Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 05:25 AM EST

PDB ID	:	6XHY
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with telithromycin, mRNA, aminoacylated A- and P-site tRNAs, and deacylated E-site tRNA at 2.60A resolution
Authors	:	Svetlov, M.S.; Syroegin, E.A.; Aleksandrova, E.V.; Atkinson, G.C.; Gregory, S.T.; Mankin, A.S.; Polikanov, Y.S.
Deposited on	:	2020-06-19
Resolution	:	2.60 Å(reported)

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

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

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

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

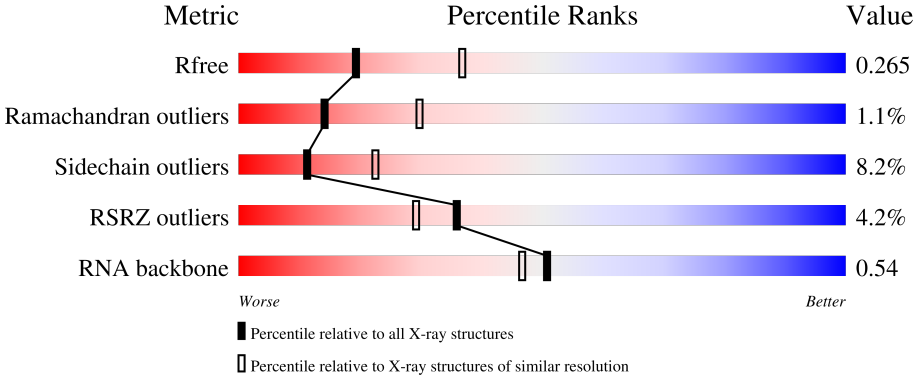
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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	2% 82% 16%
1	2A	2915	3% 79% 16%
2	1B	121	89% 10%
2	2B	121	78% 21%
3	1D	276	95% 5%

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Mol	Chain	Length	Quality of chain
3	2D	276	3% 94% 5%
4	1E	206	93% 6%
4	2E	206	3% 94% 5%
5	1F	210	90% 7%
5	2F	210	% 90% 7%
6	1G	182	% 91% 7%
6	2G	182	7% 87% 12%
7	1H	180	91% 6%
7	2H	180	14% 88% 8%
8	1I	148	87% 11%
8	2I	148	7% 91% 8%
9	1N	140	93% 7%
9	2N	140	4% 91% 9%
10	1O	122	98%
10	2O	122	2% 98%
11	1P	150	88% 11%
11	2P	150	4% 87% 12%
12	1Q	141	% 95% 5%
12	2Q	141	9% 96%
13	1R	118	95% 5%
13	2R	118	% 94% 6%
14	1S	112	87% 12%
14	2S	112	87% 12%
15	1T	146	84% 5% 10%
15	2T	146	% 86% 10%

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Mol	Chain	Length	Quality of chain
16	1U	118	94%
16	2U	118	3%, 92%, 7%
17	1V	101	93%, 6%
17	2V	101	91%, 8%
18	1W	113	92%, 7%
18	2W	113	2%, 96%
19	1X	96	94%
19	2X	96	4%, 94%
20	1Y	110	90%, 7%
20	2Y	110	6%, 91%, 6%
21	1Z	206	%, 68%, 7%, 25%
21	2Z	206	6%, 69%, 8%, 22%
22	10	85	94%
22	20	85	%, 94%
23	11	98	2%, 96%
23	21	98	7%, 93%, 6%
24	12	72	92%, 6%
24	22	72	%, 94%
25	13	60	87%, 12%
25	23	60	12%, 90%, 8%
26	14	71	76%, 17%
26	24	71	10%, 80%, 17%
27	15	60	2%, 90%, 8%
27	25	60	2%, 93%, 5%
28	16	54	78%, 20%

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Mol	Chain	Length	Quality of chain
28	26	54	6% 91% 7%
29	17	49	6% 96%
29	27	49	8% 90% 8%
30	18	65	92% 6%
30	28	65	5% 92% 6%
31	19	37	100%
31	29	37	16% 95% 5%
32	1a	1521	% 83% 15%
32	2a	1521	2% 79% 19%
33	1b	256	% 79% 11% 10%
33	2b	256	4% 78% 12% 10%
34	1c	239	3% 81% 5% 14%
34	2c	239	7% 77% 9% 14%
35	1d	209	9% 92% 7%
35	2d	209	4% 92% 8%
36	1e	162	2% 87% 9%
36	2e	162	4% 83% 9% 9%
37	1f	101	92% 7%
37	2f	101	91% 8%
38	1g	156	4% 92% 8%
38	2g	156	15% 88% 12%
39	1h	138	2% 96%
39	2h	138	15% 92% 7%
40	1i	128	5% 94% 5%
40	2i	128	35% 89% 10%

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Mol	Chain	Length	Quality of chain
41	1j	105	7% 83% 10% 8%
41	2j	105	23% 78% 13% 9%
42	1k	129	2% 82% 6% 12%
42	2k	129	6% 84% 12%
43	1l	132	2% 89% 8%
43	2l	132	4% 88% 5% 8%
44	1m	126	2% 90% 6%
44	2m	126	17% 87% 10%
45	1n	61	13% 92% 7%
45	2n	61	52% 89% 10%
46	1o	89	2% 91% 8%
46	2o	89	3% 93% 6%
47	1p	88	13% 84% 9% 7%
47	2p	88	% 83% 10% 7%
48	1q	105	4% 86% 9% 6%
48	2q	105	13% 89% 6% 6%
49	1r	88	75% 23%
49	2r	88	2% 74% 23%
50	1s	93	% 84% 5% 11%
50	2s	93	20% 83% 5% 11%
51	1t	106	15% 82% 8% 9%
51	2t	106	8% 80% 10% 9%
52	1u	27	19% 81% 15%
52	2u	27	63% 85% 15%
53	1v	24	8% 50% 46%

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Mol	Chain	Length	Quality of chain
53	2v	24	21% 50% 46%
54	1w	76	9% 61% 33%
54	2w	76	13% 61% 30% 5%
55	1x	77	78% 19%
55	2x	77	% 79% 19%
56	1y	76	49% 49% 41% 8%
56	2y	76	80% 55% 37%

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
56	PSU	2y	32	-	-	-	X
56	MIA	2y	37	-	-	-	X
56	5MU	2y	54	-	-	-	X
57	MG	1A	3354	-	-	-	X
57	MG	1A	3380	-	-	-	X
57	MG	1A	3381	-	-	-	X
57	MG	1S	201	-	-	-	X
57	MG	23	102	-	-	-	X
57	MG	2A	3033	-	-	-	X
57	MG	2A	3208	-	-	-	X
57	MG	2A	3294	-	-	-	X
57	MG	2A	3314	-	-	-	X
57	MG	2A	3398	-	-	-	X
57	MG	2A	3436	-	-	-	X
57	MG	2a	1690	-	-	-	X

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 299652 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	2871	61852	27531	11572	19878	2871	0	0	0
1	2A	2800	60322	26848	11284	19390	2800	0	0	0

