	VAL
42	1k	114	VAL
43	1l	22	SER
43	1l	33	ARG
43	1l	41	ARG
44	1m	4	ILE
44	1m	11	ARG
44	1m	15	VAL
44	1m	27	LYS
44	1m	35	GLU
44	1m	70	LEU
44	1m	102	ARG
45	1n	9	LYS
45	1n	13	THR
45	1n	32	SER
46	1o	26	GLU
46	1o	39	LEU
46	1o	84	LYS
47	1p	1	MET

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Mol	Chain	Res	Type
47	1p	5	ARG
47	1p	6	LEU
47	1p	8	ARG
47	1p	20	VAL
47	1p	21	VAL
47	1p	29	ASP
47	1p	38	TYR
47	1p	60	LEU
47	1p	61	SER
47	1p	67	THR
47	1p	72	ARG
48	1q	20	THR
48	1q	74	LEU
49	1r	25	THR
49	1r	31	LEU
49	1r	42	ARG
49	1r	82	THR
50	1s	12	ASP
50	1s	28	LYS
50	1s	30	LEU
50	1s	35	SER
50	1s	37	ARG
50	1s	48	THR
50	1s	56	GLN
50	1s	66	MET
50	1s	81	ARG
51	1t	10	LEU
51	1t	15	ARG
52	1u	15	ARG
53	1y	24	LEU
53	1y	42	SER
3	2D	3	VAL
3	2D	32	SER
3	2D	38	LYS
3	2D	69	ARG
3	2D	94	LEU
3	2D	103	ARG
3	2D	113	VAL
3	2D	116	GLN
3	2D	134	ARG
3	2D	142	VAL
3	2D	155	LEU

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Mol	Chain	Res	Type
3	2D	173	VAL
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	276	LYS
4	2E	75	VAL
4	2E	87	GLU
4	2E	89	ASP
4	2E	93	VAL
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	145	LYS
4	2E	170	LEU
4	2E	181	LEU
5	2F	13	SER
5	2F	17	ARG
5	2F	20	LEU
5	2F	33	LEU
5	2F	57	VAL
5	2F	74	ARG
5	2F	126	VAL
5	2F	140	LEU
5	2F	170	LEU
5	2F	175	THR
5	2F	176	LEU
5	2F	183	VAL
5	2F	192	LEU
5	2F	197	ASP
5	2F	201	VAL
6	2G	3	LEU
6	2G	5	VAL
6	2G	7	LEU
6	2G	15	VAL
6	2G	28	VAL
6	2G	43	LEU
6	2G	53	LEU
6	2G	58	GLN
6	2G	88	ILE
6	2G	91	ARG

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Mol	Chain	Res	Type
6	2G	113	ARG
6	2G	126	ASP
6	2G	133	LEU
6	2G	165	THR
6	2G	168	GLU
6	2G	172	LEU
7	2H	15	VAL
7	2H	38	SER
7	2H	43	VAL
7	2H	47	GLU
7	2H	49	VAL
7	2H	50	VAL
7	2H	65	HIS
7	2H	68	THR
7	2H	69	ARG
7	2H	80	SER
7	2H	95	ARG
8	2I	38	LEU
8	2I	41	GLU
8	2I	44	LEU
8	2I	50	ARG
8	2I	62	LYS
8	2I	64	GLU
8	2I	68	LEU
8	2I	74	ASN
8	2I	76	THR
8	2I	82	ARG
8	2I	86	THR
8	2I	87	LYS
8	2I	91	SER
8	2I	92	VAL
8	2I	116	LEU
8	2I	117	GLU
8	2I	123	LEU
9	2N	12	ARG
9	2N	28	THR
9	2N	33	LEU
9	2N	34	LEU
9	2N	38	HIS
9	2N	48	MET
9	2N	67	LEU
9	2N	74	ARG

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Mol	Chain	Res	Type
9	2N	99	LEU
9	2N	115	ARG
10	2O	1	MET
10	2O	64	ARG
10	2O	98	VAL
10	2O	116	SER
11	2P	76	LYS
11	2P	86	LYS
11	2P	98	GLU
11	2P	101	VAL
11	2P	106	LEU
11	2P	123	LEU
11	2P	135	LEU
12	2Q	7	MET
12	2Q	55	VAL
12	2Q	75	THR
12	2Q	109	VAL
12	2Q	111	GLU
12	2Q	130	LYS
13	2R	24	GLN
13	2R	29	LEU
13	2R	36	THR
13	2R	100	LEU
13	2R	114	VAL
13	2R	117	VAL
14	2S	12	PHE
14	2S	13	ARG
14	2S	25	ARG
14	2S	44	LYS
14	2S	78	LEU
14	2S	85	VAL
14	2S	110	LEU
15	2T	6	LEU
15	2T	16	ARG
15	2T	36	GLU
15	2T	65	LYS
15	2T	89	VAL
15	2T	108	ARG
15	2T	118	ARG
16	2U	5	LYS
16	2U	31	SER
16	2U	52	ARG

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Mol	Chain	Res	Type
16	2U	74	LEU
16	2U	77	SER
16	2U	78	THR
16	2U	83	LEU
16	2U	104	GLN
16	2U	108	GLU
17	2V	13	ARG
17	2V	19	LYS
17	2V	32	THR
17	2V	35	LEU
17	2V	46	VAL
17	2V	51	VAL
17	2V	72	VAL
17	2V	79	VAL
17	2V	96	ILE
18	2W	11	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	23	LEU
18	2W	68	ARG
19	2X	33	LYS
19	2X	57	LEU
19	2X	66	LEU
20	2Y	2	ARG
20	2Y	6	HIS
20	2Y	19	LYS
20	2Y	31	LEU
20	2Y	67	LEU
20	2Y	70	SER
20	2Y	72	VAL
20	2Y	99	CYS
21	2Z	5	LEU
21	2Z	65	GLN
21	2Z	72	ARG
21	2Z	73	GLN
21	2Z	121	HIS
21	2Z	126	VAL
21	2Z	128	VAL
21	2Z	141	VAL
21	2Z	162	GLU
21	2Z	170	THR
21	2Z	182	LYS

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Mol	Chain	Res	Type
22	20	10	THR
22	20	70	GLN
23	21	3	LYS
23	21	4	VAL
23	21	21	ARG
23	21	23	LYS
23	21	40	ARG
23	21	51	VAL
23	21	80	LEU
23	21	83	GLU
24	22	32	LEU
24	22	53	LEU
24	22	64	LEU
24	22	70	GLN
25	23	7	LYS
25	23	44	ARG
26	24	3	GLU
26	24	9	LEU
26	24	15	ILE
26	24	23	GLU
26	24	34	GLU
26	24	46	GLN
26	24	50	VAL
26	24	58	ARG
26	24	60	GLN
26	24	62	ARG
26	24	63	TYR
27	25	55	ARG
28	26	6	ARG
28	26	20	ASN
28	26	48	VAL
29	27	23	ARG
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
30	28	3	LYS
30	28	14	VAL
30	28	31	HIS
30	28	32	LEU
30	28	34	TRP
30	28	46	ARG
31	29	17	ILE

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Mol	Chain	Res	Type
33	2b	8	LYS
33	2b	12	GLU
33	2b	15	VAL
33	2b	23	ARG
33	2b	24	TRP
33	2b	28	PHE
33	2b	39	ILE
33	2b	44	LEU
33	2b	45	GLN
33	2b	52	GLU
33	2b	55	PHE
33	2b	80	ILE
33	2b	97	TRP
33	2b	98	LEU
33	2b	111	ARG
33	2b	114	ARG
33	2b	150	SER
33	2b	154	LEU
33	2b	157	ARG
33	2b	160	ASP
33	2b	163	PHE
33	2b	187	LEU
33	2b	189	ASP
33	2b	196	LEU
33	2b	222	ILE
34	2c	8	ILE
34	2c	15	THR
34	2c	33	LEU
34	2c	47	LEU
34	2c	52	LEU
34	2c	56	ASP
34	2c	105	GLU
34	2c	128	PHE
34	2c	152	ILE
34	2c	154	SER
34	2c	181	ASN
34	2c	192	THR
34	2c	195	VAL
34	2c	204	LEU
35	2d	3	ARG
35	2d	19	LEU
35	2d	49	ARG

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Mol	Chain	Res	Type
35	2d	53	ASP
35	2d	57	ARG
35	2d	76	ARG
35	2d	83	SER
35	2d	106	TYR
35	2d	108	LEU
35	2d	135	LEU
35	2d	141	ARG
35	2d	150	GLU
35	2d	157	LEU
35	2d	166	LYS
35	2d	169	LYS
35	2d	188	LEU
35	2d	190	ASP
35	2d	194	LEU
35	2d	209	ARG
36	2e	6	PHE
36	2e	31	LEU
36	2e	34	VAL
36	2e	41	VAL
36	2e	68	GLU
36	2e	75	THR
36	2e	144	THR
37	2f	22	GLU
37	2f	31	GLU
37	2f	45	LEU
37	2f	61	LEU
37	2f	64	GLN
37	2f	69	GLU
37	2f	93	SER
38	2g	6	ARG
38	2g	15	ASP
38	2g	27	ILE
38	2g	50	ILE
38	2g	75	VAL
38	2g	111	ARG
38	2g	115	ARG
38	2g	153	HIS
39	2h	19	VAL
39	2h	29	SER
39	2h	84	ARG
39	2h	85	ARG

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Mol	Chain	Res	Type
39	2h	91	ARG
39	2h	112	LEU
39	2h	121	ASP
39	2h	125	ARG
39	2h	133	LEU
40	2i	27	THR
40	2i	33	PHE
40	2i	47	LEU
40	2i	60	ASP
40	2i	75	ASP
40	2i	81	ILE
40	2i	93	ARG
40	2i	102	LEU
40	2i	104	ARG
40	2i	121	ARG
41	2j	16	LEU
41	2j	34	VAL
41	2j	38	ILE
41	2j	43	ARG
41	2j	92	THR
41	2j	95	GLU
42	2k	53	SER
42	2k	79	SER
42	2k	93	GLN
42	2k	109	VAL
42	2k	116	HIS
43	2l	33	ARG
43	2l	41	ARG
43	2l	81	SER
43	2l	89	ARG
44	2m	3	ARG
44	2m	15	VAL
44	2m	17	VAL
44	2m	48	LEU
44	2m	49	THR
44	2m	69	GLU
44	2m	102	ARG
44	2m	104	ARG
44	2m	116	THR
45	2n	13	THR
45	2n	18	VAL
45	2n	29	ARG

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Mol	Chain	Res	Type
46	2o	3	ILE
46	2o	10	LYS
46	2o	26	GLU
46	2o	38	ARG
46	2o	39	LEU
46	2o	84	LYS
47	2p	12	LYS
47	2p	20	VAL
47	2p	25	ARG
47	2p	28	ARG
47	2p	60	LEU
47	2p	69	THR
48	2q	39	SER
48	2q	93	GLN
48	2q	96	GLU
48	2q	99	SER
49	2r	31	LEU
49	2r	37	VAL
49	2r	55	ARG
49	2r	82	THR
50	2s	23	ASN
50	2s	41	VAL
50	2s	62	ILE
50	2s	64	GLU
50	2s	77	THR
50	2s	79	THR
50	2s	81	ARG
50	2s	83	HIS
51	2t	11	SER
51	2t	15	ARG
51	2t	24	LEU
51	2t	42	GLN
51	2t	55	ILE
51	2t	62	LEU
51	2t	86	ARG
51	2t	100	ILE
53	2y	6	THR
53	2y	9	GLN
53	2y	16	ILE
53	2y	24	LEU
53	2y	46	GLN
53	2y	56	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	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
8	1I	43	ASN
8	1I	54	GLN
8	1I	105	HIS
9	1N	133	GLN
15	1T	58	ASN
15	1T	123	GLN
16	1U	104	GLN
16	1U	117	GLN
19	1X	31	HIS
19	1X	82	GLN
21	1Z	73	GLN
21	1Z	151	HIS
22	10	35	ASN
23	11	56	GLN
25	13	32	GLN
26	14	20	ASN
26	14	60	GLN
33	1b	78	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	118	GLN
34	1c	176	HIS
35	1d	45	GLN
35	1d	77	ASN
35	1d	123	HIS
35	1d	129	ASN
36	1e	56	GLN
37	1f	32	ASN
37	1f	73	ASN
37	1f	84	ASN
37	1f	100	ASN
38	1g	28	ASN
38	1g	56	GLN
38	1g	96	GLN

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Mol	Chain	Res	Type
38	1g	97	GLN
38	1g	148	ASN
40	1i	3	GLN
40	1i	73	GLN
40	1i	87	GLN
41	1j	21	GLN
41	1j	56	HIS
41	1j	84	GLN
42	1k	93	GLN
43	1l	99	HIS
44	1m	92	HIS
45	1n	49	HIS
46	1o	71	GLN
47	1p	16	HIS
48	1q	16	GLN
50	1s	69	HIS
50	1s	83	HIS
53	1y	9	GLN
53	1y	38	HIS
3	2D	87	ASN
3	2D	253	GLN
4	2E	48	GLN
5	2F	69	HIS
6	2G	41	GLN
6	2G	58	GLN
8	2I	74	ASN
8	2I	133	HIS
10	2O	3	GLN
11	2P	27	HIS
12	2Q	89	ASN
13	2R	71	GLN
15	2T	58	ASN
16	2U	94	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	73	GLN
21	2Z	132	ASN
21	2Z	151	HIS
25	23	32	GLN
26	24	40	HIS
26	24	46	GLN
26	24	60	GLN

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Mol	Chain	Res	Type
29	27	36	GLN
33	2b	19	HIS
33	2b	40	HIS
33	2b	94	ASN
34	2c	37	GLN
34	2c	98	ASN
34	2c	110	ASN
34	2c	123	GLN
34	2c	136	GLN
34	2c	139	GLN
34	2c	176	HIS
34	2c	181	ASN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	129	ASN
35	2d	160	GLN
36	2e	56	GLN
37	2f	73	ASN
38	2g	13	GLN
38	2g	28	ASN
38	2g	56	GLN
39	2h	15	ASN
40	2i	3	GLN
40	2i	31	GLN
40	2i	73	GLN
41	2j	33	GLN
41	2j	62	HIS
41	2j	68	HIS
43	2l	99	HIS
44	2m	62	ASN
44	2m	77	ASN
46	2o	71	GLN
48	2q	16	GLN
48	2q	93	GLN
50	2s	57	HIS
53	2y	36	ASN
53	2y	46	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	381 (13%)	36 (1%)
1	2A	2857/2915 (98%)	455 (15%)	33 (1%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	119/121 (98%)	15 (12%)	0
32	1a	1494/1521 (98%)	231 (15%)	0
32	2a	1498/1521 (98%)	263 (17%)	0
54	1w	2/4 (50%)	1 (50%)	0
54	2w	2/4 (50%)	0	0
55	1x	2/4 (50%)	0	0
55	2x	2/4 (50%)	0	0
All	All	8959/9130 (98%)	1358 (15%)	69 (0%)

All (1358) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	154(A)	C
1	1A	181	A
1	1A	196	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	229	A
1	1A	248	G
1	1A	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

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Mol	Chain	Res	Type
1	1A	272(H)	C
1	1A	272(J)	C
1	1A	275	G
1	1A	279	C
1	1A	280	C
1	1A	311	A
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	407	G
1	1A	411	G
1	1A	412	A
1	1A	421	U
1	1A	422	A
1	1A	428	A
1	1A	429	A
1	1A	448	U
1	1A	454	A
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	494	G
1	1A	505	A
1	1A	509	C
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G

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Mol	Chain	Res	Type
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(A)	A
1	1A	652(U)	G
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	765	G
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	879	G
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	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C

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Mol	Chain	Res	Type
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1026	U
1	1A	1033	U
1	1A	1039	G
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	1067	A
1	1A	1070	A
1	1A	1071	G
1	1A	1072	C
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1093	G
1	1A	1095	A
1	1A	1096	A
1	1A	1097	U
1	1A	1098	A
1	1A	1109	C
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1128	A
1	1A	1135	C
1	1A	1136	G

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Mol	Chain	Res	Type
1	1A	1139	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	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1352	U
1	1A	1359	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1459	G
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G
1	1A	1487	G
1	1A	1493	C
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A

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Mol	Chain	Res	Type
1	1A	1525	G
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	1647	G
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A
1	1A	1816	G
1	1A	1839	G
1	1A	1847	A
1	1A	1877	A
1	1A	1887	C
1	1A	1900	A
1	1A	1906	G

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Mol	Chain	Res	Type
1	1A	1913	A
1	1A	1914	C
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
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	2099	U
1	1A	2102	U
1	1A	2103	C
1	1A	2104	G
1	1A	2107	C
1	1A	2108	C
1	1A	2110	G
1	1A	2111	C
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2119	A
1	1A	2123	G
1	1A	2125	G
1	1A	2126	A
1	1A	2127	G
1	1A	2131	G

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Mol	Chain	Res	Type
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2142	C
1	1A	2146	C
1	1A	2147	G
1	1A	2158	A
1	1A	2159	G
1	1A	2164	C
1	1A	2172	U
1	1A	2180	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
1	1A	2208	A
1	1A	2218	U
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2321	G
1	1A	2325	G
1	1A	2334	G
1	1A	2347	C
1	1A	2350	C

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Mol	Chain	Res	Type
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	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2432	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2469	A
1	1A	2476	A
1	1A	2478	A
1	1A	2498	C
1	1A	2502	G
1	1A	2504	U
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U

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Mol	Chain	Res	Type
1	1A	2733	A
1	1A	2744	G
1	1A	2757	A
1	1A	2758	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	7	G
2	1B	13	A
2	1B	30	C
2	1B	42	C
2	1B	45	A
2	1B	56	G
2	1B	73	A
2	1B	74	U
2	1B	106	G
2	1B	110	G
2	1B	120	A
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	53	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	93	G
32	1a	101	A

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Mol	Chain	Res	Type
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	150	C
32	1a	151	A
32	1a	156	G
32	1a	163	C
32	1a	165	C
32	1a	169	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	195	A
32	1a	197	A
32	1a	216	G
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	318	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
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	414	A
32	1a	423	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	458	C
32	1a	460	G
32	1a	461	A
32	1a	470	C
32	1a	475	G
32	1a	484	G
32	1a	485	G
32	1a	492	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	532	A
32	1a	536	C
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	619	U
32	1a	630	G
32	1a	632	A
32	1a	642	A
32	1a	653	A
32	1a	665	A
32	1a	673	G
32	1a	687	A
32	1a	688	G

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Mol	Chain	Res	Type
32	1a	723	U
32	1a	731	G
32	1a	755	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	810	C
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G
32	1a	836	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	874	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	983	A
32	1a	992	U
32	1a	993	G
32	1a	998	G
32	1a	1001	A
32	1a	1001(A)	G

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Mol	Chain	Res	Type
32	1a	1004	A
32	1a	1005	A
32	1a	1009	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	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1032	G
32	1a	1037	C
32	1a	1044	A
32	1a	1065	U
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1104	G
32	1a	1124	G
32	1a	1126	U
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1163	C
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U

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Mol	Chain	Res	Type
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	1240	U
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1312	G
32	1a	1320	C
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1467	G
32	1a	1487	G
32	1a	1492	A
32	1a	1493	A
32	1a	1499	A
32	1a	1503	A

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Mol	Chain	Res	Type
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
54	1w	74	C
1	2A	11	G
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	92	A
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	141	A
1	2A	149	A
1	2A	157	U
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U

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Mol	Chain	Res	Type
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	311	A
1	2A	317	G
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	352	G
1	2A	363	G
1	2A	363(B)	G
1	2A	370	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	563	G
1	2A	573	G
1	2A	575	A

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Mol	Chain	Res	Type
1	2A	586	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	609	A
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
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	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	765	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	880	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	901	A
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	1012	U
1	2A	1013	C
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1042	G
1	2A	1044	G
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1052	C
1	2A	1054	A
1	2A	1059	G
1	2A	1060	U
1	2A	1063	G
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G

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Mol	Chain	Res	Type
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	1078	U
1	2A	1079	C
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	1096	A
1	2A	1097	U
1	2A	1098	A
1	2A	1106	G
1	2A	1109	C
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1117	G
1	2A	1129	A
1	2A	1135	C
1	2A	1136	G
1	2A	1171	G
1	2A	1179	C
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1236	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A

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Mol	Chain	Res	Type
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1321	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1453	U
1	2A	1459	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1494	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A

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Mol	Chain	Res	Type
1	2A	1584	C
1	2A	1586	A
1	2A	1595	G
1	2A	1608	A
1	2A	1609	A
1	2A	1640	C
1	2A	1648	C
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1750	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1919	A
1	2A	1929	G

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Mol	Chain	Res	Type
1	2A	1930	G
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	2101	G
1	2A	2103	C
1	2A	2104	G
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2111	C
1	2A	2112	G
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2120	G
1	2A	2121	G
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G

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Mol	Chain	Res	Type
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	2140	C
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2155	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2162	G
1	2A	2163	C
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2175	C
1	2A	2176	A
1	2A	2178	C
1	2A	2182	G
1	2A	2183	C
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U

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Mol	Chain	Res	Type
1	2A	2219	G
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2383	G
1	2A	2384	G
1	2A	2385	C
1	2A	2406	U
1	2A	2410	G
1	2A	2422	A
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	2448	A
1	2A	2468	G
1	2A	2474	C
1	2A	2476	A
1	2A	2491	U

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Mol	Chain	Res	Type
1	2A	2502	G
1	2A	2505	G
1	2A	2518	A
1	2A	2529	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2585	U
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2757	A
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2779	U
1	2A	2789	C
1	2A	2802	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2880	C

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Mol	Chain	Res	Type
1	2A	2894	G
1	2A	2896	C
2	2B	2	C
2	2B	7	G
2	2B	8	U
2	2B	12	C
2	2B	32	C
2	2B	33	G
2	2B	35	U
2	2B	42	C
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	106	G
2	2B	110	G
2	2B	115	G
2	2B	120	A
32	2a	5	U
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	61	G
32	2a	78	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	151	A
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(C)	C
32	2a	189(F)	U
32	2a	194	C

Continued on next page...

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Mol	Chain	Res	Type
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	220	G
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	318	G
32	2a	319	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	438	G
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	458	C
32	2a	461	A

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Mol	Chain	Res	Type
32	2a	470	C
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	520	A
32	2a	521	G
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	589	C
32	2a	596	C
32	2a	630	G
32	2a	631	G
32	2a	632	A
32	2a	650	G
32	2a	653	A
32	2a	660	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	690	G
32	2a	702	A
32	2a	723	U
32	2a	731	G
32	2a	735	C
32	2a	749	C
32	2a	753	A
32	2a	754	C

Continued on next page...

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Mol	Chain	Res	Type
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	854	G
32	2a	859	A
32	2a	872	A
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	942	G
32	2a	943	U
32	2a	960	U
32	2a	961	U
32	2a	965	A
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C

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Mol	Chain	Res	Type
32	2a	1007	C
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	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	1037	C
32	2a	1041	A
32	2a	1044	A
32	2a	1053	G
32	2a	1054	C
32	2a	1055	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1094	G
32	2a	1101	A
32	2a	1113	C
32	2a	1122	U
32	2a	1125	U
32	2a	1128	C
32	2a	1129	C
32	2a	1130	A
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1142	G
32	2a	1147	C

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Mol	Chain	Res	Type
32	2a	1152	A
32	2a	1159	U
32	2a	1160	G
32	2a	1161	C
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	1224	G
32	2a	1227	A
32	2a	1228	C
32	2a	1236	A
32	2a	1238	A
32	2a	1248	A
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1281	U
32	2a	1282	C
32	2a	1286	A
32	2a	1287	A
32	2a	1297	C
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1316	G
32	2a	1317	C
32	2a	1319	A
32	2a	1320	C
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G

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Mol	Chain	Res	Type
32	2a	1353	G
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1383	C
32	2a	1384	C
32	2a	1397	C
32	2a	1400	5MC
32	2a	1401	G
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1446	U
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1458	G
32	2a	1459	C
32	2a	1492	A
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	1528	U
32	2a	1529	G
32	2a	1530	G

All (69) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	34	C
1	1A	196	A
1	1A	199	A
1	1A	266	G
1	1A	278	A
1	1A	573	G
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	776	G

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Mol	Chain	Res	Type
1	1A	827	U
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	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1175	U
1	1A	1210	A
1	1A	1300	U
1	1A	1379	A
1	1A	1442	G
1	1A	1608	A
1	1A	1653	G
1	1A	2126	A
1	1A	2238	G
1	1A	2406	U
1	1A	2422	A
1	1A	2439	A
1	1A	2611	U
1	1A	2689	U
1	1A	2756	U
1	1A	2893	G
1	2A	195	A
1	2A	196	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	532	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	1051	G
1	2A	1053	C
1	2A	1065	U

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Mol	Chain	Res	Type
1	2A	1067	A
1	2A	1073	A
1	2A	1076	C
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2321	G
1	2A	2406	U
1	2A	2439	A
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMG	1A	2251	1,55	18,26,27	1.06	1 (5%)	19,38,41	0.99	2 (10%)
1	5MU	1A	1915	1	19,22,23	1.47	5 (26%)	28,32,35	2.25	10 (35%)
1	2MA	1A	2503	1,57	17,25,26	0.95	0	17,37,40	0.99	2 (11%)
1	5MC	1A	1962	1	18,22,23	0.96	2 (11%)	26,32,35	1.13	4 (15%)
32	5MC	2a	1404	32	18,22,23	0.97	2 (11%)	26,32,35	1.22	4 (15%)
55	8AN	1x	76	57,55	19,24,25	1.19	2 (10%)	13,35,38	1.82	2 (15%)
43	0TD	1l	92	43	7,9,10	4.89	1 (14%)	6,11,13	2.21	3 (50%)
1	PSU	2A	1911	1	18,21,22	1.40	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	1A	1911	1	18,21,22	1.37	2 (11%)	22,30,33	1.81	3 (13%)

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	0.99	1 (5%)	26,32,35	1.13	3 (11%)
32	M2G	1a	966	32	20,27,28	1.43	3 (15%)	22,40,43	0.91	2 (9%)
32	MA6	2a	1518	32	19,26,27	0.78	0	18,38,41	1.41	2 (11%)
32	MA6	2a	1519	32	19,26,27	0.82	0	18,38,41	1.53	2 (11%)
1	OMC	1A	1920	1	19,22,23	0.82	0	26,31,34	0.93	1 (3%)
1	PSU	2A	2605	1	18,21,22	1.26	2 (11%)	22,30,33	1.91	3 (13%)
32	M2G	2a	966	32	20,27,28	1.39	3 (15%)	22,40,43	0.97	2 (9%)
1	OMG	2A	2251	1,57,55	18,26,27	0.91	1 (5%)	19,38,41	1.04	2 (10%)
32	G7M	2a	527	32,57	20,26,27	1.24	2 (10%)	17,39,42	0.66	0
32	5MC	2a	1407	32	18,22,23	0.96	2 (11%)	26,32,35	1.13	3 (11%)
32	MA6	1a	1518	32	19,26,27	0.81	0	18,38,41	1.34	2 (11%)
1	5MC	2A	1962	1,57	18,22,23	0.95	2 (11%)	26,32,35	1.13	2 (7%)
32	5MC	2a	1400	32	18,22,23	0.96	2 (11%)	26,32,35	1.30	3 (11%)
32	UR3	1a	1498	32	19,22,23	1.04	1 (5%)	26,32,35	1.58	3 (11%)
32	G7M	1a	527	32,57	20,26,27	1.19	2 (10%)	17,39,42	0.54	0
1	PSU	2A	1917	1	18,21,22	1.32	2 (11%)	22,30,33	1.83	3 (13%)
1	2MA	2A	2503	1,57	17,25,26	1.01	1 (5%)	17,37,40	1.10	2 (11%)
1	5MU	1A	1939	1,57	19,22,23	1.38	5 (26%)	28,32,35	2.26	6 (21%)
54	PPU	2w	76	1,54	32,40,41	0.91	2 (6%)	33,57,60	1.37	4 (12%)
1	5MC	1A	1942	1,57	18,22,23	1.02	2 (11%)	26,32,35	1.11	1 (3%)
54	PPU	1w	76	1,54	32,40,41	0.83	1 (3%)	33,57,60	1.28	4 (12%)
32	PSU	2a	516	32,57	18,21,22	1.30	2 (11%)	22,30,33	1.87	4 (18%)
32	MA6	1a	1519	32	19,26,27	0.80	0	18,38,41	1.43	2 (11%)
1	PSU	1A	1917	1	18,21,22	1.31	2 (11%)	22,30,33	1.85	3 (13%)
1	OMU	1A	2552	1,57	19,22,23	1.24	3 (15%)	26,31,34	1.81	6 (23%)
1	OMC	2A	1920	1	19,22,23	0.82	0	26,31,34	0.93	1 (3%)
1	5MU	2A	1915	1	19,22,23	1.46	4 (21%)	28,32,35	2.14	8 (28%)
32	5MC	1a	1404	32	18,22,23	0.92	2 (11%)	26,32,35	1.08	2 (7%)
32	5MC	1a	967	32	18,22,23	0.95	2 (11%)	26,32,35	1.11	2 (7%)
1	5MU	2A	1939	1,57	19,22,23	1.44	6 (31%)	28,32,35	2.20	6 (21%)
32	2MG	1a	1207	32	18,26,27	0.94	1 (5%)	16,38,41	1.15	3 (18%)
1	OMU	2A	2552	1,57	19,22,23	1.22	3 (15%)	26,31,34	1.86	6 (23%)
32	4OC	2a	1402	32	20,23,24	0.76	1 (5%)	26,32,35	0.93	1 (3%)
32	5MC	2a	967	32	18,22,23	0.95	1 (5%)	26,32,35	1.10	2 (7%)
43	0TD	2l	92	43	7,9,10	4.52	1 (14%)	6,11,13	4.34	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
55	8AN	2x	76	57,55	19,24,25	1.26	3 (15%)	13,35,38	1.79	2 (15%)
32	5MC	1a	1400	32	18,22,23	1.01	2 (11%)	26,32,35	1.18	2 (7%)
32	UR3	2a	1498	32	19,22,23	0.98	1 (5%)	26,32,35	1.44	2 (7%)
32	PSU	1a	516	32,57	18,21,22	1.37	2 (11%)	22,30,33	1.79	3 (13%)
32	2MG	2a	1207	32	18,26,27	0.90	0	16,38,41	1.05	1 (6%)
1	PSU	1A	2605	1	18,21,22	1.35	3 (16%)	22,30,33	2.02	4 (18%)
1	5MC	2A	1942	1	18,22,23	0.98	2 (11%)	26,32,35	1.21	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.72	1 (5%)	26,32,35	0.99	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1A	2251	1,55	-	0/5/27/28	0/3/3/3
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	2MA	1A	2503	1,57	-	2/3/25/26	0/3/3/3
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	57,55	-	1/3/25/26	0/3/3/3
43	0TD	1l	92	43	-	3/7/12/14	-
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	2/7/29/30	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
1	OMG	2A	2251	1,57,55	-	1/5/27/28	0/3/3/3
32	G7M	2a	527	32,57	-	1/3/25/26	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,57	-	2/3/25/26	0/3/3/3

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

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.50	1.69	1.82
43	2l	92	0TD	CB-SB	-11.53	1.70	1.82
32	2a	966	M2G	C2-N3	4.28	1.35	1.30
32	1a	966	M2G	C2-N3	4.26	1.35	1.30
32	1a	527	G7M	C5-C4	3.73	1.46	1.39
32	2a	527	G7M	C5-C4	3.61	1.46	1.39
1	2A	1911	PSU	C6-C5	3.58	1.39	1.35
32	1a	516	PSU	C6-C5	3.36	1.39	1.35
1	1A	1911	PSU	C6-C5	3.32	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1917	PSU	C6-C5	3.14	1.39	1.35
1	1A	1917	PSU	C6-C5	3.10	1.38	1.35
1	1A	2251	OMG	C6-N1	-3.08	1.33	1.37
32	2a	516	PSU	C6-C5	3.07	1.38	1.35
1	1A	1915	5MU	C2-N1	3.03	1.43	1.38
32	1a	1400	5MC	C6-C5	3.02	1.39	1.34
1	2A	1915	5MU	C2-N1	3.02	1.43	1.38
32	1a	1407	5MC	C6-C5	3.01	1.39	1.34
1	2A	1915	5MU	C6-C5	2.99	1.39	1.34
1	2A	1939	5MU	C6-C5	2.98	1.39	1.34
1	1A	1939	5MU	C6-C5	2.92	1.39	1.34
32	2a	967	5MC	C6-C5	2.90	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.88	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.88	1.33	1.38
32	2a	1407	5MC	C6-C5	2.86	1.39	1.34
1	1A	1942	5MC	C6-C5	2.85	1.39	1.34
1	2A	1942	5MC	C6-C5	2.80	1.39	1.34
55	1x	76	8AN	C5-C4	-2.80	1.33	1.40
32	1a	967	5MC	C6-C5	2.77	1.39	1.34
32	1a	1404	5MC	C6-C5	2.77	1.39	1.34
55	2x	76	8AN	C5-C4	-2.75	1.33	1.40
1	2A	1962	5MC	C6-C5	2.74	1.39	1.34
32	2a	1404	5MC	C6-C5	2.69	1.39	1.34
32	1a	966	M2G	C6-N1	-2.66	1.33	1.37
1	1A	1915	5MU	C4-N3	-2.65	1.33	1.38
32	2a	966	M2G	C2-N2	2.63	1.40	1.35
1	1A	1911	PSU	C4-N3	-2.60	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.59	1.34	1.38
1	1A	1915	5MU	C4-C5	2.57	1.49	1.44
32	1a	516	PSU	C4-N3	-2.57	1.34	1.38
32	2a	1400	5MC	C6-C5	2.57	1.38	1.34
1	1A	1939	5MU	C4-N3	-2.57	1.34	1.38
1	1A	1915	5MU	C6-C5	2.56	1.38	1.34
1	1A	1917	PSU	C4-N3	-2.55	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.54	1.34	1.38
32	1a	966	M2G	C2-N2	2.54	1.39	1.35
1	1A	1942	5MC	C6-N1	-2.51	1.33	1.38
55	2x	76	8AN	C6-C5	-2.49	1.34	1.43
55	1x	76	8AN	C6-C5	-2.48	1.34	1.43
1	2A	2605	PSU	C6-C5	2.48	1.38	1.35
32	2a	527	G7M	C6-N1	-2.47	1.34	1.37
1	2A	1917	PSU	C4-N3	-2.45	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2605	PSU	C4-N3	-2.45	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.43	1.33	1.38
32	2a	1400	5MC	C6-N1	-2.41	1.33	1.38
1	2A	2251	OMG	C6-N1	-2.41	1.34	1.37
1	2A	1939	5MU	C4-C5	2.40	1.48	1.44
1	2A	2552	OMU	C4-N3	-2.39	1.34	1.38
32	2a	516	PSU	C4-N3	-2.39	1.34	1.38
1	1A	1939	5MU	C6-N1	-2.39	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.37	1.34	1.38
1	1A	1962	5MC	C6-C5	2.36	1.38	1.34
1	1A	2552	OMU	C4-N3	-2.35	1.34	1.38
1	2A	1915	5MU	C4-C5	2.34	1.48	1.44
1	1A	2552	OMU	C2-N1	2.32	1.42	1.38
1	2A	1962	5MC	C6-N1	-2.32	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.30	1.34	1.37
54	1w	76	PPU	C5-C4	2.29	1.47	1.40
54	2w	76	PPU	C6-N1	2.28	1.36	1.33
1	2A	1942	5MC	C6-N1	-2.26	1.34	1.38
55	2x	76	8AN	C5-N7	-2.25	1.31	1.39
32	2a	1404	5MC	C6-N1	-2.25	1.34	1.38
54	2w	76	PPU	C5-C4	2.24	1.46	1.40
1	1A	2605	PSU	C6-C5	2.23	1.37	1.35
32	2a	966	M2G	C6-N1	-2.23	1.34	1.37
1	1A	1939	5MU	C2-N3	-2.22	1.34	1.38
1	1A	2552	OMU	C5-C4	2.21	1.48	1.43
1	2A	2503	2MA	C2-N3	2.19	1.35	1.31
32	2a	1498	UR3	C6-C5	2.17	1.40	1.35
1	1A	1939	5MU	C4-C5	2.15	1.48	1.44
1	2A	2552	OMU	C5-C4	2.15	1.48	1.43
32	1a	527	G7M	C6-N1	-2.14	1.34	1.37
1	2A	1939	5MU	C6-N1	-2.13	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.13	1.34	1.38
1	2A	1939	5MU	C2-N1	2.10	1.41	1.38
32	1a	967	5MC	C6-N1	-2.09	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.09	1.34	1.38
1	1A	2605	PSU	C2-N1	-2.06	1.33	1.36
1	2A	2552	OMU	C2-N3	-2.06	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.05	1.34	1.38
32	2a	1402	4OC	C6-C5	2.01	1.39	1.35
1	1A	1915	5MU	C6-N1	-2.01	1.34	1.38
32	1a	1402	4OC	C6-C5	2.01	1.39	1.35
32	1a	1498	UR3	C6-C5	2.00	1.39	1.35

