Full wwPDB X-ray Structure Validation Report ⓘ

Jul 18, 2023 – 12:26 AM EDT

PDB ID	:	8FC4
Title	:	Crystal structure of the A2058-N6-dimethylated Thermus thermophilus 70S ribosome in complex with protein Y, hygromycin A, and erythromycin at 2.45A resolution
Authors	:	Chen, C.-W.; Syroegin, E.A.; Svetlov, M.S.; Polikanov, Y.S.
Deposited on	:	2022-12-01
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 ⓘ symbol.

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

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

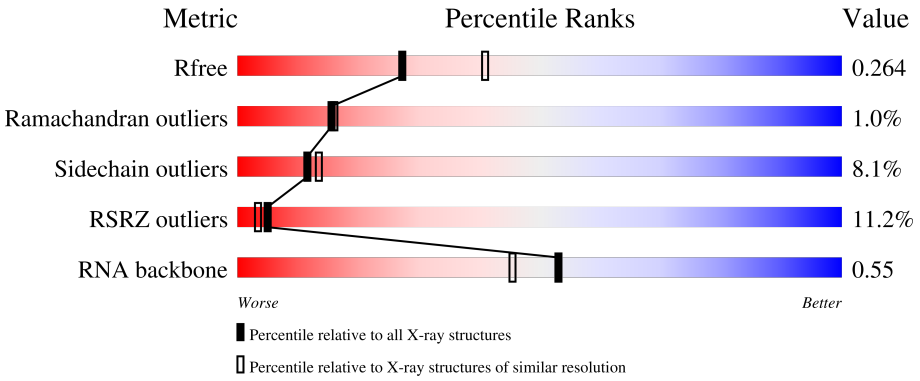
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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	6% 82% 16%
1	2A	2915	7% 80% 17%
2	1B	121	89% 10%
2	2B	121	4% 86% 13%

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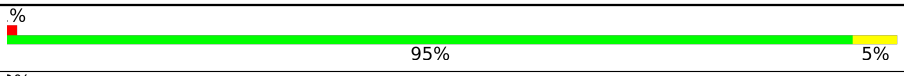
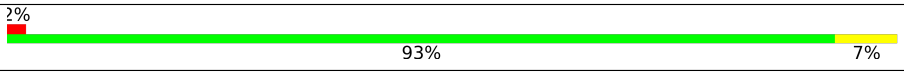
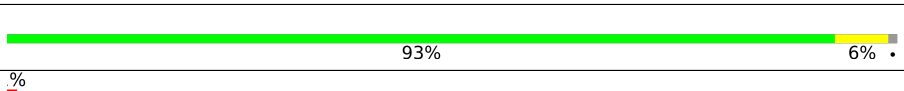
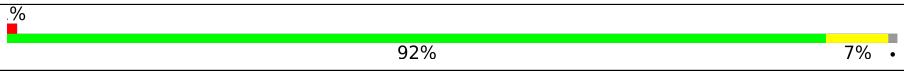
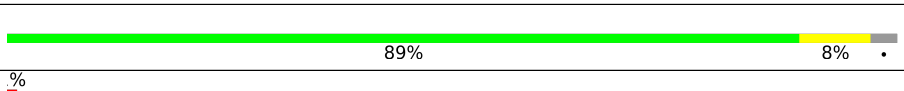
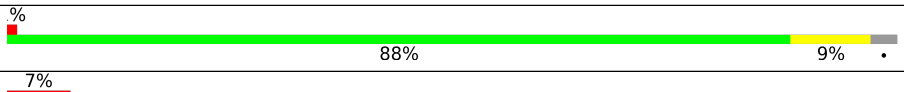
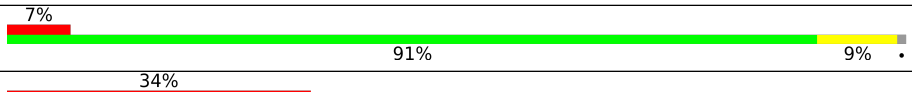
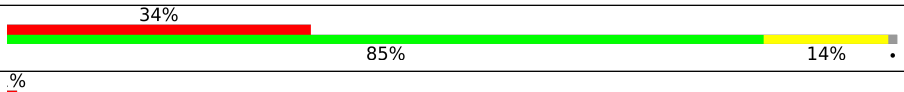
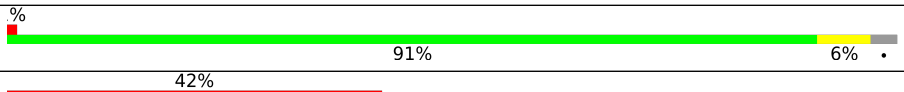
Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
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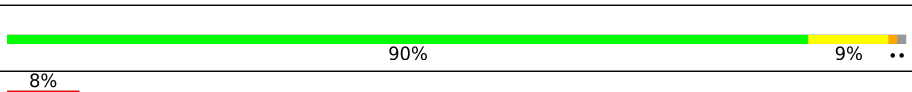
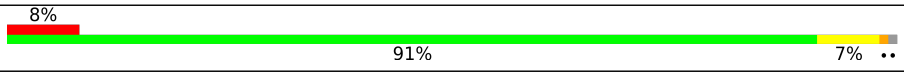
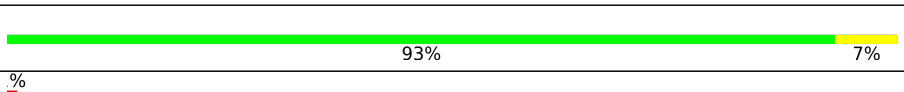
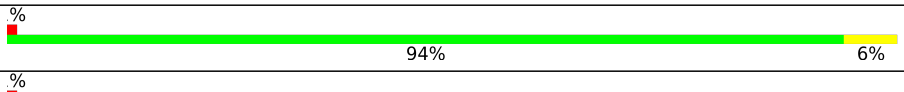
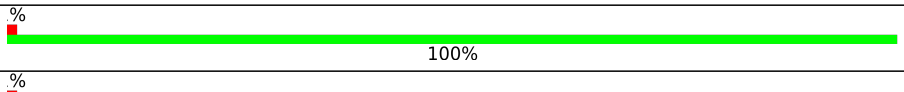
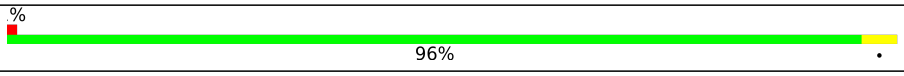
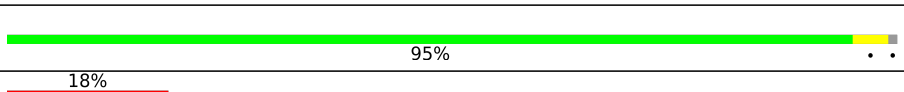
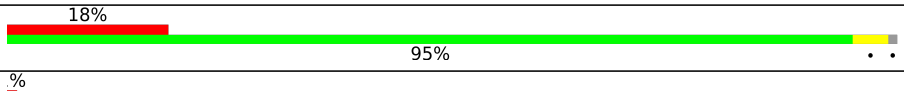
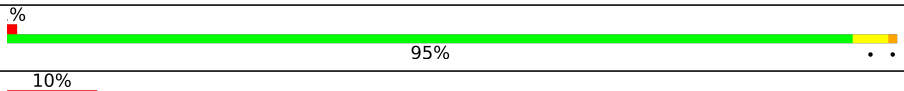
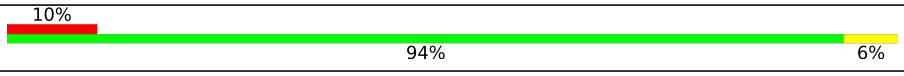
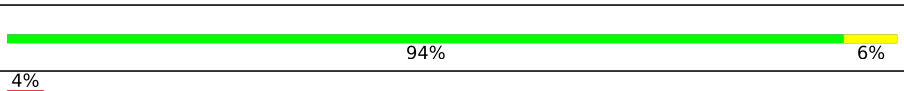
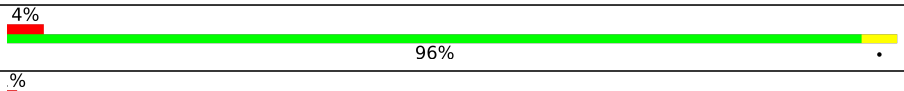
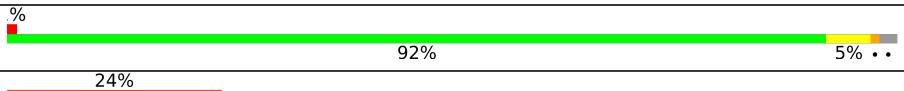
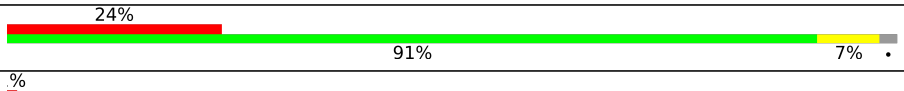
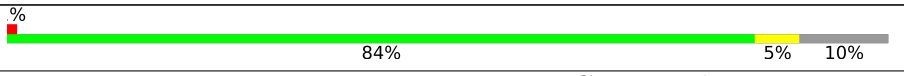
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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Mol	Chain	Length	Quality of chain
15	2T	146	2% 85% 5% 10%
16	1U	118	% 96%
16	2U	118	% 92% 6%
17	1V	101	% 93% 6%
17	2V	101	% 95%
18	1W	113	96%
18	2W	113	% 94% 5%
19	1X	96	2% 96%
19	2X	96	3% 96%
20	1Y	110	% 91% 6%
20	2Y	110	9% 93% 5%
21	1Z	206	% 90% 9%
21	2Z	206	13% 91% 7%
22	10	85	87% 9%
22	20	85	12% 87% 9%
23	11	98	4% 92% 6%
23	21	98	3% 93% 6%
24	12	72	% 93%
24	22	72	94%
25	13	60	92% 7%
25	23	60	7% 95%
26	14	71	25% 82% 14%
26	24	71	58% 80% 15%
27	15	60	2% 90% 8%
27	25	60	2% 93% 5%

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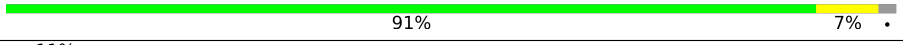
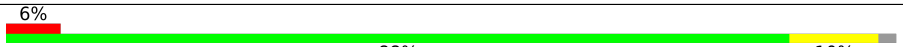
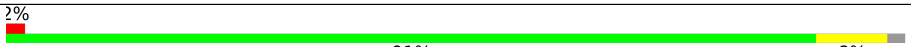
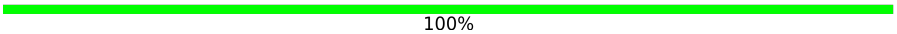
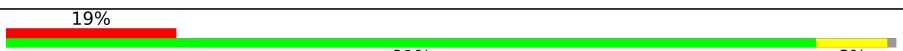
Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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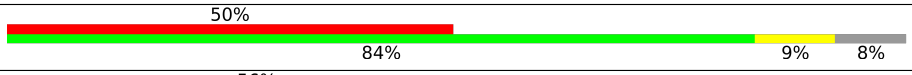
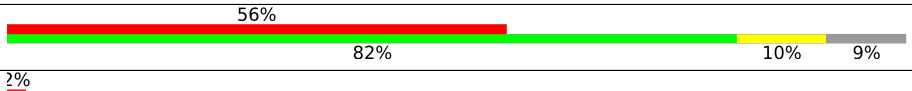
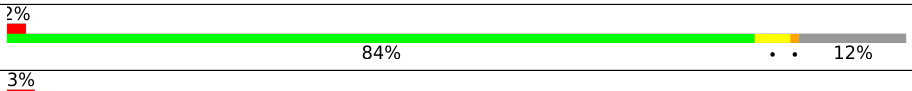
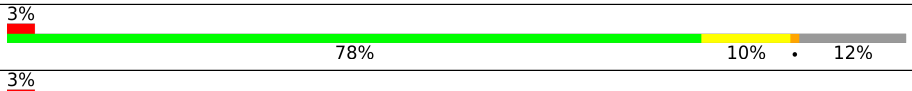
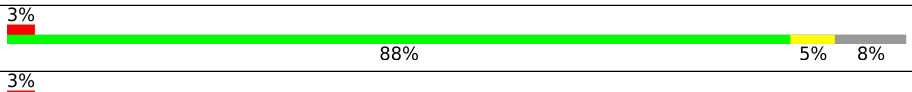
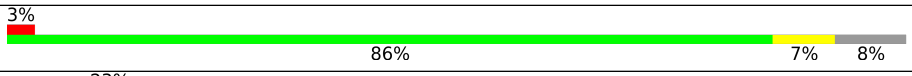
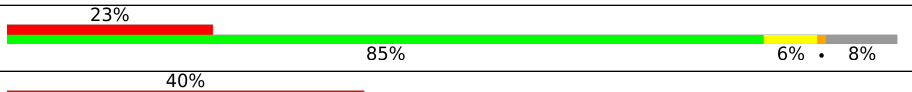
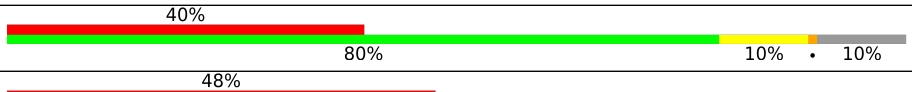
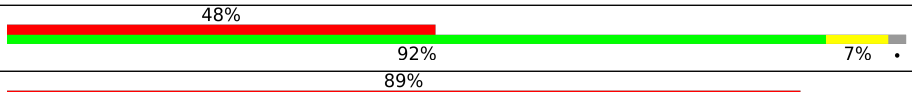
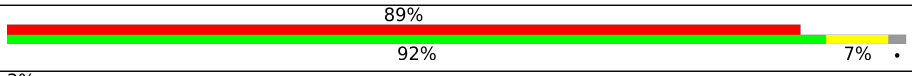
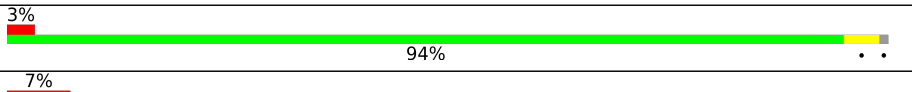
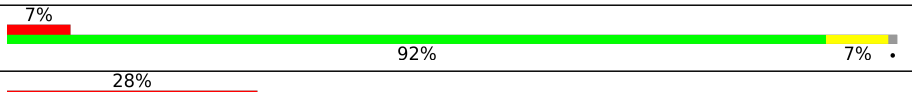
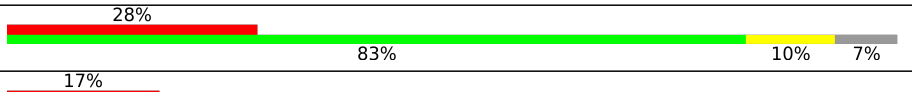
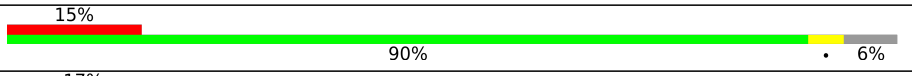
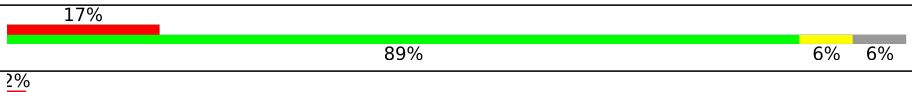
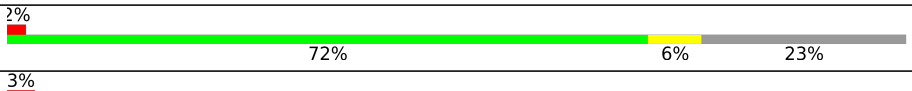
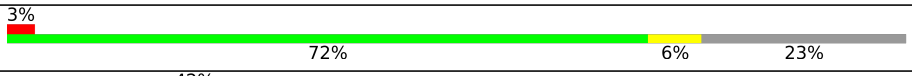
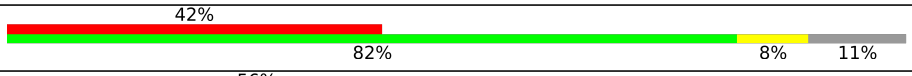
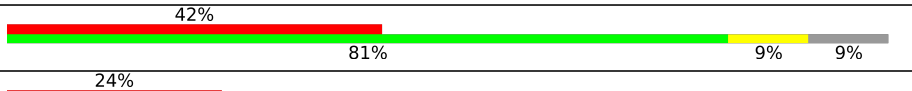
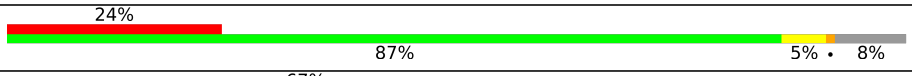
Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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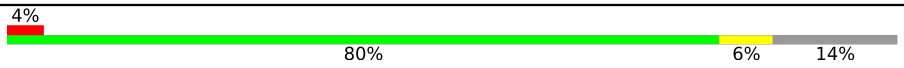
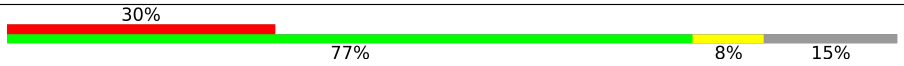
Mol	Chain	Length	Quality of chain
53	1y	113	
53	2y	113	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	1A	3279	-	-	-	X
54	MG	1F	316	-	-	-	X
54	MG	1a	1665	-	-	-	X
54	MG	1l	202	-	-	-	X
54	MG	2A	3495	-	-	-	X
54	MG	2A	3668	-	-	-	X
54	MG	2a	3025	-	-	-	X
54	MG	2a	3074	-	-	-	X
54	MG	2a	3099	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 297328 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
			61871	27542	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61760	27493	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	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1025	Total 1025	Mg 1025	0	0
54	1B	29	Total 29	Mg 29	0	0
54	1D	16	Total 16	Mg 16	0	0
54	1E	9	Total 9	Mg 9	0	0
54	1F	17	Total 17	Mg 17	0	0
54	1G	4	Total 4	Mg 4	0	0
54	1H	2	Total 2	Mg 2	0	0
54	1N	4	Total 4	Mg 4	0	0
54	1O	1	Total 1	Mg 1	0	0
54	1P	6	Total 6	Mg 6	0	0
54	1Q	5	Total 5	Mg 5	0	0
54	1R	4	Total 4	Mg 4	0	0
54	1T	4	Total 4	Mg 4	0	0
54	1U	9	Total 9	Mg 9	0	0
54	1V	6	Total 6	Mg 6	0	0
54	1W	2	Total 2	Mg 2	0	0
54	1Y	2	Total 2	Mg 2	0	0
54	1Z	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	10	8	Total Mg 8 8	0	0
54	11	6	Total Mg 6 6	0	0
54	13	4	Total Mg 4 4	0	0
54	15	8	Total Mg 8 8	0	0
54	17	5	Total Mg 5 5	0	0
54	18	2	Total Mg 2 2	0	0
54	19	2	Total Mg 2 2	0	0
54	1a	281	Total Mg 281 281	0	0
54	1b	1	Total Mg 1 1	0	0
54	1d	3	Total Mg 3 3	0	0
54	1e	3	Total Mg 3 3	0	0
54	1f	2	Total Mg 2 2	0	0
54	1g	3	Total Mg 3 3	0	0
54	1h	2	Total Mg 2 2	0	0
54	1i	1	Total Mg 1 1	0	0
54	1k	1	Total Mg 1 1	0	0
54	1l	2	Total Mg 2 2	0	0
54	1m	1	Total Mg 1 1	0	0
54	1n	1	Total Mg 1 1	0	0
54	1o	2	Total Mg 2 2	0	0
54	1t	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1y	2	Total Mg 2 2	0	0
54	2A	670	Total Mg 670 670	0	0
54	2B	14	Total Mg 14 14	0	0
54	2D	7	Total Mg 7 7	0	0
54	2E	5	Total Mg 5 5	0	0
54	2F	4	Total Mg 4 4	0	0
54	2G	1	Total Mg 1 1	0	0
54	2O	1	Total Mg 1 1	0	0
54	2P	1	Total Mg 1 1	0	0
54	2Q	4	Total Mg 4 4	0	0
54	2R	2	Total Mg 2 2	0	0
54	2T	4	Total Mg 4 4	0	0
54	2U	1	Total Mg 1 1	0	0
54	2V	1	Total Mg 1 1	0	0
54	2W	3	Total Mg 3 3	0	0
54	2Y	1	Total Mg 1 1	0	0
54	20	2	Total Mg 2 2	0	0
54	21	1	Total Mg 1 1	0	0
54	23	1	Total Mg 1 1	0	0
54	25	3	Total Mg 3 3	0	0
54	27	1	Total Mg 1 1	0	0

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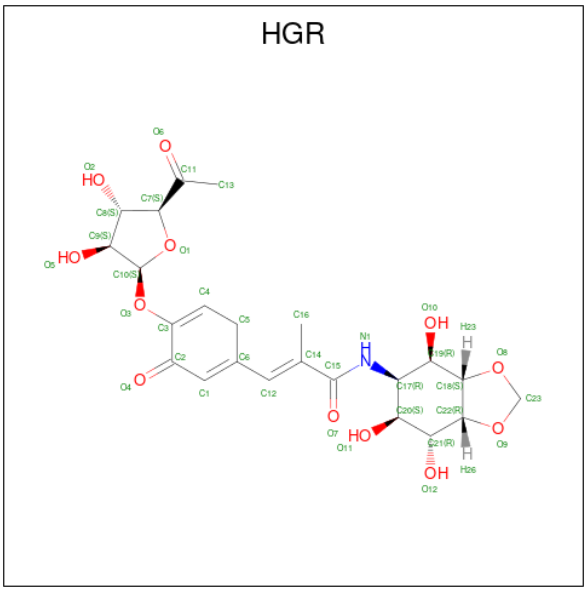
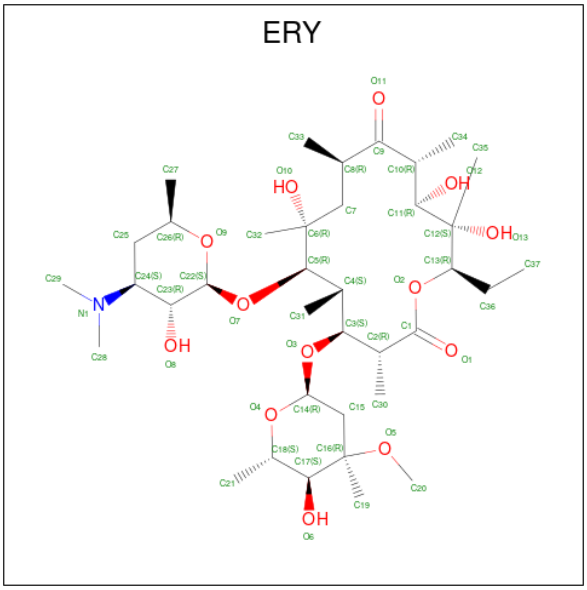
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	28	2	Total Mg 2 2	0	0
54	2a	190	Total Mg 190 190	0	0
54	2e	1	Total Mg 1 1	0	0
54	2f	1	Total Mg 1 1	0	0
54	2h	1	Total Mg 1 1	0	0
54	2j	1	Total Mg 1 1	0	0
54	2k	1	Total Mg 1 1	0	0
54	2l	1	Total Mg 1 1	0	0
54	2n	1	Total Mg 1 1	0	0
54	2r	1	Total Mg 1 1	0	0
54	2t	1	Total Mg 1 1	0	0

- Molecule 55 is Hygromycin A (three-letter code: HGR) (formula: $C_{23}H_{29}NO_{12}$) (labeled as "Ligand of Interest" by depositor).



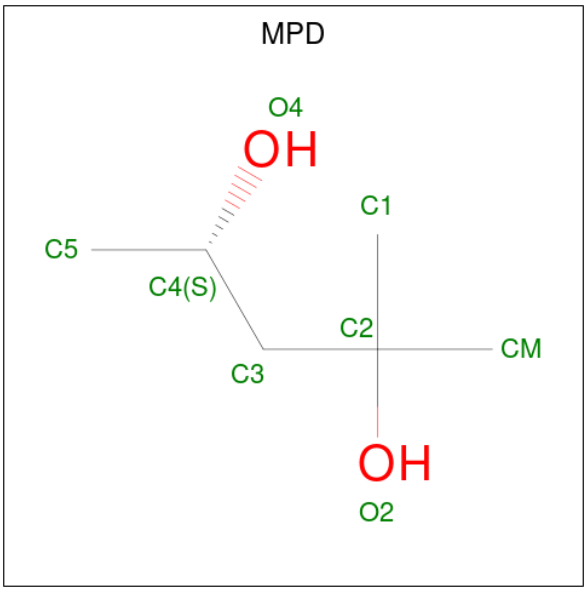
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1A	1	Total C N O 36 23 1 12	0	0
55	2A	1	Total C N O 36 23 1 12	0	0

- Molecule 56 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



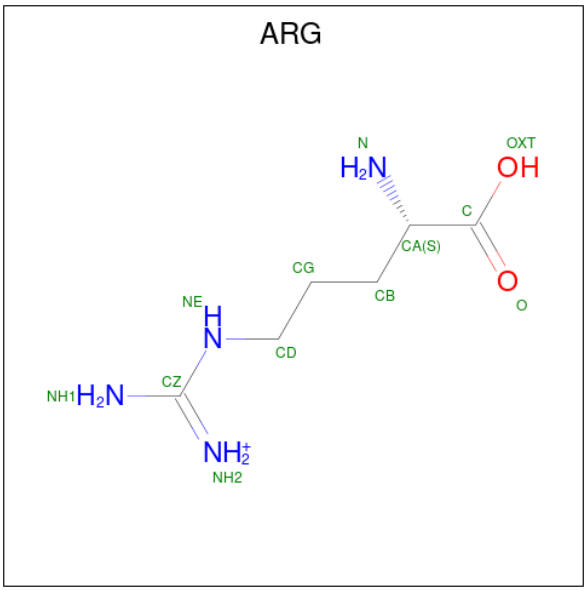
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1A	1	Total C N O 51 37 1 13	0	0
56	2A	1	Total C N O 51 37 1 13	0	0

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



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

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



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

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

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

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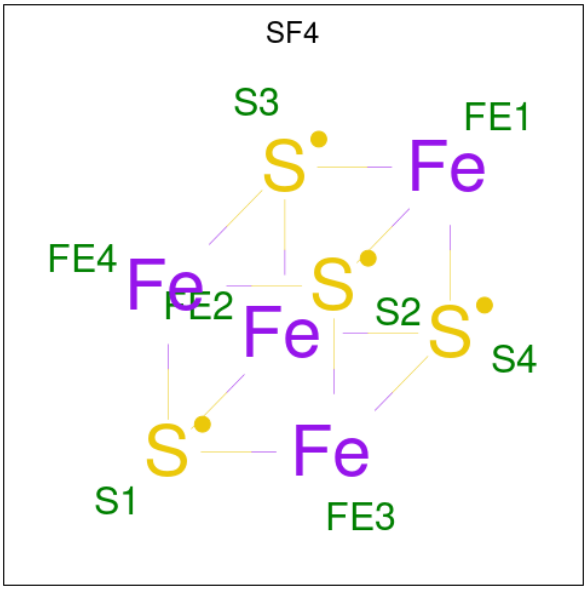
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	3899	Total O 3899 3899	0	0
61	1B	94	Total O 94 94	0	0
61	1D	118	Total O 118 118	0	0
61	1E	83	Total O 83 83	0	0
61	1F	63	Total O 63 63	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1G	15	Total O 15 15	0	0
61	1H	12	Total O 12 12	0	0
61	1I	7	Total O 7 7	0	0
61	1N	51	Total O 51 51	0	0
61	1O	27	Total O 27 27	0	0
61	1P	64	Total O 64 64	0	0
61	1Q	43	Total O 43 43	0	0
61	1R	34	Total O 34 34	0	0
61	1S	10	Total O 10 10	0	0
61	1T	38	Total O 38 38	0	0
61	1U	42	Total O 42 42	0	0
61	1V	36	Total O 36 36	0	0
61	1W	28	Total O 28 28	0	0
61	1X	27	Total O 27 27	0	0
61	1Y	17	Total O 17 17	0	0
61	1Z	10	Total O 10 10	0	0
61	10	22	Total O 22 22	0	0
61	11	26	Total O 26 26	0	0
61	12	14	Total O 14 14	0	0
61	13	23	Total O 23 23	0	0
61	14	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	15	25	Total O 25 25	0	0
61	16	20	Total O 20 20	0	0
61	17	14	Total O 14 14	0	0
61	18	24	Total O 24 24	0	0
61	19	4	Total O 4 4	0	0
61	1a	454	Total O 454 454	0	0
61	1c	2	Total O 2 2	0	0
61	1d	7	Total O 7 7	0	0
61	1e	4	Total O 4 4	0	0
61	1f	2	Total O 2 2	0	0
61	1h	1	Total O 1 1	0	0
61	1l	2	Total O 2 2	0	0
61	1m	1	Total O 1 1	0	0
61	1o	5	Total O 5 5	0	0
61	1p	4	Total O 4 4	0	0
61	1y	4	Total O 4 4	0	0
61	2A	2164	Total O 2164 2164	0	0
61	2B	45	Total O 45 45	0	0
61	2D	52	Total O 52 52	0	0
61	2E	31	Total O 31 31	0	0
61	2F	23	Total O 23 23	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2G	7	Total O 7 7	0	0
61	2H	1	Total O 1 1	0	0
61	2I	4	Total O 4 4	0	0
61	2N	5	Total O 5 5	0	0
61	2O	19	Total O 19 19	0	0
61	2P	26	Total O 26 26	0	0
61	2Q	15	Total O 15 15	0	0
61	2R	18	Total O 18 18	0	0
61	2S	5	Total O 5 5	0	0
61	2T	11	Total O 11 11	0	0
61	2U	15	Total O 15 15	0	0
61	2V	6	Total O 6 6	0	0
61	2W	18	Total O 18 18	0	0
61	2X	8	Total O 8 8	0	0
61	2Y	2	Total O 2 2	0	0
61	2Z	9	Total O 9 9	0	0
61	20	9	Total O 9 9	0	0
61	21	17	Total O 17 17	0	0
61	22	1	Total O 1 1	0	0
61	23	3	Total O 3 3	0	0
61	24	1	Total O 1 1	0	0

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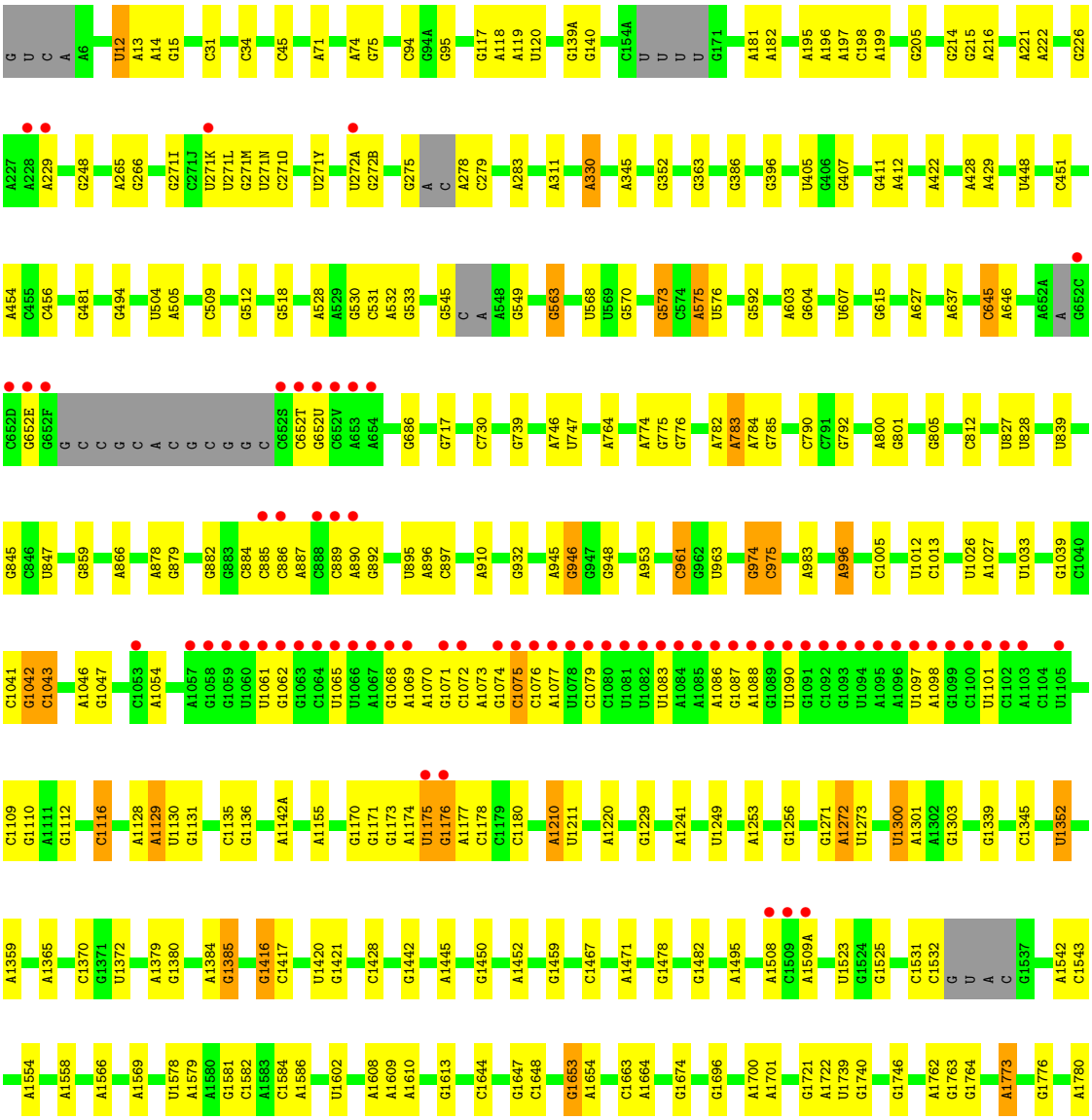
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	25	7	Total O 7 7	0	0
61	26	4	Total O 4 4	0	0
61	27	6	Total O 6 6	0	0
61	28	8	Total O 8 8	0	0
61	29	1	Total O 1 1	0	0
61	2a	322	Total O 322 322	0	0
61	2d	3	Total O 3 3	0	0
61	2e	1	Total O 1 1	0	0
61	2f	3	Total O 3 3	0	0
61	2j	2	Total O 2 2	0	0
61	2l	2	Total O 2 2	0	0
61	2n	1	Total O 1 1	0	0
61	2o	2	Total O 2 2	0	0
61	2p	1	Total O 1 1	0	0
61	2q	2	Total O 2 2	0	0
61	2r	3	Total O 3 3	0	0
61	2t	2	Total O 2 2	0	0
61	2u	1	Total O 1 1	0	0
61	2y	2	Total O 2 2	0	0

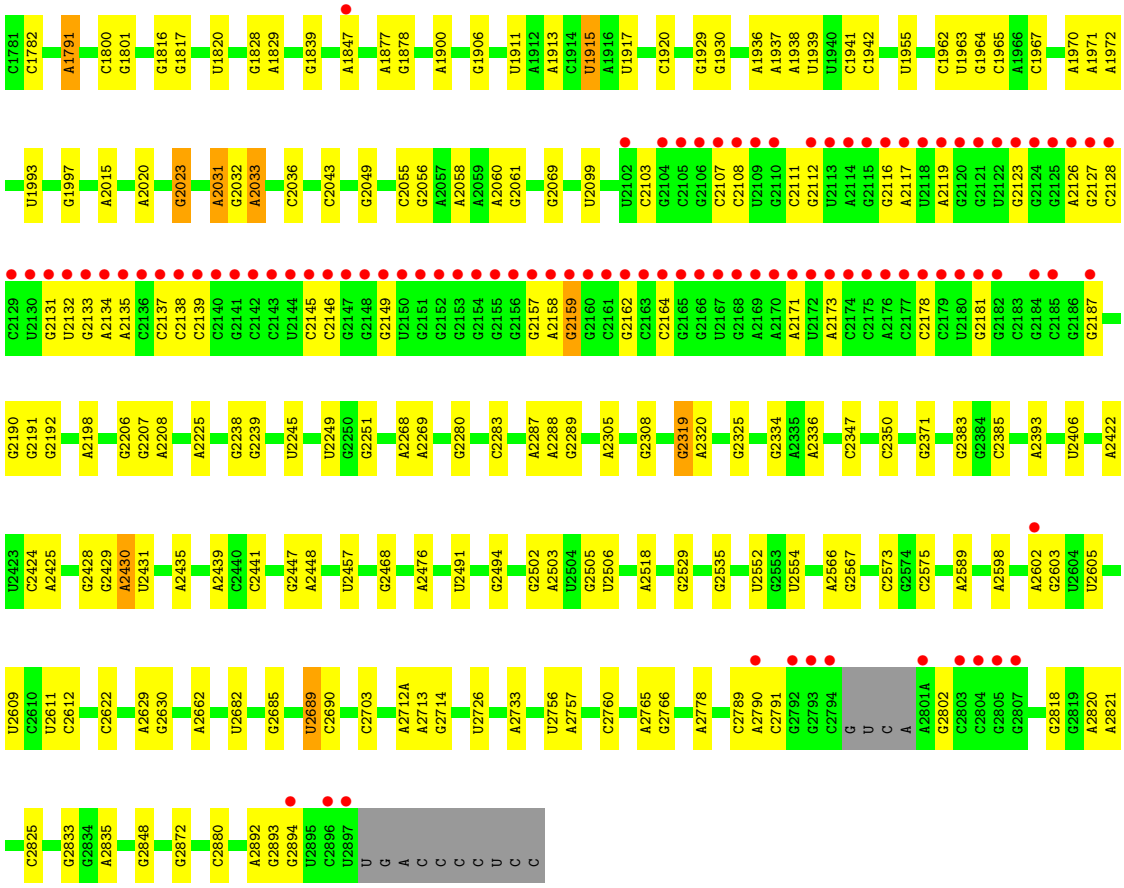
3 Residue-property plots (i)

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

- Molecule 1: 23S Ribosomal RNA

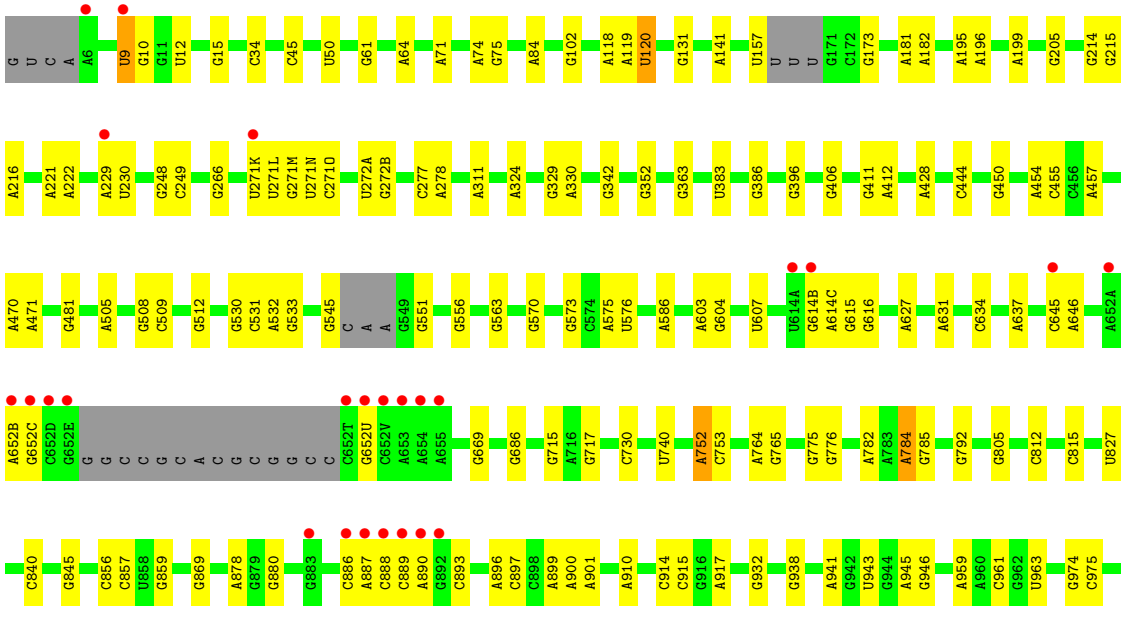
Chain 1A:

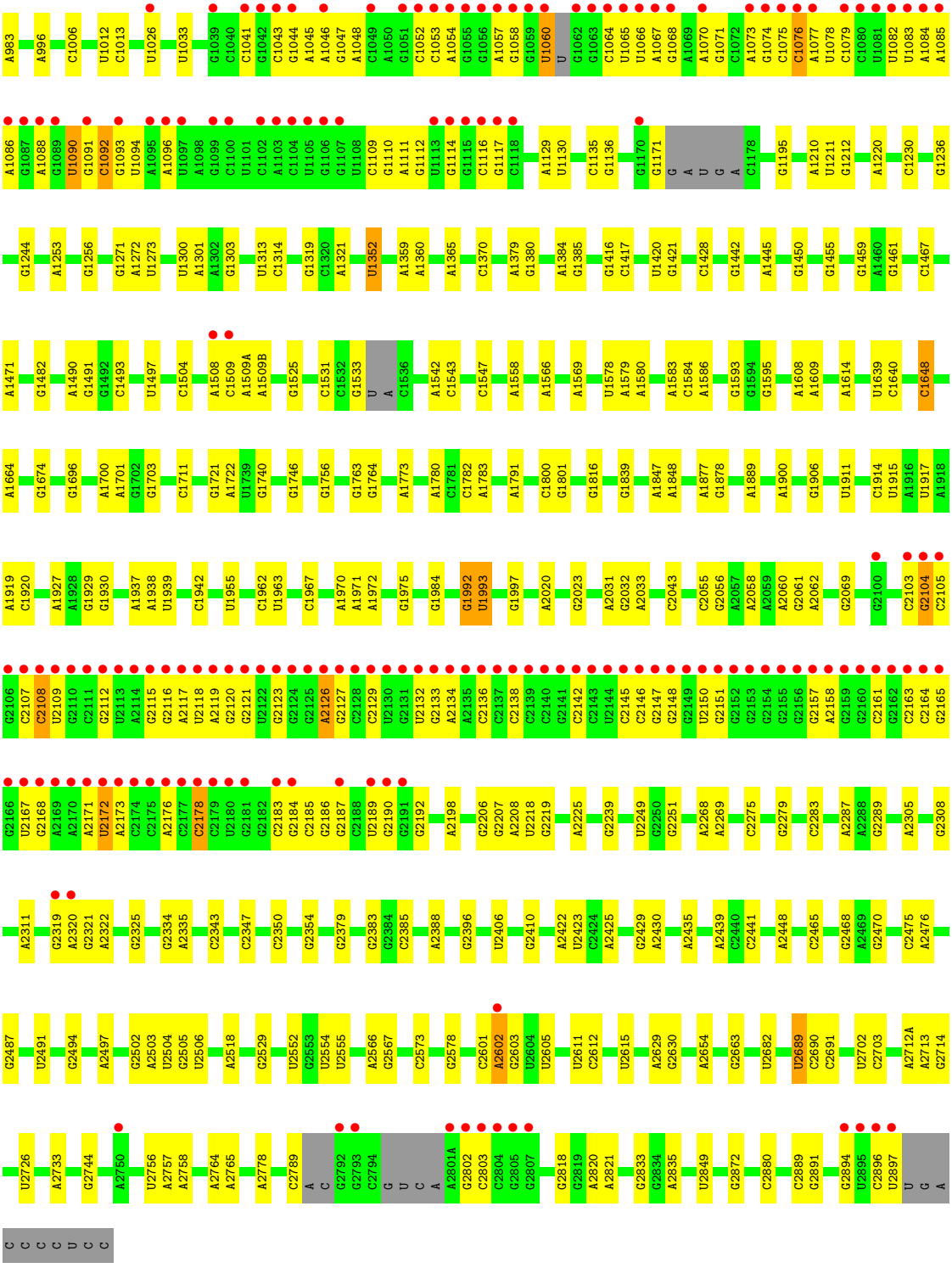




• Molecule 1: 23S Ribosomal RNA

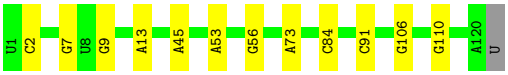
Chain 2A:





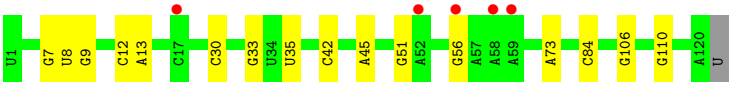
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



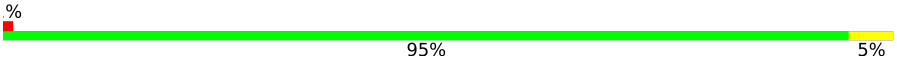
• Molecule 2: 5S Ribosomal RNA

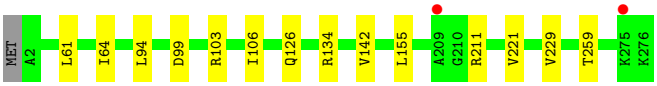
Chain 2B:



• Molecule 3: 50S ribosomal protein L2

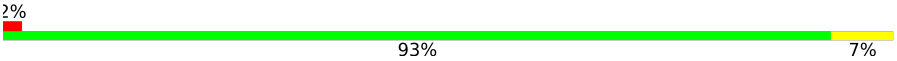
Chain 1D:

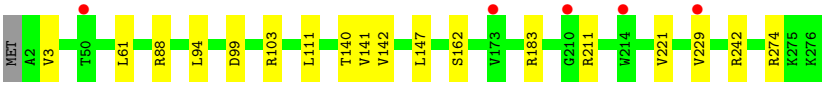




• Molecule 3: 50S ribosomal protein L2

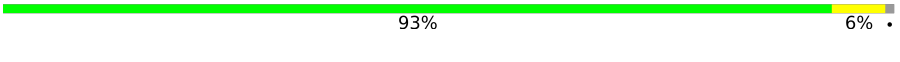
Chain 2D:

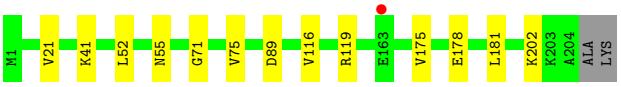




• Molecule 4: 50S ribosomal protein L3

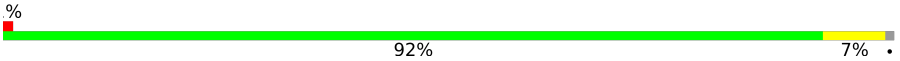
Chain 1E:

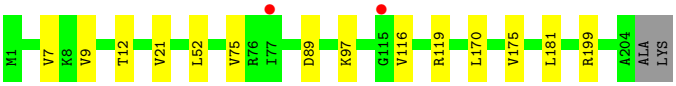




• Molecule 4: 50S ribosomal protein L3

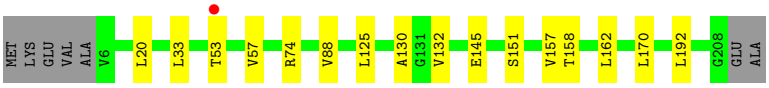
Chain 2E:





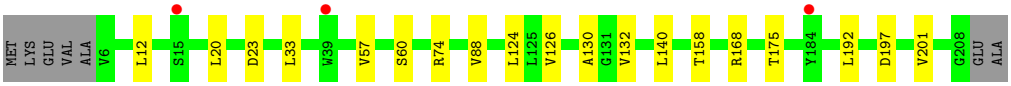
• Molecule 5: 50S ribosomal protein L4

Chain 1F:

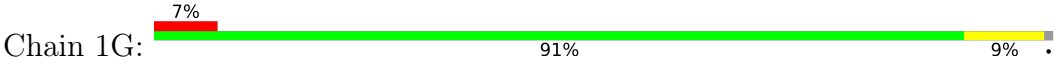


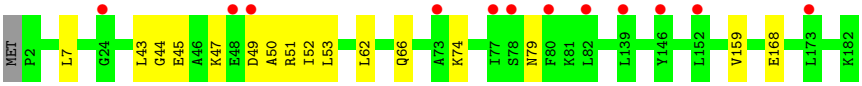
• Molecule 5: 50S ribosomal protein L4

Chain 2F:

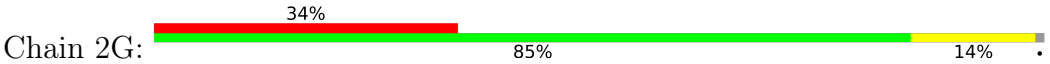


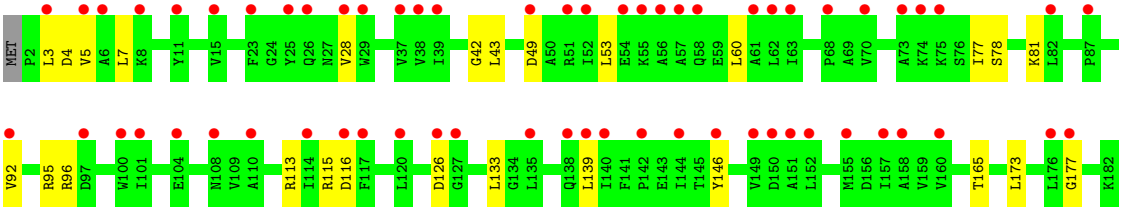
• Molecule 6: 50S ribosomal protein L5



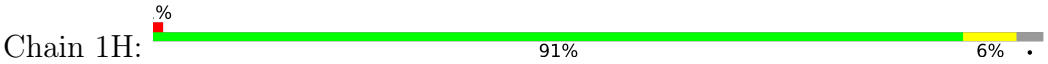


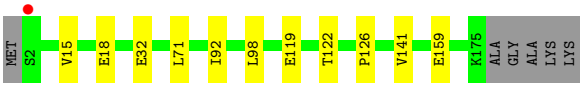
• Molecule 6: 50S ribosomal protein L5



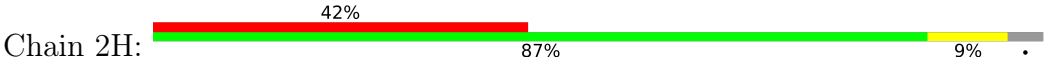


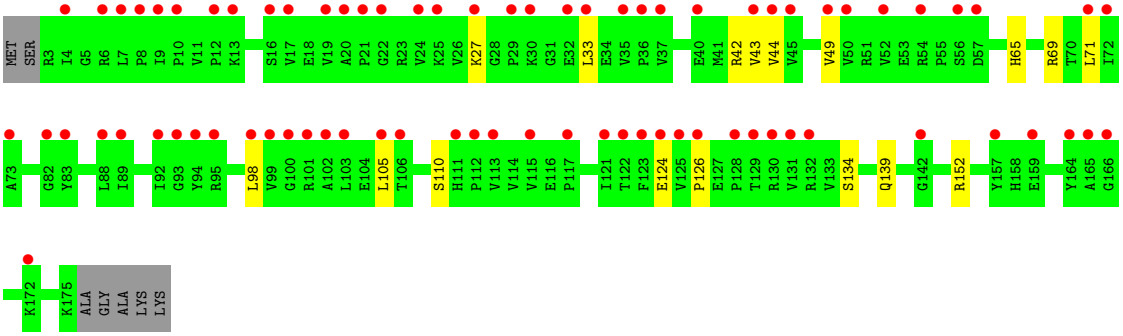
• Molecule 7: 50S ribosomal protein L6



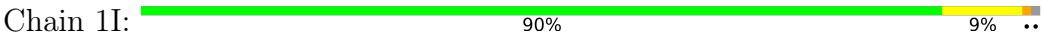


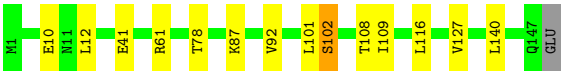
• Molecule 7: 50S ribosomal protein L6





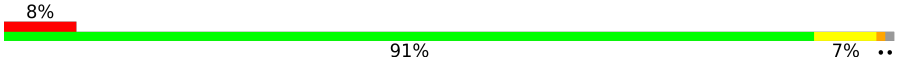
• Molecule 8: 50S ribosomal protein L9

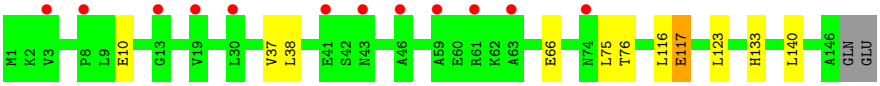




• Molecule 8: 50S ribosomal protein L9

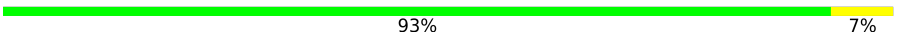
Chain 2I:





• Molecule 9: 50S ribosomal protein L13

Chain 1N:

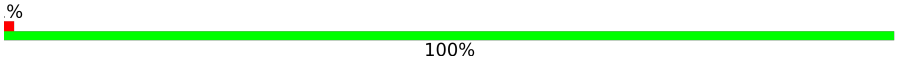


• Molecule 9: 50S ribosomal protein L13

Chain 2N:

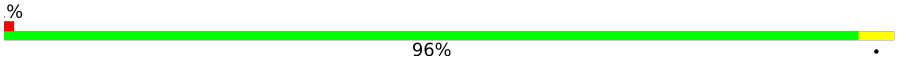
• Molecule 10: 50S ribosomal protein L14

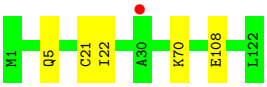
Chain 1O:



• Molecule 10: 50S ribosomal protein L14

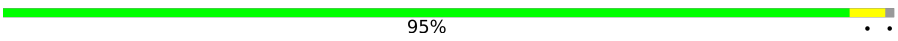
Chain 2O:

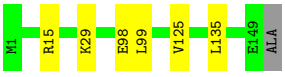




• Molecule 11: 50S ribosomal protein L15

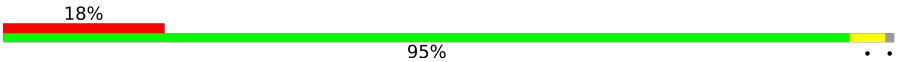
Chain 1P:

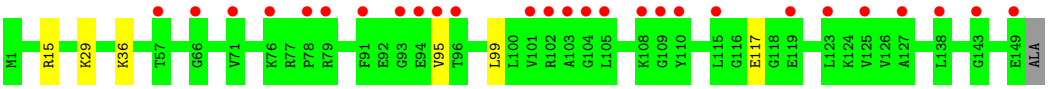




• Molecule 11: 50S ribosomal protein L15

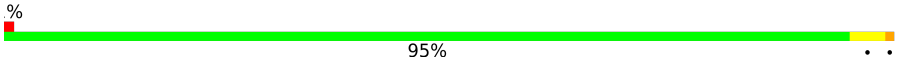
Chain 2P:

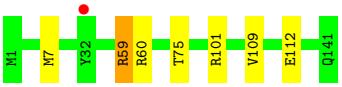




• Molecule 12: 50S ribosomal protein L16

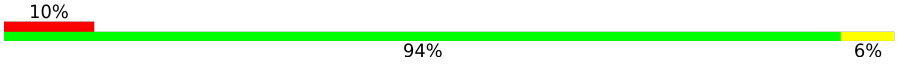
Chain 1Q:

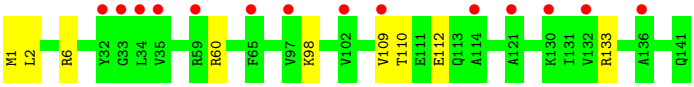




• Molecule 12: 50S ribosomal protein L16

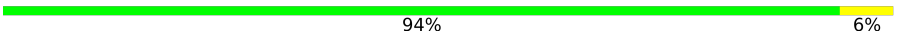
Chain 2Q:

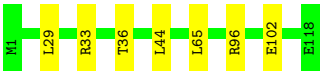




• Molecule 13: 50S ribosomal protein L17

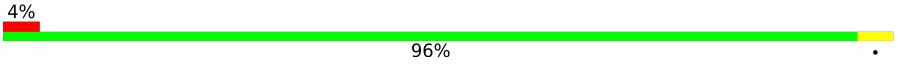
Chain 1R:

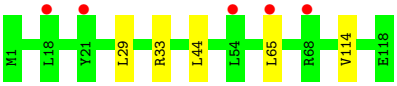




• Molecule 13: 50S ribosomal protein L17

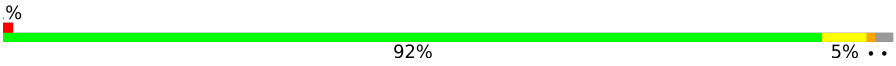
Chain 2R:





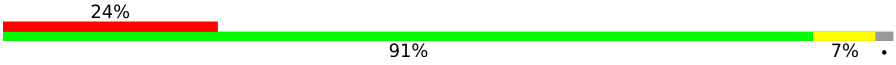
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



• Molecule 14: 50S ribosomal protein L18

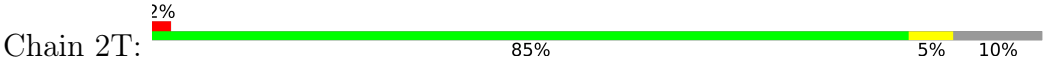
Chain 2S:

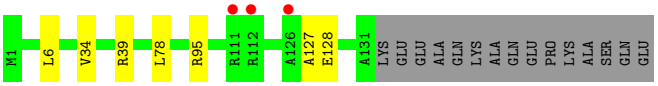


• Molecule 15: 50S ribosomal protein L19

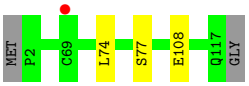
Chain 1T:

• Molecule 15: 50S ribosomal protein L19

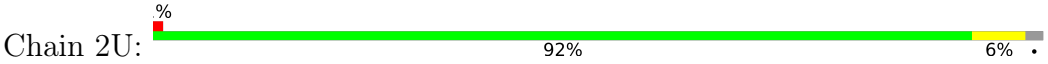




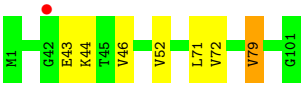
• Molecule 16: 50S ribosomal protein L20



• Molecule 16: 50S ribosomal protein L20



• Molecule 17: 50S ribosomal protein L21

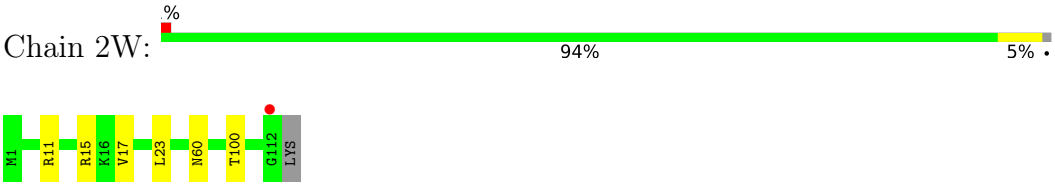


• Molecule 17: 50S ribosomal protein L21

• Molecule 18: 50S ribosomal protein L22

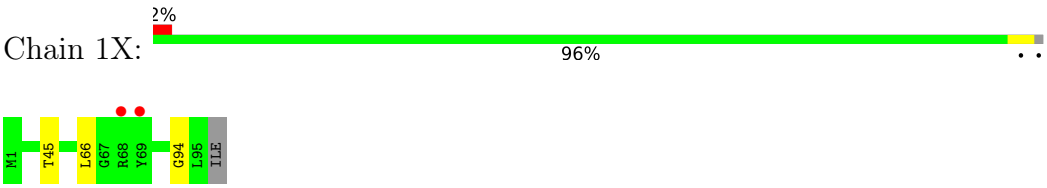
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



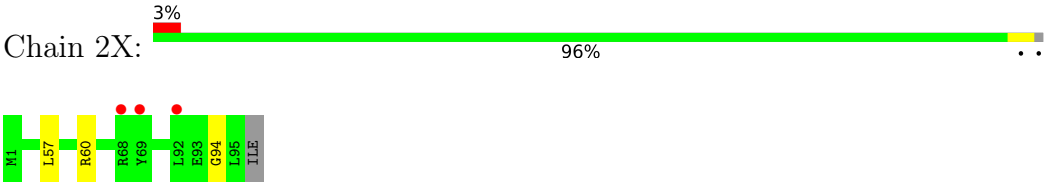
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



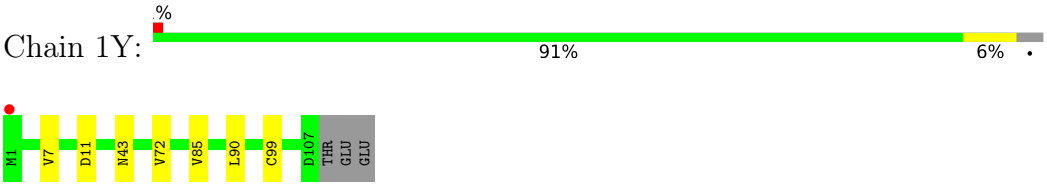
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



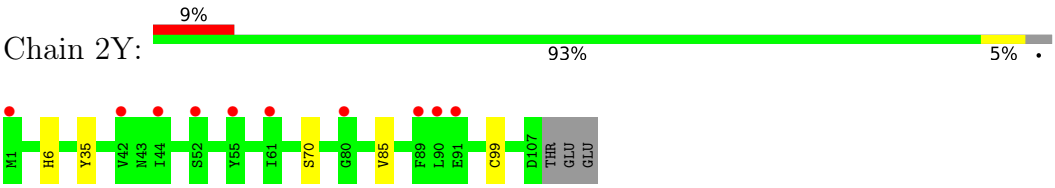
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



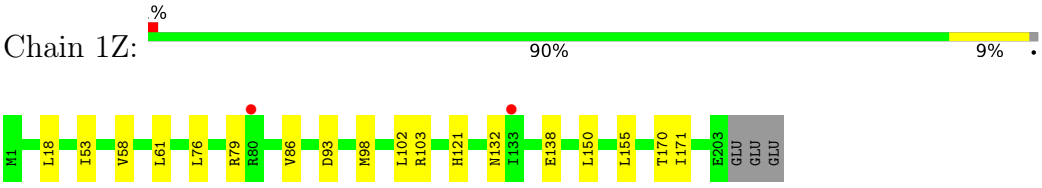
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



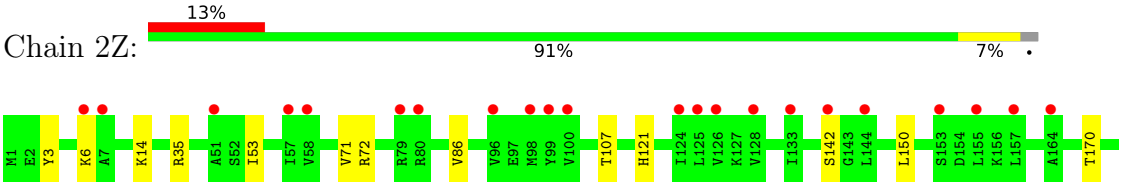
• Molecule 21: 50S ribosomal protein L25

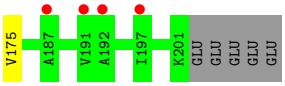
Chain 1Z:



• Molecule 21: 50S ribosomal protein L25

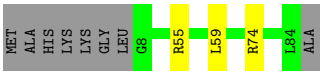
Chain 2Z:





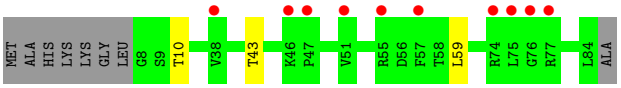
• Molecule 22: 50S ribosomal protein L27

Chain 10:



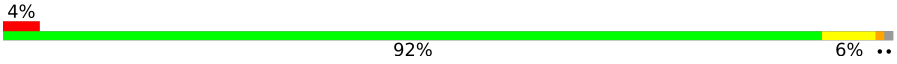
• Molecule 22: 50S ribosomal protein L27

Chain 20:



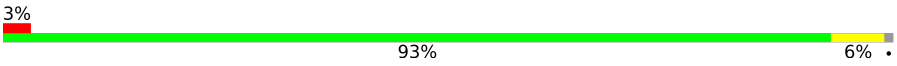
• Molecule 23: 50S ribosomal protein L28

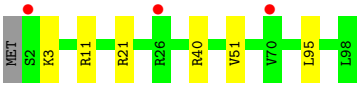
Chain 11:



• Molecule 23: 50S ribosomal protein L28

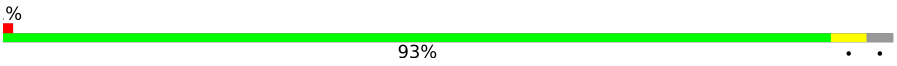
Chain 21:





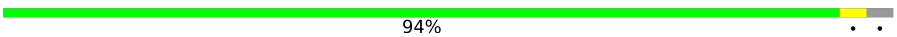
• Molecule 24: 50S ribosomal protein L29

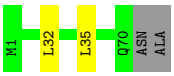
Chain 12:



• Molecule 24: 50S ribosomal protein L29

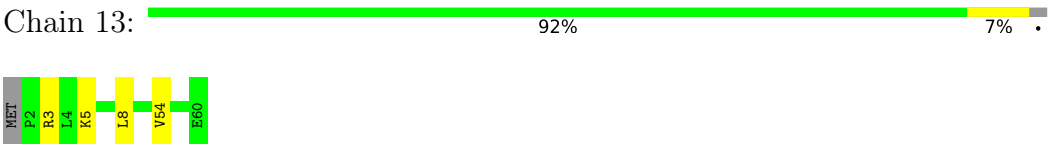
Chain 22:





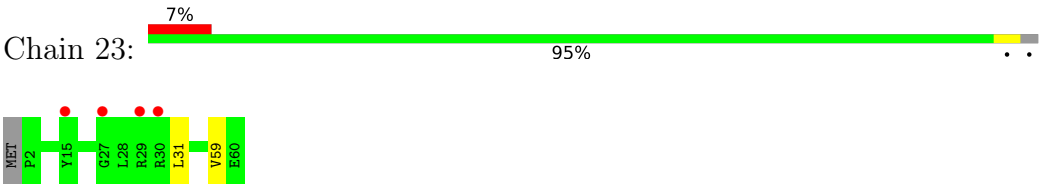
• Molecule 25: 50S ribosomal protein L30

Chain 13:



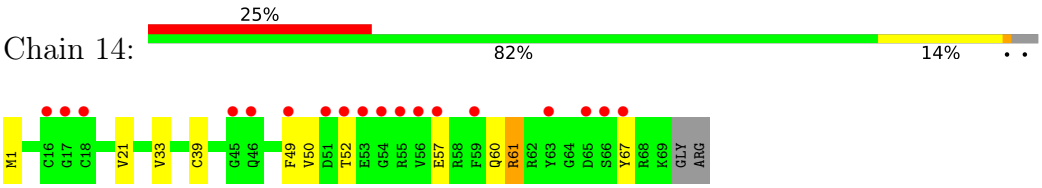
• Molecule 25: 50S ribosomal protein L30

Chain 23:



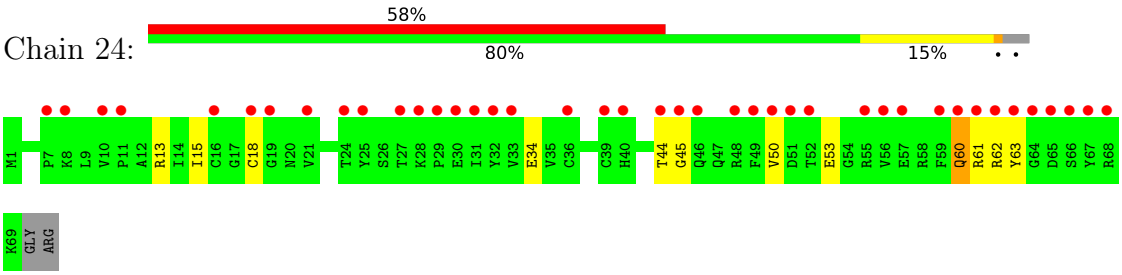
• Molecule 26: 50S ribosomal protein L31

Chain 14:



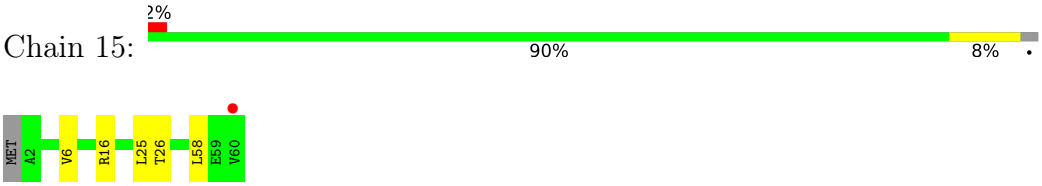
• Molecule 26: 50S ribosomal protein L31

Chain 24:



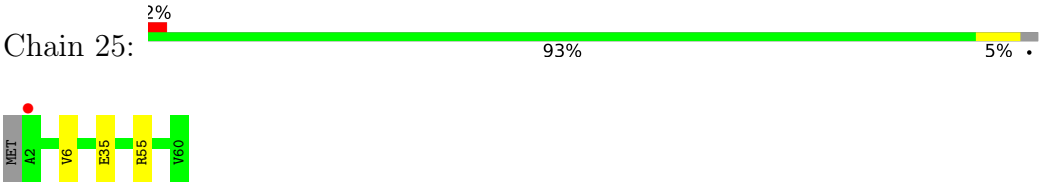
• Molecule 27: 50S ribosomal protein L32

Chain 15:



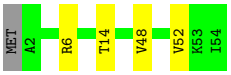
• Molecule 27: 50S ribosomal protein L32

Chain 25:



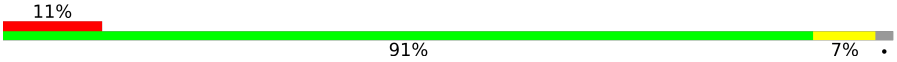
• Molecule 28: 50S ribosomal protein L33

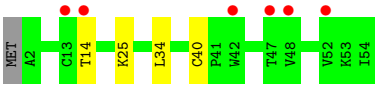
Chain 16:



• Molecule 28: 50S ribosomal protein L33

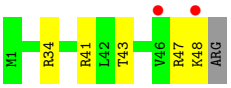
Chain 26:





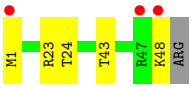
• Molecule 29: 50S ribosomal protein L34

Chain 17:



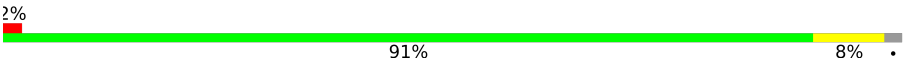
• Molecule 29: 50S ribosomal protein L34

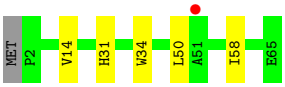
Chain 27:



• Molecule 30: 50S ribosomal protein L35

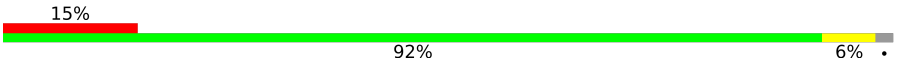
Chain 18:

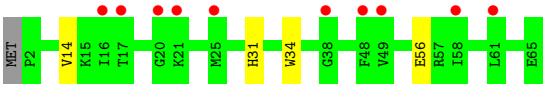




• Molecule 30: 50S ribosomal protein L35

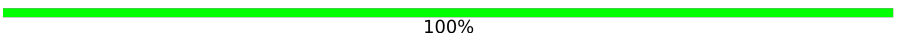
Chain 28:





• Molecule 31: 50S ribosomal protein L36

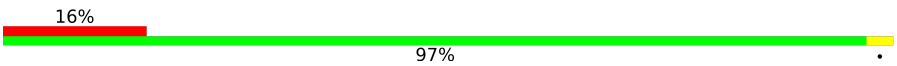
Chain 19:

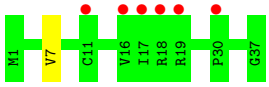


There are no outlier residues recorded for this chain.