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	120	2577	1146	476	835	120	0	0	0
2	2B	120	2575	1146	476	833	120	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	1D	275	2136	1349	423	361	3	0	0	0
3	2D	275	2136	1349	423	361	3	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	1G	181	1423	913	253	253	4	0	0	0
6	2G	181	1428	913	258	253	4	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	1I	146	1097	701	191	204	1	0	0	0
8	2I	146	1064	681	186	196	1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	1S	110	873	550	174	149	0	0	0
			Total	C	N	O			
14	2S	110	870	549	173	148	0	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	1Y	107	806	517	152	131	6	0	0	0
20	2Y	107	806	517	152	131	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	1Z	154	1240	795	222	220	3	0	0	0
21	2Z	160	1271	814	228	227	2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	11	97	755	475	148	131	1	0	0	0
23	21	97	755	475	148	131	1	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	14	69	552	349	99	99	5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	24	69	532	339	97	91	5	0	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
32	1a	1500	32246	14358	5975	10413	1500	0	0	0
32	2a	1503	32327	14396	5990	10438	1503	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	1b	231	1846	1179	331	331	5	0	0	0
33	2b	231	1825	1167	326	327	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	1c	206	1548	973	301	273	1	0	0	0
34	2c	206	1542	968	300	273	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	1d	208	1655	1038	326	284	7	0	0	0
35	2d	208	1674	1050	333	284	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	1e	148	1129	714	213	198	4	0	0	0
36	2e	148	1133	716	214	199	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	1f	100	810	514	144	149	3	0	0	0
37	2f	100	816	516	146	151	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
38	1g	155	1231	766	243	216	6	0	0	0
38	2g	155	1235	769	244	216	6	0	0	0

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
40	1i	127	983	623	193	167	0	0	0
40	2i	127	978	619	190	169	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
41	1j	97	709	440	138	131	0	0	0
41	2j	96	714	445	138	131	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	1k	114	829	516	155	155	3	0	0	0

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1m	123	958	592	198	166	2	0	0	0
44	2m	122	950	586	197	165	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	1s	83	652	417	120	113	2	0	0	0
50	2s	83	646	412	119	113	2	0	0	0

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	1t	96	728	446	156	124	2	0	0	0
51	2t	96	727	446	155	124	2	0	0	0

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
52	1u	23	199	122	48	29	0	0	0
52	2u	23	199	122	48	29	0	0	0

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
53	1v	13	277	125	51	88	13	0	0	0
53	2v	13	277	125	51	88	13	0	0	0

- Molecule 54 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
54	1w	74	1603	722	287	518	74	2	0	0	0
54	2w	72	1555	699	280	502	72	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1w	76	F3N	-	expression tag	GB 1850831943
2w	76	F3N	-	expression tag	GB 1850831943

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
55	1x	76	1635	731	296	530	76	2	0	0	0
55	2x	76	1635	731	296	530	76	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1x	76	31H	-	expression tag	GB 1848949880
2x	76	31H	-	expression tag	GB 1848949880

- Molecule 56 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
56	1y	74	1585	707	285	518	74	1	0	0	0
56	2y	73	1565	698	283	510	73	1	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	1A	1074	1074	1074	0	0
57	1B	35	35	35	0	0
57	1D	13	13	13	0	0
57	1E	12	12	12	0	0
57	1F	12	12	12	0	0
57	1G	5	5	5	0	0
57	1H	1	1	1	0	0
57	1I	1	1	1	0	0
57	1N	5	5	5	0	0
57	1O	5	5	5	0	0
57	1P	5	5	5	0	0
57	1Q	6	6	6	0	0
57	1R	6	6	6	0	0
57	1S	3	3	3	0	0
57	1T	3	3	3	0	0
57	1U	10	10	10	0	0
57	1V	6	6	6	0	0
57	1W	8	8	8	0	0
57	1X	6	6	6	0	0
57	1Y	4	4	4	0	0
57	1Z	2	2	2	0	0
57	10	8	8	8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	11	3	3	3	0	0
57	12	2	2	2	0	0
57	13	4	4	4	0	0
57	14	1	1	1	0	0
57	15	5	5	5	0	0
57	16	1	1	1	0	0
57	17	5	5	5	0	0
57	18	8	8	8	0	0
57	1a	214	214	214	0	0
57	1b	2	2	2	0	0
57	1d	1	1	1	0	0
57	1e	2	2	2	0	0
57	1f	2	2	2	0	0
57	1k	1	1	1	0	0
57	1l	2	2	2	0	0
57	1m	1	1	1	0	0
57	1n	2	2	2	0	0
57	1t	1	1	1	0	0
57	1w	8	8	8	0	0
57	1x	15	15	15	0	0
57	2A	844	844	844	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
57	2B	19	19	19	0	0
57	2D	5	5	5	0	0
57	2E	7	7	7	0	0
57	2F	6	6	6	0	0
57	2G	1	1	1	0	0
57	2N	1	1	1	0	0
57	2O	2	2	2	0	0
57	2P	2	2	2	0	0
57	2Q	4	4	4	0	0
57	2R	1	1	1	0	0
57	2T	4	4	4	0	0
57	2V	3	3	3	0	0
57	2X	2	2	2	0	0
57	20	1	1	1	0	0
57	21	1	1	1	0	0
57	23	4	4	4	0	0
57	25	3	3	3	0	0
57	27	3	3	3	0	0
57	28	4	4	4	0	0
57	2a	208	208	208	0	0
57	2d	2	2	2	0	0

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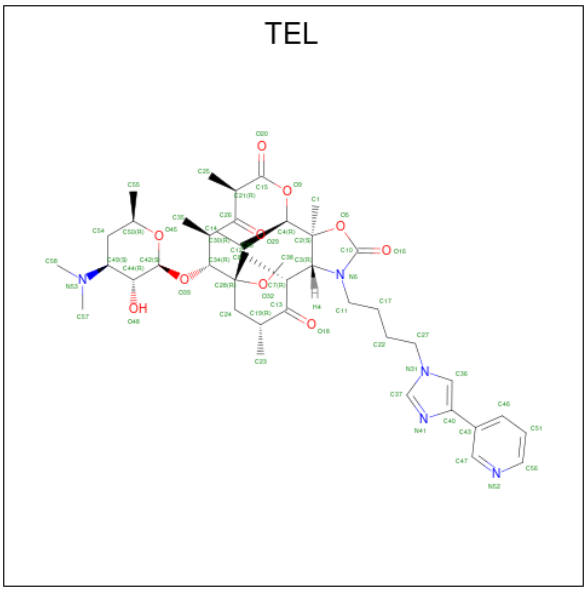
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2e	2	Total Mg 2 2	0	0
57	2f	2	Total Mg 2 2	0	0
57	2g	1	Total Mg 1 1	0	0
57	2i	1	Total Mg 1 1	0	0
57	2j	2	Total Mg 2 2	0	0
57	2l	5	Total Mg 5 5	0	0
57	2n	1	Total Mg 1 1	0	0
57	2q	1	Total Mg 1 1	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	4	Total Mg 4 4	0	0
57	2w	8	Total Mg 8 8	0	0
57	2x	5	Total Mg 5 5	0	0
57	2y	4	Total Mg 4 4	0	0

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total K 1 1	0	0
58	2x	1	Total K 1 1	0	0

- Molecule 59 is TELITHROMYCIN (three-letter code: TEL) (formula: $C_{43}H_{65}N_5O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
59	1A	1	58	43	5	10	0	0
			Total	C	N	O		
59	2A	1	58	43	5	10	0	0