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-9.72	84.85	102.44
32	1a	1498	UR3	C4-N3-C2	-6.48	118.46	124.56
1	1A	2605	PSU	N1-C2-N3	6.18	122.14	115.13
32	2a	1498	UR3	C4-N3-C2	-6.10	118.82	124.56
1	2A	1911	PSU	N1-C2-N3	5.95	121.87	115.13
1	2A	2605	PSU	N1-C2-N3	5.75	121.64	115.13
32	2a	516	PSU	N1-C2-N3	5.73	121.62	115.13
1	1A	1911	PSU	N1-C2-N3	5.72	121.61	115.13
55	1x	76	8AN	N3-C2-N1	-5.71	119.75	128.68
1	2A	1917	PSU	N1-C2-N3	5.70	121.59	115.13
1	1A	1917	PSU	N1-C2-N3	5.69	121.58	115.13
55	2x	76	8AN	N3-C2-N1	-5.64	119.86	128.68
1	2A	1939	5MU	C4-N3-C2	-5.60	120.10	127.35
1	1A	1939	5MU	C4-N3-C2	-5.59	120.11	127.35
32	1a	516	PSU	N1-C2-N3	5.47	121.32	115.13
1	2A	1939	5MU	N3-C2-N1	5.33	121.97	114.89
1	1A	2552	OMU	N3-C2-N1	5.33	121.97	114.89
1	2A	2552	OMU	N3-C2-N1	5.15	121.72	114.89
1	1A	1939	5MU	N3-C2-N1	5.08	121.64	114.89
1	2A	1939	5MU	C5-C4-N3	4.99	119.57	115.31
1	2A	1915	5MU	N3-C2-N1	4.98	121.50	114.89
1	1A	1939	5MU	C5-C4-N3	4.91	119.50	115.31
1	1A	1915	5MU	N3-C2-N1	4.90	121.39	114.89
1	1A	1915	5MU	C4-N3-C2	-4.79	121.16	127.35
1	2A	1915	5MU	C4-N3-C2	-4.68	121.29	127.35
32	1a	1519	MA6	N3-C2-N1	-4.67	121.38	128.68
32	2a	1519	MA6	N3-C2-N1	-4.65	121.40	128.68
32	2a	1518	MA6	N3-C2-N1	-4.60	121.50	128.68
1	2A	2552	OMU	C4-N3-C2	-4.51	120.64	126.58
1	1A	1939	5MU	O4-C4-C5	-4.50	119.69	124.90
1	1A	2552	OMU	C4-N3-C2	-4.45	120.72	126.58
1	1A	1915	5MU	C1'-N1-C2	4.41	125.56	117.57
32	1a	1518	MA6	N3-C2-N1	-4.39	121.82	128.68
1	1A	2605	PSU	C4-N3-C2	-4.39	120.02	126.34
1	1A	1939	5MU	C5-C6-N1	-4.33	118.88	123.34
1	1A	1915	5MU	C5-C4-N3	4.29	118.98	115.31
1	2A	1939	5MU	C5-C6-N1	-4.21	119.01	123.34
1	2A	2605	PSU	C4-N3-C2	-4.17	120.33	126.34
1	2A	1942	5MC	C5-C6-N1	-4.16	119.06	123.34
32	1a	1400	5MC	C5-C6-N1	-4.15	119.07	123.34
1	1A	2605	PSU	O2-C2-N1	-4.04	118.34	122.79
54	2w	76	PPU	N1-C6-N6	4.01	121.27	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1915	5MU	C5-C4-N3	3.99	118.72	115.31
32	2a	516	PSU	C4-N3-C2	-3.98	120.61	126.34
1	1A	1917	PSU	C4-N3-C2	-3.98	120.61	126.34
32	2a	1400	5MC	C5-C6-N1	-3.93	119.29	123.34
1	2A	1917	PSU	O2-C2-N1	-3.93	118.46	122.79
1	1A	1942	5MC	C5-C6-N1	-3.89	119.34	123.34
1	2A	1962	5MC	C5-C6-N1	-3.89	119.34	123.34
1	2A	1915	5MU	C1'-N1-C2	3.82	124.49	117.57
1	2A	1911	PSU	C4-N3-C2	-3.81	120.85	126.34
1	2A	1915	5MU	O4-C4-C5	-3.78	120.52	124.90
1	2A	1939	5MU	O4-C4-C5	-3.77	120.53	124.90
32	1a	516	PSU	C4-N3-C2	-3.74	120.95	126.34
1	1A	1915	5MU	C1'-N1-C6	-3.69	114.98	121.12
1	1A	1911	PSU	C4-N3-C2	-3.69	121.03	126.34
32	1a	967	5MC	C5-C6-N1	-3.67	119.56	123.34
32	2a	967	5MC	C5-C6-N1	-3.66	119.57	123.34
1	1A	1939	5MU	O2-C2-N1	-3.62	117.97	122.79
1	2A	2605	PSU	O2-C2-N1	-3.55	118.88	122.79
32	1a	1407	5MC	C5-C6-N1	-3.49	119.75	123.34
1	2A	1917	PSU	C4-N3-C2	-3.47	121.33	126.34
32	2a	516	PSU	O2-C2-N1	-3.43	119.01	122.79
32	1a	1404	5MC	C5-C6-N1	-3.43	119.81	123.34
32	2a	1519	MA6	C4-C5-N7	-3.41	105.84	109.40
43	1l	92	0TD	OD2-CG-CB	3.38	120.45	113.15
1	1A	1915	5MU	O4-C4-C5	-3.36	121.01	124.90
43	2l	92	0TD	OD2-CG-CB	3.30	120.28	113.15
32	2a	1404	5MC	C5-C4-N3	-3.27	118.15	121.67
54	2w	76	PPU	C4-C5-N7	-3.24	106.02	109.40
54	2w	76	PPU	N3-C2-N1	-3.23	123.62	128.68
54	1w	76	PPU	N3-C2-N1	-3.20	123.67	128.68
1	1A	1917	PSU	O2-C2-N1	-3.19	119.28	122.79
32	2a	1407	5MC	C5-C6-N1	-3.16	120.08	123.34
43	1l	92	0TD	CSB-SB-CB	-3.16	96.72	102.44
1	2A	2552	OMU	C2'-C1'-N1	-3.14	108.12	114.22
1	1A	1911	PSU	O2-C2-N1	-3.14	119.33	122.79
32	2a	1518	MA6	C4-C5-N7	-3.05	106.22	109.40
54	1w	76	PPU	C4-C5-N7	-3.05	106.22	109.40
1	2A	1911	PSU	O2-C2-N1	-3.02	119.46	122.79
32	1a	516	PSU	O2-C2-N1	-2.96	119.53	122.79
1	2A	1915	5MU	C1'-N1-C6	-2.96	116.20	121.12
1	1A	1962	5MC	C5-C6-N1	-2.95	120.30	123.34
1	2A	2552	OMU	C5-C4-N3	2.95	119.25	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1404	5MC	C5-C6-N1	-2.92	120.34	123.34
1	1A	2552	OMU	O2-C2-N1	-2.86	118.98	122.79
1	2A	2503	2MA	C8-N7-C5	2.86	108.44	102.99
54	1w	76	PPU	N1-C6-N6	2.85	120.06	117.06
32	1a	1402	4OC	C6-C5-C4	2.83	120.42	116.96
1	2A	2552	OMU	O4-C4-C5	-2.81	120.22	125.16
32	1a	1518	MA6	C4-C5-N7	-2.76	106.52	109.40
1	1A	2552	OMU	O4-C4-C5	-2.73	120.35	125.16
32	1a	1519	MA6	C4-C5-N7	-2.73	106.55	109.40
32	1a	1400	5MC	C5-C4-N3	-2.72	118.74	121.67
1	1A	1915	5MU	O2-C2-N3	-2.65	116.57	121.50
1	2A	1915	5MU	C5-C6-N1	-2.65	120.62	123.34
1	2A	2552	OMU	O2-C2-N1	-2.62	119.30	122.79
1	1A	1915	5MU	C5M-C5-C4	2.59	121.62	118.77
1	2A	2503	2MA	C5-C6-N1	2.57	118.45	114.02
32	2a	1407	5MC	C5-C4-N3	-2.55	118.92	121.67
1	1A	2503	2MA	C5-C6-N1	2.52	118.36	114.02
32	1a	1207	2MG	CM2-N2-C2	-2.50	118.35	123.86
32	2a	1207	2MG	C8-N7-C5	2.49	107.73	102.99
32	1a	1407	5MC	C5-C4-N3	-2.48	118.99	121.67
32	1a	1498	UR3	C3U-N3-C2	2.47	121.64	117.31
1	1A	1915	5MU	C5-C6-N1	-2.46	120.81	123.34
1	1A	2552	OMU	C2'-C1'-N1	-2.45	109.46	114.22
32	1a	1207	2MG	C8-N7-C5	2.45	107.66	102.99
55	2x	76	8AN	O4'-C1'-C2'	-2.44	103.35	106.93
1	1A	2552	OMU	C5-C4-N3	2.42	118.47	114.84
1	2A	1939	5MU	O2-C2-N1	-2.42	119.57	122.79
1	2A	1915	5MU	O2-C2-N3	-2.42	117.00	121.50
32	1a	1404	5MC	C5-C4-N3	-2.39	119.10	121.67
1	2A	1942	5MC	C5-C4-N3	-2.38	119.11	121.67
32	2a	966	M2G	C8-N7-C5	2.37	107.51	102.99
1	1A	2251	OMG	C8-N7-C5	2.37	107.50	102.99
1	1A	2251	OMG	C5-C6-N1	2.37	118.13	113.95
1	1A	1962	5MC	C5-C4-N3	-2.35	119.14	121.67
43	2l	92	0TD	OD1-CG-CB	-2.35	117.52	122.44
32	1a	967	5MC	C5-C4-N3	-2.34	119.15	121.67
1	1A	1920	OMC	O2-C2-N3	-2.33	118.55	122.33
55	1x	76	8AN	O4'-C1'-C2'	-2.29	103.58	106.93
32	2a	1498	UR3	C3U-N3-C4	2.29	121.17	117.89
32	2a	1404	5MC	O2-C2-N3	-2.29	118.61	122.33
1	2A	2251	OMG	C5-C6-N1	2.28	117.98	113.95
32	1a	966	M2G	C8-N7-C5	2.24	107.26	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1962	5MC	C1'-N1-C6	-2.23	117.42	121.12
54	1w	76	PPU	C10-N6-C6	-2.22	112.78	119.51
32	2a	1400	5MC	C1'-N1-C6	-2.22	117.42	121.12
32	2a	1407	5MC	O2-C2-N3	-2.22	118.72	122.33
32	2a	967	5MC	C5-C4-N3	-2.20	119.30	121.67
1	2A	1920	OMC	O2-C2-N3	-2.20	118.75	122.33
43	1l	92	0TD	OD1-CG-CB	-2.17	117.90	122.44
54	2w	76	PPU	C10-N6-C6	-2.16	112.96	119.51
1	2A	2251	OMG	C8-N7-C5	2.16	107.10	102.99
32	2a	516	PSU	O4'-C1'-C2'	2.16	108.18	105.14
32	2a	1404	5MC	CM5-C5-C6	-2.15	119.97	122.85
32	1a	1407	5MC	O2-C2-N3	-2.15	118.83	122.33
1	1A	2605	PSU	C5-C6-N1	-2.13	118.91	122.11
32	2a	1402	4OC	C6-C5-C4	2.13	119.57	116.96
32	2a	1400	5MC	C5-C4-N3	-2.11	119.39	121.67
1	1A	1962	5MC	CM5-C5-C6	-2.11	120.03	122.85
32	2a	966	M2G	C5-C6-N1	2.10	117.66	113.95
32	1a	1207	2MG	C5-C6-N1	2.09	117.65	113.95
1	2A	1962	5MC	C5-C4-N3	-2.09	119.42	121.67
32	1a	1498	UR3	C6-N1-C2	-2.08	119.92	121.79
1	1A	2503	2MA	C8-N7-C5	2.03	106.86	102.99
32	1a	966	M2G	C5-C6-N1	2.03	117.54	113.95
1	1A	1915	5MU	C5M-C5-C6	-2.02	120.16	122.85

There are no chirality outliers.

All (29) 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	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
1	2A	2251	OMG	C1'-C2'-O2'-CM2
43	2l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
54	2w	76	PPU	C3'-C4'-C5'-O5'
55	1x	76	8AN	C4'-C5'-O5'-P
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	2w	76	PPU	O4'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
55	2x	76	8AN	C4'-C5'-O5'-P
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
32	1a	527	G7M	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2
43	1l	92	0TD	SB-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD1
1	1A	2503	2MA	O4'-C4'-C5'-O5'
1	2A	2503	2MA	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2490 ligands modelled in this entry, 2480 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
58	MPD	2B	220	-	7,7,7	0.32	0	9,10,10	0.25	0
59	ARG	1F	318	-	10,11,11	0.71	1 (10%)	11,13,13	1.10	2 (18%)
61	SF4	2d	501	35	0,12,12	-	-	-		
61	SF4	1d	306	35	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
59	ARG	1B	231	-	10,11,11	0.69	0	11,13,13	1.16	2 (18%)
58	MPD	2A	3732	-	7,7,7	0.35	0	9,10,10	0.24	0
58	MPD	18	104	-	7,7,7	0.26	0	9,10,10	0.31	0
58	MPD	1a	1868	-	7,7,7	0.37	0	9,10,10	0.54	0
58	MPD	1T	208	-	7,7,7	0.27	0	9,10,10	0.32	0
58	MPD	1A	4014	-	7,7,7	0.34	0	9,10,10	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	MPD	2B	220	-	-	3/5/5/5	-
59	ARG	1F	318	-	-	2/11/11/11	-
61	SF4	2d	501	35	-	-	0/6/5/5
61	SF4	1d	306	35	-	-	0/6/5/5
59	ARG	1B	231	-	-	4/11/11/11	-
58	MPD	2A	3732	-	-	2/5/5/5	-
58	MPD	18	104	-	-	2/5/5/5	-
58	MPD	1a	1868	-	-	4/5/5/5	-
58	MPD	1T	208	-	-	5/5/5/5	-
58	MPD	1A	4014	-	-	1/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1F	318	ARG	OXT-C	-2.04	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	1F	318	ARG	OXT-C-O	-2.71	117.93	124.09
59	1B	231	ARG	OXT-C-CA	2.57	122.14	113.38
59	1B	231	ARG	OXT-C-O	-2.57	118.26	124.09
59	1F	318	ARG	OXT-C-CA	2.30	121.22	113.38

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1T	208	MPD	C1-C2-C3-C4
58	1T	208	MPD	O2-C2-C3-C4
58	1a	1868	MPD	C2-C3-C4-O4
59	1B	231	ARG	C-CA-CB-CG
59	1F	318	ARG	NE-CD-CG-CB
59	1B	231	ARG	OXT-C-CA-N
59	1B	231	ARG	O-C-CA-N
58	2B	220	MPD	O2-C2-C3-C4
58	1A	4014	MPD	C2-C3-C4-C5
58	1T	208	MPD	C2-C3-C4-C5
58	1a	1868	MPD	C2-C3-C4-C5
58	2B	220	MPD	C2-C3-C4-C5
58	2B	220	MPD	C2-C3-C4-O4
58	1T	208	MPD	CM-C2-C3-C4
58	1a	1868	MPD	C1-C2-C3-C4
58	2A	3732	MPD	C1-C2-C3-C4
58	1a	1868	MPD	O2-C2-C3-C4
58	2A	3732	MPD	O2-C2-C3-C4
58	18	104	MPD	C2-C3-C4-C5
59	1B	231	ARG	N-CA-CB-CG
59	1F	318	ARG	N-CA-CB-CG
58	1T	208	MPD	C2-C3-C4-O4
58	18	104	MPD	C2-C3-C4-O4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.56	105 (3%) 41 38	22, 38, 90, 100	0
1	2A	2856/2915 (97%)	0.35	123 (4%) 35 32	32, 55, 93, 102	0
2	1B	120/121 (99%)	0.11	0 100 100	34, 51, 67, 82	0
2	2B	120/121 (99%)	-0.04	0 100 100	59, 75, 82, 89	0
3	1D	275/276 (99%)	0.61	3 (1%) 80 80	24, 37, 52, 71	0
3	2D	275/276 (99%)	0.61	7 (2%) 57 53	30, 49, 61, 81	0
4	1E	204/206 (99%)	0.64	0 100 100	22, 41, 61, 71	0
4	2E	204/206 (99%)	0.49	0 100 100	33, 54, 68, 77	0
5	1F	203/210 (96%)	0.57	0 100 100	23, 43, 68, 84	0
5	2F	203/210 (96%)	0.40	2 (0%) 82 83	33, 64, 76, 85	0
6	1G	181/182 (99%)	0.31	8 (4%) 34 32	49, 64, 75, 84	0
6	2G	181/182 (99%)	1.27	45 (24%) 0 0	70, 79, 85, 89	0
7	1H	174/180 (96%)	0.48	2 (1%) 80 80	40, 54, 66, 72	0
7	2H	173/180 (96%)	0.95	22 (12%) 3 2	65, 77, 83, 86	0
8	1I	147/148 (99%)	0.26	2 (1%) 75 74	42, 68, 78, 82	0
8	2I	146/148 (98%)	0.39	13 (8%) 9 6	56, 73, 81, 83	0
9	1N	140/140 (100%)	0.65	0 100 100	29, 40, 59, 74	0
9	2N	140/140 (100%)	0.61	5 (3%) 42 39	45, 62, 73, 77	0
10	1O	122/122 (100%)	0.62	1 (0%) 86 86	31, 41, 59, 64	0
10	2O	122/122 (100%)	0.47	1 (0%) 86 86	43, 52, 64, 72	0
11	1P	149/150 (99%)	0.51	1 (0%) 87 88	23, 47, 67, 80	0
11	2P	149/150 (99%)	0.55	4 (2%) 54 50	39, 65, 78, 83	0
12	1Q	141/141 (100%)	0.55	0 100 100	27, 40, 52, 68	0
12	2Q	141/141 (100%)	0.63	4 (2%) 53 49	41, 63, 72, 78	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	27, 37, 54, 63	0
13	2R	118/118 (100%)	0.45	0 100 100	40, 50, 59, 71	0
14	1S	110/112 (98%)	0.39	0 100 100	40, 51, 63, 69	0
14	2S	110/112 (98%)	0.58	8 (7%) 15 11	64, 71, 76, 79	0
15	1T	131/146 (89%)	0.55	3 (2%) 60 56	34, 45, 67, 79	0
15	2T	131/146 (89%)	0.40	3 (2%) 60 56	44, 56, 72, 81	0
16	1U	116/118 (98%)	0.68	0 100 100	25, 33, 48, 67	0
16	2U	116/118 (98%)	0.53	0 100 100	40, 58, 70, 75	0
17	1V	101/101 (100%)	0.52	0 100 100	26, 43, 59, 68	0
17	2V	101/101 (100%)	0.44	1 (0%) 82 83	43, 68, 73, 80	0
18	1W	112/113 (99%)	0.68	2 (1%) 68 65	28, 34, 53, 76	0
18	2W	112/113 (99%)	0.66	4 (3%) 42 39	38, 49, 65, 85	0
19	1X	95/96 (98%)	0.64	1 (1%) 80 80	30, 39, 61, 74	0
19	2X	95/96 (98%)	0.67	5 (5%) 26 23	45, 59, 72, 78	0
20	1Y	107/110 (97%)	0.54	1 (0%) 84 85	38, 50, 65, 75	0
20	2Y	107/110 (97%)	1.00	13 (12%) 4 2	58, 68, 76, 83	0
21	1Z	203/206 (98%)	0.34	5 (2%) 57 53	42, 59, 73, 82	0
21	2Z	201/206 (97%)	0.70	20 (9%) 7 4	63, 74, 81, 84	0
22	10	83/85 (97%)	0.56	0 100 100	30, 38, 50, 62	0
22	20	83/85 (97%)	0.94	7 (8%) 11 8	45, 60, 69, 74	0
23	11	97/98 (98%)	0.74	3 (3%) 49 45	29, 45, 67, 72	0
23	21	97/98 (98%)	0.62	5 (5%) 27 24	39, 55, 73, 77	0
24	12	70/72 (97%)	0.56	1 (1%) 75 74	39, 50, 59, 81	0
24	22	70/72 (97%)	0.42	2 (2%) 51 47	61, 67, 73, 77	0
25	13	59/60 (98%)	0.59	0 100 100	27, 38, 63, 74	0
25	23	59/60 (98%)	0.55	1 (1%) 70 67	51, 60, 77, 79	0
26	14	69/71 (97%)	0.61	10 (14%) 2 1	56, 76, 88, 95	0
26	24	69/71 (97%)	1.54	21 (30%) 0 0	78, 84, 90, 93	0
27	15	59/60 (98%)	0.73	1 (1%) 70 67	25, 36, 54, 63	0
27	25	59/60 (98%)	0.44	0 100 100	35, 49, 65, 73	0
28	16	53/54 (98%)	0.43	0 100 100	33, 43, 58, 60	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.44	1 (1%) 66 64	50, 59, 65, 71	0
29	17	48/49 (97%)	0.99	6 (12%) 3 2	24, 31, 56, 61	0
29	27	48/49 (97%)	0.91	6 (12%) 3 2	35, 40, 64, 70	0
30	18	64/65 (98%)	0.53	0 100 100	30, 36, 42, 53	0
30	28	64/65 (98%)	0.83	3 (4%) 31 29	45, 54, 61, 65	0
31	19	37/37 (100%)	0.62	0 100 100	33, 42, 54, 58	0
31	29	37/37 (100%)	1.09	5 (13%) 3 2	55, 64, 72, 74	0
32	1a	1488/1521 (97%)	0.20	37 (2%) 57 53	36, 67, 89, 100	0
32	2a	1492/1521 (98%)	0.41	85 (5%) 23 20	44, 73, 91, 102	0
33	1b	231/256 (90%)	0.82	31 (13%) 3 2	63, 75, 83, 88	0
33	2b	231/256 (90%)	1.30	60 (25%) 0 0	70, 80, 86, 91	0
34	1c	206/239 (86%)	0.85	27 (13%) 3 2	62, 70, 80, 84	0
34	2c	206/239 (86%)	1.86	82 (39%) 0 0	72, 81, 85, 92	0
35	1d	208/209 (99%)	0.66	16 (7%) 13 10	56, 69, 78, 84	0
35	2d	208/209 (99%)	0.95	22 (10%) 6 4	59, 69, 77, 82	0
36	1e	148/162 (91%)	0.44	0 100 100	52, 63, 72, 80	0
36	2e	148/162 (91%)	0.84	17 (11%) 4 3	57, 70, 79, 85	0
37	1f	100/101 (99%)	0.18	1 (1%) 82 83	49, 64, 71, 79	0
37	2f	100/101 (99%)	0.28	1 (1%) 82 83	58, 67, 75, 82	0
38	1g	155/156 (99%)	0.46	11 (7%) 16 12	60, 69, 76, 81	0
38	2g	155/156 (99%)	1.28	36 (23%) 0 0	69, 79, 83, 87	0
39	1h	137/138 (99%)	0.61	7 (5%) 28 25	56, 66, 71, 78	0
39	2h	137/138 (99%)	0.94	16 (11%) 4 3	62, 71, 76, 79	0
40	1i	127/128 (99%)	1.29	32 (25%) 0 0	58, 75, 80, 82	0
40	2i	126/128 (98%)	3.21	94 (74%) 0 0	74, 82, 87, 89	0
41	1j	97/105 (92%)	1.35	17 (17%) 1 1	60, 75, 83, 89	0
41	2j	96/105 (91%)	2.43	58 (60%) 0 0	72, 82, 86, 91	0
42	1k	114/129 (88%)	0.37	3 (2%) 56 52	44, 62, 72, 77	0
42	2k	114/129 (88%)	0.74	9 (7%) 12 9	58, 70, 78, 81	0
43	1l	121/132 (91%)	0.70	10 (8%) 11 8	49, 59, 68, 76	0
43	2l	121/132 (91%)	0.63	7 (5%) 23 20	54, 63, 70, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	116/126 (92%)	0.52	9 (7%) 13 9	60, 72, 78, 80	0
44	2m	114/126 (90%)	1.65	38 (33%) 0 0	72, 81, 85, 87	0
45	1n	60/61 (98%)	1.31	12 (20%) 1 0	63, 68, 76, 79	0
45	2n	60/61 (98%)	3.07	48 (80%) 0 0	75, 80, 85, 89	0
46	1o	88/89 (98%)	0.33	1 (1%) 80 80	46, 63, 74, 76	0
46	2o	88/89 (98%)	0.67	4 (4%) 33 30	59, 69, 78, 81	0
47	1p	82/88 (93%)	1.26	17 (20%) 1 0	59, 69, 76, 83	0
47	2p	82/88 (93%)	0.91	8 (9%) 7 5	61, 68, 76, 79	0
48	1q	99/105 (94%)	0.67	10 (10%) 7 4	55, 67, 75, 80	0
48	2q	99/105 (94%)	0.73	10 (10%) 7 4	57, 67, 75, 79	0
49	1r	68/88 (77%)	0.31	1 (1%) 73 71	54, 61, 75, 82	0
49	2r	68/88 (77%)	0.57	3 (4%) 34 32	61, 69, 78, 85	0
50	1s	83/93 (89%)	0.50	5 (6%) 21 18	63, 74, 79, 82	0
50	2s	83/93 (89%)	2.06	43 (51%) 0 0	68, 82, 86, 89	0
51	1t	96/106 (90%)	1.04	17 (17%) 1 1	60, 70, 78, 82	0
51	2t	98/106 (92%)	0.67	4 (4%) 37 34	56, 67, 78, 80	0
52	1u	23/27 (85%)	1.67	8 (34%) 0 0	65, 69, 72, 74	0
52	2u	23/27 (85%)	2.63	15 (65%) 0 0	74, 79, 82, 82	0
53	1y	97/113 (85%)	0.74	5 (5%) 27 24	53, 62, 72, 76	0
53	2y	96/113 (84%)	3.99	77 (80%) 0 0	71, 80, 87, 89	0
54	1w	3/4 (75%)	-0.07	0 100 100	30, 30, 40, 55	0
54	2w	3/4 (75%)	-0.43	0 100 100	41, 41, 48, 62	0
55	1x	3/4 (75%)	0.29	0 100 100	28, 28, 30, 41	0
55	2x	3/4 (75%)	0.00	0 100 100	37, 37, 40, 55	0
56	1v	3/3 (100%)	0.94	0 100 100	25, 25, 27, 33	0
56	2v	3/3 (100%)	1.87	1 (33%) 0 0	40, 40, 44, 51	0
All	All	20796/21490 (96%)	0.62	1501 (7%) 15 11	22, 62, 85, 102	0

All (1501) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
53	2y	88	LEU	10.4
40	2i	63	ILE	9.2

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Mol	Chain	Res	Type	RSRZ
40	2i	109	VAL	9.1
53	2y	40	ILE	9.0
1	2A	2146	C	9.0
45	2n	2	ALA	9.0
44	2m	116	THR	8.6
53	2y	5	ILE	8.4
1	1A	1087	G	8.4
1	2A	2139	C	8.3
26	24	49	PHE	8.2
32	2a	1030(A)	G	8.2
53	2y	12	ILE	8.2
53	2y	10	MET	8.0
32	2a	1030(B)	C	8.0
32	2a	1036	G	8.0
34	2c	152	ILE	8.0
1	2A	2147	G	7.8
1	2A	2140	C	7.7
40	2i	72	GLY	7.7
1	2A	2153	G	7.7
1	1A	1075	C	7.5
53	2y	77	LEU	7.5
32	1a	1036	G	7.3
1	2A	2793	G	7.2
34	2c	159	GLY	7.2
21	2Z	192	ALA	7.2
32	1a	1001	A	7.1
41	2j	72	VAL	7.1
53	2y	41	LEU	7.0
34	2c	157	ILE	7.0
32	1a	1031	G	6.8
44	2m	5	ALA	6.8
20	2Y	1	MET	6.7
53	2y	39	ILE	6.7
53	2y	48	PHE	6.6
1	1A	1089	G	6.6
1	1A	1076	C	6.6
1	2A	2802	G	6.6
53	2y	52	ALA	6.6
32	1a	1030(B)	C	6.5
1	2A	2142	C	6.5
40	2i	66	ARG	6.5
1	2A	1509	C	6.5

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Mol	Chain	Res	Type	RSRZ
1	2A	2145	C	6.5
35	1d	2	GLY	6.4
53	2y	38	HIS	6.4
1	2A	2169	A	6.4
40	2i	69	GLY	6.4
35	2d	149	ALA	6.3
32	2a	1257	U	6.3
1	1A	1067	A	6.3
33	2b	118	LEU	6.3
32	1a	1001(A)	G	6.3
32	2a	1286	A	6.2
41	2j	96	ILE	6.2
34	2c	190	ARG	6.2
1	2A	2804	C	6.2
38	2g	155	ARG	6.2
21	2Z	191	VAL	6.2
53	2y	71	TYR	6.2
41	2j	67	THR	6.2
45	2n	34	TYR	6.2
53	2y	20	VAL	6.1
1	2A	2168	G	6.1
53	2y	3	MET	6.1
6	2G	39	ILE	6.1
53	2y	63	ALA	6.1
40	2i	90	PRO	6.0
1	2A	2174	C	6.0
32	2a	1033	G	6.0
1	1A	1090	U	6.0
1	2A	1046	A	6.0
40	2i	125	TYR	6.0
53	2y	64	SER	6.0
34	2c	124	ILE	6.0
44	2m	6	GLY	6.0
1	2A	2125	G	5.9
1	2A	2801(A)	A	5.9
1	1A	2141	G	5.9
33	2b	136	VAL	5.9
40	2i	10	ARG	5.9
32	2a	1001(A)	G	5.9
53	2y	78	ILE	5.9
40	2i	42	ARG	5.9
32	2a	1026	G	5.9

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Mol	Chain	Res	Type	RSRZ
53	2y	51	ASP	5.8
53	2y	4	ASN	5.8
6	2G	152	LEU	5.8
53	2y	50	ALA	5.8
53	2y	9	GLN	5.8
53	2y	11	GLU	5.7
26	24	51	ASP	5.7
38	2g	154	TYR	5.7
40	2i	67	GLY	5.7
32	2a	1034	G	5.7
53	2y	8	LYS	5.7
1	2A	2805	G	5.7
1	2A	2138	C	5.7
40	2i	102	LEU	5.7
32	1a	1030(D)	A	5.7
38	2g	156	TRP	5.6
41	2j	34	VAL	5.6
1	2A	1067	A	5.6
53	2y	42	SER	5.6
26	14	55	ARG	5.6
50	2s	10	PHE	5.6
40	2i	76	ALA	5.5
53	2y	15	ALA	5.5
44	2m	102	ARG	5.5
40	2i	50	LEU	5.5
45	2n	13	THR	5.5
48	2q	98	LEU	5.5
50	2s	82	GLY	5.5
32	1a	1026	G	5.5
42	2k	13	GLN	5.5
33	2b	97	TRP	5.5
1	2A	2124	G	5.5
1	1A	1066	U	5.4
38	2g	41	ARG	5.4
44	2m	24	GLY	5.4
1	1A	1091	G	5.4
3	2D	2	ALA	5.4
32	2a	1031	G	5.4
32	1a	1028	C	5.4
1	1A	2805	G	5.4
34	2c	196	LEU	5.4
53	2y	16	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
45	1n	51	GLY	5.3
1	2A	2154	G	5.3
1	2A	2144	U	5.3
45	1n	2	ALA	5.3
1	2A	2133	G	5.3
1	2A	2162	G	5.3
32	2a	1027	C	5.3
53	2y	67	HIS	5.3
1	1A	2792	G	5.3
7	2H	101	ARG	5.3
50	2s	69	HIS	5.2
40	2i	7	THR	5.2
40	2i	75	ASP	5.2
23	11	2	SER	5.2
1	2A	2111	C	5.2
32	2a	1001	A	5.2
32	2a	1030(C)	G	5.2
33	2b	122	PHE	5.2
41	2j	65	LEU	5.2
53	2y	37	PRO	5.2
38	2g	80	VAL	5.2
40	2i	27	THR	5.2
34	2c	189	ALA	5.2
45	2n	6	LEU	5.2
1	2A	2132	U	5.1
1	2A	2136	C	5.1
45	2n	14	PRO	5.1
53	2y	58	ASN	5.1
41	2j	27	ALA	5.1
50	2s	67	VAL	5.1
53	2y	87	LYS	5.1
41	2j	44	VAL	5.1
44	2m	87	TYR	5.1
26	24	50	VAL	5.1
1	1A	1088	A	5.1
41	2j	68	HIS	5.1
6	2G	146	TYR	5.1
20	1Y	1	MET	5.1
1	2A	2803	C	5.1
1	2A	2116	G	5.0
1	2A	2152	G	5.0
1	1A	2132	U	5.0

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Mol	Chain	Res	Type	RSRZ
34	2c	33	LEU	5.0
40	2i	74	ILE	5.0
40	2i	36	TYR	5.0
53	2y	79	ASN	5.0
40	2i	18	PHE	5.0
7	2H	128	PRO	5.0
40	2i	127	LYS	5.0
32	2a	1030	C	5.0
43	2l	18	VAL	5.0
1	2A	2141	G	5.0
33	2b	132	LYS	5.0
45	2n	12	ARG	5.0
45	2n	35	ARG	5.0
1	1A	1065	U	5.0
38	2g	83	ALA	4.9
51	1t	72	LEU	4.9
32	1a	1033	G	4.9
53	1y	95	ARG	4.9
1	1A	2140	C	4.9
45	1n	33	VAL	4.9
1	1A	1074	G	4.9
52	2u	14	TRP	4.9
45	2n	61	TRP	4.9
1	2A	2173	A	4.8
26	24	52	THR	4.8
40	2i	14	VAL	4.8
1	1A	1068	G	4.8
40	2i	56	LEU	4.8
52	2u	23	PRO	4.8
50	2s	11	VAL	4.8
1	1A	2804	C	4.8
21	2Z	155	LEU	4.8
35	2d	70	ILE	4.8
40	2i	8	GLY	4.8
32	1a	1030	C	4.8
52	2u	6	ARG	4.8
32	1a	1030(C)	G	4.8
1	2A	2126	A	4.7
32	2a	1035	A	4.7
39	2h	131	GLY	4.7
53	2y	59	GLY	4.7
40	2i	61	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
33	2b	165	VAL	4.7
40	2i	37	PHE	4.7
41	2j	38	ILE	4.7
19	2X	68	ARG	4.7
40	2i	33	PHE	4.7
50	2s	34	TRP	4.7
53	2y	24	LEU	4.7
40	2i	68	GLY	4.7
34	2c	177	THR	4.6
38	1g	85	TYR	4.6
40	1i	14	VAL	4.6
32	1a	1029	C	4.6
53	2y	23	ARG	4.6
38	2g	34	GLY	4.6
1	2A	2896	C	4.6
34	2c	87	LEU	4.6
53	2y	73	ALA	4.6
41	2j	29	ARG	4.6
53	2y	94	ALA	4.6
1	2A	1085	A	4.6
34	2c	184	TYR	4.6
40	2i	4	TYR	4.6
1	2A	2107	C	4.6
34	2c	160	ALA	4.5
7	2H	82	GLY	4.5
32	2a	1002	G	4.5
40	1i	76	ALA	4.5
38	2g	85	TYR	4.5
1	1A	2793	G	4.5
51	1t	76	ALA	4.5
32	2a	1028	C	4.5
23	11	98	LEU	4.5
40	2i	47	LEU	4.5
6	2G	136	ARG	4.5
40	2i	21	PRO	4.5
6	2G	140	ILE	4.5
1	2A	2106	G	4.5
34	1c	64	VAL	4.5
40	2i	17	VAL	4.5
52	2u	16	GLY	4.5
23	21	2	SER	4.5
1	1A	1081	U	4.5

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Mol	Chain	Res	Type	RSRZ
33	2b	121	LEU	4.5
26	14	49	PHE	4.4
34	2c	163	ALA	4.4
38	2g	25	ALA	4.4
40	2i	113	LYS	4.4
34	2c	188	LEU	4.4
35	1d	70	ILE	4.4
1	2A	2148	G	4.4
26	24	63	TYR	4.4
33	1b	128	GLU	4.4
1	1A	1080	C	4.4
1	1A	2113	U	4.4
34	2c	8	ILE	4.4
53	2y	35	ILE	4.4
53	2y	74	ILE	4.4
53	2y	19	HIS	4.4
53	2y	62	VAL	4.4
41	2j	54	PHE	4.4
41	2j	6	ILE	4.4
32	2a	1030(D)	A	4.4
34	2c	206	GLU	4.4
45	2n	10	ALA	4.4
41	2j	46	ARG	4.4
34	2c	66	VAL	4.4
1	2A	2143	C	4.3
1	1A	2144	U	4.3
1	1A	1077	A	4.3
1	1A	2794	C	4.3
32	1a	1037	C	4.3
44	1m	115	LYS	4.3
1	1A	1078	U	4.3
53	2y	7	SER	4.3
53	2y	75	ASN	4.3
32	1a	1257	U	4.3
1	2A	2165	G	4.3
40	2i	5	TYR	4.3
50	2s	71	LEU	4.3
1	2A	2110	G	4.3
32	1a	1024	G	4.3
53	2y	84	GLN	4.3
53	2y	17	ARG	4.3
45	2n	18	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	2A	2120	G	4.3
40	2i	59	PHE	4.3
20	2Y	106	LEU	4.2
33	2b	232	PRO	4.2
1	1A	2147	G	4.2
26	24	19	GLY	4.2
26	24	66	SER	4.2
1	2A	2118	U	4.2
29	27	47	ARG	4.2
40	2i	104	ARG	4.2
32	2a	1029	C	4.2
6	2G	73	ALA	4.2
1	2A	6	A	4.2
40	2i	6	GLY	4.2
32	1a	1492	A	4.2
26	24	40	HIS	4.2
1	1A	888	C	4.2
26	24	56	VAL	4.2
40	2i	88	TYR	4.2
33	2b	139	LYS	4.1
1	2A	2151	G	4.1
32	1a	1030(A)	G	4.1
40	2i	115	GLY	4.1
40	2i	108	VAL	4.1
50	2s	75	ALA	4.1
21	2Z	197	ILE	4.1
40	2i	114	TYR	4.1
39	2h	2	LEU	4.1
40	2i	92	TYR	4.1
41	2j	19	SER	4.1
41	2j	48	THR	4.1
44	2m	64	TRP	4.1
40	2i	44	VAL	4.1
42	2k	89	ALA	4.1
47	1p	19	ILE	4.1
6	2G	142	PRO	4.1
34	2c	158	GLY	4.1
38	1g	80	VAL	4.1
41	2j	89	ASP	4.0
1	2A	2108	C	4.0
52	1u	2	GLY	4.0
36	2e	13	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	2A	1083	U	4.0
1	2A	1075	C	4.0
45	2n	55	GLY	4.0
21	2Z	125	LEU	4.0
45	2n	39	LEU	4.0
8	2I	46	ALA	4.0
35	2d	48	ALA	4.0
1	1A	2145	C	4.0
1	1A	2153	G	4.0
6	2G	62	LEU	4.0
1	1A	2152	G	4.0
1	2A	229	A	4.0
1	2A	2135	A	4.0
32	1a	1000	U	4.0
53	2y	70	MET	4.0
26	24	46	GLN	4.0
33	1b	133	LYS	4.0
34	2c	195	VAL	4.0
53	2y	49	VAL	4.0
34	2c	101	LEU	4.0
1	2A	2897	U	4.0
41	2j	62	HIS	4.0
41	2j	64	GLU	4.0
41	2j	35	SER	4.0
1	1A	2142	C	3.9
33	2b	181	PHE	3.9
33	2b	133	LYS	3.9
32	1a	1447	A	3.9
38	1g	156	TRP	3.9
27	15	60	VAL	3.9
50	2s	12	ASP	3.9
53	2y	69	ASP	3.9
1	1A	2803	C	3.9
35	1d	4	TYR	3.9
40	2i	26	VAL	3.9
36	2e	109	ILE	3.9
45	2n	15	LYS	3.9
26	14	54	GLY	3.9
1	2A	2894	G	3.9
53	2y	21	ALA	3.9
1	1A	2146	C	3.9
45	2n	50	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
33	2b	44	LEU	3.9
6	2G	139	LEU	3.9
26	24	27	THR	3.8
40	2i	70	LYS	3.8
45	2n	59	ALA	3.8
1	2A	2127	G	3.8
19	2X	92	LEU	3.8
50	2s	28	LYS	3.8
33	1b	29	ALA	3.8
43	2l	19	ARG	3.8
52	2u	2	GLY	3.8
32	2a	1150	U	3.8
45	2n	54	PRO	3.8
53	2y	47	GLY	3.8
1	2A	2123	G	3.8
32	1a	1034	G	3.8
1	1A	1079	C	3.8
45	2n	57	ARG	3.8
6	2G	182	LYS	3.8
1	1A	2107	C	3.8
40	1i	114	TYR	3.8
41	2j	47	PHE	3.8
41	1j	20	ALA	3.8
41	1j	73	ASP	3.8
18	2W	60	ASN	3.8
40	2i	65	VAL	3.8
40	2i	91	ASP	3.8
33	1b	118	LEU	3.7
29	27	48	LYS	3.7
32	2a	1531	A	3.7
1	2A	1081	U	3.7
1	1A	1509	C	3.7
40	1i	28	VAL	3.7
41	2j	40	LEU	3.7
53	2y	53	THR	3.7
1	2A	1095	A	3.7
53	2y	45	PRO	3.7
40	2i	103	THR	3.7
1	1A	1175	U	3.7
7	2H	159	GLU	3.7
34	1c	94	LEU	3.7
35	1d	167	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
40	2i	57	GLY	3.7
1	2A	2137	C	3.7
1	1A	1176	G	3.7
1	2A	2119	A	3.7
53	2y	61	LEU	3.7
1	2A	1076	C	3.7
44	1m	2	ALA	3.7
50	2s	49	ILE	3.6
7	1H	2	SER	3.6
40	2i	71	SER	3.6
44	2m	23	TYR	3.6
44	2m	113	PRO	3.6
36	2e	12	LEU	3.6
1	1A	2154	G	3.6
34	2c	194	GLY	3.6
41	2j	88	LEU	3.6
41	2j	66	ARG	3.6
1	2A	888	C	3.6
1	2A	2157	G	3.6
51	1t	9	ASN	3.6
52	2u	13	ILE	3.6
1	2A	2179	C	3.6
40	1i	79	LEU	3.6
1	1A	229	A	3.6
32	1a	1035	A	3.6
45	2n	42	ILE	3.6
1	1A	1083	U	3.6
1	1A	2159	G	3.6
41	2j	45	ARG	3.6
52	2u	9	ARG	3.6
34	1c	47	LEU	3.6
6	2G	149	VAL	3.6
34	2c	4	LYS	3.6
44	2m	65	LYS	3.6
32	1a	1005	A	3.5
53	2y	46	GLN	3.5
6	2G	155	MET	3.5
32	1a	1002	G	3.5
33	2b	70	PHE	3.5
40	2i	40	LEU	3.5
6	2G	57	ALA	3.5
53	2y	6	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	1A	2139	C	3.5
1	1A	1093	G	3.5
44	2m	13	LYS	3.5
35	1d	23	GLY	3.5
45	2n	51	GLY	3.5
1	2A	2170	A	3.5
53	2y	82	GLU	3.5
34	2c	76	VAL	3.5
33	2b	38	GLY	3.5
6	2G	43	LEU	3.5
47	1p	1	MET	3.5
34	2c	153	VAL	3.5
45	2n	29	ARG	3.5
40	1i	37	PHE	3.5
21	1Z	192	ALA	3.5
53	1y	94	ALA	3.5
1	1A	2169	A	3.5
40	1i	51	ARG	3.5
40	2i	120	ARG	3.5
41	1j	72	VAL	3.5
45	2n	24	CYS	3.5
50	2s	30	LEU	3.5
26	14	46	GLN	3.5
1	1A	1063	G	3.5
40	2i	126	SER	3.5
36	2e	22	GLY	3.5
6	2G	80	PHE	3.4
45	2n	21	TYR	3.4
1	1A	1072	C	3.4
41	1j	90	LEU	3.4
51	1t	66	ALA	3.4
43	2l	13	LYS	3.4
40	2i	86	VAL	3.4
44	2m	17	VAL	3.4
1	2A	2792	G	3.4
32	1a	1286	A	3.4
40	2i	62	TYR	3.4
50	2s	80	TYR	3.4
1	1A	1064	C	3.4
7	2H	103	LEU	3.4
38	2g	81	GLY	3.4
1	1A	2115	G	3.4