• Molecule 31: 50S ribosomal protein L36

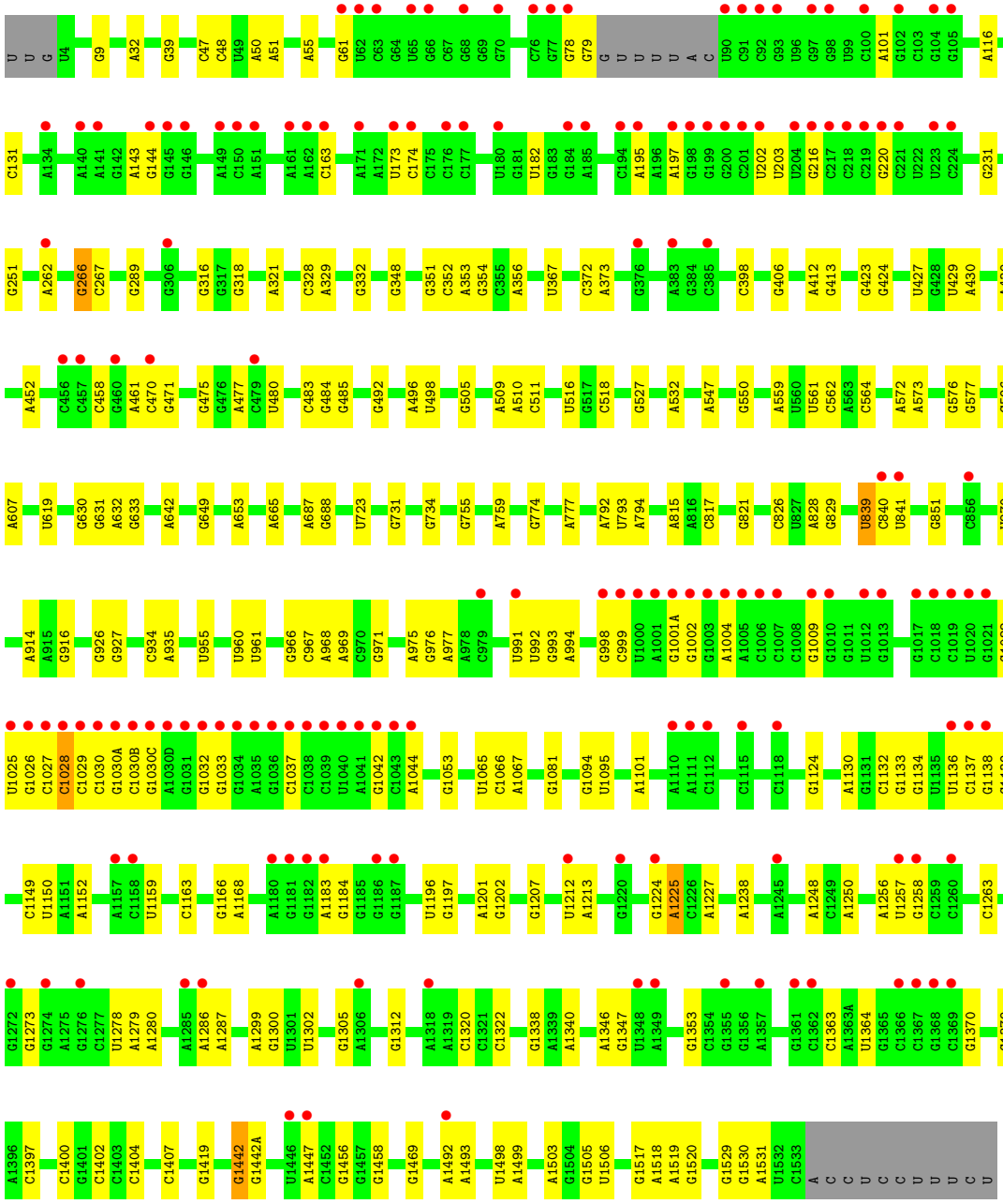
Chain 29:





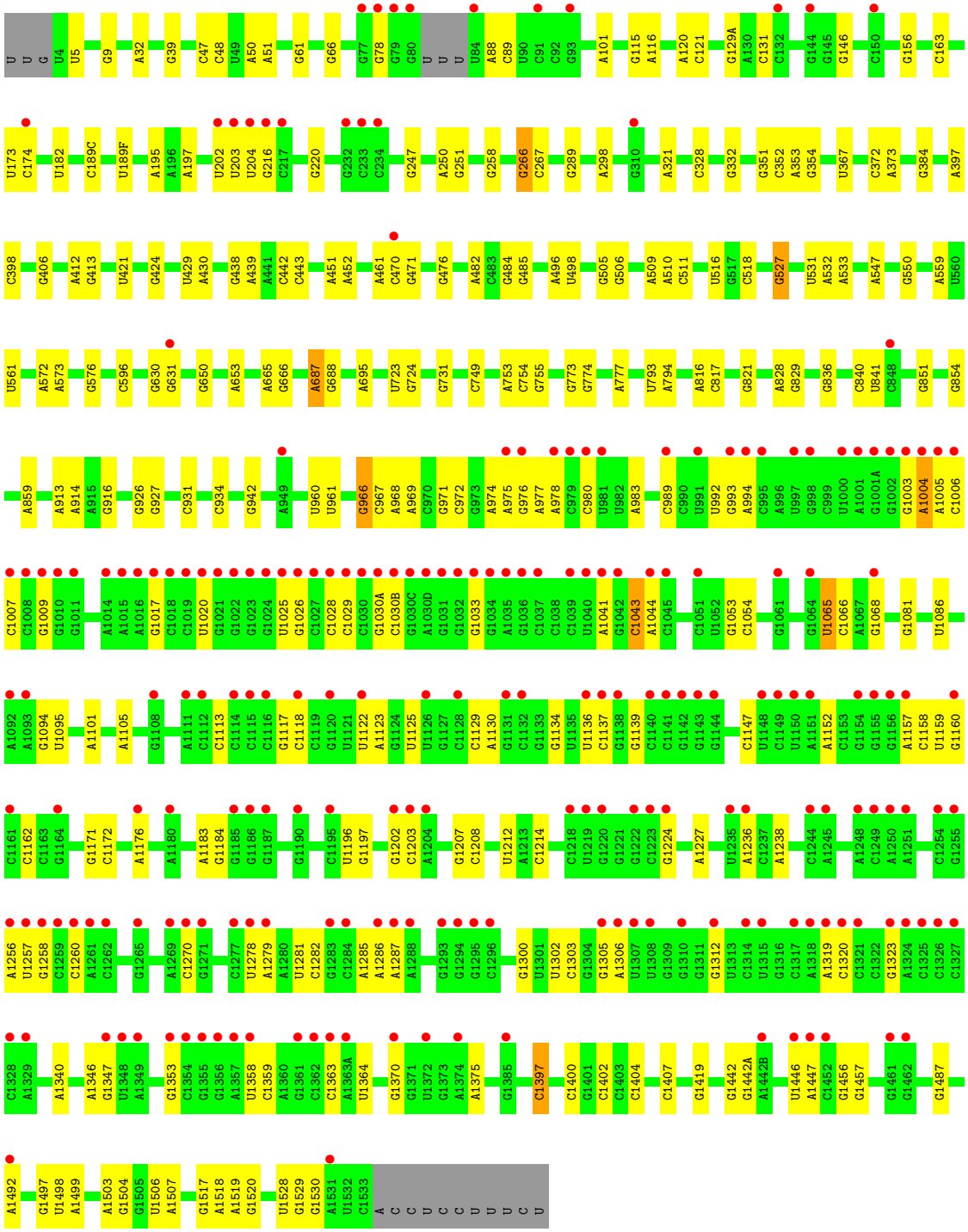
• Molecule 32: 16S Ribosomal RNA

Chain 1a:



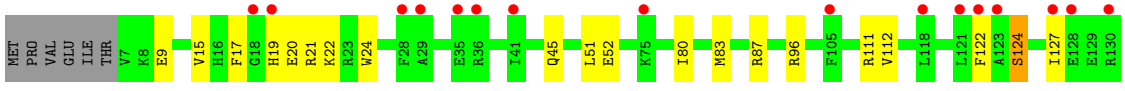
• Molecule 32: 16S Ribosomal RNA

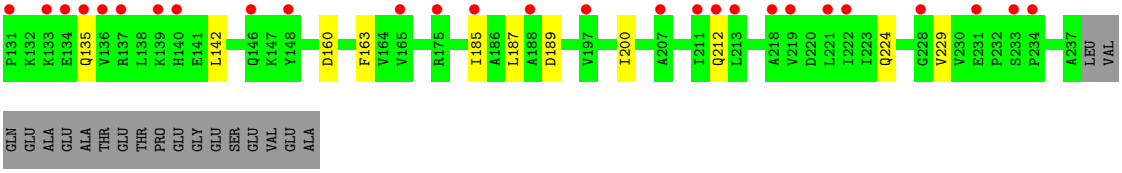
Chain 2a:



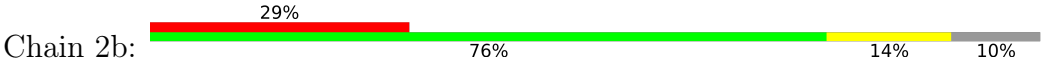
• Molecule 33: 30S ribosomal protein S2

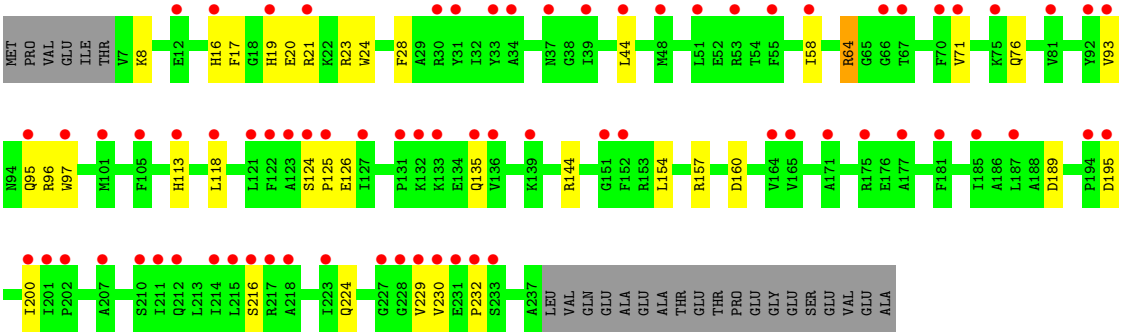
Chain 1b:



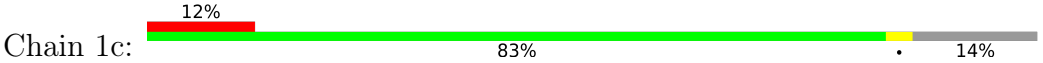


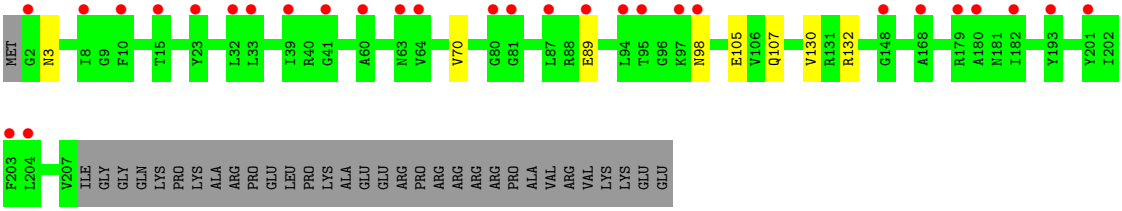
• Molecule 33: 30S ribosomal protein S2



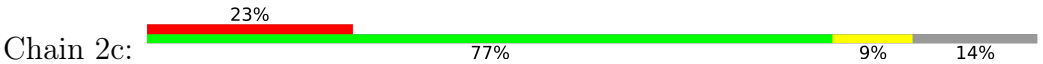


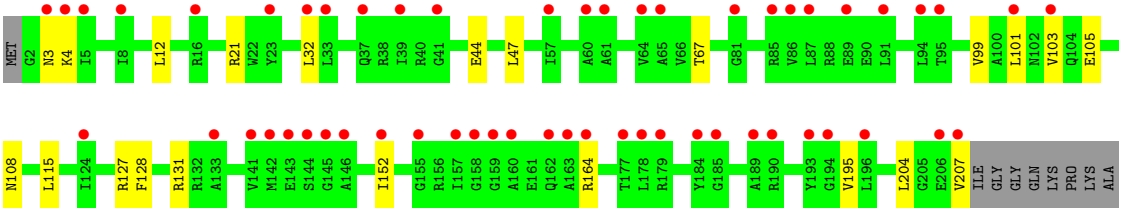
• Molecule 34: 30S ribosomal protein S3



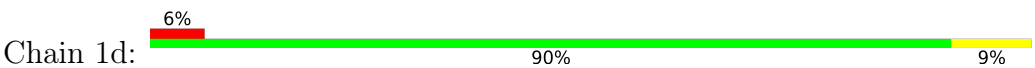


• Molecule 34: 30S ribosomal protein S3



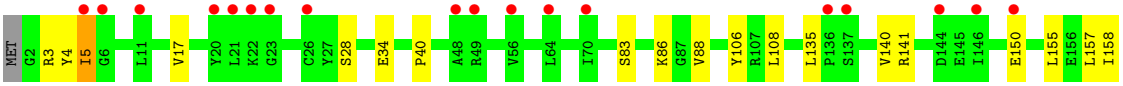


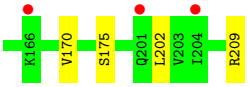
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

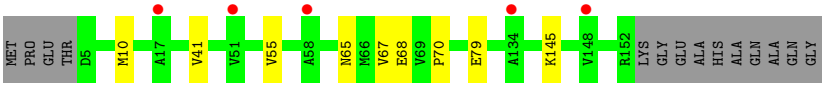
Chain 2d:





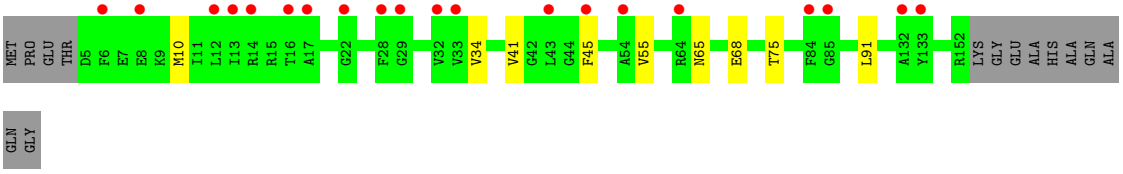
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



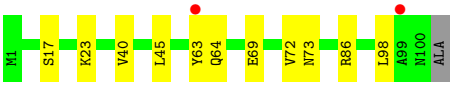
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



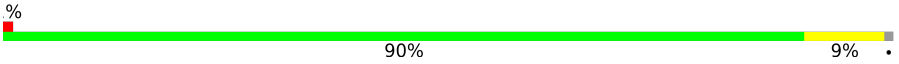
• Molecule 37: 30S ribosomal protein S6

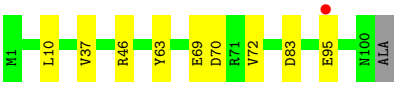
Chain 1f:



• Molecule 37: 30S ribosomal protein S6

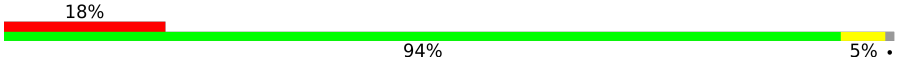
Chain 2f:

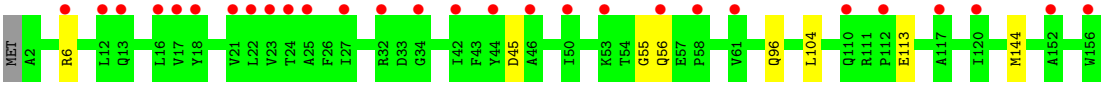




• Molecule 38: 30S ribosomal protein S7

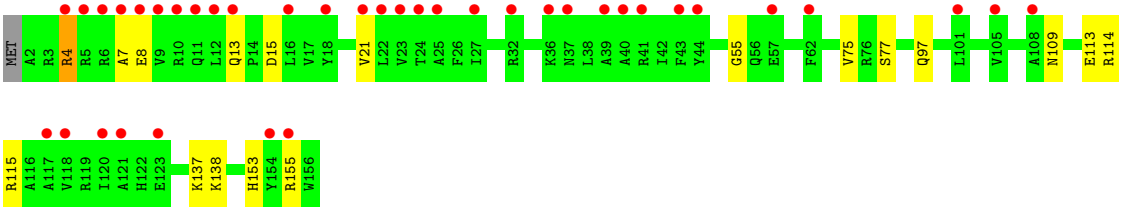
Chain 1g:





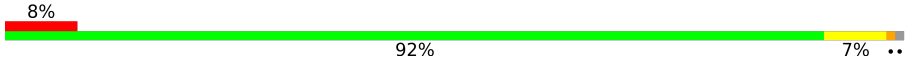
• Molecule 38: 30S ribosomal protein S7

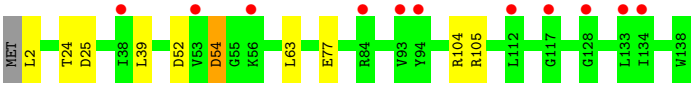
Chain 2g:



• Molecule 39: 30S ribosomal protein S8

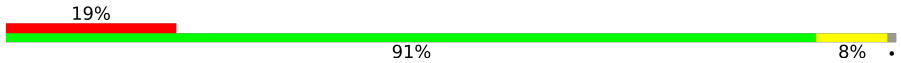
Chain 1h:

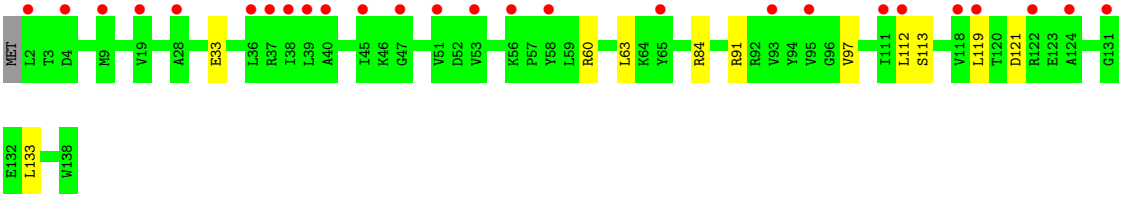




• Molecule 39: 30S ribosomal protein S8

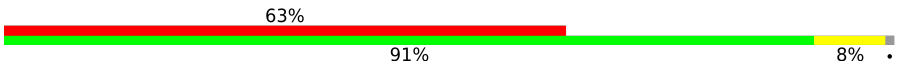
Chain 2h:

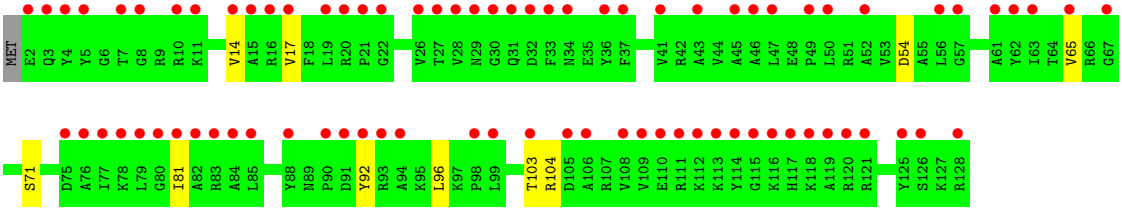




• Molecule 40: 30S ribosomal protein S9

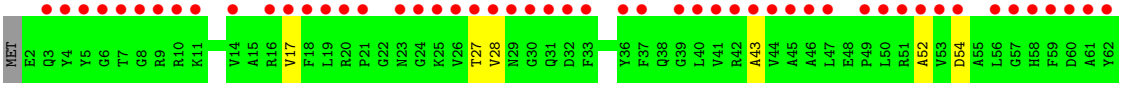
Chain 1i:

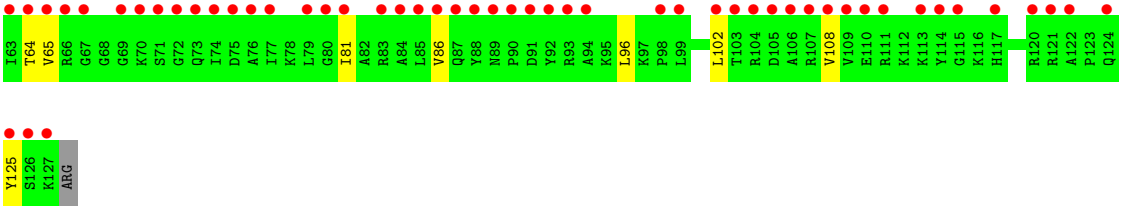




• Molecule 40: 30S ribosomal protein S9

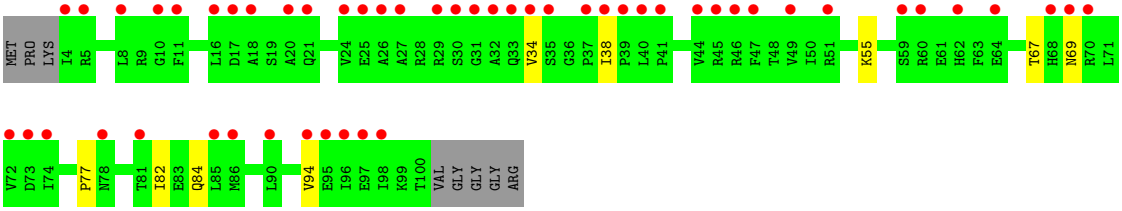
Chain 2i:





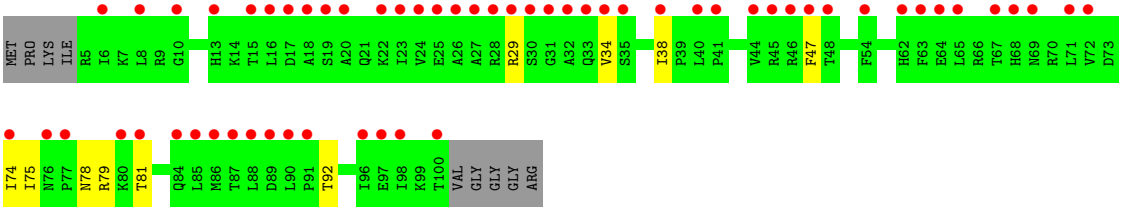
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



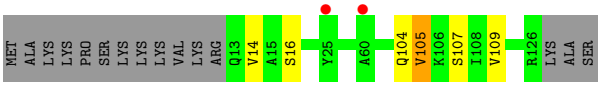
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



• Molecule 42: 30S ribosomal protein S11

Chain 1k:

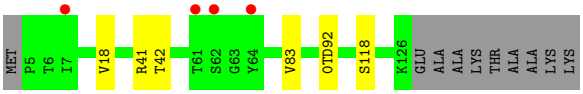


• Molecule 42: 30S ribosomal protein S11

Chain 2k:

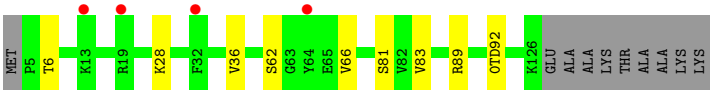
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



• Molecule 43: 30S ribosomal protein S12

Chain 2l:

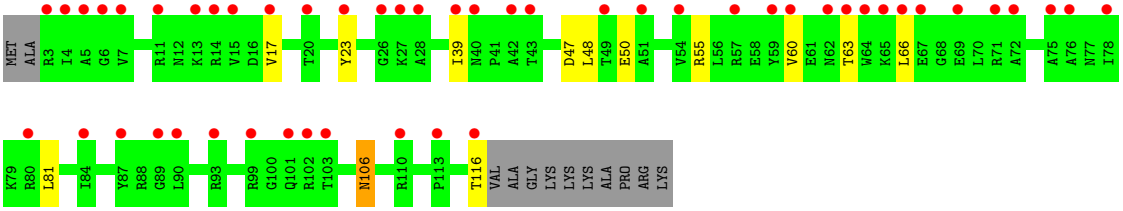


• Molecule 44: 30S ribosomal protein S13

Chain 1m:

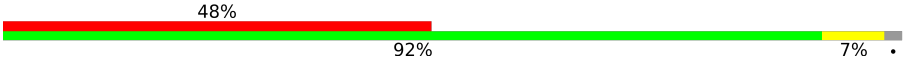
• Molecule 44: 30S ribosomal protein S13

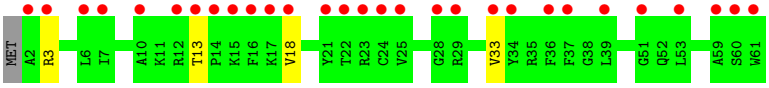
Chain 2m:



• Molecule 45: 30S ribosomal protein S14 type Z

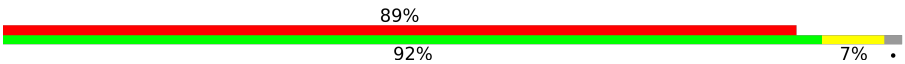
Chain 1n:

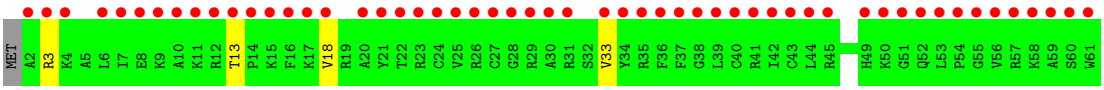




• Molecule 45: 30S ribosomal protein S14 type Z

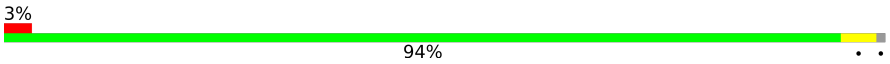
Chain 2n:





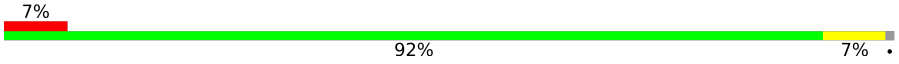
• Molecule 46: 30S ribosomal protein S15

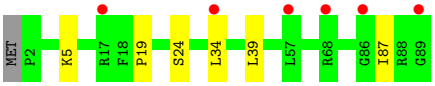
Chain 1o:



• Molecule 46: 30S ribosomal protein S15

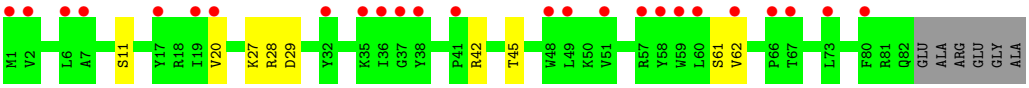
Chain 2o:





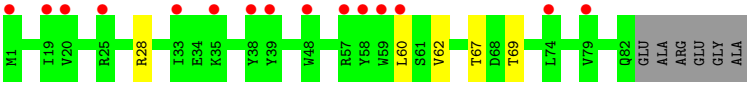
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



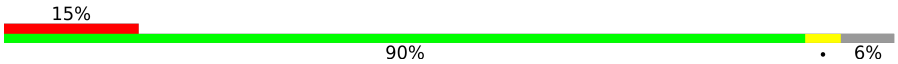
• Molecule 47: 30S ribosomal protein S16

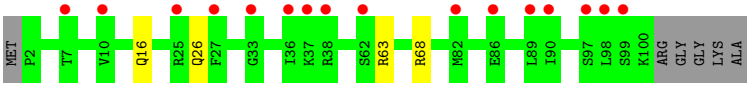
Chain 2p:



• Molecule 48: 30S ribosomal protein S17

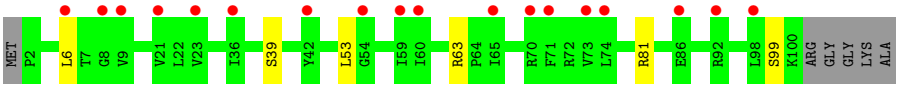
Chain 1q:





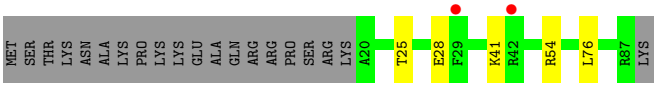
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



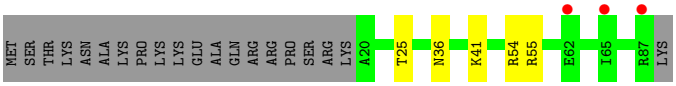
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



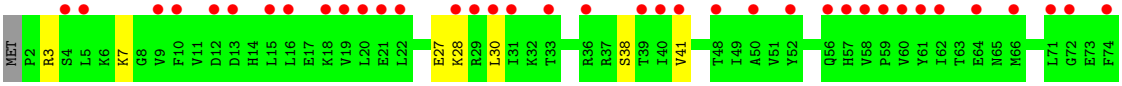
• Molecule 49: 30S ribosomal protein S18

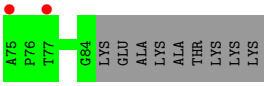
Chain 2r:



• Molecule 50: 30S ribosomal protein S19

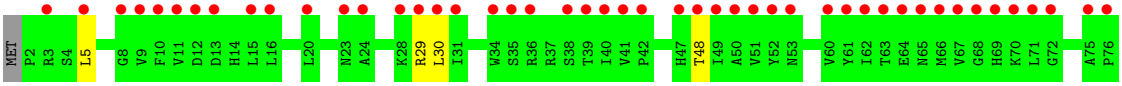
Chain 1s:

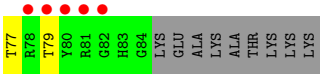




• Molecule 50: 30S ribosomal protein S19

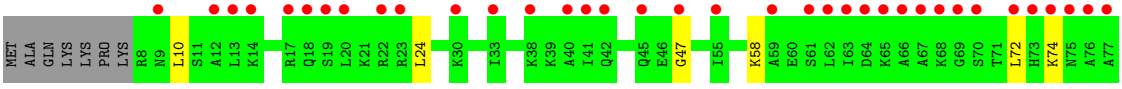
Chain 2s:

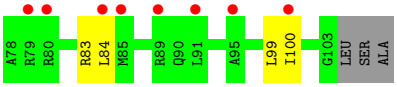




• Molecule 51: 30S ribosomal protein S20

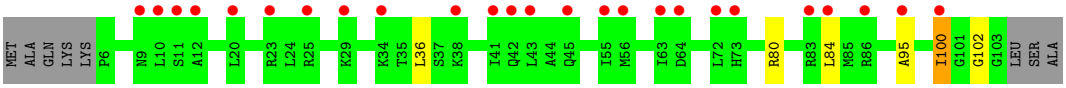
Chain 1t:





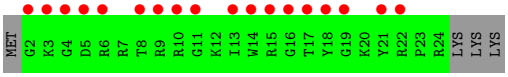
• Molecule 51: 30S ribosomal protein S20

Chain 2t:

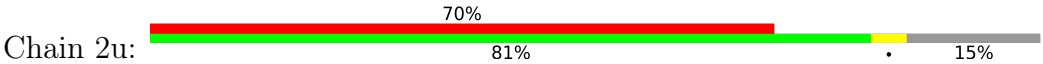


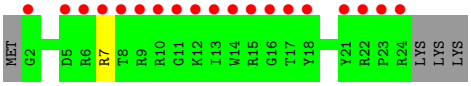
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:

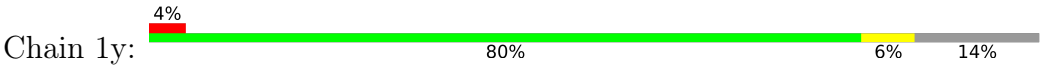


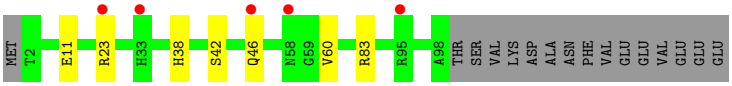
• Molecule 52: 30S ribosomal protein Thx



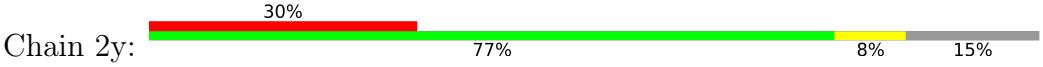


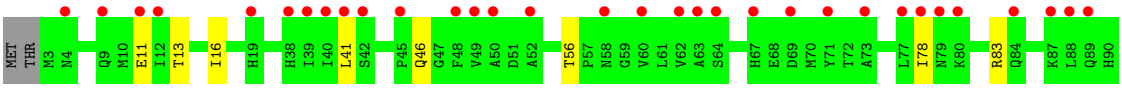
• Molecule 53: Ribosome-associated inhibitor A

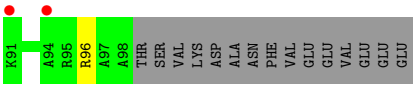




• Molecule 53: Ribosome-associated inhibitor A







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.46Å 449.56Å 619.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.72 – 2.45 161.85 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.7 (103.72-2.45) 98.7 (161.85-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.218 , 0.264 0.219 , 0.264	Depositor DCC
R_{free} test set	104449 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	52.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	297328	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.54	1/69005 (0.0%)	1.02	98/107711 (0.1%)
1	2A	0.42	2/68877 (0.0%)	0.91	59/107509 (0.1%)
2	1B	0.41	0/2876	0.91	0/4486
2	2B	0.35	0/2878	0.83	0/4490
3	1D	0.37	0/2181	0.62	0/2940
3	2D	0.33	0/2186	0.54	0/2944
4	1E	0.34	0/1592	0.55	0/2149
4	2E	0.31	0/1592	0.51	0/2149
5	1F	0.34	0/1619	0.55	0/2193
5	2F	0.31	0/1615	0.54	0/2188
6	1G	0.30	0/1451	0.47	0/1961
6	2G	0.29	0/1449	0.47	0/1957
7	1H	0.33	0/1356	0.50	0/1834
7	2H	0.29	0/1350	0.47	0/1826
8	1I	0.29	0/1109	0.49	0/1512
8	2I	0.28	0/1091	0.49	0/1490
9	1N	0.34	0/1148	0.53	0/1547
9	2N	0.29	0/1144	0.46	0/1543
10	1O	0.35	0/943	0.55	0/1269
10	2O	0.33	0/943	0.53	0/1269
11	1P	0.34	0/1152	0.54	0/1533
11	2P	0.29	0/1152	0.55	0/1533
12	1Q	0.36	0/1143	0.52	0/1527
12	2Q	0.30	0/1143	0.50	0/1527
13	1R	0.35	0/982	0.57	0/1312
13	2R	0.29	0/982	0.50	0/1312
14	1S	0.31	0/887	0.51	0/1180
14	2S	0.30	0/880	0.52	0/1172
15	1T	0.32	0/1105	0.53	0/1477
15	2T	0.30	0/1097	0.47	0/1468
16	1U	0.34	0/977	0.56	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.29	0/977	0.45	0/1301
17	1V	0.38	0/786	0.57	0/1053
17	2V	0.32	0/782	0.53	0/1049
18	1W	0.38	0/897	0.54	0/1205
18	2W	0.31	0/897	0.48	0/1205
19	1X	0.36	0/764	0.55	0/1025
19	2X	0.30	0/764	0.50	0/1025
20	1Y	0.34	0/823	0.55	0/1099
20	2Y	0.29	0/823	0.53	0/1100
21	1Z	0.31	0/1620	0.50	0/2200
21	2Z	0.30	0/1590	0.50	0/2162
22	10	0.35	0/616	0.52	0/821
22	20	0.30	0/616	0.51	0/821
23	11	0.32	0/761	0.53	0/1013
23	21	0.32	0/766	0.53	0/1018
24	12	0.30	0/590	0.50	0/781
24	22	0.27	0/594	0.42	0/785
25	13	0.35	0/474	0.53	0/635
25	23	0.32	0/469	0.51	0/630
26	14	0.31	0/559	0.54	0/754
26	24	0.32	0/549	0.53	1/741 (0.1%)
27	15	0.37	0/473	0.63	1/639 (0.2%)
27	25	0.30	0/469	0.53	0/635
28	16	0.34	0/460	0.53	0/613
28	26	0.28	0/456	0.49	0/608
29	17	0.35	0/426	0.58	0/561
29	27	0.30	0/426	0.52	0/561
30	18	0.33	0/525	0.54	0/691
30	28	0.30	0/525	0.48	0/691
31	19	0.36	0/310	0.55	0/407
31	29	0.32	0/310	0.53	0/407
32	1a	0.38	0/35795	0.89	14/55864 (0.0%)
32	2a	0.36	0/35890	0.87	22/56012 (0.0%)
33	1b	0.30	0/1876	0.48	0/2533
33	2b	0.31	0/1860	0.48	0/2518
34	1c	0.28	0/1582	0.47	0/2137
34	2c	0.29	0/1566	0.48	0/2119
35	1d	0.29	0/1695	0.47	0/2274
35	2d	0.30	0/1698	0.49	0/2277
36	1e	0.29	0/1149	0.51	0/1548
36	2e	0.29	0/1149	0.51	0/1548
37	1f	0.29	0/827	0.48	0/1120
37	2f	0.30	0/829	0.49	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.28	0/1254	0.44	0/1683
38	2g	0.29	0/1248	0.42	0/1676
39	1h	0.30	0/1118	0.49	0/1506
39	2h	0.29	0/1108	0.48	0/1494
40	1i	0.29	0/1005	0.49	0/1351
40	2i	0.29	0/985	0.48	0/1329
41	1j	0.28	0/732	0.47	0/993
41	2j	0.28	0/723	0.46	0/984
42	1k	0.29	0/849	0.51	0/1150
42	2k	0.28	0/848	0.49	0/1149
43	1l	0.30	0/937	0.53	0/1260
43	2l	0.29	0/937	0.52	0/1260
44	1m	0.25	0/924	0.46	0/1242
44	2m	0.30	0/905	0.46	0/1217
45	1n	0.30	0/501	0.47	0/664
45	2n	0.29	0/501	0.46	0/664
46	1o	0.28	0/739	0.43	0/985
46	2o	0.27	0/739	0.42	0/985
47	1p	0.27	0/697	0.52	0/939
47	2p	0.29	0/693	0.49	0/935
48	1q	0.29	0/836	0.48	0/1117
48	2q	0.30	0/836	0.48	0/1117
49	1r	0.28	0/560	0.47	0/746
49	2r	0.28	0/560	0.46	0/746
50	1s	0.27	0/663	0.51	0/895
50	2s	0.29	0/660	0.49	0/893
51	1t	0.28	0/734	0.41	0/969
51	2t	0.28	0/736	0.43	0/976
52	1u	0.28	0/203	0.49	0/266
52	2u	0.27	0/203	0.50	0/266
53	1y	0.27	0/776	0.46	0/1048
53	2y	0.29	0/761	0.45	0/1030
All	All	0.41	3/309889 (0.0%)	0.84	195/463153 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
26	24	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2104	G	N1-C2	-6.34	1.32	1.37
1	2A	2104	G	C6-N1	-5.61	1.35	1.39
1	1A	330	A	N9-C4	-5.15	1.34	1.37

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2104	G	C5-C6-O6	17.29	138.98	128.60
1	2A	2185	C	N1-C2-O2	16.48	128.79	118.90
1	2A	2104	G	N3-C2-N2	13.76	129.53	119.90
1	2A	2104	G	N1-C2-N2	-12.61	104.85	116.20
1	1A	1042	G	OP1-P-O3'	-10.75	81.55	105.20
1	1A	512	G	O4'-C1'-N9	10.55	116.64	108.20
1	1A	570	G	C5-C6-O6	-10.17	122.50	128.60
1	2A	2185	C	C5-C6-N1	10.11	126.05	121.00
1	2A	2185	C	C2-N3-C4	9.69	124.75	119.90
1	2A	2185	C	C4-C5-C6	-9.64	112.58	117.40
1	2A	2104	G	N1-C6-O6	-9.48	114.21	119.90
1	2A	1092	C	N1-C2-O2	9.40	124.54	118.90
1	2A	2104	G	C5-C6-N1	-9.40	106.80	111.50
1	2A	2104	G	C6-N1-C2	9.26	130.66	125.10
1	1A	570	G	C5-C6-N1	8.48	115.74	111.50
32	2a	1003	G	N3-C4-C5	-8.35	124.42	128.60
1	1A	1042	G	OP2-P-O3'	-8.13	87.32	105.20
1	2A	1092	C	C2-N1-C1'	8.12	127.74	118.80
1	1A	1075	C	N1-C2-O2	8.03	123.72	118.90
1	1A	2036	C	O5'-P-OP1	-8.01	98.49	105.70
1	1A	2685	G	N1-C6-O6	-7.85	115.19	119.90
1	1A	1352	U	O5'-P-OP1	-7.84	98.64	105.70
1	1A	2682	U	O5'-P-OP2	-7.70	98.78	105.70
1	1A	963	U	O5'-P-OP2	-7.58	98.88	105.70
1	2A	570	G	C5-C6-O6	-7.57	124.06	128.60
32	2a	1158	C	C2-N1-C1'	7.42	126.97	118.80
32	2a	1158	C	N1-C2-O2	7.41	123.35	118.90
1	2A	2185	C	N3-C2-O2	-7.37	116.74	121.90
1	2A	1092	C	N3-C2-O2	-7.33	116.77	121.90
1	1A	198	C	O5'-P-OP2	-7.32	99.11	105.70
1	1A	948	G	O5'-P-OP1	-7.22	99.20	105.70
1	1A	1372	U	N3-C4-O4	7.21	124.44	119.40
32	2a	754	C	C2-N1-C1'	7.17	126.69	118.80
1	1A	800	A	O5'-P-OP1	-7.13	99.28	105.70
32	2a	1004	A	O4'-C1'-N9	7.10	113.88	108.20
1	1A	1372	U	C5-C4-O4	-7.09	121.65	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1791	A	O5'-P-OP1	-7.07	99.34	105.70
1	2A	120	U	O5'-P-OP1	-7.03	99.37	105.70
1	2A	570	G	C4-C5-N7	7.03	113.61	110.80
1	2A	2178	C	N1-C2-O2	7.00	123.10	118.90
1	1A	2598	A	O5'-P-OP1	-6.94	99.45	105.70
1	1A	330	A	N1-C2-N3	6.94	132.77	129.30
32	1a	1028	C	C5-C6-N1	6.90	124.45	121.00
1	2A	1060	U	C2-N1-C1'	6.88	125.95	117.70
32	1a	1028	C	C6-N1-C2	-6.87	117.55	120.30
32	2a	1003	G	C4-N9-C1'	6.86	135.42	126.50
1	1A	2269	A	O5'-P-OP1	-6.84	99.54	105.70
1	1A	330	A	C2-N3-C4	-6.83	107.18	110.60
1	2A	2185	C	N1-C2-N3	-6.76	114.47	119.20
1	1A	1300	U	P-O3'-C3'	6.76	127.81	119.70
1	1A	2159	G	C5-C6-O6	6.71	132.63	128.60
32	2a	1158	C	C6-N1-C2	-6.68	117.63	120.30
1	1A	845	G	O4'-C1'-N9	6.63	113.50	108.20
1	2A	1614	A	O5'-P-OP1	-6.57	99.78	105.70
1	1A	2575	C	O5'-P-OP2	-6.57	99.79	105.70
32	2a	266	G	P-O3'-C3'	6.56	127.58	119.70
32	2a	1158	C	N3-C2-O2	-6.51	117.35	121.90
1	2A	1076	C	OP1-P-O3'	6.49	119.48	105.20
1	1A	2023	G	O5'-P-OP1	-6.47	99.87	105.70
1	1A	568	U	C5-C4-O4	-6.39	122.06	125.90
1	1A	1075	C	C2-N3-C4	6.38	123.09	119.90
1	2A	1783	A	O5'-P-OP1	-6.34	99.99	105.70
32	2a	1003	G	N3-C4-N9	6.28	129.77	126.00
1	1A	1176	G	OP1-P-O3'	6.26	118.98	105.20
1	1A	575	A	O5'-P-OP1	-6.26	100.06	105.70
32	2a	1003	G	C8-N9-C4	-6.26	103.89	106.40
1	2A	2185	C	C2-N1-C1'	6.24	125.66	118.80
1	1A	2848	G	O4'-C1'-N9	6.22	113.18	108.20
1	2A	1092	C	C6-N1-C2	-6.20	117.82	120.30
1	2A	2185	C	N3-C4-N4	-6.17	113.68	118.00
32	2a	754	C	N1-C2-O2	6.14	122.59	118.90
1	1A	2430	A	O5'-P-OP2	-6.14	100.18	105.70
1	1A	2159	G	C6-N1-C2	6.10	128.76	125.10
1	1A	2249	U	N3-C4-O4	-6.09	115.14	119.40
1	1A	31	C	O5'-P-OP1	-6.04	100.27	105.70
1	1A	847	U	C2-N1-C1'	6.03	124.93	117.70
1	1A	576	U	C5-C6-N1	5.98	125.69	122.70
1	1A	1776	G	O5'-P-OP2	-5.97	100.33	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	955	U	C5-C4-O4	5.94	129.46	125.90
1	2A	1352	U	O5'-P-OP1	-5.93	100.36	105.70
1	1A	1043	C	OP1-P-OP2	5.93	128.50	119.60
1	2A	570	G	N9-C4-C5	-5.91	103.03	105.40
1	1A	2589	A	O5'-P-OP1	-5.90	100.39	105.70
1	1A	2245	U	N3-C4-O4	-5.89	115.28	119.40
32	1a	955	U	C2-N3-C4	5.88	130.53	127.00
1	1A	1936	A	O4'-C1'-N9	5.88	112.90	108.20
1	1A	1602	U	N3-C4-O4	-5.87	115.29	119.40
1	1A	1653	G	C8-N9-C4	-5.85	104.06	106.40
1	2A	1075	C	N1-C2-O2	5.81	122.39	118.90
1	2A	943	U	O5'-P-OP2	-5.80	100.48	105.70
1	1A	739	G	O5'-P-OP1	-5.79	100.49	105.70
1	2A	2104	G	C2-N3-C4	-5.79	109.00	111.90
1	1A	570	G	N9-C4-C5	-5.79	103.08	105.40
1	2A	450	G	N1-C6-O6	-5.78	116.43	119.90
1	1A	783	A	C2-N3-C4	5.77	113.48	110.60
1	1A	801	G	O5'-P-OP2	-5.76	100.51	105.70
1	1A	1416	G	O4'-C1'-N9	5.74	112.79	108.20
1	1A	2689	U	P-O3'-C3'	5.72	126.57	119.70
27	15	25	LEU	C-N-CA	-5.69	107.47	121.70
1	1A	226	G	O4'-C1'-N9	5.67	112.74	108.20
1	1A	271(Y)	U	O4'-C1'-N1	5.67	112.74	108.20
1	2A	1060	U	C6-N1-C1'	-5.66	113.27	121.20
1	1A	2319	G	O4'-C1'-N9	5.66	112.73	108.20
32	2a	115	G	P-O3'-C3'	5.66	126.49	119.70
1	1A	946	G	O5'-P-OP1	-5.65	100.62	105.70
1	1A	518	G	O5'-P-OP2	-5.63	100.63	105.70
1	1A	1249	U	O5'-P-OP1	-5.63	100.64	105.70
1	1A	2430	A	C2-N3-C4	5.62	113.41	110.60
1	2A	2172	U	P-O3'-C3'	5.60	126.42	119.70
1	1A	2015	A	C8-N9-C4	5.59	108.04	105.80
1	1A	645	C	C2-N1-C1'	5.59	124.95	118.80
1	1A	570	G	C4-C5-N7	5.58	113.03	110.80
1	1A	1086	A	N1-C6-N6	-5.57	115.26	118.60
1	2A	1090	U	C5-C6-N1	5.54	125.47	122.70
32	1a	792	A	O4'-C1'-N9	5.52	112.62	108.20
1	1A	570	G	N3-C4-N9	5.52	129.31	126.00
1	2A	784	A	O4'-C1'-N9	5.49	112.59	108.20
1	2A	2689	U	N3-C2-O2	-5.49	118.36	122.20
1	1A	2033	A	OP1-P-OP2	-5.49	111.37	119.60
1	1A	117	G	C5-C6-O6	-5.48	125.31	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	512	G	O4'-C1'-N9	5.48	112.58	108.20
1	1A	2031	A	O5'-P-OP1	5.47	117.27	110.70
1	2A	383	U	O4'-C1'-N1	5.46	112.57	108.20
1	1A	2371	G	C5-C6-N1	5.45	114.22	111.50
1	1A	1075	C	N3-C2-O2	-5.42	118.11	121.90
1	2A	1060	U	N1-C2-O2	5.41	126.59	122.80
32	1a	1225	A	C6-N1-C2	5.40	121.84	118.60
1	2A	2172	U	OP1-P-O3'	5.40	117.09	105.20
1	2A	2104	G	C4-N9-C1'	5.39	133.51	126.50
1	1A	568	U	N3-C4-C5	5.39	117.83	114.60
1	2A	576	U	O5'-P-OP1	-5.37	100.87	105.70
1	1A	12	U	C2-N1-C1'	5.36	124.14	117.70
1	1A	139(A)	G	C5-N7-C8	5.36	106.98	104.30
1	1A	2825	C	C5-C4-N4	5.35	123.94	120.20
1	2A	1313	U	C2-N1-C1'	5.34	124.11	117.70
32	2a	1043	C	N1-C2-O2	5.34	122.10	118.90
32	2a	1065	U	P-O3'-C3'	5.34	126.10	119.70
1	1A	2457	U	N1-C2-O2	-5.33	119.07	122.80
1	1A	195	A	P-O3'-C3'	5.33	126.09	119.70
1	1A	1647	G	O4'-C1'-N9	-5.32	103.94	108.20
1	1A	1272	A	O5'-P-OP2	-5.32	100.91	105.70
32	2a	687	A	P-O3'-C3'	5.32	126.08	119.70
1	2A	1092	C	C6-N1-C1'	-5.31	114.43	120.80
1	2A	2689	U	P-O3'-C3'	5.31	126.07	119.70
1	1A	570	G	C2-N3-C4	5.31	114.56	111.90
1	2A	570	G	C5-C6-N1	5.29	114.15	111.50
32	1a	839	U	P-O3'-C3'	5.29	126.05	119.70
1	1A	2689	U	N3-C2-O2	-5.29	118.50	122.20
1	1A	2494	G	C2-N3-C4	5.28	114.54	111.90
1	1A	1175	U	P-O3'-C3'	5.27	126.03	119.70
1	1A	774	A	C8-N9-C4	-5.27	103.69	105.80
1	1A	1116	C	C5-C4-N4	-5.26	116.52	120.20
1	1A	1773	A	N9-C1'-C2'	-5.26	106.21	112.00
1	1A	2149	G	N3-C2-N2	-5.25	116.22	119.90
1	1A	2689	U	N1-C2-O2	5.25	126.48	122.80
32	1a	1395	C	C2-N3-C4	5.24	122.52	119.90
1	2A	845	G	O4'-C1'-N9	5.24	112.39	108.20
32	1a	1442	G	N3-C4-C5	-5.24	125.98	128.60
1	1A	1339	G	C5-C6-O6	-5.23	125.46	128.60
1	1A	1372	U	C2-N1-C1'	5.22	123.96	117.70
1	2A	1992	G	P-O3'-C3'	5.22	125.96	119.70
1	2A	2126	A	P-O3'-C3'	5.21	125.95	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2889	C	N1-C2-O2	5.20	122.02	118.90
1	1A	996	A	O5'-P-OP1	-5.20	101.02	105.70
1	1A	1210	A	P-O3'-C3'	5.18	125.92	119.70
1	1A	2622	C	N1-C2-O2	-5.17	115.80	118.90
1	1A	974	G	O5'-P-OP1	-5.15	101.06	105.70
1	2A	9	U	C5-C6-N1	5.15	125.27	122.70
1	2A	1076	C	P-O3'-C3'	5.14	125.87	119.70
1	1A	573	G	C5-C6-O6	-5.14	125.52	128.60
32	1a	1225	A	C5-C6-N6	5.13	127.80	123.70
32	1a	1028	C	C2-N3-C4	5.12	122.46	119.90
1	2A	2108	C	C2-N3-C4	5.12	122.46	119.90
1	1A	1131	G	O4'-C1'-N9	5.11	112.29	108.20
32	2a	1397	C	C2-N1-C1'	5.10	124.41	118.80
1	2A	2249	U	N3-C4-O4	-5.09	115.84	119.40
32	2a	913	A	P-O3'-C3'	5.09	125.81	119.70
1	1A	975	C	C6-N1-C2	5.09	122.33	120.30
32	2a	1043	C	C2-N3-C4	5.08	122.44	119.90
1	1A	563	G	N1-C6-O6	-5.08	116.85	119.90
26	24	60	GLN	N-CA-C	5.07	124.69	111.00
1	2A	1993	U	O5'-P-OP1	-5.07	101.14	105.70
32	2a	754	C	N3-C2-O2	-5.06	118.36	121.90
1	1A	961	C	N1-C2-O2	-5.06	115.87	118.90
1	1A	1385	G	O4'-C1'-N9	5.05	112.24	108.20
1	2A	752	A	P-O3'-C3'	5.04	125.75	119.70
32	1a	266	G	P-O3'-C3'	5.03	125.74	119.70
32	1a	78	G	O4'-C1'-N9	5.03	112.23	108.20
1	1A	1129	A	O4'-C1'-N9	5.03	112.22	108.20
32	1a	1201	A	P-O3'-C3'	5.02	125.72	119.70
1	1A	1964	G	O4'-C1'-N9	-5.02	104.19	108.20
32	2a	1003	G	C2-N3-C4	5.02	114.41	111.90
32	2a	1123	A	N1-C6-N6	-5.01	115.59	118.60
1	2A	2602	A	OP1-P-O3'	5.01	116.22	105.20
1	2A	1648	C	O5'-P-OP1	-5.01	101.19	105.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	24	18	CYS	Peptide

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%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	254 (93%)	19 (7%)	0	100	100
4	1E	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	15	16
4	2E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	29	34
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	29	34
5	2F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	29	34
6	1G	179/182 (98%)	160 (89%)	13 (7%)	6 (3%)	3	1
6	2G	179/182 (98%)	157 (88%)	18 (10%)	4 (2%)	6	4
7	1H	172/180 (96%)	160 (93%)	9 (5%)	3 (2%)	9	7
7	2H	171/180 (95%)	150 (88%)	19 (11%)	2 (1%)	13	12
8	1I	145/148 (98%)	131 (90%)	13 (9%)	1 (1%)	22	25
8	2I	144/148 (97%)	133 (92%)	9 (6%)	2 (1%)	11	9
9	1N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	2N	138/140 (99%)	127 (92%)	11 (8%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	22
11	1P	147/150 (98%)	139 (95%)	7 (5%)	1 (1%)	22	25
11	2P	147/150 (98%)	137 (93%)	8 (5%)	2 (1%)	11	9
12	1Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	22	25
12	2Q	139/141 (99%)	129 (93%)	10 (7%)	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%)	5 (5%)	1 (1%)	17	19
14	2S	108/112 (96%)	95 (88%)	12 (11%)	1 (1%)	17	19
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	19	22
15	2T	129/146 (88%)	122 (95%)	5 (4%)	2 (2%)	9	8
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	2 (2%)	2 (2%)	7	5
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	16
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	92 (99%)	0	1 (1%)	14	14
19	2X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	14	14
20	1Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
20	2Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
21	1Z	201/206 (98%)	189 (94%)	10 (5%)	2 (1%)	15	16
21	2Z	199/206 (97%)	176 (88%)	22 (11%)	1 (0%)	29	34
22	10	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
22	20	75/85 (88%)	69 (92%)	6 (8%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	14
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	14
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	8	6
26	14	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	1
26	24	67/71 (94%)	47 (70%)	18 (27%)	2 (3%)	4	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	8	6
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	17	46/49 (94%)	46 (100%)	0	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	62 (100%)	0	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%)	31 (14%)	7 (3%)	4 1
33	2b	229/256 (90%)	194 (85%)	27 (12%)	8 (4%)	3 1
34	1c	204/239 (85%)	184 (90%)	19 (9%)	1 (0%)	29 34
34	2c	204/239 (85%)	174 (85%)	26 (13%)	4 (2%)	7 5
35	1d	206/209 (99%)	193 (94%)	13 (6%)	0	100 100
35	2d	206/209 (99%)	186 (90%)	15 (7%)	5 (2%)	6 3
36	1e	146/162 (90%)	136 (93%)	9 (6%)	1 (1%)	22 25
36	2e	146/162 (90%)	138 (94%)	8 (6%)	0	100 100
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
38	1g	153/156 (98%)	150 (98%)	2 (1%)	1 (1%)	22 25
38	2g	153/156 (98%)	140 (92%)	10 (6%)	3 (2%)	7 5
39	1h	135/138 (98%)	128 (95%)	6 (4%)	1 (1%)	22 25
39	2h	135/138 (98%)	126 (93%)	9 (7%)	0	100 100
40	1i	125/128 (98%)	109 (87%)	16 (13%)	0	100 100
40	2i	124/128 (97%)	105 (85%)	15 (12%)	4 (3%)	4 1
41	1j	95/105 (90%)	79 (83%)	13 (14%)	3 (3%)	4 1
41	2j	94/105 (90%)	79 (84%)	12 (13%)	3 (3%)	4 1
42	1k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	17 19
42	2k	112/129 (87%)	102 (91%)	7 (6%)	3 (3%)	5 2
43	1l	119/132 (90%)	115 (97%)	4 (3%)	0	100 100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100 100
44	1m	114/126 (90%)	103 (90%)	9 (8%)	2 (2%)	8 6
44	2m	112/126 (89%)	97 (87%)	13 (12%)	2 (2%)	8 6
45	1n	58/61 (95%)	53 (91%)	5 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
46	1o	86/89 (97%)	77 (90%)	6 (7%)	3 (4%)	3 1
46	2o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	6 4
47	1p	80/88 (91%)	68 (85%)	11 (14%)	1 (1%)	12 11
47	2p	80/88 (91%)	70 (88%)	10 (12%)	0	100 100
48	1q	97/105 (92%)	85 (88%)	11 (11%)	1 (1%)	15 16
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100 100
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100 100
49	2r	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	10 9
50	1s	81/93 (87%)	73 (90%)	6 (7%)	2 (2%)	5 3
50	2s	81/93 (87%)	67 (83%)	13 (16%)	1 (1%)	13 12
51	1t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	4 1
51	2t	96/106 (91%)	87 (91%)	6 (6%)	3 (3%)	4 1
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2 1
53	1y	95/113 (84%)	95 (100%)	0	0	100 100
53	2y	94/113 (83%)	89 (95%)	5 (5%)	0	100 100
All	All	11629/12354 (94%)	10763 (93%)	749 (6%)	117 (1%)	15 16