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

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

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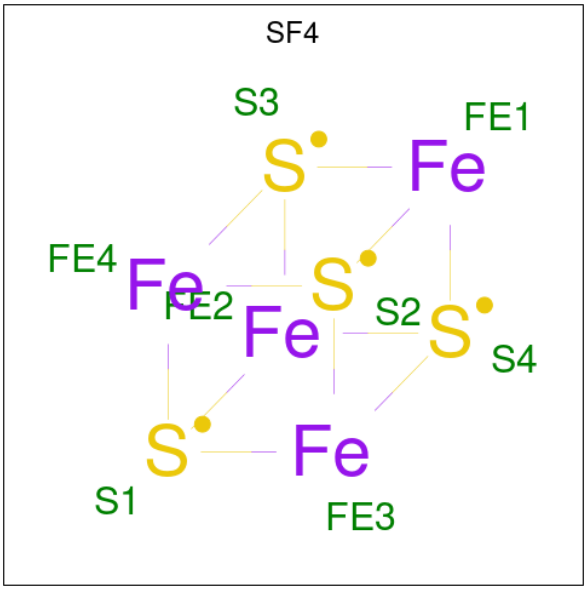
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

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



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1A	1964	Total O 1964 1964	0	0
62	1B	63	Total O 63 63	0	0
62	1D	26	Total O 26 26	0	0
62	1E	30	Total O 30 30	0	0
62	1F	12	Total O 12 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1G	5	Total O 5 5	0	0
62	1H	2	Total O 2 2	0	0
62	1N	3	Total O 3 3	0	0
62	1O	4	Total O 4 4	0	0
62	1P	20	Total O 20 20	0	0
62	1Q	6	Total O 6 6	0	0
62	1R	8	Total O 8 8	0	0
62	1S	4	Total O 4 4	0	0
62	1T	6	Total O 6 6	0	0
62	1U	11	Total O 11 11	0	0
62	1V	6	Total O 6 6	0	0
62	1W	6	Total O 6 6	0	0
62	1X	8	Total O 8 8	0	0
62	1Y	1	Total O 1 1	0	0
62	1Z	1	Total O 1 1	0	0
62	10	9	Total O 9 9	0	0
62	11	6	Total O 6 6	0	0
62	12	3	Total O 3 3	0	0
62	13	7	Total O 7 7	0	0
62	14	1	Total O 1 1	0	0
62	15	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	16	2	Total O 2 2	0	0
62	17	11	Total O 11 11	0	0
62	18	9	Total O 9 9	0	0
62	1a	219	Total O 219 219	0	0
62	1b	1	Total O 1 1	0	0
62	1e	1	Total O 1 1	0	0
62	1f	1	Total O 1 1	0	0
62	1l	3	Total O 3 3	0	0
62	1q	1	Total O 1 1	0	0
62	1v	3	Total O 3 3	0	0
62	1w	12	Total O 12 12	0	0
62	1x	13	Total O 13 13	0	0
62	1y	1	Total O 1 1	0	0
62	2A	1001	Total O 1001 1001	0	0
62	2B	20	Total O 20 20	0	0
62	2D	20	Total O 20 20	0	0
62	2E	8	Total O 8 8	0	0
62	2F	18	Total O 18 18	0	0
62	2O	3	Total O 3 3	0	0
62	2P	11	Total O 11 11	0	0
62	2Q	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2R	3	Total O 3 3	0	0
62	2T	6	Total O 6 6	0	0
62	2U	2	Total O 2 2	0	0
62	2W	2	Total O 2 2	0	0
62	2X	3	Total O 3 3	0	0
62	2Y	1	Total O 1 1	0	0
62	20	3	Total O 3 3	0	0
62	21	11	Total O 11 11	0	0
62	22	2	Total O 2 2	0	0
62	23	1	Total O 1 1	0	0
62	27	5	Total O 5 5	0	0
62	28	5	Total O 5 5	0	0
62	29	1	Total O 1 1	0	0
62	2a	153	Total O 153 153	0	0
62	2e	2	Total O 2 2	0	0
62	2g	2	Total O 2 2	0	0
62	2i	1	Total O 1 1	0	0
62	2j	3	Total O 3 3	0	0
62	2l	4	Total O 4 4	0	0
62	2p	1	Total O 1 1	0	0
62	2r	1	Total O 1 1	0	0

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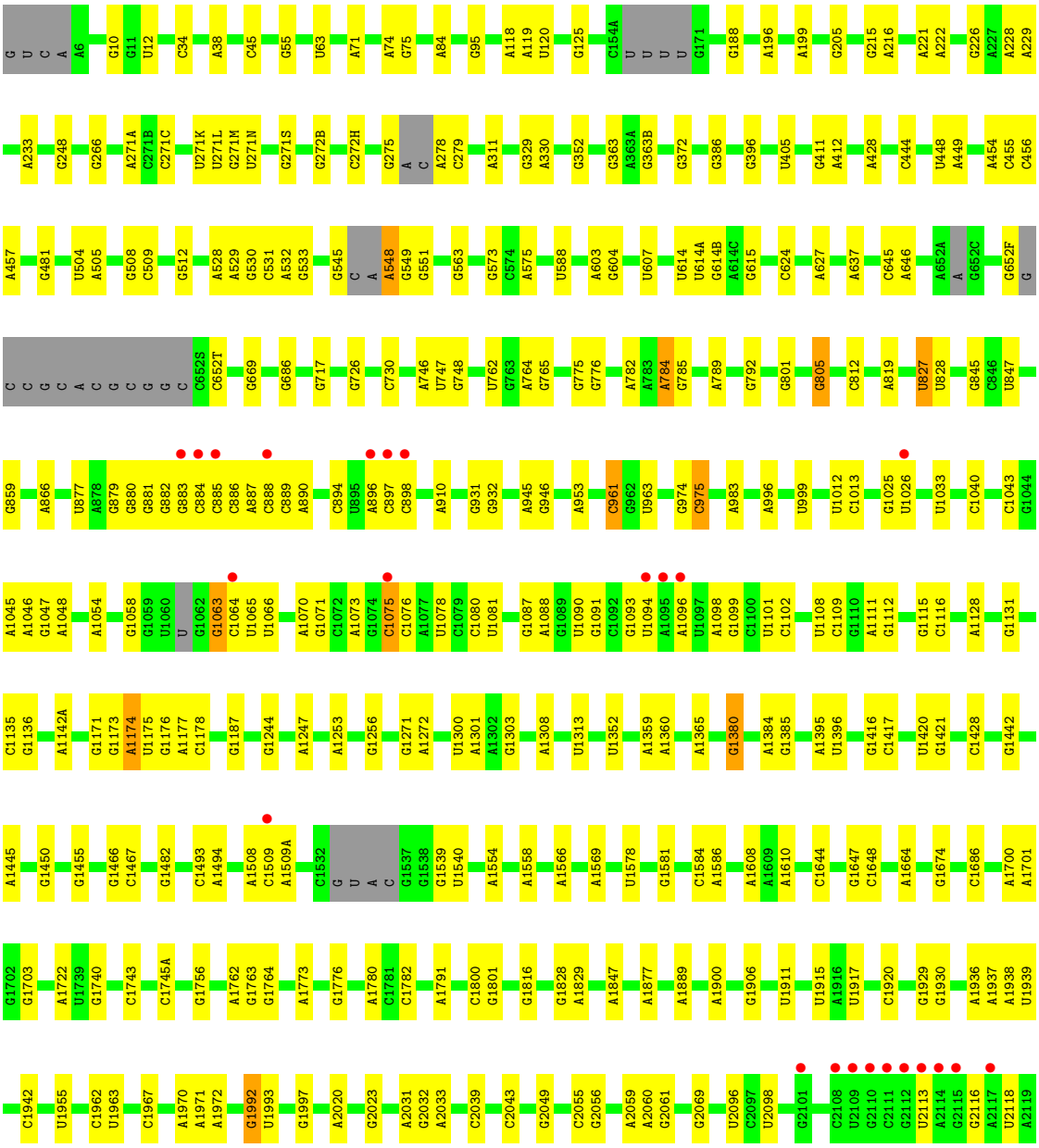
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2t	1	Total O 1 1	0	0
62	2w	2	Total O 2 2	0	0
62	2x	5	Total O 5 5	0	0
62	2y	4	Total O 4 4	0	0