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Mol	Chain	Res	Type	RSRZ
53	2y	54	ILE	3.4
7	2H	105	LEU	3.4
29	17	47	ARG	3.4
7	2H	19	VAL	3.4
1	1A	2155	G	3.4
44	2m	75	ALA	3.4
45	2n	49	HIS	3.4
36	2e	84	PHE	3.4
48	1q	27	PHE	3.4
21	1Z	51	ALA	3.4
50	2s	63	THR	3.4
32	2a	1492	A	3.4
1	2A	2149	G	3.4
32	2a	1032	G	3.4
38	2g	6	ARG	3.4
34	1c	201	TYR	3.4
38	2g	40	ALA	3.4
1	1A	2137	C	3.4
1	1A	2143	C	3.4
9	2N	140	VAL	3.4
44	2m	60	VAL	3.4
50	2s	16	LEU	3.3
44	1m	116	THR	3.3
33	2b	92	TYR	3.3
1	1A	1085	A	3.3
40	2i	30	GLY	3.3
40	2i	73	GLN	3.3
47	2p	33	ILE	3.3
44	2m	42	ALA	3.3
36	2e	20	GLN	3.3
34	1c	63	ASN	3.3
1	1A	2117	A	3.3
40	2i	79	LEU	3.3
40	2i	81	ILE	3.3
7	2H	102	ALA	3.3
40	1i	128	ARG	3.3
6	1G	48	GLU	3.3
38	2g	144	MET	3.3
50	2s	66	MET	3.3
34	2c	41	GLY	3.3
6	1G	49	ASP	3.3
40	2i	32	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	1A	2138	C	3.3
42	2k	126	ARG	3.3
38	2g	42	ILE	3.3
50	2s	15	LEU	3.3
44	2m	43	THR	3.3
1	1A	2116	G	3.3
32	2a	1003	G	3.3
52	2u	5	ASP	3.3
33	1b	165	VAL	3.3
19	2X	66	LEU	3.3
34	2c	146	ALA	3.3
36	2e	94	ALA	3.3
40	1i	63	ILE	3.3
32	1a	1032	G	3.3
6	2G	52	ILE	3.3
26	14	52	THR	3.3
38	2g	134	ALA	3.3
41	2j	74	ILE	3.3
15	1T	38	ASN	3.3
53	2y	76	GLU	3.3
45	2n	45	ARG	3.3
33	2b	124	SER	3.3
32	1a	1023	G	3.2
41	1j	85	LEU	3.2
45	2n	44	LEU	3.2
1	2A	2109	U	3.2
38	2g	78	ARG	3.2
40	2i	105	ASP	3.2
29	17	1	MET	3.2
1	2A	2164	C	3.2
40	1i	109	VAL	3.2
34	1c	80	GLY	3.2
38	1g	12	LEU	3.2
50	2s	5	LEU	3.2
34	2c	65	ALA	3.2
1	1A	2112	G	3.2
1	1A	2167	U	3.2
35	2d	146	ILE	3.2
40	2i	124	GLN	3.2
32	1a	1027	C	3.2
1	2A	2134	A	3.2
48	1q	23	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
33	2b	66	GLY	3.2
35	2d	96	LEU	3.2
38	1g	16	LEU	3.2
47	1p	73	LEU	3.2
50	2s	72	GLY	3.2
39	2h	124	ALA	3.2
34	2c	128	PHE	3.2
1	2A	2159	G	3.2
38	2g	5	ARG	3.2
26	24	67	TYR	3.2
34	1c	193	TYR	3.2
7	2H	115	VAL	3.2
6	2G	138	GLN	3.2
45	2n	7	ILE	3.2
3	2D	38	LYS	3.2
48	1q	97	SER	3.2
7	2H	36	PRO	3.2
1	1A	1102	C	3.2
40	1i	125	TYR	3.2
33	2b	120	ALA	3.2
41	2j	15	THR	3.2
1	2A	2150	U	3.2
1	2A	2172	U	3.2
15	2T	111	ARG	3.2
1	2A	1064	C	3.2
20	2Y	90	LEU	3.2
32	2a	1157	A	3.2
1	2A	1066	U	3.2
6	2G	88	ILE	3.2
33	2b	182	ILE	3.2
34	2c	149	ALA	3.1
38	2g	116	ALA	3.1
45	1n	34	TYR	3.1
26	24	54	GLY	3.1
40	2i	29	ASN	3.1
34	2c	199	LYS	3.1
45	1n	14	PRO	3.1
20	2Y	75	ILE	3.1
39	2h	134	ILE	3.1
41	2j	31	GLY	3.1
33	1b	207	ALA	3.1
41	2j	32	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
50	2s	41	VAL	3.1
53	2y	43	LYS	3.1
53	2y	72	THR	3.1
6	2G	58	GLN	3.1
44	2m	110	ARG	3.1
33	1b	131	PRO	3.1
1	2A	1084	A	3.1
35	1d	157	LEU	3.1
45	1n	61	TRP	3.1
36	2e	11	ILE	3.1
6	2G	87	PRO	3.1
34	2c	23	TYR	3.1
47	1p	39	TYR	3.1
32	2a	1223	C	3.1
1	2A	2155	G	3.1
34	2c	201	TYR	3.1
41	2j	63	PHE	3.1
43	1l	64	TYR	3.1
45	2n	36	PHE	3.1
47	2p	9	PHE	3.1
56	2v	1	MET	3.1
41	2j	25	GLU	3.1
21	2Z	80	ARG	3.1
34	1c	41	GLY	3.1
34	2c	81	GLY	3.1
36	2e	16	THR	3.1
39	2h	4	ASP	3.0
45	2n	31	ARG	3.0
50	2s	3	ARG	3.0
6	2G	92	VAL	3.0
26	14	56	VAL	3.0
1	2A	2167	U	3.0
42	2k	75	TYR	3.0
1	1A	1071	G	3.0
43	1l	63	GLY	3.0
53	2y	55	ASN	3.0
7	2H	165	ALA	3.0
40	2i	85	LEU	3.0
9	2N	9	VAL	3.0
33	1b	132	LYS	3.0
41	1j	44	VAL	3.0
47	2p	19	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
6	1G	146	TYR	3.0
33	2b	146	GLN	3.0
32	2a	998	G	3.0
47	2p	11	SER	3.0
35	2d	11	LEU	3.0
40	2i	64	THR	3.0
40	2i	28	VAL	3.0
38	2g	32	ARG	3.0
38	2g	76	ARG	3.0
40	2i	9	ARG	3.0
1	2A	2160	G	3.0
20	2Y	42	VAL	3.0
21	2Z	96	VAL	3.0
43	2l	43	VAL	3.0
29	27	1	MET	3.0
34	2c	126	ARG	3.0
40	2i	20	ARG	3.0
1	1A	1070	A	3.0
34	1c	60	ALA	3.0
34	2c	43	LEU	3.0
29	17	48	LYS	3.0
40	2i	31	GLN	3.0
1	1A	2149	G	3.0
32	2a	1006	C	3.0
35	2d	158	ILE	3.0
45	2n	37	PHE	3.0
43	1l	62	SER	3.0
32	2a	994	A	3.0
6	2G	29	TRP	3.0
34	2c	3	ASN	3.0
50	2s	60	VAL	2.9
45	2n	16	PHE	2.9
1	1A	2174	C	2.9
32	2a	1149	C	2.9
42	2k	25	TYR	2.9
50	2s	52	TYR	2.9
51	1t	62	LEU	2.9
1	1A	1847	A	2.9
32	2a	1041	A	2.9
8	2I	92	VAL	2.9
40	2i	53	VAL	2.9
1	1A	271(K)	U	2.9

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Mol	Chain	Res	Type	RSRZ
1	2A	2130	U	2.9
53	2y	89	GLN	2.9
32	1a	219	C	2.9
34	1c	160	ALA	2.9
34	2c	166	GLU	2.9
36	2e	21	ALA	2.9
1	2A	2176	A	2.9
11	2P	15	ARG	2.9
34	2c	164	ARG	2.9
1	2A	1043	C	2.9
26	24	44	THR	2.9
1	1A	2168	G	2.9
8	2I	107	VAL	2.9
42	2k	91	ARG	2.9
1	1A	2801(A)	A	2.9
1	2A	2117	A	2.9
53	2y	18	GLN	2.9
33	2b	162	ILE	2.9
53	2y	92	GLY	2.9
21	2Z	187	ALA	2.9
40	2i	106	ALA	2.9
26	24	57	GLU	2.9
52	1u	9	ARG	2.9
41	2j	33	GLN	2.9
6	2G	159	VAL	2.9
33	2b	164	VAL	2.9
41	2j	24	VAL	2.9
44	1m	74	VAL	2.9
50	2s	35	SER	2.9
1	2A	1103	A	2.9
32	2a	1111	A	2.9
7	2H	40	GLU	2.9
7	2H	129	THR	2.9
46	2o	17	ARG	2.9
53	2y	83	ARG	2.9
6	2G	37	VAL	2.9
40	2i	41	VAL	2.9
45	2n	25	VAL	2.9
33	2b	37	ASN	2.9
6	1G	80	PHE	2.9
32	2a	1023	G	2.9
1	1A	1086	A	2.9

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Mol	Chain	Res	Type	RSRZ
47	1p	41	PRO	2.9
45	2n	30	ALA	2.9
52	1u	14	TRP	2.9
40	2i	110	GLU	2.8
45	2n	33	VAL	2.8
53	1y	58	ASN	2.8
53	2y	68	GLU	2.8
35	2d	49	ARG	2.8
36	2e	14	ARG	2.8
44	2m	104	ARG	2.8
41	1j	54	PHE	2.8
41	2j	77	PRO	2.8
21	2Z	51	ALA	2.8
51	1t	67	ALA	2.8
14	2S	58	LEU	2.8
21	1Z	202	GLU	2.8
26	24	55	ARG	2.8
33	1b	36	ARG	2.8
40	1i	126	SER	2.8
41	2j	10	GLY	2.8
53	2y	80	LYS	2.8
40	2i	49	PRO	2.8
39	1h	133	LEU	2.8
53	2y	85	LEU	2.8
7	2H	95	ARG	2.8
32	1a	1003	G	2.8
32	2a	1024	G	2.8
32	2a	1156	G	2.8
47	1p	59	TRP	2.8
40	2i	116	LYS	2.8
52	2u	24	ARG	2.8
1	1A	2130	U	2.8
1	2A	34	C	2.8
8	2I	88	ILE	2.8
12	2Q	65	PHE	2.8
33	2b	39	ILE	2.8
41	1j	38	ILE	2.8
50	2s	31	ILE	2.8
23	21	26	ARG	2.8
33	2b	137	ARG	2.8
53	2y	91	LYS	2.8
32	2a	1092	A	2.8

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Mol	Chain	Res	Type	RSRZ
34	2c	37	GLN	2.8
47	1p	48	TRP	2.8
21	2Z	193	GLU	2.8
47	1p	17	TYR	2.8
1	1A	1082	U	2.8
1	1A	1963	U	2.8
14	2S	35	ILE	2.8
32	1a	1020	U	2.8
33	1b	127	ILE	2.8
41	1j	4	ILE	2.8
41	2j	98	ILE	2.8
26	24	68	ARG	2.8
41	1j	26	ALA	2.8
52	2u	10	ARG	2.8
26	24	45	GLY	2.8
26	24	7	PRO	2.8
33	2b	31	TYR	2.8
1	2A	2121	G	2.8
40	1i	10	ARG	2.8
44	2m	3	ARG	2.8
1	1A	1053	C	2.8
32	2a	848	C	2.8
34	2c	16	ARG	2.8
33	2b	71	VAL	2.8
1	1A	1069	A	2.8
32	2a	1357	A	2.8
6	2G	48	GLU	2.8
8	2I	34	GLY	2.8
46	2o	89	GLY	2.8
21	2Z	18	LEU	2.8
44	2m	11	ARG	2.8
53	2y	95	ARG	2.8
20	2Y	5	MET	2.8
50	2s	83	HIS	2.8
29	17	46	VAL	2.7
33	1b	126	GLU	2.7
26	14	59	PHE	2.7
40	1i	46	ALA	2.7
41	2j	23	ILE	2.7
52	1u	13	ILE	2.7
8	2I	38	LEU	2.7
44	2m	70	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
12	2Q	59	ARG	2.7
1	2A	2131	G	2.7
48	2q	86	GLU	2.7
40	1i	78	LYS	2.7
34	2c	155	GLY	2.7
11	2P	79	ARG	2.7
14	2S	3	ARG	2.7
33	2b	127	ILE	2.7
34	2c	85	ARG	2.7
38	1g	32	ARG	2.7
40	2i	77	ILE	2.7
40	2i	101	PHE	2.7
48	1q	90	ILE	2.7
52	2u	15	ARG	2.7
1	1A	1096	A	2.7
33	1b	19	HIS	2.7
1	2A	2166	G	2.7
32	2a	1037	C	2.7
38	2g	75	VAL	2.7
15	2T	112	ARG	2.7
1	1A	1026	U	2.7
35	2d	21	LEU	2.7
33	2b	135	GLN	2.7
6	2G	15	VAL	2.7
33	2b	81	VAL	2.7
34	2c	58	GLU	2.7
34	2c	89	GLU	2.7
40	2i	119	ALA	2.7
33	2b	58	ILE	2.7
33	2b	223	ILE	2.7
41	2j	87	THR	2.7
35	2d	157	LEU	2.7
50	2s	40	ILE	2.7
47	2p	48	TRP	2.7
35	1d	163	GLU	2.7
41	2j	37	PRO	2.7
1	1A	889	C	2.7
1	2A	645	C	2.7
1	2A	2181	G	2.7
7	2H	89	ILE	2.7
33	2b	33	TYR	2.7
40	2i	123	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
34	2c	167	TRP	2.7
45	2n	40	CYS	2.7
38	2g	77	SER	2.7
33	1b	226	ARG	2.7
33	2b	185	ILE	2.7
34	2c	94	LEU	2.7
41	1j	96	ILE	2.7
44	2m	66	LEU	2.7
47	1p	49	LEU	2.7
1	2A	1091	G	2.7
32	2a	1373	G	2.7
50	2s	76	PRO	2.7
7	2H	43	VAL	2.6
22	20	77	ARG	2.6
26	14	66	SER	2.6
38	2g	10	ARG	2.6
45	1n	59	ALA	2.6
1	2A	2178	C	2.6
6	2G	173	LEU	2.6
32	2a	1219	U	2.6
34	1c	204	LEU	2.6
40	1i	19	LEU	2.6
19	2X	69	TYR	2.6
35	1d	138	TYR	2.6
29	27	46	VAL	2.6
8	2I	86	THR	2.6
41	2j	18	ALA	2.6
50	2s	77	THR	2.6
1	1A	1094	U	2.6
32	1a	841	U	2.6
44	2m	106	ASN	2.6
45	2n	53	LEU	2.6
33	1b	135	GLN	2.6
33	2b	152	PHE	2.6
1	2A	2105	C	2.6
34	2c	162	GLN	2.6
51	1t	18	GLN	2.6
42	1k	25	TYR	2.6
6	2G	75	LYS	2.6
35	1d	3	ARG	2.6
52	1u	10	ARG	2.6
47	1p	7	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
53	2y	36	ASN	2.6
9	2N	8	GLN	2.6
32	2a	1004	A	2.6
34	1c	8	ILE	2.6
40	2i	121	ARG	2.6
43	1l	89	ARG	2.6
1	1A	1092	C	2.6
47	1p	20	VAL	2.6
6	2G	3	LEU	2.6
33	1b	213	LEU	2.6
41	2j	71	LEU	2.6
18	1W	96	ILE	2.6
39	2h	45	ILE	2.6
52	2u	22	ARG	2.6
26	14	57	GLU	2.6
32	2a	1195	C	2.6
40	2i	80	GLY	2.6
7	2H	113	VAL	2.6
14	2S	5	THR	2.6
39	1h	102	ARG	2.6
44	2m	76	ALA	2.6
1	2A	2113	U	2.6
6	1G	82	LEU	2.6
6	2G	133	LEU	2.6
34	1c	12	LEU	2.6
53	2y	14	PRO	2.6
1	2A	1056	G	2.6
32	2a	1202	G	2.6
1	1A	2136	C	2.6
1	2A	1102	C	2.6
1	2A	2161	C	2.6
44	1m	112	GLY	2.6
12	2Q	117	ALA	2.6
34	2c	187	ALA	2.6
51	2t	72	LEU	2.6
50	2s	62	ILE	2.6
1	2A	11	G	2.6
1	2A	2893	G	2.6
8	1I	14	ASP	2.6
20	2Y	50	ARG	2.6
32	2a	1180	A	2.6
35	2d	6	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
38	2g	4	ARG	2.6
32	2a	1116	C	2.6
40	2i	43	ALA	2.5
33	1b	121	LEU	2.5
34	2c	7	PRO	2.5
44	2m	84	ILE	2.5
18	2W	92	ARG	2.5
40	2i	93	ARG	2.5
22	20	3	HIS	2.5
34	1c	81	GLY	2.5
34	2c	145	GLY	2.5
38	2g	153	HIS	2.5
50	2s	38	SER	2.5
1	2A	887	A	2.5
32	2a	1224	G	2.5
32	2a	1452	C	2.5
53	2y	13	THR	2.5
44	2m	56	LEU	2.5
50	1s	56	GLN	2.5
48	2q	91	ARG	2.5
6	2G	49	ASP	2.5
6	2G	117	PHE	2.5
12	2Q	104	PHE	2.5
21	2Z	133	ILE	2.5
20	2Y	91	GLU	2.5
34	1c	10	PHE	2.5
41	2j	97	GLU	2.5
6	2G	47	LYS	2.5
7	2H	25	LYS	2.5
1	1A	1103	A	2.5
1	1A	2173	A	2.5
40	2i	13	ALA	2.5
50	2s	2	PRO	2.5
34	2c	204	LEU	2.5
50	2s	29	ARG	2.5
32	1a	78	G	2.5
32	2a	1370	G	2.5
33	1b	214	ILE	2.5
33	1b	227	GLY	2.5
34	2c	77	ILE	2.5
40	1i	33	PHE	2.5
40	2i	25	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
51	1t	73	HIS	2.5
51	1t	74	LYS	2.5
38	1g	13	GLN	2.5
50	2s	36	ARG	2.5
33	1b	184	VAL	2.5
44	1m	56	LEU	2.5
38	2g	82	GLY	2.5
44	2m	38	GLY	2.5
32	2a	1321	C	2.5
34	1c	182	ILE	2.5
15	2T	108	ARG	2.5
40	1i	66	ARG	2.5
41	2j	41	PRO	2.5
33	1b	136	VAL	2.5
33	2b	229	VAL	2.5
41	2j	49	VAL	2.5
45	2n	28	GLY	2.5
1	2A	1536	C	2.5
1	2A	2794	C	2.5
45	2n	60	SER	2.5
1	1A	2151	G	2.5
52	2u	12	LYS	2.5
33	1b	26	PRO	2.5
33	2b	171	ALA	2.5
38	2g	24	THR	2.5
40	2i	24	GLY	2.5
40	2i	19	LEU	2.5
47	1p	6	LEU	2.5
47	2p	79	VAL	2.5
33	2b	210	SER	2.5
1	2A	652(B)	A	2.5
32	2a	1005	A	2.5
34	2c	186	PHE	2.5
44	2m	115	LYS	2.5
1	2A	1104	C	2.5
1	1A	2807	G	2.5
1	2A	1816	G	2.5
32	2a	1021	G	2.5
39	2h	99	GLU	2.5
44	2m	109	THR	2.5
25	23	15	TYR	2.4
31	29	13	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
33	2b	230	VAL	2.4
34	2c	193	TYR	2.4
36	2e	133	TYR	2.4
40	2i	11	LYS	2.4
51	1t	11	SER	2.4
1	2A	652(T)	C	2.4
50	2s	64	GLU	2.4
29	27	45	ALA	2.4
51	1t	68	LYS	2.4
1	2A	2156	G	2.4
40	1i	50	LEU	2.4
6	1G	78	SER	2.4
30	28	22	VAL	2.4
32	1a	1446	U	2.4
32	2a	1358	U	2.4
3	2D	64	ILE	2.4
3	1D	275	LYS	2.4
34	2c	108	ASN	2.4
1	2A	2158	A	2.4
33	2b	131	PRO	2.4
40	2i	87	GLN	2.4
48	1q	25	ARG	2.4
52	2u	11	GLY	2.4
6	2G	50	ALA	2.4
47	1p	56	ALA	2.4
53	2y	56	THR	2.4
8	2I	35	LEU	2.4
33	2b	215	LEU	2.4
38	2g	99	LEU	2.4
7	2H	114	VAL	2.4
34	2c	207	VAL	2.4
1	2A	1026	U	2.4
1	2A	1044	G	2.4
50	2s	61	TYR	2.4
44	2m	111	LYS	2.4
35	2d	75	PHE	2.4
22	20	42	GLY	2.4
40	2i	117	HIS	2.4
32	2a	1183	A	2.4
32	2a	1363(A)	A	2.4
45	1n	22	THR	2.4
6	2G	60	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
33	1b	61	LEU	2.4
33	2b	149	LEU	2.4
41	1j	8	LEU	2.4
41	2j	85	LEU	2.4
30	28	21	LYS	2.4
35	1d	178	VAL	2.4
42	2k	14	VAL	2.4
32	1a	4	U	2.4
40	1i	83	ARG	2.4
45	2n	26	ARG	2.4
1	2A	2807	G	2.4
39	1h	101	PRO	2.4
45	2n	8	GLU	2.4
21	1Z	189	ALA	2.4
33	2b	195	ASP	2.4
45	2n	47	LEU	2.4
51	1t	53	LEU	2.4
41	2j	70	ARG	2.4
44	2m	7	VAL	2.4
32	2a	841	U	2.4
40	1i	8	GLY	2.4
34	2c	143	GLU	2.4
26	14	18	CYS	2.4
40	1i	106	ALA	2.4
51	1t	32	ALA	2.4
29	17	23	ARG	2.4
41	2j	60	ARG	2.4
39	2h	36	LEU	2.4
39	2h	112	LEU	2.4
20	2Y	93	GLY	2.4
21	2Z	100	VAL	2.4
38	2g	9	VAL	2.4
43	2l	16	GLU	2.4
5	2F	14	PRO	2.4
34	2c	202	ILE	2.4
35	2d	4	TYR	2.4
33	1b	114	ARG	2.4
44	1m	107	ALA	2.4
45	2n	48	ALA	2.4
51	1t	59	ALA	2.4
35	2d	74	GLN	2.4
41	2j	16	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
41	2j	90	LEU	2.4
32	2a	1353	G	2.3
3	1D	34	VAL	2.3
32	2a	1066	C	2.3
32	2a	1322	C	2.3
23	21	7	ILE	2.3
49	2r	87	ARG	2.3
38	1g	25	ALA	2.3
50	2s	39	THR	2.3
3	2D	276	LYS	2.3
45	2n	11	LYS	2.3
41	2j	36	GLY	2.3
46	1o	89	GLY	2.3
50	2s	53	ASN	2.3
7	2H	35	VAL	2.3
1	1A	2180	U	2.3
33	2b	144	ARG	2.3
34	2c	6	HIS	2.3
33	2b	193	ASP	2.3
34	2c	56	ASP	2.3
45	2n	23	ARG	2.3
14	2S	40	ILE	2.3
32	2a	1114	C	2.3
45	2n	52	GLN	2.3
36	2e	45	PHE	2.3
34	2c	48	TYR	2.3
39	2h	58	TYR	2.3
41	2j	26	ALA	2.3
43	1l	26	ALA	2.3
3	2D	50	THR	2.3
41	2j	59	SER	2.3
41	2j	13	HIS	2.3
40	1i	41	VAL	2.3
32	2a	1235	U	2.3
33	1b	27	LYS	2.3
1	1A	2156	G	2.3
48	2q	36	ILE	2.3
1	1A	2114	A	2.3
19	1X	69	TYR	2.3
35	2d	20	TYR	2.3
36	2e	54	ALA	2.3
47	1p	38	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
48	1q	99	SER	2.3
53	1y	98	ALA	2.3
8	1I	38	LEU	2.3
40	1i	47	LEU	2.3
44	2m	96	LEU	2.3
50	1s	15	LEU	2.3
40	1i	105	ASP	2.3
52	1u	3	LYS	2.3
8	2I	3	VAL	2.3
32	2a	1532	U	2.3
34	2c	182	ILE	2.3
48	1q	36	ILE	2.3
32	2a	1260	C	2.3
33	1b	231	GLU	2.3
38	2g	149	ARG	2.3
38	2g	152	ALA	2.3
40	1i	111	ARG	2.3
41	2j	20	ALA	2.3
14	2S	92	TYR	2.3
52	1u	17	THR	2.3
32	2a	958	A	2.3
35	2d	58	LEU	2.3
50	2s	58	VAL	2.3
34	2c	35	GLU	2.3
38	2g	31	MET	2.3
14	2S	20	ARG	2.3
20	2Y	80	GLY	2.3
35	1d	50	ARG	2.3
43	1l	7	ILE	2.3
1	1A	2158	A	2.3
1	1A	2892	A	2.3
35	1d	186	LEU	2.3
39	2h	107	LEU	2.3
41	2j	91	PRO	2.3
1	1A	272(A)	U	2.3
20	2Y	73	ARG	2.3
46	2o	68	ARG	2.3
48	1q	37	LYS	2.3
35	2d	23	GLY	2.3
36	2e	89	ILE	2.3
3	2D	272	ALA	2.3
34	2c	192	THR	2.3

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Mol	Chain	Res	Type	RSRZ
38	2g	101	LEU	2.3
47	1p	60	LEU	2.3
31	29	11	CYS	2.3
32	2a	1256	A	2.2
33	2b	30	ARG	2.2
35	1d	73	ARG	2.2
41	1j	70	ARG	2.2
43	1l	91	LYS	2.2
48	1q	28	PRO	2.2
18	2W	50	VAL	2.2
1	1A	1097	U	2.2
38	1g	11	GLN	2.2
38	2g	89	MET	2.2
41	1j	86	MET	2.2
33	1b	109	SER	2.2
34	2c	200	ALA	2.2
53	2y	25	ALA	2.2
33	1b	134	GLU	2.2
3	2D	182	LEU	2.2
26	24	32	TYR	2.2
52	1u	21	TYR	2.2
45	1n	27	CYS	2.2
21	2Z	180	VAL	2.2
23	21	70	VAL	2.2
32	2a	723	U	2.2
33	2b	101	MET	2.2
41	2j	58	ASP	2.2
48	2q	23	VAL	2.2
1	1A	2125	G	2.2
1	2A	1042	G	2.2
5	2F	64	ILE	2.2
35	2d	5	ILE	2.2
39	2h	86	ILE	2.2
50	2s	6	LYS	2.2
34	2c	79	ARG	2.2
24	12	70	GLN	2.2
53	1y	71	TYR	2.2
23	21	83	GLU	2.2
21	2Z	201	LYS	2.2
24	22	63	VAL	2.2
50	2s	9	VAL	2.2
8	2I	36	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
10	2O	41	ALA	2.2
29	27	41	ARG	2.2
41	2j	11	PHE	2.2
1	2A	614(B)	G	2.2
1	2A	2115	G	2.2
32	2a	1155	G	2.2
35	1d	174	LEU	2.2
39	1h	112	LEU	2.2
34	2c	22	TRP	2.2
36	2e	50	GLU	2.2
34	2c	185	GLY	2.2
20	2Y	4	LYS	2.2
18	1W	59	VAL	2.2
31	29	25	VAL	2.2
32	1a	999	C	2.2
32	2a	979	C	2.2
33	1b	130	ARG	2.2
34	2c	198	VAL	2.2
43	1l	43	VAL	2.2
1	2A	2114	A	2.2
32	1a	161	A	2.2
40	1i	77	ILE	2.2
48	2q	59	ILE	2.2
48	2q	90	ILE	2.2
8	2I	20	ASP	2.2
1	2A	2206	G	2.2
15	1T	37	GLY	2.2
21	2Z	199	LYS	2.2
34	2c	32	LEU	2.2
53	2y	81	LEU	2.2
32	2a	1258	G	2.2
34	1c	127	ARG	2.2
45	2n	41	ARG	2.2
33	2b	192	SER	2.2
33	2b	233	SER	2.2
17	2V	79	VAL	2.2
33	2b	48	MET	2.2
6	1G	46	ALA	2.2
6	2G	137	GLU	2.2
32	2a	1045	C	2.2
40	2i	84	ALA	2.2
9	2N	104	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
35	1d	166	LYS	2.2
45	2n	22	THR	2.2
50	2s	79	THR	2.2
34	2c	178	LEU	2.2
47	1p	46	PRO	2.2
48	1q	98	LEU	2.2
33	2b	21	ARG	2.2
1	1A	2127	G	2.2
1	1A	2893	G	2.2
1	2A	2104	G	2.2
44	2m	67	GLU	2.2
48	2q	97	SER	2.2
1	2A	1090	U	2.2
32	2a	1040	U	2.2
41	1j	34	VAL	2.2
7	2H	106	THR	2.2
21	2Z	124	ILE	2.2
38	1g	24	THR	2.2
39	1h	128	GLY	2.2
6	2G	112	PRO	2.2
11	2P	59	LEU	2.2
32	2a	1261	A	2.2
39	1h	59	LEU	2.2
33	2b	231	GLU	2.2
35	2d	150	GLU	2.2
51	1t	70	SER	2.2
6	2G	86	MET	2.1
50	1s	61	TYR	2.1
1	2A	2191	G	2.1
34	2c	106	VAL	2.1
53	2y	60	VAL	2.1
33	1b	188	ALA	2.1
6	1G	88	ILE	2.1
6	2G	144	ILE	2.1
6	2G	157	ILE	2.1
6	2G	161	THR	2.1
22	20	55	ARG	2.1
22	20	74	ARG	2.1
40	1i	9	ARG	2.1
24	22	57	ILE	2.1
34	2c	14	ILE	2.1
1	1A	2108	C	2.1