All (117) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	50	ALA
33	1b	17	PHE
33	1b	124	SER
34	1c	107	GLN
41	1j	55	LYS
6	2G	78	SER
6	2G	81	LYS
7	2H	126	PRO
8	2I	117	GLU
11	2P	36	LYS
15	2T	127	ALA
33	2b	20	GLU
35	2d	5	ILE
38	2g	55	GLY

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Mol	Chain	Res	Type
40	2i	54	ASP
41	2j	78	ASN
42	2k	89	ALA
51	2t	100	ILE
4	1E	71	GLY
5	1F	130	ALA
6	1G	44	GLY
6	1G	47	LYS
7	1H	126	PRO
21	1Z	53	ILE
33	1b	127	ILE
38	1g	55	GLY
44	1m	67	GLU
46	1o	88	ARG
50	1s	27	GLU
51	1t	47	GLY
5	2F	130	ALA
6	2G	42	GLY
19	2X	94	GLY
23	21	3	LYS
33	2b	17	PHE
35	2d	4	TYR
40	2i	43	ALA
41	2j	79	ARG
44	2m	23	TYR
46	2o	19	PRO
46	2o	87	ILE
6	1G	51	ARG
7	1H	159	GLU
8	1I	102	SER
14	1S	59	LYS
19	1X	94	GLY
26	14	39	CYS
26	14	57	GLU
33	1b	22	LYS
36	1e	70	PRO
41	1j	77	PRO
44	1m	3	ARG
51	1t	100	ILE
8	2I	10	GLU
11	2P	29	LYS
15	2T	128	GLU

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Mol	Chain	Res	Type
26	24	62	ARG
33	2b	64	ARG
33	2b	126	GLU
34	2c	4	LYS
34	2c	12	LEU
34	2c	99	VAL
35	2d	86	LYS
38	2g	7	ALA
40	2i	96	LEU
49	2r	36	ASN
50	2s	29	ARG
4	1E	52	LEU
6	1G	49	ASP
6	1G	74	LYS
11	1P	29	LYS
12	1Q	59	ARG
17	1V	43	GLU
21	1Z	79	ARG
33	1b	9	GLU
33	1b	83	MET
46	1o	19	PRO
46	1o	87	ILE
47	1p	28	ARG
51	1t	99	LEU
4	2E	52	LEU
7	2H	110	SER
33	2b	16	HIS
33	2b	21	ARG
40	2i	52	ALA
44	2m	106	ASN
51	2t	95	ALA
15	1T	126	ALA
23	11	3	LYS
26	14	61	ARG
33	1b	20	GLU
48	1q	68	ARG
50	1s	7	LYS
27	25	35	GLU
33	2b	125	PRO
34	2c	108	ASN
38	2g	4	ARG
52	2u	7	ARG

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Mol	Chain	Res	Type
7	1H	92	ILE
39	1h	54	ASP
10	2O	5	GLN
33	2b	232	PRO
42	2k	105	VAL
17	1V	79	VAL
14	2S	82	ILE
17	2V	79	VAL
51	2t	102	GLY
21	2Z	53	ILE
25	23	59	VAL
6	2G	177	GLY
26	24	45	GLY
42	2k	90	GLY
42	1k	105	VAL
35	2d	40	PRO
41	1j	82	ILE
35	2d	88	VAL
41	2j	75	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	214/218 (98%)	200 (94%)	14 (6%)	17 21
3	2D	215/218 (99%)	197 (92%)	18 (8%)	11 12
4	1E	164/166 (99%)	153 (93%)	11 (7%)	16 20
4	2E	164/166 (99%)	151 (92%)	13 (8%)	12 14
5	1F	160/166 (96%)	145 (91%)	15 (9%)	8 9
5	2F	159/166 (96%)	141 (89%)	18 (11%)	6 5
6	1G	144/156 (92%)	134 (93%)	10 (7%)	15 18
6	2G	142/156 (91%)	120 (84%)	22 (16%)	2 2
7	1H	144/148 (97%)	136 (94%)	8 (6%)	21 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	2H	143/148 (97%)	128 (90%)	15 (10%)	7 6
8	1I	111/124 (90%)	97 (87%)	14 (13%)	4 3
8	2I	108/124 (87%)	98 (91%)	10 (9%)	9 9
9	1N	119/119 (100%)	109 (92%)	10 (8%)	11 12
9	2N	118/119 (99%)	110 (93%)	8 (7%)	16 19
10	1O	100/100 (100%)	100 (100%)	0	100 100
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31 41
11	1P	115/116 (99%)	110 (96%)	5 (4%)	29 38
11	2P	115/116 (99%)	111 (96%)	4 (4%)	36 47
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18 22
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11 13
13	1R	101/101 (100%)	94 (93%)	7 (7%)	15 18
13	2R	101/101 (100%)	96 (95%)	5 (5%)	24 32
14	1S	87/88 (99%)	80 (92%)	7 (8%)	12 14
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%)	108 (96%)	5 (4%)	28 37
16	1U	93/94 (99%)	90 (97%)	3 (3%)	39 50
16	2U	93/94 (99%)	86 (92%)	7 (8%)	13 16
17	1V	81/82 (99%)	75 (93%)	6 (7%)	13 16
17	2V	80/82 (98%)	75 (94%)	5 (6%)	18 22
18	1W	90/92 (98%)	87 (97%)	3 (3%)	38 49
18	2W	90/92 (98%)	84 (93%)	6 (7%)	16 20
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46 58
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46 58
20	1Y	86/91 (94%)	79 (92%)	7 (8%)	11 13
20	2Y	86/91 (94%)	81 (94%)	5 (6%)	20 25
21	1Z	169/179 (94%)	153 (90%)	16 (10%)	8 9
21	2Z	165/179 (92%)	152 (92%)	13 (8%)	12 14
22	10	61/67 (91%)	58 (95%)	3 (5%)	25 32
22	20	61/67 (91%)	58 (95%)	3 (5%)	25 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	11	79/83 (95%)	72 (91%)	7 (9%)	9 10
23	21	81/83 (98%)	76 (94%)	5 (6%)	18 23
24	12	65/67 (97%)	62 (95%)	3 (5%)	27 35
24	22	66/67 (98%)	64 (97%)	2 (3%)	41 52
25	13	51/52 (98%)	47 (92%)	4 (8%)	12 15
25	23	50/52 (96%)	49 (98%)	1 (2%)	55 67
26	14	58/63 (92%)	49 (84%)	9 (16%)	2 2
26	24	54/63 (86%)	45 (83%)	9 (17%)	2 1
27	15	51/52 (98%)	47 (92%)	4 (8%)	12 15
27	25	50/52 (96%)	48 (96%)	2 (4%)	31 41
28	16	51/52 (98%)	47 (92%)	4 (8%)	12 15
28	26	50/52 (96%)	46 (92%)	4 (8%)	12 14
29	17	41/42 (98%)	36 (88%)	5 (12%)	5 4
29	27	41/42 (98%)	36 (88%)	5 (12%)	5 4
30	18	54/55 (98%)	49 (91%)	5 (9%)	9 9
30	28	54/55 (98%)	50 (93%)	4 (7%)	13 16
31	19	34/34 (100%)	34 (100%)	0	100 100
31	29	34/34 (100%)	33 (97%)	1 (3%)	42 53
33	1b	191/220 (87%)	166 (87%)	25 (13%)	4 3
33	2b	187/220 (85%)	158 (84%)	29 (16%)	2 2
34	1c	144/188 (77%)	137 (95%)	7 (5%)	25 32
34	2c	140/188 (74%)	122 (87%)	18 (13%)	4 3
35	1d	171/181 (94%)	152 (89%)	19 (11%)	6 5
35	2d	172/181 (95%)	153 (89%)	19 (11%)	6 5
36	1e	114/123 (93%)	106 (93%)	8 (7%)	15 18
36	2e	114/123 (93%)	105 (92%)	9 (8%)	12 14
37	1f	85/90 (94%)	74 (87%)	11 (13%)	4 3
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6 6
38	1g	120/127 (94%)	113 (94%)	7 (6%)	20 25
38	2g	119/127 (94%)	103 (87%)	16 (13%)	4 3
39	1h	116/119 (98%)	106 (91%)	10 (9%)	10 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8 8
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%)	62 (91%)	6 (9%)	10 11
41	2j	68/92 (74%)	61 (90%)	7 (10%)	7 7
42	1k	83/99 (84%)	77 (93%)	6 (7%)	14 17
42	2k	83/99 (84%)	71 (86%)	12 (14%)	3 2
43	1l	96/108 (89%)	91 (95%)	5 (5%)	23 30
43	2l	96/108 (89%)	88 (92%)	8 (8%)	11 12
44	1m	90/101 (89%)	82 (91%)	8 (9%)	9 10
44	2m	87/101 (86%)	75 (86%)	12 (14%)	3 2
45	1n	49/50 (98%)	45 (92%)	4 (8%)	11 13
45	2n	49/50 (98%)	45 (92%)	4 (8%)	11 13
46	1o	78/80 (98%)	77 (99%)	1 (1%)	69 79
46	2o	78/80 (98%)	74 (95%)	4 (5%)	24 31
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5 5
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13 16
48	1q	94/97 (97%)	91 (97%)	3 (3%)	39 50
48	2q	94/97 (97%)	88 (94%)	6 (6%)	17 21
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10 12
49	2r	59/77 (77%)	55 (93%)	4 (7%)	16 19
50	1s	68/80 (85%)	63 (93%)	5 (7%)	13 16
50	2s	67/80 (84%)	62 (92%)	5 (8%)	13 16
51	1t	71/82 (87%)	64 (90%)	7 (10%)	8 7
51	2t	70/82 (85%)	66 (94%)	4 (6%)	20 26
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	18 (100%)	0	100 100
53	1y	82/98 (84%)	75 (92%)	7 (8%)	10 12
53	2y	79/98 (81%)	70 (89%)	9 (11%)	5 5
All	All	9524/10260 (93%)	8753 (92%)	771 (8%)	11 13

All (771) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	61	LEU
3	1D	64	ILE
3	1D	94	LEU
3	1D	99	ASP
3	1D	103	ARG
3	1D	106	ILE
3	1D	126	GLN
3	1D	134	ARG
3	1D	142	VAL
3	1D	155	LEU
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	259	THR
4	1E	21	VAL
4	1E	41	LYS
4	1E	55	ASN
4	1E	75	VAL
4	1E	89	ASP
4	1E	116	VAL
4	1E	119	ARG
4	1E	175	VAL
4	1E	178	GLU
4	1E	181	LEU
4	1E	202	LYS
5	1F	20	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	125	LEU
5	1F	132	VAL
5	1F	145	GLU
5	1F	151	SER
5	1F	157	VAL
5	1F	158	THR
5	1F	162	LEU
5	1F	170	LEU
5	1F	192	LEU
6	1G	7	LEU
6	1G	43	LEU
6	1G	45	GLU

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Mol	Chain	Res	Type
6	1G	52	ILE
6	1G	53	LEU
6	1G	62	LEU
6	1G	66	GLN
6	1G	79	ASN
6	1G	159	VAL
6	1G	168	GLU
7	1H	15	VAL
7	1H	18	GLU
7	1H	32	GLU
7	1H	71	LEU
7	1H	98	LEU
7	1H	119	GLU
7	1H	122	THR
7	1H	141	VAL
8	1I	10	GLU
8	1I	12	LEU
8	1I	41	GLU
8	1I	61	ARG
8	1I	78	THR
8	1I	87	LYS
8	1I	92	VAL
8	1I	101	LEU
8	1I	102	SER
8	1I	108	THR
8	1I	109	ILE
8	1I	116	LEU
8	1I	127	VAL
8	1I	140	LEU
9	1N	8	GLN
9	1N	12	ARG
9	1N	15	LEU
9	1N	19	GLU
9	1N	33	LEU
9	1N	48	MET
9	1N	60	ILE
9	1N	61	ARG
9	1N	62	VAL
9	1N	99	LEU
11	1P	15	ARG
11	1P	98	GLU
11	1P	99	LEU

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Mol	Chain	Res	Type
11	1P	125	VAL
11	1P	135	LEU
12	1Q	7	MET
12	1Q	59	ARG
12	1Q	60	ARG
12	1Q	75	THR
12	1Q	101	ARG
12	1Q	109	VAL
12	1Q	112	GLU
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	65	LEU
13	1R	96	ARG
13	1R	102	GLU
14	1S	3	ARG
14	1S	43	GLU
14	1S	46	VAL
14	1S	52	SER
14	1S	59	LYS
14	1S	67	ARG
14	1S	73	LEU
15	1T	28	VAL
15	1T	34	VAL
15	1T	36	GLU
15	1T	49	VAL
15	1T	53	ARG
15	1T	96	ARG
15	1T	118	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	108	GLU
17	1V	44	LYS
17	1V	46	VAL
17	1V	52	VAL
17	1V	71	LEU
17	1V	72	VAL
17	1V	79	VAL
18	1W	11	ARG
18	1W	17	VAL
18	1W	23	LEU

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Mol	Chain	Res	Type
19	1X	45	THR
19	1X	66	LEU
20	1Y	7	VAL
20	1Y	11	ASP
20	1Y	43	ASN
20	1Y	72	VAL
20	1Y	85	VAL
20	1Y	90	LEU
20	1Y	99	CYS
21	1Z	18	LEU
21	1Z	58	VAL
21	1Z	61	LEU
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	93	ASP
21	1Z	98	MET
21	1Z	102	LEU
21	1Z	103	ARG
21	1Z	121	HIS
21	1Z	132	ASN
21	1Z	138	GLU
21	1Z	150	LEU
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	171	ILE
22	10	55	ARG
22	10	59	LEU
22	10	74	ARG
23	11	3	LYS
23	11	21	ARG
23	11	30	VAL
23	11	40	ARG
23	11	46	LEU
23	11	69	LYS
23	11	94	LEU
24	12	1	MET
24	12	19	VAL
24	12	53	LEU
25	13	3	ARG
25	13	5	LYS
25	13	8	LEU
25	13	54	VAL

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Mol	Chain	Res	Type
26	14	1	MET
26	14	21	VAL
26	14	33	VAL
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	60	GLN
26	14	61	ARG
26	14	67	TYR
27	15	6	VAL
27	15	16	ARG
27	15	26	THR
27	15	58	LEU
28	16	6	ARG
28	16	14	THR
28	16	48	VAL
28	16	52	VAL
29	17	34	ARG
29	17	41	ARG
29	17	43	THR
29	17	47	ARG
29	17	48	LYS
30	18	14	VAL
30	18	31	HIS
30	18	34	TRP
30	18	50	LEU
30	18	58	ILE
33	1b	15	VAL
33	1b	19	HIS
33	1b	21	ARG
33	1b	24	TRP
33	1b	45	GLN
33	1b	51	LEU
33	1b	52	GLU
33	1b	80	ILE
33	1b	87	ARG
33	1b	96	ARG
33	1b	111	ARG
33	1b	112	VAL
33	1b	122	PHE
33	1b	124	SER
33	1b	135	GLN

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Mol	Chain	Res	Type
33	1b	142	LEU
33	1b	160	ASP
33	1b	163	PHE
33	1b	185	ILE
33	1b	187	LEU
33	1b	189	ASP
33	1b	200	ILE
33	1b	212	GLN
33	1b	224	GLN
33	1b	229	VAL
34	1c	3	ASN
34	1c	70	VAL
34	1c	89	GLU
34	1c	98	ASN
34	1c	105	GLU
34	1c	130	VAL
34	1c	132	ARG
35	1d	5	ILE
35	1d	25	ARG
35	1d	58	LEU
35	1d	59	ARG
35	1d	61	LYS
35	1d	67	ILE
35	1d	77	ASN
35	1d	85	LYS
35	1d	127	THR
35	1d	135	LEU
35	1d	144	ASP
35	1d	156	GLU
35	1d	157	LEU
35	1d	168	ARG
35	1d	178	VAL
35	1d	191	ARG
35	1d	194	LEU
35	1d	196	LEU
35	1d	201	GLN
36	1e	10	MET
36	1e	41	VAL
36	1e	55	VAL
36	1e	65	ASN
36	1e	67	VAL
36	1e	68	GLU

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Mol	Chain	Res	Type
36	1e	79	GLU
36	1e	145	LYS
37	1f	17	SER
37	1f	23	LYS
37	1f	40	VAL
37	1f	45	LEU
37	1f	63	TYR
37	1f	64	GLN
37	1f	69	GLU
37	1f	72	VAL
37	1f	73	ASN
37	1f	86	ARG
37	1f	98	LEU
38	1g	6	ARG
38	1g	45	ASP
38	1g	56	GLN
38	1g	96	GLN
38	1g	104	LEU
38	1g	113	GLU
38	1g	144	MET
39	1h	2	LEU
39	1h	24	THR
39	1h	25	ASP
39	1h	39	LEU
39	1h	52	ASP
39	1h	54	ASP
39	1h	63	LEU
39	1h	77	GLU
39	1h	104	ARG
39	1h	105	ARG
40	1i	14	VAL
40	1i	17	VAL
40	1i	54	ASP
40	1i	65	VAL
40	1i	71	SER
40	1i	81	ILE
40	1i	92	TYR
40	1i	96	LEU
40	1i	103	THR
40	1i	104	ARG
41	1j	34	VAL
41	1j	38	ILE

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Mol	Chain	Res	Type
41	1j	67	THR
41	1j	69	ASN
41	1j	84	GLN
41	1j	94	VAL
42	1k	14	VAL
42	1k	16	SER
42	1k	104	GLN
42	1k	105	VAL
42	1k	107	SER
42	1k	109	VAL
43	1l	18	VAL
43	1l	41	ARG
43	1l	42	THR
43	1l	83	VAL
43	1l	118	SER
44	1m	3	ARG
44	1m	4	ILE
44	1m	11	ARG
44	1m	54	VAL
44	1m	56	LEU
44	1m	70	LEU
44	1m	73	GLU
44	1m	80	ARG
45	1n	3	ARG
45	1n	13	THR
45	1n	18	VAL
45	1n	33	VAL
46	1o	39	LEU
47	1p	11	SER
47	1p	20	VAL
47	1p	27	LYS
47	1p	29	ASP
47	1p	42	ARG
47	1p	45	THR
47	1p	61	SER
47	1p	62	VAL
48	1q	16	GLN
48	1q	26	GLN
48	1q	63	ARG
49	1r	25	THR
49	1r	28	GLU
49	1r	41	LYS

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Mol	Chain	Res	Type
49	1r	54	ARG
49	1r	76	LEU
50	1s	3	ARG
50	1s	28	LYS
50	1s	30	LEU
50	1s	38	SER
50	1s	41	VAL
51	1t	10	LEU
51	1t	24	LEU
51	1t	58	LYS
51	1t	72	LEU
51	1t	74	LYS
51	1t	83	ARG
51	1t	84	LEU
53	1y	11	GLU
53	1y	23	ARG
53	1y	38	HIS
53	1y	42	SER
53	1y	46	GLN
53	1y	60	VAL
53	1y	83	ARG
3	2D	3	VAL
3	2D	61	LEU
3	2D	88	ARG
3	2D	94	LEU
3	2D	99	ASP
3	2D	103	ARG
3	2D	111	LEU
3	2D	140	THR
3	2D	141	VAL
3	2D	142	VAL
3	2D	147	LEU
3	2D	162	SER
3	2D	183	ARG
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	274	ARG
4	2E	7	VAL
4	2E	9	VAL
4	2E	12	THR

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Mol	Chain	Res	Type
4	2E	21	VAL
4	2E	75	VAL
4	2E	89	ASP
4	2E	97	LYS
4	2E	116	VAL
4	2E	119	ARG
4	2E	170	LEU
4	2E	175	VAL
4	2E	181	LEU
4	2E	199	ARG
5	2F	12	LEU
5	2F	20	LEU
5	2F	23	ASP
5	2F	33	LEU
5	2F	57	VAL
5	2F	60	SER
5	2F	74	ARG
5	2F	88	VAL
5	2F	124	LEU
5	2F	126	VAL
5	2F	132	VAL
5	2F	140	LEU
5	2F	158	THR
5	2F	168	ARG
5	2F	175	THR
5	2F	192	LEU
5	2F	197	ASP
5	2F	201	VAL
6	2G	3	LEU
6	2G	4	ASP
6	2G	5	VAL
6	2G	7	LEU
6	2G	28	VAL
6	2G	43	LEU
6	2G	49	ASP
6	2G	53	LEU
6	2G	60	LEU
6	2G	77	ILE
6	2G	92	VAL
6	2G	95	ARG
6	2G	96	ARG
6	2G	113	ARG

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Mol	Chain	Res	Type
6	2G	115	ARG
6	2G	116	ASP
6	2G	126	ASP
6	2G	133	LEU
6	2G	139	LEU
6	2G	146	TYR
6	2G	165	THR
6	2G	173	LEU
7	2H	27	LYS
7	2H	33	LEU
7	2H	42	ARG
7	2H	43	VAL
7	2H	44	VAL
7	2H	49	VAL
7	2H	65	HIS
7	2H	69	ARG
7	2H	71	LEU
7	2H	98	LEU
7	2H	105	LEU
7	2H	124	GLU
7	2H	134	SER
7	2H	139	GLN
7	2H	152	ARG
8	2I	37	VAL
8	2I	38	LEU
8	2I	66	GLU
8	2I	75	LEU
8	2I	76	THR
8	2I	116	LEU
8	2I	117	GLU
8	2I	123	LEU
8	2I	133	HIS
8	2I	140	LEU
9	2N	12	ARG
9	2N	28	THR
9	2N	34	LEU
9	2N	46	VAL
9	2N	48	MET
9	2N	62	VAL
9	2N	87	LEU
9	2N	99	LEU
10	2O	21	CYS

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Mol	Chain	Res	Type
10	2O	22	ILE
10	2O	70	LYS
10	2O	108	GLU
11	2P	15	ARG
11	2P	95	VAL
11	2P	99	LEU
11	2P	117	GLU
12	2Q	1	MET
12	2Q	2	LEU
12	2Q	6	ARG
12	2Q	60	ARG
12	2Q	98	LYS
12	2Q	109	VAL
12	2Q	110	THR
12	2Q	112	GLU
12	2Q	133	ARG
13	2R	29	LEU
13	2R	33	ARG
13	2R	44	LEU
13	2R	65	LEU
13	2R	114	VAL
14	2S	12	PHE
14	2S	14	VAL
14	2S	35	ILE
14	2S	50	SER
14	2S	69	VAL
14	2S	78	LEU
14	2S	111	GLU
15	2T	6	LEU
15	2T	34	VAL
15	2T	39	ARG
15	2T	78	LEU
15	2T	95	ARG
16	2U	5	LYS
16	2U	31	SER
16	2U	55	ARG
16	2U	59	ARG
16	2U	74	LEU
16	2U	108	GLU
16	2U	117	GLN
17	2V	51	VAL
17	2V	53	GLU

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Mol	Chain	Res	Type
17	2V	66	ARG
17	2V	72	VAL
17	2V	79	VAL
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	60	ASN
18	2W	100	THR
19	2X	57	LEU
19	2X	60	ARG
20	2Y	6	HIS
20	2Y	35	TYR
20	2Y	70	SER
20	2Y	85	VAL
20	2Y	99	CYS
21	2Z	3	TYR
21	2Z	6	LYS
21	2Z	14	LYS
21	2Z	35	ARG
21	2Z	71	VAL
21	2Z	72	ARG
21	2Z	86	VAL
21	2Z	107	THR
21	2Z	121	HIS
21	2Z	142	SER
21	2Z	150	LEU
21	2Z	170	THR
21	2Z	175	VAL
22	20	10	THR
22	20	43	THR
22	20	59	LEU
23	21	11	ARG
23	21	21	ARG
23	21	40	ARG
23	21	51	VAL
23	21	95	LEU
24	22	32	LEU
24	22	35	LEU
25	23	31	LEU
26	24	13	ARG
26	24	15	ILE

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Mol	Chain	Res	Type
26	24	34	GLU
26	24	44	THR
26	24	50	VAL
26	24	53	GLU
26	24	60	GLN
26	24	61	ARG
26	24	63	TYR
27	25	6	VAL
27	25	55	ARG
28	26	14	THR
28	26	25	LYS
28	26	34	LEU
28	26	40	CYS
29	27	1	MET
29	27	23	ARG
29	27	24	THR
29	27	43	THR
29	27	48	LYS
30	28	14	VAL
30	28	31	HIS
30	28	34	TRP
30	28	56	GLU
31	29	7	VAL
33	2b	8	LYS
33	2b	19	HIS
33	2b	23	ARG
33	2b	24	TRP
33	2b	28	PHE
33	2b	44	LEU
33	2b	58	ILE
33	2b	64	ARG
33	2b	71	VAL
33	2b	76	GLN
33	2b	93	VAL
33	2b	95	GLN
33	2b	96	ARG
33	2b	97	TRP
33	2b	113	HIS
33	2b	118	LEU
33	2b	124	SER
33	2b	135	GLN
33	2b	144	ARG

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Mol	Chain	Res	Type
33	2b	154	LEU
33	2b	157	ARG
33	2b	160	ASP
33	2b	189	ASP
33	2b	195	ASP
33	2b	200	ILE
33	2b	216	SER
33	2b	224	GLN
33	2b	229	VAL
33	2b	230	VAL
34	2c	3	ASN
34	2c	21	ARG
34	2c	32	LEU
34	2c	44	GLU
34	2c	47	LEU
34	2c	67	THR
34	2c	101	LEU
34	2c	103	VAL
34	2c	105	GLU
34	2c	115	LEU
34	2c	127	ARG
34	2c	128	PHE
34	2c	131	ARG
34	2c	152	ILE
34	2c	164	ARG
34	2c	195	VAL
34	2c	204	LEU
34	2c	207	VAL
35	2d	3	ARG
35	2d	5	ILE
35	2d	17	VAL
35	2d	28	SER
35	2d	34	GLU
35	2d	83	SER
35	2d	106	TYR
35	2d	108	LEU
35	2d	135	LEU
35	2d	140	VAL
35	2d	141	ARG
35	2d	150	GLU
35	2d	155	LEU
35	2d	157	LEU

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Mol	Chain	Res	Type
35	2d	158	ILE
35	2d	170	VAL
35	2d	175	SER
35	2d	202	LEU
35	2d	209	ARG
36	2e	10	MET
36	2e	34	VAL
36	2e	41	VAL
36	2e	45	PHE
36	2e	55	VAL
36	2e	65	ASN
36	2e	68	GLU
36	2e	75	THR
36	2e	91	LEU
37	2f	10	LEU
37	2f	37	VAL
37	2f	46	ARG
37	2f	63	TYR
37	2f	69	GLU
37	2f	70	ASP
37	2f	72	VAL
37	2f	83	ASP
37	2f	95	GLU
38	2g	4	ARG
38	2g	8	GLU
38	2g	13	GLN
38	2g	15	ASP
38	2g	21	VAL
38	2g	75	VAL
38	2g	77	SER
38	2g	97	GLN
38	2g	109	ASN
38	2g	113	GLU
38	2g	114	ARG
38	2g	115	ARG
38	2g	137	LYS
38	2g	138	LYS
38	2g	153	HIS
38	2g	155	ARG
39	2h	33	GLU
39	2h	60	ARG
39	2h	63	LEU

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Mol	Chain	Res	Type
39	2h	84	ARG
39	2h	91	ARG
39	2h	97	VAL
39	2h	112	LEU
39	2h	113	SER
39	2h	119	LEU
39	2h	121	ASP
39	2h	133	LEU
40	2i	17	VAL
40	2i	27	THR
40	2i	28	VAL
40	2i	64	THR
40	2i	65	VAL
40	2i	81	ILE
40	2i	86	VAL
40	2i	102	LEU
40	2i	108	VAL
40	2i	125	TYR
41	2j	29	ARG
41	2j	34	VAL
41	2j	38	ILE
41	2j	47	PHE
41	2j	74	ILE
41	2j	81	THR
41	2j	92	THR
42	2k	14	VAL
42	2k	16	SER
42	2k	30	VAL
42	2k	53	SER
42	2k	63	LEU
42	2k	83	ILE
42	2k	91	ARG
42	2k	103	LEU
42	2k	105	VAL
42	2k	109	VAL
42	2k	114	VAL
42	2k	117	ASN
43	2l	6	THR
43	2l	28	LYS
43	2l	36	VAL
43	2l	62	SER
43	2l	66	VAL

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Mol	Chain	Res	Type
43	2l	81	SER
43	2l	83	VAL
43	2l	89	ARG
44	2m	17	VAL
44	2m	39	ILE
44	2m	47	ASP
44	2m	48	LEU
44	2m	50	GLU
44	2m	55	ARG
44	2m	60	VAL
44	2m	63	THR
44	2m	66	LEU
44	2m	81	LEU
44	2m	106	ASN
44	2m	116	THR
45	2n	3	ARG
45	2n	13	THR
45	2n	18	VAL
45	2n	33	VAL
46	2o	5	LYS
46	2o	24	SER
46	2o	34	LEU
46	2o	39	LEU
47	2p	28	ARG
47	2p	60	LEU
47	2p	62	VAL
47	2p	67	THR
47	2p	69	THR
48	2q	6	LEU
48	2q	39	SER
48	2q	53	LEU
48	2q	63	ARG
48	2q	81	ARG
48	2q	99	SER
49	2r	25	THR
49	2r	41	LYS
49	2r	54	ARG
49	2r	55	ARG
50	2s	5	LEU
50	2s	30	LEU
50	2s	48	THR
50	2s	77	THR

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Mol	Chain	Res	Type
50	2s	79	THR
51	2t	36	LEU
51	2t	80	ARG
51	2t	84	LEU
51	2t	100	ILE
53	2y	11	GLU
53	2y	13	THR
53	2y	16	ILE
53	2y	41	LEU
53	2y	46	GLN
53	2y	56	THR
53	2y	78	ILE
53	2y	83	ARG
53	2y	96	ARG

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	253	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
6	1G	108	ASN
6	1G	132	ASN
8	1I	104	GLN
8	1I	105	HIS
10	1O	3	GLN
10	1O	89	ASN
13	1R	24	GLN
15	1T	58	ASN
15	1T	123	GLN
18	1W	34	ASN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	34	ASN
21	1Z	73	GLN
22	10	35	ASN
23	11	56	GLN

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Mol	Chain	Res	Type
25	13	32	GLN
33	1b	40	HIS
33	1b	135	GLN
34	1c	6	HIS
34	1c	102	ASN
34	1c	108	ASN
35	1d	77	ASN
35	1d	119	GLN
35	1d	123	HIS
35	1d	129	ASN
36	1e	20	GLN
36	1e	72	GLN
37	1f	73	ASN
38	1g	28	ASN
38	1g	64	GLN
38	1g	96	GLN
38	1g	148	ASN
40	1i	3	GLN
40	1i	34	ASN
40	1i	73	GLN
41	1j	56	HIS
42	1k	93	GLN
43	1l	99	HIS
44	1m	40	ASN
46	1o	9	GLN
46	1o	28	GLN
48	1q	26	GLN
50	1s	83	HIS
51	1t	18	GLN
53	1y	18	GLN
53	1y	38	HIS
3	2D	126	GLN
3	2D	129	ASN
3	2D	143	HIS
3	2D	253	GLN
4	2E	48	GLN
5	2F	69	HIS
5	2F	75	HIS
5	2F	133	ASN
6	2G	138	GLN
8	2I	43	ASN
8	2I	104	GLN

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Mol	Chain	Res	Type
8	2I	105	HIS
9	2N	8	GLN
9	2N	131	GLN
9	2N	133	GLN
12	2Q	13	GLN
12	2Q	89	ASN
12	2Q	123	HIS
12	2Q	141	GLN
15	2T	58	ASN
15	2T	123	GLN
18	2W	34	ASN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
21	2Z	32	HIS
21	2Z	55	HIS
21	2Z	151	HIS
26	24	60	GLN
30	28	35	GLN
33	2b	37	ASN
33	2b	78	GLN
33	2b	94	ASN
33	2b	135	GLN
33	2b	224	GLN
34	2c	6	HIS
34	2c	37	GLN
34	2c	104	GLN
34	2c	136	GLN
34	2c	176	HIS
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
36	2e	20	GLN
36	2e	65	ASN
37	2f	100	ASN
38	2g	13	GLN
38	2g	28	ASN
38	2g	64	GLN
38	2g	68	ASN
38	2g	106	GLN
40	2i	3	GLN

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Mol	Chain	Res	Type
40	2i	58	HIS
40	2i	117	HIS
42	2k	93	GLN
43	2l	99	HIS
44	2m	12	ASN
44	2m	62	ASN
44	2m	77	ASN
46	2o	28	GLN
48	2q	26	GLN
50	2s	65	ASN
50	2s	83	HIS
51	2t	16	HIS
53	2y	36	ASN
53	2y	58	ASN
53	2y	89	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	416 (14%)	32 (1%)
1	2A	2856/2915 (97%)	481 (16%)	36 (1%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	119/121 (98%)	16 (13%)	0
32	1a	1494/1521 (98%)	248 (16%)	0
32	2a	1498/1521 (98%)	264 (17%)	0
All	All	8949/9114 (98%)	1437 (16%)	68 (0%)

All (1437) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	14	A
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	94	C
1	1A	95	G

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Mol	Chain	Res	Type
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	140	G
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	197	A
1	1A	205	G
1	1A	214	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	265	A
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	275	G
1	1A	279	C
1	1A	283	A
1	1A	311	A
1	1A	330	A
1	1A	345	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	422	A
1	1A	428	A
1	1A	429	A

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Mol	Chain	Res	Type
1	1A	448	U
1	1A	451	C
1	1A	454	A
1	1A	456	C
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	652(U)	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	746	A
1	1A	747	U
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G

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Mol	Chain	Res	Type
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	878	A
1	1A	879	G
1	1A	882	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	889	C
1	1A	890	A
1	1A	892	G
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	953	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1005	C
1	1A	1012	U
1	1A	1013	C
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1039	G
1	1A	1041	C
1	1A	1042	G
1	1A	1043	C
1	1A	1046	A
1	1A	1047	G

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Mol	Chain	Res	Type
1	1A	1054	A
1	1A	1061	U
1	1A	1062	G
1	1A	1065	U
1	1A	1068	G
1	1A	1069	A
1	1A	1070	A
1	1A	1071	G
1	1A	1072	C
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1079	C
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1090	U
1	1A	1097	U
1	1A	1098	A
1	1A	1101	U
1	1A	1109	C
1	1A	1110	G
1	1A	1112	G
1	1A	1116	C
1	1A	1128	A
1	1A	1129	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1155	A
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1180	C
1	1A	1210	A

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Mol	Chain	Res	Type
1	1A	1211	U
1	1A	1220	A
1	1A	1229	G
1	1A	1241	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1365	A
1	1A	1370	C
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	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	1452	A
1	1A	1459	G
1	1A	1467	C
1	1A	1471	A
1	1A	1478	G
1	1A	1482	G
1	1A	1495	A
1	1A	1508	A
1	1A	1509(A)	A
1	1A	1523	U
1	1A	1525	G
1	1A	1531	C
1	1A	1532	C
1	1A	1542	A
1	1A	1543	C

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Mol	Chain	Res	Type
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
1	1A	1581	G
1	1A	1582	C
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1613	G
1	1A	1644	C
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1721	G
1	1A	1722	A
1	1A	1739	U
1	1A	1740	G
1	1A	1746	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	1816	G
1	1A	1817	G
1	1A	1820	U
1	1A	1828	G
1	1A	1829	A
1	1A	1839	G

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Mol	Chain	Res	Type
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1915	5MU
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1941	C
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2049	G
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	2103	C
1	1A	2107	C
1	1A	2108	C
1	1A	2111	C
1	1A	2112	G
1	1A	2116	G
1	1A	2117	A
1	1A	2119	A

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Mol	Chain	Res	Type
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2128	C
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2137	C
1	1A	2138	C
1	1A	2139	C
1	1A	2145	C
1	1A	2146	C
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2162	G
1	1A	2164	C
1	1A	2171	A
1	1A	2173	A
1	1A	2178	C
1	1A	2181	G
1	1A	2187	G
1	1A	2190	G
1	1A	2191	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	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	2319	G

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Mol	Chain	Res	Type
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2383	G
1	1A	2385	C
1	1A	2393	A
1	1A	2406	U
1	1A	2422	A
1	1A	2424	C
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2447	G
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2603	G
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G

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Mol	Chain	Res	Type
1	1A	2662	A
1	1A	2689	U
1	1A	2690	C
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2760	C
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2789	C
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	7	G
2	1B	9	G
2	1B	13	A
2	1B	45	A
2	1B	53	A
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	91	C
2	1B	106	G
2	1B	110	G
32	1a	9	G
32	1a	32	A
32	1a	39	G

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Mol	Chain	Res	Type
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	55	A
32	1a	61	G
32	1a	79	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	143	A
32	1a	144	G
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	216	G
32	1a	220	G
32	1a	231	G
32	1a	247	G
32	1a	251	G
32	1a	262	A
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	316	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

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Mol	Chain	Res	Type
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	423	G
32	1a	424	G
32	1a	427	U
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	475	G
32	1a	477	A
32	1a	480	U
32	1a	483	C
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	532	A
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	564	C
32	1a	572	A
32	1a	573	A

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Mol	Chain	Res	Type
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	631	G
32	1a	632	A
32	1a	633	G
32	1a	642	A
32	1a	649	G
32	1a	653	A
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	755	G
32	1a	759	A
32	1a	774	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	826	C
32	1a	828	A
32	1a	829	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	874	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A

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Mol	Chain	Res	Type
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	991	U
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	998	G
32	1a	999	C
32	1a	1001(A)	G
32	1a	1002	G
32	1a	1004	A
32	1a	1009	G
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(C)	G
32	1a	1032	G
32	1a	1033	G
32	1a	1037	C
32	1a	1042	G
32	1a	1044	A
32	1a	1053	G
32	1a	1065	U
32	1a	1066	C
32	1a	1067	A
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U

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Mol	Chain	Res	Type
32	1a	1101	A
32	1a	1124	G
32	1a	1130	A
32	1a	1132	C
32	1a	1133	G
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1149	C
32	1a	1150	U
32	1a	1152	A
32	1a	1159	U
32	1a	1163	C
32	1a	1166	G
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1224	G
32	1a	1225	A
32	1a	1227	A
32	1a	1238	A
32	1a	1248	A
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1263	C
32	1a	1270	C
32	1a	1273	G
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A

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Mol	Chain	Res	Type
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1312	G
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
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	1379	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1447	A
32	1a	1456	G
32	1a	1458	G
32	1a	1469	G
32	1a	1492	A
32	1a	1493	A
32	1a	1499	A
32	1a	1503	A
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	10	G
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	45	C
1	2A	50	U
1	2A	61	G

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Mol	Chain	Res	Type
1	2A	64	A
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	229	A
1	2A	230	U
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	363	G

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Mol	Chain	Res	Type
1	2A	386	G
1	2A	396	G
1	2A	406	G
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	457	A
1	2A	470	A
1	2A	471	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	551	G
1	2A	556	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	631	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G

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Mol	Chain	Res	Type
1	2A	652(U)	G
1	2A	669	G
1	2A	686	G
1	2A	715	G
1	2A	717	G
1	2A	730	C
1	2A	740	U
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	792	G
1	2A	805	G
1	2A	812	C
1	2A	815	C
1	2A	827	U
1	2A	857	C
1	2A	859	G
1	2A	869	G
1	2A	878	A
1	2A	880	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	896	A
1	2A	897	C
1	2A	899	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	915	C
1	2A	917	A
1	2A	932	G

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Mol	Chain	Res	Type
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	963	U
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1026	U
1	2A	1033	U
1	2A	1041	C
1	2A	1043	C
1	2A	1044	G
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A
1	2A	1057	A
1	2A	1058	G
1	2A	1060	U
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1070	A
1	2A	1071	G
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
1	2A	1079	C

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Mol	Chain	Res	Type
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	1094	U
1	2A	1096	A
1	2A	1109	C
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1114	G
1	2A	1116	C
1	2A	1117	G
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1171	G
1	2A	1195	G
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1230	C
1	2A	1236	G
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1319	G
1	2A	1321	A

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Mol	Chain	Res	Type
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1497	U
1	2A	1504	C
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1509(B)	A
1	2A	1525	G
1	2A	1531	C
1	2A	1533	G
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	1579	A
1	2A	1580	A
1	2A	1583	A

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Mol	Chain	Res	Type
1	2A	1584	C
1	2A	1586	A
1	2A	1593	G
1	2A	1595	G
1	2A	1608	A
1	2A	1609	A
1	2A	1639	U
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	1703	G
1	2A	1711	C
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1839	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	1914	C
1	2A	1919	A
1	2A	1927	A
1	2A	1929	G

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Mol	Chain	Res	Type
1	2A	1930	G
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1975	G
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	2032	G
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	2062	A
1	2A	2069	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	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	2127	G
1	2A	2129	C

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Mol	Chain	Res	Type
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2136	C
1	2A	2138	C
1	2A	2142	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	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2163	C
1	2A	2164	C
1	2A	2165	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2173	A
1	2A	2176	A
1	2A	2178	C
1	2A	2183	C
1	2A	2184	G
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2190	G
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2219	G
1	2A	2225	A
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2275	C

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Mol	Chain	Res	Type
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2396	G
1	2A	2406	U
1	2A	2410	G
1	2A	2422	A
1	2A	2423	U
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	2465	C
1	2A	2468	G
1	2A	2470	G
1	2A	2475	C
1	2A	2476	A
1	2A	2487	G
1	2A	2491	U
1	2A	2494	G

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Mol	Chain	Res	Type
1	2A	2497	A
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2529	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2602	A
1	2A	2603	G
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2757	A
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2789	C
1	2A	2802	G
1	2A	2803	C

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Mol	Chain	Res	Type
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2849	U
1	2A	2872	G
1	2A	2880	C
1	2A	2891	G
1	2A	2894	G
1	2A	2896	C
1	2A	2897	U
2	2B	7	G
2	2B	8	U
2	2B	9	G
2	2B	12	C
2	2B	13	A
2	2B	30	C
2	2B	33	G
2	2B	35	U
2	2B	42	C
2	2B	45	A
2	2B	51	G
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	106	G
2	2B	110	G
32	2a	5	U
32	2a	9	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	61	G
32	2a	66	G
32	2a	78	G
32	2a	88	A
32	2a	89	C
32	2a	101	A

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Mol	Chain	Res	Type
32	2a	116	A
32	2a	120	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	146	G
32	2a	156	G
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(C)	C
32	2a	189(F)	U
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	247	G
32	2a	250	A
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	298	A
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
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

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Mol	Chain	Res	Type
32	2a	412	A
32	2a	413	G
32	2a	421	U
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	443	C
32	2a	451	A
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	476	G
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	506	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	550	G
32	2a	559	A
32	2a	561	U
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	596	C
32	2a	630	G
32	2a	631	G
32	2a	650	G

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Mol	Chain	Res	Type
32	2a	653	A
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	854	G
32	2a	859	A
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	942	G
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C

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Mol	Chain	Res	Type
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	978	A
32	2a	980	C
32	2a	983	A
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1007	C
32	2a	1009	G
32	2a	1017	G
32	2a	1020	U
32	2a	1025	U
32	2a	1026	G
32	2a	1028	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1033	G
32	2a	1041	A
32	2a	1043	C
32	2a	1044	A
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1105	A
32	2a	1113	C
32	2a	1117	G
32	2a	1118	C

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Mol	Chain	Res	Type
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1139	G
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1162	C
32	2a	1171	G
32	2a	1172	C
32	2a	1176	A
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1203	C
32	2a	1208	C
32	2a	1212	U
32	2a	1214	C
32	2a	1224	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1281	U
32	2a	1282	C
32	2a	1285	A
32	2a	1286	A
32	2a	1287	A

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Mol	Chain	Res	Type
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1312	G
32	2a	1319	A
32	2a	1320	C
32	2a	1323	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U
32	2a	1359	C
32	2a	1363	C
32	2a	1364	U
32	2a	1370	G
32	2a	1375	A
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1456	G
32	2a	1457	G
32	2a	1487	G
32	2a	1492	A
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1528	U
32	2a	1529	G
32	2a	1530	G

All (68) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	199	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	746	A
1	1A	764	A
1	1A	839	U
1	1A	895	U
1	1A	974	G
1	1A	1065	U
1	1A	1142(A)	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1300	U
1	1A	1301	A
1	1A	1379	A
1	1A	1442	G
1	1A	1608	A
1	1A	1653	G
1	1A	1663	C
1	1A	1929	G
1	1A	2126	A
1	1A	2288	A
1	1A	2406	U
1	1A	2430	A
1	1A	2439	A
1	1A	2602	A
1	1A	2611	U
1	1A	2689	U
1	1A	2756	U
1	1A	2893	G
1	2A	9	U
1	2A	195	A
1	2A	196	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	752	A
1	2A	764	A
1	2A	827	U
1	2A	840	C

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Mol	Chain	Res	Type
1	2A	856	C
1	2A	900	A
1	2A	1047	G
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1076	C
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	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	2601	C
1	2A	2602	A
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	PSU	1a	516	32,54	18,21,22	1.38	2 (11%)	22,30,33	1.76	3 (13%)
1	PSU	1A	1917	1	18,21,22	1.33	2 (11%)	22,30,33	1.87	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MU	1A	1915	1,54	19,22,23	1.42	5 (26%)	28,32,35	2.31	9 (32%)
32	4OC	1a	1402	32	20,23,24	0.73	0	26,32,35	0.92	1 (3%)
32	5MC	1a	1404	32	18,22,23	0.95	2 (11%)	26,32,35	1.14	2 (7%)
1	OMC	1A	1920	1	19,22,23	0.83	0	26,31,34	0.89	1 (3%)
32	MA6	2a	1518	32	19,26,27	0.80	0	18,38,41	1.40	2 (11%)
32	M2G	2a	966	32,54	20,27,28	1.46	3 (15%)	22,40,43	0.93	1 (4%)
32	G7M	2a	527	32,54	20,26,27	1.24	2 (10%)	17,39,42	0.52	0
32	5MC	2a	1400	32	18,22,23	0.97	2 (11%)	26,32,35	1.24	2 (7%)
32	M2G	1a	966	32	20,27,28	1.45	3 (15%)	22,40,43	0.93	2 (9%)
32	MA6	1a	1519	32	19,26,27	0.78	0	18,38,41	1.48	2 (11%)
1	PSU	2A	1917	1	18,21,22	1.32	2 (11%)	22,30,33	1.95	3 (13%)
1	MA6	1A	2058	1,54	19,26,27	0.78	0	18,38,41	1.61	2 (11%)
1	PSU	2A	1911	1	18,21,22	1.35	2 (11%)	22,30,33	1.93	3 (13%)
1	PSU	2A	2605	1	18,21,22	1.30	3 (16%)	22,30,33	1.96	4 (18%)
32	5MC	1a	1400	32	18,22,23	1.04	2 (11%)	26,32,35	1.22	3 (11%)
1	OMG	2A	2251	1,54	18,26,27	0.95	1 (5%)	19,38,41	1.07	2 (10%)
32	PSU	2a	516	32,54	18,21,22	1.33	2 (11%)	22,30,33	1.94	5 (22%)
1	OMC	2A	1920	1	19,22,23	0.83	0	26,31,34	1.01	1 (3%)
32	UR3	2a	1498	32,54	19,22,23	1.02	2 (10%)	26,32,35	1.39	2 (7%)
32	UR3	1a	1498	32	19,22,23	0.99	0	26,32,35	1.62	4 (15%)
1	OMG	1A	2251	1,54	18,26,27	1.05	1 (5%)	19,38,41	1.02	1 (5%)
1	5MC	1A	1962	1,54	18,22,23	0.93	2 (11%)	26,32,35	1.08	2 (7%)
1	OMU	1A	2552	1,54	19,22,23	1.26	3 (15%)	26,31,34	1.83	6 (23%)
1	5MU	2A	1915	1	19,22,23	1.45	4 (21%)	28,32,35	2.17	9 (32%)
32	4OC	2a	1402	32	20,23,24	0.77	0	26,32,35	1.09	3 (11%)
32	5MC	1a	1407	32	18,22,23	0.93	2 (11%)	26,32,35	1.11	3 (11%)
32	2MG	2a	1207	32	18,26,27	0.90	1 (5%)	16,38,41	1.16	3 (18%)
1	MA6	2A	2058	56,1	19,26,27	0.78	0	18,38,41	1.84	4 (22%)
1	PSU	1A	2605	1,54	18,21,22	1.33	2 (11%)	22,30,33	1.87	4 (18%)
32	5MC	1a	967	32	18,22,23	1.00	2 (11%)	26,32,35	1.07	2 (7%)
1	PSU	1A	1911	1	18,21,22	1.33	2 (11%)	22,30,33	1.95	5 (22%)
32	5MC	2a	1404	32	18,22,23	0.95	2 (11%)	26,32,35	1.13	2 (7%)
1	2MA	2A	2503	1,54	17,25,26	0.99	1 (5%)	17,37,40	1.03	2 (11%)
1	OMU	2A	2552	1,54	19,22,23	1.25	3 (15%)	26,31,34	1.85	6 (23%)
32	MA6	1a	1518	32	19,26,27	0.80	0	18,38,41	1.34	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	MA6	2a	1519	32	19,26,27	0.83	0	18,38,41	1.53	2 (11%)
1	5MC	2A	1942	1	18,22,23	0.96	2 (11%)	26,32,35	1.22	2 (7%)
1	5MU	2A	1939	1	19,22,23	1.40	4 (21%)	28,32,35	2.40	8 (28%)
1	2MA	1A	2503	1,54	17,25,26	1.05	2 (11%)	17,37,40	0.92	1 (5%)
32	5MC	2a	1407	32	18,22,23	0.99	1 (5%)	26,32,35	1.17	3 (11%)
1	5MC	1A	1942	1,54	18,22,23	0.97	2 (11%)	26,32,35	1.09	1 (3%)
43	0TD	1l	92	43	7,9,10	4.74	1 (14%)	6,11,13	8.27	3 (50%)
1	5MU	1A	1939	1,54	19,22,23	1.52	6 (31%)	28,32,35	2.01	6 (21%)
32	G7M	1a	527	32,54	20,26,27	1.18	2 (10%)	17,39,42	0.45	0
43	0TD	2l	92	43	7,9,10	4.75	1 (14%)	6,11,13	5.93	3 (50%)
1	5MC	2A	1962	1,54	18,22,23	0.99	2 (11%)	26,32,35	1.16	2 (7%)
32	5MC	2a	967	32	18,22,23	0.99	2 (11%)	26,32,35	1.07	2 (7%)
32	2MG	1a	1207	32	18,26,27	0.95	1 (5%)	16,38,41	1.21	2 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1,54	-	2/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	M2G	2a	966	32,54	-	0/7/29/30	0/3/3/3
32	G7M	2a	527	32,54	-	2/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	4/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	MA6	1A	2058	1,54	-	0/7/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
1	OMG	2A	2251	1,54	-	0/5/27/28	0/3/3/3
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
32	UR3	2a	1498	32,54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,54	-	1/5/27/28	0/3/3/3
1	5MC	1A	1962	1,54	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,54	-	0/9/27/28	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	MA6	2A	2058	56,1	-	0/7/29/30	0/3/3/3
1	PSU	1A	2605	1,54	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,54	-	1/3/25/26	0/3/3/3
1	OMU	2A	2552	1,54	-	0/9/27/28	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	1/7/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,54	-	2/3/25/26	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
1	5MU	1A	1939	1,54	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,54	-	1/3/25/26	0/3/3/3
43	0TD	2l	92	43	-	1/7/12/14	-
1	5MC	2A	1962	1,54	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	1/5/27/28	0/3/3/3

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.23	1.69	1.82
43	1l	92	0TD	CB-SB	-12.13	1.69	1.82
32	2a	966	M2G	C2-N3	4.59	1.36	1.30
32	1a	966	M2G	C2-N3	4.45	1.36	1.30
32	1a	516	PSU	C6-C5	3.69	1.39	1.35
32	2a	527	G7M	C5-C4	3.66	1.46	1.39
32	1a	527	G7M	C5-C4	3.61	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1917	PSU	C6-C5	3.35	1.39	1.35
32	2a	516	PSU	C6-C5	3.29	1.39	1.35
1	1A	2605	PSU	C4-N3	-3.27	1.32	1.38
1	2A	1911	PSU	C6-C5	3.22	1.39	1.35
32	1a	1400	5MC	C6-C5	3.03	1.39	1.34
1	1A	1939	5MU	C6-C5	3.02	1.39	1.34
1	1A	1915	5MU	C2-N1	3.01	1.43	1.38
1	2A	1915	5MU	C6-C5	3.00	1.39	1.34
1	2A	1962	5MC	C6-C5	2.97	1.39	1.34
1	1A	1911	PSU	C6-C5	2.91	1.38	1.35
1	2A	1915	5MU	C2-N1	2.90	1.43	1.38
32	2a	1407	5MC	C6-C5	2.89	1.39	1.34
1	1A	1939	5MU	C4-N3	-2.89	1.33	1.38
32	1a	967	5MC	C6-C5	2.88	1.39	1.34
1	2A	1939	5MU	C4-C5	2.87	1.49	1.44
1	2A	1917	PSU	C6-C5	2.87	1.38	1.35
32	2a	967	5MC	C6-C5	2.86	1.39	1.34
1	2A	1939	5MU	C6-C5	2.83	1.39	1.34
32	1a	1404	5MC	C6-C5	2.82	1.39	1.34
32	1a	966	M2G	C6-N1	-2.81	1.33	1.37
1	1A	1942	5MC	C6-C5	2.78	1.39	1.34
32	2a	1400	5MC	C6-C5	2.77	1.39	1.34
1	2A	1942	5MC	C6-C5	2.75	1.39	1.34
32	2a	1404	5MC	C6-C5	2.73	1.39	1.34
1	1A	2251	OMG	C6-N1	-2.70	1.33	1.37
1	2A	2605	PSU	C4-N3	-2.70	1.33	1.38
32	1a	966	M2G	C2-N2	2.68	1.40	1.35
32	1a	1407	5MC	C6-C5	2.64	1.38	1.34
1	1A	1917	PSU	C4-N3	-2.62	1.34	1.38
1	1A	1911	PSU	C4-N3	-2.62	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.60	1.34	1.38
32	2a	966	M2G	C2-N2	2.59	1.40	1.35
1	2A	1939	5MU	C4-N3	-2.58	1.34	1.38
1	1A	1939	5MU	C4-C5	2.56	1.49	1.44
1	2A	1915	5MU	C4-N3	-2.56	1.34	1.38
32	1a	516	PSU	C4-N3	-2.55	1.34	1.38
1	2A	2605	PSU	C6-C5	2.54	1.38	1.35
1	2A	1917	PSU	C4-N3	-2.54	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.52	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.50	1.34	1.37
1	2A	2552	OMU	C4-N3	-2.50	1.34	1.38
32	2a	516	PSU	C4-N3	-2.49	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	OMU	C4-N3	-2.46	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.45	1.33	1.38
1	1A	1915	5MU	C6-C5	2.45	1.38	1.34
1	2A	2251	OMG	C6-N1	-2.45	1.34	1.37
32	2a	527	G7M	C6-N1	-2.45	1.34	1.37
32	2a	966	M2G	C6-N1	-2.40	1.34	1.37
32	2a	1207	2MG	C6-N1	-2.36	1.34	1.37
32	1a	1400	5MC	C6-N1	-2.36	1.34	1.38
1	1A	1939	5MU	C2-N1	2.36	1.42	1.38
32	2a	1400	5MC	C6-N1	-2.36	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.34	1.34	1.38
32	1a	527	G7M	C6-N1	-2.33	1.34	1.37
1	2A	1915	5MU	C4-C5	2.29	1.48	1.44
1	1A	1915	5MU	C4-C5	2.28	1.48	1.44
1	2A	2552	OMU	C5-C4	2.28	1.48	1.43
32	2a	1498	UR3	C6-C5	2.27	1.40	1.35
1	2A	1939	5MU	C6-N1	-2.26	1.34	1.38
1	1A	2552	OMU	C5-C4	2.23	1.48	1.43
32	2a	1404	5MC	C6-N1	-2.22	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.20	1.34	1.38
1	1A	1939	5MU	C6-N1	-2.19	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.19	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.19	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.19	1.33	1.37
1	1A	2503	2MA	C2-N3	2.18	1.35	1.31
1	1A	2552	OMU	C2-N3	-2.16	1.34	1.38
1	1A	1962	5MC	C6-C5	2.13	1.38	1.34
1	1A	1939	5MU	C2-N3	-2.11	1.34	1.38
32	2a	1498	UR3	C2-N1	2.10	1.41	1.38
32	2a	967	5MC	C6-N1	-2.10	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.09	1.33	1.37
1	1A	2503	2MA	C6-N1	-2.08	1.33	1.38
32	1a	967	5MC	C6-N1	-2.08	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.07	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.02	1.34	1.38
1	2A	2503	2MA	C6-N1	-2.00	1.33	1.38
1	2A	2552	OMU	C6-C5	2.00	1.39	1.35

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-19.80	66.63	102.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-13.91	77.28	102.44
32	1a	1498	UR3	C4-N3-C2	-6.33	118.60	124.56
1	2A	1911	PSU	N1-C2-N3	6.17	122.12	115.13
1	2A	1939	5MU	C4-N3-C2	-6.14	119.40	127.35
1	2A	1917	PSU	N1-C2-N3	6.10	122.04	115.13
1	1A	1911	PSU	N1-C2-N3	6.09	122.03	115.13
32	2a	516	PSU	N1-C2-N3	6.00	121.93	115.13
1	2A	1939	5MU	N3-C2-N1	5.84	122.64	114.89
1	2A	2605	PSU	N1-C2-N3	5.80	121.70	115.13
1	1A	1917	PSU	N1-C2-N3	5.75	121.65	115.13
32	2a	1498	UR3	C4-N3-C2	-5.68	119.21	124.56
1	1A	2605	PSU	N1-C2-N3	5.67	121.55	115.13
32	1a	516	PSU	N1-C2-N3	5.54	121.41	115.13
1	1A	2058	MA6	N3-C2-N1	-5.16	120.61	128.68
1	2A	2552	OMU	N3-C2-N1	5.16	121.74	114.89
1	2A	2058	MA6	N3-C2-N1	-5.08	120.74	128.68
1	1A	1915	5MU	C1'-N1-C2	5.02	126.65	117.57
1	1A	1939	5MU	C4-N3-C2	-4.97	120.91	127.35
1	2A	1915	5MU	N3-C2-N1	4.86	121.34	114.89
1	1A	1939	5MU	N3-C2-N1	4.80	121.26	114.89
32	1a	1519	MA6	N3-C2-N1	-4.79	121.20	128.68
1	1A	2552	OMU	N3-C2-N1	4.78	121.23	114.89
1	2A	1939	5MU	C5-C4-N3	4.65	119.28	115.31
32	2a	1518	MA6	N3-C2-N1	-4.64	121.42	128.68
32	2a	1519	MA6	N3-C2-N1	-4.56	121.56	128.68
1	1A	1915	5MU	C1'-N1-C6	-4.53	113.58	121.12
32	1a	1518	MA6	N3-C2-N1	-4.52	121.62	128.68
1	1A	1915	5MU	C4-N3-C2	-4.51	121.51	127.35
32	2a	1400	5MC	C5-C6-N1	-4.44	118.77	123.34
1	2A	2552	OMU	C4-N3-C2	-4.42	120.74	126.58
1	2A	1915	5MU	C4-N3-C2	-4.40	121.65	127.35
1	1A	1915	5MU	C5-C4-N3	4.40	119.07	115.31
1	1A	1939	5MU	C5-C4-N3	4.38	119.05	115.31
1	2A	1939	5MU	C5-C6-N1	-4.38	118.83	123.34
1	2A	2605	PSU	C4-N3-C2	-4.36	120.05	126.34
1	1A	1915	5MU	N3-C2-N1	4.35	120.67	114.89
1	1A	2605	PSU	C4-N3-C2	-4.30	120.14	126.34
1	1A	1939	5MU	C5-C6-N1	-4.21	119.00	123.34
1	2A	1915	5MU	C1'-N1-C2	4.20	125.17	117.57
1	2A	1939	5MU	O2-C2-N1	-4.10	117.33	122.79
1	2A	1911	PSU	C4-N3-C2	-4.04	120.52	126.34
1	2A	1917	PSU	C4-N3-C2	-4.03	120.53	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1400	5MC	C5-C6-N1	-4.03	119.20	123.34
1	1A	1911	PSU	C4-N3-C2	-4.02	120.54	126.34
1	1A	2552	OMU	C4-N3-C2	-4.02	121.28	126.58
32	2a	516	PSU	C4-N3-C2	-4.00	120.57	126.34
1	1A	1915	5MU	O4-C4-C5	-4.00	120.27	124.90
1	1A	1917	PSU	C4-N3-C2	-3.98	120.61	126.34
1	2A	1917	PSU	O2-C2-N1	-3.93	118.47	122.79
1	1A	1911	PSU	O2-C2-N1	-3.89	118.51	122.79
1	2A	1939	5MU	O4-C4-C5	-3.87	120.41	124.90
1	2A	1942	5MC	C5-C6-N1	-3.87	119.36	123.34
1	2A	1915	5MU	C5-C4-N3	3.82	118.58	115.31
1	2A	1915	5MU	O4-C4-C5	-3.82	120.47	124.90
1	1A	1942	5MC	C5-C6-N1	-3.81	119.42	123.34
32	1a	1404	5MC	C5-C6-N1	-3.75	119.48	123.34
32	2a	1519	MA6	C4-C5-N7	-3.64	105.61	109.40
1	2A	2552	OMU	O2-C2-N1	-3.60	118.01	122.79
32	1a	516	PSU	C4-N3-C2	-3.59	121.16	126.34
32	1a	1407	5MC	C5-C6-N1	-3.55	119.69	123.34
32	2a	967	5MC	C5-C6-N1	-3.43	119.81	123.34
1	2A	1962	5MC	C5-C6-N1	-3.43	119.81	123.34
32	2a	516	PSU	O2-C2-N1	-3.39	119.06	122.79
1	2A	1915	5MU	C1'-N1-C6	-3.32	115.60	121.12
1	2A	1911	PSU	O2-C2-N1	-3.31	119.15	122.79
1	2A	2605	PSU	O2-C2-N1	-3.28	119.18	122.79
32	1a	967	5MC	C5-C6-N1	-3.27	119.97	123.34
32	2a	1404	5MC	C5-C6-N1	-3.26	119.99	123.34
43	1l	92	0TD	OD2-CG-CB	3.26	120.18	113.15
1	1A	1962	5MC	C5-C6-N1	-3.25	119.99	123.34
43	2l	92	0TD	OD2-CG-CB	3.22	120.11	113.15
1	1A	1939	5MU	O4-C4-C5	-3.20	121.20	124.90
32	2a	1407	5MC	C5-C6-N1	-3.17	120.07	123.34
1	2A	2058	MA6	C4-C5-N7	-3.14	106.13	109.40
1	1A	1917	PSU	O2-C2-N1	-3.09	119.39	122.79
1	2A	2058	MA6	N1-C6-N6	-3.00	113.90	117.06
1	1A	2552	OMU	C2'-C1'-N1	-2.99	108.41	114.22
32	1a	1519	MA6	C4-C5-N7	-2.98	106.29	109.40
32	2a	1518	MA6	C4-C5-N7	-2.92	106.36	109.40
32	2a	1404	5MC	C5-C4-N3	-2.91	118.53	121.67
1	1A	2552	OMU	O4-C4-C5	-2.90	120.06	125.16
1	1A	2605	PSU	O2-C2-N1	-2.83	119.67	122.79
1	2A	1962	5MC	C5-C4-N3	-2.79	118.66	121.67
32	2a	1407	5MC	C5-C4-N3	-2.78	118.67	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1404	5MC	C5-C4-N3	-2.76	118.69	121.67
1	1A	2058	MA6	C4-C5-N7	-2.71	106.57	109.40
1	1A	2552	OMU	C5-C4-N3	2.71	118.89	114.84
1	1A	2251	OMG	C8-N7-C5	2.70	108.14	102.99
1	2A	2552	OMU	O4-C4-C5	-2.70	120.41	125.16
32	1a	1518	MA6	C4-C5-N7	-2.67	106.62	109.40
1	2A	2552	OMU	C5-C4-N3	2.66	118.83	114.84
32	1a	1402	4OC	C6-C5-C4	2.62	120.16	116.96
1	2A	1920	OMC	O2-C2-N3	-2.61	118.09	122.33
32	1a	1400	5MC	C5-C4-N3	-2.60	118.87	121.67
1	2A	2503	2MA	C8-N7-C5	2.59	107.92	102.99
1	1A	1915	5MU	C5M-C5-C4	2.57	121.59	118.77
32	1a	1498	UR3	C3U-N3-C2	2.56	121.80	117.31
1	2A	2552	OMU	C2'-C1'-N1	-2.52	109.33	114.22
32	1a	1207	2MG	C5-C6-N1	2.52	118.39	113.95
32	1a	1498	UR3	C1'-N1-C2	2.52	121.24	116.99
32	2a	967	5MC	C5-C4-N3	-2.52	118.96	121.67
32	1a	516	PSU	O2-C2-N1	-2.50	120.04	122.79
32	2a	1407	5MC	O2-C2-N3	-2.49	118.27	122.33
32	1a	1207	2MG	C8-N7-C5	2.45	107.67	102.99
1	2A	1915	5MU	C5-C6-N1	-2.45	120.81	123.34
32	2a	516	PSU	O4'-C1'-C2'	2.42	108.55	105.14
1	2A	2503	2MA	C5-C6-N1	2.37	118.11	114.02
1	2A	2058	MA6	C1'-N9-C4	-2.37	122.48	126.64
1	1A	2605	PSU	C5-C6-N1	-2.36	118.57	122.11
32	1a	966	M2G	C5-C6-N1	2.36	118.12	113.95
32	1a	967	5MC	C5-C4-N3	-2.34	119.14	121.67
32	2a	966	M2G	C8-N7-C5	2.34	107.45	102.99
1	1A	2503	2MA	C8-N7-C5	2.34	107.44	102.99
32	2a	1402	4OC	C6-C5-C4	2.33	119.81	116.96
1	2A	1915	5MU	O2-C2-N3	-2.32	117.18	121.50
1	2A	1942	5MC	C5-C4-N3	-2.32	119.17	121.67
43	1l	92	0TD	OD1-CG-CB	-2.29	117.64	122.44
1	1A	1920	OMC	O2-C2-N3	-2.28	118.62	122.33
1	1A	1915	5MU	O2-C2-N3	-2.28	117.25	121.50
32	2a	1207	2MG	C8-N7-C5	2.28	107.33	102.99
1	2A	2251	OMG	C8-N7-C5	2.26	107.29	102.99
43	2l	92	0TD	OD1-CG-CB	-2.26	117.71	122.44
1	2A	2605	PSU	C5-C6-N1	-2.26	118.72	122.11
32	1a	1407	5MC	C5-C4-N3	-2.25	119.25	121.67
32	1a	966	M2G	C8-N7-C5	2.24	107.25	102.99
1	1A	1915	5MU	C5-C6-N1	-2.22	121.05	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1962	5MC	C1'-N1-C6	-2.21	117.44	121.12
1	2A	1939	5MU	C5M-C5-C6	-2.21	119.90	122.85
32	1a	1498	UR3	C6-N1-C2	-2.21	119.81	121.79
32	2a	1498	UR3	C3U-N3-C4	2.17	120.99	117.89
1	1A	1939	5MU	O2-C2-N1	-2.15	119.93	122.79
32	2a	1207	2MG	CM2-N2-C2	-2.14	119.13	123.86
32	2a	1207	2MG	C5-C6-N1	2.13	117.71	113.95
1	1A	1911	PSU	O4'-C1'-C2'	2.10	108.11	105.14
1	2A	1939	5MU	C5M-C5-C4	2.10	121.08	118.77
32	2a	1400	5MC	C5-C4-N3	-2.09	119.42	121.67
1	2A	1915	5MU	C6-N1-C2	-2.09	119.18	121.30
32	2a	516	PSU	C5-C6-N1	-2.08	118.99	122.11
1	1A	1911	PSU	C5-C6-N1	-2.07	119.00	122.11
32	1a	1400	5MC	O2-C2-N3	-2.07	118.97	122.33
1	1A	1917	PSU	C5-C6-N1	-2.07	119.01	122.11
1	1A	2552	OMU	O2-C2-N1	-2.06	120.05	122.79
32	1a	1407	5MC	CM5-C5-C6	-2.03	120.14	122.85
1	2A	2251	OMG	C5-C6-N1	2.01	117.50	113.95
32	2a	1402	4OC	CM2-O2'-C2'	2.01	119.80	114.52
32	2a	1402	4OC	C5-C4-N4	-2.01	118.52	122.61