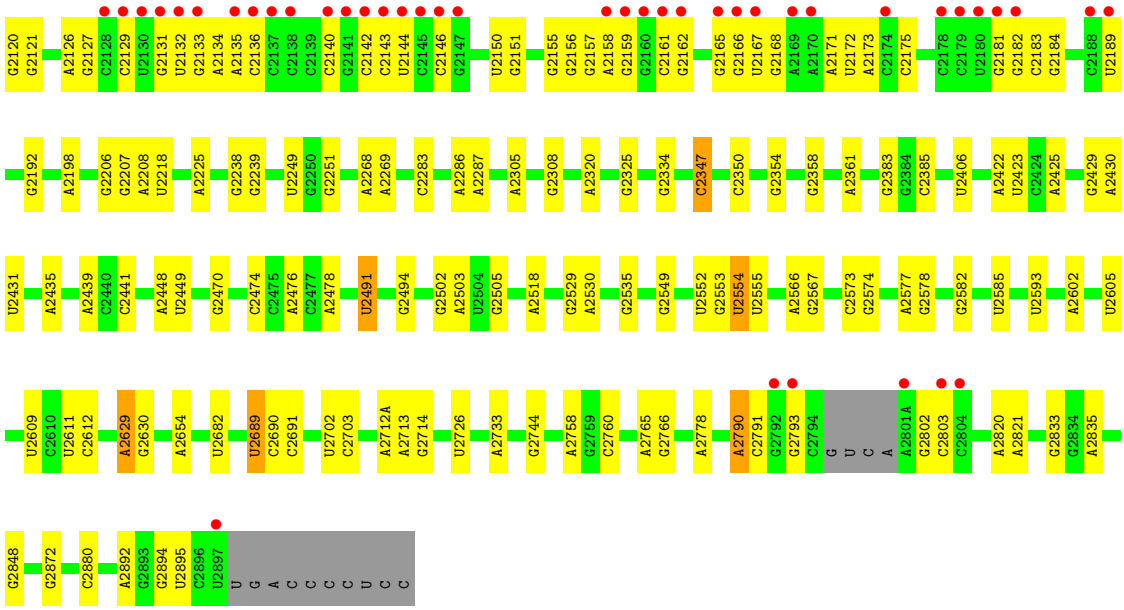
3 Residue-property plots (i)