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Mol	Chain	Res	Type	RSRZ
20	2Y	89	PHE	2.1
34	2c	82	GLU	2.1
34	2c	105	GLU	2.1
51	1t	20	LEU	2.1
1	1A	1057	A	2.1
31	29	16	VAL	2.1
33	2b	23	ARG	2.1
37	1f	90	VAL	2.1
38	2g	95	ARG	2.1
34	2c	161	GLU	2.1
40	2i	122	ALA	2.1
43	1l	61	THR	2.1
1	1A	2166	G	2.1
1	2A	10	G	2.1
1	2A	1099	G	2.1
6	2G	77	ILE	2.1
7	1H	92	ILE	2.1
23	11	68	PRO	2.1
33	2b	108	ILE	2.1
44	2m	4	ILE	2.1
34	1c	203	PHE	2.1
8	2I	31	LEU	2.1
11	2P	6	LEU	2.1
33	2b	102	LEU	2.1
41	2j	84	GLN	2.1
51	1t	10	LEU	2.1
1	2A	1079	C	2.1
32	2a	1354	C	2.1
18	2W	13	SER	2.1
1	1A	1095	A	2.1
34	2c	172	ARG	2.1
50	2s	17	GLU	2.1
8	2I	89	TYR	2.1
21	2Z	188	ALA	2.1
44	1m	117	VAL	2.1
48	2q	95	TYR	2.1
53	2y	26	LYS	2.1
42	2k	87	THR	2.1
50	1s	77	THR	2.1
15	1T	42	ILE	2.1
39	2h	138	TRP	2.1
42	2k	108	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
42	1k	125	PHE	2.1
51	2t	10	LEU	2.1
22	20	72	ARG	2.1
32	2a	1138	G	2.1
33	2b	113	HIS	2.1
33	2b	130	ARG	2.1
34	1c	38	ARG	2.1
40	2i	83	ARG	2.1
49	2r	42	ARG	2.1
43	2l	28	LYS	2.1
31	29	37	GLY	2.1
1	1A	2119	A	2.1
1	1A	2109	U	2.1
6	2G	56	ALA	2.1
14	2S	21	THR	2.1
32	1a	1040	U	2.1
34	1c	184	TYR	2.1
35	2d	26	CYS	2.1
35	2d	67	ILE	2.1
6	2G	19	LEU	2.1
34	2c	179	ARG	2.1
39	2h	56	LYS	2.1
41	1j	57	LYS	2.1
40	2i	89	ASN	2.1
1	1A	171	G	2.1
1	1A	2133	G	2.1
10	1O	1	MET	2.1
34	2c	61	ALA	2.1
32	2a	1287	A	2.1
36	2e	81	GLU	2.1
45	1n	25	VAL	2.1
7	2H	88	LEU	2.1
9	2N	116	LEU	2.1
30	28	7	HIS	2.1
34	2c	47	LEU	2.1
37	2f	61	LEU	2.1
34	1c	2	GLY	2.1
34	2c	2	GLY	2.1
44	2m	89	GLY	2.1
1	1A	2161	C	2.1
32	2a	1140	C	2.1
11	1P	15	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
29	17	45	ALA	2.1
32	2a	1187	G	2.1
33	2b	218	ALA	2.1
41	2j	43	ARG	2.1
42	1k	60	ALA	2.1
32	2a	1025	U	2.1
47	1p	53	VAL	2.1
48	2q	10	VAL	2.1
50	1s	39	THR	2.1
51	2t	6	PRO	2.1
52	2u	21	TYR	2.1
46	2o	87	ILE	2.1
6	2G	53	LEU	2.1
34	1c	175	LEU	2.1
34	2c	91	LEU	2.1
39	2h	133	LEU	2.1
26	24	64	GLY	2.1
28	26	40	CYS	2.1
34	1c	22	TRP	2.1
44	1m	114	ARG	2.1
49	1r	42	ARG	2.1
1	2A	9	U	2.0
45	2n	56	VAL	2.0
49	2r	22	VAL	2.0
1	1A	2120	G	2.0
21	2Z	171	ILE	2.0
43	2l	64	TYR	2.0
22	20	45	PHE	2.0
32	2a	1280	A	2.0
33	1b	28	PHE	2.0
33	1b	180	LEU	2.0
40	1i	99	LEU	2.0
3	1D	38	LYS	2.0
41	1j	51	ARG	2.0
51	2t	83	ARG	2.0
35	1d	111	ALA	2.0
1	1A	2150	U	2.0
19	2X	81	VAL	2.0
32	2a	204	U	2.0
39	2h	93	VAL	2.0
45	1n	18	VAL	2.0
47	2p	76	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
33	2b	214	ILE	2.0
34	1c	14	ILE	2.0
40	1i	127	LYS	2.0
40	1i	80	GLY	2.0
40	2i	39	GLY	2.0
34	1c	172	ARG	2.0
34	1c	179	ARG	2.0
40	1i	107	ARG	2.0
44	2m	59	TYR	2.0
1	2A	1087	G	2.0
32	2a	1068	G	2.0
32	2a	1250	A	2.0
21	1Z	203	GLU	2.0
38	2g	13	GLN	2.0
45	2n	27	CYS	2.0
47	2p	7	ALA	2.0
44	2m	98	VAL	2.0
32	2a	1137	C	2.0
35	2d	101	LEU	2.0
38	1g	50	ILE	2.0
43	1l	60	LEU	2.0
44	2m	19	LEU	2.0
45	1n	44	LEU	2.0
39	1h	58	TYR	2.0
21	2Z	78	LYS	2.0
32	2a	951	G	2.0
32	2a	1447	A	2.0
33	2b	125	PRO	2.0
34	1c	107	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
43	0TD	1l	92	10/11	0.86	0.16	49,59,64,67	0
1	5MU	2A	1915	21/22	0.87	0.14	79,87,90,101	0
1	5MU	1A	1915	21/22	0.89	0.19	74,79,83,87	0
1	PSU	2A	1911	20/21	0.90	0.15	67,72,77,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	2A	1917	20/21	0.90	0.15	73,77,92,95	0
43	0TD	2l	92	10/11	0.90	0.17	59,66,69,74	0
32	M2G	2a	966	25/26	0.91	0.16	63,71,84,97	0
1	PSU	1A	1917	20/21	0.92	0.18	65,69,75,77	0
32	5MC	1a	967	21/22	0.93	0.20	57,66,73,82	0
32	5MC	2a	967	21/22	0.93	0.20	66,72,78,80	0
32	2MG	2a	1207	24/25	0.93	0.21	77,81,86,93	0
32	PSU	2a	516	20/21	0.93	0.16	66,72,76,79	0
32	2MG	1a	1207	24/25	0.94	0.18	62,70,74,78	0
32	M2G	1a	966	25/26	0.94	0.18	55,61,68,71	0
1	OMC	2A	1920	21/22	0.94	0.19	65,68,71,76	0
32	5MC	2a	1404	21/22	0.94	0.18	54,61,64,66	0
32	PSU	1a	516	20/21	0.94	0.17	60,64,67,71	0
32	4OC	2a	1402	22/23	0.95	0.18	59,64,71,73	0
1	PSU	1A	1911	20/21	0.95	0.16	57,64,69,70	0
32	MA6	2a	1518	24/25	0.95	0.18	58,64,68,69	0
32	5MC	2a	1400	21/22	0.95	0.29	62,75,78,80	0
32	G7M	2a	527	24/25	0.96	0.15	60,67,70,72	0
32	5MC	2a	1407	21/22	0.96	0.17	56,64,67,69	0
32	UR3	2a	1498	21/22	0.96	0.20	52,62,66,69	0
32	4OC	1a	1402	22/23	0.96	0.19	46,53,56,64	0
32	MA6	2a	1519	24/25	0.96	0.28	49,63,67,69	0
32	MA6	1a	1518	24/25	0.96	0.22	43,47,52,53	0
1	OMG	2A	2251	24/25	0.97	0.22	38,40,43,45	0
1	OMU	2A	2552	21/22	0.97	0.20	33,40,43,46	0
1	PSU	2A	2605	20/21	0.97	0.19	32,38,43,44	0
32	G7M	1a	527	24/25	0.97	0.18	48,55,59,67	0
32	5MC	1a	1404	21/22	0.97	0.17	45,48,51,56	0
32	UR3	1a	1498	21/22	0.97	0.19	42,50,53,59	0
1	OMC	1A	1920	21/22	0.97	0.20	50,57,61,63	0
32	MA6	1a	1519	24/25	0.97	0.22	42,48,52,54	0
32	5MC	1a	1400	21/22	0.98	0.18	49,57,60,65	0
1	PSU	1A	2605	20/21	0.98	0.21	27,30,33,36	0
1	5MU	1A	1939	21/22	0.98	0.21	27,31,36,39	0
32	5MC	1a	1407	21/22	0.98	0.17	44,54,58,63	0
1	5MU	2A	1939	21/22	0.98	0.20	35,39,42,46	0
1	5MC	2A	1942	21/22	0.98	0.19	44,49,54,60	0
1	5MC	2A	1962	21/22	0.98	0.18	33,46,53,56	0
1	5MC	1A	1942	21/22	0.98	0.22	33,39,44,47	0
1	2MA	2A	2503	23/24	0.98	0.20	29,34,37,39	0
1	5MC	1A	1962	21/22	0.98	0.19	30,36,40,48	0
1	OMG	1A	2251	24/25	0.98	0.21	22,28,32,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	2MA	1A	2503	23/24	0.98	0.23	20,24,27,29	0
54	PPU	2w	76	37/38	0.98	0.23	30,36,41,44	0
55	8AN	2x	76	22/23	0.98	0.19	33,36,39,44	0
1	OMU	1A	2552	21/22	0.99	0.23	26,31,33,35	0
55	8AN	1x	76	22/23	0.99	0.22	19,26,28,32	0
54	PPU	1w	76	37/38	0.99	0.22	21,26,30,30	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	1822	1/1	0.15	0.15	89,89,89,89	0
57	MG	1A	3873	1/1	0.25	0.16	57,57,57,57	0
57	MG	1A	3905	1/1	0.33	0.09	55,55,55,55	0
57	MG	1A	3741	1/1	0.33	0.13	71,71,71,71	0
57	MG	1A	3613	1/1	0.37	0.17	72,72,72,72	0
57	MG	2A	3414	1/1	0.38	0.41	70,70,70,70	0
57	MG	2G	202	1/1	0.38	0.16	80,80,80,80	0
57	MG	1A	3934	1/1	0.39	0.26	72,72,72,72	0
57	MG	1A	3380	1/1	0.39	0.24	57,57,57,57	0
57	MG	1A	3785	1/1	0.44	0.13	66,66,66,66	0
57	MG	1A	3909	1/1	0.44	0.09	63,63,63,63	0
57	MG	1A	3874	1/1	0.44	0.29	45,45,45,45	0
57	MG	2a	3128	1/1	0.44	0.17	74,74,74,74	0
57	MG	1A	3659	1/1	0.45	0.08	51,51,51,51	0
57	MG	2a	3156	1/1	0.47	0.12	84,84,84,84	0
57	MG	1A	3208	1/1	0.48	0.25	58,58,58,58	0
57	MG	1a	1703	1/1	0.48	0.16	72,72,72,72	0
57	MG	2A	3542	1/1	0.48	0.51	70,70,70,70	0
57	MG	1A	3528	1/1	0.50	0.19	57,57,57,57	0
57	MG	1A	3968	1/1	0.50	0.20	40,40,40,40	0
57	MG	2A	3326	1/1	0.50	0.35	72,72,72,72	0
57	MG	1R	207	1/1	0.50	0.29	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	3272	1/1	0.51	0.15	78,78,78,78	0
57	MG	2A	3311	1/1	0.51	0.13	79,79,79,79	0
57	MG	1A	3857	1/1	0.52	0.17	71,71,71,71	0
57	MG	1A	3433	1/1	0.52	0.20	51,51,51,51	0
57	MG	1A	3206	1/1	0.52	0.25	68,68,68,68	0
57	MG	2A	3032	1/1	0.53	0.27	80,80,80,80	0
57	MG	1a	1775	1/1	0.53	0.11	72,72,72,72	0
57	MG	1a	1651	1/1	0.53	0.18	72,72,72,72	0
60	ZN	24	501	1/1	0.53	0.15	129,129,129,129	0
57	MG	2A	3552	1/1	0.54	0.10	59,59,59,59	0
57	MG	1A	3193	1/1	0.55	0.35	64,64,64,64	0
57	MG	2A	3572	1/1	0.55	0.20	50,50,50,50	0
57	MG	2A	3433	1/1	0.56	0.29	69,69,69,69	0
57	MG	1t	202	1/1	0.56	0.13	74,74,74,74	0
57	MG	1a	1686	1/1	0.56	0.26	72,72,72,72	0
57	MG	1A	3618	1/1	0.56	0.23	43,43,43,43	0
57	MG	1A	3504	1/1	0.57	0.15	53,53,53,53	0
57	MG	1a	1867	1/1	0.57	0.15	76,76,76,76	0
57	MG	2A	3602	1/1	0.58	0.13	68,68,68,68	0
57	MG	2A	3620	1/1	0.58	0.17	79,79,79,79	0
57	MG	2A	3474	1/1	0.58	0.15	64,64,64,64	0
57	MG	2a	3009	1/1	0.58	0.20	81,81,81,81	0
57	MG	2A	3397	1/1	0.58	0.18	66,66,66,66	0
57	MG	2A	3082	1/1	0.58	0.20	78,78,78,78	0
57	MG	1A	3596	1/1	0.58	0.18	47,47,47,47	0
57	MG	2a	3018	1/1	0.59	0.15	68,68,68,68	0
57	MG	2A	3108	1/1	0.59	0.15	72,72,72,72	0
57	MG	1B	206	1/1	0.59	0.18	53,53,53,53	0
57	MG	1a	1844	1/1	0.59	0.11	69,69,69,69	0
57	MG	2a	3005	1/1	0.60	0.15	73,73,73,73	0
57	MG	1A	3730	1/1	0.60	0.07	54,54,54,54	0
57	MG	2A	3037	1/1	0.61	0.25	69,69,69,69	0
57	MG	2A	3121	1/1	0.61	0.19	79,79,79,79	0
57	MG	2A	3161	1/1	0.61	0.31	74,74,74,74	0
57	MG	2a	3010	1/1	0.61	0.16	81,81,81,81	0
57	MG	1A	3315	1/1	0.62	0.23	58,58,58,58	0
57	MG	1A	3913	1/1	0.62	0.11	64,64,64,64	0
57	MG	2B	218	1/1	0.63	0.20	85,85,85,85	0
57	MG	1a	1796	1/1	0.63	0.06	80,80,80,80	0
57	MG	2A	3178	1/1	0.63	0.27	65,65,65,65	0
57	MG	1A	3652	1/1	0.63	0.14	43,43,43,43	0
57	MG	1A	3852	1/1	0.63	0.21	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	3740	1/1	0.63	0.18	65,65,65,65	0
57	MG	1A	3708	1/1	0.63	0.15	41,41,41,41	0
57	MG	2A	3127	1/1	0.63	0.26	78,78,78,78	0
57	MG	2A	3707	1/1	0.63	0.17	86,86,86,86	0
57	MG	1O	201	1/1	0.64	0.11	61,61,61,61	0
57	MG	1A	3981	1/1	0.64	0.28	73,73,73,73	0
57	MG	2A	3182	1/1	0.64	0.18	73,73,73,73	0
57	MG	1a	1841	1/1	0.64	0.16	74,74,74,74	0
57	MG	2A	3299	1/1	0.64	0.23	75,75,75,75	0
57	MG	2A	3481	1/1	0.64	0.24	51,51,51,51	0
57	MG	1A	3183	1/1	0.64	0.17	72,72,72,72	0
57	MG	1A	3656	1/1	0.65	0.53	75,75,75,75	0
57	MG	2A	3683	1/1	0.65	0.49	57,57,57,57	0
57	MG	1a	1858	1/1	0.65	0.14	77,77,77,77	0
57	MG	2a	3023	1/1	0.65	0.24	79,79,79,79	0
57	MG	2a	3089	1/1	0.65	0.18	83,83,83,83	0
57	MG	2A	3290	1/1	0.65	0.30	68,68,68,68	0
57	MG	1A	3952	1/1	0.65	0.19	49,49,49,49	0
57	MG	1a	1653	1/1	0.65	0.27	70,70,70,70	0
57	MG	1A	3130	1/1	0.66	0.29	60,60,60,60	0
57	MG	2A	3516	1/1	0.66	0.14	79,79,79,79	0
57	MG	2A	3045	1/1	0.66	0.16	67,67,67,67	0
57	MG	1A	3846	1/1	0.66	0.12	62,62,62,62	0
57	MG	1a	1746	1/1	0.66	0.18	67,67,67,67	0
57	MG	2A	3419	1/1	0.66	0.16	62,62,62,62	0
57	MG	1y	201	1/1	0.66	0.15	70,70,70,70	0
57	MG	2A	3655	1/1	0.66	0.10	77,77,77,77	0
57	MG	2A	3671	1/1	0.66	0.10	58,58,58,58	0
57	MG	1a	1667	1/1	0.66	0.26	65,65,65,65	0
57	MG	2A	3698	1/1	0.66	0.18	65,65,65,65	0
57	MG	2A	3699	1/1	0.66	0.12	65,65,65,65	0
57	MG	2E	303	1/1	0.67	0.55	49,49,49,49	0
57	MG	2A	3026	1/1	0.67	0.51	70,70,70,70	0
57	MG	1a	1678	1/1	0.67	0.19	78,78,78,78	0
57	MG	1a	1607	1/1	0.67	0.13	63,63,63,63	0
57	MG	2A	3253	1/1	0.67	0.17	75,75,75,75	0
57	MG	1a	1702	1/1	0.67	0.18	79,79,79,79	0
57	MG	1A	3924	1/1	0.67	0.15	61,61,61,61	0
57	MG	2A	3502	1/1	0.67	0.32	58,58,58,58	0
57	MG	1A	3296	1/1	0.67	0.17	66,66,66,66	0
57	MG	1a	1661	1/1	0.67	0.15	58,58,58,58	0
57	MG	1A	3943	1/1	0.67	0.10	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2F	301	1/1	0.68	0.16	66,66,66,66	0
57	MG	2A	3172	1/1	0.68	0.12	80,80,80,80	0
57	MG	1A	3912	1/1	0.68	0.11	56,56,56,56	0
57	MG	1A	3591	1/1	0.68	0.08	39,39,39,39	0
57	MG	1a	1795	1/1	0.68	0.12	69,69,69,69	0
57	MG	1a	1603	1/1	0.68	0.15	72,72,72,72	0
57	MG	2a	3021	1/1	0.68	0.18	74,74,74,74	0
57	MG	2A	3116	1/1	0.68	0.07	91,91,91,91	0
57	MG	1a	1802	1/1	0.68	0.14	76,76,76,76	0
57	MG	1A	3876	1/1	0.68	0.15	55,55,55,55	0
57	MG	1a	1740	1/1	0.68	0.14	91,91,91,91	0
57	MG	2A	3164	1/1	0.68	0.12	86,86,86,86	0
57	MG	2A	3604	1/1	0.69	0.15	46,46,46,46	0
57	MG	2A	3209	1/1	0.69	0.31	73,73,73,73	0
57	MG	2A	3219	1/1	0.69	0.19	69,69,69,69	0
57	MG	1A	3637	1/1	0.69	0.10	79,79,79,79	0
57	MG	1A	3663	1/1	0.69	0.13	52,52,52,52	0
57	MG	17	105	1/1	0.69	0.29	59,59,59,59	0
57	MG	1a	1676	1/1	0.69	0.16	58,58,58,58	0
57	MG	1A	3705	1/1	0.69	0.11	60,60,60,60	0
57	MG	2a	3105	1/1	0.69	0.15	65,65,65,65	0
57	MG	1A	3431	1/1	0.69	0.21	32,32,32,32	0
57	MG	1A	3211	1/1	0.69	0.19	64,64,64,64	0
57	MG	2A	3204	1/1	0.69	0.18	67,67,67,67	0
57	MG	2A	3614	1/1	0.70	0.23	38,38,38,38	0
57	MG	1a	1709	1/1	0.70	0.24	60,60,60,60	0
57	MG	2A	3495	1/1	0.70	0.10	71,71,71,71	0
57	MG	1A	3197	1/1	0.70	0.30	68,68,68,68	0
57	MG	2A	3373	1/1	0.70	0.17	44,44,44,44	0
57	MG	1A	3759	1/1	0.70	0.13	59,59,59,59	0
57	MG	2A	3267	1/1	0.70	0.45	54,54,54,54	0
57	MG	2A	3569	1/1	0.70	0.16	71,71,71,71	0
57	MG	2B	210	1/1	0.70	0.13	66,66,66,66	0
57	MG	1a	1773	1/1	0.70	0.12	75,75,75,75	0
57	MG	1A	3953	1/1	0.70	0.20	71,71,71,71	0
60	ZN	2Y	202	1/1	0.70	0.14	93,93,93,93	0
57	MG	1A	3178	1/1	0.70	0.22	55,55,55,55	0
57	MG	2A	3315	1/1	0.71	0.10	50,50,50,50	0
57	MG	1a	1863	1/1	0.71	0.20	57,57,57,57	0
57	MG	1A	3582	1/1	0.71	0.22	37,37,37,37	0
57	MG	2A	3256	1/1	0.71	0.28	62,62,62,62	0
57	MG	2a	3019	1/1	0.71	0.16	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1697	1/1	0.71	0.14	69,69,69,69	0
57	MG	2A	3415	1/1	0.71	0.21	53,53,53,53	0
57	MG	2a	3025	1/1	0.71	0.20	69,69,69,69	0
57	MG	2A	3714	1/1	0.71	0.20	67,67,67,67	0
57	MG	1A	3860	1/1	0.71	0.14	58,58,58,58	0
57	MG	2A	3423	1/1	0.71	0.18	77,77,77,77	0
57	MG	2a	3140	1/1	0.71	0.10	77,77,77,77	0
57	MG	2a	3141	1/1	0.71	0.15	72,72,72,72	0
57	MG	2a	3149	1/1	0.71	0.11	75,75,75,75	0
57	MG	2A	3024	1/1	0.71	0.17	51,51,51,51	0
57	MG	1a	1854	1/1	0.71	0.15	67,67,67,67	0
57	MG	1a	1820	1/1	0.71	0.10	60,60,60,60	0
57	MG	1e	205	1/1	0.72	0.11	70,70,70,70	0
57	MG	2B	205	1/1	0.72	0.24	72,72,72,72	0
57	MG	1A	3317	1/1	0.72	0.52	52,52,52,52	0
57	MG	2B	214	1/1	0.72	0.17	65,65,65,65	0
57	MG	10	108	1/1	0.72	0.18	64,64,64,64	0
57	MG	1a	1798	1/1	0.72	0.14	77,77,77,77	0
57	MG	11	104	1/1	0.72	0.19	64,64,64,64	0
57	MG	1a	1815	1/1	0.72	0.08	66,66,66,66	0
57	MG	2A	3508	1/1	0.72	0.22	71,71,71,71	0
57	MG	1A	3593	1/1	0.72	0.23	67,67,67,67	0
57	MG	2A	3259	1/1	0.72	0.46	57,57,57,57	0
57	MG	1A	3319	1/1	0.72	0.22	83,83,83,83	0
57	MG	1A	3518	1/1	0.72	0.10	58,58,58,58	0
57	MG	2A	3105	1/1	0.72	0.16	65,65,65,65	0
57	MG	1a	1612	1/1	0.72	0.17	90,90,90,90	0
57	MG	1a	1846	1/1	0.72	0.21	64,64,64,64	0
57	MG	1A	3691	1/1	0.72	0.23	73,73,73,73	0
57	MG	1a	1855	1/1	0.72	0.16	79,79,79,79	0
57	MG	2A	3340	1/1	0.72	0.17	75,75,75,75	0
57	MG	2A	3139	1/1	0.72	0.22	55,55,55,55	0
57	MG	2A	3159	1/1	0.72	0.93	59,59,59,59	0
57	MG	2A	3691	1/1	0.72	0.28	50,50,50,50	0
57	MG	1A	3160	1/1	0.72	0.26	52,52,52,52	0
57	MG	1A	3002	1/1	0.72	0.18	52,52,52,52	0
57	MG	1A	3646	1/1	0.72	0.28	54,54,54,54	0
57	MG	1B	217	1/1	0.73	0.16	63,63,63,63	0
57	MG	1H	201	1/1	0.73	0.14	72,72,72,72	0
57	MG	1A	3728	1/1	0.73	0.21	64,64,64,64	0
57	MG	1A	3890	1/1	0.73	0.40	37,37,37,37	0
57	MG	2A	3551	1/1	0.73	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	2A	3157	1/1	0.73	0.19	64,64,64,64	0
57	MG	1A	3750	1/1	0.73	0.10	50,50,50,50	0
57	MG	1a	1684	1/1	0.73	0.10	56,56,56,56	0
57	MG	1A	3556	1/1	0.73	0.14	56,56,56,56	0
57	MG	2A	3362	1/1	0.73	0.09	48,48,48,48	0
57	MG	2A	3001	1/1	0.73	0.22	65,65,65,65	0
57	MG	15	105	1/1	0.73	0.27	35,35,35,35	0
57	MG	1A	3287	1/1	0.73	0.16	54,54,54,54	0
57	MG	2A	3670	1/1	0.73	0.14	69,69,69,69	0
57	MG	2A	3198	1/1	0.73	0.19	75,75,75,75	0
57	MG	1a	1835	1/1	0.73	0.80	67,67,67,67	0
57	MG	1a	1838	1/1	0.73	0.38	71,71,71,71	0
57	MG	1A	3824	1/1	0.73	0.14	54,54,54,54	0
57	MG	2A	3461	1/1	0.73	0.24	56,56,56,56	0
57	MG	1A	3992	1/1	0.73	0.16	60,60,60,60	0
57	MG	1A	3843	1/1	0.73	0.11	67,67,67,67	0
57	MG	2a	3162	1/1	0.73	0.13	78,78,78,78	0
57	MG	1B	213	1/1	0.73	0.24	69,69,69,69	0
57	MG	2B	207	1/1	0.73	0.14	67,67,67,67	0
57	MG	2A	3146	1/1	0.74	0.18	70,70,70,70	0
57	MG	1A	3938	1/1	0.74	0.09	49,49,49,49	0
57	MG	2A	3663	1/1	0.74	0.13	71,71,71,71	0
57	MG	1a	1722	1/1	0.74	0.19	76,76,76,76	0
57	MG	1A	3376	1/1	0.74	0.12	65,65,65,65	0
57	MG	1A	3698	1/1	0.74	0.46	45,45,45,45	0
57	MG	2A	3075	1/1	0.74	0.20	74,74,74,74	0
57	MG	1a	1833	1/1	0.74	0.07	68,68,68,68	0
57	MG	2A	3088	1/1	0.74	0.17	65,65,65,65	0
57	MG	2a	3037	1/1	0.74	0.25	77,77,77,77	0
57	MG	2a	3061	1/1	0.74	0.14	74,74,74,74	0
57	MG	1A	3786	1/1	0.74	0.14	65,65,65,65	0
57	MG	1A	3875	1/1	0.74	0.63	62,62,62,62	0
57	MG	2B	201	1/1	0.74	0.17	79,79,79,79	0
57	MG	2a	3137	1/1	0.74	0.09	63,63,63,63	0
57	MG	1A	3853	1/1	0.74	0.15	69,69,69,69	0
57	MG	1y	202	1/1	0.74	0.14	84,84,84,84	0
57	MG	1A	3690	1/1	0.74	0.22	70,70,70,70	0
57	MG	2A	3132	1/1	0.74	0.16	65,65,65,65	0
57	MG	1A	4003	1/1	0.74	0.18	29,29,29,29	0
57	MG	2A	3607	1/1	0.74	0.12	65,65,65,65	0
57	MG	2A	3426	1/1	0.74	0.11	68,68,68,68	0
57	MG	1A	3576	1/1	0.75	0.69	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3506	1/1	0.75	0.19	76,76,76,76	0
57	MG	1a	1738	1/1	0.75	0.31	67,67,67,67	0
57	MG	2A	3445	1/1	0.75	0.25	76,76,76,76	0
57	MG	2a	3050	1/1	0.75	0.20	57,57,57,57	0
57	MG	1a	1666	1/1	0.75	0.22	74,74,74,74	0
57	MG	1A	3788	1/1	0.75	0.22	64,64,64,64	0
57	MG	1A	3900	1/1	0.75	0.25	63,63,63,63	0
57	MG	2A	3637	1/1	0.75	0.14	53,53,53,53	0
57	MG	2A	3492	1/1	0.75	0.28	78,78,78,78	0
57	MG	2a	3138	1/1	0.75	0.07	75,75,75,75	0
57	MG	1a	1602	1/1	0.75	0.16	74,74,74,74	0
57	MG	2A	3128	1/1	0.75	0.16	60,60,60,60	0
57	MG	1A	3482	1/1	0.75	0.18	32,32,32,32	0
57	MG	1a	1605	1/1	0.75	0.10	64,64,64,64	0
57	MG	1A	3986	1/1	0.75	0.24	52,52,52,52	0
57	MG	2a	3176	1/1	0.75	0.15	74,74,74,74	0
57	MG	1P	202	1/1	0.75	0.32	43,43,43,43	0
57	MG	1A	3907	1/1	0.75	0.23	29,29,29,29	0
57	MG	2A	3547	1/1	0.76	0.07	80,80,80,80	0
57	MG	2A	3031	1/1	0.76	0.23	56,56,56,56	0
57	MG	2A	3220	1/1	0.76	0.27	67,67,67,67	0
57	MG	1A	3463	1/1	0.76	0.19	46,46,46,46	0
57	MG	2A	3143	1/1	0.76	0.25	57,57,57,57	0
57	MG	1a	1642	1/1	0.76	0.14	67,67,67,67	0
57	MG	2a	3064	1/1	0.76	0.11	71,71,71,71	0
57	MG	2A	3155	1/1	0.76	0.34	66,66,66,66	0
57	MG	1A	3793	1/1	0.76	0.11	43,43,43,43	0
57	MG	1A	4011	1/1	0.76	0.27	59,59,59,59	0
57	MG	2a	3131	1/1	0.76	0.19	76,76,76,76	0
57	MG	1a	1768	1/1	0.76	0.15	62,62,62,62	0
57	MG	1a	1834	1/1	0.76	0.22	60,60,60,60	0
57	MG	1a	1658	1/1	0.76	0.11	69,69,69,69	0
57	MG	2F	303	1/1	0.76	0.19	49,49,49,49	0
57	MG	1A	3823	1/1	0.76	0.16	50,50,50,50	0
57	MG	1A	3700	1/1	0.76	0.44	60,60,60,60	0
57	MG	1a	1843	1/1	0.76	0.13	56,56,56,56	0
57	MG	2a	3167	1/1	0.76	0.12	72,72,72,72	0
57	MG	2A	3677	1/1	0.76	0.61	56,56,56,56	0
57	MG	1A	3531	1/1	0.76	0.16	50,50,50,50	0
57	MG	1a	1714	1/1	0.76	0.10	72,72,72,72	0
57	MG	1A	3263	1/1	0.77	0.32	77,77,77,77	0
57	MG	2A	3231	1/1	0.77	0.25	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3472	1/1	0.77	0.20	55,55,55,55	0
57	MG	1a	1711	1/1	0.77	0.18	76,76,76,76	0
57	MG	1a	1713	1/1	0.77	0.33	60,60,60,60	0
57	MG	1A	3614	1/1	0.77	0.15	44,44,44,44	0
57	MG	2A	3084	1/1	0.77	0.22	74,74,74,74	0
57	MG	2a	3011	1/1	0.77	0.18	65,65,65,65	0
57	MG	1V	204	1/1	0.77	0.33	64,64,64,64	0
57	MG	2a	3142	1/1	0.77	0.11	51,51,51,51	0
57	MG	2A	3723	1/1	0.77	0.24	57,57,57,57	0
57	MG	1A	3268	1/1	0.77	0.20	62,62,62,62	0
57	MG	2A	3512	1/1	0.77	0.18	40,40,40,40	0
57	MG	2A	3148	1/1	0.77	0.42	69,69,69,69	0
57	MG	2A	3658	1/1	0.77	0.17	70,70,70,70	0
58	MPD	1a	1868	8/8	0.77	0.19	53,64,70,74	0
57	MG	1a	1669	1/1	0.77	0.21	66,66,66,66	0
57	MG	1A	3677	1/1	0.77	0.07	83,83,83,83	0
57	MG	1a	1774	1/1	0.78	0.08	69,69,69,69	0
57	MG	2A	3264	1/1	0.78	0.22	60,60,60,60	0
57	MG	2A	3540	1/1	0.78	0.09	70,70,70,70	0
57	MG	1a	1866	1/1	0.78	0.15	72,72,72,72	0
57	MG	1A	3363	1/1	0.78	0.12	52,52,52,52	0
57	MG	2a	3004	1/1	0.78	0.81	76,76,76,76	0
57	MG	1a	1784	1/1	0.78	0.07	79,79,79,79	0
57	MG	1o	102	1/1	0.78	0.22	68,68,68,68	0
57	MG	2A	3301	1/1	0.78	0.16	70,70,70,70	0
57	MG	1a	1679	1/1	0.78	0.15	77,77,77,77	0
57	MG	2a	3016	1/1	0.78	0.12	80,80,80,80	0
57	MG	1a	1683	1/1	0.78	0.18	59,59,59,59	0
57	MG	1A	3572	1/1	0.78	0.22	51,51,51,51	0
57	MG	1B	221	1/1	0.78	0.13	50,50,50,50	0
57	MG	2A	3612	1/1	0.78	0.22	44,44,44,44	0
57	MG	2A	3357	1/1	0.78	0.15	51,51,51,51	0
57	MG	1a	1688	1/1	0.78	0.17	63,63,63,63	0
57	MG	2a	3045	1/1	0.78	0.26	71,71,71,71	0
57	MG	1D	301	1/1	0.78	0.36	65,65,65,65	0
57	MG	2a	3052	1/1	0.78	0.20	74,74,74,74	0
57	MG	1E	304	1/1	0.78	0.25	28,28,28,28	0
57	MG	2A	3169	1/1	0.78	0.13	56,56,56,56	0
57	MG	1A	3975	1/1	0.78	0.21	48,48,48,48	0
57	MG	2A	3175	1/1	0.78	0.21	56,56,56,56	0
57	MG	1A	3977	1/1	0.78	0.33	55,55,55,55	0
57	MG	1A	3752	1/1	0.78	0.11	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3459	1/1	0.78	0.18	23,23,23,23	0
57	MG	1T	202	1/1	0.78	0.20	69,69,69,69	0
57	MG	2a	3139	1/1	0.78	0.09	58,58,58,58	0
57	MG	2A	3452	1/1	0.78	0.22	58,58,58,58	0
57	MG	1T	204	1/1	0.78	0.12	63,63,63,63	0
57	MG	2A	3706	1/1	0.78	0.11	66,66,66,66	0
57	MG	1A	3667	1/1	0.78	0.86	72,72,72,72	0
57	MG	1A	3645	1/1	0.78	0.12	29,29,29,29	0
57	MG	2A	3230	1/1	0.78	0.20	67,67,67,67	0
57	MG	2a	3164	1/1	0.78	0.13	82,82,82,82	0
57	MG	2A	3483	1/1	0.78	0.14	64,64,64,64	0
57	MG	1A	3610	1/1	0.78	0.16	56,56,56,56	0
57	MG	2j	201	1/1	0.78	0.12	79,79,79,79	0
57	MG	2A	3251	1/1	0.78	0.25	65,65,65,65	0
59	ARG	1F	318	12/12	0.78	0.28	58,66,77,78	0
57	MG	1a	1671	1/1	0.78	0.15	62,62,62,62	0
57	MG	1A	3163	1/1	0.78	0.21	58,58,58,58	0
57	MG	1A	3480	1/1	0.79	0.24	39,39,39,39	0
57	MG	2A	3177	1/1	0.79	0.09	65,65,65,65	0
57	MG	1a	1778	1/1	0.79	0.20	72,72,72,72	0
57	MG	1A	3910	1/1	0.79	0.10	57,57,57,57	0
57	MG	1a	1647	1/1	0.79	0.20	70,70,70,70	0
57	MG	1A	3246	1/1	0.79	0.13	68,68,68,68	0
57	MG	2A	3120	1/1	0.79	0.09	65,65,65,65	0
57	MG	2A	3413	1/1	0.79	0.72	77,77,77,77	0
57	MG	2A	3560	1/1	0.79	0.12	65,65,65,65	0
57	MG	1e	203	1/1	0.79	0.21	61,61,61,61	0
57	MG	1A	3865	1/1	0.79	0.25	51,51,51,51	0
57	MG	1a	1657	1/1	0.79	0.42	72,72,72,72	0
57	MG	1A	3148	1/1	0.79	0.12	56,56,56,56	0
57	MG	1a	1660	1/1	0.79	0.14	64,64,64,64	0
57	MG	1A	3171	1/1	0.79	0.11	68,68,68,68	0
57	MG	1A	3511	1/1	0.79	0.18	35,35,35,35	0
57	MG	2A	3619	1/1	0.79	0.21	59,59,59,59	0
57	MG	1A	3038	1/1	0.79	0.20	53,53,53,53	0
57	MG	2A	3261	1/1	0.79	0.20	53,53,53,53	0
57	MG	1A	3525	1/1	0.79	0.16	64,64,64,64	0
57	MG	1A	3849	1/1	0.79	0.12	57,57,57,57	0
57	MG	2A	3475	1/1	0.79	0.19	60,60,60,60	0
57	MG	1A	3967	1/1	0.79	0.08	62,62,62,62	0
57	MG	1a	1750	1/1	0.79	0.09	82,82,82,82	0
57	MG	1A	3223	1/1	0.79	0.18	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1E	307	1/1	0.79	0.22	62,62,62,62	0
57	MG	1A	3602	1/1	0.79	0.09	71,71,71,71	0
57	MG	2a	3038	1/1	0.80	0.18	65,65,65,65	0
57	MG	2A	3206	1/1	0.80	0.21	67,67,67,67	0
57	MG	1A	3636	1/1	0.80	0.10	75,75,75,75	0
57	MG	2A	3731	1/1	0.80	0.18	63,63,63,63	0
57	MG	2A	3590	1/1	0.80	0.12	46,46,46,46	0
57	MG	2A	3463	1/1	0.80	0.25	41,41,41,41	0
57	MG	2A	3216	1/1	0.80	0.18	62,62,62,62	0
57	MG	1A	3894	1/1	0.80	0.05	65,65,65,65	0
57	MG	2a	3118	1/1	0.80	0.16	62,62,62,62	0
57	MG	1A	3775	1/1	0.80	0.21	45,45,45,45	0
57	MG	2A	3224	1/1	0.80	0.67	60,60,60,60	0
57	MG	1A	3127	1/1	0.80	0.17	40,40,40,40	0
57	MG	1A	3589	1/1	0.80	0.14	66,66,66,66	0
57	MG	2A	3367	1/1	0.80	0.11	70,70,70,70	0
57	MG	2A	3242	1/1	0.80	0.09	60,60,60,60	0
57	MG	20	102	1/1	0.80	0.09	64,64,64,64	0
57	MG	2A	3505	1/1	0.80	0.06	71,71,71,71	0
57	MG	1A	3560	1/1	0.80	0.13	57,57,57,57	0
57	MG	1A	3497	1/1	0.80	0.12	62,62,62,62	0
57	MG	1A	3695	1/1	0.80	0.40	65,65,65,65	0
57	MG	2A	3531	1/1	0.80	0.11	77,77,77,77	0
57	MG	1A	3027	1/1	0.80	0.17	70,70,70,70	0
57	MG	1a	1673	1/1	0.80	0.19	63,63,63,63	0
57	MG	1A	3829	1/1	0.80	0.17	45,45,45,45	0
57	MG	2r	101	1/1	0.80	0.10	67,67,67,67	0
57	MG	1A	3830	1/1	0.80	0.16	52,52,52,52	0
57	MG	2A	3704	1/1	0.80	0.11	64,64,64,64	0
57	MG	1A	4010	1/1	0.80	0.25	51,51,51,51	0
57	MG	1A	3634	1/1	0.80	0.22	48,48,48,48	0
57	MG	1A	3918	1/1	0.81	0.16	63,63,63,63	0
57	MG	2A	3629	1/1	0.81	0.16	71,71,71,71	0
57	MG	2A	3057	1/1	0.81	0.17	61,61,61,61	0
57	MG	1A	3430	1/1	0.81	0.17	62,62,62,62	0
57	MG	1A	3011	1/1	0.81	0.20	60,60,60,60	0
57	MG	1A	3583	1/1	0.81	0.18	60,60,60,60	0
57	MG	1A	3866	1/1	0.81	0.20	40,40,40,40	0
57	MG	1A	3059	1/1	0.81	0.31	44,44,44,44	0
57	MG	2A	3491	1/1	0.81	0.11	72,72,72,72	0
57	MG	2A	3678	1/1	0.81	0.06	77,77,77,77	0