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
1	1A	2251	OMG	C1'-C2'-O2'-CM2
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
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
32	2a	1400	5MC	C2'-C1'-N1-C6
32	1a	1207	2MG	O4'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1402	4OC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	1A	1920	OMC	C2'-C1'-N1-C2
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
1	2A	1920	OMC	C2'-C1'-N1-C2
32	2a	1400	5MC	O4'-C1'-N1-C2
32	1a	1400	5MC	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1400	5MC	C2'-C1'-N1-C2
1	1A	2503	2MA	O4'-C4'-C5'-O5'

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 2442 ligands modelled in this entry, 2427 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
56	ERY	2A	3672	1	53,53,53	0.92	1 (1%)	82,82,82	1.57	15 (18%)
60	SF4	1d	304	35	0,12,12	-	-	-		
60	SF4	2d	501	35	0,12,12	-	-	-		
57	MPD	1A	4028	-	7,7,7	0.31	0	9,10,10	0.23	0
57	MPD	2A	3673	-	7,7,7	0.29	0	9,10,10	0.21	0
55	HGR	2A	3671	-	39,39,39	2.43	9 (23%)	50,58,58	1.62	10 (20%)
57	MPD	1T	205	-	7,7,7	0.31	0	9,10,10	0.37	0
57	MPD	2A	3675	-	7,7,7	0.31	0	9,10,10	0.29	0
56	ERY	1A	4027	-	53,53,53	0.90	2 (3%)	82,82,82	1.49	12 (14%)
55	HGR	1A	4026	-	39,39,39	2.40	8 (20%)	50,58,58	1.82	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
57	MPD	1a	1882	32	7,7,7	0.49	0	9,10,10	0.66	0
57	MPD	18	103	-	7,7,7	0.26	0	9,10,10	0.50	0
58	ARG	1B	230	54	10,11,11	0.75	1 (10%)	11,13,13	1.09	2 (18%)
58	ARG	1F	318	-	10,11,11	0.73	0	11,13,13	1.04	2 (18%)
57	MPD	2A	3674	-	7,7,7	0.32	0	9,10,10	0.19	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
56	ERY	2A	3672	1	-	13/72/107/107	0/3/3/3
60	SF4	1d	304	35	-	-	0/6/5/5
60	SF4	2d	501	35	-	-	0/6/5/5
57	MPD	1A	4028	-	-	2/5/5/5	-
57	MPD	2A	3673	-	-	0/5/5/5	-
55	HGR	2A	3671	-	-	5/20/79/79	0/4/4/4
57	MPD	1T	205	-	-	0/5/5/5	-
57	MPD	2A	3675	-	-	3/5/5/5	-
56	ERY	1A	4027	-	-	4/72/107/107	0/3/3/3
55	HGR	1A	4026	-	-	5/20/79/79	0/4/4/4
57	MPD	1a	1882	32	-	2/5/5/5	-
57	MPD	18	103	-	-	2/5/5/5	-
58	ARG	1B	230	54	-	0/11/11/11	-
58	ARG	1F	318	-	-	5/11/11/11	-
57	MPD	2A	3674	-	-	3/5/5/5	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2A	3671	HGR	C12-C14	9.29	1.55	1.33
55	1A	4026	HGR	C12-C14	9.01	1.54	1.33
55	1A	4026	HGR	C5-C6	-5.30	1.39	1.50
55	2A	3671	HGR	C5-C6	-5.29	1.39	1.50
55	1A	4026	HGR	C5-C4	-5.23	1.39	1.49
56	2A	3672	ERY	O2-C1	5.21	1.46	1.34
55	2A	3671	HGR	C5-C4	-5.18	1.39	1.49
56	1A	4027	ERY	O2-C1	4.79	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2A	3671	HGR	C3-C2	-4.75	1.39	1.48
55	2A	3671	HGR	O4-C2	4.58	1.36	1.24
55	1A	4026	HGR	C3-C2	-4.45	1.39	1.48
55	1A	4026	HGR	O4-C2	4.22	1.35	1.24
55	2A	3671	HGR	C1-C6	2.87	1.39	1.35
55	1A	4026	HGR	C8-C7	-2.79	1.50	1.53
55	1A	4026	HGR	O8-C23	2.73	1.45	1.41
55	1A	4026	HGR	C1-C6	2.67	1.39	1.35
55	2A	3671	HGR	O1-C10	2.33	1.45	1.41
56	1A	4027	ERY	O2-C13	-2.28	1.42	1.46
55	2A	3671	HGR	O8-C23	2.26	1.45	1.41
58	1B	230	ARG	OXT-C	-2.19	1.23	1.30
55	2A	3671	HGR	O9-C23	2.12	1.44	1.41

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	1A	4027	ERY	O7-C5-C6	5.04	112.61	106.39
56	2A	3672	ERY	O5-C16-C15	-4.77	105.32	112.96
55	1A	4026	HGR	C4-C5-C6	4.36	121.76	112.36
55	2A	3671	HGR	C4-C5-C6	4.26	121.53	112.36
56	2A	3672	ERY	O5-C16-C17	4.14	109.95	103.81
55	1A	4026	HGR	C12-C6-C1	-3.98	115.65	119.31
56	1A	4027	ERY	O5-C16-C17	3.95	109.67	103.81
56	2A	3672	ERY	O7-C5-C6	3.95	111.26	106.39
55	2A	3671	HGR	C12-C6-C1	-3.89	115.73	119.31
56	1A	4027	ERY	C13-O2-C1	-3.88	111.28	118.18
56	1A	4027	ERY	C6-C5-C4	-3.53	109.06	114.05
55	1A	4026	HGR	O9-C22-C18	-3.41	98.33	105.97
55	1A	4026	HGR	C23-O9-C22	-3.40	101.13	106.31
56	2A	3672	ERY	O2-C1-C2	3.36	118.94	111.56
55	1A	4026	HGR	O1-C10-C9	-3.35	100.67	104.98
55	2A	3671	HGR	O8-C18-C22	-3.25	98.68	105.97
55	1A	4026	HGR	C8-C7-C11	-3.24	107.98	113.67
56	1A	4027	ERY	O2-C1-C2	3.20	118.58	111.56
55	2A	3671	HGR	O1-C10-C9	-3.17	100.89	104.98
55	1A	4026	HGR	C4-C3-C2	-3.17	118.91	121.83
56	2A	3672	ERY	C25-C24-N1	-3.15	106.78	115.67
56	2A	3672	ERY	C6-C5-C4	-3.00	109.80	114.05
56	1A	4027	ERY	C25-C24-N1	-2.98	107.25	115.67
55	1A	4026	HGR	O8-C18-C22	-2.93	99.40	105.97
55	2A	3671	HGR	O4-C2-C3	-2.89	116.78	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	1A	4027	ERY	O5-C16-C15	-2.86	108.38	112.96
55	1A	4026	HGR	C10-C9-C8	-2.85	98.68	102.30
56	2A	3672	ERY	C15-C16-C17	2.85	112.78	107.67
56	2A	3672	ERY	C13-O2-C1	-2.83	113.15	118.18
55	2A	3671	HGR	C10-C9-C8	-2.76	98.80	102.30
55	1A	4026	HGR	C1-C2-C3	2.74	121.27	115.99
56	2A	3672	ERY	C20-O5-C16	2.71	123.21	117.55
55	2A	3671	HGR	C4-C3-C2	-2.59	119.44	121.83
56	1A	4027	ERY	O7-C5-C4	-2.58	107.68	111.54
55	2A	3671	HGR	C8-C7-C11	-2.57	109.16	113.67
58	1B	230	ARG	OXT-C-O	-2.55	118.30	124.09
56	1A	4027	ERY	C20-O5-C16	2.55	122.86	117.55
58	1F	318	ARG	OXT-C-O	-2.54	118.31	124.09
56	2A	3672	ERY	C16-C17-C18	2.52	114.99	111.14
55	1A	4026	HGR	O3-C3-C2	2.51	117.33	112.56
56	2A	3672	ERY	C23-C24-N1	2.49	118.04	110.83
55	1A	4026	HGR	O3-C10-C9	2.45	110.92	106.78
55	2A	3671	HGR	C1-C2-C3	2.42	120.66	115.99
56	2A	3672	ERY	O4-C18-C21	2.37	111.82	106.70
56	2A	3672	ERY	C14-O4-C18	2.34	120.15	113.84
55	1A	4026	HGR	O4-C2-C3	-2.29	117.71	121.30
56	2A	3672	ERY	C16-C15-C14	-2.28	111.12	115.07
56	1A	4027	ERY	C2-C3-C4	-2.25	106.53	113.05
55	2A	3671	HGR	O9-C22-C18	-2.20	101.04	105.97
58	1B	230	ARG	OXT-C-CA	2.20	120.88	113.38
58	1F	318	ARG	OXT-C-CA	2.14	120.68	113.38
55	1A	4026	HGR	C9-C8-C7	-2.11	99.17	101.64
56	2A	3672	ERY	C27-C26-C25	-2.10	110.11	113.40
56	1A	4027	ERY	O2-C1-O1	-2.03	120.15	123.94
56	1A	4027	ERY	O3-C3-C4	2.01	110.65	108.22

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	1A	4026	HGR	C2-C3-O3-C10
55	2A	3671	HGR	C2-C3-O3-C10
56	1A	4027	ERY	C15-C16-O5-C20
56	1A	4027	ERY	C17-C16-O5-C20
56	2A	3672	ERY	C15-C16-O5-C20
56	2A	3672	ERY	C17-C16-O5-C20
56	2A	3672	ERY	C19-C16-O5-C20

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Mol	Chain	Res	Type	Atoms
57	18	103	MPD	C2-C3-C4-O4
56	2A	3672	ERY	C23-C24-N1-C29
56	1A	4027	ERY	C19-C16-O5-C20
58	1F	318	ARG	OXT-C-CA-N
56	2A	3672	ERY	C32-C6-C7-C8
56	2A	3672	ERY	C6-C7-C8-C33
56	2A	3672	ERY	O7-C5-C6-C7
56	2A	3672	ERY	C4-C5-C6-O10
58	1F	318	ARG	O-C-CA-N
57	2A	3675	MPD	O2-C2-C3-C4
57	18	103	MPD	C2-C3-C4-C5
57	1a	1882	MPD	C2-C3-C4-C5
57	2A	3674	MPD	C2-C3-C4-C5
55	1A	4026	HGR	C12-C14-C15-O7
55	2A	3671	HGR	C12-C14-C15-O7
55	2A	3671	HGR	C12-C14-C15-N1
58	1F	318	ARG	OXT-C-CA-CB
56	1A	4027	ERY	C23-C24-N1-C29
58	1F	318	ARG	O-C-CA-CB
55	1A	4026	HGR	C16-C14-C15-O7
55	2A	3671	HGR	C16-C14-C15-O7
55	2A	3671	HGR	C16-C14-C15-N1
58	1F	318	ARG	CA-CB-CG-CD
55	1A	4026	HGR	C12-C14-C15-N1
56	2A	3672	ERY	C4-C5-C6-C32
56	2A	3672	ERY	C25-C24-N1-C28
56	2A	3672	ERY	O9-C22-O7-C5
57	2A	3674	MPD	O2-C2-C3-C4
56	2A	3672	ERY	C23-C22-O7-C5
56	2A	3672	ERY	C6-C7-C8-C9
55	1A	4026	HGR	C16-C14-C15-N1
57	1A	4028	MPD	C2-C3-C4-C5
57	2A	3675	MPD	C2-C3-C4-C5
57	1A	4028	MPD	C2-C3-C4-O4
57	1a	1882	MPD	C2-C3-C4-O4
57	2A	3674	MPD	C2-C3-C4-O4
57	2A	3675	MPD	C2-C3-C4-O4

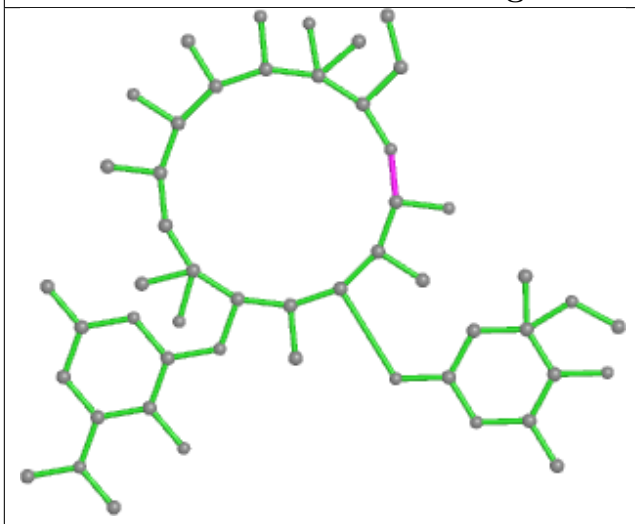
There are no ring outliers.

No monomer is involved in short contacts.

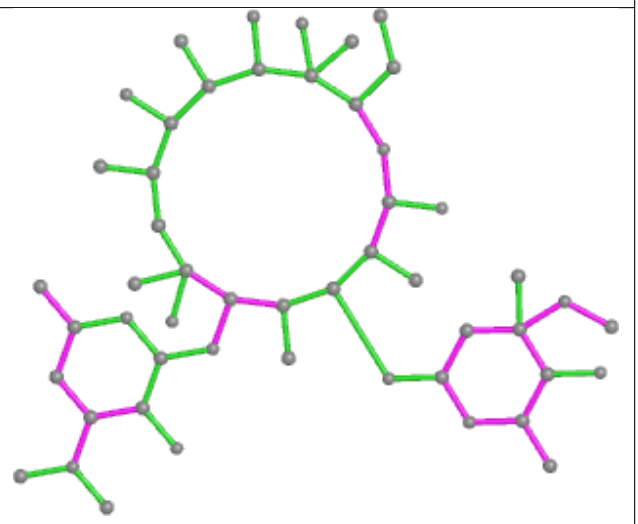
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

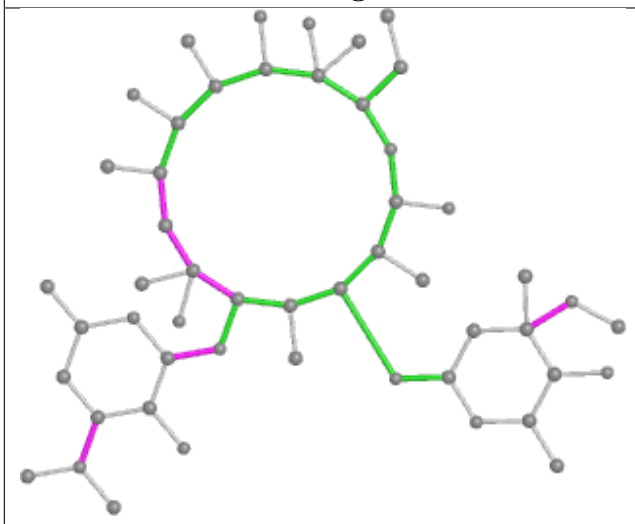
Ligand ERY 2A 3672



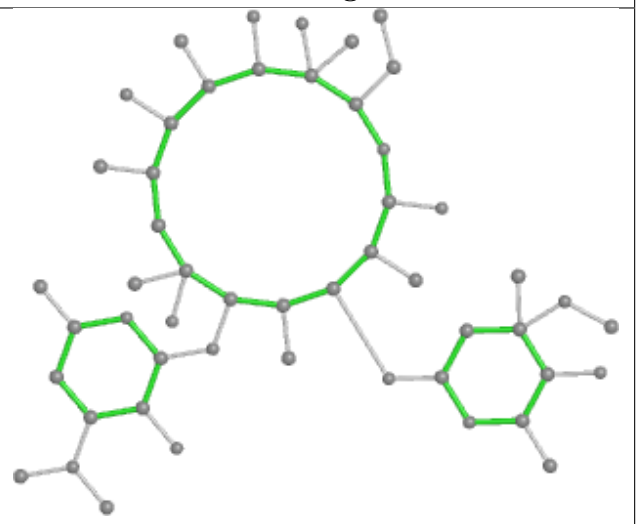
Bond lengths



Bond angles

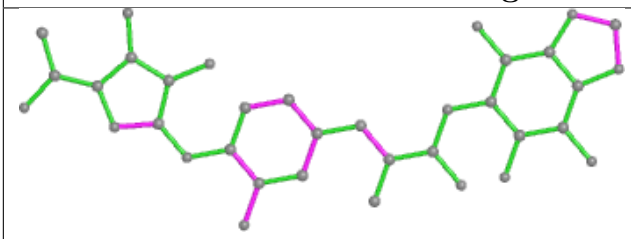


Torsions

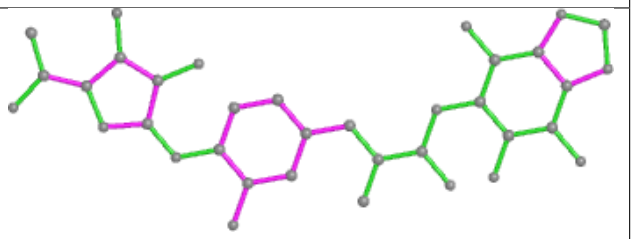


Rings

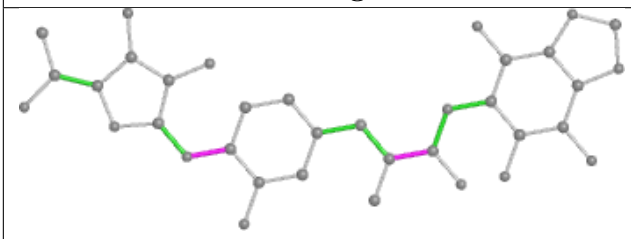
Ligand HGR 2A 3671



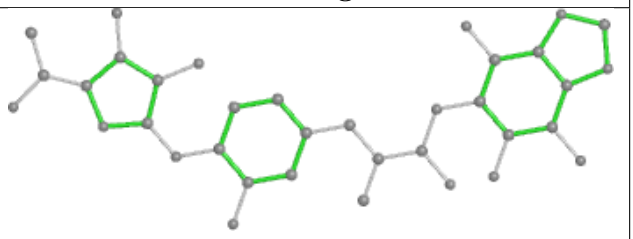
Bond lengths



Bond angles

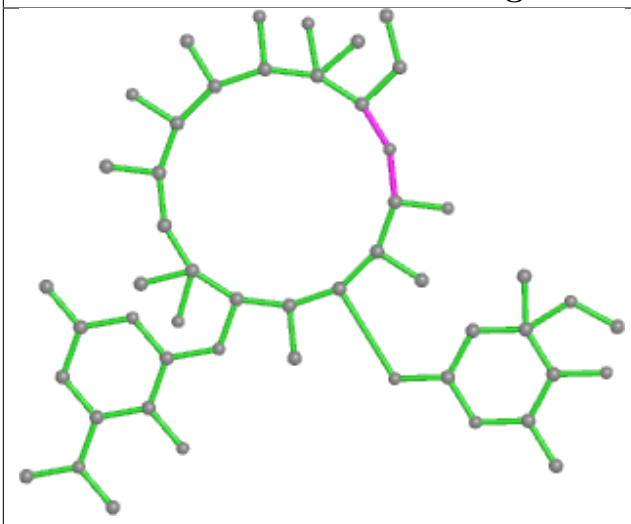


Torsions

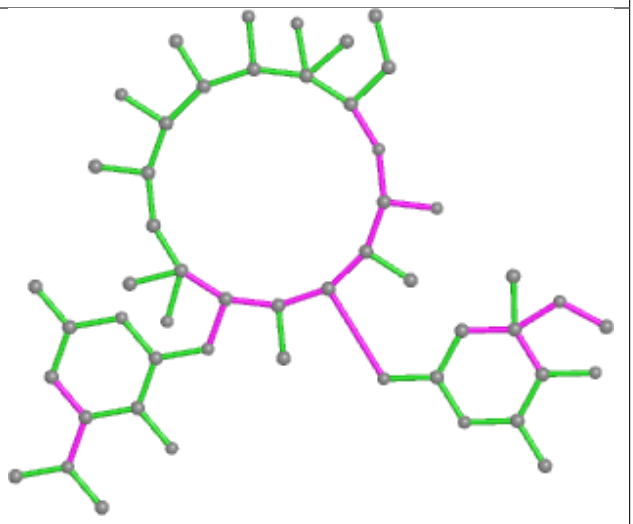


Rings

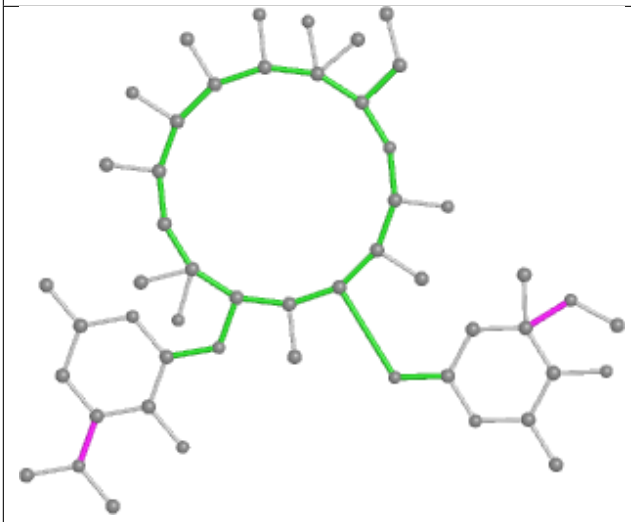
Ligand ERY 1A 4027



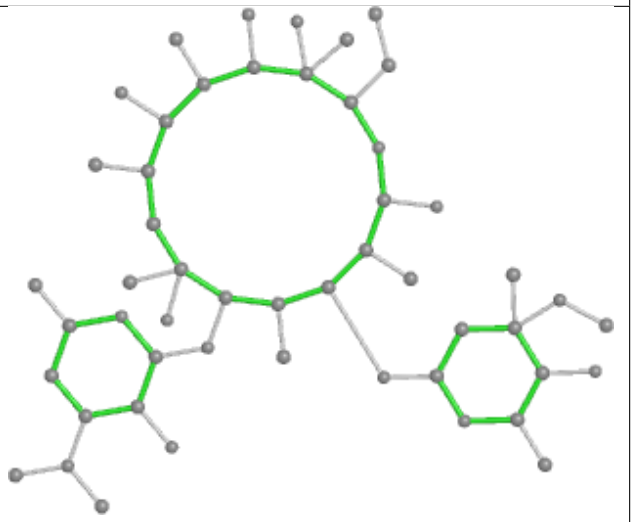
Bond lengths



Bond angles

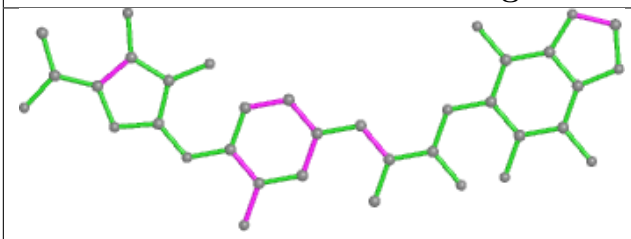


Torsions

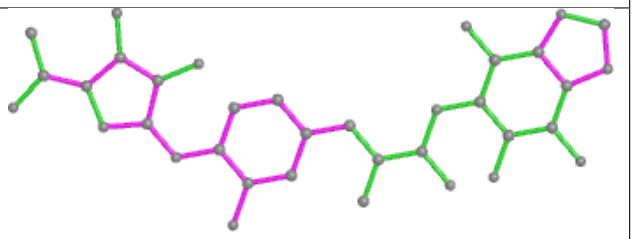


Rings

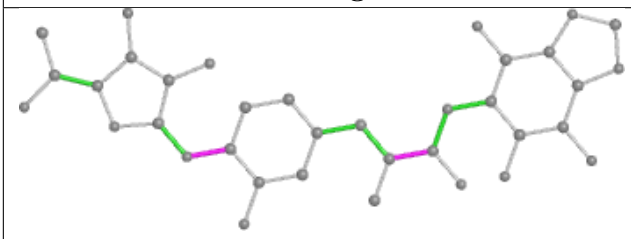
Ligand HGR 1A 4026



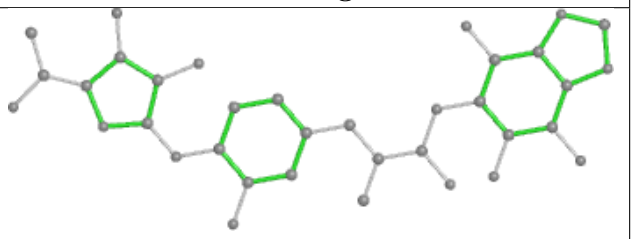
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	2860/2915 (98%)	0.77	167 (5%) 23 20	24, 41, 92, 103	0
1	2A	2855/2915 (97%)	0.70	191 (6%) 17 14	36, 58, 94, 103	0
2	1B	120/121 (99%)	0.16	0 100 100	38, 58, 68, 81	0
2	2B	120/121 (99%)	0.43	5 (4%) 36 33	62, 77, 84, 89	0
3	1D	275/276 (99%)	0.83	2 (0%) 87 88	26, 41, 54, 73	0
3	2D	275/276 (99%)	0.87	5 (1%) 68 65	35, 52, 63, 79	0
4	1E	204/206 (99%)	0.74	1 (0%) 91 92	24, 44, 66, 73	0
4	2E	204/206 (99%)	0.62	2 (0%) 82 83	37, 59, 73, 78	0
5	1F	203/210 (96%)	0.58	1 (0%) 91 92	23, 48, 71, 81	0
5	2F	203/210 (96%)	0.50	3 (1%) 73 71	36, 66, 77, 84	0
6	1G	181/182 (99%)	0.51	12 (6%) 18 14	52, 68, 79, 89	0
6	2G	181/182 (99%)	1.60	62 (34%) 0 0	75, 81, 87, 92	0
7	1H	174/180 (96%)	0.36	1 (0%) 89 89	42, 56, 66, 72	0
7	2H	173/180 (96%)	1.86	76 (43%) 0 0	66, 79, 85, 87	0
8	1I	147/148 (99%)	0.28	0 100 100	47, 72, 81, 86	0
8	2I	146/148 (98%)	0.66	12 (8%) 11 8	59, 74, 83, 86	0
9	1N	140/140 (100%)	0.65	0 100 100	30, 43, 61, 76	0
9	2N	140/140 (100%)	0.51	1 (0%) 87 88	49, 65, 75, 78	0
10	1O	122/122 (100%)	0.69	1 (0%) 86 86	30, 43, 61, 67	0
10	2O	122/122 (100%)	0.52	1 (0%) 86 86	46, 56, 67, 73	0
11	1P	149/150 (99%)	0.45	0 100 100	25, 50, 68, 79	0
11	2P	149/150 (99%)	1.16	27 (18%) 1 0	42, 67, 79, 85	0
12	1Q	141/141 (100%)	0.65	1 (0%) 87 88	31, 46, 59, 67	0
12	2Q	141/141 (100%)	0.77	14 (9%) 7 5	49, 65, 73, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.50	0 100 100	29, 41, 54, 59	0
13	2R	118/118 (100%)	0.73	5 (4%) 36 33	42, 53, 63, 69	0
14	1S	110/112 (98%)	0.43	1 (0%) 84 85	45, 58, 69, 74	0
14	2S	110/112 (98%)	1.22	27 (24%) 0 0	65, 72, 77, 81	0
15	1T	131/146 (89%)	0.44	2 (1%) 73 71	36, 50, 70, 80	0
15	2T	131/146 (89%)	0.57	3 (2%) 60 56	50, 60, 77, 81	0
16	1U	116/118 (98%)	0.68	1 (0%) 84 85	26, 36, 50, 67	0
16	2U	116/118 (98%)	0.60	1 (0%) 84 85	45, 62, 73, 80	0
17	1V	101/101 (100%)	0.42	1 (0%) 82 83	27, 47, 62, 67	0
17	2V	101/101 (100%)	0.39	1 (0%) 82 83	44, 71, 76, 78	0
18	1W	112/113 (99%)	0.63	0 100 100	29, 35, 54, 79	0
18	2W	112/113 (99%)	0.68	1 (0%) 84 85	42, 52, 68, 83	0
19	1X	95/96 (98%)	0.67	2 (2%) 63 60	33, 45, 64, 73	0
19	2X	95/96 (98%)	0.60	3 (3%) 47 44	51, 63, 75, 82	0
20	1Y	107/110 (97%)	0.41	1 (0%) 84 85	40, 52, 66, 77	0
20	2Y	107/110 (97%)	0.71	10 (9%) 8 5	59, 68, 78, 84	0
21	1Z	203/206 (98%)	0.29	2 (0%) 82 83	47, 62, 73, 81	0
21	2Z	201/206 (97%)	0.81	26 (12%) 3 2	65, 75, 81, 88	0
22	10	77/85 (90%)	0.62	0 100 100	35, 44, 58, 62	0
22	20	77/85 (90%)	0.89	10 (12%) 3 2	53, 65, 75, 79	0
23	11	97/98 (98%)	0.68	4 (4%) 37 34	34, 49, 69, 76	0
23	21	97/98 (98%)	0.68	3 (3%) 49 45	43, 57, 74, 78	0
24	12	70/72 (97%)	0.56	1 (1%) 75 74	42, 54, 65, 74	0
24	22	70/72 (97%)	0.32	0 100 100	61, 69, 76, 77	0
25	13	59/60 (98%)	0.59	0 100 100	34, 42, 66, 71	0
25	23	59/60 (98%)	0.73	4 (6%) 17 13	53, 63, 75, 81	0
26	14	69/71 (97%)	1.20	18 (26%) 0 0	64, 79, 86, 92	0
26	24	69/71 (97%)	2.65	41 (59%) 0 0	80, 86, 92, 95	0
27	15	59/60 (98%)	0.67	1 (1%) 70 67	25, 39, 60, 70	0
27	25	59/60 (98%)	0.56	1 (1%) 70 67	39, 53, 72, 77	0
28	16	53/54 (98%)	0.40	0 100 100	40, 48, 60, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.72	6 (11%) 5 3	55, 61, 69, 73	0
29	17	48/49 (97%)	0.95	2 (4%) 36 33	26, 34, 60, 66	0
29	27	48/49 (97%)	0.96	3 (6%) 20 16	35, 44, 64, 71	0
30	18	64/65 (98%)	0.73	1 (1%) 72 69	33, 40, 46, 64	0
30	28	64/65 (98%)	1.07	10 (15%) 2 1	47, 56, 63, 67	0
31	19	37/37 (100%)	0.63	0 100 100	37, 45, 60, 61	0
31	29	37/37 (100%)	1.24	6 (16%) 1 1	59, 67, 75, 81	0
32	1a	1488/1521 (97%)	0.75	162 (10%) 5 3	41, 72, 91, 100	0
32	2a	1492/1521 (98%)	0.83	216 (14%) 2 1	50, 76, 92, 101	0
33	1b	231/256 (90%)	1.01	43 (18%) 1 0	66, 77, 85, 91	0
33	2b	231/256 (90%)	1.73	74 (32%) 0 0	72, 82, 88, 91	0
34	1c	206/239 (86%)	0.87	29 (14%) 2 1	63, 75, 83, 88	0
34	2c	206/239 (86%)	1.48	55 (26%) 0 0	73, 81, 86, 92	0
35	1d	208/209 (99%)	0.68	13 (6%) 20 16	58, 72, 79, 84	0
35	2d	208/209 (99%)	0.78	21 (10%) 7 4	62, 71, 79, 82	0
36	1e	148/162 (91%)	0.56	5 (3%) 45 41	56, 67, 74, 86	0
36	2e	148/162 (91%)	0.80	20 (13%) 3 2	61, 73, 80, 87	0
37	1f	100/101 (99%)	0.27	2 (2%) 65 62	59, 71, 77, 78	0
37	2f	100/101 (99%)	0.35	1 (1%) 82 83	60, 69, 75, 77	0
38	1g	155/156 (99%)	1.00	28 (18%) 1 0	67, 74, 79, 85	0
38	2g	155/156 (99%)	1.26	38 (24%) 0 0	73, 79, 84, 86	0
39	1h	137/138 (99%)	0.82	11 (8%) 12 9	58, 70, 76, 78	0
39	2h	137/138 (99%)	1.08	26 (18%) 1 0	63, 73, 78, 84	0
40	1i	127/128 (99%)	2.52	81 (63%) 0 0	66, 79, 83, 86	0
40	2i	126/128 (98%)	3.54	103 (81%) 0 0	73, 83, 87, 89	0
41	1j	97/105 (92%)	2.17	52 (53%) 0 0	67, 79, 84, 85	0
41	2j	96/105 (91%)	2.91	59 (61%) 0 0	74, 83, 87, 89	0
42	1k	114/129 (88%)	0.43	2 (1%) 68 65	48, 65, 75, 75	0
42	2k	114/129 (88%)	0.44	4 (3%) 44 40	58, 72, 80, 84	0
43	1l	121/132 (91%)	0.61	4 (3%) 46 43	52, 62, 71, 77	0
43	2l	121/132 (91%)	0.51	4 (3%) 46 43	52, 69, 76, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	116/126 (92%)	1.29	29 (25%) 0 0	65, 77, 82, 83	0
44	2m	114/126 (90%)	2.06	50 (43%) 0 0	77, 83, 86, 88	0
45	1n	60/61 (98%)	2.14	29 (48%) 0 0	70, 75, 81, 85	0
45	2n	60/61 (98%)	3.67	54 (90%) 0 0	75, 82, 87, 92	0
46	1o	88/89 (98%)	0.49	3 (3%) 45 41	51, 67, 75, 80	0
46	2o	88/89 (98%)	0.52	6 (6%) 17 13	60, 71, 78, 83	0
47	1p	82/88 (93%)	1.66	25 (30%) 0 0	64, 73, 80, 86	0
47	2p	82/88 (93%)	1.28	15 (18%) 1 0	62, 70, 77, 80	0
48	1q	99/105 (94%)	1.08	16 (16%) 1 1	59, 70, 76, 83	0
48	2q	99/105 (94%)	1.18	18 (18%) 1 0	59, 72, 78, 81	0
49	1r	68/88 (77%)	0.43	2 (2%) 51 47	61, 67, 77, 84	0
49	2r	68/88 (77%)	0.35	3 (4%) 34 32	62, 71, 79, 83	0
50	1s	83/93 (89%)	1.83	39 (46%) 0 0	73, 79, 84, 88	0
50	2s	83/93 (89%)	2.67	52 (62%) 0 0	77, 85, 89, 91	0
51	1t	96/106 (90%)	2.10	44 (45%) 0 0	66, 73, 81, 83	0
51	2t	98/106 (92%)	1.38	25 (25%) 0 0	59, 71, 82, 83	0
52	1u	23/27 (85%)	3.02	18 (78%) 0 0	73, 76, 78, 79	0
52	2u	23/27 (85%)	3.87	19 (82%) 0 0	78, 81, 82, 84	0
53	1y	97/113 (85%)	0.76	5 (5%) 27 24	58, 67, 75, 77	0
53	2y	96/113 (84%)	1.65	34 (35%) 0 0	69, 78, 84, 86	0
All	All	20764/21468 (96%)	0.86	2322 (11%) 5 3	23, 65, 87, 103	0

All (2322) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	652(C)	G	14.0
1	2A	652(C)	G	12.7
1	1A	653	A	12.5
1	1A	652(V)	C	11.9
1	2A	652(V)	C	11.2
1	1A	652(D)	C	10.6
1	2A	653	A	10.5
1	2A	654	A	10.3
1	1A	1509	C	9.8
40	2i	109	VAL	9.6

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Mol	Chain	Res	Type	RSRZ
45	2n	13	THR	9.5
1	2A	652(U)	G	9.5
6	2G	62	LEU	9.4
1	2A	652(D)	C	9.4
1	2A	2140	C	9.2
32	2a	1030(B)	C	8.9
1	2A	2147	G	8.8
1	2A	2162	G	8.8
1	2A	652(E)	G	8.8
1	1A	652(U)	G	8.7
1	2A	2124	G	8.7
1	2A	2174	C	8.6
32	2a	1030(A)	G	8.6
1	1A	1089	G	8.6
1	2A	1046	A	8.4
44	2m	7	VAL	8.4
6	2G	3	LEU	8.4
52	2u	14	TRP	8.3
26	24	49	PHE	8.2
1	1A	652(S)	C	8.1
1	2A	2141	G	8.1
1	2A	652(T)	C	8.1
41	2j	96	ILE	8.0
1	1A	652(E)	G	8.0
1	2A	229	A	7.9
32	2a	1001(A)	G	7.9
1	2A	2169	A	7.8
32	1a	1031	G	7.7
32	2a	1257	U	7.7
33	2b	44	LEU	7.7
40	2i	63	ILE	7.6
1	1A	1091	G	7.6
1	2A	2126	A	7.6
40	2i	88	TYR	7.6
1	1A	2132	U	7.6
1	2A	2176	A	7.5
32	1a	1001	A	7.5
32	2a	1001	A	7.5
1	2A	2138	C	7.4
32	2a	1033	G	7.4
40	2i	18	PHE	7.4
1	2A	2123	G	7.4

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Mol	Chain	Res	Type	RSRZ
1	1A	1066	U	7.4
53	2y	88	LEU	7.3
50	2s	63	THR	7.3
1	1A	2147	G	7.3
1	2A	2107	C	7.3
1	1A	654	A	7.3
44	2m	28	ALA	7.2
1	2A	2125	G	7.2
1	2A	2127	G	7.2
1	2A	1509	C	7.1
1	2A	888	C	7.1
1	1A	2141	G	7.1
32	1a	1030(B)	C	7.0
32	1a	1030(D)	A	7.0
1	2A	2793	G	7.0
1	1A	2107	C	7.0
52	2u	16	GLY	7.0
1	1A	2123	G	6.9
33	2b	214	ILE	6.9
1	1A	1080	C	6.9
45	2n	12	ARG	6.9
40	2i	17	VAL	6.9
41	2j	19	SER	6.9
32	1a	1030(C)	G	6.8
45	2n	38	GLY	6.8
50	2s	10	PHE	6.8
1	2A	2142	C	6.8
32	2a	1286	A	6.8
1	1A	652(F)	G	6.8
40	2i	127	LYS	6.8
7	2H	102	ALA	6.8
1	1A	2161	C	6.7
1	1A	2792	G	6.7
26	24	63	TYR	6.7
41	2j	72	VAL	6.6
52	2u	15	ARG	6.6
32	2a	1031	G	6.6
41	2j	44	VAL	6.6
32	2a	1030(C)	G	6.6
32	1a	1257	U	6.5
41	2j	62	HIS	6.5
6	2G	87	PRO	6.5

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Mol	Chain	Res	Type	RSRZ
40	2i	62	TYR	6.5
40	2i	76	ALA	6.5
1	2A	1085	A	6.5
1	1A	1067	A	6.5
1	1A	2142	C	6.5
1	2A	2106	G	6.5
1	2A	2168	G	6.5
1	2A	2173	A	6.5
41	2j	100	THR	6.4
40	2i	69	GLY	6.4
1	2A	2165	G	6.4
34	2c	155	GLY	6.4
41	2j	27	ALA	6.4
1	2A	2153	G	6.4
40	1i	28	VAL	6.4
40	2i	44	VAL	6.4
38	2g	5	ARG	6.3
40	2i	75	ASP	6.3
34	2c	157	ILE	6.3
1	1A	1076	C	6.3
32	1a	1001(A)	G	6.3
34	2c	177	THR	6.3
1	1A	1087	G	6.2
1	1A	2169	A	6.2
1	2A	2120	G	6.2
6	1G	48	GLU	6.2
1	2A	2116	G	6.2
52	2u	13	ILE	6.2
26	24	29	PRO	6.2
1	1A	2116	G	6.2
1	2A	2139	C	6.2
45	1n	18	VAL	6.1
45	2n	16	PHE	6.1
41	2j	67	THR	6.1
1	1A	652(T)	C	6.1
32	2a	1034	G	6.1
40	2i	105	ASP	6.1
44	2m	84	ILE	6.1
1	2A	652(B)	A	6.1
7	2H	165	ALA	6.1
33	2b	132	LYS	6.1
1	2A	1075	C	6.1

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Mol	Chain	Res	Type	RSRZ
34	2c	8	ILE	6.1
45	1n	15	LYS	6.1
40	2i	90	PRO	6.0
1	2A	2172	U	6.0
50	2s	40	ILE	6.0
7	2H	35	VAL	6.0
40	2i	108	VAL	6.0
1	1A	2140	C	6.0
1	2A	1076	C	6.0
1	2A	2151	G	6.0
1	1A	2159	G	6.0
1	2A	2136	C	6.0
26	24	64	GLY	6.0
50	1s	58	VAL	6.0
40	2i	45	ALA	6.0
1	1A	2124	G	5.9
1	1A	2805	G	5.9
32	1a	1036	G	5.9
1	1A	1093	G	5.9
40	1i	15	ALA	5.9
1	2A	2118	U	5.9
40	2i	7	THR	5.9
50	2s	42	PRO	5.9
50	2s	41	VAL	5.8
52	1u	14	TRP	5.8
1	2A	2146	C	5.8
1	1A	1075	C	5.8
1	2A	2155	G	5.8
26	24	56	VAL	5.8
45	2n	15	LYS	5.8
1	2A	2177	C	5.8
1	2A	2121	G	5.8
1	2A	2119	A	5.8
14	2S	92	TYR	5.8
32	1a	1000	U	5.7
34	2c	33	LEU	5.7
6	2G	39	ILE	5.7
1	2A	2170	A	5.7
32	2a	1032	G	5.7
40	2i	36	TYR	5.7
26	24	67	TYR	5.7
40	2i	86	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2161	C	5.6
1	2A	2110	G	5.6
45	1n	14	PRO	5.6
21	2Z	125	LEU	5.6
51	1t	76	ALA	5.6
1	2A	2145	C	5.6
40	2i	40	LEU	5.6
26	24	68	ARG	5.6
48	1q	98	LEU	5.6
33	2b	231	GLU	5.6
23	11	2	SER	5.6
7	2H	103	LEU	5.5
1	1A	2127	G	5.5
41	2j	98	ILE	5.5
32	1a	999	C	5.5
32	1a	1028	C	5.5
40	2i	42	ARG	5.5
41	2j	34	VAL	5.5
52	1u	4	GLY	5.5
1	1A	1068	G	5.5
45	2n	14	PRO	5.5
41	2j	20	ALA	5.5
6	2G	58	GLN	5.4
32	2a	1036	G	5.4
33	2b	232	PRO	5.4
7	2H	115	VAL	5.4
1	1A	1092	C	5.4
32	2a	1028	C	5.4
33	2b	70	PHE	5.4
44	1m	2	ALA	5.4
41	2j	38	ILE	5.4
11	2P	103	ALA	5.4
50	2s	11	VAL	5.4
32	2a	1029	C	5.4
26	24	52	THR	5.4
1	2A	1080	C	5.4
32	2a	1030	C	5.4
1	1A	1090	U	5.4
1	2A	1083	U	5.4
45	1n	61	TRP	5.3
1	2A	1067	A	5.3
1	1A	1065	U	5.3

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Mol	Chain	Res	Type	RSRZ
1	2A	2150	U	5.3
50	2s	16	LEU	5.3
33	1b	123	ALA	5.3
50	2s	62	ILE	5.3
32	1a	1034	G	5.3
52	2u	6	ARG	5.3
26	14	18	CYS	5.3
1	1A	2176	A	5.3
1	1A	2174	C	5.3
51	1t	18	GLN	5.3
52	2u	23	PRO	5.3
11	2P	109	GLY	5.2
41	2j	87	THR	5.2
50	2s	79	THR	5.2
45	2n	2	ALA	5.2
1	1A	2143	C	5.2
40	2i	102	LEU	5.2
32	2a	1041	A	5.2
26	24	10	VAL	5.2
32	2a	1002	G	5.2
33	2b	131	PRO	5.2
40	2i	74	ILE	5.2
1	2A	1079	C	5.2
45	2n	33	VAL	5.2
50	1s	72	GLY	5.2
50	2s	80	TYR	5.2
1	1A	1088	A	5.1
1	2A	2175	C	5.1
41	1j	10	GLY	5.1
45	2n	61	TRP	5.1
33	2b	228	GLY	5.1
40	2i	72	GLY	5.1
45	2n	54	PRO	5.1
1	2A	2802	G	5.1
53	2y	40	ILE	5.1
44	2m	42	ALA	5.1
7	2H	101	ARG	5.1
40	2i	103	THR	5.0
1	2A	2801(A)	A	5.0
40	2i	92	TYR	5.0
1	1A	2153	G	5.0
7	2H	98	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
44	2m	15	VAL	5.0
26	24	45	GLY	5.0
33	1b	228	GLY	5.0
45	2n	29	ARG	5.0
40	1i	63	ILE	5.0
40	1i	19	LEU	5.0
1	2A	2805	G	5.0
1	1A	1079	C	5.0
38	2g	41	ARG	5.0
41	2j	24	VAL	5.0
45	2n	18	VAL	5.0
1	1A	1059	G	5.0
1	2A	2148	G	5.0
32	2a	1026	G	5.0
33	1b	36	ARG	5.0
35	2d	23	GLY	5.0
1	1A	2150	U	5.0
33	2b	216	SER	5.0
41	2j	29	ARG	5.0
40	2i	29	ASN	5.0
32	2a	1045	C	5.0
1	2A	887	A	5.0
6	2G	157	ILE	4.9
26	24	30	GLU	4.9
33	2b	185	ILE	4.9
40	1i	77	ILE	4.9
1	2A	652(A)	A	4.9
32	1a	1005	A	4.9
1	1A	2113	U	4.9
40	2i	85	LEU	4.9
50	2s	71	LEU	4.9
1	1A	2125	G	4.9
32	2a	1021	G	4.9
33	1b	122	PHE	4.9
1	2A	1064	C	4.9
1	2A	2117	A	4.9
40	2i	104	ARG	4.9
1	2A	2133	G	4.9
1	2A	2154	G	4.9
45	2n	27	CYS	4.9
47	1p	19	ILE	4.9
32	1a	1029	C	4.9

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Mol	Chain	Res	Type	RSRZ
40	1i	81	ILE	4.9
32	2a	1030(D)	A	4.8
1	2A	2167	U	4.8
32	2a	1235	U	4.8
1	2A	1043	C	4.8
50	2s	9	VAL	4.8
32	2a	1024	G	4.8
48	1q	27	PHE	4.8
47	1p	73	LEU	4.8
1	1A	1083	U	4.8
51	1t	73	HIS	4.8
1	2A	2166	G	4.8
40	2i	26	VAL	4.8
53	2y	63	ALA	4.8
1	1A	2173	A	4.8
51	1t	72	LEU	4.8
1	2A	1044	G	4.8
1	1A	2163	C	4.8
40	2i	50	LEU	4.7
50	2s	15	LEU	4.7
1	1A	2117	A	4.7
32	1a	220	G	4.7
33	2b	136	VAL	4.7
45	2n	3	ARG	4.7
1	1A	1053	C	4.7
39	1h	38	ILE	4.7
39	2h	2	LEU	4.7
40	2i	8	GLY	4.7
40	2i	53	VAL	4.7
45	2n	25	VAL	4.7
1	2A	2104	G	4.7
41	2j	40	LEU	4.7
1	1A	1072	C	4.7
11	2P	110	TYR	4.7
47	2p	59	TRP	4.7
32	1a	1447	A	4.7
51	1t	75	ASN	4.7
1	1A	1074	G	4.7
32	1a	1030(A)	G	4.7
32	1a	1032	G	4.7
1	2A	2111	C	4.7
31	29	16	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
41	2j	31	GLY	4.7
1	1A	2126	A	4.7
39	1h	134	ILE	4.7
41	1j	4	ILE	4.7
41	2j	65	LEU	4.7
1	1A	2166	G	4.7
26	14	63	TYR	4.7
32	1a	1020	U	4.7
1	2A	645	C	4.7
32	2a	1027	C	4.7
34	2c	159	GLY	4.7
6	2G	29	TRP	4.7
40	1i	119	ALA	4.7
41	2j	89	ASP	4.7
40	1i	79	LEU	4.7
32	2a	1040	U	4.6
40	2i	65	VAL	4.6
44	2m	5	ALA	4.6
51	1t	67	ALA	4.6
50	2s	69	HIS	4.6
33	2b	92	TYR	4.6
1	2A	2152	G	4.6
45	1n	22	THR	4.6
50	2s	51	VAL	4.6
1	1A	2129	C	4.6
1	2A	1041	C	4.6
34	1c	94	LEU	4.6
1	1A	2165	G	4.6
33	2b	218	ALA	4.6
38	2g	40	ALA	4.6
41	2j	26	ALA	4.6
32	2a	1008	C	4.6
1	2A	2132	U	4.6
32	2a	1202	G	4.6
51	1t	66	ALA	4.6
40	2i	115	GLY	4.6
1	2A	2179	C	4.5
1	1A	2144	U	4.5
26	24	27	THR	4.5
6	2G	5	VAL	4.5
40	1i	5	TYR	4.5
32	2a	1035	A	4.5

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Mol	Chain	Res	Type	RSRZ
32	2a	1157	A	4.5
41	1j	86	MET	4.5
41	1j	41	PRO	4.5
45	1n	2	ALA	4.5
26	14	17	GLY	4.5
1	1A	2149	G	4.5
1	2A	1095	A	4.5
1	2A	1081	U	4.5
26	24	66	SER	4.5
32	2a	1150	U	4.5
26	24	50	VAL	4.5
1	2A	2131	G	4.5
32	1a	1002	G	4.5
32	1a	1286	A	4.5
1	1A	888	C	4.5
14	2S	20	ARG	4.5
40	2i	41	VAL	4.5
44	1m	98	VAL	4.5
45	2n	6	LEU	4.5
40	1i	33	PHE	4.5
41	2j	77	PRO	4.5
44	1m	87	TYR	4.5
50	2s	66	MET	4.5
26	24	19	GLY	4.5
14	2S	31	SER	4.5
1	1A	2793	G	4.5
32	1a	198	G	4.5
20	2Y	42	VAL	4.5
32	1a	1030	C	4.5
45	2n	24	CYS	4.5
36	2e	13	ILE	4.5
40	1i	26	VAL	4.5
19	2X	92	LEU	4.5
38	1g	12	LEU	4.5
1	1A	2108	C	4.5
1	2A	2164	C	4.5
32	2a	1326	C	4.5
33	2b	227	GLY	4.5
44	2m	26	GLY	4.5
12	2Q	32	TYR	4.4
40	1i	46	ALA	4.4
45	2n	10	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	1A	2155	G	4.4
41	2j	23	ILE	4.4
33	2b	171	ALA	4.4
50	2s	12	ASP	4.4
32	2a	1357	A	4.4
40	2i	61	ALA	4.4
45	2n	53	LEU	4.4
1	1A	2803	C	4.4
1	1A	2115	G	4.4
35	1d	2	GLY	4.4
34	1c	63	ASN	4.4
40	1i	109	VAL	4.4
1	1A	1064	C	4.4
32	1a	1037	C	4.4
1	2A	1056	G	4.4
38	2g	22	LEU	4.4
44	2m	75	ALA	4.4
1	1A	1078	U	4.4
40	2i	114	TYR	4.4
7	2H	19	VAL	4.4
20	2Y	1	MET	4.4
26	14	49	PHE	4.4
33	2b	122	PHE	4.4
45	1n	13	THR	4.4
52	2u	17	THR	4.4
1	2A	1103	A	4.3
1	1A	2148	G	4.3
45	2n	55	GLY	4.3
50	2s	68	GLY	4.3
45	2n	30	ALA	4.3
40	1i	113	LYS	4.3
44	2m	65	LYS	4.3
26	24	51	ASP	4.3
40	2i	14	VAL	4.3
41	1j	44	VAL	4.3
41	1j	24	VAL	4.3
32	2a	1354	C	4.3
47	1p	1	MET	4.3
45	2n	35	ARG	4.3
1	2A	1086	A	4.3
32	2a	1236	A	4.3
51	1t	12	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
40	2i	111	ARG	4.3
44	2m	87	TYR	4.3
40	1i	14	VAL	4.3
1	1A	2181	G	4.3
1	2A	2159	G	4.3
52	2u	5	ASP	4.3
41	2j	18	ALA	4.3
52	2u	22	ARG	4.3
47	2p	79	VAL	4.3
32	1a	998	G	4.3
1	1A	2602	A	4.2
32	1a	1136	U	4.2
52	2u	11	GLY	4.2
33	2b	37	ASN	4.2
1	1A	2151	G	4.2
32	2a	1283	G	4.2
40	2i	31	GLN	4.2
26	14	66	SER	4.2
1	1A	1176	G	4.2
1	1A	2139	C	4.2
32	2a	994	A	4.2
32	2a	1003	G	4.2
52	1u	18	TYR	4.2
45	1n	16	PHE	4.2
1	1A	1081	U	4.2
1	1A	2168	G	4.2
41	2j	84	GLN	4.2
44	1m	42	ALA	4.2
1	2A	1084	A	4.2
52	1u	5	ASP	4.2
1	1A	1063	G	4.2
40	2i	4	TYR	4.2
7	2H	132	ARG	4.2
21	2Z	96	VAL	4.2
38	1g	24	THR	4.2
50	2s	65	ASN	4.2
40	1i	84	ALA	4.2
1	1A	2130	U	4.1
40	2i	91	ASP	4.1
44	2m	43	THR	4.1
41	2j	47	PHE	4.1
33	2b	223	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	1A	1082	U	4.1
1	1A	2156	G	4.1
32	1a	1258	G	4.1
32	2a	1009	G	4.1
36	2e	12	LEU	4.1
40	2i	89	ASN	4.1
7	2H	37	VAL	4.1
34	2c	61	ALA	4.1
51	1t	69	GLY	4.1
11	2P	125	VAL	4.1
44	1m	91	ARG	4.1
44	2m	51	ALA	4.1
50	1s	19	VAL	4.1
41	2j	68	HIS	4.1
1	2A	1104	C	4.1
1	2A	2130	U	4.1
40	2i	73	GLN	4.1
52	2u	9	ARG	4.1
52	2u	8	THR	4.1
34	2c	160	ALA	4.1
41	1j	27	ALA	4.1
32	1a	1033	G	4.1
40	1i	11	LYS	4.1
51	1t	74	LYS	4.1
1	2A	2105	C	4.1
21	2Z	80	ARG	4.1
32	2a	1006	C	4.1
33	2b	118	LEU	4.1
23	21	2	SER	4.1
45	2n	43	CYS	4.1
7	2H	24	VAL	4.1
1	1A	2122	U	4.1
32	1a	217	C	4.1
32	1a	218	C	4.1
44	2m	102	ARG	4.1
45	2n	31	ARG	4.1
1	2A	2191	G	4.0
41	1j	16	LEU	4.0
1	2A	2122	U	4.0
32	2a	1148	U	4.0
51	1t	30	LYS	4.0
26	24	44	THR	4.0

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Mol	Chain	Res	Type	RSRZ
32	1a	470	C	4.0
32	1a	1137	C	4.0
33	2b	66	GLY	4.0
14	2S	29	PHE	4.0
39	2h	112	LEU	4.0
50	2s	49	ILE	4.0
50	2s	39	THR	4.0
1	2A	2178	C	4.0
32	1a	219	C	4.0
1	1A	2114	A	4.0
1	2A	2134	A	4.0
32	1a	1044	A	4.0
7	2H	21	PRO	4.0
53	2y	11	GLU	4.0
41	2j	6	ILE	4.0
26	24	39	CYS	4.0
38	2g	32	ARG	4.0
33	2b	48	MET	4.0
38	2g	154	TYR	4.0
8	2I	59	ALA	4.0
33	1b	29	ALA	4.0
52	2u	12	LYS	4.0
1	1A	2120	G	4.0
1	1A	2137	C	4.0
1	1A	2157	G	4.0
1	1A	2794	C	4.0
32	2a	998	G	4.0
32	2a	1220	G	4.0
47	1p	6	LEU	4.0
40	2i	57	GLY	4.0
41	1j	72	VAL	4.0
33	1b	131	PRO	4.0
1	2A	2602	A	4.0
35	1d	157	LEU	4.0
40	1i	125	TYR	4.0
40	1i	78	LYS	4.0
1	2A	2792	G	4.0
38	1g	34	GLY	4.0
47	1p	59	TRP	4.0
34	2c	65	ALA	4.0
40	2i	67	GLY	4.0
1	2A	2108	C	3.9

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Mol	Chain	Res	Type	RSRZ
33	1b	121	LEU	3.9
40	1i	120	ARG	3.9
41	1j	17	ASP	3.9
44	2m	39	ILE	3.9
32	2a	981	U	3.9
40	2i	5	TYR	3.9
40	2i	30	GLY	3.9
52	2u	2	GLY	3.9
41	1j	69	ASN	3.9
50	2s	5	LEU	3.9
32	2a	91	C	3.9
26	24	61	ARG	3.9
6	2G	82	LEU	3.9
38	2g	27	ILE	3.9
1	1A	2804	C	3.9
47	1p	67	THR	3.9
40	1i	45	ALA	3.9
40	1i	76	ALA	3.9
40	1i	30	GLY	3.9
40	2i	71	SER	3.9
41	2j	76	ASN	3.9
40	2i	87	GLN	3.9
47	2p	58	TYR	3.9
50	2s	67	VAL	3.9
40	2i	37	PHE	3.9
1	1A	2167	U	3.9
32	1a	1019	C	3.9
32	2a	1223	C	3.9
45	1n	12	ARG	3.9
39	1h	128	GLY	3.9
40	1i	31	GLN	3.9
40	1i	114	TYR	3.9
42	1k	25	TYR	3.9
1	2A	1106	G	3.9
1	2A	2149	G	3.9
40	2i	59	PHE	3.9
45	2n	42	ILE	3.9
50	1s	62	ILE	3.9
32	1a	1040	U	3.9
53	2y	9	GLN	3.9
1	2A	2171	A	3.9
6	2G	152	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
41	2j	71	LEU	3.9
38	2g	13	GLN	3.9
26	24	11	PRO	3.9
39	2h	93	VAL	3.9
41	2j	8	LEU	3.9
50	1s	61	TYR	3.9
51	1t	84	LEU	3.9
1	1A	2119	A	3.8
33	2b	201	ILE	3.8
51	1t	68	LYS	3.8
1	2A	1059	G	3.8
32	1a	1274	G	3.8
1	2A	1088	A	3.8
51	1t	55	ILE	3.8
21	2Z	153	SER	3.8
51	1t	45	GLN	3.8
32	1a	1186	G	3.8
48	2q	9	VAL	3.8
34	2c	184	TYR	3.8
41	1j	20	ALA	3.8
41	1j	38	ILE	3.8
32	2a	1151	A	3.8
32	2a	1312	G	3.8
34	1c	87	LEU	3.8
1	2A	889	C	3.8
41	1j	46	ARG	3.8
6	1G	146	TYR	3.8
38	2g	25	ALA	3.8
1	1A	1508	A	3.8
50	2s	36	ARG	3.8
1	1A	1071	G	3.8
32	2a	80	G	3.8
32	2a	1140	C	3.8
34	2c	206	GLU	3.8
32	2a	1358	U	3.8
41	2j	46	ARG	3.8
48	2q	54	GLY	3.8
52	1u	10	ARG	3.8
33	2b	113	HIS	3.8
34	2c	86	VAL	3.8
34	2c	101	LEU	3.8
40	1i	47	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
40	2i	27	THR	3.8
32	2a	1260	C	3.8
52	1u	2	GLY	3.8
1	2A	1057	A	3.8
7	2H	113	VAL	3.8
34	2c	152	ILE	3.7
38	2g	120	ILE	3.7
40	2i	20	ARG	3.7
50	2s	52	TYR	3.7
44	1m	96	LEU	3.7
51	1t	13	LEU	3.7
40	1i	112	LYS	3.7
34	2c	190	ARG	3.7
38	2g	6	ARG	3.7
48	1q	25	ARG	3.7
51	1t	41	ILE	3.7
1	1A	2145	C	3.7
39	2h	122	ARG	3.7
7	2H	45	VAL	3.7
32	2a	1255	G	3.7
41	2j	91	PRO	3.7
32	2a	1111	A	3.7
1	2A	2163	C	3.7
34	2c	196	LEU	3.7
26	24	33	VAL	3.7
34	2c	64	VAL	3.7
44	1m	97	PRO	3.7
40	1i	80	GLY	3.7
52	1u	8	THR	3.7
1	1A	2131	G	3.7
32	1a	1021	G	3.7
32	2a	1138	G	3.7
51	1t	63	ILE	3.7
45	1n	34	TYR	3.7
1	2A	2137	C	3.7
34	2c	145	GLY	3.7
40	1i	67	GLY	3.7
50	1s	77	THR	3.7
51	1t	17	ARG	3.7
1	1A	1085	A	3.7
1	2A	1066	U	3.7
32	1a	1187	G	3.7