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

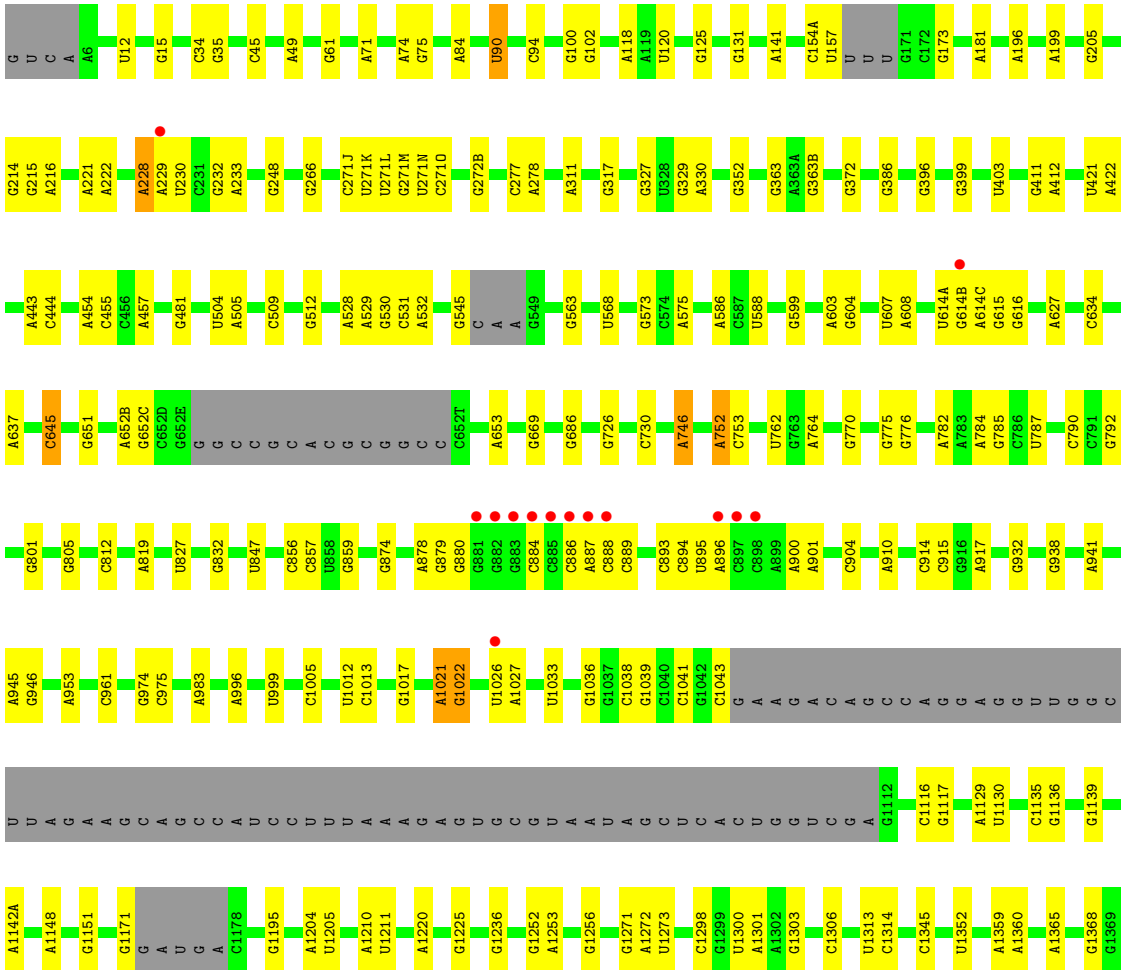
Chain 1A: 2% 82% 16%

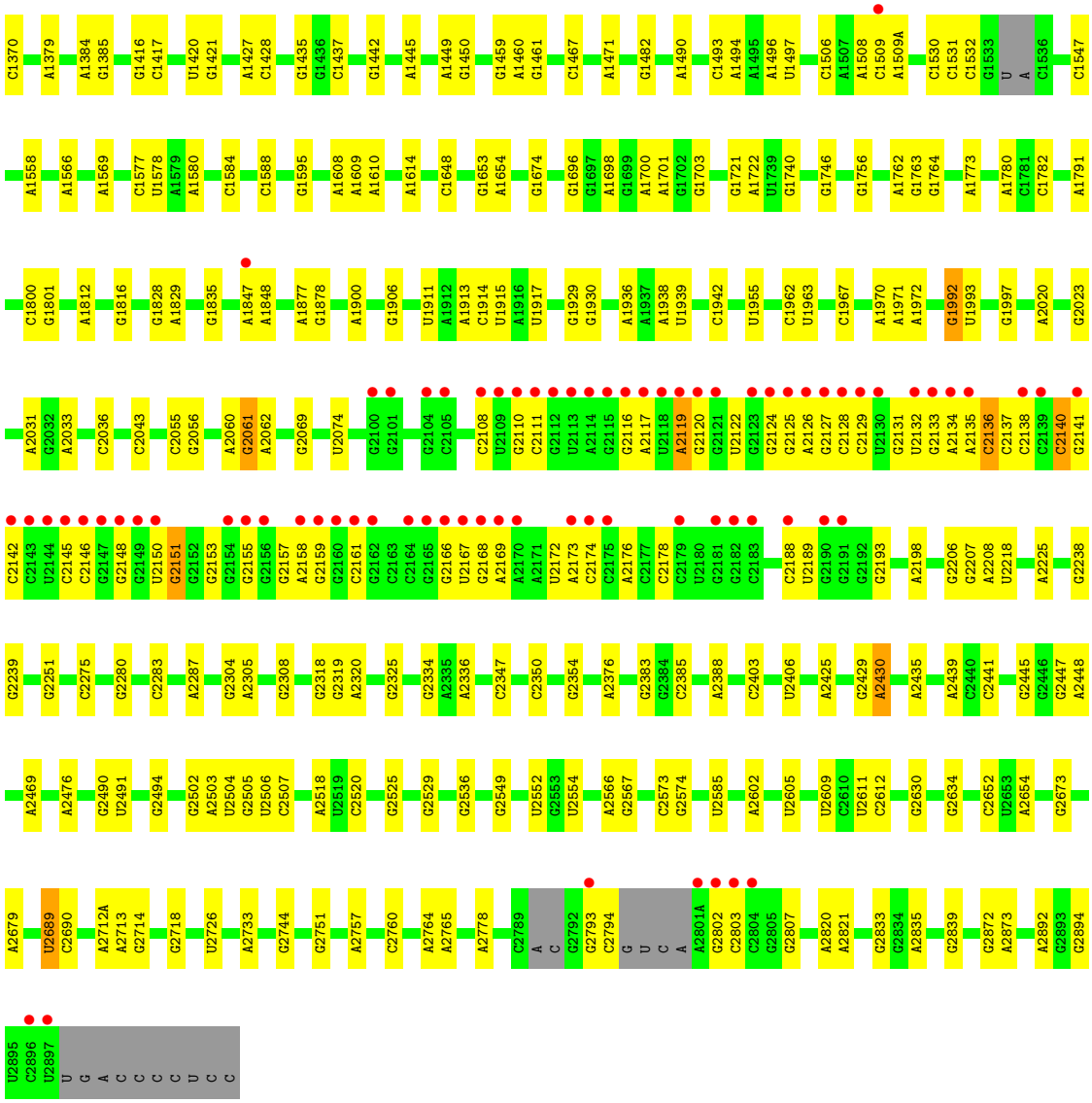




• Molecule 1: 23S Ribosomal RNA

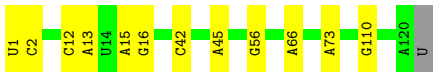
Chain 2A:





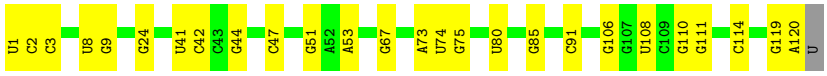
- Molecule 2: 5S Ribosomal RNA

Chain 1B:



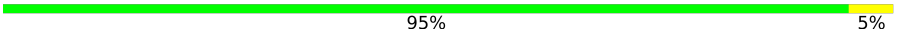
- Molecule 2: 5S Ribosomal RNA

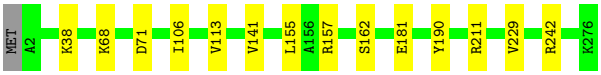
Chain 2B:



- Molecule 3: 50S ribosomal protein L2

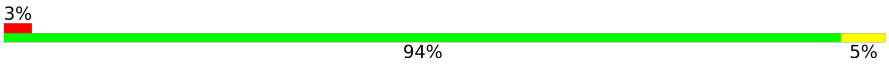
Chain 1D:

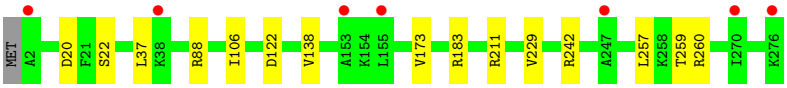




• Molecule 3: 50S ribosomal protein L2

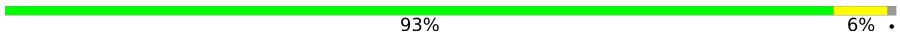
Chain 2D:





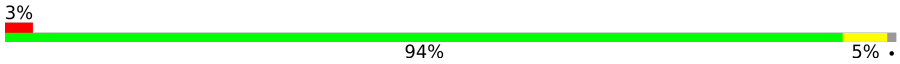
• Molecule 4: 50S ribosomal protein L3

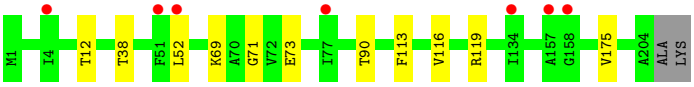
Chain 1E:



• Molecule 4: 50S ribosomal protein L3

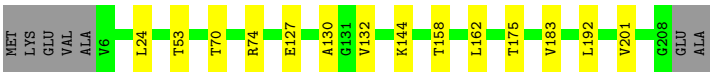
Chain 2E:





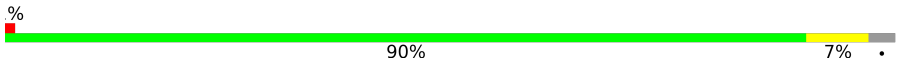
• Molecule 5: 50S ribosomal protein L4

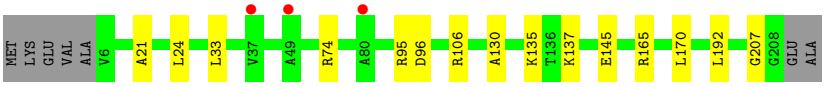
Chain 1F:



• Molecule 5: 50S ribosomal protein L4

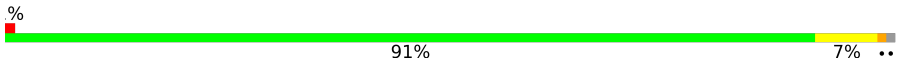
Chain 2F:

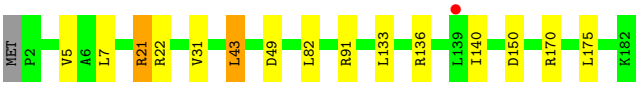




• Molecule 6: 50S ribosomal protein L5

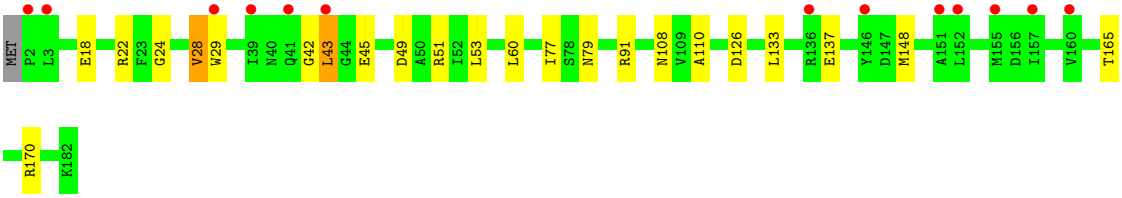
Chain 1G:





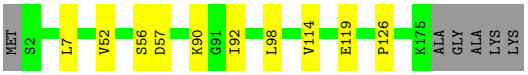
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



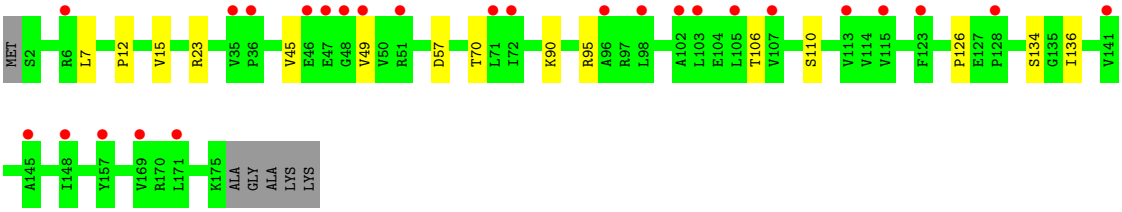
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



• Molecule 7: 50S ribosomal protein L6

Chain 2H:

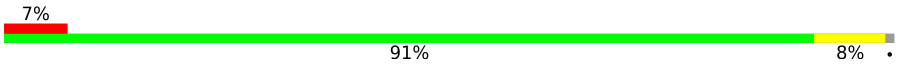


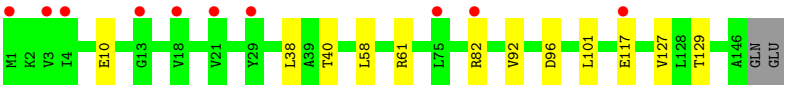
• Molecule 8: 50S ribosomal protein L9

Chain 1I:

• Molecule 8: 50S ribosomal protein L9

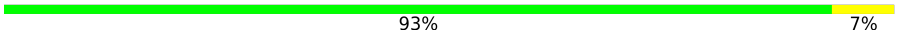
Chain 2I:

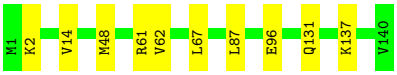




• Molecule 9: 50S ribosomal protein L13

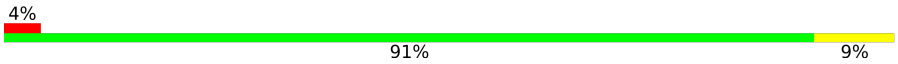
Chain 1N:

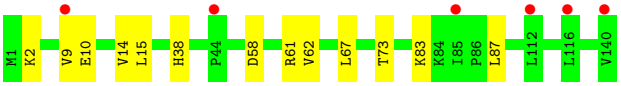




• Molecule 9: 50S ribosomal protein L13

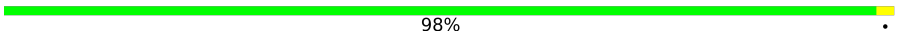
Chain 2N:

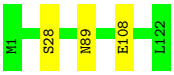




• Molecule 10: 50S ribosomal protein L14

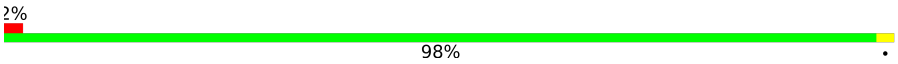
Chain 1O:





• Molecule 10: 50S ribosomal protein L14

Chain 2O:

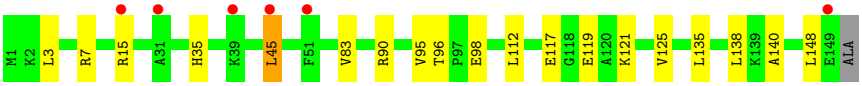


• Molecule 11: 50S ribosomal protein L15

Chain 1P:

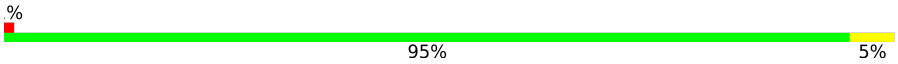
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



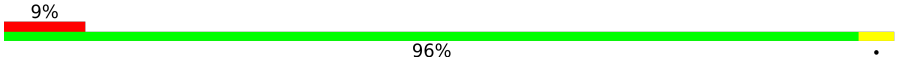
• Molecule 12: 50S ribosomal protein L16

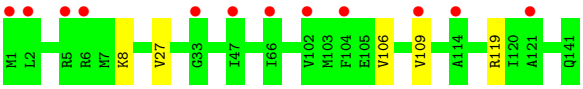
Chain 1Q:



• Molecule 12: 50S ribosomal protein L16

Chain 2Q:





• Molecule 13: 50S ribosomal protein L17

Chain 1R: 95% 5%

M1 L29 R33 T36 L67 L79 V114 E118

• Molecule 13: 50S ribosomal protein L17

Chain 2R: % 94% 6%

M1 S6 S15 L29 R33 V66 L67 L79 V114 E118

• Molecule 14: 50S ribosomal protein L18

Chain 1S: 87% 12%

MET ALA R3 E8 V14 R15 N16 R17 V46 T47 L48 V49 Q68 R71 A72 L73 L78 L110 E111 F112

• Molecule 14: 50S ribosomal protein L18

Chain 2S: 87% 12%

MET ALA R3 L4 T5 R20 R25 I35 Y36 E43 L58 E64 Q68 K83 Q84 V85 K93 F112

• Molecule 15: 50S ribosomal protein L19

Chain 1T: 84% 5% 10%

M1 E21 V28 G37 R51 V89 R96 N104 E128 A131 LYS GLU GLU ALA GLN LYS ALA GLN GLU PRO LYS ALA SER GLN GLU

• Molecule 15: 50S ribosomal protein L19

Chain 2T: % 86% 10%

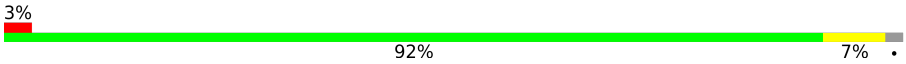
M1 L9 T17 V49 R96 R108 R111 A131 LYS GLU GLU ALA GLN LYS ALA GLN GLU PRO LYS ALA SER GLN GLU