57	MG	1a	1794	1/1	0.81	0.15	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3055	1/1	0.81	0.09	68,68,68,68	0
57	MG	2A	3188	1/1	0.81	0.14	63,63,63,63	0
57	MG	1A	3444	1/1	0.81	0.13	42,42,42,42	0
57	MG	2a	3066	1/1	0.81	0.25	65,65,65,65	0
57	MG	2a	3087	1/1	0.81	0.14	55,55,55,55	0
57	MG	1A	3808	1/1	0.81	0.11	73,73,73,73	0
57	MG	2a	3096	1/1	0.81	0.18	63,63,63,63	0
57	MG	2A	3507	1/1	0.81	0.18	44,44,44,44	0
57	MG	2A	3339	1/1	0.81	0.20	73,73,73,73	0
57	MG	2a	3122	1/1	0.81	0.16	63,63,63,63	0
57	MG	1A	3330	1/1	0.81	0.13	58,58,58,58	0
57	MG	2A	3122	1/1	0.81	0.35	44,44,44,44	0
57	MG	2A	3525	1/1	0.81	0.21	75,75,75,75	0
57	MG	2A	3529	1/1	0.81	0.11	75,75,75,75	0
57	MG	1A	3124	1/1	0.81	0.18	63,63,63,63	0
57	MG	1A	3155	1/1	0.81	0.19	71,71,71,71	0
57	MG	1A	3247	1/1	0.81	0.13	64,64,64,64	0
57	MG	2A	3394	1/1	0.81	0.13	75,75,75,75	0
57	MG	2A	3221	1/1	0.81	0.42	52,52,52,52	0
57	MG	2A	3403	1/1	0.81	0.19	78,78,78,78	0
57	MG	2A	3406	1/1	0.81	0.18	74,74,74,74	0
57	MG	1A	3611	1/1	0.81	0.71	61,61,61,61	0
57	MG	1A	3490	1/1	0.81	0.07	71,71,71,71	0
57	MG	1A	3672	1/1	0.81	0.21	69,69,69,69	0
57	MG	2A	3233	1/1	0.81	0.18	65,65,65,65	0
57	MG	1A	3424	1/1	0.81	0.28	53,53,53,53	0
57	MG	2A	3250	1/1	0.81	0.13	68,68,68,68	0
57	MG	1a	1743	1/1	0.81	0.17	74,74,74,74	0
57	MG	1A	3683	1/1	0.81	0.12	79,79,79,79	0
57	MG	1A	3856	1/1	0.81	0.16	45,45,45,45	0
57	MG	2A	3051	1/1	0.82	0.21	68,68,68,68	0
57	MG	1a	1619	1/1	0.82	0.12	55,55,55,55	0
57	MG	1a	1624	1/1	0.82	0.13	60,60,60,60	0
57	MG	2A	3580	1/1	0.82	0.18	52,52,52,52	0
57	MG	1A	3436	1/1	0.82	0.09	61,61,61,61	0
57	MG	2a	3015	1/1	0.82	0.12	61,61,61,61	0
57	MG	1A	3821	1/1	0.82	0.13	62,62,62,62	0
57	MG	1A	3151	1/1	0.82	0.52	62,62,62,62	0
57	MG	1a	1652	1/1	0.82	0.10	74,74,74,74	0
57	MG	2A	3107	1/1	0.82	0.12	62,62,62,62	0
57	MG	1A	3190	1/1	0.82	0.56	61,61,61,61	0
57	MG	2A	3229	1/1	0.82	0.15	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	1a	1737	1/1	0.82	0.10	67,67,67,67	0
57	MG	2A	3437	1/1	0.82	0.11	48,48,48,48	0
57	MG	2a	3043	1/1	0.82	0.09	74,74,74,74	0
57	MG	1A	3826	1/1	0.82	0.12	47,47,47,47	0
57	MG	1a	1852	1/1	0.82	0.11	61,61,61,61	0
57	MG	1A	3048	1/1	0.82	0.49	51,51,51,51	0
57	MG	2A	3245	1/1	0.82	0.27	57,57,57,57	0
57	MG	2A	3465	1/1	0.82	0.11	54,54,54,54	0
57	MG	1A	3010	1/1	0.82	0.20	52,52,52,52	0
57	MG	2A	3672	1/1	0.82	0.05	62,62,62,62	0
57	MG	2a	3080	1/1	0.82	0.19	62,62,62,62	0
57	MG	1R	205	1/1	0.82	0.16	56,56,56,56	0
57	MG	1a	1860	1/1	0.82	0.20	68,68,68,68	0
57	MG	2a	3093	1/1	0.82	0.22	69,69,69,69	0
57	MG	1A	3969	1/1	0.82	0.14	49,49,49,49	0
57	MG	2A	3687	1/1	0.82	0.07	67,67,67,67	0
57	MG	2a	3114	1/1	0.82	0.14	59,59,59,59	0
57	MG	1a	1756	1/1	0.82	0.11	58,58,58,58	0
57	MG	2A	3485	1/1	0.82	0.13	59,59,59,59	0
57	MG	1A	3893	1/1	0.82	0.20	35,35,35,35	0
57	MG	1A	3838	1/1	0.82	0.14	37,37,37,37	0
57	MG	2A	3153	1/1	0.82	0.22	62,62,62,62	0
57	MG	1A	3272	1/1	0.82	0.20	67,67,67,67	0
57	MG	2A	3713	1/1	0.82	0.13	68,68,68,68	0
57	MG	1A	3776	1/1	0.82	0.20	45,45,45,45	0
57	MG	1a	1675	1/1	0.82	0.17	60,60,60,60	0
57	MG	1A	3778	1/1	0.82	0.18	63,63,63,63	0
57	MG	1A	3781	1/1	0.82	0.28	59,59,59,59	0
57	MG	2A	3514	1/1	0.82	0.20	68,68,68,68	0
57	MG	2A	3167	1/1	0.82	0.24	42,42,42,42	0
57	MG	1A	3320	1/1	0.82	0.15	64,64,64,64	0
57	MG	1A	3535	1/1	0.82	0.12	78,78,78,78	0
57	MG	1a	1797	1/1	0.82	0.11	70,70,70,70	0
57	MG	1B	203	1/1	0.82	0.16	68,68,68,68	0
57	MG	1A	3673	1/1	0.82	0.12	69,69,69,69	0
57	MG	1A	3279	1/1	0.82	0.30	75,75,75,75	0
57	MG	1A	3863	1/1	0.82	0.22	35,35,35,35	0
57	MG	2V	201	1/1	0.82	0.31	69,69,69,69	0
57	MG	2A	3380	1/1	0.82	0.18	47,47,47,47	0
57	MG	2A	3312	1/1	0.83	0.17	39,39,39,39	0
57	MG	1A	3501	1/1	0.83	0.10	69,69,69,69	0
57	MG	2A	3524	1/1	0.83	0.14	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3544	1/1	0.83	0.11	48,48,48,48	0
57	MG	1A	3608	1/1	0.83	0.12	46,46,46,46	0
57	MG	11	102	1/1	0.83	0.57	59,59,59,59	0
57	MG	2A	3350	1/1	0.83	0.13	52,52,52,52	0
57	MG	1A	3671	1/1	0.83	0.18	55,55,55,55	0
57	MG	2O	202	1/1	0.83	0.12	76,76,76,76	0
57	MG	2Q	203	1/1	0.83	0.74	62,62,62,62	0
57	MG	2A	3546	1/1	0.83	0.19	66,66,66,66	0
57	MG	1A	3996	1/1	0.83	0.12	58,58,58,58	0
57	MG	2A	3363	1/1	0.83	0.18	43,43,43,43	0
57	MG	15	107	1/1	0.83	0.15	71,71,71,71	0
57	MG	2A	3557	1/1	0.83	0.06	54,54,54,54	0
57	MG	1a	1800	1/1	0.83	0.12	68,68,68,68	0
57	MG	2A	3563	1/1	0.83	0.10	59,59,59,59	0
57	MG	2A	3375	1/1	0.83	0.17	43,43,43,43	0
57	MG	2A	3571	1/1	0.83	0.24	44,44,44,44	0
57	MG	2A	3184	1/1	0.83	0.44	60,60,60,60	0
57	MG	2A	3573	1/1	0.83	0.14	47,47,47,47	0
57	MG	2A	3044	1/1	0.83	0.13	67,67,67,67	0
57	MG	2A	3582	1/1	0.83	0.47	63,63,63,63	0
57	MG	2A	3584	1/1	0.83	0.08	58,58,58,58	0
57	MG	2a	3030	1/1	0.83	0.26	58,58,58,58	0
57	MG	1A	4001	1/1	0.83	0.17	34,34,34,34	0
57	MG	2A	3599	1/1	0.83	0.17	41,41,41,41	0
57	MG	2a	3039	1/1	0.83	0.09	76,76,76,76	0
57	MG	1A	3847	1/1	0.83	0.19	39,39,39,39	0
57	MG	2A	3404	1/1	0.83	0.17	50,50,50,50	0
57	MG	1A	3551	1/1	0.83	0.14	51,51,51,51	0
57	MG	1a	1691	1/1	0.83	0.13	69,69,69,69	0
57	MG	1a	1827	1/1	0.83	0.11	77,77,77,77	0
57	MG	1a	1604	1/1	0.83	0.13	72,72,72,72	0
57	MG	1A	3850	1/1	0.83	0.17	49,49,49,49	0
57	MG	2A	3626	1/1	0.83	0.09	54,54,54,54	0
57	MG	2a	3067	1/1	0.83	0.12	71,71,71,71	0
57	MG	1A	3554	1/1	0.83	0.18	65,65,65,65	0
57	MG	2A	3636	1/1	0.83	0.08	60,60,60,60	0
57	MG	1A	3298	1/1	0.83	0.26	82,82,82,82	0
57	MG	2A	3647	1/1	0.83	0.10	66,66,66,66	0
57	MG	2a	3095	1/1	0.83	0.40	71,71,71,71	0
57	MG	2A	3652	1/1	0.83	0.14	62,62,62,62	0
57	MG	1B	207	1/1	0.83	0.21	69,69,69,69	0
57	MG	2A	3113	1/1	0.83	0.15	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	3435	1/1	0.83	0.11	54,54,54,54	0
57	MG	2A	3449	1/1	0.83	0.17	92,92,92,92	0
57	MG	1A	3058	1/1	0.83	0.25	49,49,49,49	0
57	MG	1A	3625	1/1	0.83	0.21	37,37,37,37	0
57	MG	2a	3132	1/1	0.83	0.19	62,62,62,62	0
57	MG	2A	3675	1/1	0.83	0.11	64,64,64,64	0
57	MG	1A	3632	1/1	0.83	0.54	45,45,45,45	0
57	MG	1A	3442	1/1	0.83	0.14	55,55,55,55	0
57	MG	1A	3241	1/1	0.83	0.23	38,38,38,38	0
57	MG	1A	3448	1/1	0.83	0.14	49,49,49,49	0
57	MG	2A	3138	1/1	0.83	0.36	63,63,63,63	0
57	MG	2a	3148	1/1	0.83	0.15	69,69,69,69	0
57	MG	1N	203	1/1	0.83	0.10	61,61,61,61	0
57	MG	1A	3956	1/1	0.83	0.18	48,48,48,48	0
57	MG	2A	3703	1/1	0.83	0.12	67,67,67,67	0
57	MG	1A	3529	1/1	0.83	0.15	56,56,56,56	0
57	MG	1A	3590	1/1	0.83	0.11	48,48,48,48	0
57	MG	2A	3268	1/1	0.83	0.21	61,61,61,61	0
57	MG	2f	202	1/1	0.83	0.14	75,75,75,75	0
57	MG	2A	3271	1/1	0.83	0.12	61,61,61,61	0
57	MG	1e	202	1/1	0.83	0.36	73,73,73,73	0
57	MG	1a	1769	1/1	0.83	0.07	69,69,69,69	0
57	MG	1A	3500	1/1	0.83	0.11	58,58,58,58	0
57	MG	1a	1668	1/1	0.83	0.19	58,58,58,58	0
57	MG	1A	3532	1/1	0.83	0.17	53,53,53,53	0
57	MG	2A	3249	1/1	0.84	0.28	69,69,69,69	0
57	MG	2A	3436	1/1	0.84	0.12	53,53,53,53	0
57	MG	2a	3006	1/1	0.84	0.14	55,55,55,55	0
57	MG	1G	202	1/1	0.84	0.16	60,60,60,60	0
57	MG	2A	3442	1/1	0.84	0.16	75,75,75,75	0
57	MG	1A	3994	1/1	0.84	0.21	37,37,37,37	0
57	MG	1A	3862	1/1	0.84	0.12	56,56,56,56	0
57	MG	1A	3392	1/1	0.84	0.15	38,38,38,38	0
57	MG	2A	3456	1/1	0.84	0.26	78,78,78,78	0
57	MG	2A	3154	1/1	0.84	0.36	52,52,52,52	0
57	MG	2A	3033	1/1	0.84	0.21	68,68,68,68	0
57	MG	2A	3035	1/1	0.84	0.11	70,70,70,70	0
57	MG	1A	3076	1/1	0.84	0.41	55,55,55,55	0
57	MG	1a	1609	1/1	0.84	0.16	60,60,60,60	0
57	MG	1A	3630	1/1	0.84	0.21	57,57,57,57	0
57	MG	2A	3050	1/1	0.84	0.36	61,61,61,61	0
57	MG	2A	3653	1/1	0.84	0.14	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	2A	3276	1/1	0.84	0.25	69,69,69,69	0
57	MG	1a	1758	1/1	0.84	0.15	71,71,71,71	0
57	MG	1a	1618	1/1	0.84	0.11	62,62,62,62	0
57	MG	2A	3064	1/1	0.84	0.18	57,57,57,57	0
57	MG	2A	3069	1/1	0.84	0.24	65,65,65,65	0
57	MG	2a	3059	1/1	0.84	0.24	70,70,70,70	0
57	MG	2a	3060	1/1	0.84	0.17	75,75,75,75	0
57	MG	1A	3966	1/1	0.84	0.19	62,62,62,62	0
57	MG	2a	3062	1/1	0.84	0.22	83,83,83,83	0
57	MG	2A	3179	1/1	0.84	0.10	73,73,73,73	0
57	MG	2A	3321	1/1	0.84	0.17	61,61,61,61	0
57	MG	1A	3461	1/1	0.84	0.21	63,63,63,63	0
57	MG	2a	3079	1/1	0.84	0.16	59,59,59,59	0
57	MG	2A	3509	1/1	0.84	0.13	54,54,54,54	0
57	MG	2A	3685	1/1	0.84	0.14	59,59,59,59	0
57	MG	2A	3183	1/1	0.84	0.21	78,78,78,78	0
57	MG	1A	3851	1/1	0.84	0.08	63,63,63,63	0
57	MG	1A	3103	1/1	0.84	0.14	45,45,45,45	0
57	MG	2A	3193	1/1	0.84	0.25	73,73,73,73	0
57	MG	2A	3700	1/1	0.84	0.13	70,70,70,70	0
57	MG	2A	3093	1/1	0.84	0.17	57,57,57,57	0
57	MG	2A	3201	1/1	0.84	0.14	74,74,74,74	0
57	MG	1a	1776	1/1	0.84	0.12	59,59,59,59	0
57	MG	1W	201	1/1	0.84	0.37	55,55,55,55	0
57	MG	2A	3711	1/1	0.84	0.12	78,78,78,78	0
57	MG	10	101	1/1	0.84	0.22	43,43,43,43	0
57	MG	2A	3211	1/1	0.84	0.18	70,70,70,70	0
57	MG	2A	3389	1/1	0.84	0.14	76,76,76,76	0
57	MG	2A	3110	1/1	0.84	0.23	63,63,63,63	0
57	MG	10	106	1/1	0.84	0.07	44,44,44,44	0
57	MG	2A	3553	1/1	0.84	0.17	39,39,39,39	0
57	MG	1A	3657	1/1	0.84	0.22	26,26,26,26	0
57	MG	2A	3558	1/1	0.84	0.10	73,73,73,73	0
57	MG	2B	212	1/1	0.84	0.28	68,68,68,68	0
57	MG	1A	3758	1/1	0.84	0.16	33,33,33,33	0
57	MG	1A	3933	1/1	0.84	0.11	62,62,62,62	0
57	MG	2A	3409	1/1	0.84	0.14	56,56,56,56	0
57	MG	2E	304	1/1	0.84	0.19	43,43,43,43	0
57	MG	1A	3982	1/1	0.84	0.18	50,50,50,50	0
57	MG	1a	1799	1/1	0.84	0.08	66,66,66,66	0
57	MG	1A	3789	1/1	0.84	0.11	43,43,43,43	0
57	MG	1a	1716	1/1	0.84	0.14	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3446	1/1	0.84	0.11	83,83,83,83	0
58	MPD	2B	220	8/8	0.84	0.18	63,66,74,77	0
57	MG	1a	1733	1/1	0.84	0.09	56,56,56,56	0
57	MG	2X	101	1/1	0.84	0.18	52,52,52,52	0
57	MG	2A	3585	1/1	0.84	0.14	58,58,58,58	0
57	MG	2A	3061	1/1	0.85	0.16	46,46,46,46	0
57	MG	2R	201	1/1	0.85	0.24	51,51,51,51	0
57	MG	1A	3751	1/1	0.85	0.10	50,50,50,50	0
57	MG	1E	305	1/1	0.85	0.10	50,50,50,50	0
57	MG	20	101	1/1	0.85	0.12	63,63,63,63	0
57	MG	2A	3074	1/1	0.85	0.49	55,55,55,55	0
57	MG	1A	3318	1/1	0.85	0.34	65,65,65,65	0
57	MG	1E	308	1/1	0.85	0.15	36,36,36,36	0
57	MG	1A	3386	1/1	0.85	0.22	29,29,29,29	0
57	MG	1a	1630	1/1	0.85	0.37	67,67,67,67	0
57	MG	1a	1635	1/1	0.85	0.22	65,65,65,65	0
57	MG	2A	3228	1/1	0.85	0.26	73,73,73,73	0
57	MG	1A	3641	1/1	0.85	0.17	45,45,45,45	0
57	MG	2A	3106	1/1	0.85	0.11	62,62,62,62	0
57	MG	2A	3610	1/1	0.85	0.16	50,50,50,50	0
57	MG	1A	3452	1/1	0.85	0.21	71,71,71,71	0
57	MG	2A	3441	1/1	0.85	0.35	70,70,70,70	0
57	MG	1a	1735	1/1	0.85	0.18	70,70,70,70	0
57	MG	1A	3568	1/1	0.85	0.27	52,52,52,52	0
57	MG	1A	3456	1/1	0.85	0.18	53,53,53,53	0
57	MG	2a	3031	1/1	0.85	0.14	69,69,69,69	0
57	MG	1A	3575	1/1	0.85	0.19	54,54,54,54	0
57	MG	1A	3102	1/1	0.85	0.21	38,38,38,38	0
57	MG	1A	3420	1/1	0.85	0.14	32,32,32,32	0
57	MG	2A	3640	1/1	0.85	0.17	41,41,41,41	0
57	MG	1A	3713	1/1	0.85	0.12	44,44,44,44	0
57	MG	1a	1754	1/1	0.85	0.19	67,67,67,67	0
57	MG	1a	1861	1/1	0.85	0.19	74,74,74,74	0
57	MG	1T	205	1/1	0.85	0.15	57,57,57,57	0
57	MG	1A	3722	1/1	0.85	0.15	60,60,60,60	0
57	MG	2A	3662	1/1	0.85	0.31	58,58,58,58	0
57	MG	1a	1759	1/1	0.85	0.18	67,67,67,67	0
57	MG	2A	3669	1/1	0.85	0.12	53,53,53,53	0
57	MG	1d	303	1/1	0.85	0.24	77,77,77,77	0
57	MG	2A	3270	1/1	0.85	0.16	64,64,64,64	0
57	MG	2A	3486	1/1	0.85	0.07	59,59,59,59	0
57	MG	2a	3071	1/1	0.85	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1761	1/1	0.85	0.16	70,70,70,70	0
57	MG	1a	1762	1/1	0.85	0.11	60,60,60,60	0
57	MG	2a	3081	1/1	0.85	0.27	75,75,75,75	0
57	MG	2a	3083	1/1	0.85	0.14	67,67,67,67	0
57	MG	1e	204	1/1	0.85	0.13	70,70,70,70	0
57	MG	2A	3281	1/1	0.85	0.14	72,72,72,72	0
57	MG	1A	3792	1/1	0.85	0.13	51,51,51,51	0
57	MG	1A	3372	1/1	0.85	0.35	74,74,74,74	0
57	MG	1a	1772	1/1	0.85	0.15	69,69,69,69	0
57	MG	2a	3100	1/1	0.85	0.23	63,63,63,63	0
57	MG	10	102	1/1	0.85	0.81	47,47,47,47	0
57	MG	2a	3112	1/1	0.85	0.11	50,50,50,50	0
57	MG	1A	3062	1/1	0.85	0.11	68,68,68,68	0
57	MG	1x	101	1/1	0.85	0.18	47,47,47,47	0
57	MG	2a	3120	1/1	0.85	0.08	80,80,80,80	0
57	MG	1A	3549	1/1	0.85	0.17	39,39,39,39	0
57	MG	2A	3521	1/1	0.85	0.15	66,66,66,66	0
57	MG	2A	3005	1/1	0.85	0.34	63,63,63,63	0
57	MG	2A	3171	1/1	0.85	0.45	53,53,53,53	0
57	MG	1A	4012	1/1	0.85	0.29	64,64,64,64	0
57	MG	1A	3514	1/1	0.85	0.30	65,65,65,65	0
57	MG	2A	3532	1/1	0.85	0.10	67,67,67,67	0
57	MG	1A	3950	1/1	0.85	0.37	82,82,82,82	0
57	MG	1a	1791	1/1	0.85	0.18	66,66,66,66	0
57	MG	2A	3545	1/1	0.85	0.12	78,78,78,78	0
57	MG	1A	3742	1/1	0.85	0.28	59,59,59,59	0
57	MG	1B	212	1/1	0.85	0.23	72,72,72,72	0
57	MG	2B	209	1/1	0.85	0.17	71,71,71,71	0
57	MG	2A	3549	1/1	0.85	0.18	65,65,65,65	0
57	MG	1A	3746	1/1	0.85	0.15	50,50,50,50	0
57	MG	1A	3592	1/1	0.85	0.17	69,69,69,69	0
57	MG	2a	3170	1/1	0.85	0.21	59,59,59,59	0
57	MG	2a	3171	1/1	0.85	0.18	75,75,75,75	0
57	MG	1A	3962	1/1	0.85	0.11	54,54,54,54	0
57	MG	2B	219	1/1	0.85	0.13	69,69,69,69	0
57	MG	1A	3963	1/1	0.85	0.15	60,60,60,60	0
57	MG	1a	1693	1/1	0.85	0.25	70,70,70,70	0
57	MG	1D	315	1/1	0.85	0.18	74,74,74,74	0
57	MG	2A	3399	1/1	0.85	0.20	79,79,79,79	0
57	MG	2A	3565	1/1	0.85	0.09	63,63,63,63	0
57	MG	2I	201	1/1	0.85	0.11	74,74,74,74	0
57	MG	2A	3401	1/1	0.85	0.13	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	3761	1/1	0.86	0.12	29,29,29,29	0
57	MG	2A	3191	1/1	0.86	0.22	71,71,71,71	0
57	MG	2A	3598	1/1	0.86	0.14	74,74,74,74	0
57	MG	1A	3567	1/1	0.86	0.21	50,50,50,50	0
57	MG	2A	3194	1/1	0.86	0.12	62,62,62,62	0
57	MG	1a	1662	1/1	0.86	0.10	75,75,75,75	0
57	MG	2A	3199	1/1	0.86	0.13	59,59,59,59	0
57	MG	1A	3454	1/1	0.86	0.14	55,55,55,55	0
57	MG	1A	3777	1/1	0.86	0.09	39,39,39,39	0
57	MG	1a	1780	1/1	0.86	0.16	64,64,64,64	0
57	MG	1A	3619	1/1	0.86	0.08	57,57,57,57	0
57	MG	2A	3210	1/1	0.86	0.17	65,65,65,65	0
57	MG	1A	3569	1/1	0.86	0.15	52,52,52,52	0
57	MG	1T	201	1/1	0.86	0.17	68,68,68,68	0
57	MG	2a	3026	1/1	0.86	0.13	75,75,75,75	0
57	MG	1A	3083	1/1	0.86	0.24	55,55,55,55	0
57	MG	1A	3974	1/1	0.86	0.19	44,44,44,44	0
57	MG	1A	3234	1/1	0.86	0.29	57,57,57,57	0
57	MG	2A	3646	1/1	0.86	0.11	61,61,61,61	0
57	MG	1A	3787	1/1	0.86	0.15	69,69,69,69	0
57	MG	1A	3978	1/1	0.86	0.25	40,40,40,40	0
57	MG	1W	202	1/1	0.86	0.21	52,52,52,52	0
57	MG	1W	203	1/1	0.86	0.33	48,48,48,48	0
57	MG	2A	3657	1/1	0.86	0.13	45,45,45,45	0
57	MG	2A	3469	1/1	0.86	0.11	62,62,62,62	0
57	MG	1A	3697	1/1	0.86	0.18	57,57,57,57	0
57	MG	1A	3352	1/1	0.86	0.12	36,36,36,36	0
57	MG	2A	3086	1/1	0.86	0.17	51,51,51,51	0
57	MG	1A	3985	1/1	0.86	0.31	72,72,72,72	0
57	MG	2A	3090	1/1	0.86	0.21	66,66,66,66	0
57	MG	1A	3361	1/1	0.86	0.21	39,39,39,39	0
57	MG	1a	1829	1/1	0.86	0.15	46,46,46,46	0
57	MG	1A	3886	1/1	0.86	0.14	63,63,63,63	0
57	MG	1a	1698	1/1	0.86	0.22	68,68,68,68	0
57	MG	1A	3479	1/1	0.86	0.18	30,30,30,30	0
57	MG	2A	3684	1/1	0.86	0.11	40,40,40,40	0
57	MG	1A	3800	1/1	0.86	0.12	48,48,48,48	0
57	MG	2A	3111	1/1	0.86	0.12	58,58,58,58	0
57	MG	1a	1706	1/1	0.86	0.24	62,62,62,62	0
57	MG	2A	3697	1/1	0.86	0.11	84,84,84,84	0
57	MG	1A	3530	1/1	0.86	0.12	30,30,30,30	0
57	MG	1A	3711	1/1	0.86	0.56	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	1601	1/1	0.86	0.43	80,80,80,80	0
57	MG	2a	3102	1/1	0.86	0.16	66,66,66,66	0
57	MG	1A	3644	1/1	0.86	0.18	59,59,59,59	0
57	MG	2A	3125	1/1	0.86	0.08	85,85,85,85	0
57	MG	1A	3087	1/1	0.86	0.09	56,56,56,56	0
57	MG	1a	1718	1/1	0.86	0.25	77,77,77,77	0
57	MG	2a	3119	1/1	0.86	0.09	65,65,65,65	0
57	MG	1a	1719	1/1	0.86	0.18	58,58,58,58	0
57	MG	1A	3035	1/1	0.86	0.24	54,54,54,54	0
57	MG	1A	3485	1/1	0.86	0.18	24,24,24,24	0
57	MG	2A	3720	1/1	0.86	0.09	77,77,77,77	0
57	MG	1A	3055	1/1	0.86	0.16	58,58,58,58	0
57	MG	1A	3835	1/1	0.86	0.28	61,61,61,61	0
57	MG	1A	3836	1/1	0.86	0.07	46,46,46,46	0
57	MG	1A	3179	1/1	0.86	0.15	77,77,77,77	0
57	MG	1e	201	1/1	0.86	0.14	76,76,76,76	0
57	MG	1A	3929	1/1	0.86	0.13	44,44,44,44	0
57	MG	1A	3383	1/1	0.86	0.28	62,62,62,62	0
57	MG	1a	1626	1/1	0.86	0.18	57,57,57,57	0
57	MG	1B	222	1/1	0.86	0.19	35,35,35,35	0
57	MG	1h	201	1/1	0.86	0.24	59,59,59,59	0
57	MG	2a	3161	1/1	0.86	0.14	70,70,70,70	0
57	MG	1l	3102	1/1	0.86	0.18	75,75,75,75	0
57	MG	1n	102	1/1	0.86	0.14	53,53,53,53	0
57	MG	1A	3552	1/1	0.86	0.14	52,52,52,52	0
57	MG	1A	3022	1/1	0.86	0.15	49,49,49,49	0
57	MG	1A	3668	1/1	0.86	0.23	41,41,41,41	0
57	MG	2a	3172	1/1	0.86	0.15	68,68,68,68	0
57	MG	2A	3391	1/1	0.86	0.16	65,65,65,65	0
57	MG	1A	3947	1/1	0.86	0.17	63,63,63,63	0
57	MG	1A	3670	1/1	0.86	0.10	59,59,59,59	0
57	MG	1A	3212	1/1	0.86	0.18	56,56,56,56	0
57	MG	2A	3574	1/1	0.86	0.12	54,54,54,54	0
57	MG	2R	202	1/1	0.86	0.23	62,62,62,62	0
57	MG	1F	314	1/1	0.86	0.12	42,42,42,42	0
57	MG	2A	3006	1/1	0.86	0.12	51,51,51,51	0
57	MG	1A	3397	1/1	0.86	0.16	42,42,42,42	0
57	MG	1D	313	1/1	0.87	0.31	33,33,33,33	0
57	MG	1a	1692	1/1	0.87	0.33	64,64,64,64	0
57	MG	2A	3173	1/1	0.87	0.14	52,52,52,52	0
57	MG	2a	3034	1/1	0.87	0.19	68,68,68,68	0
57	MG	2A	3539	1/1	0.87	0.19	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3405	1/1	0.87	0.12	72,72,72,72	0
57	MG	2A	3682	1/1	0.87	0.17	59,59,59,59	0
57	MG	2A	3097	1/1	0.87	0.24	58,58,58,58	0
57	MG	2A	3544	1/1	0.87	0.09	64,64,64,64	0
57	MG	2a	3049	1/1	0.87	0.27	66,66,66,66	0
57	MG	2A	3099	1/1	0.87	0.28	66,66,66,66	0
57	MG	2a	3051	1/1	0.87	0.17	69,69,69,69	0
57	MG	1a	1645	1/1	0.87	0.19	63,63,63,63	0
57	MG	1A	3832	1/1	0.87	0.17	53,53,53,53	0
57	MG	1A	3245	1/1	0.87	0.21	54,54,54,54	0
57	MG	2A	3550	1/1	0.87	0.27	73,73,73,73	0
57	MG	1A	3186	1/1	0.87	0.11	78,78,78,78	0
57	MG	1A	3685	1/1	0.87	0.13	72,72,72,72	0
57	MG	1A	3080	1/1	0.87	0.23	55,55,55,55	0
57	MG	2A	3430	1/1	0.87	0.13	59,59,59,59	0
57	MG	2A	3431	1/1	0.87	0.22	41,41,41,41	0
57	MG	1A	3301	1/1	0.87	0.43	35,35,35,35	0
57	MG	2a	3077	1/1	0.87	0.32	69,69,69,69	0
57	MG	1A	3257	1/1	0.87	0.09	54,54,54,54	0
57	MG	2A	3277	1/1	0.87	0.18	50,50,50,50	0
57	MG	1A	3095	1/1	0.87	0.15	41,41,41,41	0
57	MG	18	102	1/1	0.87	0.36	40,40,40,40	0
57	MG	1A	3958	1/1	0.87	0.15	50,50,50,50	0
57	MG	2A	3446	1/1	0.87	0.42	47,47,47,47	0
57	MG	1A	3012	1/1	0.87	0.12	41,41,41,41	0
57	MG	2A	3304	1/1	0.87	0.11	73,73,73,73	0
57	MG	2A	3306	1/1	0.87	0.19	65,65,65,65	0
57	MG	2A	3583	1/1	0.87	0.10	48,48,48,48	0
57	MG	1A	3200	1/1	0.87	0.28	63,63,63,63	0
57	MG	1A	3084	1/1	0.87	0.33	51,51,51,51	0
57	MG	2a	3111	1/1	0.87	0.19	71,71,71,71	0
57	MG	1a	1725	1/1	0.87	0.26	66,66,66,66	0
57	MG	2A	3596	1/1	0.87	0.06	51,51,51,51	0
57	MG	2A	3467	1/1	0.87	0.13	66,66,66,66	0
57	MG	2D	304	1/1	0.87	0.39	58,58,58,58	0
57	MG	2A	3047	1/1	0.87	0.16	79,79,79,79	0
57	MG	2A	3600	1/1	0.87	0.20	53,53,53,53	0
57	MG	1A	3753	1/1	0.87	0.18	44,44,44,44	0
57	MG	2A	3334	1/1	0.87	0.10	64,64,64,64	0
57	MG	2G	201	1/1	0.87	0.18	77,77,77,77	0
57	MG	2a	3134	1/1	0.87	0.15	77,77,77,77	0
57	MG	1A	3756	1/1	0.87	0.21	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3218	1/1	0.87	0.13	53,53,53,53	0
57	MG	2A	3349	1/1	0.87	0.12	51,51,51,51	0
57	MG	1B	210	1/1	0.87	0.22	60,60,60,60	0
57	MG	2A	3355	1/1	0.87	0.17	65,65,65,65	0
57	MG	1A	3328	1/1	0.87	0.23	62,62,62,62	0
57	MG	2A	3152	1/1	0.87	0.16	61,61,61,61	0
57	MG	1A	3709	1/1	0.87	0.13	44,44,44,44	0
57	MG	2a	3151	1/1	0.87	0.13	54,54,54,54	0
57	MG	2A	3631	1/1	0.87	0.12	44,44,44,44	0
57	MG	2A	3500	1/1	0.87	0.15	63,63,63,63	0
57	MG	29	101	1/1	0.87	0.37	66,66,66,66	0
57	MG	2a	3002	1/1	0.87	0.25	60,60,60,60	0
57	MG	1A	3710	1/1	0.87	0.08	62,62,62,62	0
57	MG	2A	3073	1/1	0.87	0.11	51,51,51,51	0
57	MG	1A	3763	1/1	0.87	0.16	60,60,60,60	0
57	MG	1g	202	1/1	0.87	0.13	68,68,68,68	0
57	MG	2A	3384	1/1	0.87	0.17	49,49,49,49	0
57	MG	2A	3511	1/1	0.87	0.19	75,75,75,75	0
57	MG	1A	3395	1/1	0.87	0.17	31,31,31,31	0
57	MG	2A	3513	1/1	0.87	0.14	35,35,35,35	0
57	MG	2t	201	1/1	0.87	0.17	46,46,46,46	0
58	MPD	1A	4014	8/8	0.87	0.16	55,58,65,69	0
57	MG	2A	3234	1/1	0.87	0.30	66,66,66,66	0
57	MG	1l	3101	1/1	0.87	0.25	73,73,73,73	0
57	MG	2A	3395	1/1	0.87	0.12	61,61,61,61	0
57	MG	1A	3674	1/1	0.87	0.12	69,69,69,69	0
57	MG	1Y	201	1/1	0.87	0.19	57,57,57,57	0
57	MG	2A	3303	1/1	0.88	0.13	67,67,67,67	0
57	MG	1A	3369	1/1	0.88	0.15	32,32,32,32	0
57	MG	2A	3134	1/1	0.88	0.25	68,68,68,68	0
57	MG	2A	3136	1/1	0.88	0.23	66,66,66,66	0
57	MG	1A	3493	1/1	0.88	0.16	34,34,34,34	0
57	MG	1A	3548	1/1	0.88	0.30	40,40,40,40	0
57	MG	2P	201	1/1	0.88	0.09	61,61,61,61	0
57	MG	1A	3839	1/1	0.88	0.13	40,40,40,40	0
57	MG	1a	1739	1/1	0.88	0.13	60,60,60,60	0
57	MG	2A	3329	1/1	0.88	0.15	33,33,33,33	0
57	MG	1g	201	1/1	0.88	0.20	67,67,67,67	0
57	MG	1A	3841	1/1	0.88	0.37	59,59,59,59	0
57	MG	1a	1636	1/1	0.88	0.23	65,65,65,65	0
57	MG	1a	1637	1/1	0.88	0.15	44,44,44,44	0
57	MG	25	101	1/1	0.88	0.10	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	1a	1640	1/1	0.88	0.28	69,69,69,69	0
57	MG	1A	3494	1/1	0.88	0.08	48,48,48,48	0
57	MG	1A	3014	1/1	0.88	0.23	62,62,62,62	0
57	MG	2A	3564	1/1	0.88	0.09	32,32,32,32	0
57	MG	1F	311	1/1	0.88	0.15	55,55,55,55	0
57	MG	1A	3275	1/1	0.88	0.54	36,36,36,36	0
57	MG	2A	3364	1/1	0.88	0.13	35,35,35,35	0
57	MG	2A	3166	1/1	0.88	0.11	68,68,68,68	0
57	MG	1F	317	1/1	0.88	0.12	51,51,51,51	0
57	MG	1G	201	1/1	0.88	0.09	65,65,65,65	0
57	MG	1A	3232	1/1	0.88	0.27	76,76,76,76	0
57	MG	1A	3281	1/1	0.88	0.23	46,46,46,46	0
57	MG	1H	202	1/1	0.88	0.17	53,53,53,53	0
57	MG	2A	3009	1/1	0.88	0.35	47,47,47,47	0
57	MG	2A	3017	1/1	0.88	0.21	56,56,56,56	0
57	MG	2A	3586	1/1	0.88	0.09	57,57,57,57	0
57	MG	2a	3029	1/1	0.88	0.14	70,70,70,70	0
57	MG	1A	3326	1/1	0.88	0.20	45,45,45,45	0
57	MG	1A	3688	1/1	0.88	0.07	53,53,53,53	0
57	MG	1A	3762	1/1	0.88	0.18	62,62,62,62	0
57	MG	1A	3563	1/1	0.88	0.12	52,52,52,52	0
57	MG	1a	1777	1/1	0.88	0.14	75,75,75,75	0
57	MG	1A	3327	1/1	0.88	0.10	61,61,61,61	0
57	MG	2A	3190	1/1	0.88	0.18	74,74,74,74	0
57	MG	2a	3044	1/1	0.88	0.19	71,71,71,71	0
57	MG	1A	3063	1/1	0.88	0.21	52,52,52,52	0
57	MG	2A	3408	1/1	0.88	0.09	68,68,68,68	0
57	MG	2A	3041	1/1	0.88	0.30	72,72,72,72	0
57	MG	2A	3411	1/1	0.88	0.17	35,35,35,35	0
57	MG	2A	3042	1/1	0.88	0.20	48,48,48,48	0
57	MG	1A	3696	1/1	0.88	0.33	44,44,44,44	0
57	MG	2a	3056	1/1	0.88	0.18	77,77,77,77	0
57	MG	2a	3057	1/1	0.88	0.10	68,68,68,68	0
57	MG	2a	3058	1/1	0.88	0.07	79,79,79,79	0
57	MG	1A	3516	1/1	0.88	0.13	53,53,53,53	0
57	MG	1a	1674	1/1	0.88	0.19	69,69,69,69	0
57	MG	1A	3570	1/1	0.88	0.08	63,63,63,63	0
57	MG	2A	3205	1/1	0.88	0.15	61,61,61,61	0
57	MG	1A	3979	1/1	0.88	0.10	85,85,85,85	0
57	MG	2a	3065	1/1	0.88	0.39	65,65,65,65	0
57	MG	2A	3208	1/1	0.88	0.20	59,59,59,59	0
57	MG	2A	3644	1/1	0.88	0.09	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3053	1/1	0.88	0.16	73,73,73,73	0
57	MG	2a	3073	1/1	0.88	0.18	71,71,71,71	0
57	MG	2a	3075	1/1	0.88	0.15	50,50,50,50	0
57	MG	2A	3054	1/1	0.88	0.18	65,65,65,65	0
57	MG	2A	3648	1/1	0.88	0.10	60,60,60,60	0
57	MG	1A	3783	1/1	0.88	0.23	67,67,67,67	0
57	MG	2A	3060	1/1	0.88	0.73	54,54,54,54	0
57	MG	1A	3262	1/1	0.88	0.30	55,55,55,55	0
57	MG	2A	3062	1/1	0.88	0.19	56,56,56,56	0
57	MG	1A	3704	1/1	0.88	0.17	67,67,67,67	0
57	MG	2A	3068	1/1	0.88	0.36	54,54,54,54	0
57	MG	2A	3223	1/1	0.88	0.18	62,62,62,62	0
57	MG	2A	3455	1/1	0.88	0.10	65,65,65,65	0
57	MG	1A	3344	1/1	0.88	0.22	47,47,47,47	0
57	MG	2A	3460	1/1	0.88	0.20	62,62,62,62	0
57	MG	2a	3103	1/1	0.88	0.11	61,61,61,61	0
57	MG	2A	3226	1/1	0.88	0.33	54,54,54,54	0
57	MG	2A	3673	1/1	0.88	0.11	54,54,54,54	0