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Mol	Chain	Res	Type	RSRZ
32	2a	216	G	3.7
32	2a	1361	G	3.7
38	2g	36	LYS	3.7
33	1b	218	ALA	3.7
40	1i	110	GLU	3.7
32	1a	1035	A	3.7
32	2a	1224	G	3.7
32	2a	1256	A	3.7
32	2a	1323	G	3.7
52	2u	21	TYR	3.7
31	29	30	PRO	3.7
41	1j	59	SER	3.7
40	2i	66	ARG	3.7
45	2n	44	LEU	3.7
44	2m	103	THR	3.7
32	2a	1149	C	3.7
6	2G	140	ILE	3.6
7	2H	9	ILE	3.6
6	2G	142	PRO	3.6
33	2b	33	TYR	3.6
21	2Z	155	LEU	3.6
1	2A	1042	G	3.6
32	1a	1024	G	3.6
1	2A	2143	C	3.6
41	2j	74	ILE	3.6
15	2T	111	ARG	3.6
5	2F	15	SER	3.6
40	2i	21	PRO	3.6
53	2y	42	SER	3.6
26	24	65	ASP	3.6
32	1a	197	A	3.6
20	2Y	89	PHE	3.6
41	1j	74	ILE	3.6
50	2s	31	ILE	3.6
32	1a	1446	U	3.6
45	2n	4	LYS	3.6
7	2H	128	PRO	3.6
39	2h	119	LEU	3.6
41	2j	16	LEU	3.6
7	2H	20	ALA	3.6
33	2b	93	VAL	3.6
38	2g	39	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
51	2t	95	ALA	3.6
32	2a	1363(A)	A	3.6
1	2A	1115	G	3.6
1	1A	2128	C	3.6
1	2A	2109	U	3.6
32	2a	1039	C	3.6
32	2a	1203	C	3.6
40	1i	117	HIS	3.6
40	2i	124	GLN	3.6
44	2m	64	TRP	3.6
8	2I	3	VAL	3.6
1	1A	2170	A	3.6
35	2d	204	ILE	3.6
51	1t	70	SER	3.6
1	2A	2115	G	3.6
32	1a	144	G	3.6
32	1a	1026	G	3.6
33	1b	118	LEU	3.6
29	17	46	VAL	3.6
40	1i	118	LYS	3.6
32	2a	1023	G	3.6
47	1p	32	TYR	3.6
38	1g	156	TRP	3.6
14	2S	12	PHE	3.5
32	1a	1212	U	3.5
53	2y	77	LEU	3.5
11	2P	93	GLY	3.5
32	2a	470	C	3.5
32	2a	1452	C	3.5
39	2h	47	GLY	3.5
44	2m	6	GLY	3.5
40	2i	46	ALA	3.5
1	2A	2181	G	3.5
34	2c	23	TYR	3.5
44	2m	4	ILE	3.5
1	1A	1086	A	3.5
33	1b	207	ALA	3.5
41	2j	15	THR	3.5
1	2A	1026	U	3.5
39	2h	131	GLY	3.5
1	1A	229	A	3.5
1	1A	1077	A	3.5

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Mol	Chain	Res	Type	RSRZ
44	2m	116	THR	3.5
32	2a	1259	C	3.5
40	1i	108	VAL	3.5
41	1j	30	SER	3.5
47	1p	2	VAL	3.5
48	2q	73	VAL	3.5
52	1u	21	TYR	3.5
40	1i	37	PHE	3.5
44	1m	22	ILE	3.5
51	1t	23	ARG	3.5
52	1u	13	ILE	3.5
32	1a	204	U	3.5
32	2a	1219	U	3.5
41	1j	85	LEU	3.5
44	1m	56	LEU	3.5
12	2Q	114	ALA	3.5
32	2a	1092	A	3.5
11	2P	101	VAL	3.5
1	1A	2138	C	3.5
1	1A	2164	C	3.5
33	1b	127	ILE	3.5
33	2b	58	ILE	3.5
48	1q	36	ILE	3.5
6	2G	74	LYS	3.5
33	1b	139	LYS	3.5
7	2H	129	THR	3.5
32	1a	1361	G	3.5
32	2a	1154	G	3.5
53	2y	64	SER	3.5
7	2H	8	PRO	3.5
43	2l	19	ARG	3.5
47	1p	20	VAL	3.5
50	2s	23	ASN	3.5
38	1g	27	ILE	3.5
26	24	57	GLU	3.5
36	2e	14	ARG	3.5
41	1j	68	HIS	3.5
42	1k	60	ALA	3.5
47	1p	48	TRP	3.5
32	1a	145	G	3.5
32	1a	306	G	3.5
6	2G	177	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
32	1a	457	C	3.4
33	1b	211	ILE	3.4
45	2n	52	GLN	3.4
50	2s	75	ALA	3.4
26	24	16	CYS	3.4
32	2a	1155	G	3.4
32	1a	1318	A	3.4
38	2g	44	TYR	3.4
44	2m	23	TYR	3.4
1	1A	889	C	3.4
32	2a	1037	C	3.4
34	2c	87	LEU	3.4
45	1n	6	LEU	3.4
47	2p	74	LEU	3.4
34	2c	81	GLY	3.4
36	2e	22	GLY	3.4
40	2i	28	VAL	3.4
1	1A	2112	G	3.4
6	2G	75	LYS	3.4
40	2i	33	PHE	3.4
45	2n	36	PHE	3.4
41	2j	17	ASP	3.4
47	1p	17	TYR	3.4
7	2H	71	LEU	3.4
40	2i	79	LEU	3.4
40	1i	115	GLY	3.4
46	1o	89	GLY	3.4
39	1h	93	VAL	3.4
41	1j	94	VAL	3.4
42	2k	14	VAL	3.4
20	2Y	44	ILE	3.4
33	2b	152	PHE	3.4
47	1p	58	TYR	3.4
48	2q	98	LEU	3.4
1	2A	2112	G	3.4
1	2A	2319	G	3.4
32	2a	1293	G	3.4
32	2a	1531	A	3.4
34	1c	41	GLY	3.4
38	1g	117	ALA	3.4
39	2h	40	ALA	3.4
47	1p	66	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
26	24	31	ILE	3.4
6	2G	25	TYR	3.4
33	2b	210	SER	3.4
40	1i	116	LYS	3.4
51	1t	9	ASN	3.4
41	1j	32	ALA	3.4
1	1A	2106	G	3.4
32	2a	174	C	3.4
41	1j	73	ASP	3.4
33	1b	165	VAL	3.4
34	2c	194	GLY	3.4
38	1g	16	LEU	3.4
47	2p	19	ILE	3.4
1	1A	271(K)	U	3.4
33	2b	95	GLN	3.4
35	2d	26	CYS	3.4
45	2n	34	TYR	3.4
32	1a	92	C	3.4
32	1a	1006	C	3.4
32	2a	1137	C	3.4
40	2i	93	ARG	3.4
40	2i	120	ARG	3.4
47	2p	57	ARG	3.4
45	2n	28	GLY	3.3
12	2Q	34	LEU	3.3
26	24	59	PHE	3.3
44	2m	101	GLN	3.3
41	2j	85	LEU	3.3
48	2q	71	PHE	3.3
53	2y	87	LYS	3.3
1	1A	1103	A	3.3
1	1A	2175	C	3.3
1	2A	2803	C	3.3
34	1c	81	GLY	3.3
41	2j	97	GLU	3.3
32	1a	199	G	3.3
21	2Z	133	ILE	3.3
48	2q	59	ILE	3.3
33	2b	207	ALA	3.3
45	1n	17	LYS	3.3
25	23	15	TYR	3.3
38	1g	18	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
26	24	40	HIS	3.3
51	1t	47	GLY	3.3
7	2H	72	ILE	3.3
33	1b	222	ILE	3.3
33	2b	215	LEU	3.3
1	1A	2152	G	3.3
44	1m	24	GLY	3.3
7	2H	44	VAL	3.3
34	2c	207	VAL	3.3
39	1h	53	VAL	3.3
1	1A	1084	A	3.3
1	2A	1118	C	3.3
1	2A	1508	A	3.3
6	1G	80	PHE	3.3
32	2a	1321	C	3.3
41	2j	45	ARG	3.3
51	1t	100	ILE	3.3
1	2A	2160	G	3.3
7	2H	166	GLY	3.3
32	1a	78	G	3.3
39	2h	65	TYR	3.3
40	2i	80	GLY	3.3
45	1n	33	VAL	3.3
21	2Z	51	ALA	3.3
35	2d	48	ALA	3.3
40	1i	106	ALA	3.3
41	1j	18	ALA	3.3
53	2y	48	PHE	3.3
33	1b	75	LYS	3.3
1	2A	2187	G	3.3
32	1a	1138	G	3.3
32	2a	1064	G	3.3
51	1t	80	ARG	3.3
6	2G	38	VAL	3.3
34	1c	64	VAL	3.3
50	2s	38	SER	3.3
36	2e	84	PHE	3.3
38	2g	24	THR	3.3
1	2A	1082	U	3.3
32	1a	1043	C	3.3
40	2i	121	ARG	3.3
14	2S	36	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
33	2b	233	SER	3.3
44	1m	115	LYS	3.3
6	2G	160	VAL	3.3
45	2n	56	VAL	3.3
32	1a	105	G	3.2
41	1j	90	LEU	3.2
6	2G	73	ALA	3.2
41	1j	11	PHE	3.2
32	2a	1020	U	3.2
52	1u	19	GLY	3.2
34	1c	148	GLY	3.2
44	1m	108	ARG	3.2
53	2y	38	HIS	3.2
1	1A	1175	U	3.2
1	1A	2160	G	3.2
1	1A	2162	G	3.2
1	2A	1055	G	3.2
1	2A	1091	G	3.2
1	2A	2157	G	3.2
6	2G	49	ASP	3.2
45	1n	36	PHE	3.2
53	2y	73	ALA	3.2
45	2n	58	LYS	3.2
1	2A	1070	A	3.2
1	2A	2114	A	3.2
32	1a	1041	A	3.2
50	2s	61	TYR	3.2
12	2Q	59	ARG	3.2
50	1s	9	VAL	3.2
15	1T	38	ASN	3.2
32	2a	1446	U	3.2
43	1l	7	ILE	3.2
40	1i	126	SER	3.2
32	1a	1366	C	3.2
50	1s	29	ARG	3.2
1	1A	2790	A	3.2
44	1m	112	GLY	3.2
32	2a	203	U	3.2
32	2a	1025	U	3.2
34	1c	39	ILE	3.2
51	2t	25	ARG	3.2
1	2A	2128	C	3.2

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Mol	Chain	Res	Type	RSRZ
32	1a	221	C	3.2
32	2a	1287	A	3.2
14	2S	102	ALA	3.2
1	2A	614(A)	U	3.2
6	2G	63	ILE	3.2
45	2n	11	LYS	3.2
33	2b	151	GLY	3.2
45	2n	8	GLU	3.2
48	1q	33	GLY	3.2
50	2s	82	GLY	3.2
1	1A	2121	G	3.2
32	2a	1186	G	3.2
32	2a	1356	G	3.2
32	2a	1114	C	3.2
38	2g	117	ALA	3.2
53	2y	80	LYS	3.2
7	2H	54	ARG	3.2
32	2a	1005	A	3.2
40	1i	16	ARG	3.2
32	2a	1278	U	3.2
53	2y	78	ILE	3.2
7	2H	40	GLU	3.2
50	2s	35	SER	3.2
7	2H	36	PRO	3.2
38	1g	56	GLN	3.2
40	2i	98	PRO	3.2
41	2j	13	HIS	3.2
33	2b	133	LYS	3.2
11	2P	79	ARG	3.2
34	2c	60	ALA	3.1
45	1n	59	ALA	3.1
48	1q	7	THR	3.1
1	1A	2179	C	3.1
1	2A	1087	G	3.1
1	2A	2156	G	3.1
32	2a	1187	G	3.1
1	1A	2158	A	3.1
1	1A	2171	A	3.1
38	1g	42	ILE	3.1
12	2Q	33	GLY	3.1
7	2H	6	ARG	3.1
40	1i	111	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
40	2i	122	ALA	3.1
44	1m	63	THR	3.1
45	1n	10	ALA	3.1
1	1A	1097	U	3.1
32	2a	1314	C	3.1
34	2c	41	GLY	3.1
34	2c	158	GLY	3.1
35	2d	70	ILE	3.1
1	1A	2133	G	3.1
32	1a	1003	G	3.1
32	1a	1182	G	3.1
40	2i	9	ARG	3.1
6	2G	92	VAL	3.1
11	2P	108	LYS	3.1
28	26	14	THR	3.1
50	1s	4	SER	3.1
50	2s	8	GLY	3.1
6	2G	52	ILE	3.1
49	2r	87	ARG	3.1
32	1a	174	C	3.1
32	1a	1004	A	3.1
32	1a	1023	G	3.1
32	1a	1224	G	3.1
32	2a	1042	G	3.1
6	1G	152	LEU	3.1
39	2h	124	ALA	3.1
40	2i	43	ALA	3.1
1	2A	1105	U	3.1
51	1t	85	MET	3.1
52	1u	3	LYS	3.1
26	14	65	ASP	3.1
50	1s	12	ASP	3.1
1	1A	1062	G	3.1
32	2a	1142	G	3.1
32	2a	1305	G	3.1
40	1i	7	THR	3.1
40	1i	56	LEU	3.1
40	1i	83	ARG	3.1
41	2j	32	ALA	3.1
47	1p	49	LEU	3.1
50	1s	30	LEU	3.1
51	1t	62	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
45	2n	40	CYS	3.1
52	1u	16	GLY	3.1
32	2a	1315	U	3.1
35	1d	166	LYS	3.1
32	1a	1027	C	3.1
32	2a	1141	C	3.1
14	2S	3	ARG	3.1
1	1A	1098	A	3.1
1	1A	2801(A)	A	3.1
1	2A	6	A	3.1
32	2a	1004	A	3.1
33	2b	51	LEU	3.1
34	1c	32	LEU	3.1
40	1i	99	LEU	3.1
44	1m	90	LEU	3.1
45	1n	28	GLY	3.1
44	2m	72	ALA	3.1
6	1G	78	SER	3.1
7	2H	25	LYS	3.1
7	2H	125	VAL	3.1
27	15	60	VAL	3.1
34	2c	141	VAL	3.1
38	2g	118	VAL	3.1
1	1A	2154	G	3.1
32	1a	1009	G	3.1
1	1A	1105	U	3.1
40	1i	10	ARG	3.1
32	2a	1327	C	3.1
13	2R	65	LEU	3.1
33	2b	123	ALA	3.1
34	2c	94	LEU	3.1
32	2a	1447	A	3.0
1	1A	1058	G	3.0
41	1j	47	PHE	3.0
44	2m	78	ILE	3.0
45	2n	21	TYR	3.0
1	1A	2185	C	3.0
32	1a	1018	C	3.0
32	2a	1363	C	3.0
40	2i	58	HIS	3.0
47	1p	7	ALA	3.0
51	2t	73	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
39	2h	118	VAL	3.0
40	1i	41	VAL	3.0
1	2A	2135	A	3.0
7	2H	157	TYR	3.0
36	2e	133	TYR	3.0
1	2A	1099	G	3.0
35	1d	180	GLY	3.0
6	2G	139	LEU	3.0
45	2n	26	ARG	3.0
45	2n	57	ARG	3.0
26	14	56	VAL	3.0
30	28	21	LYS	3.0
32	2a	132	C	3.0
32	2a	217	C	3.0
50	2s	70	LYS	3.0
1	1A	2109	U	3.0
34	1c	2	GLY	3.0
45	1n	21	TYR	3.0
33	1b	233	SER	3.0
34	2c	85	ARG	3.0
44	2m	11	ARG	3.0
53	2y	67	HIS	3.0
32	1a	184	G	3.0
50	2s	28	LYS	3.0
40	2i	64	THR	3.0
47	1p	60	LEU	3.0
48	2q	74	LEU	3.0
53	2y	49	VAL	3.0
35	1d	69	GLY	3.0
41	1j	98	ILE	3.0
33	2b	53	ARG	3.0
40	2i	83	ARG	3.0
33	1b	19	HIS	3.0
11	2P	105	LEU	3.0
33	2b	187	LEU	3.0
51	2t	20	LEU	3.0
1	1A	2894	G	3.0
14	2S	69	VAL	3.0
32	2a	976	G	3.0
32	2a	1061	G	3.0
1	1A	1102	C	3.0
1	2A	2896	C	3.0

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Mol	Chain	Res	Type	RSRZ
32	1a	177	C	3.0
32	2a	1328	C	3.0
33	2b	217	ARG	3.0
34	2c	162	GLN	3.0
1	1A	2180	U	3.0
32	2a	1122	U	3.0
41	2j	28	ARG	3.0
51	2t	100	ILE	3.0
21	2Z	142	SER	3.0
32	2a	1442(B)	A	3.0
6	2G	135	LEU	3.0
48	2q	6	LEU	3.0
40	2i	49	PRO	3.0
23	21	70	VAL	3.0
44	2m	93	ARG	3.0
51	2t	83	ARG	3.0
32	2a	79	G	3.0
6	1G	77	ILE	3.0
12	2Q	65	PHE	3.0
7	2H	16	SER	3.0
33	2b	124	SER	3.0
32	2a	1324	A	3.0
36	2e	16	THR	3.0
50	1s	5	LEU	3.0
53	2y	52	ALA	3.0
50	1s	60	VAL	2.9
1	2A	2113	U	2.9
32	1a	1025	U	2.9
44	1m	25	ILE	2.9
1	2A	1102	C	2.9
7	1H	2	SER	2.9
31	29	19	ARG	2.9
33	2b	125	PRO	2.9
38	2g	16	LEU	2.9
40	2i	56	LEU	2.9
41	2j	88	LEU	2.9
1	1A	1069	A	2.9
7	2H	50	VAL	2.9
14	2S	14	VAL	2.9
38	2g	21	VAL	2.9
38	1g	53	LYS	2.9
41	2j	80	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
41	2j	35	SER	2.9
33	1b	175	ARG	2.9
52	1u	6	ARG	2.9
1	2A	1063	G	2.9
6	2G	110	ALA	2.9
21	2Z	7	ALA	2.9
33	2b	67	THR	2.9
36	1e	134	ALA	2.9
44	2m	69	GLU	2.9
51	1t	59	ALA	2.9
34	1c	23	TYR	2.9
32	2a	1248	A	2.9
7	2H	123	PHE	2.9
32	1a	223	U	2.9
53	1y	58	ASN	2.9
32	2a	1018	C	2.9
33	2b	31	TYR	2.9
29	27	47	ARG	2.9
34	2c	142	MET	2.9
40	2i	10	ARG	2.9
44	2m	80	ARG	2.9
52	2u	10	ARG	2.9
1	1A	1057	A	2.9
26	14	46	GLN	2.9
32	2a	949	A	2.9
1	2A	271(K)	U	2.9
7	2H	121	ILE	2.9
45	2n	37	PHE	2.9
34	1c	80	GLY	2.9
45	2n	9	LYS	2.9
44	2m	113	PRO	2.9
51	1t	77	ALA	2.9
1	1A	885	C	2.9
44	2m	110	ARG	2.9
50	1s	56	GLN	2.9
1	2A	1170	G	2.9
32	2a	1015	A	2.9
38	2g	37	ASN	2.9
47	1p	37	GLY	2.9
50	2s	53	ASN	2.9
33	1b	128	GLU	2.9
38	2g	101	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
44	1m	48	LEU	2.9
45	2n	45	ARG	2.9
50	2s	3	ARG	2.9
33	2b	16	HIS	2.9
19	2X	69	TYR	2.9
32	1a	100	C	2.9
53	2y	71	TYR	2.9
26	24	18	CYS	2.9
1	2A	1117	G	2.9
32	1a	68	G	2.9
32	1a	1013	G	2.9
1	2A	2158	A	2.9
7	2H	95	ARG	2.9
32	1a	162	A	2.9
26	24	46	GLN	2.9
33	2b	34	ALA	2.9
33	2b	121	LEU	2.9
34	1c	95	THR	2.9
44	2m	49	THR	2.9
40	1i	4	TYR	2.9
1	2A	1052	C	2.8
7	2H	82	GLY	2.8
32	1a	201	C	2.8
32	1a	1112	C	2.8
33	2b	81	VAL	2.8
38	1g	17	VAL	2.8
41	1j	49	VAL	2.8
48	2q	23	VAL	2.8
6	2G	138	GLN	2.8
29	27	48	LYS	2.8
34	2c	37	GLN	2.8
40	2i	77	ILE	2.8
47	1p	41	PRO	2.8
1	2A	1051	G	2.8
7	2H	33	LEU	2.8
32	2a	1269	A	2.8
45	2n	22	THR	2.8
44	2m	67	GLU	2.8
20	2Y	55	TYR	2.8
33	1b	219	VAL	2.8
1	1A	2136	C	2.8
1	1A	2178	C	2.8

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Mol	Chain	Res	Type	RSRZ
32	1a	840	C	2.8
32	2a	1362	C	2.8
1	1A	272(A)	U	2.8
40	1i	49	PRO	2.8
40	1i	94	ALA	2.8
7	2H	7	LEU	2.8
1	1A	1099	G	2.8
1	1A	2134	A	2.8
40	2i	32	ASP	2.8
1	2A	614(B)	G	2.8
7	2H	22	GLY	2.8
32	1a	200	G	2.8
41	1j	5	ARG	2.8
7	2H	56	SER	2.8
1	1A	2177	C	2.8
32	2a	204	U	2.8
50	1s	74	PHE	2.8
37	1f	99	ALA	2.8
7	2H	13	LYS	2.8
13	2R	68	ARG	2.8
40	2i	54	ASP	2.8
33	1b	18	GLY	2.8
48	1q	99	SER	2.8
21	2Z	100	VAL	2.8
44	2m	60	VAL	2.8
32	1a	991	U	2.8
38	2g	62	PHE	2.8
45	1n	7	ILE	2.8
32	2a	979	C	2.8
32	2a	1116	C	2.8
32	2a	1249	C	2.8
34	1c	168	ALA	2.8
34	1c	180	ALA	2.8
41	1j	26	ALA	2.8
28	26	13	CYS	2.8
47	2p	1	MET	2.8
8	2I	19	VAL	2.8
32	1a	1285	A	2.8
32	2a	1306	A	2.8
33	1b	136	VAL	2.8
39	2h	95	VAL	2.8
40	1i	17	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2894	G	2.8
32	1a	216	G	2.8
32	2a	1258	G	2.8
38	2g	4	ARG	2.8
53	1y	95	ARG	2.8
32	1a	63	C	2.8
39	2h	36	LEU	2.8
41	1j	97	GLU	2.8
44	2m	90	LEU	2.8
49	1r	42	ARG	2.8
33	2b	165	VAL	2.8
47	1p	51	VAL	2.8
50	1s	41	VAL	2.8
1	2A	890	A	2.8
32	1a	185	A	2.8
7	2H	83	TYR	2.8
33	2b	12	GLU	2.8
34	1c	182	ILE	2.8
34	2c	163	ALA	2.8
47	1p	80	PHE	2.8
51	1t	95	ALA	2.8
1	1A	2187	G	2.8
6	2G	176	LEU	2.8
11	2P	138	LEU	2.8
1	1A	886	C	2.8
32	1a	224	C	2.8
32	1a	1115	C	2.8
41	2j	30	SER	2.8
50	2s	78	ARG	2.8
33	2b	164	VAL	2.7
45	1n	25	VAL	2.7
32	1a	202	U	2.7
32	1a	1349	A	2.7
32	2a	1204	A	2.7
32	2a	1279	A	2.7
32	2a	1307	U	2.7
51	2t	9	ASN	2.7
52	1u	11	GLY	2.7
33	1b	188	ALA	2.7
39	2h	28	ALA	2.7
40	1i	52	ALA	2.7
40	2i	94	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
14	2S	54	LEU	2.7
40	1i	20	ARG	2.7
1	1A	2110	G	2.7
1	1A	2182	G	2.7
32	1a	1017	G	2.7
32	1a	1007	C	2.7
48	1q	10	VAL	2.7
1	2A	2180	U	2.7
6	2G	151	ALA	2.7
14	2S	66	ALA	2.7
26	14	67	TYR	2.7
33	2b	105	PHE	2.7
39	2h	37	ARG	2.7
40	1i	82	ALA	2.7
44	1m	109	THR	2.7
50	1s	52	TYR	2.7
53	2y	50	ALA	2.7
50	2s	20	LEU	2.7
39	2h	4	ASP	2.7
1	1A	2146	C	2.7
32	1a	460	G	2.7
32	2a	1310	G	2.7
7	2H	93	GLY	2.7
36	1e	51	VAL	2.7
38	1g	21	VAL	2.7
44	1m	53	VAL	2.7
34	2c	16	ARG	2.7
35	2d	49	ARG	2.7
1	2A	2895	U	2.7
26	14	52	THR	2.7
6	2G	146	TYR	2.7
26	14	59	PHE	2.7
43	1l	61	THR	2.7
34	2c	32	LEU	2.7
1	2A	655	A	2.7
45	2n	49	HIS	2.7
40	2i	6	GLY	2.7
19	2X	68	ARG	2.7
22	20	74	ARG	2.7
32	1a	1369	C	2.7
32	2a	1112	C	2.7
40	1i	121	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
41	1j	45	ARG	2.7
48	2q	86	GLU	2.7
1	1A	2897	U	2.7
6	2G	61	ALA	2.7
30	18	51	ALA	2.7
32	2a	1000	U	2.7
40	2i	11	LYS	2.7
40	2i	70	LYS	2.7
44	1m	49	THR	2.7
44	2m	20	THR	2.7
51	2t	34	LYS	2.7
34	2c	91	LEU	2.7
38	1g	13	GLN	2.7
41	1j	96	ILE	2.7
51	1t	33	ILE	2.7
53	2y	39	ILE	2.7
8	2I	43	ASN	2.7
32	2a	1180	A	2.7
35	1d	124	GLY	2.7
1	2A	2129	C	2.7
1	2A	1060	U	2.7
36	1e	17	ALA	2.7
44	1m	21	TYR	2.7
33	2b	139	LYS	2.7
51	1t	64	ASP	2.7
34	2c	133	ALA	2.7
1	1A	1060	U	2.7
7	2H	4	ILE	2.7
7	2H	88	LEU	2.7
21	2Z	197	ILE	2.7
34	2c	164	ARG	2.7
32	1a	77	G	2.7
32	2a	1011	G	2.7
34	2c	185	GLY	2.7
32	2a	975	A	2.6
32	2a	1250	A	2.6
11	2P	95	VAL	2.6
40	2i	107	ARG	2.6
1	1A	1094	U	2.6
29	17	48	LYS	2.6
34	2c	124	ILE	2.6
44	2m	89	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
47	2p	38	TYR	2.6
32	1a	98	G	2.6
26	24	55	ARG	2.6
45	2n	50	LYS	2.6
46	2o	68	ARG	2.6
51	1t	22	ARG	2.6
34	2c	144	SER	2.6
1	1A	890	A	2.6
32	2a	1288	A	2.6
34	1c	60	ALA	2.6
50	1s	33	THR	2.6
33	1b	41	ILE	2.6
46	2o	89	GLY	2.6
1	2A	886	C	2.6
2	2B	17	C	2.6
7	2H	126	PRO	2.6
32	1a	456	C	2.6
32	2a	1019	C	2.6
32	2a	1325	C	2.6
53	1y	46	GLN	2.6
43	2l	64	TYR	2.6
11	2P	102	ARG	2.6
40	1i	93	ARG	2.6
50	1s	66	MET	2.6
50	2s	81	ARG	2.6
51	1t	14	LYS	2.6
32	1a	70	G	2.6
32	2a	1120	G	2.6
32	2a	1462	G	2.6
38	2g	108	ALA	2.6
40	1i	8	GLY	2.6
40	1i	57	GLY	2.6
44	2m	40	ASN	2.6
1	2A	2189	U	2.6
6	1G	139	LEU	2.6
40	2i	3	GLN	2.6
50	1s	64	GLU	2.6
51	2t	84	LEU	2.6
11	2P	91	PHE	2.6
14	2S	35	ILE	2.6
38	1g	50	ILE	2.6
1	2A	2804	C	2.6

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Mol	Chain	Res	Type	RSRZ
32	2a	1051	C	2.6
32	2a	1218	C	2.6
39	2h	9	MET	2.6
47	2p	39	TYR	2.6
45	2n	60	SER	2.6
7	2H	49	VAL	2.6
7	2H	100	GLY	2.6
7	2H	142	GLY	2.6
7	2H	106	THR	2.6
44	1m	107	ALA	2.6
23	11	98	LEU	2.6
32	2a	631	G	2.6
32	2a	1022	G	2.6
32	2a	1294	G	2.6
33	1b	213	LEU	2.6
34	2c	4	LYS	2.6
32	2a	1308	U	2.6
44	2m	66	LEU	2.6
7	2H	10	PRO	2.6
21	2Z	124	ILE	2.6
1	2A	2103	C	2.6
13	2R	21	TYR	2.6
32	1a	194	C	2.6
32	2a	1320	C	2.6
44	2m	13	LYS	2.6
38	1g	32	ARG	2.6
38	2g	105	VAL	2.6
50	1s	75	ALA	2.6
39	2h	38	ILE	2.6
41	2j	63	PHE	2.6
48	2q	60	ILE	2.6
1	1A	1095	A	2.6
1	1A	1847	A	2.6
1	2A	1077	A	2.6
32	1a	1492	A	2.6
32	2a	1329	A	2.6
5	2F	184	TYR	2.6
6	2G	108	ASN	2.6
33	2b	230	VAL	2.6
38	1g	61	VAL	2.6
52	1u	17	THR	2.6
32	2a	1126	U	2.6

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Mol	Chain	Res	Type	RSRZ
32	2a	1136	U	2.6
38	1g	112	PRO	2.6
33	2b	200	ILE	2.6
34	1c	10	PHE	2.6
35	2d	146	ILE	2.6
38	2g	43	PHE	2.6
45	2n	7	ILE	2.6
48	2q	36	ILE	2.6
50	2s	34	TRP	2.6
14	2S	16	ASN	2.6
7	2H	57	ASP	2.6
32	2a	1318	A	2.6
41	1j	51	ARG	2.6
41	1j	70	ARG	2.6
51	2t	11	SER	2.6
53	2y	79	ASN	2.6
14	2S	100	ALA	2.5
38	1g	46	ALA	2.5
50	2s	24	ALA	2.5
7	2H	112	PRO	2.5
45	1n	39	LEU	2.5
51	2t	10	LEU	2.5
48	2q	65	ILE	2.5
53	2y	12	ILE	2.5
40	2i	16	ARG	2.5
44	2m	62	ASN	2.5
6	2G	155	MET	2.5
41	2j	25	GLU	2.5
2	2B	52	A	2.5
32	1a	1183	A	2.5
21	2Z	187	ALA	2.5
26	24	24	THR	2.5
40	2i	84	ALA	2.5
44	1m	18	ALA	2.5
9	2N	46	VAL	2.5
26	24	7	PRO	2.5
13	2R	18	LEU	2.5
33	1b	135	GLN	2.5
34	1c	204	LEU	2.5
50	1s	22	LEU	2.5
1	2A	2144	U	2.5
26	24	62	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
40	1i	128	ARG	2.5
26	14	57	GLU	2.5
48	2q	8	GLY	2.5
50	2s	64	GLU	2.5
33	2b	75	LYS	2.5
50	1s	18	LYS	2.5
32	2a	1016	A	2.5
32	2a	1319	A	2.5
34	2c	95	THR	2.5
35	2d	201	GLN	2.5
38	2g	11	GLN	2.5
40	2i	125	TYR	2.5
40	1i	98	PRO	2.5
50	1s	48	THR	2.5
53	2y	45	PRO	2.5
19	1X	68	ARG	2.5
38	1g	6	ARG	2.5
32	2a	1007	C	2.5
40	1i	2	GLU	2.5
45	2n	39	LEU	2.5
6	2G	150	ASP	2.5
30	28	48	PHE	2.5
33	2b	39	ILE	2.5
40	2i	81	ILE	2.5
47	1p	36	ILE	2.5
11	2P	149	GLU	2.5
34	2c	143	GLU	2.5
40	1i	90	PRO	2.5
32	1a	134	A	2.5
32	1a	1110	A	2.5
40	1i	91	ASP	2.5
1	2A	1116	C	2.5
32	1a	1260	C	2.5
41	1j	62	HIS	2.5
1	2A	892	G	2.5
1	2A	2100	G	2.5
1	2A	2184	G	2.5
33	2b	211	ILE	2.5
51	1t	61	SER	2.5
33	2b	212	GLN	2.5
41	2j	86	MET	2.5
45	1n	29	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
46	2o	17	ARG	2.5
6	2G	55	LYS	2.5
33	2b	194	PRO	2.5
40	2i	106	ALA	2.5
40	1i	75	ASP	2.5
41	2j	81	THR	2.5
50	1s	39	THR	2.5
7	2H	105	LEU	2.5
8	2I	30	LEU	2.5
34	2c	178	LEU	2.5
38	2g	9	VAL	2.5
40	1i	65	VAL	2.5
52	2u	18	TYR	2.5
53	2y	41	LEU	2.5
50	2s	47	HIS	2.5
1	1A	1096	A	2.5
32	1a	383	A	2.5
7	2H	89	ILE	2.5
35	2d	5	ILE	2.5
51	1t	42	GLN	2.5
15	2T	112	ARG	2.5
31	29	18	ARG	2.5
51	1t	79	ARG	2.5
32	1a	1368	G	2.5
35	2d	166	LYS	2.5
53	2y	91	LYS	2.5
8	2I	74	ASN	2.5
7	2H	52	VAL	2.5
45	1n	53	LEU	2.5
33	1b	231	GLU	2.5
38	2g	57	GLU	2.5
47	1p	62	VAL	2.5
32	2a	1348	U	2.5
1	2A	1049	C	2.5
32	1a	150	C	2.5
32	2a	1010	G	2.5
32	2a	1068	G	2.5
32	2a	1385	G	2.5
41	2j	48	THR	2.5
53	1y	33	HIS	2.4
53	2y	19	HIS	2.4
6	1G	173	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
21	2Z	157	LEU	2.4
23	11	46	LEU	2.4
26	14	55	ARG	2.4
39	2h	39	LEU	2.4
40	1i	85	LEU	2.4
44	1m	93	ARG	2.4
47	2p	33	ILE	2.4
32	2a	1254	C	2.4
33	1b	234	PRO	2.4
33	2b	202	PRO	2.4
23	21	26	ARG	2.4
33	2b	19	HIS	2.4
41	1j	21	GLN	2.4
50	2s	29	ARG	2.4
11	2P	115	LEU	2.4
32	1a	61	G	2.4
32	2a	1222	G	2.4
46	2o	34	LEU	2.4
12	2Q	102	VAL	2.4
30	28	49	VAL	2.4
1	2A	1113	U	2.4
35	1d	138	TYR	2.4
39	2h	58	TYR	2.4
40	1i	92	TYR	2.4
6	2G	117	PHE	2.4
7	2H	92	ILE	2.4
34	2c	57	ILE	2.4
20	1Y	1	MET	2.4
41	1j	39	PRO	2.4
45	1n	51	GLY	2.4
1	2A	1096	A	2.4
52	1u	9	ARG	2.4
6	1G	73	ALA	2.4
7	2H	111	HIS	2.4
11	2P	57	THR	2.4
32	1a	1362	C	2.4
32	1a	146	G	2.4
32	1a	841	U	2.4
32	2a	78	G	2.4
32	2a	232	G	2.4
26	14	16	CYS	2.4
44	1m	4	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
50	1s	28	LYS	2.4
34	1c	203	PHE	2.4
36	2e	45	PHE	2.4
38	2g	10	ARG	2.4
50	1s	10	PHE	2.4
22	20	76	GLY	2.4
22	20	47	PRO	2.4
34	2c	189	ALA	2.4
38	2g	121	ALA	2.4
32	1a	385	C	2.4
32	2a	1492	A	2.4
49	2r	62	GLU	2.4
41	1j	40	LEU	2.4
48	1q	97	SER	2.4
50	1s	20	LEU	2.4
36	2e	32	VAL	2.4
14	1S	17	ARG	2.4
35	1d	3	ARG	2.4
42	2k	13	GLN	2.4
52	1u	22	ARG	2.4
26	14	45	GLY	2.4
30	28	16	ILE	2.4
33	1b	185	ILE	2.4
46	1o	78	TYR	2.4
30	28	38	GLY	2.4
1	2A	1089	G	2.4
32	2a	1295	G	2.4
6	2G	104	GLU	2.4
34	2c	89	GLU	2.4
50	1s	57	HIS	2.4
7	2H	27	LYS	2.4
14	2S	5	THR	2.4
51	1t	40	ALA	2.4
1	1A	1509(A)	A	2.4
1	2A	2183	C	2.4
14	2S	56	LEU	2.4
32	1a	161	A	2.4
32	1a	1039	C	2.4
32	2a	1244	C	2.4
32	2a	1261	A	2.4
32	2a	1349	A	2.4
34	1c	33	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
41	1j	8	LEU	2.4
50	1s	71	LEU	2.4
41	1j	60	ARG	2.4
7	2H	131	VAL	2.4
53	2y	84	GLN	2.4
20	2Y	80	GLY	2.4
32	2a	991	U	2.4
40	1i	29	ASN	2.4
50	2s	72	GLY	2.4
6	2G	144	ILE	2.4
21	1Z	133	ILE	2.4
26	14	53	GLU	2.4
34	1c	89	GLU	2.4
35	1d	4	TYR	2.4
39	2h	111	ILE	2.4
41	2j	54	PHE	2.4
47	1p	38	TYR	2.4
48	2q	42	TYR	2.4
39	1h	56	LYS	2.4
40	1i	32	ASP	2.4
45	2n	20	ALA	2.4
50	2s	50	ALA	2.4
1	2A	883	G	2.4
32	1a	376	G	2.4
32	1a	1010	G	2.4
32	1a	1272	G	2.4
32	2a	1143	G	2.4
32	2a	1265	G	2.4
44	2m	71	ARG	2.4
26	24	60	GLN	2.4
32	1a	1245	A	2.4
32	2a	1115	C	2.4
32	1a	173	U	2.4
11	2P	76	LYS	2.4
14	2S	33	LYS	2.4
26	24	8	LYS	2.4
33	2b	127	ILE	2.4
34	2c	39	ILE	2.4
50	1s	31	ILE	2.4
7	2H	130	ARG	2.4
40	2i	60	ASP	2.4
47	2p	25	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
30	28	17	THR	2.4
40	1i	3	GLN	2.4
1	2A	1062	G	2.3
41	2j	10	GLY	2.3
45	2n	51	GLY	2.3
6	2G	70	VAL	2.3
33	2b	71	VAL	2.3
44	2m	54	VAL	2.3
1	2A	1097	U	2.3
1	2A	1100	C	2.3
32	1a	1111	A	2.3
32	1a	1158	C	2.3
32	2a	995	C	2.3
32	2a	1296	C	2.3
32	2a	1374	A	2.3
4	2E	77	ILE	2.3
22	20	55	ARG	2.3
30	28	25	MET	2.3
41	1j	37	PRO	2.3
48	1q	90	ILE	2.3
50	1s	59	PRO	2.3
33	2b	55	PHE	2.3
38	2g	155	ARG	2.3
34	1c	193	TYR	2.3
41	2j	33	GLN	2.3
40	1i	61	ALA	2.3
42	2k	87	THR	2.3
40	2i	25	LYS	2.3
8	2I	13	GLY	2.3
46	2o	57	LEU	2.3
1	2A	2190	G	2.3
32	2a	1355	G	2.3
6	2G	126	ASP	2.3
45	1n	23	ARG	2.3
45	2n	23	ARG	2.3
47	1p	57	ARG	2.3
48	2q	92	ARG	2.3
11	2P	94	GLU	2.3
41	2j	64	GLU	2.3
51	2t	56	MET	2.3
32	1a	141	A	2.3
15	2T	126	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
22	20	46	LYS	2.3
33	1b	133	LYS	2.3
34	2c	146	ALA	2.3
44	2m	76	ALA	2.3
45	2n	17	LYS	2.3
38	2g	12	LEU	2.3
41	2j	90	LEU	2.3
41	1j	29	ARG	2.3
45	1n	3	ARG	2.3
5	2F	39	TRP	2.3
6	2G	54	GLU	2.3
48	1q	86	GLU	2.3
47	2p	20	VAL	2.3
12	2Q	130	LYS	2.3
21	2Z	6	LYS	2.3
43	2l	13	LYS	2.3
51	2t	38	LYS	2.3
1	1A	2104	G	2.3
1	1A	2184	G	2.3
1	2A	1114	G	2.3
32	1a	1276	G	2.3
32	2a	93	G	2.3
51	2t	55	ILE	2.3
33	1b	105	PHE	2.3
1	1A	2135	A	2.3
11	2P	127	ALA	2.3
32	1a	151	A	2.3
32	1a	1157	A	2.3
38	1g	25	ALA	2.3
43	1l	64	TYR	2.3
3	2D	210	GLY	2.3
6	2G	127	GLY	2.3
36	2e	85	GLY	2.3
14	2S	13	ARG	2.3
35	2d	11	LEU	2.3
37	2f	95	GLU	2.3
40	2i	47	LEU	2.3
50	1s	15	LEU	2.3
51	1t	20	LEU	2.3
34	1c	97	LYS	2.3
53	2y	89	GLN	2.3
21	2Z	126	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
41	2j	41	PRO	2.3
47	2p	48	TRP	2.3
50	2s	60	VAL	2.3
50	2s	76	PRO	2.3
1	1A	1061	U	2.3
49	2r	65	ILE	2.3
6	2G	57	ALA	2.3
34	1c	15	THR	2.3
35	2d	150	GLU	2.3
38	2g	123	GLU	2.3
40	2i	126	SER	2.3
1	2A	1093	G	2.3
2	2B	56	G	2.3
32	2a	1156	G	2.3
34	1c	201	TYR	2.3
48	2q	70	ARG	2.3
50	1s	36	ARG	2.3
53	1y	23	ARG	2.3
35	2d	22	LYS	2.3
38	1g	22	LEU	2.3
6	2G	149	VAL	2.3
7	2H	99	VAL	2.3
32	2a	202	U	2.3
6	2G	100	TRP	2.3
36	2e	8	GLU	2.3
44	1m	26	GLY	2.3
46	2o	86	GLY	2.3
52	1u	15	ARG	2.3
10	2O	30	ALA	2.3
14	2S	93	LYS	2.3
49	1r	29	PHE	2.3
14	2S	21	THR	2.3
26	14	51	ASP	2.3
50	2s	48	THR	2.3
32	2a	980	C	2.3
32	2a	989	C	2.3
40	1i	36	TYR	2.3
2	2B	58	A	2.3
32	1a	102	G	2.3
32	2a	1131	G	2.3
32	2a	1347	G	2.3
32	2a	1370	G	2.3

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Mol	Chain	Res	Type	RSRZ
8	2I	41	GLU	2.3
7	2H	43	VAL	2.3
12	2Q	109	VAL	2.3
33	2b	229	VAL	2.3
1	1A	1101	U	2.3
21	2Z	98	MET	2.3
32	2a	997	U	2.3
52	2u	24	ARG	2.3
45	1n	60	SER	2.3
6	2G	56	ALA	2.3
36	1e	58	ALA	2.3
38	1g	152	ALA	2.3
50	1s	50	ALA	2.3
5	1F	53	THR	2.3
38	1g	44	TYR	2.3
44	2m	59	TYR	2.3
50	1s	16	LEU	2.3
32	1a	262	A	2.2
40	2i	113	LYS	2.2
32	2a	1160	G	2.2
3	2D	229	VAL	2.2
21	2Z	58	VAL	2.2
1	2A	2897	U	2.2
30	28	20	GLY	2.2
39	2h	19	VAL	2.2
44	1m	117	VAL	2.2
6	1G	49	ASP	2.2
35	1d	71	SER	2.2
24	12	13	ALA	2.2
33	1b	134	GLU	2.2
38	2g	8	GLU	2.2
44	2m	63	THR	2.2
40	2i	117	HIS	2.2
6	2G	120	LEU	2.2
20	2Y	90	LEU	2.2
44	2m	3	ARG	2.2
7	2H	29	PRO	2.2
1	1A	2896	C	2.2
32	2a	234	C	2.2
32	2a	1161	C	2.2
26	24	36	CYS	2.2
1	2A	1054	A	2.2

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Mol	Chain	Res	Type	RSRZ
21	2Z	191	VAL	2.2
32	1a	140	A	2.2
32	1a	1180	A	2.2
33	2b	135	GLN	2.2
36	2e	33	VAL	2.2
39	2h	51	VAL	2.2
39	2h	53	VAL	2.2
32	1a	90	U	2.2
32	2a	1372	U	2.2
48	1q	82	MET	2.2
1	2A	1107	G	2.2
7	2H	124	GLU	2.2
32	1a	66	G	2.2
33	1b	35	GLU	2.2
6	2G	158	ALA	2.2
7	2H	73	ALA	2.2
12	2Q	121	ALA	2.2
36	2e	132	ALA	2.2
51	2t	41	ILE	2.2
14	2S	57	LYS	2.2
25	23	30	ARG	2.2
30	28	61	LEU	2.2
40	1i	50	LEU	2.2
40	2i	19	LEU	2.2
35	2d	20	TYR	2.2
35	2d	136	PRO	2.2
26	14	54	GLY	2.2
32	2a	1128	C	2.2
32	2a	1270	C	2.2
41	1j	95	GLU	2.2
28	26	48	VAL	2.2
1	2A	2750	A	2.2
31	29	11	CYS	2.2
35	2d	56	VAL	2.2
41	2j	22	LYS	2.2
48	2q	21	VAL	2.2
51	1t	19	SER	2.2
14	2S	17	ARG	2.2
21	2Z	192	ALA	2.2
27	25	2	ALA	2.2
34	2c	5	ILE	2.2
38	2g	7	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
6	2G	23	PHE	2.2
32	2a	1190	G	2.2
32	2a	1353	G	2.2
32	2a	1461	G	2.2
36	2e	43	LEU	2.2
39	1h	133	LEU	2.2
40	1i	21	PRO	2.2
51	1t	91	LEU	2.2
7	2H	32	GLU	2.2
11	2P	119	GLU	2.2
35	1d	102	ASP	2.2
41	1j	31	GLY	2.2
21	2Z	99	TYR	2.2
47	2p	35	LYS	2.2
21	2Z	128	VAL	2.2
32	1a	979	C	2.2
33	1b	137	ARG	2.2
33	2b	30	ARG	2.2
35	2d	137	SER	2.2
44	2m	57	ARG	2.2
32	1a	1348	U	2.2
3	1D	209	ALA	2.2
35	2d	144	ASP	2.2
41	2j	69	ASN	2.2
51	1t	65	LYS	2.2
32	2a	144	G	2.2
32	2a	1017	G	2.2
33	2b	97	TRP	2.2
44	2m	14	ARG	2.2
48	1q	38	ARG	2.2
15	1T	106	SER	2.2
1	1A	2172	U	2.2
1	2A	1065	U	2.2
12	2Q	132	VAL	2.2
21	2Z	164	ALA	2.2
32	1a	856	C	2.2
32	2a	1132	C	2.2
51	2t	45	GLN	2.2
30	28	58	ILE	2.2
33	2b	195	ASP	2.2
36	2e	6	PHE	2.2
51	2t	29	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
11	2P	78	PRO	2.2
11	2P	104	GLY	2.2
39	1h	112	LEU	2.2
51	2t	72	LEU	2.2
21	1Z	80	ARG	2.2
25	23	29	ARG	2.2
51	2t	86	ARG	2.2
1	2A	1068	G	2.2
12	1Q	32	TYR	2.2
32	1a	97	G	2.2
32	2a	77	G	2.2
33	1b	148	TYR	2.2
12	2Q	35	VAL	2.2
17	2V	5	VAL	2.2
28	26	52	VAL	2.2
33	2b	101	MET	2.2
32	1a	180	U	2.2
38	1g	23	VAL	2.2
53	2y	62	VAL	2.2
40	2i	52	ALA	2.2
44	1m	33	ALA	2.2
3	2D	50	THR	2.2
23	11	7	ILE	2.2
32	1a	76	C	2.2
32	2a	233	C	2.2
34	1c	8	ILE	2.2
44	1m	39	ILE	2.2
22	20	77	ARG	2.2
35	2d	6	GLY	2.2
40	2i	24	GLY	2.2
32	2a	1251	A	2.2
47	2p	60	LEU	2.2
20	2Y	52	SER	2.2
33	1b	140	HIS	2.1
7	2H	164	TYR	2.1
1	2A	1039	G	2.1
1	2A	1074	G	2.1
26	24	21	VAL	2.1
32	1a	93	G	2.1
32	1a	1042	G	2.1
32	2a	310	G	2.1
32	2a	993	G	2.1

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Mol	Chain	Res	Type	RSRZ
53	2y	69	ASP	2.1
6	1G	24	GLY	2.1
17	1V	42	GLY	2.1
36	2e	29	GLY	2.1
40	1i	27	THR	2.1
52	2u	7	ARG	2.1
36	2e	28	PHE	2.1
38	1g	58	PRO	2.1
41	1j	64	GLU	2.1
35	2d	64	LEU	2.1
3	1D	275	LYS	2.1
6	2G	8	LYS	2.1
48	1q	37	LYS	2.1
32	2a	1245	A	2.1
41	1j	35	SER	2.1
6	2G	28	VAL	2.1
33	1b	130	ARG	2.1
40	1i	88	TYR	2.1
51	1t	89	ARG	2.1
3	2D	214	TRP	2.1
8	2I	63	ALA	2.1
12	2Q	136	ALA	2.1
36	2e	54	ALA	2.1
53	2y	60	VAL	2.1
11	2P	96	THR	2.1
14	2S	47	THR	2.1
28	26	42	TRP	2.1
40	1i	22	GLY	2.1
1	2A	1058	G	2.1
32	2a	1108	G	2.1
32	2a	1185	G	2.1
50	2s	30	LEU	2.1
1	1A	2105	C	2.1
1	2A	1053	C	2.1
32	1a	1118	C	2.1
32	2a	1118	C	2.1
1	2A	1073	A	2.1
6	2G	97	ASP	2.1
6	2G	116	ASP	2.1
7	2H	159	GLU	2.1
32	1a	195	A	2.1
40	2i	23	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
18	2W	112	GLY	2.1
11	2P	71	VAL	2.1
26	24	32	TYR	2.1
33	1b	197	VAL	2.1
33	2b	177	ALA	2.1
34	2c	193	TYR	2.1
39	2h	56	LYS	2.1
47	1p	35	LYS	2.1
40	1i	103	THR	2.1
7	2H	12	PRO	2.1
33	2b	181	PHE	2.1
40	2i	99	LEU	2.1
48	1q	89	LEU	2.1
6	2G	51	ARG	2.1
32	1a	104	G	2.1
20	2Y	91	GLU	2.1
21	2Z	79	ARG	2.1
48	1q	62	SER	2.1
32	1a	163	C	2.1
32	2a	1317	C	2.1
51	2t	64	ASP	2.1
51	1t	38	LYS	2.1
4	2E	115	GLY	2.1
11	2P	66	GLY	2.1
11	2P	143	GLY	2.1
32	1a	171	A	2.1
32	2a	978	A	2.1
8	2I	46	ALA	2.1
33	1b	212	GLN	2.1
34	2c	103	VAL	2.1
38	1g	110	GLN	2.1
40	1i	62	TYR	2.1
42	2k	104	GLN	2.1
45	2n	59	ALA	2.1
51	2t	42	GLN	2.1
14	2S	91	PRO	2.1
21	2Z	57	ILE	2.1
8	2I	61	ARG	2.1
14	2S	4	LEU	2.1
21	2Z	144	LEU	2.1
22	20	57	PHE	2.1
45	1n	37	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
7	2H	30	LYS	2.1
43	1l	62	SER	2.1
53	2y	4	ASN	2.1
25	23	27	GLY	2.1
32	1a	91	C	2.1
32	1a	479	C	2.1
32	2a	848	C	2.1
39	1h	117	GLY	2.1
46	1o	86	GLY	2.1
1	2A	9	U	2.1
6	2G	15	VAL	2.1
7	2H	17	VAL	2.1
22	20	38	VAL	2.1
14	2S	7	TYR	2.1
32	2a	1014	A	2.1
32	2a	1044	A	2.1
32	2a	1176	A	2.1
41	1j	34	VAL	2.1
34	1c	179	ARG	2.1
35	1d	50	ARG	2.1
40	2i	51	ARG	2.1
41	1j	81	THR	2.1
44	2m	17	VAL	2.1
20	2Y	61	ILE	2.1
39	2h	45	ILE	2.1
40	1i	105	ASP	2.1
50	2s	13	ASP	2.1
6	1G	82	LEU	2.1
33	1b	221	LEU	2.1
35	1d	58	LEU	2.1
34	1c	98	ASN	2.1
41	1j	33	GLN	2.1
1	1A	1100	C	2.1
29	27	1	MET	2.1
32	2a	150	C	2.1
32	2a	1262	C	2.1
32	2a	1277	C	2.1
41	1j	25	GLU	2.1
32	1a	1220	G	2.1
36	2e	17	ALA	2.1
39	1h	84	ARG	2.1
1	1A	2118	U	2.1

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Mol	Chain	Res	Type	RSRZ
3	2D	173	VAL	2.1
6	2G	37	VAL	2.1
7	2H	117	PRO	2.1
51	2t	12	ALA	2.1
12	2Q	97	VAL	2.1
22	20	51	VAL	2.1
36	1e	148	VAL	2.1
38	2g	23	VAL	2.1
39	1h	94	TYR	2.1
50	1s	13	ASP	2.1
1	1A	228	A	2.1
6	2G	114	ILE	2.1
31	29	17	ILE	2.1
32	1a	149	A	2.1
32	1a	1357	A	2.1
51	2t	63	ILE	2.1
11	2P	123	LEU	2.1
22	20	75	LEU	2.1
35	2d	21	LEU	2.1
43	2l	32	PHE	2.1
40	1i	34	ASN	2.1
41	1j	78	ASN	2.1
6	2G	26	GLN	2.1
16	1U	69	CYS	2.1
33	1b	146	GLN	2.1
50	1s	21	GLU	2.1
7	2H	172	LYS	2.1
33	2b	21	ARG	2.1
6	2G	6	ALA	2.0
32	2a	1284	C	2.0
53	2y	94	ALA	2.0
1	1A	2102	U	2.0
28	26	47	THR	2.0
6	2G	11	TYR	2.0
6	2G	101	ILE	2.0
7	2H	94	TYR	2.0
16	2U	31	SER	2.0
26	24	25	TYR	2.0
32	2a	1144	G	2.0
32	2a	1164	G	2.0
32	2a	1271	G	2.0
38	2g	18	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
50	1s	40	ILE	2.0
13	2R	54	LEU	2.0
32	1a	1306	A	2.0
51	2t	43	LEU	2.0
44	2m	27	LYS	2.0
26	24	48	ARG	2.0
36	2e	64	ARG	2.0
44	2m	99	ARG	2.0
51	2t	23	ARG	2.0
45	1n	24	CYS	2.0
40	1i	43	ALA	2.0
32	1a	62	U	2.0
32	1a	176	C	2.0
32	1a	1012	U	2.0
32	1a	1038	C	2.0
32	1a	1367	C	2.0
32	2a	84	U	2.0
32	2a	1195	C	2.0
34	2c	3	ASN	2.0
37	1f	63	TYR	2.0
38	1g	120	ILE	2.0
1	1A	2807	G	2.0
33	1b	28	PHE	2.0
33	2b	175	ARG	2.0
34	2c	179	ARG	2.0
1	2A	2320	A	2.0
8	2I	8	PRO	2.0
40	2i	110	GLU	2.0
7	2H	122	THR	2.0
32	1a	65	U	2.0
53	2y	58	ASN	2.0
40	2i	39	GLY	2.0
45	2n	41	ARG	2.0
19	1X	69	TYR	2.0
4	1E	163	GLU	2.0
10	1O	108	GLU	2.0
1	2A	2807	G	2.0
2	2B	59	A	2.0
26	24	28	LYS	2.0
32	1a	606	G	2.0
32	1a	1181	G	2.0
32	1a	1355	G	2.0