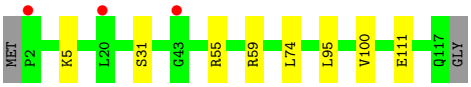
• Molecule 16: 50S ribosomal protein L20

Chain 1U: 94%

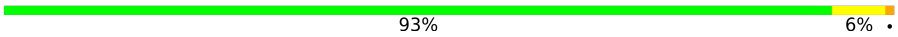
MET P2 R50 L74 S77 T78 L95 Q117 GLY

• Molecule 16: 50S ribosomal protein L20

Chain 2U: 



• Molecule 17: 50S ribosomal protein L21

Chain 1V: 

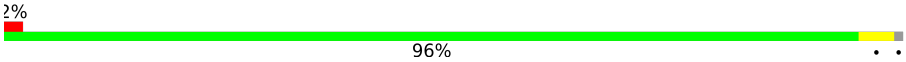
• Molecule 17: 50S ribosomal protein L21

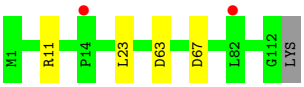
Chain 2V:

• Molecule 18: 50S ribosomal protein L22

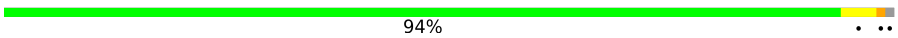
Chain 1W:

• Molecule 18: 50S ribosomal protein L22

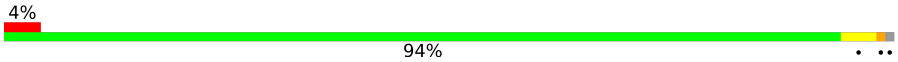
Chain 2W: 

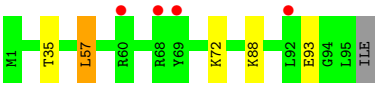


• Molecule 19: 50S ribosomal protein L23

Chain 1X: 

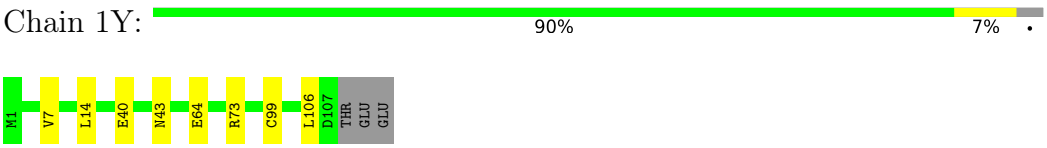
• Molecule 19: 50S ribosomal protein L23

Chain 2X: 



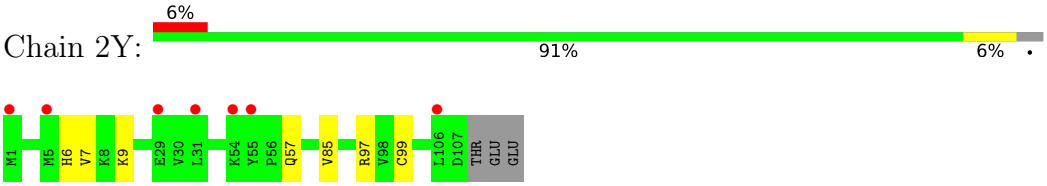
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



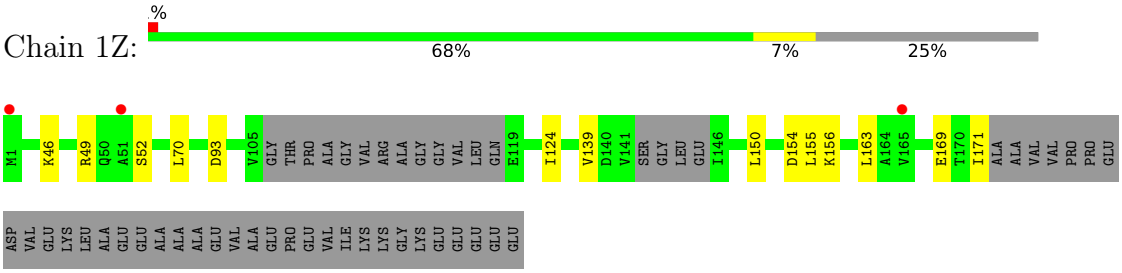
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



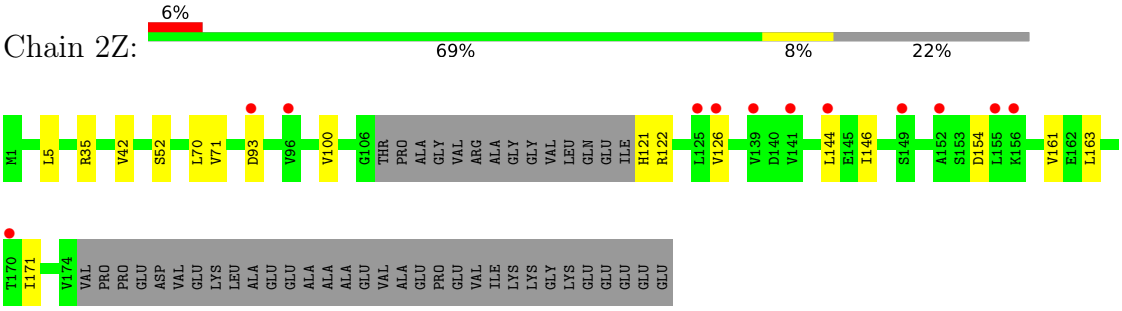
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



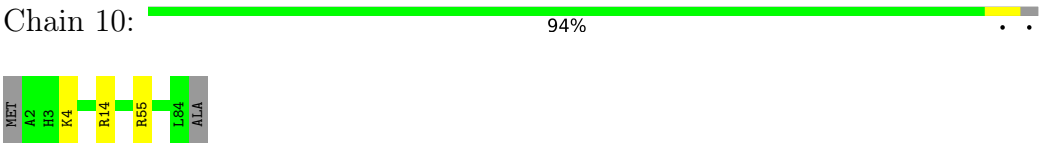
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



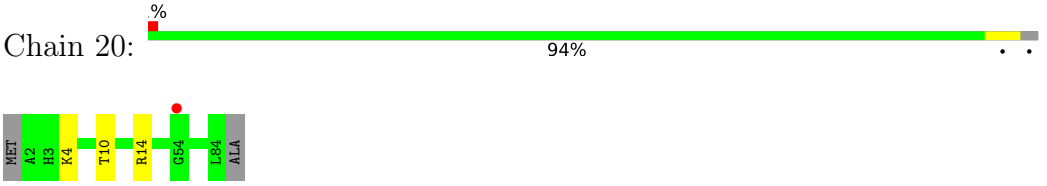
• Molecule 22: 50S ribosomal protein L27

Chain 10:



• Molecule 22: 50S ribosomal protein L27

Chain 20:



• Molecule 23: 50S ribosomal protein L28

Chain 11: 2% 96%

• Molecule 23: 50S ribosomal protein L28

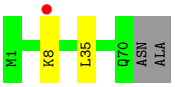
Chain 21: 7% 93% 6%

• Molecule 24: 50S ribosomal protein L29

Chain 12: 92% 6%

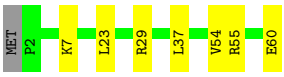
• Molecule 24: 50S ribosomal protein L29