57	MG	1A	3987	1/1	0.88	0.21	77,77,77,77	0
57	MG	1A	3643	1/1	0.88	0.22	56,56,56,56	0
57	MG	1a	1689	1/1	0.88	0.30	65,65,65,65	0
57	MG	2A	3468	1/1	0.88	0.07	65,65,65,65	0
57	MG	1A	3526	1/1	0.88	0.17	54,54,54,54	0
57	MG	1A	3887	1/1	0.88	0.10	63,63,63,63	0
57	MG	2a	3125	1/1	0.88	0.13	58,58,58,58	0
57	MG	1A	3998	1/1	0.88	0.06	54,54,54,54	0
57	MG	1a	1695	1/1	0.88	0.17	66,66,66,66	0
57	MG	2A	3480	1/1	0.88	0.17	56,56,56,56	0
57	MG	2A	3244	1/1	0.88	0.14	60,60,60,60	0
57	MG	1A	3345	1/1	0.88	0.15	42,42,42,42	0
57	MG	2A	3247	1/1	0.88	0.10	59,59,59,59	0
57	MG	1A	3348	1/1	0.88	0.25	26,26,26,26	0
57	MG	2A	3701	1/1	0.88	0.16	55,55,55,55	0
57	MG	2A	3095	1/1	0.88	0.13	46,46,46,46	0
57	MG	1a	1699	1/1	0.88	0.11	70,70,70,70	0
57	MG	2a	3144	1/1	0.88	0.11	67,67,67,67	0
57	MG	1A	3199	1/1	0.88	0.23	41,41,41,41	0
57	MG	1A	3714	1/1	0.88	0.18	29,29,29,29	0
57	MG	1A	3814	1/1	0.88	0.35	75,75,75,75	0
57	MG	1A	3715	1/1	0.88	0.12	59,59,59,59	0
57	MG	2a	3160	1/1	0.88	0.06	71,71,71,71	0
57	MG	1A	3822	1/1	0.88	0.17	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	3721	1/1	0.88	0.23	46,46,46,46	0
57	MG	1A	3044	1/1	0.88	0.29	68,68,68,68	0
57	MG	2A	3726	1/1	0.88	0.08	64,64,64,64	0
57	MG	1a	1857	1/1	0.88	0.25	59,59,59,59	0
57	MG	1A	3269	1/1	0.88	0.13	45,45,45,45	0
57	MG	1A	3827	1/1	0.88	0.27	58,58,58,58	0
57	MG	1A	3533	1/1	0.88	0.25	69,69,69,69	0
57	MG	2a	3179	1/1	0.88	0.19	77,77,77,77	0
57	MG	2a	3182	1/1	0.88	0.12	59,59,59,59	0
57	MG	1A	3534	1/1	0.88	0.23	57,57,57,57	0
57	MG	2A	3280	1/1	0.88	0.18	61,61,61,61	0
57	MG	1A	3595	1/1	0.88	0.17	47,47,47,47	0
57	MG	1a	1727	1/1	0.88	0.15	54,54,54,54	0
57	MG	2A	3296	1/1	0.88	0.30	69,69,69,69	0
57	MG	1a	1732	1/1	0.88	0.28	85,85,85,85	0
57	MG	2A	3130	1/1	0.88	0.32	54,54,54,54	0
57	MG	2D	305	1/1	0.88	0.40	55,55,55,55	0
57	MG	2A	3535	1/1	0.88	0.28	37,37,37,37	0
57	MG	2A	3536	1/1	0.88	0.14	67,67,67,67	0
57	MG	1A	3093	1/1	0.89	0.21	57,57,57,57	0
57	MG	2A	3617	1/1	0.89	0.18	82,82,82,82	0
57	MG	1A	3999	1/1	0.89	0.19	47,47,47,47	0
57	MG	2A	3274	1/1	0.89	0.24	51,51,51,51	0
57	MG	1A	3194	1/1	0.89	0.24	65,65,65,65	0
57	MG	2A	3627	1/1	0.89	0.17	37,37,37,37	0
57	MG	1A	4002	1/1	0.89	0.21	71,71,71,71	0
57	MG	2A	3278	1/1	0.89	0.14	55,55,55,55	0
57	MG	1A	3008	1/1	0.89	0.12	38,38,38,38	0
57	MG	2A	3471	1/1	0.89	0.17	69,69,69,69	0
57	MG	2A	3014	1/1	0.89	0.14	54,54,54,54	0
57	MG	2A	3283	1/1	0.89	0.31	56,56,56,56	0
57	MG	1a	1677	1/1	0.89	0.42	66,66,66,66	0
57	MG	1A	3458	1/1	0.89	0.25	42,42,42,42	0
57	MG	10	107	1/1	0.89	0.18	65,65,65,65	0
57	MG	1A	3919	1/1	0.89	0.17	45,45,45,45	0
57	MG	1A	3923	1/1	0.89	0.19	47,47,47,47	0
57	MG	1A	3842	1/1	0.89	0.22	71,71,71,71	0
57	MG	11	105	1/1	0.89	0.12	43,43,43,43	0
57	MG	1A	3061	1/1	0.89	0.19	35,35,35,35	0
57	MG	2a	3048	1/1	0.89	0.23	69,69,69,69	0
57	MG	2A	3660	1/1	0.89	0.15	42,42,42,42	0
57	MG	1A	3640	1/1	0.89	0.11	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	1B	208	1/1	0.89	0.36	65,65,65,65	0
57	MG	2A	3664	1/1	0.89	0.12	56,56,56,56	0
57	MG	1A	3177	1/1	0.89	0.10	52,52,52,52	0
57	MG	2A	3323	1/1	0.89	0.17	43,43,43,43	0
57	MG	1a	1801	1/1	0.89	0.12	58,58,58,58	0
57	MG	2A	3046	1/1	0.89	0.13	63,63,63,63	0
57	MG	18	103	1/1	0.89	0.06	54,54,54,54	0
57	MG	2A	3335	1/1	0.89	0.13	65,65,65,65	0
57	MG	1a	1809	1/1	0.89	0.19	60,60,60,60	0
57	MG	1a	1812	1/1	0.89	0.15	70,70,70,70	0
57	MG	1a	1696	1/1	0.89	0.32	71,71,71,71	0
57	MG	1a	1819	1/1	0.89	0.13	80,80,80,80	0
57	MG	2A	3517	1/1	0.89	0.10	77,77,77,77	0
57	MG	1A	3408	1/1	0.89	0.10	68,68,68,68	0
57	MG	2a	3068	1/1	0.89	0.07	71,71,71,71	0
57	MG	2a	3069	1/1	0.89	0.31	70,70,70,70	0
57	MG	2A	3523	1/1	0.89	0.13	64,64,64,64	0
57	MG	2A	3058	1/1	0.89	0.25	67,67,67,67	0
57	MG	1A	3465	1/1	0.89	0.18	62,62,62,62	0
57	MG	1a	1823	1/1	0.89	0.07	74,74,74,74	0
57	MG	2A	3530	1/1	0.89	0.18	72,72,72,72	0
57	MG	1A	3471	1/1	0.89	0.18	55,55,55,55	0
57	MG	1a	1700	1/1	0.89	0.32	60,60,60,60	0
57	MG	2A	3533	1/1	0.89	0.48	68,68,68,68	0
57	MG	2a	3086	1/1	0.89	0.14	78,78,78,78	0
57	MG	2A	3368	1/1	0.89	0.14	32,32,32,32	0
57	MG	1A	3419	1/1	0.89	0.10	76,76,76,76	0
57	MG	1A	3649	1/1	0.89	0.12	53,53,53,53	0
57	MG	1B	225	1/1	0.89	0.05	53,53,53,53	0
57	MG	2A	3541	1/1	0.89	0.13	79,79,79,79	0
57	MG	1A	3141	1/1	0.89	0.16	64,64,64,64	0
57	MG	2A	3543	1/1	0.89	0.08	59,59,59,59	0
57	MG	2A	3721	1/1	0.89	0.11	73,73,73,73	0
57	MG	2A	3722	1/1	0.89	0.25	75,75,75,75	0
57	MG	2A	3387	1/1	0.89	0.12	63,63,63,63	0
57	MG	1A	3423	1/1	0.89	0.20	38,38,38,38	0
57	MG	2A	3728	1/1	0.89	0.11	56,56,56,56	0
57	MG	1a	1615	1/1	0.89	0.10	63,63,63,63	0
57	MG	1A	3957	1/1	0.89	0.09	54,54,54,54	0
57	MG	1A	3009	1/1	0.89	0.16	32,32,32,32	0
57	MG	1A	3537	1/1	0.89	0.24	56,56,56,56	0
57	MG	2a	3124	1/1	0.89	0.13	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3110	1/1	0.89	0.27	56,56,56,56	0
57	MG	2a	3126	1/1	0.89	0.06	76,76,76,76	0
57	MG	1A	3666	1/1	0.89	0.07	41,41,41,41	0
57	MG	1A	3799	1/1	0.89	0.20	30,30,30,30	0
57	MG	1a	1726	1/1	0.89	0.20	57,57,57,57	0
57	MG	2B	216	1/1	0.89	0.24	83,83,83,83	0
57	MG	1A	3868	1/1	0.89	0.17	67,67,67,67	0
57	MG	1A	3185	1/1	0.89	0.27	60,60,60,60	0
57	MG	1A	3971	1/1	0.89	0.09	49,49,49,49	0
57	MG	1A	3367	1/1	0.89	0.14	42,42,42,42	0
57	MG	1a	1644	1/1	0.89	0.14	61,61,61,61	0
57	MG	1A	3117	1/1	0.89	0.21	37,37,37,37	0
57	MG	1A	3226	1/1	0.89	0.46	38,38,38,38	0
57	MG	1a	1649	1/1	0.89	0.16	44,44,44,44	0
57	MG	2A	3235	1/1	0.89	0.15	72,72,72,72	0
57	MG	1A	3881	1/1	0.89	0.21	45,45,45,45	0
57	MG	2a	3153	1/1	0.89	0.20	60,60,60,60	0
57	MG	1A	3373	1/1	0.89	0.18	53,53,53,53	0
57	MG	2a	3159	1/1	0.89	0.10	70,70,70,70	0
57	MG	2O	201	1/1	0.89	0.20	66,66,66,66	0
57	MG	2A	3581	1/1	0.89	0.17	48,48,48,48	0
57	MG	1A	3555	1/1	0.89	0.20	60,60,60,60	0
57	MG	2a	3163	1/1	0.89	0.19	81,81,81,81	0
57	MG	2Q	202	1/1	0.89	0.35	65,65,65,65	0
57	MG	1R	204	1/1	0.89	0.20	39,39,39,39	0
57	MG	2a	3169	1/1	0.89	0.10	72,72,72,72	0
57	MG	1A	3747	1/1	0.89	0.12	52,52,52,52	0
57	MG	1A	3983	1/1	0.89	0.38	57,57,57,57	0
57	MG	2U	201	1/1	0.89	0.17	62,62,62,62	0
57	MG	1h	202	1/1	0.89	0.17	67,67,67,67	0
57	MG	2V	202	1/1	0.89	0.44	49,49,49,49	0
57	MG	1i	201	1/1	0.89	0.15	68,68,68,68	0
57	MG	1A	3375	1/1	0.89	0.13	38,38,38,38	0
57	MG	2A	3443	1/1	0.89	0.08	61,61,61,61	0
57	MG	1a	1760	1/1	0.89	0.09	55,55,55,55	0
57	MG	1A	3615	1/1	0.89	0.25	24,24,24,24	0
57	MG	1A	3558	1/1	0.89	0.15	55,55,55,55	0
57	MG	2a	3003	1/1	0.89	0.16	56,56,56,56	0
58	MPD	2A	3732	8/8	0.89	0.16	51,60,66,69	0
57	MG	1A	3324	1/1	0.89	0.17	30,30,30,30	0
57	MG	2A	3454	1/1	0.89	0.15	82,82,82,82	0
57	MG	1A	3156	1/1	0.89	0.18	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	3757	1/1	0.89	0.21	50,50,50,50	0
57	MG	1A	3599	1/1	0.90	0.08	62,62,62,62	0
57	MG	2A	3140	1/1	0.90	0.15	50,50,50,50	0
57	MG	2A	3345	1/1	0.90	0.12	67,67,67,67	0
57	MG	2A	3554	1/1	0.90	0.12	47,47,47,47	0
57	MG	1a	1610	1/1	0.90	0.25	60,60,60,60	0
57	MG	1A	3930	1/1	0.90	0.12	54,54,54,54	0
57	MG	1A	3410	1/1	0.90	0.10	38,38,38,38	0
57	MG	23	101	1/1	0.90	0.17	59,59,59,59	0
57	MG	1B	218	1/1	0.90	0.29	53,53,53,53	0
57	MG	1A	3411	1/1	0.90	0.26	56,56,56,56	0
57	MG	1a	1620	1/1	0.90	0.12	55,55,55,55	0
57	MG	1a	1621	1/1	0.90	0.18	61,61,61,61	0
57	MG	1A	3545	1/1	0.90	0.23	56,56,56,56	0
57	MG	1A	3755	1/1	0.90	0.23	59,59,59,59	0
57	MG	1A	3944	1/1	0.90	0.10	57,57,57,57	0
57	MG	2a	3007	1/1	0.90	0.25	56,56,56,56	0
57	MG	2A	3163	1/1	0.90	0.11	74,74,74,74	0
57	MG	2A	3379	1/1	0.90	0.19	70,70,70,70	0
57	MG	1a	1633	1/1	0.90	0.15	40,40,40,40	0
57	MG	2a	3013	1/1	0.90	0.29	71,71,71,71	0
57	MG	2A	3165	1/1	0.90	0.47	60,60,60,60	0
57	MG	1A	3945	1/1	0.90	0.17	62,62,62,62	0
57	MG	1a	1745	1/1	0.90	0.16	66,66,66,66	0
57	MG	1A	3415	1/1	0.90	0.15	48,48,48,48	0
57	MG	1o	101	1/1	0.90	0.15	73,73,73,73	0
57	MG	1A	3948	1/1	0.90	0.12	48,48,48,48	0
57	MG	2a	3024	1/1	0.90	0.12	65,65,65,65	0
57	MG	2A	3593	1/1	0.90	0.09	61,61,61,61	0
57	MG	1t	201	1/1	0.90	0.14	57,57,57,57	0
57	MG	1a	1752	1/1	0.90	0.11	55,55,55,55	0
57	MG	1A	3844	1/1	0.90	0.14	37,37,37,37	0
57	MG	1A	3676	1/1	0.90	0.07	74,74,74,74	0
57	MG	2a	3033	1/1	0.90	0.28	64,64,64,64	0
57	MG	1A	3049	1/1	0.90	0.30	44,44,44,44	0
57	MG	2A	3603	1/1	0.90	0.10	59,59,59,59	0
57	MG	1A	3550	1/1	0.90	0.13	58,58,58,58	0
57	MG	2A	3606	1/1	0.90	0.20	38,38,38,38	0
57	MG	2A	3002	1/1	0.90	0.16	53,53,53,53	0
57	MG	1F	313	1/1	0.90	0.54	45,45,45,45	0
57	MG	2A	3185	1/1	0.90	0.17	66,66,66,66	0
57	MG	2a	3046	1/1	0.90	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3047	1/1	0.90	0.17	82,82,82,82	0
57	MG	1a	1648	1/1	0.90	0.20	68,68,68,68	0
57	MG	1A	3030	1/1	0.90	0.16	31,31,31,31	0
57	MG	1a	1765	1/1	0.90	0.11	61,61,61,61	0
57	MG	1a	1650	1/1	0.90	0.20	49,49,49,49	0
57	MG	2A	3417	1/1	0.90	0.10	50,50,50,50	0
57	MG	2A	3023	1/1	0.90	0.20	61,61,61,61	0
57	MG	2A	3196	1/1	0.90	0.23	64,64,64,64	0
57	MG	2A	3424	1/1	0.90	0.19	37,37,37,37	0
57	MG	1A	3616	1/1	0.90	0.25	27,27,27,27	0
57	MG	2A	3427	1/1	0.90	0.15	48,48,48,48	0
57	MG	1A	3236	1/1	0.90	0.19	34,34,34,34	0
57	MG	1A	3764	1/1	0.90	0.18	27,27,27,27	0
57	MG	1A	3191	1/1	0.90	0.14	61,61,61,61	0
57	MG	1A	3621	1/1	0.90	0.17	24,24,24,24	0
57	MG	1A	3623	1/1	0.90	0.12	53,53,53,53	0
57	MG	2A	3649	1/1	0.90	0.12	42,42,42,42	0
57	MG	2A	3438	1/1	0.90	0.08	46,46,46,46	0
57	MG	2A	3207	1/1	0.90	0.50	53,53,53,53	0
57	MG	1A	3040	1/1	0.90	0.14	64,64,64,64	0
57	MG	2A	3039	1/1	0.90	0.19	49,49,49,49	0
57	MG	1A	3371	1/1	0.90	0.19	64,64,64,64	0
57	MG	1a	1665	1/1	0.90	0.47	65,65,65,65	0
57	MG	2A	3661	1/1	0.90	0.12	44,44,44,44	0
57	MG	2a	3078	1/1	0.90	0.43	65,65,65,65	0
57	MG	1a	1782	1/1	0.90	0.10	71,71,71,71	0
57	MG	2A	3451	1/1	0.90	0.10	64,64,64,64	0
57	MG	1P	203	1/1	0.90	0.19	72,72,72,72	0
57	MG	2a	3082	1/1	0.90	0.21	66,66,66,66	0
57	MG	1a	1787	1/1	0.90	0.22	75,75,75,75	0
57	MG	1A	3699	1/1	0.90	0.08	40,40,40,40	0
57	MG	1a	1792	1/1	0.90	0.10	83,83,83,83	0
57	MG	2A	3457	1/1	0.90	0.07	61,61,61,61	0
57	MG	1a	1793	1/1	0.90	0.16	66,66,66,66	0
57	MG	1A	3278	1/1	0.90	0.29	47,47,47,47	0
57	MG	1A	3323	1/1	0.90	0.36	74,74,74,74	0
57	MG	1A	3150	1/1	0.90	0.12	41,41,41,41	0
57	MG	1A	3437	1/1	0.90	0.23	68,68,68,68	0
57	MG	1A	3508	1/1	0.90	0.13	62,62,62,62	0
57	MG	1A	3218	1/1	0.90	0.21	39,39,39,39	0
57	MG	1A	3377	1/1	0.90	0.24	63,63,63,63	0
57	MG	1A	3379	1/1	0.90	0.17	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	3113	1/1	0.90	0.08	62,62,62,62	0
57	MG	1A	3283	1/1	0.90	0.15	62,62,62,62	0
57	MG	1A	3802	1/1	0.90	0.09	59,59,59,59	0
57	MG	2A	3072	1/1	0.90	0.45	51,51,51,51	0
57	MG	1A	3803	1/1	0.90	0.09	40,40,40,40	0
57	MG	1A	3993	1/1	0.90	0.12	70,70,70,70	0
57	MG	1a	1816	1/1	0.90	0.08	73,73,73,73	0
57	MG	2A	3702	1/1	0.90	0.13	47,47,47,47	0
57	MG	2A	3076	1/1	0.90	0.17	58,58,58,58	0
57	MG	1a	1685	1/1	0.90	0.10	56,56,56,56	0
57	MG	1A	3381	1/1	0.90	0.16	48,48,48,48	0
57	MG	2A	3493	1/1	0.90	0.14	60,60,60,60	0
57	MG	2A	3085	1/1	0.90	0.25	77,77,77,77	0
57	MG	2a	3135	1/1	0.90	0.12	62,62,62,62	0
57	MG	10	105	1/1	0.90	0.23	56,56,56,56	0
57	MG	1A	3718	1/1	0.90	0.04	72,72,72,72	0
57	MG	2A	3719	1/1	0.90	0.23	58,58,58,58	0
57	MG	1a	1825	1/1	0.90	0.20	67,67,67,67	0
57	MG	1A	3252	1/1	0.90	0.13	47,47,47,47	0
57	MG	2A	3094	1/1	0.90	0.20	53,53,53,53	0
57	MG	1A	3906	1/1	0.90	0.07	54,54,54,54	0
57	MG	2A	3096	1/1	0.90	0.21	52,52,52,52	0
57	MG	1a	1830	1/1	0.90	0.14	77,77,77,77	0
57	MG	2A	3729	1/1	0.90	0.16	69,69,69,69	0
57	MG	1A	3455	1/1	0.90	0.20	52,52,52,52	0
57	MG	2A	3104	1/1	0.90	0.23	47,47,47,47	0
57	MG	1A	3292	1/1	0.90	0.15	49,49,49,49	0
57	MG	1A	3336	1/1	0.90	0.17	31,31,31,31	0
57	MG	1a	1836	1/1	0.90	0.14	58,58,58,58	0
57	MG	1a	1837	1/1	0.90	0.22	72,72,72,72	0
57	MG	15	102	1/1	0.90	0.40	51,51,51,51	0
57	MG	2A	3286	1/1	0.90	0.20	67,67,67,67	0
57	MG	1A	4004	1/1	0.90	0.22	56,56,56,56	0
57	MG	2a	3168	1/1	0.90	0.19	64,64,64,64	0
57	MG	1A	3733	1/1	0.90	0.12	45,45,45,45	0
57	MG	2A	3298	1/1	0.90	0.31	78,78,78,78	0
57	MG	1A	3293	1/1	0.90	0.37	39,39,39,39	0
57	MG	2A	3118	1/1	0.90	0.19	37,37,37,37	0
57	MG	2D	310	1/1	0.90	0.11	66,66,66,66	0
57	MG	1A	3460	1/1	0.90	0.20	30,30,30,30	0
57	MG	1B	202	1/1	0.90	0.33	60,60,60,60	0
57	MG	2f	201	1/1	0.90	0.22	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3184	1/1	0.90	0.20	55,55,55,55	0
57	MG	1a	1707	1/1	0.90	0.29	64,64,64,64	0
57	MG	2p	101	1/1	0.90	0.16	61,61,61,61	0
57	MG	1A	3405	1/1	0.90	0.13	69,69,69,69	0
57	MG	1A	3090	1/1	0.90	0.12	45,45,45,45	0
57	MG	2A	3320	1/1	0.90	0.08	51,51,51,51	0
58	MPD	1T	208	8/8	0.90	0.22	68,70,74,81	0
57	MG	1A	3925	1/1	0.90	0.12	54,54,54,54	0
57	MG	1B	209	1/1	0.90	0.16	41,41,41,41	0
57	MG	1A	3927	1/1	0.90	0.14	58,58,58,58	0
57	MG	2A	3135	1/1	0.90	0.09	37,37,37,37	0
57	MG	1a	1864	1/1	0.90	0.21	57,57,57,57	0
57	MG	1a	1608	1/1	0.90	0.10	61,61,61,61	0
57	MG	1A	3153	1/1	0.91	0.51	52,52,52,52	0
57	MG	2A	3295	1/1	0.91	0.19	65,65,65,65	0
57	MG	1G	204	1/1	0.91	0.24	65,65,65,65	0
57	MG	2A	3297	1/1	0.91	0.36	60,60,60,60	0
57	MG	1a	1817	1/1	0.91	0.06	83,83,83,83	0
57	MG	2A	3162	1/1	0.91	0.18	65,65,65,65	0
57	MG	1A	3701	1/1	0.91	0.80	69,69,69,69	0
57	MG	2A	3038	1/1	0.91	0.20	49,49,49,49	0
57	MG	1a	1628	1/1	0.91	0.36	65,65,65,65	0
57	MG	1a	1821	1/1	0.91	0.10	68,68,68,68	0
57	MG	2A	3309	1/1	0.91	0.14	39,39,39,39	0
57	MG	1A	3467	1/1	0.91	0.17	52,52,52,52	0
57	MG	1a	1631	1/1	0.91	0.15	43,43,43,43	0
57	MG	2A	3665	1/1	0.91	0.10	51,51,51,51	0
57	MG	2A	3668	1/1	0.91	0.26	57,57,57,57	0
57	MG	1A	3658	1/1	0.91	0.11	47,47,47,47	0
57	MG	1A	3911	1/1	0.91	0.08	66,66,66,66	0
57	MG	1A	3837	1/1	0.91	0.21	56,56,56,56	0
57	MG	1A	3707	1/1	0.91	0.10	38,38,38,38	0
57	MG	2A	3325	1/1	0.91	0.06	65,65,65,65	0
57	MG	1A	3094	1/1	0.91	0.18	57,57,57,57	0
57	MG	2A	3676	1/1	0.91	0.37	65,65,65,65	0
57	MG	1A	3995	1/1	0.91	0.07	61,61,61,61	0
57	MG	1R	206	1/1	0.91	0.21	53,53,53,53	0
57	MG	1A	3773	1/1	0.91	0.20	45,45,45,45	0
57	MG	1a	1646	1/1	0.91	0.20	60,60,60,60	0
57	MG	1A	3662	1/1	0.91	0.13	54,54,54,54	0
57	MG	1a	1839	1/1	0.91	0.09	44,44,44,44	0
57	MG	1A	3476	1/1	0.91	0.23	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3063	1/1	0.91	0.21	48,48,48,48	0
57	MG	2a	3063	1/1	0.91	0.06	78,78,78,78	0
57	MG	2A	3351	1/1	0.91	0.17	37,37,37,37	0
57	MG	2A	3352	1/1	0.91	0.14	51,51,51,51	0
57	MG	1A	3477	1/1	0.91	0.16	28,28,28,28	0
57	MG	1A	3712	1/1	0.91	0.23	38,38,38,38	0
57	MG	1U	203	1/1	0.91	0.22	37,37,37,37	0
57	MG	1a	1848	1/1	0.91	0.06	65,65,65,65	0
57	MG	1A	3617	1/1	0.91	0.24	32,32,32,32	0
57	MG	1a	1853	1/1	0.91	0.13	52,52,52,52	0
57	MG	1V	206	1/1	0.91	0.31	59,59,59,59	0
57	MG	2A	3370	1/1	0.91	0.13	46,46,46,46	0
57	MG	1A	3848	1/1	0.91	0.12	41,41,41,41	0
57	MG	2A	3712	1/1	0.91	0.23	68,68,68,68	0
57	MG	2A	3374	1/1	0.91	0.18	70,70,70,70	0
57	MG	1A	3085	1/1	0.91	0.26	37,37,37,37	0
57	MG	1a	1751	1/1	0.91	0.14	42,42,42,42	0
57	MG	1A	3571	1/1	0.91	0.20	22,22,22,22	0
57	MG	2A	3381	1/1	0.91	0.23	55,55,55,55	0
57	MG	1A	3401	1/1	0.91	0.20	29,29,29,29	0
57	MG	1a	1755	1/1	0.91	0.16	47,47,47,47	0
57	MG	2a	3090	1/1	0.91	0.26	67,67,67,67	0
57	MG	1A	3942	1/1	0.91	0.07	60,60,60,60	0
57	MG	2A	3727	1/1	0.91	0.11	69,69,69,69	0
57	MG	2A	3390	1/1	0.91	0.23	53,53,53,53	0
57	MG	2a	3099	1/1	0.91	0.11	75,75,75,75	0
57	MG	2A	3092	1/1	0.91	0.12	68,68,68,68	0
57	MG	2A	3730	1/1	0.91	0.17	68,68,68,68	0
57	MG	1A	3403	1/1	0.91	0.22	29,29,29,29	0
57	MG	1B	205	1/1	0.91	0.10	50,50,50,50	0
57	MG	1d	302	1/1	0.91	0.08	71,71,71,71	0
57	MG	1A	3157	1/1	0.91	0.22	36,36,36,36	0
57	MG	2B	208	1/1	0.91	0.07	69,69,69,69	0
57	MG	1A	3004	1/1	0.91	0.09	41,41,41,41	0
57	MG	2A	3222	1/1	0.91	0.27	65,65,65,65	0
57	MG	1A	3409	1/1	0.91	0.16	22,22,22,22	0
57	MG	1A	3187	1/1	0.91	0.29	68,68,68,68	0
57	MG	1A	3088	1/1	0.91	0.17	35,35,35,35	0
57	MG	2B	217	1/1	0.91	0.16	68,68,68,68	0
57	MG	1A	3684	1/1	0.91	0.21	68,68,68,68	0
57	MG	2A	3568	1/1	0.91	0.05	75,75,75,75	0
57	MG	2a	3127	1/1	0.91	0.35	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	102	1/1	0.91	0.23	73,73,73,73	0
57	MG	2A	3410	1/1	0.91	0.15	32,32,32,32	0
57	MG	1A	3413	1/1	0.91	0.14	70,70,70,70	0
57	MG	2A	3109	1/1	0.91	0.23	74,74,74,74	0
57	MG	1A	3744	1/1	0.91	0.25	42,42,42,42	0
57	MG	2A	3576	1/1	0.91	0.13	58,58,58,58	0
57	MG	2F	302	1/1	0.91	0.61	47,47,47,47	0
57	MG	1A	3805	1/1	0.91	0.21	47,47,47,47	0
57	MG	1A	3871	1/1	0.91	0.13	37,37,37,37	0
57	MG	2A	3115	1/1	0.91	0.35	50,50,50,50	0
57	MG	1a	1680	1/1	0.91	0.10	63,63,63,63	0
57	MG	2A	3117	1/1	0.91	0.13	54,54,54,54	0
57	MG	2a	3147	1/1	0.91	0.08	77,77,77,77	0
57	MG	2A	3246	1/1	0.91	0.36	46,46,46,46	0
57	MG	1A	3959	1/1	0.91	0.21	55,55,55,55	0
57	MG	2A	3589	1/1	0.91	0.19	49,49,49,49	0
57	MG	1A	3686	1/1	0.91	0.19	46,46,46,46	0
57	MG	2a	3154	1/1	0.91	0.05	80,80,80,80	0
57	MG	1A	3810	1/1	0.91	0.26	36,36,36,36	0
57	MG	2a	3158	1/1	0.91	0.06	55,55,55,55	0
57	MG	1A	3811	1/1	0.91	0.34	48,48,48,48	0
57	MG	2R	203	1/1	0.91	0.16	62,62,62,62	0
57	MG	2T	204	1/1	0.91	0.13	59,59,59,59	0
57	MG	2A	3252	1/1	0.91	0.11	65,65,65,65	0
57	MG	1a	1786	1/1	0.91	0.10	68,68,68,68	0
57	MG	2A	3255	1/1	0.91	0.15	40,40,40,40	0
57	MG	1A	3007	1/1	0.91	0.21	33,33,33,33	0
57	MG	1A	3816	1/1	0.91	0.62	37,37,37,37	0
57	MG	1A	3417	1/1	0.91	0.27	22,22,22,22	0
57	MG	2A	3444	1/1	0.91	0.13	70,70,70,70	0
57	MG	1A	3001	1/1	0.91	0.15	36,36,36,36	0
57	MG	28	101	1/1	0.91	0.13	65,65,65,65	0
57	MG	2a	3174	1/1	0.91	0.17	66,66,66,66	0
57	MG	1A	3888	1/1	0.91	0.08	57,57,57,57	0
57	MG	2A	3448	1/1	0.91	0.27	61,61,61,61	0
57	MG	1A	3224	1/1	0.91	0.23	40,40,40,40	0
57	MG	2A	3003	1/1	0.91	0.14	64,64,64,64	0
57	MG	1F	312	1/1	0.91	0.27	37,37,37,37	0
57	MG	1a	1611	1/1	0.91	0.14	69,69,69,69	0
57	MG	1A	3366	1/1	0.91	0.22	77,77,77,77	0
57	MG	2A	3012	1/1	0.91	0.17	68,68,68,68	0
57	MG	1A	3119	1/1	0.91	0.28	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	2x	101	1/1	0.91	0.17	44,44,44,44	0
57	MG	1F	316	1/1	0.91	0.57	53,53,53,53	0
57	MG	2A	3634	1/1	0.91	0.13	49,49,49,49	0
57	MG	2a	3014	1/1	0.91	0.25	57,57,57,57	0
57	MG	1a	1701	1/1	0.91	0.16	72,72,72,72	0
57	MG	1A	3389	1/1	0.91	0.16	40,40,40,40	0
59	ARG	1B	231	12/12	0.91	0.21	40,47,58,61	0
57	MG	1A	3464	1/1	0.91	0.11	57,57,57,57	0
57	MG	1a	1705	1/1	0.91	0.20	63,63,63,63	0
57	MG	2A	3289	1/1	0.91	0.29	65,65,65,65	0
57	MG	1A	3922	1/1	0.92	0.07	62,62,62,62	0
57	MG	1A	4013	1/1	0.92	0.17	61,61,61,61	0
57	MG	1A	3562	1/1	0.92	0.17	62,62,62,62	0
57	MG	2A	3618	1/1	0.92	0.27	31,31,31,31	0
57	MG	2A	3440	1/1	0.92	0.14	53,53,53,53	0
57	MG	2a	3017	1/1	0.92	0.12	49,49,49,49	0
57	MG	1a	1710	1/1	0.92	0.21	64,64,64,64	0
57	MG	1A	3353	1/1	0.92	0.15	62,62,62,62	0
57	MG	2a	3020	1/1	0.92	0.14	49,49,49,49	0
57	MG	1B	204	1/1	0.92	0.33	60,60,60,60	0
57	MG	2a	3022	1/1	0.92	0.13	58,58,58,58	0
57	MG	1A	3388	1/1	0.92	0.14	29,29,29,29	0
57	MG	1A	3926	1/1	0.92	0.14	69,69,69,69	0
57	MG	2A	3632	1/1	0.92	0.15	48,48,48,48	0
57	MG	1A	3840	1/1	0.92	0.07	51,51,51,51	0
57	MG	2a	3028	1/1	0.92	0.13	57,57,57,57	0
57	MG	1A	3519	1/1	0.92	0.19	24,24,24,24	0
57	MG	1A	3522	1/1	0.92	0.13	62,62,62,62	0
57	MG	2A	3638	1/1	0.92	0.17	58,58,58,58	0
57	MG	1a	1859	1/1	0.92	0.27	71,71,71,71	0
57	MG	1a	1724	1/1	0.92	0.12	63,63,63,63	0
57	MG	2A	3645	1/1	0.92	0.13	34,34,34,34	0
57	MG	1A	3694	1/1	0.92	0.23	50,50,50,50	0
57	MG	1A	3356	1/1	0.92	0.19	33,33,33,33	0
57	MG	2a	3040	1/1	0.92	0.13	72,72,72,72	0
57	MG	2A	3269	1/1	0.92	0.22	45,45,45,45	0
57	MG	1A	3937	1/1	0.92	0.13	26,26,26,26	0
57	MG	2A	3458	1/1	0.92	0.23	64,64,64,64	0
57	MG	1A	3766	1/1	0.92	0.14	38,38,38,38	0
57	MG	2A	3119	1/1	0.92	0.11	36,36,36,36	0
57	MG	1a	1617	1/1	0.92	0.10	67,67,67,67	0
57	MG	1A	3771	1/1	0.92	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3626	1/1	0.92	0.18	23,23,23,23	0
57	MG	1A	3470	1/1	0.92	0.17	33,33,33,33	0
57	MG	1A	3358	1/1	0.92	0.19	32,32,32,32	0
57	MG	2A	3470	1/1	0.92	0.08	56,56,56,56	0
57	MG	1a	1623	1/1	0.92	0.11	54,54,54,54	0
57	MG	1B	228	1/1	0.92	0.09	58,58,58,58	0
57	MG	2A	3666	1/1	0.92	0.09	32,32,32,32	0
57	MG	2A	3473	1/1	0.92	0.10	71,71,71,71	0
57	MG	2A	3285	1/1	0.92	0.24	53,53,53,53	0
57	MG	1a	1625	1/1	0.92	0.13	58,58,58,58	0
57	MG	1A	3473	1/1	0.92	0.21	63,63,63,63	0
57	MG	1a	1749	1/1	0.92	0.12	54,54,54,54	0
57	MG	2A	3292	1/1	0.92	0.29	76,76,76,76	0
57	MG	2A	3484	1/1	0.92	0.17	35,35,35,35	0
57	MG	1A	3474	1/1	0.92	0.21	28,28,28,28	0
57	MG	1A	3779	1/1	0.92	0.10	55,55,55,55	0
57	MG	1A	3578	1/1	0.92	0.14	52,52,52,52	0
57	MG	2A	3679	1/1	0.92	0.08	77,77,77,77	0
57	MG	1A	3638	1/1	0.92	0.26	62,62,62,62	0
57	MG	1a	1634	1/1	0.92	0.10	49,49,49,49	0
57	MG	2A	3300	1/1	0.92	0.26	66,66,66,66	0
57	MG	2A	3496	1/1	0.92	0.12	56,56,56,56	0
57	MG	1E	306	1/1	0.92	0.19	25,25,25,25	0
57	MG	2A	3690	1/1	0.92	0.12	46,46,46,46	0
57	MG	1A	3005	1/1	0.92	0.22	23,23,23,23	0
57	MG	2A	3504	1/1	0.92	0.12	55,55,55,55	0
57	MG	2A	3151	1/1	0.92	0.13	43,43,43,43	0
57	MG	1A	3290	1/1	0.92	0.20	61,61,61,61	0
57	MG	1A	3584	1/1	0.92	0.17	47,47,47,47	0
57	MG	1A	3587	1/1	0.92	0.18	23,23,23,23	0
57	MG	1A	3960	1/1	0.92	0.14	30,30,30,30	0
57	MG	1a	1764	1/1	0.92	0.07	70,70,70,70	0
57	MG	2a	3091	1/1	0.92	0.17	69,69,69,69	0
57	MG	1A	3588	1/1	0.92	0.11	49,49,49,49	0
57	MG	1a	1766	1/1	0.92	0.14	71,71,71,71	0
57	MG	1A	3070	1/1	0.92	0.12	38,38,38,38	0
57	MG	1A	3964	1/1	0.92	0.10	58,58,58,58	0
57	MG	1A	3439	1/1	0.92	0.09	55,55,55,55	0
57	MG	1A	3325	1/1	0.92	0.15	37,37,37,37	0
57	MG	2A	3008	1/1	0.92	0.20	41,41,41,41	0
57	MG	2A	3716	1/1	0.92	0.13	66,66,66,66	0
57	MG	2a	3110	1/1	0.92	0.13	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3655	1/1	0.92	0.18	16,16,16,16	0
57	MG	2A	3528	1/1	0.92	0.08	63,63,63,63	0
57	MG	1A	3250	1/1	0.92	0.16	48,48,48,48	0
57	MG	1A	3238	1/1	0.92	0.29	44,44,44,44	0
57	MG	2A	3342	1/1	0.92	0.24	42,42,42,42	0
57	MG	1A	3973	1/1	0.92	0.34	52,52,52,52	0
57	MG	1A	3594	1/1	0.92	0.11	42,42,42,42	0
57	MG	1a	1779	1/1	0.92	0.13	50,50,50,50	0
57	MG	1A	3882	1/1	0.92	0.12	59,59,59,59	0
57	MG	2A	3027	1/1	0.92	0.11	36,36,36,36	0
57	MG	1A	3885	1/1	0.92	0.14	42,42,42,42	0
57	MG	1A	3277	1/1	0.92	0.18	49,49,49,49	0
57	MG	2B	204	1/1	0.92	0.13	75,75,75,75	0
57	MG	2A	3359	1/1	0.92	0.18	34,34,34,34	0
57	MG	1a	1785	1/1	0.92	0.10	75,75,75,75	0
57	MG	1A	3240	1/1	0.92	0.10	50,50,50,50	0
57	MG	1A	3333	1/1	0.92	0.26	51,51,51,51	0
57	MG	1A	3600	1/1	0.92	0.28	31,31,31,31	0
57	MG	2A	3189	1/1	0.92	0.15	48,48,48,48	0
57	MG	2A	3548	1/1	0.92	0.12	73,73,73,73	0
57	MG	1A	3892	1/1	0.92	0.21	28,28,28,28	0
57	MG	1A	3601	1/1	0.92	0.35	35,35,35,35	0
57	MG	1A	3303	1/1	0.92	0.20	49,49,49,49	0
57	MG	1A	3898	1/1	0.92	0.27	57,57,57,57	0
57	MG	2A	3195	1/1	0.92	0.16	51,51,51,51	0
57	MG	1T	206	1/1	0.92	0.12	71,71,71,71	0
57	MG	2D	309	1/1	0.92	0.15	35,35,35,35	0
57	MG	1A	3989	1/1	0.92	0.15	54,54,54,54	0
57	MG	1A	3990	1/1	0.92	0.10	38,38,38,38	0
57	MG	2A	3200	1/1	0.92	0.14	48,48,48,48	0
57	MG	1A	3991	1/1	0.92	0.09	57,57,57,57	0
57	MG	1V	207	1/1	0.92	0.14	59,59,59,59	0
57	MG	1A	3603	1/1	0.92	0.20	59,59,59,59	0
57	MG	1A	3902	1/1	0.92	0.08	46,46,46,46	0
57	MG	1A	3903	1/1	0.92	0.31	41,41,41,41	0
57	MG	2A	3570	1/1	0.92	0.12	56,56,56,56	0
57	MG	1a	1682	1/1	0.92	0.13	68,68,68,68	0
57	MG	1A	3414	1/1	0.92	0.16	37,37,37,37	0
57	MG	2a	3166	1/1	0.92	0.08	70,70,70,70	0