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Mol	Chain	Res	Type	RSRZ
32	2a	1093	A	2.0
6	2G	68	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
32	2MG	2a	1207	24/25	0.86	0.23	84,88,92,94	0
43	0TD	2l	92	10/11	0.86	0.14	65,71,73,88	0
1	PSU	2A	1911	20/21	0.87	0.17	69,75,90,93	0
1	5MU	2A	1915	21/22	0.87	0.15	75,84,90,98	0
1	5MU	1A	1915	21/22	0.88	0.17	71,78,84,93	0
32	M2G	2a	966	25/26	0.88	0.18	61,71,84,86	0
1	PSU	1A	1917	20/21	0.90	0.19	61,71,79,79	0
32	5MC	2a	967	21/22	0.90	0.21	70,75,82,86	0
32	5MC	1a	967	21/22	0.90	0.25	67,74,81,82	0
1	PSU	2A	1917	20/21	0.90	0.16	79,83,89,94	0
32	5MC	2a	1404	21/22	0.91	0.20	58,63,65,66	0
32	PSU	2a	516	20/21	0.92	0.10	77,81,87,92	0
32	4OC	2a	1402	22/23	0.92	0.20	58,67,73,75	0
32	2MG	1a	1207	24/25	0.92	0.15	73,79,81,86	0
1	PSU	1A	1911	20/21	0.92	0.17	51,71,76,78	0
32	PSU	1a	516	20/21	0.93	0.18	63,66,72,76	0
1	OMC	2A	1920	21/22	0.93	0.17	68,72,75,80	0
32	MA6	2a	1518	24/25	0.93	0.20	60,69,73,74	0
32	M2G	1a	966	25/26	0.93	0.23	64,68,75,82	0
32	G7M	2a	527	24/25	0.94	0.17	64,71,76,79	0
43	0TD	1l	92	10/11	0.94	0.13	51,62,67,73	0
32	5MC	2a	1407	21/22	0.94	0.19	62,67,70,77	0
32	UR3	1a	1498	21/22	0.94	0.20	49,56,60,66	0
32	MA6	1a	1519	24/25	0.94	0.22	48,54,60,65	0
32	UR3	2a	1498	21/22	0.95	0.19	64,67,71,74	0
32	5MC	2a	1400	21/22	0.95	0.23	70,74,78,80	0
32	MA6	2a	1519	24/25	0.95	0.24	57,67,71,74	0
1	OMC	1A	1920	21/22	0.95	0.24	52,60,67,69	0
1	5MC	2A	1962	21/22	0.96	0.23	43,50,58,64	0
1	OMG	2A	2251	24/25	0.96	0.23	40,44,47,47	0
1	2MA	2A	2503	23/24	0.96	0.24	34,38,43,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OMU	2A	2552	21/22	0.96	0.23	39,44,49,53	0
1	PSU	2A	2605	20/21	0.96	0.24	35,44,50,51	0
32	4OC	1a	1402	22/23	0.96	0.18	51,58,66,79	0
32	5MC	1a	1407	21/22	0.96	0.20	49,58,61,69	0
32	G7M	1a	527	24/25	0.96	0.21	50,60,64,65	0
1	5MC	2A	1942	21/22	0.96	0.22	47,57,61,64	0
1	5MC	1A	1962	21/22	0.97	0.20	29,38,44,49	0
32	5MC	1a	1404	21/22	0.97	0.17	51,56,60,62	0
1	MA6	1A	2058	24/25	0.97	0.23	20,28,38,43	0
1	PSU	1A	2605	20/21	0.97	0.25	27,33,38,41	0
32	MA6	1a	1518	24/25	0.97	0.23	49,53,57,59	0
1	5MC	1A	1942	21/22	0.97	0.23	34,40,42,51	0
1	MA6	2A	2058	24/25	0.97	0.23	34,41,49,52	0
32	5MC	1a	1400	21/22	0.97	0.18	55,60,66,69	0
1	2MA	1A	2503	23/24	0.98	0.23	21,29,32,33	0
1	OMU	1A	2552	21/22	0.98	0.24	31,35,38,43	0
1	5MU	1A	1939	21/22	0.98	0.21	27,32,36,38	0
1	OMG	1A	2251	24/25	0.98	0.22	22,29,32,34	0
1	5MU	2A	1939	21/22	0.98	0.23	36,40,46,48	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	4018	1/1	0.12	0.10	68,68,68,68	0
54	MG	1a	1802	1/1	0.28	0.35	84,84,84,84	0
54	MG	2A	3569	1/1	0.29	0.10	78,78,78,78	0
54	MG	1A	3842	1/1	0.32	0.17	70,70,70,70	0
54	MG	1A	3481	1/1	0.33	0.15	68,68,68,68	0
54	MG	2A	3475	1/1	0.37	0.11	83,83,83,83	0
54	MG	1A	3929	1/1	0.40	0.11	60,60,60,60	0
54	MG	2a	3039	1/1	0.40	0.27	94,94,94,94	0
54	MG	1A	4000	1/1	0.41	0.14	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3653	1/1	0.41	0.15	77,77,77,77	0
54	MG	2A	3594	1/1	0.42	0.28	85,85,85,85	0
54	MG	1a	1873	1/1	0.42	0.19	83,83,83,83	0
54	MG	1A	3322	1/1	0.43	0.32	69,69,69,69	0
54	MG	1a	1663	1/1	0.43	0.20	66,66,66,66	0
54	MG	2a	3020	1/1	0.44	0.10	86,86,86,86	0
54	MG	2A	3078	1/1	0.47	0.21	69,69,69,69	0
54	MG	2A	3443	1/1	0.48	0.18	79,79,79,79	0
54	MG	1d	303	1/1	0.48	0.20	74,74,74,74	0
54	MG	1a	1658	1/1	0.49	0.38	75,75,75,75	0
54	MG	1A	3687	1/1	0.50	0.09	56,56,56,56	0
54	MG	1A	3676	1/1	0.51	0.10	57,57,57,57	0
54	MG	1A	3463	1/1	0.51	0.20	83,83,83,83	0
54	MG	2A	3148	1/1	0.51	0.31	73,73,73,73	0
54	MG	2A	3523	1/1	0.52	0.24	60,60,60,60	0
54	MG	2A	3566	1/1	0.52	0.35	86,86,86,86	0
54	MG	1f	201	1/1	0.53	0.27	80,80,80,80	0
54	MG	1A	3872	1/1	0.55	0.21	67,67,67,67	0
54	MG	1A	3894	1/1	0.56	0.15	60,60,60,60	0
54	MG	1A	3991	1/1	0.57	0.10	81,81,81,81	0
54	MG	2A	3669	1/1	0.57	0.32	60,60,60,60	0
54	MG	1A	3484	1/1	0.57	0.13	59,59,59,59	0
54	MG	2A	3080	1/1	0.57	0.24	79,79,79,79	0
54	MG	1a	1863	1/1	0.58	0.33	74,74,74,74	0
54	MG	2A	3108	1/1	0.58	0.25	66,66,66,66	0
54	MG	2a	3068	1/1	0.58	0.09	81,81,81,81	0
54	MG	2A	3477	1/1	0.59	0.17	86,86,86,86	0
54	MG	1a	1701	1/1	0.59	0.16	72,72,72,72	0
54	MG	11	105	1/1	0.59	0.20	66,66,66,66	0
54	MG	2A	3210	1/1	0.60	0.34	71,71,71,71	0
54	MG	2a	3085	1/1	0.60	0.19	76,76,76,76	0
54	MG	2a	3159	1/1	0.60	0.17	74,74,74,74	0
54	MG	1A	3680	1/1	0.61	0.16	63,63,63,63	0
54	MG	1A	3844	1/1	0.61	0.08	54,54,54,54	0
54	MG	1A	3861	1/1	0.61	0.18	63,63,63,63	0
54	MG	1a	1679	1/1	0.61	0.23	66,66,66,66	0
54	MG	2A	3585	1/1	0.62	0.20	60,60,60,60	0
54	MG	1A	3429	1/1	0.62	0.25	75,75,75,75	0
54	MG	1A	3243	1/1	0.62	0.19	74,74,74,74	0
54	MG	1A	3804	1/1	0.62	0.10	78,78,78,78	0
54	MG	2A	3243	1/1	0.63	0.37	73,73,73,73	0
54	MG	2A	3510	1/1	0.63	0.16	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3895	1/1	0.63	0.25	58,58,58,58	0
54	MG	1A	3397	1/1	0.63	0.17	57,57,57,57	0
54	MG	2B	213	1/1	0.63	0.12	65,65,65,65	0
54	MG	1A	3544	1/1	0.64	0.15	50,50,50,50	0
54	MG	2a	3116	1/1	0.64	0.23	70,70,70,70	0
54	MG	2A	3047	1/1	0.64	0.12	63,63,63,63	0
54	MG	2a	3025	1/1	0.65	0.47	83,83,83,83	0
54	MG	2A	3359	1/1	0.65	0.22	80,80,80,80	0
54	MG	2A	3515	1/1	0.65	0.19	49,49,49,49	0
54	MG	1A	3089	1/1	0.65	0.24	56,56,56,56	0
54	MG	1l	202	1/1	0.65	0.46	78,78,78,78	0
54	MG	1A	3596	1/1	0.65	0.25	66,66,66,66	0
54	MG	2A	3399	1/1	0.66	0.17	69,69,69,69	0
54	MG	2A	3402	1/1	0.66	0.20	62,62,62,62	0
54	MG	1a	1648	1/1	0.66	0.15	71,71,71,71	0
54	MG	2A	3184	1/1	0.66	0.28	61,61,61,61	0
54	MG	1y	201	1/1	0.66	0.19	73,73,73,73	0
54	MG	2A	3106	1/1	0.66	0.16	70,70,70,70	0
54	MG	1A	3279	1/1	0.66	0.42	55,55,55,55	0
54	MG	2A	3147	1/1	0.67	0.35	79,79,79,79	0
54	MG	1a	1692	1/1	0.67	0.16	62,62,62,62	0
54	MG	2a	3097	1/1	0.67	0.14	64,64,64,64	0
54	MG	2a	3101	1/1	0.67	0.11	78,78,78,78	0
54	MG	2A	3175	1/1	0.67	0.24	47,47,47,47	0
54	MG	1A	3027	1/1	0.67	0.21	64,64,64,64	0
54	MG	1l	102	1/1	0.68	0.29	56,56,56,56	0
54	MG	1A	3066	1/1	0.68	0.14	67,67,67,67	0
54	MG	1o	101	1/1	0.68	0.23	74,74,74,74	0
54	MG	1A	3330	1/1	0.68	0.19	56,56,56,56	0
54	MG	2A	3017	1/1	0.68	0.24	56,56,56,56	0
54	MG	1A	3993	1/1	0.69	0.20	71,71,71,71	0
54	MG	2A	3601	1/1	0.69	0.11	77,77,77,77	0
54	MG	1A	3300	1/1	0.69	0.20	52,52,52,52	0
54	MG	1A	4001	1/1	0.69	0.17	80,80,80,80	0
54	MG	2A	3459	1/1	0.69	0.22	72,72,72,72	0
54	MG	1g	201	1/1	0.69	0.21	69,69,69,69	0
54	MG	1A	3188	1/1	0.69	0.14	65,65,65,65	0
54	MG	2a	3040	1/1	0.69	0.17	71,71,71,71	0
54	MG	1B	205	1/1	0.69	0.24	64,64,64,64	0
54	MG	2a	3071	1/1	0.69	0.16	62,62,62,62	0
54	MG	2a	3074	1/1	0.69	0.57	70,70,70,70	0
54	MG	1A	3712	1/1	0.69	0.26	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1735	1/1	0.69	0.30	68,68,68,68	0
54	MG	1A	3291	1/1	0.69	0.17	82,82,82,82	0
54	MG	15	106	1/1	0.69	0.22	48,48,48,48	0
54	MG	2a	3149	1/1	0.69	0.17	80,80,80,80	0
54	MG	2A	3363	1/1	0.69	0.21	75,75,75,75	0
54	MG	2A	3589	1/1	0.70	0.17	73,73,73,73	0
54	MG	1A	3277	1/1	0.70	0.19	75,75,75,75	0
54	MG	1a	1665	1/1	0.70	0.50	76,76,76,76	0
54	MG	1A	3531	1/1	0.70	0.10	58,58,58,58	0
54	MG	1a	1638	1/1	0.70	0.24	71,71,71,71	0
54	MG	1H	201	1/1	0.70	0.10	67,67,67,67	0
54	MG	1a	1702	1/1	0.70	0.40	78,78,78,78	0
54	MG	2A	3570	1/1	0.70	0.24	76,76,76,76	0
54	MG	1A	3308	1/1	0.70	0.21	73,73,73,73	0
54	MG	2a	3057	1/1	0.71	0.11	66,66,66,66	0
54	MG	1A	3268	1/1	0.71	0.23	58,58,58,58	0
54	MG	1a	1771	1/1	0.71	0.14	74,74,74,74	0
54	MG	1A	3979	1/1	0.71	0.27	57,57,57,57	0
54	MG	1A	3194	1/1	0.71	0.34	65,65,65,65	0
54	MG	2a	3092	1/1	0.71	0.11	67,67,67,67	0
54	MG	1A	3136	1/1	0.71	0.33	46,46,46,46	0
54	MG	1a	1649	1/1	0.71	0.32	57,57,57,57	0
54	MG	2A	3405	1/1	0.71	0.16	67,67,67,67	0
54	MG	2A	3179	1/1	0.71	0.30	69,69,69,69	0
54	MG	1A	3257	1/1	0.71	0.30	68,68,68,68	0
54	MG	1A	3310	1/1	0.72	0.09	77,77,77,77	0
54	MG	1a	1623	1/1	0.72	0.21	57,57,57,57	0
54	MG	1A	3090	1/1	0.72	0.28	46,46,46,46	0
54	MG	2A	3556	1/1	0.72	0.21	48,48,48,48	0
54	MG	2a	3003	1/1	0.72	0.20	69,69,69,69	0
54	MG	2A	3407	1/1	0.72	0.14	65,65,65,65	0
54	MG	2A	3237	1/1	0.72	0.17	42,42,42,42	0
54	MG	1A	3964	1/1	0.72	0.12	68,68,68,68	0
54	MG	1A	4024	1/1	0.72	0.19	69,69,69,69	0
54	MG	2a	3150	1/1	0.72	0.10	69,69,69,69	0
54	MG	1i	201	1/1	0.72	0.12	70,70,70,70	0
58	ARG	1F	318	12/12	0.72	0.27	60,69,76,80	0
54	MG	2A	3520	1/1	0.73	0.21	54,54,54,54	0
54	MG	1A	3669	1/1	0.73	0.16	35,35,35,35	0
54	MG	2A	3091	1/1	0.73	0.16	57,57,57,57	0
54	MG	2A	3371	1/1	0.73	0.23	71,71,71,71	0
54	MG	1a	1604	1/1	0.73	0.17	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3400	1/1	0.73	0.14	72,72,72,72	0
54	MG	1a	1683	1/1	0.73	0.17	83,83,83,83	0
54	MG	1a	1620	1/1	0.73	0.20	56,56,56,56	0
54	MG	1A	3961	1/1	0.73	0.31	64,64,64,64	0
54	MG	1A	3061	1/1	0.73	0.18	67,67,67,67	0
54	MG	2a	3102	1/1	0.73	0.10	63,63,63,63	0
54	MG	1A	3590	1/1	0.73	0.18	51,51,51,51	0
54	MG	2a	3118	1/1	0.73	0.08	77,77,77,77	0
54	MG	2a	3119	1/1	0.73	0.18	68,68,68,68	0
54	MG	1A	3256	1/1	0.73	0.30	60,60,60,60	0
54	MG	1A	3165	1/1	0.73	0.26	73,73,73,73	0
54	MG	1a	1823	1/1	0.73	0.17	86,86,86,86	0
54	MG	1A	3661	1/1	0.73	0.09	64,64,64,64	0
54	MG	1B	225	1/1	0.74	0.14	74,74,74,74	0
54	MG	1a	1615	1/1	0.74	0.11	63,63,63,63	0
54	MG	2A	3425	1/1	0.74	0.19	70,70,70,70	0
54	MG	2A	3201	1/1	0.74	0.22	71,71,71,71	0
54	MG	1a	1858	1/1	0.74	0.09	66,66,66,66	0
54	MG	1a	1667	1/1	0.74	0.16	79,79,79,79	0
54	MG	2A	3616	1/1	0.74	0.17	53,53,53,53	0
54	MG	1D	314	1/1	0.74	0.30	70,70,70,70	0
54	MG	2B	212	1/1	0.74	0.11	69,69,69,69	0
54	MG	1A	3465	1/1	0.74	0.10	43,43,43,43	0
54	MG	20	102	1/1	0.74	0.22	69,69,69,69	0
54	MG	1R	203	1/1	0.74	0.22	48,48,48,48	0
54	MG	2a	3131	1/1	0.74	0.27	66,66,66,66	0
54	MG	1A	3609	1/1	0.74	0.09	37,37,37,37	0
54	MG	1A	3998	1/1	0.74	0.28	52,52,52,52	0
54	MG	1A	3711	1/1	0.74	0.21	59,59,59,59	0
54	MG	2h	201	1/1	0.74	0.13	74,74,74,74	0
54	MG	1a	1659	1/1	0.74	0.10	72,72,72,72	0
54	MG	1a	1785	1/1	0.75	0.12	79,79,79,79	0
54	MG	2A	3218	1/1	0.75	0.26	63,63,63,63	0
54	MG	2A	3087	1/1	0.75	0.27	63,63,63,63	0
54	MG	1A	3884	1/1	0.75	0.24	52,52,52,52	0
54	MG	2A	3299	1/1	0.75	0.15	80,80,80,80	0
54	MG	1a	1622	1/1	0.75	0.33	62,62,62,62	0
54	MG	1a	1854	1/1	0.75	0.15	67,67,67,67	0
54	MG	1A	3355	1/1	0.75	0.15	70,70,70,70	0
54	MG	1a	1859	1/1	0.75	0.10	69,69,69,69	0
54	MG	2A	3543	1/1	0.75	0.08	70,70,70,70	0
54	MG	1a	1601	1/1	0.75	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3034	1/1	0.75	0.13	68,68,68,68	0
54	MG	1A	3570	1/1	0.75	0.20	59,59,59,59	0
54	MG	2a	3053	1/1	0.75	0.14	63,63,63,63	0
54	MG	2a	3166	1/1	0.75	0.30	90,90,90,90	0
54	MG	2a	3170	1/1	0.75	0.15	69,69,69,69	0
54	MG	1A	3201	1/1	0.75	0.24	56,56,56,56	0
54	MG	2A	3413	1/1	0.75	0.24	72,72,72,72	0
54	MG	1A	3288	1/1	0.76	0.17	61,61,61,61	0
54	MG	2a	3090	1/1	0.76	0.09	69,69,69,69	0
54	MG	1A	3012	1/1	0.76	0.24	42,42,42,42	0
54	MG	2A	3554	1/1	0.76	0.11	81,81,81,81	0
54	MG	2a	3099	1/1	0.76	0.50	70,70,70,70	0
54	MG	2A	3166	1/1	0.76	0.18	64,64,64,64	0
54	MG	2A	3273	1/1	0.76	0.27	43,43,43,43	0
54	MG	1A	3585	1/1	0.76	0.18	47,47,47,47	0
54	MG	2a	3028	1/1	0.76	0.22	74,74,74,74	0
54	MG	2a	3035	1/1	0.76	0.15	66,66,66,66	0
54	MG	1A	3875	1/1	0.76	0.17	44,44,44,44	0
54	MG	1A	3327	1/1	0.76	0.17	68,68,68,68	0
54	MG	2a	3048	1/1	0.76	0.10	71,71,71,71	0
54	MG	2A	3192	1/1	0.76	0.13	65,65,65,65	0
54	MG	2A	3495	1/1	0.76	0.46	73,73,73,73	0
54	MG	2A	3032	1/1	0.76	0.29	63,63,63,63	0
54	MG	1a	1674	1/1	0.76	0.31	61,61,61,61	0
54	MG	2A	3212	1/1	0.76	0.17	60,60,60,60	0
54	MG	2A	3105	1/1	0.77	0.17	53,53,53,53	0
54	MG	1a	1634	1/1	0.77	0.33	78,78,78,78	0
54	MG	1a	1847	1/1	0.77	0.09	63,63,63,63	0
54	MG	1B	208	1/1	0.77	0.19	64,64,64,64	0
54	MG	1B	222	1/1	0.77	0.09	55,55,55,55	0
54	MG	1A	3944	1/1	0.77	0.16	50,50,50,50	0
54	MG	2A	3461	1/1	0.77	0.09	76,76,76,76	0
54	MG	1A	3808	1/1	0.77	0.21	62,62,62,62	0
54	MG	1A	3450	1/1	0.77	0.23	56,56,56,56	0
54	MG	1A	3166	1/1	0.77	0.17	66,66,66,66	0
54	MG	1T	202	1/1	0.77	0.10	75,75,75,75	0
54	MG	2a	3070	1/1	0.77	0.28	71,71,71,71	0
54	MG	1A	3196	1/1	0.77	0.33	64,64,64,64	0
54	MG	2A	3203	1/1	0.77	0.09	67,67,67,67	0
54	MG	2a	3078	1/1	0.77	0.21	68,68,68,68	0
54	MG	1A	3693	1/1	0.77	0.11	69,69,69,69	0
54	MG	15	104	1/1	0.77	0.22	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3874	1/1	0.77	0.14	47,47,47,47	0
54	MG	1a	1688	1/1	0.77	0.14	72,72,72,72	0
54	MG	2A	3559	1/1	0.77	0.10	63,63,63,63	0
54	MG	1A	3656	1/1	0.77	0.33	49,49,49,49	0
54	MG	1A	3011	1/1	0.77	0.25	55,55,55,55	0
54	MG	1A	3742	1/1	0.77	0.13	60,60,60,60	0
54	MG	1a	1619	1/1	0.77	0.10	71,71,71,71	0
54	MG	1A	4023	1/1	0.77	0.16	70,70,70,70	0
54	MG	1A	3798	1/1	0.77	0.21	65,65,65,65	0
54	MG	2a	3146	1/1	0.77	0.19	81,81,81,81	0
54	MG	2A	3375	1/1	0.77	0.21	68,68,68,68	0
54	MG	2A	3383	1/1	0.77	0.19	62,62,62,62	0
54	MG	2A	3663	1/1	0.77	0.20	58,58,58,58	0
54	MG	2A	3391	1/1	0.77	0.15	60,60,60,60	0
54	MG	2A	3085	1/1	0.77	0.23	64,64,64,64	0
54	MG	2a	3187	1/1	0.77	0.20	73,73,73,73	0
54	MG	1a	1790	1/1	0.77	0.11	75,75,75,75	0
54	MG	2l	201	1/1	0.77	0.22	72,72,72,72	0
54	MG	1A	3190	1/1	0.77	0.10	84,84,84,84	0
54	MG	1a	1631	1/1	0.78	0.30	62,62,62,62	0
54	MG	1A	3651	1/1	0.78	0.20	45,45,45,45	0
54	MG	1A	3994	1/1	0.78	0.12	60,60,60,60	0
54	MG	1a	1645	1/1	0.78	0.12	64,64,64,64	0
54	MG	2A	3410	1/1	0.78	0.09	67,67,67,67	0
54	MG	1A	3153	1/1	0.78	0.18	67,67,67,67	0
54	MG	1a	1696	1/1	0.78	0.21	80,80,80,80	0
54	MG	1a	1699	1/1	0.78	0.17	69,69,69,69	0
54	MG	2A	3451	1/1	0.78	0.26	62,62,62,62	0
54	MG	1a	1880	1/1	0.78	0.20	74,74,74,74	0
54	MG	1A	3086	1/1	0.78	0.37	40,40,40,40	0
54	MG	2A	3465	1/1	0.78	0.24	70,70,70,70	0
54	MG	1a	1657	1/1	0.78	0.29	61,61,61,61	0
54	MG	1a	1716	1/1	0.78	0.24	54,54,54,54	0
54	MG	2a	3009	1/1	0.78	0.08	66,66,66,66	0
54	MG	2A	3486	1/1	0.78	0.17	69,69,69,69	0
54	MG	2A	3305	1/1	0.78	0.20	56,56,56,56	0
54	MG	2A	3306	1/1	0.78	0.13	79,79,79,79	0
54	MG	2A	3128	1/1	0.78	0.09	61,61,61,61	0
54	MG	1A	3473	1/1	0.78	0.14	58,58,58,58	0
54	MG	1A	3807	1/1	0.78	0.23	61,61,61,61	0
54	MG	1A	3973	1/1	0.78	0.14	71,71,71,71	0
54	MG	1A	3701	1/1	0.78	0.14	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3217	1/1	0.78	0.33	62,62,62,62	0
54	MG	2A	3181	1/1	0.78	0.22	64,64,64,64	0
54	MG	1A	3394	1/1	0.79	0.13	72,72,72,72	0
54	MG	1a	1720	1/1	0.79	0.31	82,82,82,82	0
54	MG	2a	3069	1/1	0.79	0.27	71,71,71,71	0
54	MG	1A	3910	1/1	0.79	0.09	52,52,52,52	0
54	MG	1a	1739	1/1	0.79	0.22	48,48,48,48	0
54	MG	2A	3572	1/1	0.79	0.14	61,61,61,61	0
54	MG	1A	3311	1/1	0.79	0.20	49,49,49,49	0
54	MG	2A	3199	1/1	0.79	0.24	70,70,70,70	0
54	MG	1A	3935	1/1	0.79	0.26	64,64,64,64	0
54	MG	1A	3317	1/1	0.79	0.19	41,41,41,41	0
54	MG	1A	3222	1/1	0.79	0.10	71,71,71,71	0
54	MG	2A	3629	1/1	0.79	0.18	39,39,39,39	0
54	MG	2a	3100	1/1	0.79	0.12	68,68,68,68	0
54	MG	2A	3649	1/1	0.79	0.21	56,56,56,56	0
54	MG	1a	1815	1/1	0.79	0.23	79,79,79,79	0
54	MG	1A	3458	1/1	0.79	0.12	44,44,44,44	0
54	MG	1A	3966	1/1	0.79	0.10	54,54,54,54	0
54	MG	1A	3307	1/1	0.79	0.20	52,52,52,52	0
54	MG	1A	3603	1/1	0.79	0.23	74,74,74,74	0
54	MG	2a	3132	1/1	0.79	0.34	67,67,67,67	0
54	MG	2a	3136	1/1	0.79	0.13	76,76,76,76	0
54	MG	1F	316	1/1	0.79	0.46	59,59,59,59	0
54	MG	1a	1632	1/1	0.79	0.19	60,60,60,60	0
54	MG	1a	1693	1/1	0.79	0.23	72,72,72,72	0
54	MG	2A	3126	1/1	0.79	0.29	66,66,66,66	0
54	MG	1A	3141	1/1	0.79	0.16	55,55,55,55	0
54	MG	2a	3169	1/1	0.79	0.09	86,86,86,86	0
54	MG	1A	3080	1/1	0.79	0.23	70,70,70,70	0
54	MG	1A	3359	1/1	0.79	0.16	41,41,41,41	0
54	MG	2A	3379	1/1	0.79	0.15	64,64,64,64	0
54	MG	2A	3163	1/1	0.79	0.17	65,65,65,65	0
54	MG	1A	3384	1/1	0.79	0.16	43,43,43,43	0
54	MG	2A	3111	1/1	0.80	0.19	60,60,60,60	0
54	MG	1A	3454	1/1	0.80	0.20	78,78,78,78	0
54	MG	1A	3252	1/1	0.80	0.47	52,52,52,52	0
54	MG	2A	3005	1/1	0.80	0.38	63,63,63,63	0
54	MG	2A	3276	1/1	0.80	0.27	70,70,70,70	0
54	MG	2A	3456	1/1	0.80	0.45	66,66,66,66	0
54	MG	2a	3086	1/1	0.80	0.19	74,74,74,74	0
54	MG	2A	3297	1/1	0.80	0.10	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3809	1/1	0.80	0.14	53,53,53,53	0
54	MG	1A	3335	1/1	0.80	0.28	60,60,60,60	0
54	MG	2A	3668	1/1	0.80	0.44	77,77,77,77	0
54	MG	1W	202	1/1	0.80	0.17	45,45,45,45	0
54	MG	2A	3355	1/1	0.80	0.38	59,59,59,59	0
54	MG	2A	3478	1/1	0.80	0.17	68,68,68,68	0
54	MG	2T	203	1/1	0.80	0.09	77,77,77,77	0
54	MG	2a	3117	1/1	0.80	0.11	78,78,78,78	0
54	MG	2A	3045	1/1	0.80	0.15	68,68,68,68	0
54	MG	1A	3795	1/1	0.80	0.19	62,62,62,62	0
54	MG	2a	3007	1/1	0.80	0.15	62,62,62,62	0
54	MG	1A	3990	1/1	0.80	0.15	50,50,50,50	0
54	MG	2a	3012	1/1	0.80	0.31	70,70,70,70	0
54	MG	2a	3145	1/1	0.80	0.11	75,75,75,75	0
54	MG	1a	1876	1/1	0.80	0.14	71,71,71,71	0
54	MG	1A	3448	1/1	0.80	0.21	36,36,36,36	0
54	MG	1A	3803	1/1	0.80	0.15	69,69,69,69	0
54	MG	1A	3058	1/1	0.80	0.16	62,62,62,62	0
54	MG	2A	3393	1/1	0.80	0.17	72,72,72,72	0
54	MG	1B	227	1/1	0.80	0.16	76,76,76,76	0
54	MG	1a	1806	1/1	0.80	0.14	72,72,72,72	0
54	MG	2A	3211	1/1	0.80	0.19	73,73,73,73	0
54	MG	1A	3947	1/1	0.80	0.09	67,67,67,67	0
54	MG	2a	3067	1/1	0.80	0.09	78,78,78,78	0
57	MPD	2A	3673	8/8	0.80	0.36	45,57,63,63	0
54	MG	2A	3216	1/1	0.80	0.30	61,61,61,61	0
54	MG	1A	3951	1/1	0.81	0.19	62,62,62,62	0
54	MG	1B	204	1/1	0.81	0.21	63,63,63,63	0
54	MG	1A	3745	1/1	0.81	0.09	58,58,58,58	0
54	MG	1a	1820	1/1	0.81	0.13	72,72,72,72	0
54	MG	2A	3253	1/1	0.81	0.18	74,74,74,74	0
54	MG	2A	3271	1/1	0.81	0.10	54,54,54,54	0
54	MG	1A	3762	1/1	0.81	0.17	52,52,52,52	0
54	MG	1a	1837	1/1	0.81	0.12	83,83,83,83	0
54	MG	1a	1840	1/1	0.81	0.16	83,83,83,83	0
54	MG	1A	3788	1/1	0.81	0.23	34,34,34,34	0
54	MG	1A	3607	1/1	0.81	0.21	68,68,68,68	0
54	MG	2A	3102	1/1	0.81	0.26	59,59,59,59	0
54	MG	2A	3347	1/1	0.81	0.24	64,64,64,64	0
54	MG	1a	1855	1/1	0.81	0.15	82,82,82,82	0
54	MG	1a	1856	1/1	0.81	0.14	59,59,59,59	0
54	MG	2A	3360	1/1	0.81	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3211	1/1	0.81	0.33	57,57,57,57	0
54	MG	2A	3586	1/1	0.81	0.14	54,54,54,54	0
54	MG	1A	3985	1/1	0.81	0.17	65,65,65,65	0
54	MG	1A	3697	1/1	0.81	0.11	54,54,54,54	0
54	MG	1a	1700	1/1	0.81	0.31	78,78,78,78	0
54	MG	2a	3106	1/1	0.81	0.16	76,76,76,76	0
54	MG	2A	3603	1/1	0.81	0.33	79,79,79,79	0
54	MG	2A	3140	1/1	0.81	0.40	56,56,56,56	0
54	MG	1a	1874	1/1	0.81	0.08	76,76,76,76	0
54	MG	1A	3646	1/1	0.81	0.17	48,48,48,48	0
54	MG	2A	3155	1/1	0.81	0.14	55,55,55,55	0
54	MG	1A	3900	1/1	0.81	0.16	57,57,57,57	0
54	MG	1A	3529	1/1	0.81	0.18	52,52,52,52	0
54	MG	1A	3679	1/1	0.81	0.15	55,55,55,55	0
54	MG	1A	3726	1/1	0.81	0.14	63,63,63,63	0
54	MG	1A	3941	1/1	0.81	0.13	65,65,65,65	0
54	MG	1A	4014	1/1	0.81	0.20	53,53,53,53	0
54	MG	1A	3731	1/1	0.81	0.16	73,73,73,73	0
54	MG	2a	3161	1/1	0.81	0.08	80,80,80,80	0
54	MG	1a	1787	1/1	0.81	0.19	78,78,78,78	0
54	MG	2A	3003	1/1	0.81	0.26	67,67,67,67	0
54	MG	1a	1788	1/1	0.81	0.10	88,88,88,88	0
54	MG	2A	3006	1/1	0.81	0.14	57,57,57,57	0
54	MG	2A	3016	1/1	0.81	0.17	73,73,73,73	0
54	MG	1A	3130	1/1	0.81	0.21	50,50,50,50	0
54	MG	2a	3033	1/1	0.81	0.09	79,79,79,79	0
54	MG	2A	3215	1/1	0.81	0.29	77,77,77,77	0
54	MG	2a	3064	1/1	0.82	0.13	83,83,83,83	0
54	MG	1A	3180	1/1	0.82	0.13	70,70,70,70	0
54	MG	1a	1624	1/1	0.82	0.10	56,56,56,56	0
54	MG	2A	3019	1/1	0.82	0.49	58,58,58,58	0
54	MG	1A	3664	1/1	0.82	0.31	58,58,58,58	0
54	MG	1A	3345	1/1	0.82	0.22	59,59,59,59	0
54	MG	1A	3671	1/1	0.82	0.19	69,69,69,69	0
54	MG	2A	3587	1/1	0.82	0.26	64,64,64,64	0
54	MG	2A	3046	1/1	0.82	0.21	66,66,66,66	0
54	MG	1A	3672	1/1	0.82	0.19	37,37,37,37	0
54	MG	2A	3055	1/1	0.82	0.43	63,63,63,63	0
54	MG	1A	3786	1/1	0.82	0.16	59,59,59,59	0
54	MG	1A	3422	1/1	0.82	0.23	55,55,55,55	0
54	MG	2A	3084	1/1	0.82	0.15	60,60,60,60	0
54	MG	2A	3421	1/1	0.82	0.12	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1725	1/1	0.82	0.24	61,61,61,61	0
54	MG	2A	3433	1/1	0.82	0.17	73,73,73,73	0
54	MG	1A	3324	1/1	0.82	0.20	62,62,62,62	0
54	MG	1A	3549	1/1	0.82	0.17	64,64,64,64	0
54	MG	1A	3620	1/1	0.82	0.19	71,71,71,71	0
54	MG	1A	3631	1/1	0.82	0.13	36,36,36,36	0
54	MG	1A	3805	1/1	0.82	0.14	47,47,47,47	0
54	MG	1A	3035	1/1	0.82	0.30	54,54,54,54	0
54	MG	2a	3006	1/1	0.82	0.34	75,75,75,75	0
54	MG	1A	3575	1/1	0.82	0.14	68,68,68,68	0
54	MG	2a	3008	1/1	0.82	0.23	65,65,65,65	0
54	MG	2A	3285	1/1	0.82	0.24	43,43,43,43	0
54	MG	1a	1613	1/1	0.82	0.12	68,68,68,68	0
54	MG	1a	1804	1/1	0.82	0.15	70,70,70,70	0
54	MG	2A	3139	1/1	0.82	0.18	57,57,57,57	0
54	MG	1A	3584	1/1	0.82	0.33	45,45,45,45	0
54	MG	1t	201	1/1	0.82	0.22	62,62,62,62	0
54	MG	2A	3350	1/1	0.82	0.09	66,66,66,66	0
54	MG	1A	3032	1/1	0.82	0.21	57,57,57,57	0
54	MG	1a	1817	1/1	0.82	0.21	84,84,84,84	0
54	MG	2e	201	1/1	0.82	0.29	76,76,76,76	0
54	MG	2A	3158	1/1	0.82	0.13	56,56,56,56	0
54	MG	1A	3725	1/1	0.82	0.23	56,56,56,56	0
54	MG	1A	3848	1/1	0.82	0.17	44,44,44,44	0
54	MG	2a	3059	1/1	0.82	0.14	74,74,74,74	0
54	MG	1A	3719	1/1	0.83	0.14	59,59,59,59	0
54	MG	1A	3897	1/1	0.83	0.20	58,58,58,58	0
54	MG	2A	3311	1/1	0.83	0.17	56,56,56,56	0
54	MG	2A	3318	1/1	0.83	0.23	44,44,44,44	0
54	MG	2A	3320	1/1	0.83	0.34	76,76,76,76	0
54	MG	2A	3534	1/1	0.83	0.26	42,42,42,42	0
54	MG	2A	3537	1/1	0.83	0.10	72,72,72,72	0
54	MG	1A	3333	1/1	0.83	0.18	37,37,37,37	0
54	MG	1A	3195	1/1	0.83	0.19	59,59,59,59	0
54	MG	2A	3157	1/1	0.83	0.22	51,51,51,51	0
54	MG	1A	3925	1/1	0.83	0.12	45,45,45,45	0
54	MG	1a	1673	1/1	0.83	0.14	63,63,63,63	0
54	MG	1a	1813	1/1	0.83	0.12	70,70,70,70	0
54	MG	2A	3173	1/1	0.83	0.13	61,61,61,61	0
54	MG	2a	3079	1/1	0.83	0.08	76,76,76,76	0
54	MG	2a	3080	1/1	0.83	0.42	57,57,57,57	0
54	MG	1A	3495	1/1	0.83	0.20	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3930	1/1	0.83	0.08	61,61,61,61	0
54	MG	1a	1606	1/1	0.83	0.14	66,66,66,66	0
54	MG	1A	3734	1/1	0.83	0.09	74,74,74,74	0
54	MG	2A	3043	1/1	0.83	0.57	84,84,84,84	0
54	MG	1a	1689	1/1	0.83	0.17	73,73,73,73	0
54	MG	1A	3649	1/1	0.83	0.34	68,68,68,68	0
54	MG	1A	3294	1/1	0.83	0.13	69,69,69,69	0
54	MG	2A	3608	1/1	0.83	0.13	67,67,67,67	0
54	MG	1A	3846	1/1	0.83	0.14	41,41,41,41	0
54	MG	2a	3107	1/1	0.83	0.15	71,71,71,71	0
54	MG	2a	3109	1/1	0.83	0.19	62,62,62,62	0
54	MG	2a	3115	1/1	0.83	0.14	68,68,68,68	0
54	MG	1a	1698	1/1	0.83	0.12	75,75,75,75	0
54	MG	1A	3400	1/1	0.83	0.14	64,64,64,64	0
54	MG	2A	3657	1/1	0.83	0.22	58,58,58,58	0
54	MG	1A	3954	1/1	0.83	0.22	47,47,47,47	0
54	MG	1A	3403	1/1	0.83	0.19	33,33,33,33	0
54	MG	2A	3422	1/1	0.83	0.26	79,79,79,79	0
54	MG	1A	3963	1/1	0.83	0.13	67,67,67,67	0
54	MG	1a	1715	1/1	0.83	0.26	76,76,76,76	0
54	MG	2A	3435	1/1	0.83	0.11	78,78,78,78	0
54	MG	1A	3866	1/1	0.83	0.15	56,56,56,56	0
54	MG	2A	3248	1/1	0.83	0.36	65,65,65,65	0
54	MG	2a	3004	1/1	0.83	0.24	57,57,57,57	0
54	MG	1A	3606	1/1	0.83	0.17	49,49,49,49	0
54	MG	1A	3663	1/1	0.83	0.31	58,58,58,58	0
54	MG	2A	3272	1/1	0.83	0.16	52,52,52,52	0
54	MG	1A	3797	1/1	0.83	0.15	59,59,59,59	0
54	MG	1A	3247	1/1	0.83	0.24	60,60,60,60	0
54	MG	1a	1767	1/1	0.83	0.10	80,80,80,80	0
54	MG	1A	3172	1/1	0.83	0.39	55,55,55,55	0
54	MG	1V	205	1/1	0.83	0.17	67,67,67,67	0
54	MG	2A	3487	1/1	0.83	0.08	71,71,71,71	0
54	MG	2A	3494	1/1	0.83	0.11	74,74,74,74	0
54	MG	2A	3448	1/1	0.84	0.16	66,66,66,66	0
54	MG	2A	3618	1/1	0.84	0.10	67,67,67,67	0
54	MG	1a	1694	1/1	0.84	0.23	84,84,84,84	0
54	MG	2A	3029	1/1	0.84	0.29	52,52,52,52	0
54	MG	1A	3965	1/1	0.84	0.15	65,65,65,65	0
54	MG	1A	3433	1/1	0.84	0.21	29,29,29,29	0
54	MG	1D	313	1/1	0.84	0.47	74,74,74,74	0
54	MG	2A	3326	1/1	0.84	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3044	1/1	0.84	0.17	53,53,53,53	0
54	MG	1A	3435	1/1	0.84	0.17	79,79,79,79	0
54	MG	1A	3440	1/1	0.84	0.22	43,43,43,43	0
54	MG	1A	3909	1/1	0.84	0.14	63,63,63,63	0
54	MG	1Q	205	1/1	0.84	0.20	54,54,54,54	0
54	MG	1A	3988	1/1	0.84	0.16	60,60,60,60	0
54	MG	2A	3368	1/1	0.84	0.19	66,66,66,66	0
54	MG	1a	1719	1/1	0.84	0.16	74,74,74,74	0
54	MG	2A	3208	1/1	0.84	0.13	56,56,56,56	0
54	MG	1A	3283	1/1	0.84	0.83	57,57,57,57	0
54	MG	1A	3329	1/1	0.84	0.13	60,60,60,60	0
54	MG	1A	3260	1/1	0.84	0.17	50,50,50,50	0
54	MG	1A	3108	1/1	0.84	0.24	35,35,35,35	0
54	MG	2A	3396	1/1	0.84	0.08	71,71,71,71	0
54	MG	1A	3763	1/1	0.84	0.36	67,67,67,67	0
54	MG	2a	3139	1/1	0.84	0.11	67,67,67,67	0
54	MG	1A	3274	1/1	0.84	0.30	62,62,62,62	0
54	MG	2A	3562	1/1	0.84	0.10	88,88,88,88	0
54	MG	1A	3864	1/1	0.84	0.17	63,63,63,63	0
54	MG	1A	3110	1/1	0.84	0.31	48,48,48,48	0
54	MG	1A	3699	1/1	0.84	0.18	67,67,67,67	0
54	MG	2a	3056	1/1	0.84	0.24	69,69,69,69	0
54	MG	1A	3952	1/1	0.84	0.19	52,52,52,52	0
54	MG	1a	1680	1/1	0.84	0.23	55,55,55,55	0
54	MG	1A	3469	1/1	0.84	0.14	60,60,60,60	0
54	MG	1A	3957	1/1	0.84	0.12	33,33,33,33	0
54	MG	1A	3472	1/1	0.84	0.23	58,58,58,58	0
54	MG	1a	1690	1/1	0.84	0.28	73,73,73,73	0
54	MG	1A	3002	1/1	0.84	0.19	52,52,52,52	0
54	MG	2n	101	1/1	0.84	0.09	78,78,78,78	0
57	MPD	1a	1882	8/8	0.84	0.17	62,65,70,72	0
54	MG	1A	3357	1/1	0.84	0.12	56,56,56,56	0
54	MG	2A	3444	1/1	0.84	0.27	74,74,74,74	0
54	MG	1A	3960	1/1	0.85	0.12	58,58,58,58	0
54	MG	2A	3123	1/1	0.85	0.21	43,43,43,43	0
54	MG	1d	301	1/1	0.85	0.32	78,78,78,78	0
54	MG	2a	3046	1/1	0.85	0.15	81,81,81,81	0
54	MG	1A	3293	1/1	0.85	0.10	71,71,71,71	0
54	MG	2a	3049	1/1	0.85	0.12	75,75,75,75	0
54	MG	2A	3324	1/1	0.85	0.17	53,53,53,53	0
54	MG	1a	1753	1/1	0.85	0.14	79,79,79,79	0
54	MG	1a	1758	1/1	0.85	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
54	MG	2a	3058	1/1	0.85	0.16	58,58,58,58	0
54	MG	1h	201	1/1	0.85	0.35	66,66,66,66	0
54	MG	2a	3062	1/1	0.85	0.19	84,84,84,84	0
54	MG	1A	4019	1/1	0.85	0.17	49,49,49,49	0
54	MG	1A	3962	1/1	0.85	0.14	51,51,51,51	0
54	MG	1a	1774	1/1	0.85	0.16	66,66,66,66	0
54	MG	1A	3250	1/1	0.85	0.20	41,41,41,41	0
54	MG	1A	3657	1/1	0.85	0.18	60,60,60,60	0
54	MG	2A	3565	1/1	0.85	0.17	58,58,58,58	0
54	MG	2a	3073	1/1	0.85	0.17	62,62,62,62	0
54	MG	2A	3369	1/1	0.85	0.20	59,59,59,59	0
54	MG	1A	3660	1/1	0.85	0.12	65,65,65,65	0
54	MG	1A	3927	1/1	0.85	0.21	34,34,34,34	0
54	MG	1a	1796	1/1	0.85	0.10	65,65,65,65	0
54	MG	1a	1800	1/1	0.85	0.15	68,68,68,68	0
54	MG	1B	209	1/1	0.85	0.28	71,71,71,71	0
54	MG	2A	3183	1/1	0.85	0.33	54,54,54,54	0
54	MG	2A	3588	1/1	0.85	0.14	53,53,53,53	0
54	MG	1a	1684	1/1	0.85	0.16	81,81,81,81	0
54	MG	1A	3737	1/1	0.85	0.16	57,57,57,57	0
54	MG	1B	224	1/1	0.85	0.13	56,56,56,56	0
54	MG	1A	3800	1/1	0.85	0.17	66,66,66,66	0
54	MG	2A	3037	1/1	0.85	0.09	83,83,83,83	0
54	MG	2a	3103	1/1	0.85	0.14	74,74,74,74	0
54	MG	2a	3105	1/1	0.85	0.16	72,72,72,72	0
54	MG	2A	3406	1/1	0.85	0.18	38,38,38,38	0
54	MG	1A	3010	1/1	0.85	0.20	67,67,67,67	0
54	MG	2A	3622	1/1	0.85	0.27	64,64,64,64	0
54	MG	1A	3132	1/1	0.85	0.10	70,70,70,70	0
54	MG	2A	3630	1/1	0.85	0.26	50,50,50,50	0
54	MG	2A	3643	1/1	0.85	0.08	76,76,76,76	0
54	MG	2A	3648	1/1	0.85	0.14	70,70,70,70	0
54	MG	1a	1821	1/1	0.85	0.14	72,72,72,72	0
54	MG	1A	3393	1/1	0.85	0.11	57,57,57,57	0
54	MG	2A	3660	1/1	0.85	0.19	75,75,75,75	0
54	MG	2a	3133	1/1	0.85	0.24	79,79,79,79	0
54	MG	1F	313	1/1	0.85	0.16	45,45,45,45	0
54	MG	1A	3720	1/1	0.85	0.13	54,54,54,54	0
54	MG	2A	3058	1/1	0.85	0.20	51,51,51,51	0
54	MG	2A	3064	1/1	0.85	0.25	48,48,48,48	0
54	MG	1G	201	1/1	0.85	0.13	73,73,73,73	0
54	MG	2Q	203	1/1	0.85	0.49	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3949	1/1	0.85	0.17	37,37,37,37	0
54	MG	1P	204	1/1	0.85	0.17	52,52,52,52	0
54	MG	1a	1646	1/1	0.85	0.13	65,65,65,65	0
54	MG	2a	3167	1/1	0.85	0.10	64,64,64,64	0
54	MG	1a	1703	1/1	0.85	0.26	75,75,75,75	0
54	MG	1A	3765	1/1	0.85	0.15	58,58,58,58	0
54	MG	1A	3772	1/1	0.85	0.23	53,53,53,53	0
54	MG	2A	3277	1/1	0.85	0.23	40,40,40,40	0
54	MG	2f	201	1/1	0.85	0.22	51,51,51,51	0
54	MG	2A	3282	1/1	0.85	0.13	48,48,48,48	0
54	MG	1a	1650	1/1	0.85	0.23	52,52,52,52	0
54	MG	1A	3836	1/1	0.85	0.07	60,60,60,60	0
54	MG	1A	3837	1/1	0.85	0.15	57,57,57,57	0
54	MG	2A	3110	1/1	0.85	0.30	62,62,62,62	0
54	MG	2A	3489	1/1	0.85	0.07	76,76,76,76	0
59	ZN	24	501	1/1	0.85	0.17	121,121,121,121	0
54	MG	1a	1661	1/1	0.86	0.38	70,70,70,70	0
54	MG	1A	3342	1/1	0.86	0.19	52,52,52,52	0
54	MG	1e	201	1/1	0.86	0.27	52,52,52,52	0
54	MG	2A	3339	1/1	0.86	0.12	71,71,71,71	0
54	MG	2A	3530	1/1	0.86	0.17	54,54,54,54	0
54	MG	1a	1759	1/1	0.86	0.17	66,66,66,66	0
54	MG	11	106	1/1	0.86	0.17	40,40,40,40	0
54	MG	2a	3054	1/1	0.86	0.18	68,68,68,68	0
54	MG	2A	3540	1/1	0.86	0.14	48,48,48,48	0
54	MG	1g	202	1/1	0.86	0.11	69,69,69,69	0
54	MG	1A	3411	1/1	0.86	0.18	31,31,31,31	0
54	MG	1A	3312	1/1	0.86	0.25	38,38,38,38	0
54	MG	2a	3060	1/1	0.86	0.11	71,71,71,71	0
54	MG	2a	3061	1/1	0.86	0.11	78,78,78,78	0
54	MG	1a	1778	1/1	0.86	0.08	86,86,86,86	0
54	MG	19	102	1/1	0.86	0.14	71,71,71,71	0
54	MG	1A	3050	1/1	0.86	0.18	44,44,44,44	0
54	MG	1A	3430	1/1	0.86	0.16	43,43,43,43	0
54	MG	1A	3703	1/1	0.86	0.19	53,53,53,53	0
54	MG	2A	3378	1/1	0.86	0.14	49,49,49,49	0
54	MG	1A	3773	1/1	0.86	0.12	36,36,36,36	0
54	MG	2A	3573	1/1	0.86	0.25	64,64,64,64	0
54	MG	2A	3584	1/1	0.86	0.10	76,76,76,76	0
54	MG	1a	1687	1/1	0.86	0.30	73,73,73,73	0
54	MG	2A	3384	1/1	0.86	0.15	69,69,69,69	0
54	MG	1A	3781	1/1	0.86	0.16	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3197	1/1	0.86	0.23	73,73,73,73	0
54	MG	1A	3933	1/1	0.86	0.13	60,60,60,60	0
54	MG	2a	3087	1/1	0.86	0.24	80,80,80,80	0
54	MG	2a	3089	1/1	0.86	0.19	70,70,70,70	0
54	MG	1a	1807	1/1	0.86	0.21	57,57,57,57	0
54	MG	1A	3853	1/1	0.86	0.23	65,65,65,65	0
54	MG	1E	308	1/1	0.86	0.25	62,62,62,62	0
54	MG	1A	3939	1/1	0.86	0.23	54,54,54,54	0
54	MG	2A	3612	1/1	0.86	0.21	80,80,80,80	0
54	MG	1A	3156	1/1	0.86	0.17	61,61,61,61	0
54	MG	1A	3305	1/1	0.86	0.33	41,41,41,41	0
54	MG	1G	202	1/1	0.86	0.11	56,56,56,56	0
54	MG	1a	1829	1/1	0.86	0.12	66,66,66,66	0
54	MG	1a	1831	1/1	0.86	0.25	73,73,73,73	0
54	MG	1a	1833	1/1	0.86	0.14	63,63,63,63	0
54	MG	1A	3997	1/1	0.86	0.21	38,38,38,38	0
54	MG	1a	1839	1/1	0.86	0.26	61,61,61,61	0
54	MG	2A	3065	1/1	0.86	0.13	52,52,52,52	0
54	MG	2A	3437	1/1	0.86	0.16	75,75,75,75	0
54	MG	1a	1644	1/1	0.86	0.13	70,70,70,70	0
54	MG	1N	204	1/1	0.86	0.15	62,62,62,62	0
54	MG	1A	3502	1/1	0.86	0.26	60,60,60,60	0
54	MG	2B	202	1/1	0.86	0.15	75,75,75,75	0
54	MG	2B	208	1/1	0.86	0.11	88,88,88,88	0
54	MG	1A	3208	1/1	0.86	0.38	67,67,67,67	0
54	MG	1A	3193	1/1	0.86	0.29	44,44,44,44	0
54	MG	2a	3141	1/1	0.86	0.28	78,78,78,78	0
54	MG	2B	214	1/1	0.86	0.17	71,71,71,71	0
54	MG	2F	302	1/1	0.86	0.18	55,55,55,55	0
54	MG	2O	3701	1/1	0.86	0.23	71,71,71,71	0
54	MG	1A	3014	1/1	0.86	0.30	63,63,63,63	0
54	MG	2a	3157	1/1	0.86	0.13	66,66,66,66	0
54	MG	2R	202	1/1	0.86	0.31	55,55,55,55	0
54	MG	2A	3460	1/1	0.86	0.14	64,64,64,64	0
54	MG	1a	1652	1/1	0.86	0.29	51,51,51,51	0
54	MG	2A	3463	1/1	0.86	0.18	59,59,59,59	0
54	MG	1A	3881	1/1	0.86	0.09	54,54,54,54	0
54	MG	2A	3287	1/1	0.86	0.18	41,41,41,41	0
54	MG	1A	3547	1/1	0.86	0.30	55,55,55,55	0
54	MG	1A	3185	1/1	0.86	0.25	56,56,56,56	0
54	MG	2A	3303	1/1	0.86	0.44	58,58,58,58	0
54	MG	1a	1875	1/1	0.86	0.18	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1742	1/1	0.86	0.08	64,64,64,64	0
54	MG	2a	3022	1/1	0.86	0.21	73,73,73,73	0
54	MG	2a	3024	1/1	0.86	0.35	68,68,68,68	0
54	MG	2A	3114	1/1	0.86	0.20	74,74,74,74	0
54	MG	1a	1743	1/1	0.86	0.16	80,80,80,80	0
54	MG	2A	3499	1/1	0.86	0.23	52,52,52,52	0
54	MG	1A	3532	1/1	0.87	0.06	52,52,52,52	0
54	MG	2A	3232	1/1	0.87	0.30	58,58,58,58	0
54	MG	2A	3233	1/1	0.87	0.22	62,62,62,62	0
54	MG	1a	1662	1/1	0.87	0.17	68,68,68,68	0
54	MG	1A	4016	1/1	0.87	0.15	45,45,45,45	0
54	MG	1A	3938	1/1	0.87	0.14	59,59,59,59	0
54	MG	1A	3253	1/1	0.87	0.33	49,49,49,49	0
54	MG	1a	1670	1/1	0.87	0.36	69,69,69,69	0
54	MG	2A	3544	1/1	0.87	0.11	51,51,51,51	0
54	MG	2A	3552	1/1	0.87	0.07	79,79,79,79	0
54	MG	1a	1736	1/1	0.87	0.18	58,58,58,58	0
54	MG	2A	3011	1/1	0.87	0.29	43,43,43,43	0
54	MG	1G	203	1/1	0.87	0.34	77,77,77,77	0
54	MG	1A	3723	1/1	0.87	0.20	35,35,35,35	0
54	MG	1a	1621	1/1	0.87	0.28	67,67,67,67	0
54	MG	2A	3025	1/1	0.87	0.31	55,55,55,55	0
54	MG	1A	3850	1/1	0.87	0.24	64,64,64,64	0
54	MG	2A	3290	1/1	0.87	0.22	54,54,54,54	0
54	MG	1a	1756	1/1	0.87	0.22	65,65,65,65	0
54	MG	2a	3017	1/1	0.87	0.19	66,66,66,66	0
54	MG	2a	3111	1/1	0.87	0.20	69,69,69,69	0
54	MG	1A	3494	1/1	0.87	0.17	32,32,32,32	0
54	MG	1A	3601	1/1	0.87	0.22	52,52,52,52	0
54	MG	2A	3436	1/1	0.87	0.17	67,67,67,67	0
54	MG	1B	207	1/1	0.87	0.19	49,49,49,49	0
54	MG	1A	3779	1/1	0.87	0.17	29,29,29,29	0
54	MG	1A	3914	1/1	0.87	0.18	36,36,36,36	0
54	MG	1W	201	1/1	0.87	0.28	41,41,41,41	0
54	MG	2a	3037	1/1	0.87	0.12	68,68,68,68	0
54	MG	2a	3134	1/1	0.87	0.18	70,70,70,70	0
54	MG	1a	1691	1/1	0.87	0.20	61,61,61,61	0
54	MG	2a	3137	1/1	0.87	0.07	59,59,59,59	0
54	MG	1A	3915	1/1	0.87	0.11	61,61,61,61	0
54	MG	10	103	1/1	0.87	0.28	60,60,60,60	0
54	MG	10	105	1/1	0.87	0.10	47,47,47,47	0
54	MG	2A	3344	1/1	0.87	0.25	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3051	1/1	0.87	0.16	81,81,81,81	0
54	MG	2A	3187	1/1	0.87	0.36	64,64,64,64	0
54	MG	1A	3102	1/1	0.87	0.13	46,46,46,46	0
54	MG	2a	3055	1/1	0.87	0.13	68,68,68,68	0
54	MG	2A	3073	1/1	0.87	0.19	60,60,60,60	0
54	MG	1A	3100	1/1	0.87	0.16	62,62,62,62	0
54	MG	1A	3655	1/1	0.87	0.17	57,57,57,57	0
54	MG	2A	3633	1/1	0.87	0.21	70,70,70,70	0
54	MG	2A	3082	1/1	0.87	0.22	52,52,52,52	0
54	MG	2A	3366	1/1	0.87	0.28	66,66,66,66	0
54	MG	1B	228	1/1	0.87	0.06	65,65,65,65	0
54	MG	2a	3063	1/1	0.87	0.26	80,80,80,80	0
54	MG	2A	3651	1/1	0.87	0.10	65,65,65,65	0
54	MG	2j	201	1/1	0.87	0.40	86,86,86,86	0
54	MG	2A	3652	1/1	0.87	0.17	55,55,55,55	0
54	MG	1A	3999	1/1	0.87	0.22	34,34,34,34	0
57	MPD	1A	4028	8/8	0.87	0.17	50,52,60,64	0
54	MG	1A	3479	1/1	0.87	0.11	45,45,45,45	0
54	MG	2A	3662	1/1	0.87	0.27	62,62,62,62	0
54	MG	1A	3452	1/1	0.87	0.25	63,63,63,63	0
54	MG	1a	1712	1/1	0.87	0.27	73,73,73,73	0
54	MG	1A	3625	1/1	0.88	0.23	51,51,51,51	0
54	MG	1A	3729	1/1	0.88	0.15	42,42,42,42	0
54	MG	2A	3061	1/1	0.88	0.14	55,55,55,55	0
54	MG	1A	3626	1/1	0.88	0.20	37,37,37,37	0
54	MG	1A	4003	1/1	0.88	0.20	55,55,55,55	0
54	MG	2a	3029	1/1	0.88	0.09	68,68,68,68	0
54	MG	1A	4009	1/1	0.88	0.11	48,48,48,48	0
54	MG	2A	3284	1/1	0.88	0.09	59,59,59,59	0
54	MG	1A	3630	1/1	0.88	0.08	58,58,58,58	0
54	MG	1A	3486	1/1	0.88	0.16	39,39,39,39	0
54	MG	2A	3288	1/1	0.88	0.16	75,75,75,75	0
54	MG	1A	3640	1/1	0.88	0.20	58,58,58,58	0
54	MG	1A	3937	1/1	0.88	0.15	61,61,61,61	0
54	MG	1A	3841	1/1	0.88	0.17	48,48,48,48	0
54	MG	1A	3686	1/1	0.88	0.05	70,70,70,70	0
54	MG	2A	3539	1/1	0.88	0.10	59,59,59,59	0
54	MG	1A	3751	1/1	0.88	0.17	46,46,46,46	0
54	MG	1A	3754	1/1	0.88	0.17	50,50,50,50	0
54	MG	1A	3290	1/1	0.88	0.12	66,66,66,66	0
54	MG	2A	3550	1/1	0.88	0.29	56,56,56,56	0
54	MG	1A	3688	1/1	0.88	0.22	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3319	1/1	0.88	0.19	62,62,62,62	0
54	MG	1A	3388	1/1	0.88	0.14	65,65,65,65	0
54	MG	1a	1861	1/1	0.88	0.11	64,64,64,64	0
54	MG	1A	3696	1/1	0.88	0.23	60,60,60,60	0
54	MG	1a	1713	1/1	0.88	0.09	71,71,71,71	0
54	MG	2A	3116	1/1	0.88	0.39	50,50,50,50	0
54	MG	1A	3191	1/1	0.88	0.19	43,43,43,43	0
54	MG	2A	3349	1/1	0.88	0.10	80,80,80,80	0
54	MG	1A	3774	1/1	0.88	0.09	59,59,59,59	0
54	MG	1A	3275	1/1	0.88	0.20	48,48,48,48	0
54	MG	1A	3873	1/1	0.88	0.21	34,34,34,34	0
54	MG	1D	309	1/1	0.88	0.17	53,53,53,53	0
54	MG	1D	310	1/1	0.88	0.21	48,48,48,48	0
54	MG	1a	1642	1/1	0.88	0.12	75,75,75,75	0
54	MG	2A	3149	1/1	0.88	0.32	53,53,53,53	0
54	MG	2A	3151	1/1	0.88	0.32	56,56,56,56	0
54	MG	2a	3082	1/1	0.88	0.51	63,63,63,63	0
54	MG	1A	3129	1/1	0.88	0.40	52,52,52,52	0
54	MG	2A	3597	1/1	0.88	0.22	39,39,39,39	0
54	MG	1A	3784	1/1	0.88	0.15	38,38,38,38	0
54	MG	1A	3278	1/1	0.88	0.23	60,60,60,60	0
54	MG	2A	3161	1/1	0.88	0.34	62,62,62,62	0
54	MG	1F	305	1/1	0.88	0.20	40,40,40,40	0
54	MG	2a	3094	1/1	0.88	0.40	67,67,67,67	0
54	MG	2A	3614	1/1	0.88	0.18	53,53,53,53	0
54	MG	1a	1754	1/1	0.88	0.24	61,61,61,61	0
54	MG	2A	3385	1/1	0.88	0.26	61,61,61,61	0
54	MG	1A	3109	1/1	0.88	0.17	42,42,42,42	0
54	MG	1A	3888	1/1	0.88	0.29	65,65,65,65	0
54	MG	1A	3892	1/1	0.88	0.09	41,41,41,41	0
54	MG	1a	1654	1/1	0.88	0.12	68,68,68,68	0
54	MG	2A	3182	1/1	0.88	0.35	58,58,58,58	0
54	MG	2A	3002	1/1	0.88	0.12	56,56,56,56	0
54	MG	2A	3403	1/1	0.88	0.09	68,68,68,68	0
54	MG	2a	3110	1/1	0.88	0.24	67,67,67,67	0
54	MG	1A	3604	1/1	0.88	0.23	54,54,54,54	0
54	MG	2a	3114	1/1	0.88	0.13	78,78,78,78	0
54	MG	1A	3982	1/1	0.88	0.21	66,66,66,66	0
54	MG	1a	1775	1/1	0.88	0.16	60,60,60,60	0
54	MG	2A	3658	1/1	0.88	0.24	71,71,71,71	0
54	MG	2A	3198	1/1	0.88	0.16	78,78,78,78	0
54	MG	1A	3717	1/1	0.88	0.12	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3419	1/1	0.88	0.28	60,60,60,60	0
54	MG	1N	203	1/1	0.88	0.09	69,69,69,69	0
54	MG	1A	3986	1/1	0.88	0.20	57,57,57,57	0
54	MG	2A	3670	1/1	0.88	0.26	73,73,73,73	0
54	MG	2A	3205	1/1	0.88	0.52	59,59,59,59	0
54	MG	2B	205	1/1	0.88	0.18	77,77,77,77	0
54	MG	1A	3545	1/1	0.88	0.22	47,47,47,47	0
54	MG	1A	3799	1/1	0.88	0.12	69,69,69,69	0
54	MG	2a	3142	1/1	0.88	0.10	66,66,66,66	0
54	MG	1A	3901	1/1	0.88	0.17	41,41,41,41	0
54	MG	1a	1798	1/1	0.88	0.07	78,78,78,78	0
54	MG	2D	304	1/1	0.88	0.25	44,44,44,44	0
54	MG	2D	307	1/1	0.88	0.35	62,62,62,62	0
54	MG	2E	305	1/1	0.88	0.32	76,76,76,76	0
54	MG	2A	3441	1/1	0.88	0.12	65,65,65,65	0
54	MG	2a	3160	1/1	0.88	0.16	64,64,64,64	0
54	MG	2A	3213	1/1	0.88	0.43	67,67,67,67	0
54	MG	1A	3138	1/1	0.88	0.11	48,48,48,48	0
54	MG	1A	3801	1/1	0.88	0.06	72,72,72,72	0
54	MG	1A	3173	1/1	0.88	0.38	63,63,63,63	0
54	MG	2A	3452	1/1	0.88	0.17	43,43,43,43	0
54	MG	2a	3171	1/1	0.88	0.15	78,78,78,78	0
54	MG	21	101	1/1	0.88	0.15	75,75,75,75	0
54	MG	2A	3220	1/1	0.88	0.29	41,41,41,41	0
54	MG	1a	1678	1/1	0.88	0.33	67,67,67,67	0
54	MG	1A	3568	1/1	0.88	0.27	54,54,54,54	0
54	MG	1Y	202	1/1	0.88	0.19	58,58,58,58	0
54	MG	10	101	1/1	0.88	0.13	50,50,50,50	0
54	MG	2A	3049	1/1	0.88	0.31	74,74,74,74	0
56	ERY	2A	3672	51/51	0.88	0.34	43,60,66,72	0
54	MG	2a	3010	1/1	0.88	0.14	70,70,70,70	0
54	MG	2A	3053	1/1	0.88	0.22	61,61,61,61	0
54	MG	2a	3016	1/1	0.88	0.21	56,56,56,56	0
58	ARG	1B	230	12/12	0.88	0.20	39,54,61,64	0
54	MG	2A	3254	1/1	0.88	0.27	60,60,60,60	0
59	ZN	14	501	1/1	0.88	0.13	118,118,118,118	0
54	MG	2a	3019	1/1	0.88	0.33	55,55,55,55	0
54	MG	13	103	1/1	0.89	0.14	73,73,73,73	0
54	MG	2T	201	1/1	0.89	0.17	62,62,62,62	0
54	MG	2A	3167	1/1	0.89	0.15	59,59,59,59	0
54	MG	2A	3168	1/1	0.89	0.33	52,52,52,52	0
54	MG	1A	3685	1/1	0.89	0.19	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	15	105	1/1	0.89	0.25	51,51,51,51	0
54	MG	1A	3904	1/1	0.89	0.14	58,58,58,58	0
54	MG	1A	3073	1/1	0.89	0.21	40,40,40,40	0
54	MG	1e	202	1/1	0.89	0.15	61,61,61,61	0
54	MG	1A	3793	1/1	0.89	0.12	37,37,37,37	0
54	MG	1A	3117	1/1	0.89	0.12	40,40,40,40	0
54	MG	1A	3105	1/1	0.89	0.19	60,60,60,60	0
54	MG	2A	3190	1/1	0.89	0.22	54,54,54,54	0
54	MG	2A	3449	1/1	0.89	0.15	53,53,53,53	0
54	MG	1a	1609	1/1	0.89	0.23	69,69,69,69	0
54	MG	2A	3194	1/1	0.89	0.17	73,73,73,73	0
54	MG	1A	3314	1/1	0.89	0.26	44,44,44,44	0
54	MG	1A	3926	1/1	0.89	0.13	53,53,53,53	0
54	MG	1n	101	1/1	0.89	0.13	63,63,63,63	0
54	MG	1a	1616	1/1	0.89	0.11	62,62,62,62	0
54	MG	1a	1730	1/1	0.89	0.21	77,77,77,77	0
54	MG	1A	3499	1/1	0.89	0.19	35,35,35,35	0
54	MG	2A	3474	1/1	0.89	0.20	55,55,55,55	0
54	MG	1A	3501	1/1	0.89	0.17	29,29,29,29	0
54	MG	1a	1737	1/1	0.89	0.11	91,91,91,91	0
54	MG	1A	3610	1/1	0.89	0.12	65,65,65,65	0
54	MG	2A	3481	1/1	0.89	0.08	74,74,74,74	0
54	MG	2A	3482	1/1	0.89	0.14	54,54,54,54	0
54	MG	2a	3047	1/1	0.89	0.16	74,74,74,74	0
54	MG	1A	3232	1/1	0.89	0.20	39,39,39,39	0
54	MG	1A	3519	1/1	0.89	0.13	53,53,53,53	0
54	MG	1A	3708	1/1	0.89	0.12	49,49,49,49	0
54	MG	2A	3493	1/1	0.89	0.18	74,74,74,74	0
54	MG	1A	3142	1/1	0.89	0.22	49,49,49,49	0
54	MG	1A	3627	1/1	0.89	0.14	50,50,50,50	0
54	MG	2A	3021	1/1	0.89	0.17	47,47,47,47	0
54	MG	2A	3023	1/1	0.89	0.39	64,64,64,64	0
54	MG	1A	3033	1/1	0.89	0.15	47,47,47,47	0
54	MG	2A	3516	1/1	0.89	0.13	66,66,66,66	0
54	MG	2A	3518	1/1	0.89	0.06	83,83,83,83	0
54	MG	1A	3831	1/1	0.89	0.18	68,68,68,68	0
54	MG	2A	3522	1/1	0.89	0.31	49,49,49,49	0
54	MG	1A	3833	1/1	0.89	0.51	39,39,39,39	0
54	MG	2A	3529	1/1	0.89	0.11	67,67,67,67	0
54	MG	2A	3249	1/1	0.89	0.21	61,61,61,61	0
54	MG	1D	301	1/1	0.89	0.29	48,48,48,48	0
54	MG	1A	3390	1/1	0.89	0.27	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3637	1/1	0.89	0.20	49,49,49,49	0
54	MG	1A	3536	1/1	0.89	0.09	50,50,50,50	0
54	MG	1a	1780	1/1	0.89	0.18	65,65,65,65	0
54	MG	1A	3326	1/1	0.89	0.31	43,43,43,43	0
54	MG	1A	3456	1/1	0.89	0.21	62,62,62,62	0
54	MG	2A	3279	1/1	0.89	0.22	50,50,50,50	0
54	MG	1A	3299	1/1	0.89	0.21	57,57,57,57	0
54	MG	2A	3051	1/1	0.89	0.20	51,51,51,51	0
54	MG	1F	308	1/1	0.89	0.35	59,59,59,59	0
54	MG	1a	1792	1/1	0.89	0.18	65,65,65,65	0
54	MG	2A	3056	1/1	0.89	0.21	45,45,45,45	0
54	MG	2a	3088	1/1	0.89	0.27	57,57,57,57	0
54	MG	1F	310	1/1	0.89	0.22	40,40,40,40	0
54	MG	2A	3060	1/1	0.89	0.43	65,65,65,65	0
54	MG	1F	312	1/1	0.89	0.72	51,51,51,51	0
54	MG	2A	3062	1/1	0.89	0.23	44,44,44,44	0
54	MG	2A	3063	1/1	0.89	0.16	52,52,52,52	0
54	MG	2A	3582	1/1	0.89	0.10	61,61,61,61	0
54	MG	1A	3396	1/1	0.89	0.18	48,48,48,48	0
54	MG	1A	3550	1/1	0.89	0.28	60,60,60,60	0
54	MG	2A	3313	1/1	0.89	0.14	62,62,62,62	0
54	MG	2A	3068	1/1	0.89	0.18	52,52,52,52	0
54	MG	1A	3553	1/1	0.89	0.21	49,49,49,49	0
54	MG	2A	3076	1/1	0.89	0.16	52,52,52,52	0
54	MG	1A	3860	1/1	0.89	0.13	47,47,47,47	0
54	MG	1A	3563	1/1	0.89	0.28	70,70,70,70	0
54	MG	1a	1812	1/1	0.89	0.13	57,57,57,57	0
54	MG	1A	3276	1/1	0.89	0.24	38,38,38,38	0
54	MG	1a	1668	1/1	0.89	0.34	79,79,79,79	0
54	MG	2A	3611	1/1	0.89	0.16	46,46,46,46	0
54	MG	1A	3969	1/1	0.89	0.14	66,66,66,66	0
54	MG	1A	3569	1/1	0.89	0.09	47,47,47,47	0
54	MG	2A	3092	1/1	0.89	0.30	77,77,77,77	0
54	MG	1A	3662	1/1	0.89	0.12	32,32,32,32	0
54	MG	2a	3122	1/1	0.89	0.16	63,63,63,63	0
54	MG	2A	3619	1/1	0.89	0.10	78,78,78,78	0
54	MG	1a	1675	1/1	0.89	0.41	66,66,66,66	0
54	MG	1A	3154	1/1	0.89	0.19	63,63,63,63	0
54	MG	2A	3364	1/1	0.89	0.12	58,58,58,58	0
54	MG	1A	3067	1/1	0.89	0.21	50,50,50,50	0
54	MG	2A	3634	1/1	0.89	0.16	57,57,57,57	0
54	MG	1R	204	1/1	0.89	0.23	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1681	1/1	0.89	0.31	52,52,52,52	0
54	MG	1a	1682	1/1	0.89	0.24	56,56,56,56	0
54	MG	2A	3373	1/1	0.89	0.18	46,46,46,46	0
54	MG	1A	3576	1/1	0.89	0.17	58,58,58,58	0
54	MG	2A	3118	1/1	0.89	0.16	42,42,42,42	0
54	MG	1a	1844	1/1	0.89	0.20	61,61,61,61	0
54	MG	2A	3659	1/1	0.89	0.09	84,84,84,84	0
54	MG	1A	3583	1/1	0.89	0.17	70,70,70,70	0
54	MG	1A	3157	1/1	0.89	0.26	42,42,42,42	0
54	MG	2A	3137	1/1	0.89	0.26	62,62,62,62	0
54	MG	2a	3164	1/1	0.89	0.07	78,78,78,78	0
54	MG	2A	3386	1/1	0.89	0.20	62,62,62,62	0
54	MG	2A	3138	1/1	0.89	0.34	54,54,54,54	0
54	MG	1A	3478	1/1	0.89	0.13	56,56,56,56	0
54	MG	2B	201	1/1	0.89	0.16	67,67,67,67	0
54	MG	1A	3775	1/1	0.89	0.15	55,55,55,55	0
54	MG	2a	3175	1/1	0.89	0.13	70,70,70,70	0
54	MG	2a	3177	1/1	0.89	0.14	64,64,64,64	0
54	MG	2a	3179	1/1	0.89	0.22	68,68,68,68	0
54	MG	2a	3185	1/1	0.89	0.14	69,69,69,69	0
54	MG	2B	203	1/1	0.89	0.23	59,59,59,59	0
54	MG	1A	3893	1/1	0.89	0.21	58,58,58,58	0
54	MG	1A	3996	1/1	0.89	0.37	56,56,56,56	0
54	MG	2B	210	1/1	0.89	0.27	71,71,71,71	0
54	MG	2B	211	1/1	0.89	0.21	88,88,88,88	0
54	MG	2A	3401	1/1	0.89	0.16	68,68,68,68	0
54	MG	1A	3777	1/1	0.89	0.21	67,67,67,67	0
54	MG	10	106	1/1	0.89	0.15	58,58,58,58	0
54	MG	1a	1870	1/1	0.89	0.18	59,59,59,59	0
54	MG	1a	1871	1/1	0.89	0.08	81,81,81,81	0
54	MG	1A	3678	1/1	0.89	0.14	69,69,69,69	0
57	MPD	2A	3674	8/8	0.89	0.15	64,71,73,74	0
54	MG	1A	3412	1/1	0.89	0.16	45,45,45,45	0
54	MG	1A	3339	1/1	0.89	0.20	24,24,24,24	0
54	MG	2Q	201	1/1	0.89	0.17	61,61,61,61	0
54	MG	2A	3416	1/1	0.89	0.14	73,73,73,73	0
54	MG	1A	3174	1/1	0.90	0.14	45,45,45,45	0
54	MG	2A	3265	1/1	0.90	0.15	50,50,50,50	0
54	MG	1A	3702	1/1	0.90	0.17	66,66,66,66	0
54	MG	1A	3608	1/1	0.90	0.24	46,46,46,46	0
54	MG	2A	3509	1/1	0.90	0.07	63,63,63,63	0
54	MG	1a	1664	1/1	0.90	0.16	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3816	1/1	0.90	0.13	29,29,29,29	0
54	MG	1a	1666	1/1	0.90	0.10	67,67,67,67	0
54	MG	1A	3820	1/1	0.90	0.17	40,40,40,40	0
54	MG	1A	3705	1/1	0.90	0.12	53,53,53,53	0
54	MG	2a	3031	1/1	0.90	0.16	66,66,66,66	0
54	MG	1a	1814	1/1	0.90	0.10	65,65,65,65	0
54	MG	1A	3152	1/1	0.90	0.18	39,39,39,39	0
54	MG	2A	3526	1/1	0.90	0.13	59,59,59,59	0
54	MG	1A	3313	1/1	0.90	0.22	38,38,38,38	0
54	MG	1A	3611	1/1	0.90	0.19	60,60,60,60	0
54	MG	2a	3041	1/1	0.90	0.26	68,68,68,68	0
54	MG	1A	3615	1/1	0.90	0.25	44,44,44,44	0
54	MG	1A	3213	1/1	0.90	0.44	50,50,50,50	0
54	MG	1a	1824	1/1	0.90	0.21	61,61,61,61	0
54	MG	1A	3121	1/1	0.90	0.21	47,47,47,47	0
54	MG	1A	3401	1/1	0.90	0.22	48,48,48,48	0
54	MG	1A	3847	1/1	0.90	0.22	48,48,48,48	0
54	MG	1a	1834	1/1	0.90	0.22	71,71,71,71	0
54	MG	1a	1836	1/1	0.90	0.12	80,80,80,80	0
54	MG	2A	3315	1/1	0.90	0.11	66,66,66,66	0
54	MG	1A	3062	1/1	0.90	0.32	46,46,46,46	0
54	MG	1A	3405	1/1	0.90	0.19	38,38,38,38	0
54	MG	1A	3521	1/1	0.90	0.15	70,70,70,70	0
54	MG	2A	3563	1/1	0.90	0.21	61,61,61,61	0
54	MG	2A	3107	1/1	0.90	0.19	59,59,59,59	0
54	MG	1A	3635	1/1	0.90	0.21	42,42,42,42	0
54	MG	2A	3568	1/1	0.90	0.13	60,60,60,60	0
54	MG	1A	3223	1/1	0.90	0.14	64,64,64,64	0
54	MG	1a	1852	1/1	0.90	0.11	48,48,48,48	0
54	MG	1A	3280	1/1	0.90	0.17	51,51,51,51	0
54	MG	2A	3115	1/1	0.90	0.39	51,51,51,51	0
54	MG	2A	3576	1/1	0.90	0.11	57,57,57,57	0
54	MG	1A	3416	1/1	0.90	0.20	30,30,30,30	0
54	MG	1A	3869	1/1	0.90	0.09	55,55,55,55	0
54	MG	2A	3120	1/1	0.90	0.14	56,56,56,56	0
54	MG	2A	3121	1/1	0.90	0.12	58,58,58,58	0
54	MG	1A	3229	1/1	0.90	0.23	39,39,39,39	0
54	MG	1A	3748	1/1	0.90	0.06	50,50,50,50	0
54	MG	1A	3541	1/1	0.90	0.19	62,62,62,62	0
54	MG	2A	3135	1/1	0.90	0.14	64,64,64,64	0
54	MG	13	102	1/1	0.90	0.28	53,53,53,53	0
54	MG	1a	1866	1/1	0.90	0.18	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3752	1/1	0.90	0.21	46,46,46,46	0
54	MG	2A	3607	1/1	0.90	0.23	65,65,65,65	0
54	MG	1A	3287	1/1	0.90	0.26	45,45,45,45	0
54	MG	2A	3141	1/1	0.90	0.16	54,54,54,54	0
54	MG	2A	3142	1/1	0.90	0.44	56,56,56,56	0
54	MG	1A	3755	1/1	0.90	0.26	64,64,64,64	0
54	MG	1A	3189	1/1	0.90	0.24	48,48,48,48	0
54	MG	1A	3084	1/1	0.90	0.27	52,52,52,52	0
54	MG	1A	4007	1/1	0.90	0.10	63,63,63,63	0
54	MG	2A	3388	1/1	0.90	0.19	49,49,49,49	0
54	MG	2A	3624	1/1	0.90	0.32	66,66,66,66	0
54	MG	2A	3627	1/1	0.90	0.24	55,55,55,55	0
54	MG	1a	1877	1/1	0.90	0.07	72,72,72,72	0
54	MG	1A	3052	1/1	0.90	0.25	43,43,43,43	0
54	MG	1A	3767	1/1	0.90	0.12	66,66,66,66	0
54	MG	1a	1608	1/1	0.90	0.14	63,63,63,63	0
54	MG	2A	3162	1/1	0.90	0.20	50,50,50,50	0
54	MG	1A	3771	1/1	0.90	0.15	54,54,54,54	0
54	MG	1a	1610	1/1	0.90	0.15	62,62,62,62	0
54	MG	1A	3437	1/1	0.90	0.10	61,61,61,61	0
54	MG	1A	3336	1/1	0.90	0.21	40,40,40,40	0
54	MG	2A	3654	1/1	0.90	0.17	53,53,53,53	0
54	MG	1A	3562	1/1	0.90	0.15	62,62,62,62	0
54	MG	2A	3174	1/1	0.90	0.12	59,59,59,59	0
54	MG	2a	3125	1/1	0.90	0.23	69,69,69,69	0
54	MG	1A	3160	1/1	0.90	0.31	45,45,45,45	0
54	MG	1A	3567	1/1	0.90	0.18	43,43,43,43	0
54	MG	2A	3661	1/1	0.90	0.12	71,71,71,71	0
54	MG	1A	3037	1/1	0.90	0.17	51,51,51,51	0
54	MG	1A	3913	1/1	0.90	0.24	31,31,31,31	0
54	MG	2A	3666	1/1	0.90	0.25	87,87,87,87	0
54	MG	1a	1740	1/1	0.90	0.20	65,65,65,65	0
54	MG	1A	3004	1/1	0.90	0.22	46,46,46,46	0
54	MG	1A	3346	1/1	0.90	0.19	31,31,31,31	0
54	MG	2A	3001	1/1	0.90	0.13	64,64,64,64	0
54	MG	1a	1747	1/1	0.90	0.12	71,71,71,71	0
54	MG	1B	221	1/1	0.90	0.13	63,63,63,63	0
54	MG	1A	3170	1/1	0.90	0.48	62,62,62,62	0
54	MG	2a	3151	1/1	0.90	0.17	74,74,74,74	0
54	MG	1a	1755	1/1	0.90	0.11	66,66,66,66	0
54	MG	1A	3303	1/1	0.90	0.19	43,43,43,43	0
54	MG	1A	3790	1/1	0.90	0.23	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3447	1/1	0.90	0.25	43,43,43,43	0
54	MG	1A	3461	1/1	0.90	0.11	34,34,34,34	0
54	MG	2A	3206	1/1	0.90	0.19	44,44,44,44	0
54	MG	2A	3450	1/1	0.90	0.18	38,38,38,38	0
54	MG	2D	305	1/1	0.90	0.13	72,72,72,72	0
54	MG	1a	1761	1/1	0.90	0.12	77,77,77,77	0
54	MG	1a	1643	1/1	0.90	0.22	79,79,79,79	0
54	MG	1A	3113	1/1	0.90	0.44	61,61,61,61	0
54	MG	2G	201	1/1	0.90	0.11	81,81,81,81	0
54	MG	1A	3369	1/1	0.90	0.14	70,70,70,70	0
54	MG	2P	201	1/1	0.90	0.14	70,70,70,70	0
54	MG	1A	3588	1/1	0.90	0.11	72,72,72,72	0
54	MG	1a	1776	1/1	0.90	0.16	68,68,68,68	0
54	MG	1a	1777	1/1	0.90	0.18	51,51,51,51	0
54	MG	1A	3378	1/1	0.90	0.13	43,43,43,43	0
54	MG	2A	3466	1/1	0.90	0.16	61,61,61,61	0
54	MG	2k	201	1/1	0.90	0.27	67,67,67,67	0
54	MG	2T	204	1/1	0.90	0.20	60,60,60,60	0
54	MG	1A	3076	1/1	0.90	0.17	34,34,34,34	0
54	MG	2A	3223	1/1	0.90	0.17	55,55,55,55	0
54	MG	25	103	1/1	0.90	0.14	61,61,61,61	0
57	MPD	1T	205	8/8	0.90	0.16	65,69,78,79	0
54	MG	1a	1782	1/1	0.90	0.23	64,64,64,64	0
54	MG	1A	3387	1/1	0.90	0.19	40,40,40,40	0
54	MG	1A	3205	1/1	0.90	0.14	65,65,65,65	0
54	MG	1A	3389	1/1	0.90	0.12	54,54,54,54	0
54	MG	1A	3945	1/1	0.90	0.10	41,41,41,41	0
54	MG	1A	3273	1/1	0.90	0.12	55,55,55,55	0
54	MG	1F	311	1/1	0.90	0.27	47,47,47,47	0
54	MG	20	101	1/1	0.91	0.22	57,57,57,57	0
54	MG	2A	3221	1/1	0.91	0.25	58,58,58,58	0
54	MG	2A	3052	1/1	0.91	0.46	60,60,60,60	0
54	MG	2A	3230	1/1	0.91	0.09	63,63,63,63	0
54	MG	28	101	1/1	0.91	0.10	52,52,52,52	0
54	MG	1A	3757	1/1	0.91	0.32	55,55,55,55	0
54	MG	2A	3476	1/1	0.91	0.18	65,65,65,65	0
54	MG	2a	3005	1/1	0.91	0.24	65,65,65,65	0
54	MG	1A	3761	1/1	0.91	0.13	44,44,44,44	0
54	MG	2A	3234	1/1	0.91	0.27	43,43,43,43	0
54	MG	1A	4020	1/1	0.91	0.20	33,33,33,33	0
54	MG	2A	3242	1/1	0.91	0.19	56,56,56,56	0
54	MG	2A	3485	1/1	0.91	0.22	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	11	103	1/1	0.91	0.18	57,57,57,57	0
54	MG	2a	3014	1/1	0.91	0.18	75,75,75,75	0
54	MG	1A	3476	1/1	0.91	0.27	26,26,26,26	0
54	MG	1A	3071	1/1	0.91	0.13	39,39,39,39	0
54	MG	1B	202	1/1	0.91	0.22	67,67,67,67	0
54	MG	1A	3368	1/1	0.91	0.23	46,46,46,46	0
54	MG	1A	3214	1/1	0.91	0.17	37,37,37,37	0
54	MG	1B	206	1/1	0.91	0.47	64,64,64,64	0
54	MG	2A	3501	1/1	0.91	0.14	61,61,61,61	0
54	MG	2a	3026	1/1	0.91	0.44	64,64,64,64	0
54	MG	2A	3502	1/1	0.91	0.19	49,49,49,49	0
54	MG	2A	3507	1/1	0.91	0.15	58,58,58,58	0
54	MG	1a	1825	1/1	0.91	0.17	56,56,56,56	0
54	MG	2A	3071	1/1	0.91	0.14	55,55,55,55	0
54	MG	2a	3034	1/1	0.91	0.25	72,72,72,72	0
54	MG	2A	3511	1/1	0.91	0.22	54,54,54,54	0
54	MG	2A	3072	1/1	0.91	0.30	55,55,55,55	0
54	MG	1A	3768	1/1	0.91	0.12	50,50,50,50	0
54	MG	15	107	1/1	0.91	0.08	56,56,56,56	0
54	MG	17	105	1/1	0.91	0.24	50,50,50,50	0
54	MG	18	102	1/1	0.91	0.11	65,65,65,65	0
54	MG	1a	1835	1/1	0.91	0.20	69,69,69,69	0
54	MG	2A	3524	1/1	0.91	0.09	54,54,54,54	0
54	MG	1A	3374	1/1	0.91	0.17	40,40,40,40	0
54	MG	2a	3050	1/1	0.91	0.06	77,77,77,77	0
54	MG	1a	1695	1/1	0.91	0.17	57,57,57,57	0
54	MG	2a	3052	1/1	0.91	0.26	63,63,63,63	0
54	MG	1A	3320	1/1	0.91	0.28	59,59,59,59	0
54	MG	1a	1602	1/1	0.91	0.19	75,75,75,75	0
54	MG	1a	1843	1/1	0.91	0.13	49,49,49,49	0
54	MG	2A	3095	1/1	0.91	0.16	63,63,63,63	0
54	MG	2A	3098	1/1	0.91	0.35	76,76,76,76	0
54	MG	1B	216	1/1	0.91	0.14	63,63,63,63	0
54	MG	2A	3307	1/1	0.91	0.16	57,57,57,57	0
54	MG	2A	3549	1/1	0.91	0.08	69,69,69,69	0
54	MG	2A	3308	1/1	0.91	0.18	44,44,44,44	0
54	MG	2A	3309	1/1	0.91	0.14	72,72,72,72	0
54	MG	1A	3030	1/1	0.91	0.16	30,30,30,30	0
54	MG	1A	3700	1/1	0.91	0.18	49,49,49,49	0
54	MG	1A	3258	1/1	0.91	0.32	56,56,56,56	0
54	MG	2A	3316	1/1	0.91	0.19	63,63,63,63	0
54	MG	1A	3125	1/1	0.91	0.19	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1705	1/1	0.91	0.33	62,62,62,62	0
54	MG	1A	3865	1/1	0.91	0.15	38,38,38,38	0
54	MG	2A	3321	1/1	0.91	0.16	51,51,51,51	0
54	MG	1A	3959	1/1	0.91	0.19	30,30,30,30	0
54	MG	2a	3077	1/1	0.91	0.18	64,64,64,64	0
54	MG	1a	1714	1/1	0.91	0.18	76,76,76,76	0
54	MG	2A	3333	1/1	0.91	0.30	75,75,75,75	0
54	MG	1A	3580	1/1	0.91	0.18	39,39,39,39	0
54	MG	2A	3340	1/1	0.91	0.16	60,60,60,60	0
54	MG	1a	1617	1/1	0.91	0.14	81,81,81,81	0
54	MG	1a	1867	1/1	0.91	0.23	66,66,66,66	0
54	MG	1D	305	1/1	0.91	0.18	47,47,47,47	0
54	MG	1A	3500	1/1	0.91	0.22	32,32,32,32	0
54	MG	1A	3871	1/1	0.91	0.22	49,49,49,49	0
54	MG	1A	3267	1/1	0.91	0.16	36,36,36,36	0
54	MG	2a	3091	1/1	0.91	0.31	52,52,52,52	0
54	MG	1a	1731	1/1	0.91	0.16	55,55,55,55	0
54	MG	1A	3008	1/1	0.91	0.14	45,45,45,45	0
54	MG	1A	3512	1/1	0.91	0.13	65,65,65,65	0
54	MG	2A	3600	1/1	0.91	0.19	27,27,27,27	0
54	MG	1a	1625	1/1	0.91	0.41	67,67,67,67	0
54	MG	1A	3789	1/1	0.91	0.09	49,49,49,49	0
54	MG	1A	3451	1/1	0.91	0.20	61,61,61,61	0
54	MG	1A	3178	1/1	0.91	0.15	57,57,57,57	0
54	MG	1a	1636	1/1	0.91	0.10	57,57,57,57	0
54	MG	1A	3658	1/1	0.91	0.28	58,58,58,58	0
54	MG	1f	202	1/1	0.91	0.25	55,55,55,55	0
54	MG	1a	1752	1/1	0.91	0.19	65,65,65,65	0
54	MG	2A	3382	1/1	0.91	0.22	69,69,69,69	0
54	MG	1a	1639	1/1	0.91	0.20	35,35,35,35	0
54	MG	2A	3156	1/1	0.91	0.20	48,48,48,48	0
54	MG	1g	203	1/1	0.91	0.06	73,73,73,73	0
54	MG	1A	3600	1/1	0.91	0.15	45,45,45,45	0
54	MG	1A	3453	1/1	0.91	0.09	69,69,69,69	0
54	MG	1A	3602	1/1	0.91	0.18	55,55,55,55	0
54	MG	1A	3302	1/1	0.91	0.18	49,49,49,49	0
54	MG	2A	3164	1/1	0.91	0.18	60,60,60,60	0
54	MG	2a	3123	1/1	0.91	0.12	80,80,80,80	0
54	MG	2a	3124	1/1	0.91	0.28	80,80,80,80	0
54	MG	2A	3642	1/1	0.91	0.24	53,53,53,53	0
54	MG	2a	3126	1/1	0.91	0.18	77,77,77,77	0
54	MG	2a	3129	1/1	0.91	0.26	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3130	1/1	0.91	0.18	71,71,71,71	0
54	MG	2A	3398	1/1	0.91	0.18	68,68,68,68	0
54	MG	1A	3077	1/1	0.91	0.15	43,43,43,43	0
54	MG	1o	102	1/1	0.91	0.30	56,56,56,56	0
54	MG	1A	3666	1/1	0.91	0.13	59,59,59,59	0
54	MG	1a	1766	1/1	0.91	0.10	75,75,75,75	0
54	MG	1G	204	1/1	0.91	0.12	57,57,57,57	0
54	MG	2a	3138	1/1	0.91	0.10	80,80,80,80	0
54	MG	1A	3238	1/1	0.91	0.50	44,44,44,44	0
54	MG	1A	3739	1/1	0.91	0.16	59,59,59,59	0
54	MG	1A	3038	1/1	0.91	0.15	40,40,40,40	0
54	MG	1A	3040	1/1	0.91	0.19	39,39,39,39	0
54	MG	1Q	203	1/1	0.91	0.24	55,55,55,55	0
54	MG	1A	3249	1/1	0.91	0.19	46,46,46,46	0
54	MG	1a	1779	1/1	0.91	0.13	70,70,70,70	0
54	MG	1a	1660	1/1	0.91	0.14	49,49,49,49	0
54	MG	1A	3041	1/1	0.91	0.28	55,55,55,55	0
54	MG	1a	1784	1/1	0.91	0.11	63,63,63,63	0
54	MG	2A	3432	1/1	0.91	0.31	57,57,57,57	0
54	MG	2A	3196	1/1	0.91	0.43	64,64,64,64	0
54	MG	1A	3251	1/1	0.91	0.21	34,34,34,34	0
54	MG	2A	3026	1/1	0.91	0.26	46,46,46,46	0
54	MG	1T	201	1/1	0.91	0.14	49,49,49,49	0
54	MG	2B	206	1/1	0.91	0.19	73,73,73,73	0
54	MG	2B	207	1/1	0.91	0.14	67,67,67,67	0
54	MG	2A	3440	1/1	0.91	0.16	76,76,76,76	0
54	MG	2B	209	1/1	0.91	0.22	85,85,85,85	0
54	MG	1A	3821	1/1	0.91	0.12	40,40,40,40	0
54	MG	2A	3442	1/1	0.91	0.12	73,73,73,73	0
54	MG	2a	3180	1/1	0.91	0.11	92,92,92,92	0
54	MG	2a	3183	1/1	0.91	0.14	80,80,80,80	0
54	MG	1a	1789	1/1	0.91	0.08	84,84,84,84	0
54	MG	2A	3036	1/1	0.91	0.20	56,56,56,56	0
54	MG	2A	3445	1/1	0.91	0.17	66,66,66,66	0
54	MG	1U	209	1/1	0.91	0.39	61,61,61,61	0
54	MG	2A	3209	1/1	0.91	0.12	57,57,57,57	0
54	MG	2A	3038	1/1	0.91	0.17	57,57,57,57	0
54	MG	1A	3822	1/1	0.91	0.18	49,49,49,49	0
54	MG	2F	301	1/1	0.91	0.19	45,45,45,45	0
54	MG	1V	206	1/1	0.91	0.13	66,66,66,66	0
56	ERY	1A	4027	51/51	0.91	0.27	37,52,58,63	0
54	MG	1A	3029	1/1	0.91	0.23	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3454	1/1	0.91	0.07	66,66,66,66	0
54	MG	2A	3455	1/1	0.91	0.12	69,69,69,69	0
54	MG	1A	3928	1/1	0.91	0.12	44,44,44,44	0
54	MG	1A	3617	1/1	0.91	0.09	61,61,61,61	0
54	MG	1A	3834	1/1	0.91	0.15	34,34,34,34	0
57	MPD	2A	3675	8/8	0.91	0.22	60,65,67,69	0
54	MG	2A	3219	1/1	0.91	0.20	78,78,78,78	0
54	MG	2A	3462	1/1	0.91	0.06	86,86,86,86	0
54	MG	1A	4017	1/1	0.91	0.29	42,42,42,42	0
54	MG	2U	201	1/1	0.91	0.29	80,80,80,80	0
54	MG	1A	3091	1/1	0.92	0.19	39,39,39,39	0
54	MG	1A	3586	1/1	0.92	0.16	42,42,42,42	0
54	MG	2A	3088	1/1	0.92	0.23	51,51,51,51	0
54	MG	1A	3184	1/1	0.92	0.26	37,37,37,37	0
54	MG	1A	3885	1/1	0.92	0.20	47,47,47,47	0
54	MG	1A	3207	1/1	0.92	0.41	52,52,52,52	0
54	MG	2A	3519	1/1	0.92	0.20	58,58,58,58	0
54	MG	2A	3097	1/1	0.92	0.21	50,50,50,50	0
54	MG	1A	3674	1/1	0.92	0.27	31,31,31,31	0
54	MG	2A	3100	1/1	0.92	0.18	40,40,40,40	0
54	MG	1a	1842	1/1	0.92	0.14	72,72,72,72	0
54	MG	1A	3594	1/1	0.92	0.25	40,40,40,40	0
54	MG	2a	3030	1/1	0.92	0.19	71,71,71,71	0
54	MG	1A	4010	1/1	0.92	0.18	48,48,48,48	0
54	MG	1A	3677	1/1	0.92	0.23	35,35,35,35	0
54	MG	1a	1850	1/1	0.92	0.33	68,68,68,68	0
54	MG	2A	3535	1/1	0.92	0.27	63,63,63,63	0
54	MG	2A	3317	1/1	0.92	0.21	43,43,43,43	0
54	MG	1A	4015	1/1	0.92	0.12	59,59,59,59	0
54	MG	1A	3778	1/1	0.92	0.21	55,55,55,55	0
54	MG	1A	3493	1/1	0.92	0.19	40,40,40,40	0
54	MG	1A	3358	1/1	0.92	0.17	43,43,43,43	0
54	MG	1A	3419	1/1	0.92	0.21	31,31,31,31	0
54	MG	1A	3111	1/1	0.92	0.26	43,43,43,43	0
54	MG	2A	3331	1/1	0.92	0.25	41,41,41,41	0
54	MG	2A	3332	1/1	0.92	0.21	47,47,47,47	0
54	MG	1A	3905	1/1	0.92	0.17	51,51,51,51	0
54	MG	2A	3557	1/1	0.92	0.15	67,67,67,67	0
54	MG	2A	3337	1/1	0.92	0.12	58,58,58,58	0
54	MG	1A	3907	1/1	0.92	0.15	39,39,39,39	0
54	MG	2A	3122	1/1	0.92	0.44	66,66,66,66	0
54	MG	1A	4025	1/1	0.92	0.13	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3125	1/1	0.92	0.14	56,56,56,56	0
54	MG	2A	3348	1/1	0.92	0.19	54,54,54,54	0
54	MG	1a	1710	1/1	0.92	0.25	56,56,56,56	0
54	MG	1a	1869	1/1	0.92	0.18	61,61,61,61	0
54	MG	2A	3571	1/1	0.92	0.10	78,78,78,78	0
54	MG	2A	3129	1/1	0.92	0.48	62,62,62,62	0
54	MG	2A	3130	1/1	0.92	0.27	55,55,55,55	0
54	MG	2A	3574	1/1	0.92	0.05	75,75,75,75	0
54	MG	2a	3065	1/1	0.92	0.21	61,61,61,61	0
54	MG	1A	3425	1/1	0.92	0.21	27,27,27,27	0
54	MG	2A	3361	1/1	0.92	0.20	35,35,35,35	0
54	MG	2A	3583	1/1	0.92	0.19	59,59,59,59	0
54	MG	1A	3363	1/1	0.92	0.13	47,47,47,47	0
54	MG	1A	3367	1/1	0.92	0.14	35,35,35,35	0
54	MG	1A	3691	1/1	0.92	0.08	65,65,65,65	0
54	MG	1A	3509	1/1	0.92	0.20	53,53,53,53	0
54	MG	2a	3075	1/1	0.92	0.35	61,61,61,61	0
54	MG	2a	3076	1/1	0.92	0.32	70,70,70,70	0
54	MG	1A	3916	1/1	0.92	0.19	32,32,32,32	0
54	MG	1A	3099	1/1	0.92	0.25	49,49,49,49	0
54	MG	1B	213	1/1	0.92	0.14	52,52,52,52	0
54	MG	1a	1726	1/1	0.92	0.12	77,77,77,77	0
54	MG	2A	3598	1/1	0.92	0.10	57,57,57,57	0
54	MG	1a	1727	1/1	0.92	0.23	56,56,56,56	0
54	MG	1A	3255	1/1	0.92	0.19	60,60,60,60	0
54	MG	1B	217	1/1	0.92	0.12	57,57,57,57	0
54	MG	1a	1618	1/1	0.92	0.11	69,69,69,69	0
54	MG	1B	218	1/1	0.92	0.18	39,39,39,39	0
54	MG	2A	3609	1/1	0.92	0.20	63,63,63,63	0
54	MG	1B	220	1/1	0.92	0.10	70,70,70,70	0
54	MG	1A	3164	1/1	0.92	0.18	36,36,36,36	0
54	MG	2a	3093	1/1	0.92	0.36	63,63,63,63	0
54	MG	1A	3527	1/1	0.92	0.18	28,28,28,28	0
54	MG	1B	223	1/1	0.92	0.18	60,60,60,60	0
54	MG	1A	3613	1/1	0.92	0.16	45,45,45,45	0
54	MG	1l	201	1/1	0.92	0.31	75,75,75,75	0
54	MG	2A	3397	1/1	0.92	0.11	72,72,72,72	0
54	MG	1A	3439	1/1	0.92	0.17	38,38,38,38	0
54	MG	1a	1748	1/1	0.92	0.20	62,62,62,62	0
54	MG	2a	3104	1/1	0.92	0.22	54,54,54,54	0
54	MG	2A	3628	1/1	0.92	0.16	57,57,57,57	0
54	MG	2A	3172	1/1	0.92	0.34	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1626	1/1	0.92	0.19	57,57,57,57	0
54	MG	2A	3632	1/1	0.92	0.18	60,60,60,60	0
54	MG	1a	1627	1/1	0.92	0.11	73,73,73,73	0
54	MG	1a	1628	1/1	0.92	0.22	61,61,61,61	0
54	MG	1A	3377	1/1	0.92	0.20	59,59,59,59	0
54	MG	1A	3082	1/1	0.92	0.17	45,45,45,45	0
54	MG	2A	3647	1/1	0.92	0.12	61,61,61,61	0
54	MG	1A	3707	1/1	0.92	0.17	67,67,67,67	0
54	MG	2A	3409	1/1	0.92	0.25	79,79,79,79	0
54	MG	1a	1635	1/1	0.92	0.20	38,38,38,38	0
54	MG	2A	3412	1/1	0.92	0.07	67,67,67,67	0
54	MG	1A	3533	1/1	0.92	0.14	64,64,64,64	0
54	MG	1a	1765	1/1	0.92	0.20	60,60,60,60	0
54	MG	1A	3534	1/1	0.92	0.24	30,30,30,30	0
54	MG	1A	3449	1/1	0.92	0.33	44,44,44,44	0
54	MG	1a	1769	1/1	0.92	0.14	65,65,65,65	0
54	MG	1A	3628	1/1	0.92	0.43	68,68,68,68	0
54	MG	1A	3380	1/1	0.92	0.10	46,46,46,46	0
54	MG	1E	306	1/1	0.92	0.13	38,38,38,38	0
54	MG	1A	3039	1/1	0.92	0.19	54,54,54,54	0
54	MG	1A	3824	1/1	0.92	0.16	55,55,55,55	0
54	MG	1a	1647	1/1	0.92	0.20	52,52,52,52	0
54	MG	1A	3633	1/1	0.92	0.18	29,29,29,29	0
54	MG	2A	3033	1/1	0.92	0.22	60,60,60,60	0
54	MG	1A	3192	1/1	0.92	0.30	39,39,39,39	0
54	MG	1A	3149	1/1	0.92	0.27	38,38,38,38	0
54	MG	1a	1651	1/1	0.92	0.12	53,53,53,53	0
54	MG	1A	3638	1/1	0.92	0.20	29,29,29,29	0
54	MG	2A	3041	1/1	0.92	0.17	58,58,58,58	0
54	MG	1a	1786	1/1	0.92	0.11	67,67,67,67	0
54	MG	1a	1653	1/1	0.92	0.10	65,65,65,65	0
54	MG	2A	3217	1/1	0.92	0.25	45,45,45,45	0
54	MG	2a	3152	1/1	0.92	0.21	72,72,72,72	0
54	MG	2a	3154	1/1	0.92	0.24	56,56,56,56	0
54	MG	1A	3150	1/1	0.92	0.30	39,39,39,39	0
54	MG	1A	3642	1/1	0.92	0.18	36,36,36,36	0
54	MG	1A	3645	1/1	0.92	0.26	55,55,55,55	0
54	MG	2A	3048	1/1	0.92	0.17	60,60,60,60	0
54	MG	1a	1791	1/1	0.92	0.07	77,77,77,77	0
54	MG	1A	3269	1/1	0.92	0.36	72,72,72,72	0
54	MG	2A	3231	1/1	0.92	0.24	40,40,40,40	0
54	MG	1A	3845	1/1	0.92	0.41	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3647	1/1	0.92	0.23	49,49,49,49	0
54	MG	1A	3392	1/1	0.92	0.10	50,50,50,50	0
54	MG	2F	303	1/1	0.92	0.25	54,54,54,54	0
54	MG	1A	3746	1/1	0.92	0.20	46,46,46,46	0
54	MG	1A	3460	1/1	0.92	0.16	31,31,31,31	0
54	MG	2A	3471	1/1	0.92	0.22	43,43,43,43	0
54	MG	1A	3334	1/1	0.92	0.36	60,60,60,60	0
54	MG	1A	3031	1/1	0.92	0.24	22,22,22,22	0
54	MG	2Q	204	1/1	0.92	0.09	69,69,69,69	0
54	MG	1A	3079	1/1	0.92	0.37	42,42,42,42	0
54	MG	1A	3863	1/1	0.92	0.14	29,29,29,29	0
54	MG	1a	1669	1/1	0.92	0.27	68,68,68,68	0
54	MG	2A	3264	1/1	0.92	0.14	47,47,47,47	0
54	MG	1A	3337	1/1	0.92	0.18	47,47,47,47	0
54	MG	2A	3483	1/1	0.92	0.07	75,75,75,75	0
54	MG	1A	3987	1/1	0.92	0.14	62,62,62,62	0
54	MG	2r	101	1/1	0.92	0.09	79,79,79,79	0
54	MG	1A	3399	1/1	0.92	0.12	63,63,63,63	0
54	MG	1T	203	1/1	0.92	0.12	64,64,64,64	0
54	MG	2A	3275	1/1	0.92	0.31	73,73,73,73	0
54	MG	1A	3759	1/1	0.92	0.22	48,48,48,48	0
54	MG	1A	3239	1/1	0.92	0.17	45,45,45,45	0
54	MG	1A	3022	1/1	0.92	0.11	55,55,55,55	0
54	MG	1A	3198	1/1	0.92	0.32	59,59,59,59	0
54	MG	1A	3404	1/1	0.92	0.13	34,34,34,34	0
54	MG	2A	3083	1/1	0.92	0.14	57,57,57,57	0
54	MG	2A	3506	1/1	0.92	0.17	64,64,64,64	0
54	MG	1A	3480	1/1	0.92	0.28	58,58,58,58	0
54	MG	2a	3011	1/1	0.92	0.20	71,71,71,71	0
54	MG	1A	3328	1/1	0.93	0.17	47,47,47,47	0
54	MG	1A	3891	1/1	0.93	0.06	67,67,67,67	0
54	MG	1A	3612	1/1	0.93	0.19	48,48,48,48	0
54	MG	1a	1795	1/1	0.93	0.09	72,72,72,72	0
54	MG	2A	3226	1/1	0.93	0.27	39,39,39,39	0
54	MG	1a	1671	1/1	0.93	0.27	62,62,62,62	0
54	MG	1a	1797	1/1	0.93	0.11	71,71,71,71	0
54	MG	2A	3473	1/1	0.93	0.30	58,58,58,58	0
54	MG	1a	1672	1/1	0.93	0.13	73,73,73,73	0
54	MG	1Z	301	1/1	0.93	0.27	61,61,61,61	0
54	MG	2a	3002	1/1	0.93	0.23	69,69,69,69	0
54	MG	1a	1801	1/1	0.93	0.13	60,60,60,60	0
54	MG	1A	3187	1/1	0.93	0.24	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3239	1/1	0.93	0.18	44,44,44,44	0
54	MG	2A	3480	1/1	0.93	0.07	53,53,53,53	0
54	MG	1a	1803	1/1	0.93	0.08	70,70,70,70	0
54	MG	1A	3782	1/1	0.93	0.16	36,36,36,36	0
54	MG	2A	3247	1/1	0.93	0.24	63,63,63,63	0
54	MG	1a	1677	1/1	0.93	0.14	70,70,70,70	0
54	MG	2A	3057	1/1	0.93	0.20	40,40,40,40	0
54	MG	1A	3413	1/1	0.93	0.18	42,42,42,42	0
54	MG	1A	3896	1/1	0.93	0.24	62,62,62,62	0
54	MG	2A	3491	1/1	0.93	0.28	58,58,58,58	0
54	MG	2A	3262	1/1	0.93	0.23	57,57,57,57	0
54	MG	10	108	1/1	0.93	0.19	76,76,76,76	0
54	MG	1A	4013	1/1	0.93	0.23	50,50,50,50	0
54	MG	2A	3267	1/1	0.93	0.26	41,41,41,41	0
54	MG	2a	3023	1/1	0.93	0.13	55,55,55,55	0
54	MG	1A	3538	1/1	0.93	0.19	57,57,57,57	0
54	MG	1a	1816	1/1	0.93	0.08	65,65,65,65	0
54	MG	2A	3505	1/1	0.93	0.14	68,68,68,68	0
54	MG	1A	3898	1/1	0.93	0.16	39,39,39,39	0
54	MG	1a	1818	1/1	0.93	0.34	80,80,80,80	0
54	MG	1A	3034	1/1	0.93	0.14	54,54,54,54	0
54	MG	1a	1685	1/1	0.93	0.18	51,51,51,51	0
54	MG	1A	3467	1/1	0.93	0.18	31,31,31,31	0
54	MG	1A	3210	1/1	0.93	0.34	45,45,45,45	0
54	MG	1A	3007	1/1	0.93	0.19	39,39,39,39	0
54	MG	1A	3381	1/1	0.93	0.18	26,26,26,26	0
54	MG	2A	3286	1/1	0.93	0.15	79,79,79,79	0
54	MG	1a	1830	1/1	0.93	0.16	74,74,74,74	0
54	MG	1A	3908	1/1	0.93	0.09	61,61,61,61	0
54	MG	2a	3045	1/1	0.93	0.07	75,75,75,75	0
54	MG	1A	3629	1/1	0.93	0.18	44,44,44,44	0
54	MG	2A	3291	1/1	0.93	0.18	47,47,47,47	0
54	MG	1A	3426	1/1	0.93	0.25	41,41,41,41	0
54	MG	2A	3528	1/1	0.93	0.08	69,69,69,69	0
54	MG	1A	3704	1/1	0.93	0.27	67,67,67,67	0
54	MG	2A	3302	1/1	0.93	0.07	54,54,54,54	0
54	MG	2A	3531	1/1	0.93	0.10	50,50,50,50	0
54	MG	2A	3533	1/1	0.93	0.15	57,57,57,57	0
54	MG	1A	3477	1/1	0.93	0.23	66,66,66,66	0
54	MG	2A	3304	1/1	0.93	0.17	61,61,61,61	0
54	MG	1A	3554	1/1	0.93	0.16	25,25,25,25	0
54	MG	1A	3561	1/1	0.93	0.25	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3093	1/1	0.93	0.33	52,52,52,52	0
54	MG	2A	3542	1/1	0.93	0.21	51,51,51,51	0
54	MG	1A	3709	1/1	0.93	0.48	54,54,54,54	0
54	MG	1a	1605	1/1	0.93	0.21	68,68,68,68	0
54	MG	1A	3636	1/1	0.93	0.15	52,52,52,52	0
54	MG	2A	3099	1/1	0.93	0.23	53,53,53,53	0
54	MG	1A	3428	1/1	0.93	0.17	33,33,33,33	0
54	MG	1A	3081	1/1	0.93	0.22	40,40,40,40	0
54	MG	2A	3103	1/1	0.93	0.23	47,47,47,47	0
54	MG	1a	1848	1/1	0.93	0.26	63,63,63,63	0
54	MG	1A	3639	1/1	0.93	0.13	60,60,60,60	0
54	MG	1a	1851	1/1	0.93	0.13	68,68,68,68	0
54	MG	1A	3309	1/1	0.93	0.26	51,51,51,51	0
54	MG	2A	3322	1/1	0.93	0.09	49,49,49,49	0
54	MG	1A	3431	1/1	0.93	0.15	45,45,45,45	0
54	MG	1A	3167	1/1	0.93	0.25	40,40,40,40	0
54	MG	2A	3329	1/1	0.93	0.10	76,76,76,76	0
54	MG	2A	3330	1/1	0.93	0.10	77,77,77,77	0
54	MG	1A	3936	1/1	0.93	0.24	40,40,40,40	0
54	MG	1A	3151	1/1	0.93	0.21	52,52,52,52	0
54	MG	1A	3823	1/1	0.93	0.20	48,48,48,48	0
54	MG	2A	3117	1/1	0.93	0.21	54,54,54,54	0
54	MG	2a	3084	1/1	0.93	0.30	66,66,66,66	0
54	MG	1a	1717	1/1	0.93	0.21	66,66,66,66	0
54	MG	2A	3580	1/1	0.93	0.20	39,39,39,39	0
54	MG	1a	1718	1/1	0.93	0.24	65,65,65,65	0
54	MG	1A	3572	1/1	0.93	0.14	55,55,55,55	0
54	MG	1A	3827	1/1	0.93	0.28	43,43,43,43	0
54	MG	1a	1868	1/1	0.93	0.18	51,51,51,51	0
54	MG	2A	3124	1/1	0.93	0.19	72,72,72,72	0
54	MG	1a	1722	1/1	0.93	0.25	64,64,64,64	0
54	MG	1a	1724	1/1	0.93	0.22	65,65,65,65	0
54	MG	2A	3127	1/1	0.93	0.24	41,41,41,41	0
54	MG	2A	3593	1/1	0.93	0.10	65,65,65,65	0
54	MG	1A	3730	1/1	0.93	0.14	32,32,32,32	0
54	MG	2A	3595	1/1	0.93	0.16	47,47,47,47	0
54	MG	1a	1872	1/1	0.93	0.25	64,64,64,64	0
54	MG	2A	3362	1/1	0.93	0.21	54,54,54,54	0
54	MG	1A	3488	1/1	0.93	0.22	51,51,51,51	0
54	MG	2A	3132	1/1	0.93	0.24	61,61,61,61	0
54	MG	2A	3602	1/1	0.93	0.15	46,46,46,46	0
54	MG	1A	3340	1/1	0.93	0.11	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3367	1/1	0.93	0.21	37,37,37,37	0
54	MG	2a	3108	1/1	0.93	0.23	53,53,53,53	0
54	MG	1A	3134	1/1	0.93	0.15	46,46,46,46	0
54	MG	1A	3950	1/1	0.93	0.14	45,45,45,45	0
54	MG	2A	3610	1/1	0.93	0.17	49,49,49,49	0
54	MG	2A	3370	1/1	0.93	0.17	49,49,49,49	0
54	MG	1a	1733	1/1	0.93	0.19	67,67,67,67	0
54	MG	1a	1734	1/1	0.93	0.11	62,62,62,62	0
54	MG	1a	1881	1/1	0.93	0.24	61,61,61,61	0
54	MG	2A	3617	1/1	0.93	0.19	42,42,42,42	0
54	MG	1b	301	1/1	0.93	0.07	82,82,82,82	0
54	MG	2A	3146	1/1	0.93	0.10	65,65,65,65	0
54	MG	1A	3654	1/1	0.93	0.23	72,72,72,72	0
54	MG	1A	3839	1/1	0.93	0.17	57,57,57,57	0
54	MG	1a	1629	1/1	0.93	0.32	69,69,69,69	0
54	MG	1a	1630	1/1	0.93	0.20	71,71,71,71	0
54	MG	2a	3127	1/1	0.93	0.20	71,71,71,71	0
54	MG	2A	3153	1/1	0.93	0.37	71,71,71,71	0
54	MG	1A	3135	1/1	0.93	0.25	50,50,50,50	0
54	MG	1A	3743	1/1	0.93	0.09	65,65,65,65	0
54	MG	1A	3496	1/1	0.93	0.29	35,35,35,35	0
54	MG	1F	304	1/1	0.93	0.40	42,42,42,42	0
54	MG	2A	3641	1/1	0.93	0.17	69,69,69,69	0
54	MG	2A	3159	1/1	0.93	0.31	47,47,47,47	0
54	MG	1A	3447	1/1	0.93	0.17	66,66,66,66	0
54	MG	2A	3646	1/1	0.93	0.05	71,71,71,71	0
54	MG	1a	1637	1/1	0.93	0.12	71,71,71,71	0
54	MG	2a	3140	1/1	0.93	0.07	68,68,68,68	0
54	MG	1A	3094	1/1	0.93	0.18	38,38,38,38	0
54	MG	1A	3587	1/1	0.93	0.32	57,57,57,57	0
54	MG	1A	3351	1/1	0.93	0.19	39,39,39,39	0
54	MG	1A	3137	1/1	0.93	0.15	36,36,36,36	0
54	MG	2A	3653	1/1	0.93	0.17	55,55,55,55	0
54	MG	1A	3508	1/1	0.93	0.14	41,41,41,41	0
54	MG	1A	3756	1/1	0.93	0.28	56,56,56,56	0
54	MG	1A	3126	1/1	0.93	0.17	34,34,34,34	0
54	MG	1a	1764	1/1	0.93	0.09	71,71,71,71	0
54	MG	1A	3970	1/1	0.93	0.18	50,50,50,50	0
54	MG	2a	3158	1/1	0.93	0.19	68,68,68,68	0
54	MG	2A	3177	1/1	0.93	0.17	44,44,44,44	0
54	MG	1A	3599	1/1	0.93	0.22	49,49,49,49	0
54	MG	2A	3414	1/1	0.93	0.27	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3664	1/1	0.93	0.33	69,69,69,69	0
54	MG	2A	3415	1/1	0.93	0.22	57,57,57,57	0
54	MG	2A	3667	1/1	0.93	0.18	61,61,61,61	0
54	MG	1A	3978	1/1	0.93	0.24	60,60,60,60	0
54	MG	1A	3510	1/1	0.93	0.22	51,51,51,51	0
54	MG	1a	1770	1/1	0.93	0.22	57,57,57,57	0
54	MG	2a	3172	1/1	0.93	0.09	78,78,78,78	0
54	MG	2A	3007	1/1	0.93	0.19	49,49,49,49	0
54	MG	2A	3423	1/1	0.93	0.15	62,62,62,62	0
54	MG	2A	3009	1/1	0.93	0.11	43,43,43,43	0
54	MG	2A	3428	1/1	0.93	0.17	68,68,68,68	0
54	MG	2A	3010	1/1	0.93	0.17	74,74,74,74	0
54	MG	2A	3191	1/1	0.93	0.23	36,36,36,36	0
54	MG	1A	3159	1/1	0.93	0.15	34,34,34,34	0
54	MG	2A	3012	1/1	0.93	0.16	64,64,64,64	0
54	MG	1A	3298	1/1	0.93	0.23	38,38,38,38	0
54	MG	1P	203	1/1	0.93	0.19	34,34,34,34	0
54	MG	1A	3868	1/1	0.93	0.20	55,55,55,55	0
54	MG	1A	3520	1/1	0.93	0.20	29,29,29,29	0
54	MG	1A	3325	1/1	0.93	0.14	40,40,40,40	0
54	MG	2D	302	1/1	0.93	0.23	44,44,44,44	0
54	MG	1A	3989	1/1	0.93	0.14	28,28,28,28	0
54	MG	1A	3522	1/1	0.93	0.24	51,51,51,51	0
54	MG	2A	3446	1/1	0.93	0.11	66,66,66,66	0
54	MG	2A	3027	1/1	0.93	0.17	58,58,58,58	0
54	MG	1A	3128	1/1	0.93	0.29	50,50,50,50	0
54	MG	1A	3457	1/1	0.93	0.09	50,50,50,50	0
54	MG	1A	3186	1/1	0.93	0.27	41,41,41,41	0
54	MG	1U	208	1/1	0.93	0.17	40,40,40,40	0
54	MG	1A	3681	1/1	0.93	0.23	51,51,51,51	0
54	MG	1A	3683	1/1	0.93	0.11	44,44,44,44	0
54	MG	1A	3459	1/1	0.93	0.12	60,60,60,60	0
54	MG	2A	3039	1/1	0.93	0.24	64,64,64,64	0
59	ZN	1n	102	1/1	0.93	0.10	84,84,84,84	0
54	MG	2A	3040	1/1	0.93	0.19	47,47,47,47	0
54	MG	2E	303	1/1	0.94	0.09	50,50,50,50	0
54	MG	1a	1760	1/1	0.94	0.21	70,70,70,70	0
54	MG	1A	3906	1/1	0.94	0.17	34,34,34,34	0
54	MG	2A	3018	1/1	0.94	0.67	45,45,45,45	0
54	MG	1A	3634	1/1	0.94	0.27	34,34,34,34	0
54	MG	1A	3051	1/1	0.94	0.19	47,47,47,47	0
54	MG	1B	210	1/1	0.94	0.08	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3453	1/1	0.94	0.20	65,65,65,65	0
54	MG	2A	3024	1/1	0.94	0.07	65,65,65,65	0
54	MG	1A	3101	1/1	0.94	0.15	38,38,38,38	0
54	MG	1B	214	1/1	0.94	0.40	59,59,59,59	0
54	MG	2A	3458	1/1	0.94	0.20	64,64,64,64	0
54	MG	1B	215	1/1	0.94	0.13	65,65,65,65	0
54	MG	2T	202	1/1	0.94	0.15	70,70,70,70	0
54	MG	2A	3028	1/1	0.94	0.19	31,31,31,31	0
54	MG	1A	3802	1/1	0.94	0.24	69,69,69,69	0
54	MG	1a	1772	1/1	0.94	0.09	72,72,72,72	0
54	MG	1A	3710	1/1	0.94	0.15	45,45,45,45	0
54	MG	1A	3177	1/1	0.94	0.21	28,28,28,28	0
54	MG	1A	3487	1/1	0.94	0.23	58,58,58,58	0
54	MG	25	101	1/1	0.94	0.23	49,49,49,49	0
54	MG	25	102	1/1	0.94	0.31	50,50,50,50	0
54	MG	2A	3470	1/1	0.94	0.20	50,50,50,50	0
54	MG	2A	3229	1/1	0.94	0.17	57,57,57,57	0
54	MG	1A	3204	1/1	0.94	0.29	60,60,60,60	0
54	MG	1A	3489	1/1	0.94	0.19	58,58,58,58	0
54	MG	1A	3641	1/1	0.94	0.18	34,34,34,34	0
54	MG	1A	3810	1/1	0.94	0.23	44,44,44,44	0
54	MG	1a	1781	1/1	0.94	0.30	47,47,47,47	0
54	MG	2A	3236	1/1	0.94	0.15	44,44,44,44	0
54	MG	1A	3811	1/1	0.94	0.12	68,68,68,68	0
54	MG	1a	1783	1/1	0.94	0.12	74,74,74,74	0
54	MG	2A	3241	1/1	0.94	0.08	60,60,60,60	0
54	MG	1a	1640	1/1	0.94	0.12	72,72,72,72	0
54	MG	1A	3813	1/1	0.94	0.18	63,63,63,63	0
54	MG	1A	3814	1/1	0.94	0.43	53,53,53,53	0
54	MG	1A	3932	1/1	0.94	0.12	51,51,51,51	0
54	MG	1A	3815	1/1	0.94	0.18	68,68,68,68	0
54	MG	2a	3018	1/1	0.94	0.17	51,51,51,51	0
54	MG	1A	3934	1/1	0.94	0.07	50,50,50,50	0
54	MG	1A	3722	1/1	0.94	0.15	30,30,30,30	0
54	MG	2a	3021	1/1	0.94	0.10	51,51,51,51	0
54	MG	2A	3258	1/1	0.94	0.10	49,49,49,49	0
54	MG	1A	3819	1/1	0.94	0.10	48,48,48,48	0
54	MG	2A	3496	1/1	0.94	0.12	63,63,63,63	0
54	MG	2A	3498	1/1	0.94	0.21	43,43,43,43	0
54	MG	2A	3263	1/1	0.94	0.17	66,66,66,66	0
54	MG	1A	3292	1/1	0.94	0.18	43,43,43,43	0
54	MG	1D	316	1/1	0.94	0.26	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1E	304	1/1	0.94	0.20	29,29,29,29	0
54	MG	2A	3269	1/1	0.94	0.17	68,68,68,68	0
54	MG	1E	305	1/1	0.94	0.22	31,31,31,31	0
54	MG	1A	3571	1/1	0.94	0.18	60,60,60,60	0
54	MG	1a	1799	1/1	0.94	0.09	82,82,82,82	0
54	MG	1E	307	1/1	0.94	0.20	26,26,26,26	0
54	MG	2A	3513	1/1	0.94	0.09	50,50,50,50	0
54	MG	1a	1656	1/1	0.94	0.20	68,68,68,68	0
54	MG	1A	3434	1/1	0.94	0.22	32,32,32,32	0
54	MG	2a	3042	1/1	0.94	0.23	62,62,62,62	0
54	MG	1E	309	1/1	0.94	0.19	61,61,61,61	0
54	MG	2A	3067	1/1	0.94	0.19	37,37,37,37	0
54	MG	1A	3001	1/1	0.94	0.13	42,42,42,42	0
54	MG	1A	3942	1/1	0.94	0.06	54,54,54,54	0
54	MG	1A	3943	1/1	0.94	0.36	58,58,58,58	0
54	MG	1a	1811	1/1	0.94	0.10	74,74,74,74	0
54	MG	2A	3075	1/1	0.94	0.22	47,47,47,47	0
54	MG	1A	3648	1/1	0.94	0.37	36,36,36,36	0
54	MG	1A	3825	1/1	0.94	0.14	64,64,64,64	0
54	MG	1A	3436	1/1	0.94	0.18	35,35,35,35	0
54	MG	2A	3298	1/1	0.94	0.20	57,57,57,57	0
54	MG	1A	3828	1/1	0.94	0.19	38,38,38,38	0
54	MG	1F	314	1/1	0.94	0.47	75,75,75,75	0
54	MG	1A	3829	1/1	0.94	0.21	42,42,42,42	0
54	MG	2A	3536	1/1	0.94	0.11	50,50,50,50	0
54	MG	1A	3578	1/1	0.94	0.23	63,63,63,63	0
54	MG	1A	3497	1/1	0.94	0.16	48,48,48,48	0
54	MG	1A	3582	1/1	0.94	0.32	48,48,48,48	0
54	MG	1a	1822	1/1	0.94	0.10	71,71,71,71	0
54	MG	1A	3103	1/1	0.94	0.22	41,41,41,41	0
54	MG	1A	3085	1/1	0.94	0.17	35,35,35,35	0
54	MG	1A	3838	1/1	0.94	0.13	46,46,46,46	0
54	MG	2A	3312	1/1	0.94	0.10	62,62,62,62	0
54	MG	2A	3551	1/1	0.94	0.13	54,54,54,54	0
54	MG	1a	1826	1/1	0.94	0.11	65,65,65,65	0
54	MG	1a	1827	1/1	0.94	0.08	66,66,66,66	0
54	MG	1A	3009	1/1	0.94	0.18	35,35,35,35	0
54	MG	1P	201	1/1	0.94	0.29	38,38,38,38	0
54	MG	2A	3558	1/1	0.94	0.07	80,80,80,80	0
54	MG	2A	3101	1/1	0.94	0.12	42,42,42,42	0
54	MG	2A	3561	1/1	0.94	0.09	72,72,72,72	0
54	MG	1A	3840	1/1	0.94	0.15	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3060	1/1	0.94	0.23	55,55,55,55	0
54	MG	1Q	202	1/1	0.94	0.15	37,37,37,37	0
54	MG	1A	3301	1/1	0.94	0.22	34,34,34,34	0
54	MG	1A	3750	1/1	0.94	0.15	51,51,51,51	0
54	MG	1A	3045	1/1	0.94	0.22	32,32,32,32	0
54	MG	2A	3327	1/1	0.94	0.21	56,56,56,56	0
54	MG	1A	3968	1/1	0.94	0.15	71,71,71,71	0
54	MG	1A	3395	1/1	0.94	0.21	45,45,45,45	0
54	MG	2A	3112	1/1	0.94	0.26	51,51,51,51	0
54	MG	1A	3162	1/1	0.94	0.27	36,36,36,36	0
54	MG	1A	3595	1/1	0.94	0.28	67,67,67,67	0
54	MG	2A	3334	1/1	0.94	0.41	55,55,55,55	0
54	MG	1T	204	1/1	0.94	0.05	70,70,70,70	0
54	MG	1A	3976	1/1	0.94	0.16	40,40,40,40	0
54	MG	2a	3095	1/1	0.94	0.41	62,62,62,62	0
54	MG	2a	3096	1/1	0.94	0.33	70,70,70,70	0
54	MG	1A	3977	1/1	0.94	0.06	63,63,63,63	0
54	MG	2A	3341	1/1	0.94	0.31	71,71,71,71	0
54	MG	1A	3665	1/1	0.94	0.18	54,54,54,54	0
54	MG	1A	3515	1/1	0.94	0.18	65,65,65,65	0
54	MG	1A	3980	1/1	0.94	0.19	26,26,26,26	0
54	MG	1A	3855	1/1	0.94	0.15	56,56,56,56	0
54	MG	2A	3592	1/1	0.94	0.10	59,59,59,59	0
54	MG	1A	3983	1/1	0.94	0.15	54,54,54,54	0
54	MG	1A	3516	1/1	0.94	0.09	64,64,64,64	0
54	MG	2A	3356	1/1	0.94	0.11	89,89,89,89	0
54	MG	2A	3357	1/1	0.94	0.19	50,50,50,50	0
54	MG	1A	3163	1/1	0.94	0.17	38,38,38,38	0
54	MG	10	102	1/1	0.94	0.62	44,44,44,44	0
54	MG	1A	3398	1/1	0.94	0.24	50,50,50,50	0
54	MG	2a	3113	1/1	0.94	0.17	81,81,81,81	0
54	MG	10	104	1/1	0.94	0.14	53,53,53,53	0
54	MG	1A	3047	1/1	0.94	0.30	58,58,58,58	0
54	MG	2A	3606	1/1	0.94	0.16	42,42,42,42	0
54	MG	1A	3093	1/1	0.94	0.15	56,56,56,56	0
54	MG	10	107	1/1	0.94	0.15	57,57,57,57	0
54	MG	1a	1707	1/1	0.94	0.10	75,75,75,75	0
54	MG	2a	3121	1/1	0.94	0.20	70,70,70,70	0
54	MG	1A	3766	1/1	0.94	0.13	47,47,47,47	0
54	MG	1A	3226	1/1	0.94	0.23	39,39,39,39	0
54	MG	1A	3605	1/1	0.94	0.26	25,25,25,25	0
54	MG	2A	3613	1/1	0.94	0.07	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3870	1/1	0.94	0.16	59,59,59,59	0
54	MG	2A	3372	1/1	0.94	0.07	61,61,61,61	0
54	MG	1A	3353	1/1	0.94	0.17	40,40,40,40	0
54	MG	2A	3143	1/1	0.94	0.09	49,49,49,49	0
54	MG	2A	3376	1/1	0.94	0.10	62,62,62,62	0
54	MG	1A	3228	1/1	0.94	0.14	39,39,39,39	0
54	MG	1A	3116	1/1	0.94	0.13	61,61,61,61	0
54	MG	1A	3406	1/1	0.94	0.16	42,42,42,42	0
54	MG	1a	1878	1/1	0.94	0.16	61,61,61,61	0
54	MG	1a	1879	1/1	0.94	0.14	72,72,72,72	0
54	MG	1A	3408	1/1	0.94	0.16	33,33,33,33	0
54	MG	2A	3631	1/1	0.94	0.08	62,62,62,62	0
54	MG	1A	3879	1/1	0.94	0.15	53,53,53,53	0
54	MG	1a	1721	1/1	0.94	0.24	69,69,69,69	0
54	MG	1A	3064	1/1	0.94	0.23	41,41,41,41	0
54	MG	2a	3143	1/1	0.94	0.05	81,81,81,81	0
54	MG	2a	3144	1/1	0.94	0.06	78,78,78,78	0
54	MG	15	108	1/1	0.94	0.14	74,74,74,74	0
54	MG	1A	3883	1/1	0.94	0.19	35,35,35,35	0
54	MG	1A	3234	1/1	0.94	0.14	34,34,34,34	0
54	MG	1A	3236	1/1	0.94	0.69	42,42,42,42	0
54	MG	1a	1729	1/1	0.94	0.23	46,46,46,46	0
54	MG	1A	4012	1/1	0.94	0.07	60,60,60,60	0
54	MG	2A	3165	1/1	0.94	0.30	66,66,66,66	0
54	MG	2a	3156	1/1	0.94	0.23	67,67,67,67	0
54	MG	2A	3650	1/1	0.94	0.16	37,37,37,37	0
54	MG	1A	3542	1/1	0.94	0.24	50,50,50,50	0
54	MG	1A	3890	1/1	0.94	0.22	30,30,30,30	0
54	MG	1A	3169	1/1	0.94	0.20	35,35,35,35	0
54	MG	2A	3171	1/1	0.94	0.32	51,51,51,51	0
54	MG	2a	3162	1/1	0.94	0.25	69,69,69,69	0
54	MG	2A	3655	1/1	0.94	0.18	47,47,47,47	0
54	MG	2A	3656	1/1	0.94	0.24	39,39,39,39	0
54	MG	1h	202	1/1	0.94	0.28	66,66,66,66	0
54	MG	1A	3096	1/1	0.94	0.23	42,42,42,42	0
54	MG	1a	1607	1/1	0.94	0.17	64,64,64,64	0
54	MG	1A	3421	1/1	0.94	0.18	60,60,60,60	0
54	MG	2A	3176	1/1	0.94	0.40	39,39,39,39	0
54	MG	1A	3548	1/1	0.94	0.14	56,56,56,56	0
54	MG	1A	3282	1/1	0.94	0.24	35,35,35,35	0
54	MG	2a	3178	1/1	0.94	0.19	73,73,73,73	0
54	MG	2A	3180	1/1	0.94	0.21	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3665	1/1	0.94	0.29	72,72,72,72	0
54	MG	1a	1611	1/1	0.94	0.39	53,53,53,53	0
54	MG	2a	3184	1/1	0.94	0.44	66,66,66,66	0
54	MG	1a	1612	1/1	0.94	0.23	65,65,65,65	0
54	MG	2a	3186	1/1	0.94	0.13	76,76,76,76	0
54	MG	1A	3424	1/1	0.94	0.24	65,65,65,65	0
54	MG	2a	3189	1/1	0.94	0.31	78,78,78,78	0
54	MG	1y	202	1/1	0.94	0.12	74,74,74,74	0
54	MG	1A	4022	1/1	0.94	0.22	51,51,51,51	0
54	MG	2A	3426	1/1	0.94	0.18	61,61,61,61	0
54	MG	2A	3188	1/1	0.94	0.27	25,25,25,25	0
54	MG	2A	3429	1/1	0.94	0.19	37,37,37,37	0
54	MG	1a	1749	1/1	0.94	0.07	73,73,73,73	0
54	MG	1a	1751	1/1	0.94	0.11	61,61,61,61	0
54	MG	2A	3434	1/1	0.94	0.19	52,52,52,52	0
55	HGR	2A	3671	36/36	0.94	0.26	35,44,51,55	0
54	MG	1A	3791	1/1	0.94	0.28	49,49,49,49	0
54	MG	1A	3551	1/1	0.94	0.21	53,53,53,53	0
54	MG	2A	3195	1/1	0.94	0.15	64,64,64,64	0
54	MG	2A	3438	1/1	0.94	0.03	72,72,72,72	0
57	MPD	18	103	8/8	0.94	0.26	35,42,47,49	0
54	MG	1A	3794	1/1	0.94	0.14	56,56,56,56	0
54	MG	1A	3372	1/1	0.94	0.18	38,38,38,38	0
54	MG	1A	3903	1/1	0.94	0.17	42,42,42,42	0
54	MG	2A	3200	1/1	0.94	0.17	58,58,58,58	0
54	MG	1A	3021	1/1	0.94	0.22	43,43,43,43	0
54	MG	1A	3557	1/1	0.94	0.17	37,37,37,37	0
54	MG	2A	3014	1/1	0.94	0.15	60,60,60,60	0
54	MG	2E	301	1/1	0.94	0.28	44,44,44,44	0
54	MG	2E	302	1/1	0.94	0.21	42,42,42,42	0
59	ZN	2n	102	1/1	0.94	0.05	95,95,95,95	0
54	MG	1A	3266	1/1	0.95	0.20	39,39,39,39	0
54	MG	1A	3344	1/1	0.95	0.25	29,29,29,29	0
54	MG	2A	3134	1/1	0.95	0.15	42,42,42,42	0
54	MG	1A	3857	1/1	0.95	0.11	44,44,44,44	0
54	MG	2A	3323	1/1	0.95	0.20	50,50,50,50	0
54	MG	1a	1633	1/1	0.95	0.10	63,63,63,63	0
54	MG	1A	3858	1/1	0.95	0.18	57,57,57,57	0
54	MG	1A	3224	1/1	0.95	0.24	30,30,30,30	0
54	MG	1A	3770	1/1	0.95	0.27	58,58,58,58	0
54	MG	1F	301	1/1	0.95	0.16	35,35,35,35	0
54	MG	1A	3155	1/1	0.95	0.32	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1757	1/1	0.95	0.18	73,73,73,73	0
54	MG	1A	3348	1/1	0.95	0.31	58,58,58,58	0
54	MG	1A	3349	1/1	0.95	0.17	30,30,30,30	0
54	MG	1a	1641	1/1	0.95	0.20	56,56,56,56	0
54	MG	2A	3538	1/1	0.95	0.26	65,65,65,65	0
54	MG	2a	3027	1/1	0.95	0.21	76,76,76,76	0
54	MG	2A	3338	1/1	0.95	0.21	44,44,44,44	0
54	MG	1A	3535	1/1	0.95	0.32	45,45,45,45	0
54	MG	1A	3464	1/1	0.95	0.21	60,60,60,60	0
54	MG	2A	3152	1/1	0.95	0.24	57,57,57,57	0
54	MG	2a	3032	1/1	0.95	0.09	71,71,71,71	0
54	MG	2A	3342	1/1	0.95	0.20	46,46,46,46	0
54	MG	2A	3548	1/1	0.95	0.25	38,38,38,38	0
54	MG	1A	3684	1/1	0.95	0.11	63,63,63,63	0
54	MG	2A	3346	1/1	0.95	0.14	42,42,42,42	0
54	MG	1A	3176	1/1	0.95	0.19	37,37,37,37	0
54	MG	1A	3540	1/1	0.95	0.20	25,25,25,25	0
54	MG	1a	1768	1/1	0.95	0.08	68,68,68,68	0
54	MG	2A	3555	1/1	0.95	0.34	42,42,42,42	0
54	MG	2a	3044	1/1	0.95	0.08	79,79,79,79	0
54	MG	1F	315	1/1	0.95	0.16	49,49,49,49	0
54	MG	2A	3352	1/1	0.95	0.23	67,67,67,67	0
54	MG	2A	3354	1/1	0.95	0.24	68,68,68,68	0
54	MG	1A	3025	1/1	0.95	0.14	35,35,35,35	0
54	MG	1A	3614	1/1	0.95	0.15	46,46,46,46	0
54	MG	1A	3068	1/1	0.95	0.29	53,53,53,53	0
54	MG	1a	1773	1/1	0.95	0.13	74,74,74,74	0
54	MG	1A	3616	1/1	0.95	0.23	61,61,61,61	0
54	MG	1A	3470	1/1	0.95	0.12	64,64,64,64	0
54	MG	1A	3199	1/1	0.95	0.11	37,37,37,37	0
54	MG	1A	3698	1/1	0.95	0.13	37,37,37,37	0
54	MG	1a	1655	1/1	0.95	0.19	47,47,47,47	0
54	MG	1A	3200	1/1	0.95	0.18	47,47,47,47	0
54	MG	1A	3792	1/1	0.95	0.20	49,49,49,49	0
54	MG	1P	202	1/1	0.95	0.16	37,37,37,37	0
54	MG	1A	3886	1/1	0.95	0.29	41,41,41,41	0
54	MG	1A	3475	1/1	0.95	0.15	38,38,38,38	0
54	MG	2A	3577	1/1	0.95	0.07	75,75,75,75	0
54	MG	1A	3889	1/1	0.95	0.22	45,45,45,45	0
54	MG	2A	3581	1/1	0.95	0.21	43,43,43,43	0
54	MG	1A	3070	1/1	0.95	0.28	42,42,42,42	0
54	MG	2A	3020	1/1	0.95	0.40	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3360	1/1	0.95	0.13	42,42,42,42	0
54	MG	1A	3418	1/1	0.95	0.23	22,22,22,22	0
54	MG	2A	3377	1/1	0.95	0.17	67,67,67,67	0
54	MG	1A	3119	1/1	0.95	0.26	35,35,35,35	0
54	MG	1A	3365	1/1	0.95	0.14	41,41,41,41	0
54	MG	2A	3380	1/1	0.95	0.08	52,52,52,52	0
54	MG	1A	3632	1/1	0.95	0.22	22,22,22,22	0
54	MG	1A	3556	1/1	0.95	0.19	34,34,34,34	0
54	MG	1A	3120	1/1	0.95	0.38	45,45,45,45	0
54	MG	1a	1794	1/1	0.95	0.08	70,70,70,70	0
54	MG	1U	204	1/1	0.95	0.38	59,59,59,59	0
54	MG	2A	3387	1/1	0.95	0.16	41,41,41,41	0
54	MG	2a	3081	1/1	0.95	0.11	72,72,72,72	0
54	MG	1A	4002	1/1	0.95	0.10	67,67,67,67	0
54	MG	2a	3083	1/1	0.95	0.21	68,68,68,68	0
54	MG	2A	3389	1/1	0.95	0.22	52,52,52,52	0
54	MG	1A	3319	1/1	0.95	0.16	29,29,29,29	0
54	MG	2A	3035	1/1	0.95	0.21	67,67,67,67	0
54	MG	2A	3605	1/1	0.95	0.29	67,67,67,67	0
54	MG	2A	3394	1/1	0.95	0.10	52,52,52,52	0
54	MG	1A	4005	1/1	0.95	0.16	31,31,31,31	0
54	MG	2A	3197	1/1	0.95	0.41	61,61,61,61	0
54	MG	1A	3246	1/1	0.95	0.31	37,37,37,37	0
54	MG	1A	3321	1/1	0.95	0.32	33,33,33,33	0
54	MG	1a	1676	1/1	0.95	0.26	66,66,66,66	0
54	MG	1A	3714	1/1	0.95	0.28	52,52,52,52	0
54	MG	2A	3202	1/1	0.95	0.22	44,44,44,44	0
54	MG	1A	4011	1/1	0.95	0.12	40,40,40,40	0
54	MG	1A	3565	1/1	0.95	0.17	37,37,37,37	0
54	MG	1a	1805	1/1	0.95	0.20	69,69,69,69	0
54	MG	2A	3207	1/1	0.95	0.17	45,45,45,45	0
54	MG	1A	3373	1/1	0.95	0.24	24,24,24,24	0
54	MG	2A	3620	1/1	0.95	0.17	47,47,47,47	0
54	MG	1A	3059	1/1	0.95	0.26	30,30,30,30	0
54	MG	1a	1809	1/1	0.95	0.08	70,70,70,70	0
54	MG	1a	1810	1/1	0.95	0.06	63,63,63,63	0
54	MG	1A	3490	1/1	0.95	0.27	23,23,23,23	0
54	MG	1A	3026	1/1	0.95	0.18	35,35,35,35	0
54	MG	1A	3643	1/1	0.95	0.13	29,29,29,29	0
54	MG	1A	3147	1/1	0.95	0.18	34,34,34,34	0
54	MG	2A	3420	1/1	0.95	0.14	51,51,51,51	0
54	MG	1A	3911	1/1	0.95	0.19	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3912	1/1	0.95	0.15	21,21,21,21	0
54	MG	2A	3635	1/1	0.95	0.16	57,57,57,57	0
54	MG	2A	3636	1/1	0.95	0.07	60,60,60,60	0
54	MG	2A	3638	1/1	0.95	0.25	64,64,64,64	0
54	MG	1A	4021	1/1	0.95	0.24	56,56,56,56	0
54	MG	2A	3424	1/1	0.95	0.16	49,49,49,49	0
54	MG	1A	3727	1/1	0.95	0.21	42,42,42,42	0
54	MG	2a	3120	1/1	0.95	0.17	53,53,53,53	0
54	MG	1A	3818	1/1	0.95	0.23	39,39,39,39	0
54	MG	2A	3427	1/1	0.95	0.15	61,61,61,61	0
54	MG	1A	3728	1/1	0.95	0.16	36,36,36,36	0
54	MG	2A	3225	1/1	0.95	0.23	61,61,61,61	0
54	MG	1A	3379	1/1	0.95	0.21	19,19,19,19	0
54	MG	1A	3013	1/1	0.95	0.20	20,20,20,20	0
54	MG	1B	203	1/1	0.95	0.16	56,56,56,56	0
54	MG	2a	3128	1/1	0.95	0.27	75,75,75,75	0
54	MG	1A	3289	1/1	0.95	0.23	53,53,53,53	0
54	MG	2A	3066	1/1	0.95	0.21	56,56,56,56	0
54	MG	1A	3498	1/1	0.95	0.17	28,28,28,28	0
54	MG	1A	3736	1/1	0.95	0.31	56,56,56,56	0
54	MG	2A	3069	1/1	0.95	0.19	28,28,28,28	0
54	MG	1a	1828	1/1	0.95	0.10	74,74,74,74	0
54	MG	1A	3212	1/1	0.95	0.31	39,39,39,39	0
54	MG	17	101	1/1	0.95	0.25	42,42,42,42	0
54	MG	17	103	1/1	0.95	0.30	43,43,43,43	0
54	MG	1A	3652	1/1	0.95	0.15	37,37,37,37	0
54	MG	2A	3244	1/1	0.95	0.32	52,52,52,52	0
54	MG	2A	3245	1/1	0.95	0.27	49,49,49,49	0
54	MG	1A	3386	1/1	0.95	0.15	30,30,30,30	0
54	MG	2A	3079	1/1	0.95	0.26	54,54,54,54	0
54	MG	1a	1706	1/1	0.95	0.35	71,71,71,71	0
54	MG	2A	3251	1/1	0.95	0.18	67,67,67,67	0
54	MG	1A	3015	1/1	0.95	0.11	35,35,35,35	0
54	MG	2a	3147	1/1	0.95	0.13	46,46,46,46	0
54	MG	1a	1708	1/1	0.95	0.15	76,76,76,76	0
54	MG	1a	1709	1/1	0.95	0.11	74,74,74,74	0
54	MG	2A	3261	1/1	0.95	0.24	43,43,43,43	0
54	MG	1A	3744	1/1	0.95	0.17	38,38,38,38	0
54	MG	2A	3457	1/1	0.95	0.11	62,62,62,62	0
54	MG	1A	3063	1/1	0.95	0.13	40,40,40,40	0
54	MG	1A	3443	1/1	0.95	0.24	27,27,27,27	0
54	MG	1A	3835	1/1	0.95	0.17	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1845	1/1	0.95	0.07	77,77,77,77	0
54	MG	1a	1846	1/1	0.95	0.07	77,77,77,77	0
54	MG	2A	3270	1/1	0.95	0.19	44,44,44,44	0
54	MG	2A	3464	1/1	0.95	0.23	63,63,63,63	0
54	MG	2a	3163	1/1	0.95	0.13	54,54,54,54	0
54	MG	2A	3094	1/1	0.95	0.26	52,52,52,52	0
54	MG	2a	3165	1/1	0.95	0.12	64,64,64,64	0
54	MG	1A	3055	1/1	0.95	0.20	36,36,36,36	0
54	MG	2D	301	1/1	0.95	0.37	50,50,50,50	0
54	MG	2a	3168	1/1	0.95	0.21	55,55,55,55	0
54	MG	2A	3468	1/1	0.95	0.24	55,55,55,55	0
54	MG	2A	3469	1/1	0.95	0.18	44,44,44,44	0
54	MG	1A	3218	1/1	0.95	0.28	44,44,44,44	0
54	MG	1B	219	1/1	0.95	0.16	40,40,40,40	0
54	MG	1A	3391	1/1	0.95	0.25	32,32,32,32	0
54	MG	1A	3589	1/1	0.95	0.21	29,29,29,29	0
54	MG	1A	3057	1/1	0.95	0.36	43,43,43,43	0
54	MG	1A	3259	1/1	0.95	0.29	32,32,32,32	0
54	MG	1A	3517	1/1	0.95	0.15	43,43,43,43	0
54	MG	2a	3182	1/1	0.95	0.05	81,81,81,81	0
54	MG	1a	1723	1/1	0.95	0.30	64,64,64,64	0
54	MG	1a	1614	1/1	0.95	0.32	33,33,33,33	0
54	MG	1a	1860	1/1	0.95	0.13	56,56,56,56	0
54	MG	1A	3946	1/1	0.95	0.14	61,61,61,61	0
54	MG	2A	3289	1/1	0.95	0.26	47,47,47,47	0
54	MG	2a	3188	1/1	0.95	0.44	76,76,76,76	0
54	MG	1B	226	1/1	0.95	0.14	55,55,55,55	0
54	MG	1a	1864	1/1	0.95	0.17	65,65,65,65	0
54	MG	2A	3293	1/1	0.95	0.18	50,50,50,50	0
54	MG	2A	3294	1/1	0.95	0.29	64,64,64,64	0
54	MG	2A	3295	1/1	0.95	0.32	59,59,59,59	0
54	MG	1A	3133	1/1	0.95	0.11	35,35,35,35	0
54	MG	2A	3113	1/1	0.95	0.21	48,48,48,48	0
54	MG	1A	3948	1/1	0.95	0.14	32,32,32,32	0
54	MG	1B	229	1/1	0.95	0.07	60,60,60,60	0
54	MG	2t	201	1/1	0.95	0.13	55,55,55,55	0
55	HGR	1A	4026	36/36	0.95	0.24	20,30,38,44	0
54	MG	2W	201	1/1	0.95	0.16	50,50,50,50	0
54	MG	2W	202	1/1	0.95	0.15	61,61,61,61	0
54	MG	1A	3338	1/1	0.95	0.26	70,70,70,70	0
54	MG	1D	302	1/1	0.95	0.20	54,54,54,54	0
54	MG	1A	3668	1/1	0.95	0.08	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3119	1/1	0.95	0.15	47,47,47,47	0
54	MG	1D	308	1/1	0.95	0.19	41,41,41,41	0
54	MG	1A	3261	1/1	0.95	0.22	40,40,40,40	0
54	MG	1A	3263	1/1	0.95	0.20	48,48,48,48	0
54	MG	1a	1738	1/1	0.95	0.15	71,71,71,71	0
54	MG	1A	3953	1/1	0.95	0.11	45,45,45,45	0
54	MG	1A	3524	1/1	0.95	0.16	28,28,28,28	0
54	MG	1A	3852	1/1	0.95	0.11	47,47,47,47	0
54	MG	1E	301	1/1	0.95	0.17	34,34,34,34	0
54	MG	1a	1744	1/1	0.95	0.15	70,70,70,70	0
54	MG	1a	1746	1/1	0.95	0.07	55,55,55,55	0
54	MG	2A	3517	1/1	0.96	0.28	63,63,63,63	0
54	MG	1A	3505	1/1	0.96	0.09	45,45,45,45	0
54	MG	1k	201	1/1	0.96	0.24	49,49,49,49	0
54	MG	1A	3023	1/1	0.96	0.18	37,37,37,37	0
54	MG	2A	3521	1/1	0.96	0.13	54,54,54,54	0
54	MG	2A	3150	1/1	0.96	0.34	60,60,60,60	0
54	MG	1a	1762	1/1	0.96	0.18	56,56,56,56	0
54	MG	1a	1763	1/1	0.96	0.14	67,67,67,67	0
54	MG	1A	3024	1/1	0.96	0.23	29,29,29,29	0
54	MG	2A	3527	1/1	0.96	0.05	63,63,63,63	0
54	MG	2a	3015	1/1	0.96	0.12	59,59,59,59	0
54	MG	2A	3154	1/1	0.96	0.31	61,61,61,61	0
54	MG	1A	3161	1/1	0.96	0.18	36,36,36,36	0
54	MG	1A	3511	1/1	0.96	0.23	33,33,33,33	0
54	MG	1A	3747	1/1	0.96	0.26	34,34,34,34	0
54	MG	2A	3532	1/1	0.96	0.17	40,40,40,40	0
54	MG	1A	3216	1/1	0.96	0.36	43,43,43,43	0
54	MG	2A	3343	1/1	0.96	0.17	67,67,67,67	0
54	MG	1A	3513	1/1	0.96	0.21	49,49,49,49	0
54	MG	2A	3345	1/1	0.96	0.12	45,45,45,45	0
54	MG	2A	3160	1/1	0.96	0.25	59,59,59,59	0
54	MG	1A	3955	1/1	0.96	0.12	65,65,65,65	0
54	MG	1A	3114	1/1	0.96	0.24	33,33,33,33	0
54	MG	1A	3591	1/1	0.96	0.22	32,32,32,32	0
54	MG	1F	302	1/1	0.96	0.19	31,31,31,31	0
54	MG	2A	3351	1/1	0.96	0.11	52,52,52,52	0
54	MG	1F	303	1/1	0.96	0.26	42,42,42,42	0
54	MG	2A	3546	1/1	0.96	0.23	51,51,51,51	0
54	MG	2A	3353	1/1	0.96	0.33	56,56,56,56	0
54	MG	2A	3008	1/1	0.96	0.27	46,46,46,46	0
54	MG	1A	3592	1/1	0.96	0.20	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3036	1/1	0.96	0.29	48,48,48,48	0
54	MG	1A	3043	1/1	0.96	0.23	19,19,19,19	0
54	MG	2a	3038	1/1	0.96	0.24	82,82,82,82	0
54	MG	2A	3169	1/1	0.96	0.14	41,41,41,41	0
54	MG	2A	3553	1/1	0.96	0.24	62,62,62,62	0
54	MG	1A	3219	1/1	0.96	0.17	48,48,48,48	0
54	MG	1A	3304	1/1	0.96	0.20	47,47,47,47	0
54	MG	2a	3043	1/1	0.96	0.28	66,66,66,66	0
54	MG	1A	3598	1/1	0.96	0.32	70,70,70,70	0
54	MG	1A	3760	1/1	0.96	0.20	31,31,31,31	0
54	MG	1A	3856	1/1	0.96	0.10	37,37,37,37	0
54	MG	1A	3347	1/1	0.96	0.19	32,32,32,32	0
54	MG	2A	3560	1/1	0.96	0.11	56,56,56,56	0
54	MG	1A	3221	1/1	0.96	0.13	35,35,35,35	0
54	MG	1A	3859	1/1	0.96	0.23	39,39,39,39	0
54	MG	1F	317	1/1	0.96	0.18	47,47,47,47	0
54	MG	1A	3971	1/1	0.96	0.13	48,48,48,48	0
54	MG	1A	3972	1/1	0.96	0.23	47,47,47,47	0
54	MG	1A	3098	1/1	0.96	0.20	20,20,20,20	0
54	MG	1A	3350	1/1	0.96	0.23	28,28,28,28	0
54	MG	2A	3186	1/1	0.96	0.15	46,46,46,46	0
54	MG	2A	3374	1/1	0.96	0.17	69,69,69,69	0
54	MG	1A	3675	1/1	0.96	0.10	43,43,43,43	0
54	MG	1H	202	1/1	0.96	0.20	46,46,46,46	0
54	MG	1N	202	1/1	0.96	0.13	40,40,40,40	0
54	MG	2A	3575	1/1	0.96	0.15	75,75,75,75	0
54	MG	1A	3526	1/1	0.96	0.16	28,28,28,28	0
54	MG	1A	3265	1/1	0.96	0.25	36,36,36,36	0
54	MG	2A	3578	1/1	0.96	0.04	65,65,65,65	0
54	MG	1O	201	1/1	0.96	0.22	61,61,61,61	0
54	MG	1A	3769	1/1	0.96	0.15	39,39,39,39	0
54	MG	1A	3867	1/1	0.96	0.09	54,54,54,54	0
54	MG	1A	3528	1/1	0.96	0.17	35,35,35,35	0
54	MG	1A	3984	1/1	0.96	0.10	55,55,55,55	0
54	MG	1P	206	1/1	0.96	0.09	77,77,77,77	0
54	MG	1A	3118	1/1	0.96	0.21	30,30,30,30	0
54	MG	1A	3354	1/1	0.96	0.22	30,30,30,30	0
54	MG	1A	3044	1/1	0.96	0.17	34,34,34,34	0
54	MG	1A	3682	1/1	0.96	0.09	38,38,38,38	0
54	MG	2A	3591	1/1	0.96	0.29	60,60,60,60	0
54	MG	1A	3225	1/1	0.96	0.13	44,44,44,44	0
54	MG	1A	3407	1/1	0.96	0.19	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3395	1/1	0.96	0.24	54,54,54,54	0
54	MG	1a	1808	1/1	0.96	0.12	57,57,57,57	0
54	MG	1A	3466	1/1	0.96	0.17	55,55,55,55	0
54	MG	1A	3992	1/1	0.96	0.14	45,45,45,45	0
54	MG	1A	3876	1/1	0.96	0.15	62,62,62,62	0
54	MG	1U	202	1/1	0.96	0.19	39,39,39,39	0
54	MG	1A	3146	1/1	0.96	0.16	45,45,45,45	0
54	MG	1U	205	1/1	0.96	0.20	42,42,42,42	0
54	MG	2A	3604	1/1	0.96	0.11	71,71,71,71	0
54	MG	1A	3880	1/1	0.96	0.16	28,28,28,28	0
54	MG	1a	1686	1/1	0.96	0.10	54,54,54,54	0
54	MG	1A	3780	1/1	0.96	0.14	43,43,43,43	0
54	MG	2A	3059	1/1	0.96	0.21	41,41,41,41	0
54	MG	2A	3408	1/1	0.96	0.13	68,68,68,68	0
54	MG	1A	3882	1/1	0.96	0.20	39,39,39,39	0
54	MG	1A	3409	1/1	0.96	0.22	26,26,26,26	0
54	MG	2A	3411	1/1	0.96	0.14	68,68,68,68	0
54	MG	1A	3227	1/1	0.96	0.20	48,48,48,48	0
54	MG	1A	3689	1/1	0.96	0.17	63,63,63,63	0
54	MG	1A	3690	1/1	0.96	0.25	68,68,68,68	0
54	MG	1A	3887	1/1	0.96	0.24	28,28,28,28	0
54	MG	1A	4004	1/1	0.96	0.15	53,53,53,53	0
54	MG	2A	3417	1/1	0.96	0.28	33,33,33,33	0
54	MG	2A	3418	1/1	0.96	0.27	51,51,51,51	0
54	MG	2A	3621	1/1	0.96	0.19	49,49,49,49	0
54	MG	1A	3787	1/1	0.96	0.16	37,37,37,37	0
54	MG	2A	3623	1/1	0.96	0.33	71,71,71,71	0
54	MG	1A	3083	1/1	0.96	0.16	37,37,37,37	0
54	MG	2A	3625	1/1	0.96	0.21	72,72,72,72	0
54	MG	2A	3626	1/1	0.96	0.06	62,62,62,62	0
54	MG	1A	4008	1/1	0.96	0.25	40,40,40,40	0
54	MG	1A	3692	1/1	0.96	0.08	63,63,63,63	0
54	MG	1A	3316	1/1	0.96	0.18	46,46,46,46	0
54	MG	2A	3235	1/1	0.96	0.11	59,59,59,59	0
54	MG	1A	3694	1/1	0.96	0.21	68,68,68,68	0
54	MG	2A	3074	1/1	0.96	0.19	42,42,42,42	0
54	MG	1a	1832	1/1	0.96	0.08	63,63,63,63	0
54	MG	1A	3069	1/1	0.96	0.19	44,44,44,44	0
54	MG	1A	3618	1/1	0.96	0.33	36,36,36,36	0
54	MG	2A	3430	1/1	0.96	0.19	60,60,60,60	0
54	MG	2A	3431	1/1	0.96	0.23	45,45,45,45	0
54	MG	2A	3639	1/1	0.96	0.13	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1704	1/1	0.96	0.29	66,66,66,66	0
54	MG	1A	3124	1/1	0.96	0.26	26,26,26,26	0
54	MG	1A	3621	1/1	0.96	0.23	64,64,64,64	0
54	MG	2A	3645	1/1	0.96	0.16	64,64,64,64	0
54	MG	1A	3796	1/1	0.96	0.15	21,21,21,21	0
54	MG	1A	3622	1/1	0.96	0.24	40,40,40,40	0
54	MG	1A	3623	1/1	0.96	0.18	32,32,32,32	0
54	MG	2A	3086	1/1	0.96	0.43	65,65,65,65	0
54	MG	2A	3439	1/1	0.96	0.22	56,56,56,56	0
54	MG	2A	3252	1/1	0.96	0.22	52,52,52,52	0
54	MG	1A	3624	1/1	0.96	0.15	40,40,40,40	0
54	MG	2a	3135	1/1	0.96	0.20	58,58,58,58	0
54	MG	1a	1711	1/1	0.96	0.15	61,61,61,61	0
54	MG	2A	3255	1/1	0.96	0.22	56,56,56,56	0
54	MG	2A	3256	1/1	0.96	0.17	69,69,69,69	0
54	MG	2A	3257	1/1	0.96	0.27	49,49,49,49	0
54	MG	2A	3089	1/1	0.96	0.21	36,36,36,36	0
54	MG	2A	3090	1/1	0.96	0.11	73,73,73,73	0
54	MG	1A	3233	1/1	0.96	0.12	56,56,56,56	0
54	MG	1A	3420	1/1	0.96	0.24	28,28,28,28	0
54	MG	1A	3036	1/1	0.96	0.23	34,34,34,34	0
54	MG	1A	3370	1/1	0.96	0.17	34,34,34,34	0
54	MG	1A	3046	1/1	0.96	0.27	19,19,19,19	0
54	MG	2A	3268	1/1	0.96	0.24	33,33,33,33	0
54	MG	2A	3096	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	3483	1/1	0.96	0.13	58,58,58,58	0
54	MG	17	104	1/1	0.96	0.41	59,59,59,59	0
54	MG	1a	1853	1/1	0.96	0.14	65,65,65,65	0
54	MG	2a	3153	1/1	0.96	0.07	85,85,85,85	0
54	MG	1A	3806	1/1	0.96	0.24	38,38,38,38	0
54	MG	1A	3237	1/1	0.96	0.22	38,38,38,38	0
54	MG	19	101	1/1	0.96	0.21	61,61,61,61	0
54	MG	1a	1857	1/1	0.96	0.13	62,62,62,62	0
54	MG	1A	3555	1/1	0.96	0.18	37,37,37,37	0
54	MG	2B	204	1/1	0.96	0.17	57,57,57,57	0
54	MG	2A	3280	1/1	0.96	0.13	66,66,66,66	0
54	MG	1A	3104	1/1	0.96	0.33	35,35,35,35	0
54	MG	1A	3376	1/1	0.96	0.14	45,45,45,45	0
54	MG	1A	3020	1/1	0.96	0.42	47,47,47,47	0
54	MG	1a	1862	1/1	0.96	0.19	49,49,49,49	0
54	MG	1A	3285	1/1	0.96	0.20	34,34,34,34	0
54	MG	1A	3005	1/1	0.96	0.20	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3919	1/1	0.96	0.14	40,40,40,40	0
54	MG	1B	212	1/1	0.96	0.14	44,44,44,44	0
54	MG	1A	3923	1/1	0.96	0.15	47,47,47,47	0
54	MG	2A	3292	1/1	0.96	0.20	38,38,38,38	0
54	MG	1A	3924	1/1	0.96	0.28	41,41,41,41	0
54	MG	2a	3173	1/1	0.96	0.20	63,63,63,63	0
54	MG	1A	3721	1/1	0.96	0.15	38,38,38,38	0
54	MG	1A	3491	1/1	0.96	0.14	51,51,51,51	0
54	MG	1A	3817	1/1	0.96	0.23	41,41,41,41	0
54	MG	1A	3432	1/1	0.96	0.15	32,32,32,32	0
54	MG	1A	3724	1/1	0.96	0.19	46,46,46,46	0
54	MG	1A	3019	1/1	0.96	0.16	29,29,29,29	0
54	MG	1A	3206	1/1	0.96	0.18	43,43,43,43	0
54	MG	1a	1741	1/1	0.96	0.21	45,45,45,45	0
54	MG	1A	3383	1/1	0.96	0.23	61,61,61,61	0
54	MG	1A	3182	1/1	0.96	0.14	31,31,31,31	0
54	MG	2F	304	1/1	0.96	0.26	48,48,48,48	0
54	MG	1A	3183	1/1	0.96	0.14	33,33,33,33	0
54	MG	2A	3492	1/1	0.96	0.23	50,50,50,50	0
54	MG	1A	3438	1/1	0.96	0.27	37,37,37,37	0
54	MG	1A	3826	1/1	0.96	0.19	34,34,34,34	0
54	MG	1A	3092	1/1	0.96	0.16	45,45,45,45	0
54	MG	1d	302	1/1	0.96	0.31	71,71,71,71	0
54	MG	2A	3497	1/1	0.96	0.16	64,64,64,64	0
54	MG	2A	3133	1/1	0.96	0.18	50,50,50,50	0
54	MG	1A	3732	1/1	0.96	0.20	32,32,32,32	0
54	MG	1A	3940	1/1	0.96	0.05	51,51,51,51	0
54	MG	2A	3136	1/1	0.96	0.32	72,72,72,72	0
54	MG	2A	3503	1/1	0.96	0.22	56,56,56,56	0
54	MG	2V	201	1/1	0.96	0.39	59,59,59,59	0
54	MG	1A	3158	1/1	0.96	0.50	45,45,45,45	0
54	MG	1A	3830	1/1	0.96	0.20	35,35,35,35	0
54	MG	2W	203	1/1	0.96	0.17	66,66,66,66	0
54	MG	1D	304	1/1	0.96	0.13	47,47,47,47	0
54	MG	2A	3508	1/1	0.96	0.13	66,66,66,66	0
54	MG	1A	3579	1/1	0.96	0.17	53,53,53,53	0
54	MG	1A	3441	1/1	0.96	0.34	50,50,50,50	0
54	MG	1A	3503	1/1	0.96	0.18	23,23,23,23	0
54	MG	2A	3512	1/1	0.96	0.33	74,74,74,74	0
54	MG	27	101	1/1	0.96	0.26	49,49,49,49	0
54	MG	1A	3740	1/1	0.96	0.12	33,33,33,33	0
59	ZN	1Y	203	1/1	0.96	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	28	102	1/1	0.96	0.24	62,62,62,62	0
54	MG	2a	3001	1/1	0.96	0.23	52,52,52,52	0
59	ZN	2Y	202	1/1	0.96	0.13	80,80,80,80	0
54	MG	2A	3144	1/1	0.96	0.27	61,61,61,61	0
54	MG	1D	312	1/1	0.96	0.18	47,47,47,47	0
54	MG	1A	3209	1/1	0.97	0.32	45,45,45,45	0
54	MG	2A	3514	1/1	0.97	0.07	50,50,50,50	0
54	MG	2A	3030	1/1	0.97	0.21	45,45,45,45	0
54	MG	1A	3471	1/1	0.97	0.08	54,54,54,54	0
54	MG	1U	207	1/1	0.97	0.17	48,48,48,48	0
54	MG	1A	3017	1/1	0.97	0.15	35,35,35,35	0
54	MG	1A	3758	1/1	0.97	0.16	30,30,30,30	0
54	MG	1V	202	1/1	0.97	0.19	35,35,35,35	0
54	MG	2A	3259	1/1	0.97	0.17	51,51,51,51	0
54	MG	2A	3390	1/1	0.97	0.14	66,66,66,66	0
54	MG	2A	3260	1/1	0.97	0.27	57,57,57,57	0
54	MG	1V	204	1/1	0.97	0.20	61,61,61,61	0
54	MG	1A	3581	1/1	0.97	0.24	23,23,23,23	0
54	MG	1A	3131	1/1	0.97	0.28	58,58,58,58	0
54	MG	1A	3474	1/1	0.97	0.16	44,44,44,44	0
54	MG	1A	3967	1/1	0.97	0.26	67,67,67,67	0
54	MG	1Y	201	1/1	0.97	0.22	63,63,63,63	0
54	MG	1a	1750	1/1	0.97	0.18	45,45,45,45	0
54	MG	1A	3695	1/1	0.97	0.20	24,24,24,24	0
54	MG	1A	3168	1/1	0.97	0.24	44,44,44,44	0
54	MG	1A	3054	1/1	0.97	0.32	31,31,31,31	0
54	MG	1A	3241	1/1	0.97	0.30	35,35,35,35	0
54	MG	1A	3242	1/1	0.97	0.16	30,30,30,30	0
54	MG	2A	3050	1/1	0.97	0.18	47,47,47,47	0
54	MG	1A	3899	1/1	0.97	0.14	36,36,36,36	0
54	MG	2a	3098	1/1	0.97	0.35	63,63,63,63	0
54	MG	1A	3975	1/1	0.97	0.14	31,31,31,31	0
54	MG	1A	3530	1/1	0.97	0.17	27,27,27,27	0
54	MG	2A	3541	1/1	0.97	0.16	43,43,43,43	0
54	MG	1A	3095	1/1	0.97	0.25	39,39,39,39	0
54	MG	2A	3281	1/1	0.97	0.17	39,39,39,39	0
54	MG	2D	303	1/1	0.97	0.38	62,62,62,62	0
54	MG	1A	3902	1/1	0.97	0.06	54,54,54,54	0
54	MG	2A	3545	1/1	0.97	0.17	49,49,49,49	0
54	MG	2D	306	1/1	0.97	0.19	32,32,32,32	0
54	MG	2A	3283	1/1	0.97	0.20	73,73,73,73	0
54	MG	1A	3245	1/1	0.97	0.20	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1D	303	1/1	0.97	0.17	41,41,41,41	0
54	MG	11	104	1/1	0.97	0.17	51,51,51,51	0
54	MG	1A	3215	1/1	0.97	0.15	45,45,45,45	0
54	MG	1A	3981	1/1	0.97	0.20	33,33,33,33	0
54	MG	13	101	1/1	0.97	0.13	35,35,35,35	0
54	MG	1A	3171	1/1	0.97	0.20	43,43,43,43	0
54	MG	1a	1865	1/1	0.97	0.11	69,69,69,69	0
54	MG	2A	3170	1/1	0.97	0.21	54,54,54,54	0
54	MG	1A	3593	1/1	0.97	0.30	64,64,64,64	0
54	MG	13	104	1/1	0.97	0.16	45,45,45,45	0
54	MG	1A	3706	1/1	0.97	0.36	51,51,51,51	0
54	MG	2A	3296	1/1	0.97	0.17	43,43,43,43	0
54	MG	1A	3248	1/1	0.97	0.23	39,39,39,39	0
54	MG	1A	3106	1/1	0.97	0.17	38,38,38,38	0
54	MG	1A	3650	1/1	0.97	0.18	34,34,34,34	0
54	MG	2A	3300	1/1	0.97	0.21	39,39,39,39	0
54	MG	2A	3301	1/1	0.97	0.16	46,46,46,46	0
54	MG	1D	315	1/1	0.97	0.13	63,63,63,63	0
54	MG	2A	3178	1/1	0.97	0.39	54,54,54,54	0
54	MG	1A	3087	1/1	0.97	0.31	45,45,45,45	0
54	MG	17	102	1/1	0.97	0.19	41,41,41,41	0
54	MG	1A	3597	1/1	0.97	0.11	47,47,47,47	0
54	MG	1E	303	1/1	0.97	0.18	37,37,37,37	0
54	MG	2A	3077	1/1	0.97	0.27	44,44,44,44	0
54	MG	1A	3286	1/1	0.97	0.31	36,36,36,36	0
54	MG	2A	3185	1/1	0.97	0.20	43,43,43,43	0
54	MG	18	101	1/1	0.97	0.25	40,40,40,40	0
54	MG	1A	3444	1/1	0.97	0.17	33,33,33,33	0
54	MG	2A	3314	1/1	0.97	0.14	69,69,69,69	0
54	MG	2A	3081	1/1	0.97	0.04	70,70,70,70	0
54	MG	1A	3783	1/1	0.97	0.14	35,35,35,35	0
54	MG	1A	3716	1/1	0.97	0.12	41,41,41,41	0
54	MG	1A	3917	1/1	0.97	0.18	40,40,40,40	0
54	MG	2A	3193	1/1	0.97	0.18	47,47,47,47	0
54	MG	1A	3918	1/1	0.97	0.20	26,26,26,26	0
54	MG	1a	1603	1/1	0.97	0.18	50,50,50,50	0
54	MG	1A	3445	1/1	0.97	0.17	20,20,20,20	0
54	MG	2a	3148	1/1	0.97	0.18	56,56,56,56	0
54	MG	1A	3921	1/1	0.97	0.16	52,52,52,52	0
54	MG	2A	3590	1/1	0.97	0.28	60,60,60,60	0
54	MG	1A	3922	1/1	0.97	0.14	19,19,19,19	0
54	MG	1A	3361	1/1	0.97	0.17	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3492	1/1	0.97	0.21	28,28,28,28	0
54	MG	1F	307	1/1	0.97	0.21	37,37,37,37	0
54	MG	2a	3155	1/1	0.97	0.27	56,56,56,56	0
54	MG	1a	1793	1/1	0.97	0.14	66,66,66,66	0
54	MG	1A	3854	1/1	0.97	0.11	50,50,50,50	0
54	MG	2A	3204	1/1	0.97	0.23	62,62,62,62	0
54	MG	1A	3546	1/1	0.97	0.15	33,33,33,33	0
54	MG	1A	3362	1/1	0.97	0.13	57,57,57,57	0
54	MG	1A	3088	1/1	0.97	0.21	36,36,36,36	0
54	MG	1A	3364	1/1	0.97	0.17	33,33,33,33	0
54	MG	1A	3122	1/1	0.97	0.18	34,34,34,34	0
54	MG	1A	3931	1/1	0.97	0.12	62,62,62,62	0
54	MG	1m	201	1/1	0.97	0.09	71,71,71,71	0
54	MG	2A	3467	1/1	0.97	0.14	58,58,58,58	0
54	MG	1A	3048	1/1	0.97	0.17	26,26,26,26	0
54	MG	1A	3254	1/1	0.97	0.18	39,39,39,39	0
54	MG	2A	3214	1/1	0.97	0.10	61,61,61,61	0
54	MG	1A	3140	1/1	0.97	0.16	30,30,30,30	0
54	MG	2A	3472	1/1	0.97	0.24	40,40,40,40	0
54	MG	1A	3455	1/1	0.97	0.19	21,21,21,21	0
54	MG	1A	3179	1/1	0.97	0.12	37,37,37,37	0
54	MG	1A	3074	1/1	0.97	0.22	31,31,31,31	0
54	MG	2a	3176	1/1	0.97	0.04	68,68,68,68	0
54	MG	1A	3559	1/1	0.97	0.27	53,53,53,53	0
54	MG	1A	3673	1/1	0.97	0.16	49,49,49,49	0
54	MG	1A	3332	1/1	0.97	0.23	25,25,25,25	0
54	MG	2A	3479	1/1	0.97	0.11	60,60,60,60	0
54	MG	2A	3222	1/1	0.97	0.20	41,41,41,41	0
54	MG	1A	3181	1/1	0.97	0.32	42,42,42,42	0
54	MG	2A	3224	1/1	0.97	0.23	26,26,26,26	0
54	MG	1A	3506	1/1	0.97	0.15	35,35,35,35	0
54	MG	2A	3484	1/1	0.97	0.25	57,57,57,57	0
54	MG	1A	3564	1/1	0.97	0.08	32,32,32,32	0
54	MG	2A	3228	1/1	0.97	0.17	46,46,46,46	0
54	MG	1A	3297	1/1	0.97	0.11	41,41,41,41	0
54	MG	2a	3190	1/1	0.97	0.16	57,57,57,57	0
54	MG	2A	3488	1/1	0.97	0.24	46,46,46,46	0
54	MG	1A	3566	1/1	0.97	0.17	52,52,52,52	0
54	MG	2A	3490	1/1	0.97	0.20	30,30,30,30	0
54	MG	1A	3042	1/1	0.97	0.18	36,36,36,36	0
54	MG	1A	3144	1/1	0.97	0.26	35,35,35,35	0
54	MG	1B	201	1/1	0.97	0.21	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3877	1/1	0.97	0.10	50,50,50,50	0
54	MG	2A	3015	1/1	0.97	0.16	38,38,38,38	0
54	MG	2A	3637	1/1	0.97	0.16	60,60,60,60	0
54	MG	1A	3878	1/1	0.97	0.13	44,44,44,44	0
54	MG	1A	3127	1/1	0.97	0.18	38,38,38,38	0
54	MG	2A	3640	1/1	0.97	0.23	61,61,61,61	0
54	MG	1A	3230	1/1	0.97	0.20	41,41,41,41	0
54	MG	2A	3240	1/1	0.97	0.19	50,50,50,50	0
54	MG	2A	3500	1/1	0.97	0.12	61,61,61,61	0
54	MG	1a	1728	1/1	0.97	0.18	45,45,45,45	0
54	MG	1A	3264	1/1	0.97	0.23	53,53,53,53	0
54	MG	1A	3006	1/1	0.97	0.21	26,26,26,26	0
54	MG	2A	3504	1/1	0.97	0.23	41,41,41,41	0
54	MG	1A	3573	1/1	0.97	0.17	49,49,49,49	0
54	MG	1a	1732	1/1	0.97	0.12	46,46,46,46	0
54	MG	1A	3468	1/1	0.97	0.17	31,31,31,31	0
54	MG	1A	3753	1/1	0.97	0.32	60,60,60,60	0
54	MG	1U	201	1/1	0.97	0.25	35,35,35,35	0
54	MG	2A	3250	1/1	0.97	0.38	49,49,49,49	0
54	MG	1A	3115	1/1	0.97	0.27	35,35,35,35	0
54	MG	2A	3381	1/1	0.97	0.10	58,58,58,58	0
59	ZN	29	501	1/1	0.97	0.12	72,72,72,72	0
54	MG	2a	3072	1/1	0.97	0.13	77,77,77,77	0
60	SF4	2d	501	8/8	0.97	0.11	69,84,87,92	0
54	MG	1A	3415	1/1	0.98	0.28	30,30,30,30	0
54	MG	1a	1838	1/1	0.98	0.17	58,58,58,58	0
54	MG	2A	3274	1/1	0.98	0.35	44,44,44,44	0
54	MG	1R	202	1/1	0.98	0.12	39,39,39,39	0
54	MG	1A	3715	1/1	0.98	0.24	43,43,43,43	0
54	MG	2A	3404	1/1	0.98	0.18	62,62,62,62	0
54	MG	1a	1841	1/1	0.98	0.12	64,64,64,64	0
54	MG	1A	3143	1/1	0.98	0.18	46,46,46,46	0
54	MG	1A	3417	1/1	0.98	0.24	26,26,26,26	0
54	MG	1A	3718	1/1	0.98	0.13	39,39,39,39	0
54	MG	1A	3075	1/1	0.98	0.16	42,42,42,42	0
54	MG	1A	3525	1/1	0.98	0.21	27,27,27,27	0
54	MG	1A	3306	1/1	0.98	0.29	35,35,35,35	0
54	MG	1a	1745	1/1	0.98	0.19	57,57,57,57	0
54	MG	1a	1849	1/1	0.98	0.10	65,65,65,65	0
54	MG	2A	3054	1/1	0.98	0.12	66,66,66,66	0
54	MG	1A	3375	1/1	0.98	0.14	29,29,29,29	0
54	MG	1B	211	1/1	0.98	0.20	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3145	1/1	0.98	0.22	26,26,26,26	0
54	MG	1U	206	1/1	0.98	0.27	36,36,36,36	0
54	MG	2A	3547	1/1	0.98	0.14	29,29,29,29	0
54	MG	1A	3053	1/1	0.98	0.24	34,34,34,34	0
54	MG	1A	3956	1/1	0.98	0.17	30,30,30,30	0
54	MG	1A	3423	1/1	0.98	0.15	26,26,26,26	0
54	MG	1V	201	1/1	0.98	0.21	29,29,29,29	0
54	MG	1A	3958	1/1	0.98	0.15	33,33,33,33	0
54	MG	1V	203	1/1	0.98	0.14	45,45,45,45	0
54	MG	1A	3281	1/1	0.98	0.22	43,43,43,43	0
54	MG	1A	3341	1/1	0.98	0.22	40,40,40,40	0
54	MG	1A	3202	1/1	0.98	0.14	57,57,57,57	0
54	MG	1A	3343	1/1	0.98	0.21	60,60,60,60	0
54	MG	1A	3382	1/1	0.98	0.17	20,20,20,20	0
54	MG	2A	3070	1/1	0.98	0.34	48,48,48,48	0
54	MG	1A	3203	1/1	0.98	0.19	47,47,47,47	0
54	MG	1A	3537	1/1	0.98	0.25	30,30,30,30	0
54	MG	2a	3112	1/1	0.98	0.12	67,67,67,67	0
54	MG	1A	3733	1/1	0.98	0.12	45,45,45,45	0
54	MG	1A	3220	1/1	0.98	0.14	28,28,28,28	0
54	MG	2A	3564	1/1	0.98	0.25	64,64,64,64	0
54	MG	1A	3539	1/1	0.98	0.14	51,51,51,51	0
54	MG	2A	3189	1/1	0.98	0.30	40,40,40,40	0
54	MG	2A	3567	1/1	0.98	0.13	80,80,80,80	0
54	MG	2Q	202	1/1	0.98	0.50	56,56,56,56	0
54	MG	2A	3310	1/1	0.98	0.29	57,57,57,57	0
54	MG	1A	3812	1/1	0.98	0.14	48,48,48,48	0
54	MG	2R	201	1/1	0.98	0.17	47,47,47,47	0
54	MG	1A	3667	1/1	0.98	0.21	48,48,48,48	0
54	MG	1A	3738	1/1	0.98	0.15	37,37,37,37	0
54	MG	1A	3385	1/1	0.98	0.14	34,34,34,34	0
54	MG	1A	3482	1/1	0.98	0.15	38,38,38,38	0
54	MG	1A	3670	1/1	0.98	0.20	26,26,26,26	0
54	MG	11	101	1/1	0.98	0.28	48,48,48,48	0
54	MG	1A	3240	1/1	0.98	0.21	37,37,37,37	0
54	MG	1A	3018	1/1	0.98	0.19	34,34,34,34	0
54	MG	1D	306	1/1	0.98	0.21	17,17,17,17	0
54	MG	2A	3579	1/1	0.98	0.20	69,69,69,69	0
54	MG	2Y	201	1/1	0.98	0.35	68,68,68,68	0
54	MG	1D	307	1/1	0.98	0.20	43,43,43,43	0
54	MG	1A	3485	1/1	0.98	0.18	34,34,34,34	0
54	MG	1A	3315	1/1	0.98	0.20	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	23	101	1/1	0.98	0.19	57,57,57,57	0
54	MG	1A	3262	1/1	0.98	0.10	77,77,77,77	0
54	MG	2A	3325	1/1	0.98	0.17	66,66,66,66	0
54	MG	1D	311	1/1	0.98	0.36	32,32,32,32	0
54	MG	1A	3175	1/1	0.98	0.20	31,31,31,31	0
54	MG	2A	3328	1/1	0.98	0.18	43,43,43,43	0
54	MG	15	101	1/1	0.98	0.21	34,34,34,34	0
54	MG	15	102	1/1	0.98	0.17	38,38,38,38	0
54	MG	1e	203	1/1	0.98	0.17	73,73,73,73	0
54	MG	15	103	1/1	0.98	0.16	24,24,24,24	0
54	MG	1A	3749	1/1	0.98	0.19	23,23,23,23	0
54	MG	1A	3318	1/1	0.98	0.25	39,39,39,39	0
54	MG	2A	3335	1/1	0.98	0.16	43,43,43,43	0
54	MG	2A	3336	1/1	0.98	0.18	65,65,65,65	0
54	MG	2A	3596	1/1	0.98	0.20	41,41,41,41	0
54	MG	1A	3352	1/1	0.98	0.24	20,20,20,20	0
54	MG	1A	3078	1/1	0.98	0.26	36,36,36,36	0
54	MG	2A	3599	1/1	0.98	0.20	38,38,38,38	0
54	MG	1A	3552	1/1	0.98	0.13	29,29,29,29	0
54	MG	1E	302	1/1	0.98	0.46	45,45,45,45	0
54	MG	1A	3244	1/1	0.98	0.30	60,60,60,60	0
54	MG	1A	3442	1/1	0.98	0.25	26,26,26,26	0
54	MG	2A	3104	1/1	0.98	0.18	39,39,39,39	0
54	MG	1A	3016	1/1	0.98	0.23	37,37,37,37	0
54	MG	1A	3832	1/1	0.98	0.15	21,21,21,21	0
54	MG	1A	3356	1/1	0.98	0.28	27,27,27,27	0
54	MG	1A	3619	1/1	0.98	0.20	34,34,34,34	0
54	MG	2A	3109	1/1	0.98	0.32	36,36,36,36	0
54	MG	1a	1697	1/1	0.98	0.22	51,51,51,51	0
54	MG	1A	3072	1/1	0.98	0.22	34,34,34,34	0
54	MG	1A	3446	1/1	0.98	0.13	35,35,35,35	0
54	MG	2A	3227	1/1	0.98	0.15	35,35,35,35	0
54	MG	1A	3995	1/1	0.98	0.21	21,21,21,21	0
54	MG	2A	3615	1/1	0.98	0.04	72,72,72,72	0
54	MG	1A	3560	1/1	0.98	0.14	44,44,44,44	0
54	MG	1A	3323	1/1	0.98	0.20	35,35,35,35	0
54	MG	1A	3097	1/1	0.98	0.15	36,36,36,36	0
54	MG	2a	3174	1/1	0.98	0.16	59,59,59,59	0
54	MG	1F	306	1/1	0.98	0.17	29,29,29,29	0
54	MG	2A	3358	1/1	0.98	0.21	67,67,67,67	0
54	MG	1A	3295	1/1	0.98	0.19	27,27,27,27	0
54	MG	1A	3296	1/1	0.98	0.20	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1F	309	1/1	0.98	0.15	39,39,39,39	0
54	MG	1A	3402	1/1	0.98	0.23	34,34,34,34	0
54	MG	1A	3843	1/1	0.98	0.16	31,31,31,31	0
54	MG	2A	3238	1/1	0.98	0.19	50,50,50,50	0
54	MG	2A	3365	1/1	0.98	0.14	66,66,66,66	0
54	MG	1A	3139	1/1	0.98	0.18	32,32,32,32	0
54	MG	1A	3504	1/1	0.98	0.19	31,31,31,31	0
54	MG	1A	3270	1/1	0.98	0.20	40,40,40,40	0
54	MG	1A	3272	1/1	0.98	0.22	33,33,33,33	0
54	MG	1A	3507	1/1	0.98	0.18	29,29,29,29	0
54	MG	1A	3849	1/1	0.98	0.12	50,50,50,50	0
54	MG	1A	3107	1/1	0.98	0.26	33,33,33,33	0
54	MG	1A	3851	1/1	0.98	0.24	28,28,28,28	0
54	MG	2A	3131	1/1	0.98	0.27	49,49,49,49	0
54	MG	1A	3366	1/1	0.98	0.16	56,56,56,56	0
54	MG	1a	1819	1/1	0.98	0.21	60,60,60,60	0
54	MG	1A	3331	1/1	0.98	0.24	36,36,36,36	0
54	MG	2A	3022	1/1	0.98	0.22	58,58,58,58	0
54	MG	1A	3574	1/1	0.98	0.23	61,61,61,61	0
54	MG	1A	3056	1/1	0.98	0.15	34,34,34,34	0
54	MG	1N	201	1/1	0.98	0.12	40,40,40,40	0
54	MG	2A	3644	1/1	0.98	0.21	60,60,60,60	0
54	MG	1A	3410	1/1	0.98	0.20	31,31,31,31	0
54	MG	1A	3577	1/1	0.98	0.21	42,42,42,42	0
54	MG	1A	3049	1/1	0.98	0.14	54,54,54,54	0
54	MG	1A	3514	1/1	0.98	0.14	47,47,47,47	0
54	MG	1A	3231	1/1	0.98	0.36	37,37,37,37	0
54	MG	2A	3031	1/1	0.98	0.16	36,36,36,36	0
54	MG	2A	3145	1/1	0.98	0.13	66,66,66,66	0
54	MG	1A	3462	1/1	0.98	0.26	49,49,49,49	0
54	MG	2a	3066	1/1	0.98	0.04	76,76,76,76	0
54	MG	1A	3862	1/1	0.98	0.17	41,41,41,41	0
54	MG	1A	3644	1/1	0.98	0.20	77,77,77,77	0
54	MG	2A	3392	1/1	0.98	0.31	41,41,41,41	0
54	MG	2A	3266	1/1	0.98	0.24	38,38,38,38	0
59	ZN	15	109	1/1	0.98	0.12	52,52,52,52	0
54	MG	1P	205	1/1	0.98	0.19	58,58,58,58	0
54	MG	1A	3371	1/1	0.98	0.17	23,23,23,23	0
54	MG	1A	3414	1/1	0.98	0.20	25,25,25,25	0
59	ZN	25	104	1/1	0.98	0.16	65,65,65,65	0
59	ZN	26	501	1/1	0.98	0.14	64,64,64,64	0
54	MG	1A	3713	1/1	0.98	0.31	50,50,50,50	0