57	MG	1A	3609	1/1	0.92	0.29	32,32,32,32	0
57	MG	1A	3997	1/1	0.92	0.67	42,42,42,42	0
57	MG	2A	3214	1/1	0.92	0.18	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	10	103	1/1	0.92	0.17	47,47,47,47	0
57	MG	1A	3343	1/1	0.92	0.17	30,30,30,30	0
57	MG	1A	3047	1/1	0.92	0.20	41,41,41,41	0
57	MG	1A	4000	1/1	0.92	0.18	42,42,42,42	0
57	MG	1A	3280	1/1	0.92	0.27	80,80,80,80	0
57	MG	1a	1824	1/1	0.92	0.28	76,76,76,76	0
57	MG	2A	3412	1/1	0.92	0.16	48,48,48,48	0
57	MG	1A	3029	1/1	0.92	0.13	41,41,41,41	0
57	MG	1A	3680	1/1	0.92	0.17	37,37,37,37	0
57	MG	1A	3834	1/1	0.92	0.15	49,49,49,49	0
57	MG	2A	3595	1/1	0.92	0.08	70,70,70,70	0
57	MG	1A	4007	1/1	0.92	0.11	48,48,48,48	0
57	MG	2A	3418	1/1	0.92	0.23	56,56,56,56	0
57	MG	15	101	1/1	0.92	0.18	41,41,41,41	0
57	MG	2a	3001	1/1	0.92	0.19	46,46,46,46	0
57	MG	1A	4008	1/1	0.92	0.17	68,68,68,68	0
58	MPD	18	104	8/8	0.92	0.25	32,40,42,51	0
57	MG	15	104	1/1	0.92	0.20	38,38,38,38	0
57	MG	1A	4009	1/1	0.92	0.24	68,68,68,68	0
57	MG	1A	3512	1/1	0.92	0.19	24,24,24,24	0
57	MG	1A	3264	1/1	0.92	0.32	45,45,45,45	0
57	MG	18	101	1/1	0.92	0.11	42,42,42,42	0
60	ZN	14	501	1/1	0.92	0.07	105,105,105,105	0
57	MG	2A	3608	1/1	0.92	0.15	36,36,36,36	0
57	MG	1a	1840	1/1	0.92	0.17	76,76,76,76	0
57	MG	1A	3768	1/1	0.93	0.16	50,50,50,50	0
57	MG	2A	3656	1/1	0.93	0.11	52,52,52,52	0
57	MG	1A	3478	1/1	0.93	0.17	28,28,28,28	0
57	MG	1A	3585	1/1	0.93	0.15	72,72,72,72	0
57	MG	1A	3932	1/1	0.93	0.19	44,44,44,44	0
57	MG	2A	3330	1/1	0.93	0.13	42,42,42,42	0
57	MG	1A	3242	1/1	0.93	0.40	47,47,47,47	0
57	MG	2a	3036	1/1	0.93	0.18	67,67,67,67	0
57	MG	2A	3499	1/1	0.93	0.10	78,78,78,78	0
57	MG	1A	3639	1/1	0.93	0.29	39,39,39,39	0
57	MG	1A	3393	1/1	0.93	0.20	26,26,26,26	0
57	MG	1a	1741	1/1	0.93	0.15	67,67,67,67	0
57	MG	2a	3042	1/1	0.93	0.11	78,78,78,78	0
57	MG	2A	3341	1/1	0.93	0.21	59,59,59,59	0
57	MG	2A	3066	1/1	0.93	0.16	44,44,44,44	0
57	MG	1A	3099	1/1	0.93	0.19	47,47,47,47	0
57	MG	1A	3484	1/1	0.93	0.23	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	3855	1/1	0.93	0.09	36,36,36,36	0
57	MG	1a	1850	1/1	0.93	0.11	70,70,70,70	0
57	MG	1a	1747	1/1	0.93	0.10	66,66,66,66	0
57	MG	2A	3353	1/1	0.93	0.21	47,47,47,47	0
57	MG	2A	3515	1/1	0.93	0.17	56,56,56,56	0
57	MG	2A	3354	1/1	0.93	0.16	39,39,39,39	0
57	MG	2a	3053	1/1	0.93	0.11	67,67,67,67	0
57	MG	1A	3702	1/1	0.93	0.13	48,48,48,48	0
57	MG	2A	3356	1/1	0.93	0.09	49,49,49,49	0
57	MG	2A	3203	1/1	0.93	0.18	63,63,63,63	0
57	MG	2A	3358	1/1	0.93	0.23	35,35,35,35	0
57	MG	1a	1654	1/1	0.93	0.14	41,41,41,41	0
57	MG	1A	3543	1/1	0.93	0.20	52,52,52,52	0
57	MG	1A	3121	1/1	0.93	0.30	62,62,62,62	0
57	MG	1A	3489	1/1	0.93	0.17	38,38,38,38	0
57	MG	1A	3443	1/1	0.93	0.15	24,24,24,24	0
57	MG	1A	3864	1/1	0.93	0.20	34,34,34,34	0
57	MG	1a	1663	1/1	0.93	0.28	61,61,61,61	0
57	MG	2A	3534	1/1	0.93	0.12	57,57,57,57	0
57	MG	1a	1862	1/1	0.93	0.14	67,67,67,67	0
57	MG	1A	3321	1/1	0.93	0.39	70,70,70,70	0
57	MG	2A	3537	1/1	0.93	0.18	37,37,37,37	0
57	MG	1A	3654	1/1	0.93	0.16	59,59,59,59	0
57	MG	2A	3376	1/1	0.93	0.14	40,40,40,40	0
57	MG	1a	1865	1/1	0.93	0.24	59,59,59,59	0
57	MG	11	101	1/1	0.93	0.31	44,44,44,44	0
57	MG	1A	3790	1/1	0.93	0.23	33,33,33,33	0
57	MG	1A	3039	1/1	0.93	0.21	41,41,41,41	0
57	MG	2A	3102	1/1	0.93	0.15	33,33,33,33	0
57	MG	1A	3125	1/1	0.93	0.20	31,31,31,31	0
57	MG	1A	3796	1/1	0.93	0.14	56,56,56,56	0
57	MG	1A	3286	1/1	0.93	0.16	50,50,50,50	0
57	MG	1A	3553	1/1	0.93	0.17	41,41,41,41	0
57	MG	1A	3801	1/1	0.93	0.17	30,30,30,30	0
57	MG	2a	3088	1/1	0.93	0.14	74,74,74,74	0
57	MG	1A	3126	1/1	0.93	0.26	43,43,43,43	0
57	MG	2A	3725	1/1	0.93	0.10	56,56,56,56	0
57	MG	1A	3717	1/1	0.93	0.07	52,52,52,52	0
57	MG	2a	3092	1/1	0.93	0.18	60,60,60,60	0
57	MG	2A	3232	1/1	0.93	0.14	69,69,69,69	0
57	MG	17	104	1/1	0.93	0.22	53,53,53,53	0
57	MG	1B	230	1/1	0.93	0.07	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	3097	1/1	0.93	0.24	60,60,60,60	0
57	MG	1a	1681	1/1	0.93	0.19	72,72,72,72	0
57	MG	17	106	1/1	0.93	0.12	58,58,58,58	0
57	MG	2a	3101	1/1	0.93	0.21	61,61,61,61	0
57	MG	2A	3561	1/1	0.93	0.16	63,63,63,63	0
57	MG	2B	203	1/1	0.93	0.10	77,77,77,77	0
57	MG	1A	3660	1/1	0.93	0.44	36,36,36,36	0
57	MG	2a	3108	1/1	0.93	0.12	52,52,52,52	0
57	MG	1D	309	1/1	0.93	0.45	47,47,47,47	0
57	MG	1n	101	1/1	0.93	0.21	78,78,78,78	0
57	MG	1A	3661	1/1	0.93	0.09	64,64,64,64	0
57	MG	1A	3503	1/1	0.93	0.10	49,49,49,49	0
57	MG	1a	1687	1/1	0.93	0.17	45,45,45,45	0
57	MG	2a	3115	1/1	0.93	0.12	66,66,66,66	0
57	MG	1o	103	1/1	0.93	0.08	61,61,61,61	0
57	MG	2A	3126	1/1	0.93	0.26	49,49,49,49	0
57	MG	2B	215	1/1	0.93	0.15	68,68,68,68	0
57	MG	1A	3289	1/1	0.93	0.19	42,42,42,42	0
57	MG	1A	3891	1/1	0.93	0.12	20,20,20,20	0
57	MG	1a	1790	1/1	0.93	0.11	74,74,74,74	0
57	MG	1A	3665	1/1	0.93	0.23	49,49,49,49	0
57	MG	2A	3260	1/1	0.93	0.19	32,32,32,32	0
57	MG	2A	3133	1/1	0.93	0.21	65,65,65,65	0
57	MG	2a	3129	1/1	0.93	0.21	69,69,69,69	0
57	MG	2a	3130	1/1	0.93	0.22	73,73,73,73	0
57	MG	2D	308	1/1	0.93	0.28	69,69,69,69	0
57	MG	2A	3263	1/1	0.93	0.26	64,64,64,64	0
57	MG	1A	3054	1/1	0.93	0.21	44,44,44,44	0
57	MG	1A	3192	1/1	0.93	0.18	48,48,48,48	0
57	MG	1A	3108	1/1	0.93	0.19	44,44,44,44	0
57	MG	1A	3233	1/1	0.93	0.28	66,66,66,66	0
57	MG	1A	3564	1/1	0.93	0.31	45,45,45,45	0
57	MG	1A	3174	1/1	0.93	0.26	62,62,62,62	0
57	MG	1F	315	1/1	0.93	0.23	60,60,60,60	0
57	MG	1A	3109	1/1	0.93	0.36	44,44,44,44	0
57	MG	2A	3010	1/1	0.93	0.13	65,65,65,65	0
57	MG	2a	3145	1/1	0.93	0.13	52,52,52,52	0
57	MG	2A	3150	1/1	0.93	0.33	63,63,63,63	0
57	MG	1a	1616	1/1	0.93	0.13	65,65,65,65	0
57	MG	2A	3601	1/1	0.93	0.11	42,42,42,42	0
57	MG	2A	3279	1/1	0.93	0.28	53,53,53,53	0
57	MG	1A	3081	1/1	0.93	0.58	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3447	1/1	0.93	0.16	62,62,62,62	0
57	MG	1A	3382	1/1	0.93	0.17	61,61,61,61	0
57	MG	2A	3282	1/1	0.93	0.37	58,58,58,58	0
57	MG	1A	3988	1/1	0.93	0.17	53,53,53,53	0
57	MG	1a	1810	1/1	0.93	0.14	72,72,72,72	0
57	MG	1A	3307	1/1	0.93	0.33	45,45,45,45	0
57	MG	1A	3620	1/1	0.93	0.20	54,54,54,54	0
57	MG	2W	202	1/1	0.93	0.39	56,56,56,56	0
57	MG	2A	3615	1/1	0.93	0.16	59,59,59,59	0
57	MG	2A	3616	1/1	0.93	0.20	64,64,64,64	0
57	MG	1A	3681	1/1	0.93	0.07	49,49,49,49	0
57	MG	1N	202	1/1	0.93	0.20	45,45,45,45	0
57	MG	1a	1818	1/1	0.93	0.10	68,68,68,68	0
57	MG	1A	3427	1/1	0.93	0.15	34,34,34,34	0
57	MG	2A	3621	1/1	0.93	0.22	60,60,60,60	0
57	MG	2A	3624	1/1	0.93	0.17	71,71,71,71	0
57	MG	1A	3429	1/1	0.93	0.11	44,44,44,44	0
57	MG	2a	3175	1/1	0.93	0.11	65,65,65,65	0
57	MG	1A	3916	1/1	0.93	0.11	31,31,31,31	0
57	MG	1A	3351	1/1	0.93	0.13	31,31,31,31	0
57	MG	2A	3630	1/1	0.93	0.09	57,57,57,57	0
57	MG	1a	1717	1/1	0.93	0.10	81,81,81,81	0
57	MG	2A	3170	1/1	0.93	0.14	52,52,52,52	0
57	MG	2A	3633	1/1	0.93	0.14	56,56,56,56	0
57	MG	2A	3302	1/1	0.93	0.27	46,46,46,46	0
57	MG	1R	203	1/1	0.93	0.55	47,47,47,47	0
57	MG	1A	3387	1/1	0.93	0.19	24,24,24,24	0
57	MG	1A	3629	1/1	0.93	0.11	56,56,56,56	0
57	MG	1A	3581	1/1	0.93	0.14	47,47,47,47	0
57	MG	2A	3310	1/1	0.93	0.09	64,64,64,64	0
57	MG	1A	3111	1/1	0.93	0.27	36,36,36,36	0
57	MG	2A	3477	1/1	0.93	0.11	64,64,64,64	0
57	MG	1a	1831	1/1	0.93	0.11	80,80,80,80	0
57	MG	1A	3693	1/1	0.93	0.30	56,56,56,56	0
57	MG	2A	3181	1/1	0.93	0.28	46,46,46,46	0
57	MG	2A	3650	1/1	0.93	0.12	45,45,45,45	0
57	MG	2A	3651	1/1	0.93	0.15	76,76,76,76	0
57	MG	1A	3046	1/1	0.93	0.33	51,51,51,51	0
57	MG	2A	3322	1/1	0.93	0.20	75,75,75,75	0
57	MG	1A	3079	1/1	0.94	0.21	37,37,37,37	0
57	MG	1A	3097	1/1	0.94	0.40	42,42,42,42	0
57	MG	1A	3266	1/1	0.94	0.19	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	3215	1/1	0.94	0.37	38,38,38,38	0
57	MG	2A	3137	1/1	0.94	0.29	45,45,45,45	0
57	MG	1a	1728	1/1	0.94	0.12	77,77,77,77	0
57	MG	1b	301	1/1	0.94	0.22	78,78,78,78	0
57	MG	1d	301	1/1	0.94	0.15	73,73,73,73	0
57	MG	2U	202	1/1	0.94	0.07	84,84,84,84	0
57	MG	2A	3141	1/1	0.94	0.17	37,37,37,37	0
57	MG	1a	1730	1/1	0.94	0.15	32,32,32,32	0
57	MG	2V	203	1/1	0.94	0.24	72,72,72,72	0
57	MG	1A	3720	1/1	0.94	0.15	60,60,60,60	0
57	MG	1A	3216	1/1	0.94	0.15	52,52,52,52	0
57	MG	2Y	201	1/1	0.94	0.26	64,64,64,64	0
57	MG	2A	3149	1/1	0.94	0.11	51,51,51,51	0
57	MG	1B	219	1/1	0.94	0.21	66,66,66,66	0
57	MG	1a	1613	1/1	0.94	0.19	29,29,29,29	0
57	MG	1A	3931	1/1	0.94	0.18	48,48,48,48	0
57	MG	25	102	1/1	0.94	0.18	70,70,70,70	0
57	MG	1A	3647	1/1	0.94	0.33	49,49,49,49	0
57	MG	1f	201	1/1	0.94	0.33	72,72,72,72	0
57	MG	1A	3724	1/1	0.94	0.17	57,57,57,57	0
57	MG	2A	3156	1/1	0.94	0.19	66,66,66,66	0
57	MG	1A	3271	1/1	0.94	0.13	39,39,39,39	0
57	MG	1A	3441	1/1	0.94	0.10	53,53,53,53	0
57	MG	1A	3731	1/1	0.94	0.29	55,55,55,55	0
57	MG	1D	306	1/1	0.94	0.17	22,22,22,22	0
57	MG	1D	307	1/1	0.94	0.20	39,39,39,39	0
57	MG	1D	308	1/1	0.94	0.31	38,38,38,38	0
57	MG	1m	201	1/1	0.94	0.08	67,67,67,67	0
57	MG	2A	3578	1/1	0.94	0.09	52,52,52,52	0
57	MG	1A	3940	1/1	0.94	0.25	57,57,57,57	0
57	MG	1A	3941	1/1	0.94	0.20	58,58,58,58	0
57	MG	2A	3168	1/1	0.94	0.17	51,51,51,51	0
57	MG	1A	3051	1/1	0.94	0.41	32,32,32,32	0
57	MG	2A	3365	1/1	0.94	0.18	37,37,37,37	0
57	MG	2A	3366	1/1	0.94	0.21	64,64,64,64	0
57	MG	1D	316	1/1	0.94	0.11	57,57,57,57	0
57	MG	2A	3588	1/1	0.94	0.17	50,50,50,50	0
57	MG	1A	3734	1/1	0.94	0.17	22,22,22,22	0
57	MG	1A	3736	1/1	0.94	0.14	50,50,50,50	0
57	MG	2A	3592	1/1	0.94	0.15	34,34,34,34	0
57	MG	1a	1757	1/1	0.94	0.24	55,55,55,55	0
57	MG	2A	3174	1/1	0.94	0.17	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	3385	1/1	0.94	0.14	32,32,32,32	0
57	MG	2a	3027	1/1	0.94	0.11	73,73,73,73	0
57	MG	2A	3597	1/1	0.94	0.15	37,37,37,37	0
57	MG	1A	3946	1/1	0.94	0.19	65,65,65,65	0
57	MG	2A	3377	1/1	0.94	0.08	72,72,72,72	0
57	MG	2A	3378	1/1	0.94	0.11	40,40,40,40	0
57	MG	1A	3513	1/1	0.94	0.18	37,37,37,37	0
57	MG	1x	102	1/1	0.94	0.17	32,32,32,32	0
57	MG	1F	307	1/1	0.94	0.21	37,37,37,37	0
57	MG	2A	3382	1/1	0.94	0.10	40,40,40,40	0
57	MG	2A	3383	1/1	0.94	0.18	34,34,34,34	0
57	MG	1a	1638	1/1	0.94	0.23	67,67,67,67	0
57	MG	2A	3385	1/1	0.94	0.11	78,78,78,78	0
57	MG	1A	3221	1/1	0.94	0.28	38,38,38,38	0
57	MG	1A	3586	1/1	0.94	0.23	56,56,56,56	0
57	MG	2A	3613	1/1	0.94	0.16	60,60,60,60	0
57	MG	1A	3445	1/1	0.94	0.14	51,51,51,51	0
57	MG	2A	3186	1/1	0.94	0.28	74,74,74,74	0
57	MG	2A	3187	1/1	0.94	0.27	53,53,53,53	0
57	MG	1A	3845	1/1	0.94	0.18	30,30,30,30	0
57	MG	1A	3034	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3329	1/1	0.94	0.23	30,30,30,30	0
57	MG	2A	3011	1/1	0.94	0.16	33,33,33,33	0
57	MG	2A	3192	1/1	0.94	0.13	66,66,66,66	0
57	MG	1A	3182	1/1	0.94	0.11	51,51,51,51	0
57	MG	1A	3523	1/1	0.94	0.10	44,44,44,44	0
57	MG	1A	3524	1/1	0.94	0.14	31,31,31,31	0
57	MG	1A	3390	1/1	0.94	0.20	40,40,40,40	0
57	MG	2A	3197	1/1	0.94	0.18	53,53,53,53	0
57	MG	1A	3332	1/1	0.94	0.19	26,26,26,26	0
57	MG	1A	3131	1/1	0.94	0.51	32,32,32,32	0
57	MG	1A	3965	1/1	0.94	0.18	56,56,56,56	0
57	MG	1a	1656	1/1	0.94	0.19	58,58,58,58	0
57	MG	2A	3202	1/1	0.94	0.14	65,65,65,65	0
57	MG	1A	3669	1/1	0.94	0.09	61,61,61,61	0
57	MG	1A	3230	1/1	0.94	0.25	37,37,37,37	0
57	MG	1A	3598	1/1	0.94	0.16	56,56,56,56	0
57	MG	1A	3858	1/1	0.94	0.10	45,45,45,45	0
57	MG	2A	3420	1/1	0.94	0.17	55,55,55,55	0
57	MG	2A	3422	1/1	0.94	0.10	78,78,78,78	0
57	MG	2a	3070	1/1	0.94	0.24	62,62,62,62	0
57	MG	1Q	205	1/1	0.94	0.23	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1789	1/1	0.94	0.08	78,78,78,78	0
57	MG	1A	3396	1/1	0.94	0.11	41,41,41,41	0
57	MG	1a	1664	1/1	0.94	0.21	68,68,68,68	0
57	MG	1A	3134	1/1	0.94	0.18	49,49,49,49	0
57	MG	2A	3212	1/1	0.94	0.24	66,66,66,66	0
57	MG	2A	3213	1/1	0.94	0.15	53,53,53,53	0
57	MG	2A	3654	1/1	0.94	0.13	69,69,69,69	0
57	MG	1A	3082	1/1	0.94	0.60	48,48,48,48	0
57	MG	2A	3215	1/1	0.94	0.18	52,52,52,52	0
57	MG	1A	3462	1/1	0.94	0.15	57,57,57,57	0
57	MG	2A	3217	1/1	0.94	0.14	69,69,69,69	0
57	MG	1A	3976	1/1	0.94	0.17	59,59,59,59	0
57	MG	1A	3142	1/1	0.94	0.18	53,53,53,53	0
57	MG	1A	3678	1/1	0.94	0.12	29,29,29,29	0
57	MG	1a	1672	1/1	0.94	0.07	69,69,69,69	0
57	MG	1T	203	1/1	0.94	0.20	58,58,58,58	0
57	MG	2A	3055	1/1	0.94	0.19	47,47,47,47	0
57	MG	1A	3679	1/1	0.94	0.05	38,38,38,38	0
57	MG	2A	3667	1/1	0.94	0.22	54,54,54,54	0
57	MG	1A	3774	1/1	0.94	0.12	42,42,42,42	0
57	MG	2A	3227	1/1	0.94	0.62	51,51,51,51	0
57	MG	2A	3450	1/1	0.94	0.15	45,45,45,45	0
57	MG	1A	3347	1/1	0.94	0.27	52,52,52,52	0
57	MG	1a	1806	1/1	0.94	0.29	82,82,82,82	0
57	MG	1A	3407	1/1	0.94	0.13	27,27,27,27	0
57	MG	1A	3542	1/1	0.94	0.14	36,36,36,36	0
57	MG	1a	1811	1/1	0.94	0.21	70,70,70,70	0
57	MG	1V	205	1/1	0.94	0.13	55,55,55,55	0
57	MG	1a	1813	1/1	0.94	0.11	70,70,70,70	0
57	MG	2A	3459	1/1	0.94	0.23	43,43,43,43	0
57	MG	2A	3681	1/1	0.94	0.12	70,70,70,70	0
57	MG	1A	3144	1/1	0.94	0.28	69,69,69,69	0
57	MG	2A	3241	1/1	0.94	0.34	54,54,54,54	0
57	MG	2a	3117	1/1	0.94	0.18	69,69,69,69	0
57	MG	2A	3071	1/1	0.94	0.36	50,50,50,50	0
57	MG	2A	3243	1/1	0.94	0.36	47,47,47,47	0
57	MG	2A	3686	1/1	0.94	0.13	43,43,43,43	0
57	MG	2A	3466	1/1	0.94	0.12	71,71,71,71	0
57	MG	1A	3612	1/1	0.94	0.13	33,33,33,33	0
57	MG	1A	3780	1/1	0.94	0.10	30,30,30,30	0
57	MG	2A	3692	1/1	0.94	0.20	39,39,39,39	0
57	MG	2A	3693	1/1	0.94	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3694	1/1	0.94	0.28	65,65,65,65	0
57	MG	2A	3696	1/1	0.94	0.22	70,70,70,70	0
57	MG	1A	3189	1/1	0.94	0.16	42,42,42,42	0
57	MG	1A	3782	1/1	0.94	0.13	26,26,26,26	0
57	MG	2A	3248	1/1	0.94	0.14	55,55,55,55	0
57	MG	2a	3133	1/1	0.94	0.14	66,66,66,66	0
57	MG	1A	3105	1/1	0.94	0.13	68,68,68,68	0
57	MG	2A	3077	1/1	0.94	0.12	52,52,52,52	0
57	MG	2A	3079	1/1	0.94	0.29	44,44,44,44	0
57	MG	2A	3080	1/1	0.94	0.70	50,50,50,50	0
57	MG	1A	3015	1/1	0.94	0.18	32,32,32,32	0
57	MG	1A	3065	1/1	0.94	0.17	43,43,43,43	0
57	MG	1A	3067	1/1	0.94	0.42	33,33,33,33	0
57	MG	1A	3042	1/1	0.94	0.22	18,18,18,18	0
57	MG	2a	3143	1/1	0.94	0.14	53,53,53,53	0
57	MG	2A	3087	1/1	0.94	0.23	52,52,52,52	0
57	MG	1a	1690	1/1	0.94	0.19	57,57,57,57	0
57	MG	1A	3116	1/1	0.94	0.23	23,23,23,23	0
57	MG	2A	3487	1/1	0.94	0.14	52,52,52,52	0
57	MG	2A	3091	1/1	0.94	0.15	53,53,53,53	0
57	MG	1a	1828	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3418	1/1	0.94	0.25	28,28,28,28	0
57	MG	2A	3494	1/1	0.94	0.16	57,57,57,57	0
57	MG	1A	3895	1/1	0.94	0.18	31,31,31,31	0
57	MG	2a	3157	1/1	0.94	0.11	73,73,73,73	0
57	MG	1a	1694	1/1	0.94	0.25	67,67,67,67	0
57	MG	1A	3896	1/1	0.94	0.12	32,32,32,32	0
57	MG	1A	3071	1/1	0.94	0.61	54,54,54,54	0
57	MG	2A	3098	1/1	0.94	0.21	72,72,72,72	0
57	MG	1A	3481	1/1	0.94	0.22	47,47,47,47	0
57	MG	2A	3100	1/1	0.94	0.15	71,71,71,71	0
57	MG	1A	3073	1/1	0.94	0.30	51,51,51,51	0
57	MG	2a	3165	1/1	0.94	0.12	67,67,67,67	0
57	MG	1A	3797	1/1	0.94	0.08	60,60,60,60	0
57	MG	1A	3422	1/1	0.94	0.29	31,31,31,31	0
57	MG	1A	3627	1/1	0.94	0.12	71,71,71,71	0
57	MG	1A	3559	1/1	0.94	0.14	63,63,63,63	0
57	MG	1A	3312	1/1	0.94	0.19	64,64,64,64	0
57	MG	1a	1842	1/1	0.94	0.07	88,88,88,88	0
57	MG	15	106	1/1	0.94	0.09	52,52,52,52	0
57	MG	1A	3631	1/1	0.94	0.23	49,49,49,49	0
57	MG	2A	3112	1/1	0.94	0.19	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3520	1/1	0.94	0.10	44,44,44,44	0
57	MG	2a	3177	1/1	0.94	0.27	61,61,61,61	0
57	MG	2A	3291	1/1	0.94	0.34	65,65,65,65	0
57	MG	2a	3181	1/1	0.94	0.19	70,70,70,70	0
57	MG	2A	3522	1/1	0.94	0.20	71,71,71,71	0
57	MG	1A	3561	1/1	0.94	0.12	53,53,53,53	0
57	MG	1a	1847	1/1	0.94	0.10	55,55,55,55	0
57	MG	1a	1708	1/1	0.94	0.15	70,70,70,70	0
57	MG	1A	3807	1/1	0.94	0.18	48,48,48,48	0
57	MG	1A	3486	1/1	0.94	0.14	57,57,57,57	0
57	MG	1A	3915	1/1	0.94	0.25	55,55,55,55	0
57	MG	1A	3254	1/1	0.94	0.32	36,36,36,36	0
57	MG	1A	3316	1/1	0.94	0.19	60,60,60,60	0
57	MG	1a	1856	1/1	0.94	0.11	61,61,61,61	0
57	MG	19	101	1/1	0.94	0.14	62,62,62,62	0
57	MG	1A	3032	1/1	0.94	0.15	62,62,62,62	0
57	MG	1A	3920	1/1	0.94	0.10	47,47,47,47	0
57	MG	2A	3307	1/1	0.94	0.08	65,65,65,65	0
57	MG	2A	3538	1/1	0.94	0.09	57,57,57,57	0
57	MG	2A	3308	1/1	0.94	0.11	64,64,64,64	0
57	MG	1A	3078	1/1	0.94	0.45	44,44,44,44	0
57	MG	1a	1720	1/1	0.94	0.19	50,50,50,50	0
57	MG	1A	3496	1/1	0.94	0.18	27,27,27,27	0
57	MG	2A	3078	1/1	0.95	0.21	63,63,63,63	0
57	MG	1A	3917	1/1	0.95	0.05	50,50,50,50	0
57	MG	1A	3727	1/1	0.95	0.13	55,55,55,55	0
57	MG	2A	3081	1/1	0.95	0.14	43,43,43,43	0
57	MG	1A	3521	1/1	0.95	0.22	23,23,23,23	0
57	MG	1a	1832	1/1	0.95	0.13	70,70,70,70	0
57	MG	1A	3335	1/1	0.95	0.20	26,26,26,26	0
57	MG	1a	1704	1/1	0.95	0.33	66,66,66,66	0
57	MG	1A	3921	1/1	0.95	0.14	62,62,62,62	0
57	MG	1A	3113	1/1	0.95	0.20	43,43,43,43	0
57	MG	2A	3237	1/1	0.95	0.30	46,46,46,46	0
57	MG	2A	3089	1/1	0.95	0.13	76,76,76,76	0
57	MG	2A	3429	1/1	0.95	0.20	69,69,69,69	0
57	MG	1A	3341	1/1	0.95	0.12	55,55,55,55	0
57	MG	1A	3342	1/1	0.95	0.19	35,35,35,35	0
57	MG	1A	3735	1/1	0.95	0.20	46,46,46,46	0
57	MG	1A	3253	1/1	0.95	0.13	55,55,55,55	0
57	MG	1A	3738	1/1	0.95	0.21	52,52,52,52	0
57	MG	1a	1712	1/1	0.95	0.18	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3439	1/1	0.95	0.39	56,56,56,56	0
57	MG	2A	3623	1/1	0.95	0.13	66,66,66,66	0
57	MG	1B	216	1/1	0.95	0.19	44,44,44,44	0
57	MG	1A	3928	1/1	0.95	0.18	22,22,22,22	0
57	MG	1a	1845	1/1	0.95	0.31	77,77,77,77	0
57	MG	1a	1715	1/1	0.95	0.30	63,63,63,63	0
57	MG	1A	3294	1/1	0.95	0.22	41,41,41,41	0
57	MG	1A	3149	1/1	0.95	0.30	44,44,44,44	0
57	MG	1B	220	1/1	0.95	0.15	69,69,69,69	0
57	MG	1a	1851	1/1	0.95	0.13	44,44,44,44	0
57	MG	1a	1606	1/1	0.95	0.19	57,57,57,57	0
57	MG	2a	3032	1/1	0.95	0.13	73,73,73,73	0
57	MG	2A	3635	1/1	0.95	0.18	60,60,60,60	0
57	MG	1A	3346	1/1	0.95	0.14	50,50,50,50	0
57	MG	1A	3297	1/1	0.95	0.24	65,65,65,65	0
57	MG	1B	224	1/1	0.95	0.18	65,65,65,65	0
57	MG	2A	3639	1/1	0.95	0.20	33,33,33,33	0
57	MG	1A	3068	1/1	0.95	0.18	33,33,33,33	0
57	MG	2A	3642	1/1	0.95	0.14	22,22,22,22	0
57	MG	2a	3041	1/1	0.95	0.31	61,61,61,61	0
57	MG	2A	3453	1/1	0.95	0.08	37,37,37,37	0
57	MG	1B	226	1/1	0.95	0.11	47,47,47,47	0
57	MG	1B	227	1/1	0.95	0.18	66,66,66,66	0
57	MG	1A	3299	1/1	0.95	0.52	44,44,44,44	0
57	MG	1a	1729	1/1	0.95	0.12	53,53,53,53	0
57	MG	1a	1614	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3300	1/1	0.95	0.42	54,54,54,54	0
57	MG	1A	3069	1/1	0.95	0.20	35,35,35,35	0
57	MG	2A	3275	1/1	0.95	0.40	58,58,58,58	0
57	MG	1D	302	1/1	0.95	0.40	34,34,34,34	0
57	MG	1a	1736	1/1	0.95	0.13	72,72,72,72	0
57	MG	1D	303	1/1	0.95	0.21	41,41,41,41	0
57	MG	1D	305	1/1	0.95	0.36	44,44,44,44	0
57	MG	1A	3354	1/1	0.95	0.12	34,34,34,34	0
57	MG	1A	3538	1/1	0.95	0.13	26,26,26,26	0
57	MG	1A	3606	1/1	0.95	0.45	42,42,42,42	0
57	MG	1A	3355	1/1	0.95	0.20	25,25,25,25	0
57	MG	1d	304	1/1	0.95	0.10	70,70,70,70	0
57	MG	1a	1744	1/1	0.95	0.13	42,42,42,42	0
57	MG	1A	3118	1/1	0.95	0.19	38,38,38,38	0
57	MG	1A	3188	1/1	0.95	0.22	37,37,37,37	0
57	MG	1A	3265	1/1	0.95	0.28	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	3479	1/1	0.95	0.16	46,46,46,46	0
57	MG	1a	1748	1/1	0.95	0.11	72,72,72,72	0
57	MG	2A	3293	1/1	0.95	0.23	55,55,55,55	0
57	MG	2A	3482	1/1	0.95	0.07	71,71,71,71	0
57	MG	1D	317	1/1	0.95	0.10	45,45,45,45	0
57	MG	1A	3760	1/1	0.95	0.32	50,50,50,50	0
57	MG	1a	1632	1/1	0.95	0.17	63,63,63,63	0
57	MG	2a	3072	1/1	0.95	0.19	64,64,64,64	0
57	MG	1A	3362	1/1	0.95	0.18	14,14,14,14	0
57	MG	2a	3074	1/1	0.95	0.06	75,75,75,75	0
57	MG	1a	1753	1/1	0.95	0.09	67,67,67,67	0
57	MG	2a	3076	1/1	0.95	0.14	69,69,69,69	0
57	MG	2A	3488	1/1	0.95	0.06	74,74,74,74	0
57	MG	2A	3489	1/1	0.95	0.07	73,73,73,73	0
57	MG	2A	3142	1/1	0.95	0.34	49,49,49,49	0
57	MG	1A	3313	1/1	0.95	0.20	60,60,60,60	0
57	MG	2A	3144	1/1	0.95	0.32	45,45,45,45	0
57	MG	2A	3145	1/1	0.95	0.19	47,47,47,47	0
57	MG	1A	3364	1/1	0.95	0.24	27,27,27,27	0
57	MG	1A	3421	1/1	0.95	0.08	67,67,67,67	0
57	MG	2A	3498	1/1	0.95	0.14	67,67,67,67	0
57	MG	1A	3765	1/1	0.95	0.14	43,43,43,43	0
57	MG	2A	3689	1/1	0.95	0.16	63,63,63,63	0
57	MG	1A	3483	1/1	0.95	0.17	29,29,29,29	0
57	MG	2A	3501	1/1	0.95	0.15	60,60,60,60	0
57	MG	1A	3767	1/1	0.95	0.15	32,32,32,32	0
57	MG	1a	1641	1/1	0.95	0.10	69,69,69,69	0
57	MG	1A	3859	1/1	0.95	0.17	40,40,40,40	0
57	MG	1A	3066	1/1	0.95	0.28	41,41,41,41	0
57	MG	2A	3313	1/1	0.95	0.18	66,66,66,66	0
57	MG	1A	3229	1/1	0.95	0.15	40,40,40,40	0
57	MG	2A	3317	1/1	0.95	0.16	59,59,59,59	0
57	MG	2A	3318	1/1	0.95	0.20	38,38,38,38	0
57	MG	1A	3133	1/1	0.95	0.14	51,51,51,51	0
57	MG	1A	3120	1/1	0.95	0.25	55,55,55,55	0
57	MG	1A	3689	1/1	0.95	0.28	50,50,50,50	0
57	MG	2a	3107	1/1	0.95	0.11	80,80,80,80	0
57	MG	1A	3159	1/1	0.95	0.15	35,35,35,35	0
57	MG	2A	3324	1/1	0.95	0.18	55,55,55,55	0
57	MG	2A	3518	1/1	0.95	0.14	30,30,30,30	0
57	MG	1A	3622	1/1	0.95	0.11	52,52,52,52	0
57	MG	1A	3869	1/1	0.95	0.18	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	3870	1/1	0.95	0.17	27,27,27,27	0
57	MG	1A	3692	1/1	0.95	0.23	41,41,41,41	0
57	MG	2a	3116	1/1	0.95	0.11	71,71,71,71	0
57	MG	1A	3972	1/1	0.95	0.15	20,20,20,20	0
57	MG	2A	3718	1/1	0.95	0.26	63,63,63,63	0
57	MG	1N	204	1/1	0.95	0.10	51,51,51,51	0
57	MG	2A	3526	1/1	0.95	0.17	45,45,45,45	0
57	MG	1A	3135	1/1	0.95	0.33	47,47,47,47	0
57	MG	2a	3123	1/1	0.95	0.17	57,57,57,57	0
57	MG	1A	3138	1/1	0.95	0.17	43,43,43,43	0
57	MG	1A	3495	1/1	0.95	0.16	60,60,60,60	0
57	MG	1a	1781	1/1	0.95	0.10	72,72,72,72	0
57	MG	2A	3343	1/1	0.95	0.18	58,58,58,58	0
57	MG	1Q	203	1/1	0.95	0.23	53,53,53,53	0
57	MG	2A	3346	1/1	0.95	0.14	58,58,58,58	0
57	MG	1a	1783	1/1	0.95	0.11	79,79,79,79	0
57	MG	2A	3016	1/1	0.95	0.16	76,76,76,76	0
57	MG	1A	3322	1/1	0.95	0.24	62,62,62,62	0
57	MG	2A	3018	1/1	0.95	0.71	44,44,44,44	0
57	MG	2B	202	1/1	0.95	0.18	75,75,75,75	0
57	MG	2A	3019	1/1	0.95	0.59	48,48,48,48	0
57	MG	2A	3021	1/1	0.95	0.14	35,35,35,35	0
57	MG	2A	3022	1/1	0.95	0.42	44,44,44,44	0
57	MG	2B	206	1/1	0.95	0.13	65,65,65,65	0
57	MG	1A	3878	1/1	0.95	0.15	50,50,50,50	0
57	MG	1A	3169	1/1	0.95	0.09	64,64,64,64	0
57	MG	1A	3499	1/1	0.95	0.23	63,63,63,63	0
57	MG	1A	3884	1/1	0.95	0.18	31,31,31,31	0
57	MG	2A	3029	1/1	0.95	0.19	31,31,31,31	0
57	MG	1A	3566	1/1	0.95	0.20	48,48,48,48	0
57	MG	2a	3146	1/1	0.95	0.17	52,52,52,52	0
57	MG	1A	3378	1/1	0.95	0.25	44,44,44,44	0
57	MG	1A	3052	1/1	0.95	0.42	42,42,42,42	0
57	MG	2A	3034	1/1	0.95	0.49	58,58,58,58	0
57	MG	1A	3635	1/1	0.95	0.35	39,39,39,39	0
57	MG	2a	3152	1/1	0.95	0.10	59,59,59,59	0
57	MG	1A	3889	1/1	0.95	0.10	57,57,57,57	0
57	MG	1A	3502	1/1	0.95	0.09	52,52,52,52	0
57	MG	1A	3791	1/1	0.95	0.31	52,52,52,52	0
57	MG	1T	207	1/1	0.95	0.20	58,58,58,58	0
57	MG	1A	3123	1/1	0.95	0.28	54,54,54,54	0
57	MG	1A	3203	1/1	0.95	0.29	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	2E	301	1/1	0.95	0.34	42,42,42,42	0
57	MG	1A	3795	1/1	0.95	0.08	59,59,59,59	0
57	MG	1A	3282	1/1	0.95	0.06	67,67,67,67	0
57	MG	2E	305	1/1	0.95	0.06	54,54,54,54	0
57	MG	1A	3243	1/1	0.95	0.49	44,44,44,44	0
57	MG	1a	1803	1/1	0.95	0.05	69,69,69,69	0
57	MG	1a	1805	1/1	0.95	0.08	71,71,71,71	0
57	MG	1A	3897	1/1	0.95	0.17	26,26,26,26	0
57	MG	1a	1807	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3384	1/1	0.95	0.17	36,36,36,36	0
57	MG	2A	3056	1/1	0.95	0.16	55,55,55,55	0
57	MG	1A	3577	1/1	0.95	0.24	65,65,65,65	0
57	MG	1A	3143	1/1	0.95	0.17	41,41,41,41	0
57	MG	2a	3173	1/1	0.95	0.25	65,65,65,65	0
57	MG	2Q	201	1/1	0.95	0.13	52,52,52,52	0
57	MG	1A	3072	1/1	0.95	0.12	39,39,39,39	0
57	MG	2A	3577	1/1	0.95	0.27	60,60,60,60	0
57	MG	1A	3904	1/1	0.95	0.36	43,43,43,43	0
57	MG	2a	3178	1/1	0.95	0.28	69,69,69,69	0
57	MG	2A	3579	1/1	0.95	0.06	46,46,46,46	0
57	MG	2A	3392	1/1	0.95	0.18	31,31,31,31	0
57	MG	2T	201	1/1	0.95	0.13	73,73,73,73	0
57	MG	2a	3183	1/1	0.95	0.12	70,70,70,70	0
57	MG	2T	203	1/1	0.95	0.12	68,68,68,68	0
57	MG	1A	3331	1/1	0.95	0.20	30,30,30,30	0
57	MG	1A	3449	1/1	0.95	0.17	51,51,51,51	0
57	MG	2A	3396	1/1	0.95	0.09	70,70,70,70	0
57	MG	1A	3716	1/1	0.95	0.14	33,33,33,33	0
57	MG	1A	3908	1/1	0.95	0.15	46,46,46,46	0
57	MG	1A	3517	1/1	0.95	0.06	56,56,56,56	0
57	MG	1A	3650	1/1	0.95	0.22	48,48,48,48	0
57	MG	2A	3070	1/1	0.95	0.48	48,48,48,48	0
57	MG	1A	3651	1/1	0.95	0.10	30,30,30,30	0
57	MG	1A	3145	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3653	1/1	0.95	0.17	23,23,23,23	0
57	MG	1A	3819	1/1	0.95	0.08	57,57,57,57	0
57	MG	1A	3147	1/1	0.95	0.18	40,40,40,40	0
57	MG	1B	201	1/1	0.95	0.15	61,61,61,61	0
57	MG	27	101	1/1	0.95	0.37	46,46,46,46	0
57	MG	27	102	1/1	0.95	0.17	42,42,42,42	0
57	MG	15	103	1/1	0.95	0.32	33,33,33,33	0
60	ZN	29	102	1/1	0.95	0.17	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	ZN	2n	501	1/1	0.95	0.07	95,95,95,95	0
57	MG	1a	1643	1/1	0.96	0.40	59,59,59,59	0
57	MG	1P	201	1/1	0.96	0.48	37,37,37,37	0
57	MG	1A	3817	1/1	0.96	0.17	29,29,29,29	0
57	MG	2A	3519	1/1	0.96	0.09	62,62,62,62	0
57	MG	1A	3488	1/1	0.96	0.17	30,30,30,30	0
57	MG	1Q	201	1/1	0.96	0.13	36,36,36,36	0
57	MG	1A	3267	1/1	0.96	0.16	76,76,76,76	0
57	MG	1Q	204	1/1	0.96	0.22	39,39,39,39	0
57	MG	1A	3675	1/1	0.96	0.08	62,62,62,62	0
57	MG	1R	201	1/1	0.96	0.22	41,41,41,41	0
57	MG	2A	3371	1/1	0.96	0.15	64,64,64,64	0
57	MG	2A	3527	1/1	0.96	0.14	72,72,72,72	0
57	MG	1A	3041	1/1	0.96	0.23	29,29,29,29	0
57	MG	1A	3309	1/1	0.96	0.18	34,34,34,34	0
57	MG	1A	3749	1/1	0.96	0.16	44,44,44,44	0
57	MG	2a	3054	1/1	0.96	0.09	49,49,49,49	0
57	MG	1A	3196	1/1	0.96	0.35	56,56,56,56	0
57	MG	1A	3828	1/1	0.96	0.12	41,41,41,41	0
57	MG	1A	3270	1/1	0.96	0.23	43,43,43,43	0
57	MG	2A	3695	1/1	0.96	0.15	62,62,62,62	0
57	MG	1d	305	1/1	0.96	0.05	85,85,85,85	0
57	MG	1A	3349	1/1	0.96	0.10	60,60,60,60	0
57	MG	2A	3103	1/1	0.96	0.14	67,67,67,67	0
57	MG	1A	3350	1/1	0.96	0.14	52,52,52,52	0
57	MG	1A	3754	1/1	0.96	0.15	36,36,36,36	0
57	MG	1a	1767	1/1	0.96	0.17	53,53,53,53	0
57	MG	1A	3235	1/1	0.96	0.36	40,40,40,40	0
57	MG	1A	3391	1/1	0.96	0.17	37,37,37,37	0
57	MG	1f	202	1/1	0.96	0.17	51,51,51,51	0
57	MG	1a	1770	1/1	0.96	0.20	67,67,67,67	0
57	MG	1A	4006	1/1	0.96	0.20	35,35,35,35	0
57	MG	2A	3709	1/1	0.96	0.19	65,65,65,65	0
57	MG	2A	3710	1/1	0.96	0.15	62,62,62,62	0
57	MG	1A	3172	1/1	0.96	0.15	33,33,33,33	0
57	MG	2A	3393	1/1	0.96	0.13	38,38,38,38	0
57	MG	2A	3239	1/1	0.96	0.44	58,58,58,58	0
57	MG	2A	3240	1/1	0.96	0.50	44,44,44,44	0
57	MG	1A	3624	1/1	0.96	0.18	30,30,30,30	0
57	MG	2A	3717	1/1	0.96	0.21	48,48,48,48	0
57	MG	1A	3687	1/1	0.96	0.24	59,59,59,59	0
57	MG	1A	3274	1/1	0.96	0.35	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	3447	1/1	0.96	0.21	58,58,58,58	0
57	MG	1A	3096	1/1	0.96	0.21	47,47,47,47	0
57	MG	1A	3176	1/1	0.96	0.26	38,38,38,38	0
57	MG	2A	3556	1/1	0.96	0.18	34,34,34,34	0
57	MG	2a	3084	1/1	0.96	0.33	59,59,59,59	0
57	MG	2a	3085	1/1	0.96	0.20	51,51,51,51	0
57	MG	2A	3724	1/1	0.96	0.17	69,69,69,69	0
57	MG	1A	3507	1/1	0.96	0.15	51,51,51,51	0
57	MG	1n	103	1/1	0.96	0.27	67,67,67,67	0
57	MG	1A	3064	1/1	0.96	0.27	54,54,54,54	0
57	MG	2A	3123	1/1	0.96	0.23	43,43,43,43	0
57	MG	1A	3453	1/1	0.96	0.13	61,61,61,61	0
57	MG	1A	3398	1/1	0.96	0.17	27,27,27,27	0
57	MG	1A	3098	1/1	0.96	0.48	35,35,35,35	0
57	MG	10	104	1/1	0.96	0.08	59,59,59,59	0
57	MG	2A	3129	1/1	0.96	0.13	66,66,66,66	0
57	MG	1A	3769	1/1	0.96	0.12	44,44,44,44	0
57	MG	2a	3098	1/1	0.96	0.14	63,63,63,63	0
57	MG	2A	3416	1/1	0.96	0.15	43,43,43,43	0
57	MG	1A	3770	1/1	0.96	0.24	28,28,28,28	0
57	MG	1A	3360	1/1	0.96	0.12	45,45,45,45	0
57	MG	2A	3262	1/1	0.96	0.70	50,50,50,50	0
57	MG	1A	3457	1/1	0.96	0.22	52,52,52,52	0
57	MG	1A	3936	1/1	0.96	0.15	34,34,34,34	0
57	MG	2a	3106	1/1	0.96	0.09	67,67,67,67	0
57	MG	2A	3266	1/1	0.96	0.33	63,63,63,63	0
57	MG	1B	211	1/1	0.96	0.17	39,39,39,39	0
57	MG	2a	3109	1/1	0.96	0.13	85,85,85,85	0
57	MG	1A	3404	1/1	0.96	0.20	24,24,24,24	0
57	MG	1A	3854	1/1	0.96	0.24	31,31,31,31	0
57	MG	1B	214	1/1	0.96	0.12	57,57,57,57	0
57	MG	13	103	1/1	0.96	0.12	45,45,45,45	0
57	MG	1A	3939	1/1	0.96	0.13	46,46,46,46	0
57	MG	2A	3273	1/1	0.96	0.26	55,55,55,55	0
57	MG	2D	303	1/1	0.96	0.49	45,45,45,45	0
57	MG	2A	3435	1/1	0.96	0.12	76,76,76,76	0
57	MG	1A	3056	1/1	0.96	0.23	28,28,28,28	0
57	MG	2D	307	1/1	0.96	0.53	49,49,49,49	0
57	MG	1A	3580	1/1	0.96	0.13	60,60,60,60	0
57	MG	1A	3075	1/1	0.96	0.25	39,39,39,39	0
57	MG	1A	3703	1/1	0.96	0.11	29,29,29,29	0
57	MG	1A	3154	1/1	0.96	0.32	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3147	1/1	0.96	0.13	40,40,40,40	0
57	MG	1A	3136	1/1	0.96	0.14	37,37,37,37	0
57	MG	1a	1804	1/1	0.96	0.09	60,60,60,60	0
57	MG	1A	3861	1/1	0.96	0.17	25,25,25,25	0
57	MG	1A	3248	1/1	0.96	0.16	43,43,43,43	0
57	MG	2A	3284	1/1	0.96	0.26	67,67,67,67	0
57	MG	1A	3057	1/1	0.96	0.17	47,47,47,47	0
57	MG	1a	1808	1/1	0.96	0.10	72,72,72,72	0
57	MG	2A	3287	1/1	0.96	0.33	70,70,70,70	0
57	MG	1A	3368	1/1	0.96	0.19	33,33,33,33	0
57	MG	2A	3605	1/1	0.96	0.15	44,44,44,44	0
57	MG	1A	3951	1/1	0.96	0.17	43,43,43,43	0
57	MG	1A	3784	1/1	0.96	0.17	35,35,35,35	0
57	MG	1A	3037	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3954	1/1	0.96	0.09	45,45,45,45	0
57	MG	2A	3160	1/1	0.96	0.40	45,45,45,45	0
57	MG	1a	1814	1/1	0.96	0.15	73,73,73,73	0
57	MG	1A	3370	1/1	0.96	0.16	33,33,33,33	0
57	MG	1A	3416	1/1	0.96	0.18	27,27,27,27	0
57	MG	1A	3472	1/1	0.96	0.24	42,42,42,42	0
57	MG	2A	3036	1/1	0.96	0.20	50,50,50,50	0
57	MG	1A	3158	1/1	0.96	0.21	45,45,45,45	0
57	MG	1A	3872	1/1	0.96	0.14	49,49,49,49	0
57	MG	1A	3222	1/1	0.96	0.18	37,37,37,37	0
57	MG	2a	3150	1/1	0.96	0.20	71,71,71,71	0
57	MG	1D	311	1/1	0.96	0.37	43,43,43,43	0
57	MG	2A	3622	1/1	0.96	0.09	57,57,57,57	0
57	MG	2A	3305	1/1	0.96	0.25	52,52,52,52	0
57	MG	1D	312	1/1	0.96	0.16	54,54,54,54	0
57	MG	1A	3255	1/1	0.96	0.23	37,37,37,37	0
57	MG	1A	3374	1/1	0.96	0.21	38,38,38,38	0
57	MG	1A	3256	1/1	0.96	0.12	27,27,27,27	0
57	MG	1a	1826	1/1	0.96	0.12	65,65,65,65	0
57	MG	1A	3794	1/1	0.96	0.27	40,40,40,40	0
57	MG	2A	3176	1/1	0.96	0.20	65,65,65,65	0
57	MG	1E	301	1/1	0.96	0.15	36,36,36,36	0
57	MG	2A	3476	1/1	0.96	0.05	63,63,63,63	0
57	MG	2A	3052	1/1	0.96	0.17	66,66,66,66	0
57	MG	28	102	1/1	0.96	0.21	62,62,62,62	0
57	MG	1A	3106	1/1	0.96	0.27	33,33,33,33	0
57	MG	2A	3180	1/1	0.96	0.11	55,55,55,55	0
57	MG	1A	3024	1/1	0.96	0.19	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	1A	3539	1/1	0.96	0.12	37,37,37,37	0
57	MG	1A	3970	1/1	0.96	0.13	50,50,50,50	0
57	MG	2A	3641	1/1	0.96	0.12	41,41,41,41	0
57	MG	1A	3798	1/1	0.96	0.30	46,46,46,46	0
57	MG	1F	303	1/1	0.96	0.14	32,32,32,32	0
57	MG	2A	3059	1/1	0.96	0.15	44,44,44,44	0
57	MG	1A	3540	1/1	0.96	0.15	33,33,33,33	0
57	MG	1F	308	1/1	0.96	0.27	35,35,35,35	0
57	MG	1A	3725	1/1	0.96	0.07	30,30,30,30	0
57	MG	2A	3333	1/1	0.96	0.19	58,58,58,58	0
57	MG	1A	3162	1/1	0.96	0.25	45,45,45,45	0
57	MG	2a	3180	1/1	0.96	0.17	72,72,72,72	0
57	MG	1A	3426	1/1	0.96	0.21	25,25,25,25	0
57	MG	1a	1731	1/1	0.96	0.24	48,48,48,48	0
57	MG	1A	3339	1/1	0.96	0.18	35,35,35,35	0
57	MG	2e	201	1/1	0.96	0.23	73,73,73,73	0
57	MG	1A	3804	1/1	0.96	0.10	38,38,38,38	0
57	MG	2A	3497	1/1	0.96	0.13	35,35,35,35	0
57	MG	1a	1734	1/1	0.96	0.12	45,45,45,45	0
57	MG	1A	3604	1/1	0.96	0.14	35,35,35,35	0
57	MG	2A	3344	1/1	0.96	0.16	56,56,56,56	0
57	MG	1A	3013	1/1	0.96	0.18	19,19,19,19	0
57	MG	1A	3980	1/1	0.96	0.16	58,58,58,58	0
57	MG	1A	3546	1/1	0.96	0.25	58,58,58,58	0
57	MG	1A	3809	1/1	0.96	0.22	27,27,27,27	0
57	MG	2A	3506	1/1	0.96	0.23	28,28,28,28	0
57	MG	1A	3547	1/1	0.96	0.26	55,55,55,55	0
57	MG	1A	3166	1/1	0.96	0.47	42,42,42,42	0
57	MG	1a	1742	1/1	0.96	0.14	37,37,37,37	0
57	MG	2A	3510	1/1	0.96	0.12	55,55,55,55	0
57	MG	1A	3813	1/1	0.96	0.35	35,35,35,35	0
60	ZN	1Y	202	1/1	0.96	0.21	60,60,60,60	0
57	MG	1a	1639	1/1	0.96	0.19	74,74,74,74	0
57	MG	2a	3035	1/1	0.96	0.12	41,41,41,41	0
57	MG	1A	3899	1/1	0.96	0.23	30,30,30,30	0
60	ZN	26	501	1/1	0.96	0.19	62,62,62,62	0
57	MG	1A	3031	1/1	0.96	0.12	42,42,42,42	0
57	MG	1A	3487	1/1	0.96	0.18	29,29,29,29	0
57	MG	1A	3244	1/1	0.97	0.23	44,44,44,44	0
57	MG	1A	3205	1/1	0.97	0.56	38,38,38,38	0
57	MG	1R	202	1/1	0.97	0.13	39,39,39,39	0
57	MG	2A	3043	1/1	0.97	0.16	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3935	1/1	0.97	0.13	29,29,29,29	0
57	MG	2A	3407	1/1	0.97	0.12	61,61,61,61	0
57	MG	1A	3060	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3288	1/1	0.97	0.19	33,33,33,33	0
57	MG	1A	3541	1/1	0.97	0.23	36,36,36,36	0
57	MG	1A	3020	1/1	0.97	0.30	38,38,38,38	0
57	MG	1A	3128	1/1	0.97	0.27	34,34,34,34	0
57	MG	1A	3729	1/1	0.97	0.14	36,36,36,36	0
57	MG	1A	3867	1/1	0.97	0.21	29,29,29,29	0
57	MG	2A	3705	1/1	0.97	0.10	76,76,76,76	0
57	MG	1A	3181	1/1	0.97	0.34	37,37,37,37	0
57	MG	1A	3214	1/1	0.97	0.42	49,49,49,49	0
57	MG	2A	3708	1/1	0.97	0.13	62,62,62,62	0
57	MG	1A	3338	1/1	0.97	0.20	40,40,40,40	0
57	MG	1A	3077	1/1	0.97	0.31	40,40,40,40	0
57	MG	1U	201	1/1	0.97	0.26	38,38,38,38	0
57	MG	2A	3559	1/1	0.97	0.06	69,69,69,69	0
57	MG	1U	202	1/1	0.97	0.32	40,40,40,40	0
57	MG	2A	3421	1/1	0.97	0.18	41,41,41,41	0
57	MG	2A	3562	1/1	0.97	0.40	57,57,57,57	0
57	MG	1a	1849	1/1	0.97	0.12	58,58,58,58	0
57	MG	1A	3340	1/1	0.97	0.24	26,26,26,26	0
57	MG	1U	205	1/1	0.97	0.32	38,38,38,38	0
57	MG	2A	3288	1/1	0.97	0.28	62,62,62,62	0
57	MG	1a	1655	1/1	0.97	0.18	60,60,60,60	0
57	MG	2A	3428	1/1	0.97	0.16	33,33,33,33	0
57	MG	1V	201	1/1	0.97	0.44	36,36,36,36	0
57	MG	2A	3065	1/1	0.97	0.94	48,48,48,48	0
57	MG	1V	202	1/1	0.97	0.46	35,35,35,35	0
57	MG	2A	3432	1/1	0.97	0.12	51,51,51,51	0
57	MG	2A	3575	1/1	0.97	0.16	31,31,31,31	0
57	MG	2A	3067	1/1	0.97	0.14	22,22,22,22	0
57	MG	2A	3434	1/1	0.97	0.18	38,38,38,38	0
57	MG	2A	3294	1/1	0.97	0.12	40,40,40,40	0
57	MG	1A	3112	1/1	0.97	0.48	41,41,41,41	0
57	MG	1A	3737	1/1	0.97	0.20	44,44,44,44	0
57	MG	1A	3026	1/1	0.97	0.29	34,34,34,34	0
57	MG	1A	3739	1/1	0.97	0.10	61,61,61,61	0
57	MG	1A	3806	1/1	0.97	0.13	50,50,50,50	0
57	MG	1A	3879	1/1	0.97	0.17	34,34,34,34	0
57	MG	1A	3955	1/1	0.97	0.18	28,28,28,28	0
57	MG	1A	3220	1/1	0.97	0.23	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3587	1/1	0.97	0.09	49,49,49,49	0
57	MG	1a	1763	1/1	0.97	0.14	65,65,65,65	0
57	MG	1Z	301	1/1	0.97	0.17	62,62,62,62	0
57	MG	2B	211	1/1	0.97	0.19	69,69,69,69	0
57	MG	1A	3114	1/1	0.97	0.24	38,38,38,38	0
57	MG	2B	213	1/1	0.97	0.22	74,74,74,74	0
57	MG	2A	3591	1/1	0.97	0.12	50,50,50,50	0
57	MG	1A	3883	1/1	0.97	0.17	51,51,51,51	0
57	MG	1a	1670	1/1	0.97	0.27	61,61,61,61	0
57	MG	2A	3594	1/1	0.97	0.27	59,59,59,59	0
57	MG	1A	3440	1/1	0.97	0.15	46,46,46,46	0
57	MG	1A	3115	1/1	0.97	0.24	36,36,36,36	0
57	MG	1A	3023	1/1	0.97	0.27	34,34,34,34	0
57	MG	1A	3137	1/1	0.97	0.13	23,23,23,23	0
57	MG	1B	229	1/1	0.97	0.10	77,77,77,77	0
57	MG	1A	3557	1/1	0.97	0.16	42,42,42,42	0
57	MG	2A	3314	1/1	0.97	0.12	37,37,37,37	0
57	MG	1A	3815	1/1	0.97	0.15	16,16,16,16	0
57	MG	2A	3316	1/1	0.97	0.19	23,23,23,23	0
57	MG	1A	3304	1/1	0.97	0.25	56,56,56,56	0
57	MG	2E	302	1/1	0.97	0.26	60,60,60,60	0
57	MG	1A	3306	1/1	0.97	0.21	38,38,38,38	0
57	MG	2A	3319	1/1	0.97	0.14	39,39,39,39	0
57	MG	1D	304	1/1	0.97	0.15	40,40,40,40	0
57	MG	2A	3462	1/1	0.97	0.15	39,39,39,39	0
57	MG	1A	3225	1/1	0.97	0.34	36,36,36,36	0
57	MG	1A	3820	1/1	0.97	0.12	53,53,53,53	0
57	MG	2F	304	1/1	0.97	0.28	53,53,53,53	0
57	MG	2F	305	1/1	0.97	0.61	50,50,50,50	0
57	MG	1A	3394	1/1	0.97	0.24	27,27,27,27	0
57	MG	1A	3308	1/1	0.97	0.24	33,33,33,33	0
57	MG	1A	3505	1/1	0.97	0.19	25,25,25,25	0
57	MG	1A	3100	1/1	0.97	0.25	36,36,36,36	0
57	MG	2A	3327	1/1	0.97	0.15	61,61,61,61	0
57	MG	1A	3825	1/1	0.97	0.20	31,31,31,31	0
57	MG	1A	3310	1/1	0.97	0.23	14,14,14,14	0
57	MG	1D	314	1/1	0.97	0.09	69,69,69,69	0
57	MG	2A	3101	1/1	0.97	0.08	51,51,51,51	0
57	MG	1a	1788	1/1	0.97	0.14	66,66,66,66	0
57	MG	2A	3336	1/1	0.97	0.26	60,60,60,60	0
57	MG	2a	3136	1/1	0.97	0.14	67,67,67,67	0
57	MG	2A	3337	1/1	0.97	0.19	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3625	1/1	0.97	0.07	44,44,44,44	0
57	MG	2T	202	1/1	0.97	0.26	68,68,68,68	0
57	MG	1A	3311	1/1	0.97	0.17	35,35,35,35	0
57	MG	1A	3901	1/1	0.97	0.14	15,15,15,15	0
57	MG	1A	3510	1/1	0.97	0.21	21,21,21,21	0
57	MG	1A	3399	1/1	0.97	0.22	26,26,26,26	0
57	MG	1A	3400	1/1	0.97	0.20	26,26,26,26	0
57	MG	1A	3831	1/1	0.97	0.22	54,54,54,54	0
57	MG	1A	3140	1/1	0.97	0.17	34,34,34,34	0
57	MG	2W	201	1/1	0.97	0.41	48,48,48,48	0
57	MG	1A	3633	1/1	0.97	0.18	33,33,33,33	0
57	MG	2A	3347	1/1	0.97	0.10	59,59,59,59	0
57	MG	2A	3348	1/1	0.97	0.17	61,61,61,61	0
57	MG	1A	3402	1/1	0.97	0.16	27,27,27,27	0
57	MG	2A	3490	1/1	0.97	0.11	69,69,69,69	0
57	MG	1F	302	1/1	0.97	0.24	37,37,37,37	0
57	MG	1A	3573	1/1	0.97	0.18	23,23,23,23	0
57	MG	2a	3155	1/1	0.97	0.12	66,66,66,66	0
57	MG	2A	3114	1/1	0.97	0.07	49,49,49,49	0
57	MG	1F	305	1/1	0.97	0.33	36,36,36,36	0
57	MG	2A	3643	1/1	0.97	0.09	49,49,49,49	0
57	MG	1F	306	1/1	0.97	0.29	39,39,39,39	0
57	MG	1A	3101	1/1	0.97	0.29	39,39,39,39	0
57	MG	1A	3357	1/1	0.97	0.22	26,26,26,26	0
57	MG	1F	310	1/1	0.97	0.19	30,30,30,30	0
57	MG	1A	3231	1/1	0.97	0.16	30,30,30,30	0
57	MG	1A	3406	1/1	0.97	0.14	47,47,47,47	0
57	MG	2A	3361	1/1	0.97	0.18	37,37,37,37	0
57	MG	1A	3914	1/1	0.97	0.08	49,49,49,49	0
57	MG	1A	3579	1/1	0.97	0.06	40,40,40,40	0
57	MG	2A	3124	1/1	0.97	0.81	47,47,47,47	0
57	MG	1A	3164	1/1	0.97	0.27	47,47,47,47	0
57	MG	2A	3236	1/1	0.97	0.31	59,59,59,59	0
57	MG	1A	3642	1/1	0.97	0.16	37,37,37,37	0
57	MG	2a	3012	1/1	0.97	0.13	50,50,50,50	0
57	MG	2A	3238	1/1	0.97	0.09	60,60,60,60	0
57	MG	1A	3089	1/1	0.97	0.26	33,33,33,33	0
57	MG	2A	3659	1/1	0.97	0.16	79,79,79,79	0
57	MG	1A	3167	1/1	0.97	0.24	33,33,33,33	0
57	MG	1A	3028	1/1	0.97	0.28	30,30,30,30	0
57	MG	1G	203	1/1	0.97	0.18	44,44,44,44	0
57	MG	2A	3131	1/1	0.97	0.19	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3466	1/1	0.97	0.12	47,47,47,47	0
57	MG	1A	3104	1/1	0.97	0.30	41,41,41,41	0
57	MG	1a	1622	1/1	0.97	0.13	49,49,49,49	0
57	MG	1A	3527	1/1	0.97	0.15	30,30,30,30	0
57	MG	1A	3468	1/1	0.97	0.17	52,52,52,52	0
57	MG	1a	1721	1/1	0.97	0.25	69,69,69,69	0
57	MG	2A	3025	1/1	0.97	0.12	46,46,46,46	0
57	MG	1A	3276	1/1	0.97	0.55	43,43,43,43	0
57	MG	2k	201	1/1	0.97	0.12	57,57,57,57	0
57	MG	1a	1723	1/1	0.97	0.27	68,68,68,68	0
57	MG	1A	3091	1/1	0.97	0.21	39,39,39,39	0
57	MG	2A	3674	1/1	0.97	0.12	51,51,51,51	0
57	MG	2A	3386	1/1	0.97	0.16	62,62,62,62	0
57	MG	2x	102	1/1	0.97	0.14	52,52,52,52	0
57	MG	2A	3030	1/1	0.97	0.14	60,60,60,60	0
57	MG	2A	3388	1/1	0.97	0.17	41,41,41,41	0
57	MG	1a	1627	1/1	0.97	0.13	49,49,49,49	0
57	MG	2A	3258	1/1	0.97	0.29	42,42,42,42	0
57	MG	2A	3680	1/1	0.97	0.04	76,76,76,76	0
57	MG	1A	3239	1/1	0.97	0.27	33,33,33,33	0
57	MG	1A	4005	1/1	0.97	0.10	53,53,53,53	0
57	MG	1A	3033	1/1	0.97	0.17	46,46,46,46	0
57	MG	1A	3202	1/1	0.97	0.44	41,41,41,41	0
57	MG	1A	3053	1/1	0.97	0.13	41,41,41,41	0
60	ZN	15	108	1/1	0.97	0.21	49,49,49,49	0
60	ZN	1n	104	1/1	0.97	0.15	68,68,68,68	0
57	MG	1A	3204	1/1	0.97	0.29	39,39,39,39	0
57	MG	2A	3265	1/1	0.97	0.14	23,23,23,23	0
57	MG	2A	3398	1/1	0.97	0.10	66,66,66,66	0
57	MG	1A	3719	1/1	0.97	0.09	33,33,33,33	0
57	MG	2A	3400	1/1	0.97	0.23	65,65,65,65	0
57	MG	1A	3475	1/1	0.98	0.18	44,44,44,44	0
57	MG	1A	3428	1/1	0.98	0.16	14,14,14,14	0
57	MG	1A	3161	1/1	0.98	0.22	29,29,29,29	0
57	MG	1A	3045	1/1	0.98	0.16	23,23,23,23	0
57	MG	1A	3273	1/1	0.98	0.21	32,32,32,32	0
57	MG	1A	3207	1/1	0.98	0.49	32,32,32,32	0
57	MG	1a	1659	1/1	0.98	0.26	50,50,50,50	0
57	MG	2A	3028	1/1	0.98	0.16	44,44,44,44	0
57	MG	2a	3094	1/1	0.98	0.30	67,67,67,67	0
57	MG	1A	3706	1/1	0.98	0.10	39,39,39,39	0
57	MG	2A	3225	1/1	0.98	0.22	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	3434	1/1	0.98	0.30	63,63,63,63	0
57	MG	2A	3328	1/1	0.98	0.10	37,37,37,37	0
57	MG	1A	3314	1/1	0.98	0.17	30,30,30,30	0
57	MG	1E	302	1/1	0.98	0.41	37,37,37,37	0
57	MG	2A	3332	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	3648	1/1	0.98	0.16	54,54,54,54	0
57	MG	11	103	1/1	0.98	0.16	52,52,52,52	0
57	MG	2a	3104	1/1	0.98	0.26	61,61,61,61	0
57	MG	1A	3536	1/1	0.98	0.20	31,31,31,31	0
57	MG	1A	3019	1/1	0.98	0.22	29,29,29,29	0
57	MG	13	101	1/1	0.98	0.18	35,35,35,35	0
57	MG	2A	3555	1/1	0.98	0.19	31,31,31,31	0
57	MG	1A	3210	1/1	0.98	0.24	33,33,33,33	0
57	MG	1A	3438	1/1	0.98	0.21	15,15,15,15	0
57	MG	2A	3040	1/1	0.98	0.17	23,23,23,23	0
57	MG	2W	203	1/1	0.98	0.17	54,54,54,54	0
57	MG	1F	301	1/1	0.98	0.26	34,34,34,34	0
57	MG	1A	3003	1/1	0.98	0.20	23,23,23,23	0
57	MG	1A	3122	1/1	0.98	0.11	46,46,46,46	0
57	MG	1F	304	1/1	0.98	0.29	33,33,33,33	0
57	MG	1A	3025	1/1	0.98	0.25	40,40,40,40	0
57	MG	1A	3597	1/1	0.98	0.24	39,39,39,39	0
57	MG	1A	3359	1/1	0.98	0.16	22,22,22,22	0
57	MG	2A	3566	1/1	0.98	0.16	23,23,23,23	0
57	MG	2a	3121	1/1	0.98	0.07	77,77,77,77	0
57	MG	2A	3567	1/1	0.98	0.18	56,56,56,56	0
57	MG	2A	3048	1/1	0.98	0.17	48,48,48,48	0
57	MG	2A	3049	1/1	0.98	0.12	40,40,40,40	0
57	MG	17	101	1/1	0.98	0.15	45,45,45,45	0
57	MG	17	102	1/1	0.98	0.16	35,35,35,35	0
57	MG	17	103	1/1	0.98	0.24	38,38,38,38	0
57	MG	2A	3688	1/1	0.98	0.26	55,55,55,55	0
57	MG	1A	3168	1/1	0.98	0.15	28,28,28,28	0
57	MG	1F	309	1/1	0.98	0.26	34,34,34,34	0
57	MG	1A	3491	1/1	0.98	0.12	32,32,32,32	0
57	MG	2A	3464	1/1	0.98	0.05	53,53,53,53	0
57	MG	2a	3008	1/1	0.98	0.06	68,68,68,68	0
57	MG	1a	1771	1/1	0.98	0.15	60,60,60,60	0
57	MG	1A	3152	1/1	0.98	0.24	34,34,34,34	0
57	MG	2A	3254	1/1	0.98	0.33	42,42,42,42	0
57	MG	2A	3360	1/1	0.98	0.23	31,31,31,31	0
57	MG	1A	3217	1/1	0.98	0.11	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	3170	1/1	0.98	0.13	32,32,32,32	0
57	MG	1A	3219	1/1	0.98	0.30	38,38,38,38	0
57	MG	2A	3158	1/1	0.98	0.21	46,46,46,46	0
57	MG	1A	3726	1/1	0.98	0.19	35,35,35,35	0
57	MG	1A	3664	1/1	0.98	0.16	46,46,46,46	0
57	MG	1A	3251	1/1	0.98	0.08	69,69,69,69	0
57	MG	1A	3607	1/1	0.98	0.26	35,35,35,35	0
57	MG	2A	3369	1/1	0.98	0.14	33,33,33,33	0
57	MG	2A	3478	1/1	0.98	0.14	58,58,58,58	0
57	MG	1A	3021	1/1	0.98	0.14	36,36,36,36	0
57	MG	1A	3450	1/1	0.98	0.21	26,26,26,26	0
57	MG	1A	3732	1/1	0.98	0.22	30,30,30,30	0
57	MG	1A	3451	1/1	0.98	0.16	26,26,26,26	0
57	MG	1A	3092	1/1	0.98	0.20	14,14,14,14	0
57	MG	1N	201	1/1	0.98	0.11	41,41,41,41	0
57	MG	1A	3173	1/1	0.98	0.23	37,37,37,37	0
57	MG	1A	3291	1/1	0.98	0.21	44,44,44,44	0
57	MG	2A	3715	1/1	0.98	0.23	63,63,63,63	0
57	MG	1A	3050	1/1	0.98	0.24	31,31,31,31	0
57	MG	1A	3195	1/1	0.98	0.24	39,39,39,39	0
57	MG	1A	3175	1/1	0.98	0.37	41,41,41,41	0
57	MG	1A	3412	1/1	0.98	0.18	27,27,27,27	0
57	MG	1A	3877	1/1	0.98	0.15	30,30,30,30	0
57	MG	1A	3509	1/1	0.98	0.22	21,21,21,21	0
57	MG	1Q	202	1/1	0.98	0.24	34,34,34,34	0
57	MG	1A	3949	1/1	0.98	0.17	45,45,45,45	0
57	MG	1A	3295	1/1	0.98	0.26	58,58,58,58	0
57	MG	1A	3743	1/1	0.98	0.10	25,25,25,25	0
57	MG	2A	3609	1/1	0.98	0.15	44,44,44,44	0
57	MG	2A	3083	1/1	0.98	0.16	43,43,43,43	0
57	MG	2A	3611	1/1	0.98	0.13	26,26,26,26	0
57	MG	1A	3258	1/1	0.98	0.20	53,53,53,53	0
57	MG	1A	3812	1/1	0.98	0.23	39,39,39,39	0
57	MG	1A	3745	1/1	0.98	0.20	26,26,26,26	0
57	MG	1A	3259	1/1	0.98	0.23	38,38,38,38	0
57	MG	1B	215	1/1	0.98	0.20	49,49,49,49	0
57	MG	2A	3503	1/1	0.98	0.15	37,37,37,37	0
57	MG	1A	3565	1/1	0.98	0.18	22,22,22,22	0
57	MG	1a	1629	1/1	0.98	0.09	72,72,72,72	0
57	MG	1A	3748	1/1	0.98	0.20	54,54,54,54	0
57	MG	1A	3682	1/1	0.98	0.10	43,43,43,43	0
57	MG	1A	3818	1/1	0.98	0.14	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3260	1/1	0.98	0.37	34,34,34,34	0
57	MG	1A	3961	1/1	0.98	0.13	37,37,37,37	0
57	MG	2A	3402	1/1	0.98	0.15	64,64,64,64	0
57	MG	1A	3043	1/1	0.98	0.27	17,17,17,17	0
57	MG	1B	223	1/1	0.98	0.17	45,45,45,45	0
57	MG	2A	3628	1/1	0.98	0.14	38,38,38,38	0
57	MG	1A	3515	1/1	0.98	0.20	22,22,22,22	0
57	MG	1A	3227	1/1	0.98	0.36	36,36,36,36	0
57	MG	1A	3198	1/1	0.98	0.29	41,41,41,41	0
57	MG	1A	3628	1/1	0.98	0.15	43,43,43,43	0
57	MG	2A	3004	1/1	0.98	0.16	33,33,33,33	0
57	MG	2D	301	1/1	0.98	0.52	39,39,39,39	0
57	MG	2D	302	1/1	0.98	0.35	50,50,50,50	0
57	MG	1U	204	1/1	0.98	0.30	29,29,29,29	0
57	MG	1A	3017	1/1	0.98	0.28	34,34,34,34	0
57	MG	1A	3086	1/1	0.98	0.15	41,41,41,41	0
57	MG	2D	306	1/1	0.98	0.25	37,37,37,37	0
57	MG	1A	3520	1/1	0.98	0.14	33,33,33,33	0
57	MG	1A	3574	1/1	0.98	0.23	36,36,36,36	0
57	MG	1A	3305	1/1	0.98	0.18	22,22,22,22	0
57	MG	1A	3469	1/1	0.98	0.17	26,26,26,26	0
57	MG	2A	3013	1/1	0.98	0.14	22,22,22,22	0
57	MG	1A	3201	1/1	0.98	0.29	41,41,41,41	0
57	MG	2A	3015	1/1	0.98	0.33	40,40,40,40	0
60	ZN	19	102	1/1	0.98	0.23	44,44,44,44	0
57	MG	1A	3107	1/1	0.98	0.18	30,30,30,30	0
57	MG	1A	3425	1/1	0.98	0.23	29,29,29,29	0
57	MG	1A	3180	1/1	0.98	0.20	33,33,33,33	0
60	ZN	25	103	1/1	0.98	0.23	57,57,57,57	0
57	MG	1A	3146	1/1	0.98	0.44	37,37,37,37	0
57	MG	2A	3020	1/1	0.98	0.24	40,40,40,40	0
57	MG	2A	3425	1/1	0.98	0.16	37,37,37,37	0
57	MG	1A	3772	1/1	0.99	0.13	30,30,30,30	0
57	MG	2A	3331	1/1	0.99	0.17	32,32,32,32	0
57	MG	1V	203	1/1	0.99	0.18	42,42,42,42	0
57	MG	1A	3209	1/1	0.99	0.16	22,22,22,22	0
57	MG	1E	303	1/1	0.99	0.22	35,35,35,35	0
57	MG	2A	3372	1/1	0.99	0.14	42,42,42,42	0
57	MG	1A	3432	1/1	0.99	0.20	30,30,30,30	0
57	MG	1A	3132	1/1	0.99	0.28	32,32,32,32	0
57	MG	1A	3723	1/1	0.99	0.19	26,26,26,26	0
57	MG	2A	3338	1/1	0.99	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3261	1/1	0.99	0.50	35,35,35,35	0
57	MG	1A	3165	1/1	0.99	0.23	29,29,29,29	0
57	MG	1A	3833	1/1	0.99	0.20	22,22,22,22	0
57	MG	1A	3006	1/1	0.99	0.13	23,23,23,23	0
57	MG	1A	3249	1/1	0.99	0.25	29,29,29,29	0
57	MG	1A	3213	1/1	0.99	0.39	34,34,34,34	0
57	MG	1A	3334	1/1	0.99	0.21	30,30,30,30	0
57	MG	1A	3237	1/1	0.99	0.17	35,35,35,35	0
57	MG	1A	3605	1/1	0.99	0.31	35,35,35,35	0
57	MG	2E	306	1/1	0.99	0.19	33,33,33,33	0
57	MG	1A	3984	1/1	0.99	0.19	16,16,16,16	0
57	MG	1A	3036	1/1	0.99	0.18	32,32,32,32	0
57	MG	1A	3337	1/1	0.99	0.21	15,15,15,15	0
57	MG	1A	3018	1/1	0.99	0.15	29,29,29,29	0
57	MG	2A	3007	1/1	0.99	0.11	42,42,42,42	0
57	MG	1A	3284	1/1	0.99	0.23	23,23,23,23	0
57	MG	1A	3302	1/1	0.99	0.19	30,30,30,30	0
57	MG	1A	3285	1/1	0.99	0.16	17,17,17,17	0
57	MG	1A	3129	1/1	0.99	0.40	39,39,39,39	0
57	MG	1A	3492	1/1	0.99	0.18	21,21,21,21	0
57	MG	1D	310	1/1	0.99	0.21	35,35,35,35	0
60	ZN	16	501	1/1	0.99	0.23	44,44,44,44	0
57	MG	1A	3228	1/1	0.99	0.15	42,42,42,42	0
57	MG	1A	3074	1/1	0.99	0.32	37,37,37,37	0
57	MG	1A	3365	1/1	0.99	0.16	17,17,17,17	0
57	MG	1A	3016	1/1	0.99	0.26	34,34,34,34	0
57	MG	1A	3880	1/1	0.99	0.13	45,45,45,45	0
57	MG	2A	3257	1/1	0.99	0.18	23,23,23,23	0
57	MG	1A	3139	1/1	0.99	0.20	33,33,33,33	0
57	MG	1A	3498	1/1	0.99	0.22	46,46,46,46	0
61	SF4	1d	306	8/8	0.99	0.15	63,67,73,74	0
61	SF4	2d	501	8/8	0.99	0.14	68,78,79,82	0

6.5 Other polymers (i)

There are no such residues in this entry.