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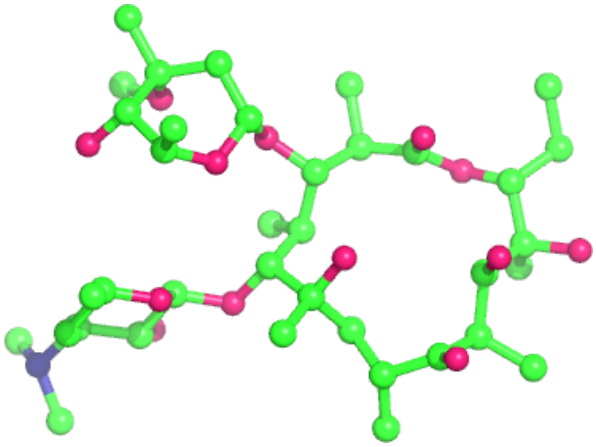
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3525	1/1	0.98	0.29	40,40,40,40	0
60	SF4	1d	304	8/8	0.98	0.13	60,68,72,73	0
54	MG	1Q	204	1/1	0.98	0.13	43,43,43,43	0
54	MG	1A	3543	1/1	0.99	0.20	26,26,26,26	0
54	MG	1A	3148	1/1	0.99	0.15	42,42,42,42	0
54	MG	2A	3278	1/1	0.99	0.22	47,47,47,47	0
54	MG	1A	3558	1/1	0.99	0.20	30,30,30,30	0
54	MG	1A	3785	1/1	0.99	0.25	26,26,26,26	0
54	MG	1A	3284	1/1	0.99	0.16	27,27,27,27	0
54	MG	1A	3920	1/1	0.99	0.25	30,30,30,30	0
54	MG	1A	3123	1/1	0.99	0.13	30,30,30,30	0
54	MG	1Q	201	1/1	0.99	0.19	38,38,38,38	0
54	MG	1A	3659	1/1	0.99	0.24	31,31,31,31	0
54	MG	2A	3004	1/1	0.99	0.19	42,42,42,42	0
54	MG	1A	3735	1/1	0.99	0.19	33,33,33,33	0
54	MG	1A	4006	1/1	0.99	0.26	18,18,18,18	0
54	MG	1A	3003	1/1	0.99	0.27	31,31,31,31	0
54	MG	2a	3013	1/1	0.99	0.15	53,53,53,53	0
54	MG	1R	201	1/1	0.99	0.18	41,41,41,41	0
54	MG	1A	3523	1/1	0.99	0.14	57,57,57,57	0
54	MG	1A	3235	1/1	0.99	0.20	33,33,33,33	0
54	MG	1A	3271	1/1	0.99	0.35	35,35,35,35	0
54	MG	1A	3112	1/1	0.99	0.26	37,37,37,37	0
54	MG	2A	3013	1/1	0.99	0.28	27,27,27,27	0
54	MG	1A	3776	1/1	0.99	0.14	30,30,30,30	0
54	MG	2a	3181	1/1	0.99	0.19	59,59,59,59	0
54	MG	2A	3042	1/1	0.99	0.26	28,28,28,28	0
59	ZN	19	103	1/1	0.99	0.19	49,49,49,49	0
54	MG	1A	3741	1/1	0.99	0.18	35,35,35,35	0
54	MG	1A	3028	1/1	0.99	0.21	34,34,34,34	0
54	MG	1A	3065	1/1	0.99	0.18	34,34,34,34	0
54	MG	1A	3427	1/1	0.99	0.32	51,51,51,51	0
54	MG	1U	203	1/1	0.99	0.25	37,37,37,37	0
54	MG	1A	3974	1/1	0.99	0.11	47,47,47,47	0
54	MG	1A	3518	1/1	0.99	0.16	46,46,46,46	0
54	MG	2E	304	1/1	0.99	0.25	43,43,43,43	0
54	MG	2A	3246	1/1	0.99	0.21	32,32,32,32	0
54	MG	1A	3764	1/1	1.00	0.16	30,30,30,30	0
59	ZN	16	501	1/1	1.00	0.20	48,48,48,48	0

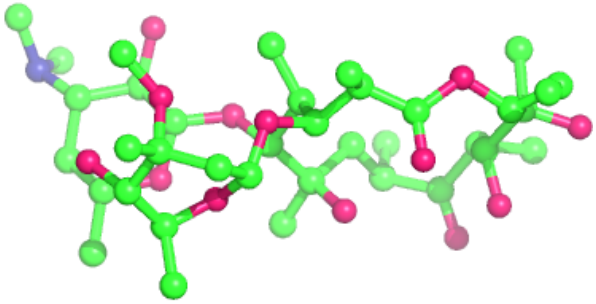
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

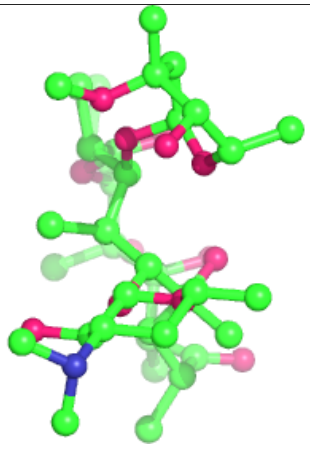
orientation to approximate a three-dimensional view.

Electron density around ERY 2A 3672:

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

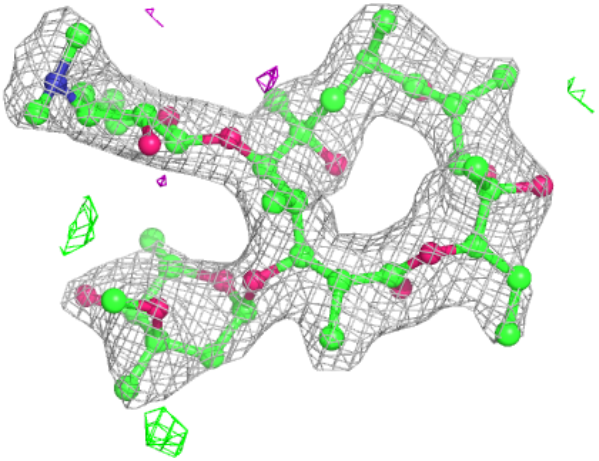


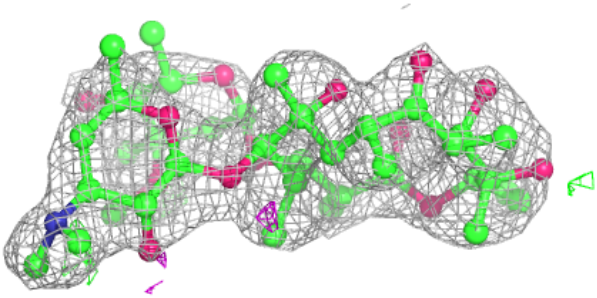


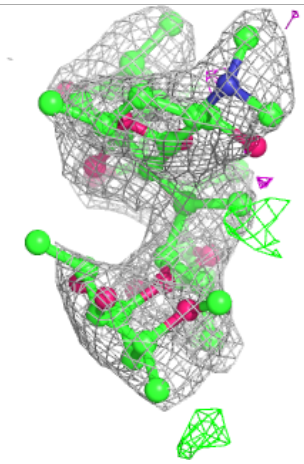


Electron density around ERY 1A 4027:

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

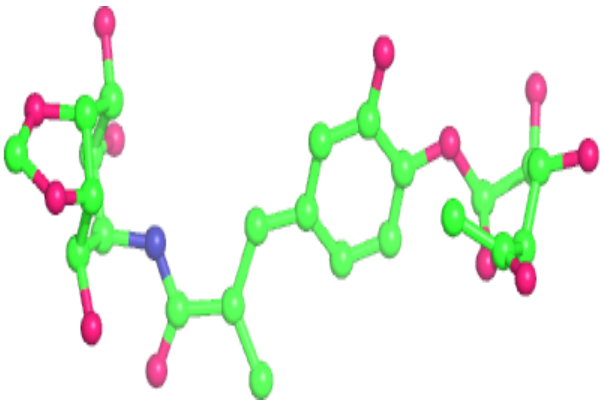


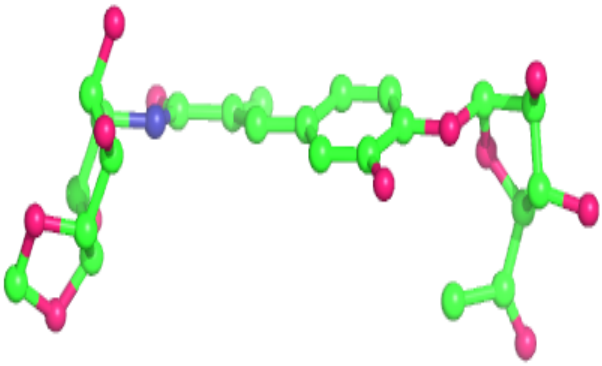


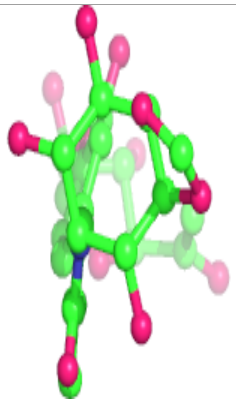


Electron density around HGR 2A 3671:

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

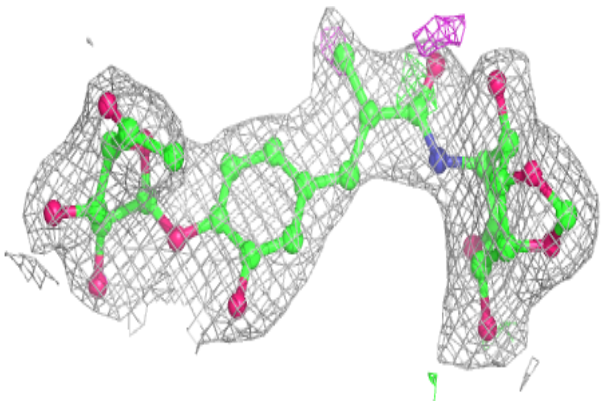


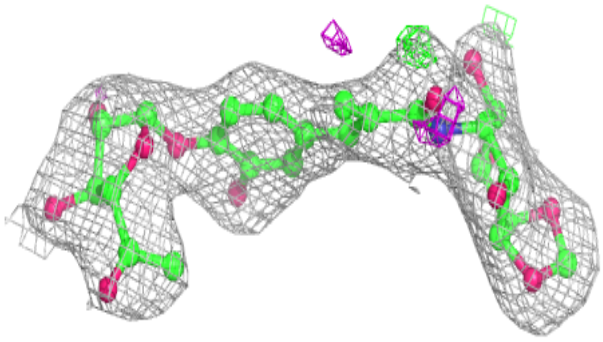


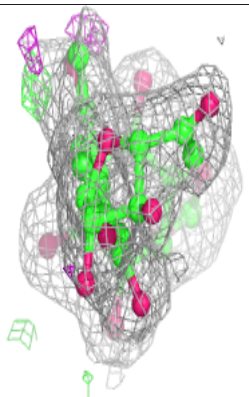


Electron density around HGR 1A 4026:

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







6.5 Other polymers (i)

There are no such residues in this entry.