Chain 22: % 94%



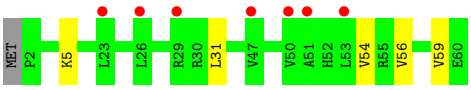
• Molecule 25: 50S ribosomal protein L30

Chain 13: 87% 12%



• Molecule 25: 50S ribosomal protein L30

Chain 23: 12% 90% 8%

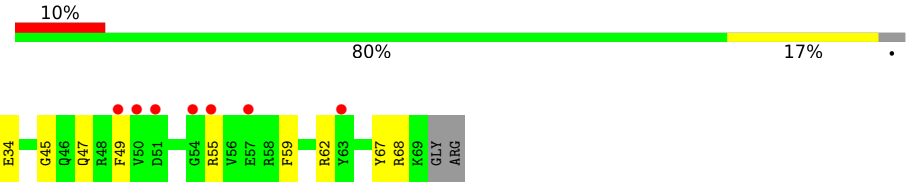


• Molecule 26: 50S ribosomal protein L31

Chain 14: 76% 17%

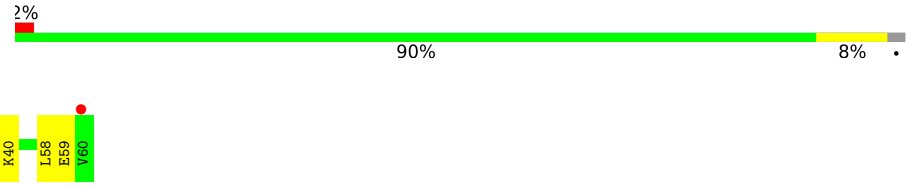
• Molecule 26: 50S ribosomal protein L31

Chain 24:



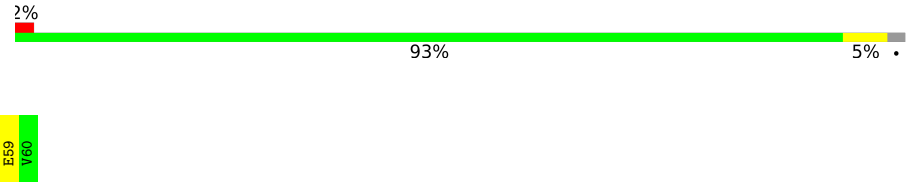
• Molecule 27: 50S ribosomal protein L32

Chain 15:



• Molecule 27: 50S ribosomal protein L32

Chain 25:

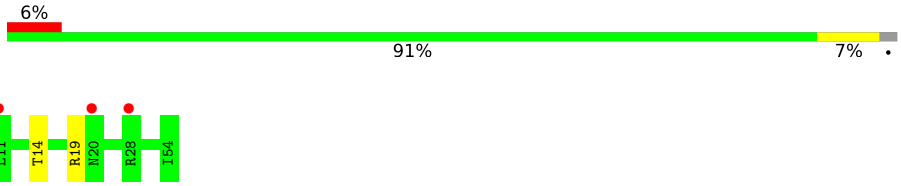


• Molecule 28: 50S ribosomal protein L33

Chain 16:

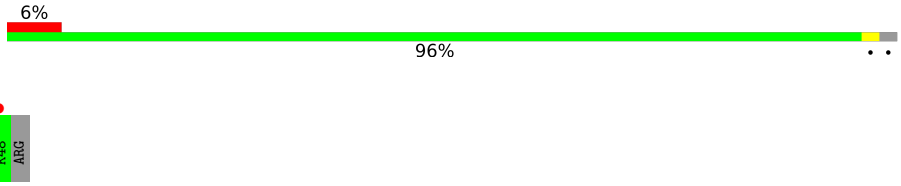
• Molecule 28: 50S ribosomal protein L33

Chain 26:



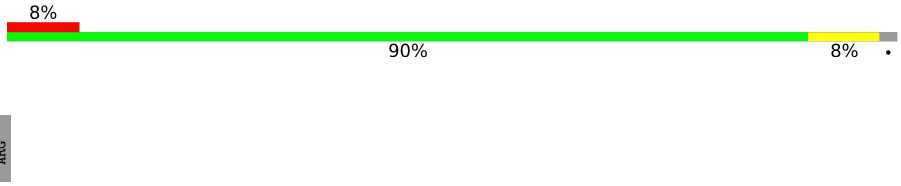
• Molecule 29: 50S ribosomal protein L34

Chain 17:



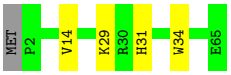
• Molecule 29: 50S ribosomal protein L34

Chain 27:



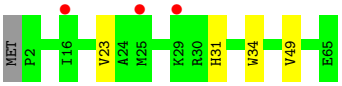
• Molecule 30: 50S ribosomal protein L35

Chain 18: 92% 6% •



• Molecule 30: 50S ribosomal protein L35

Chain 28: 5% 92% 6% •



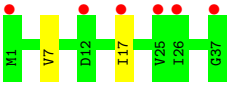
• Molecule 31: 50S ribosomal protein L36

Chain 19: 100%

There are no outlier residues recorded for this chain.

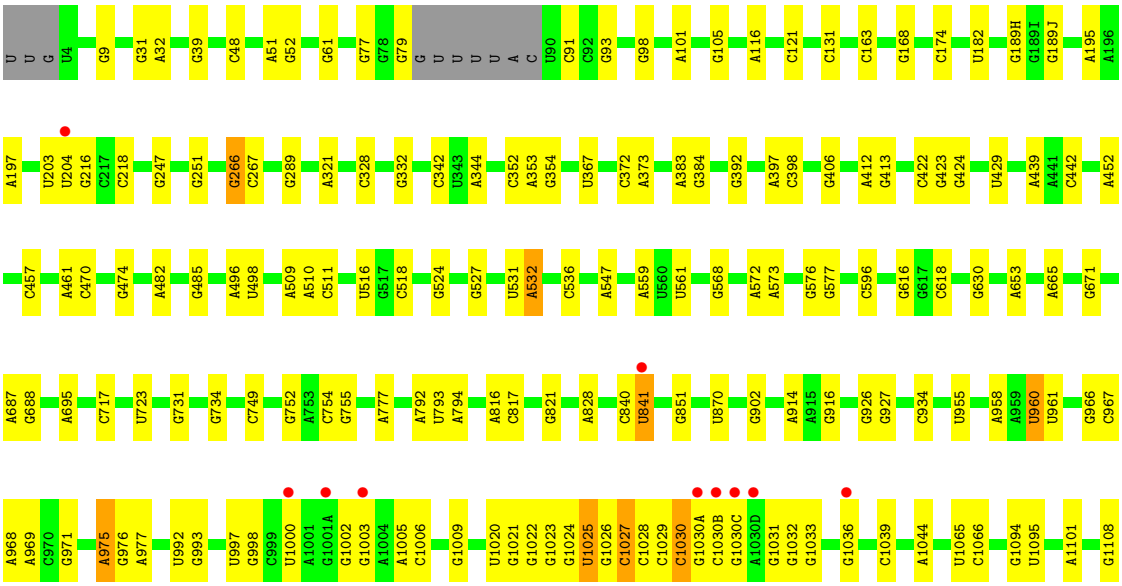
• Molecule 31: 50S ribosomal protein L36

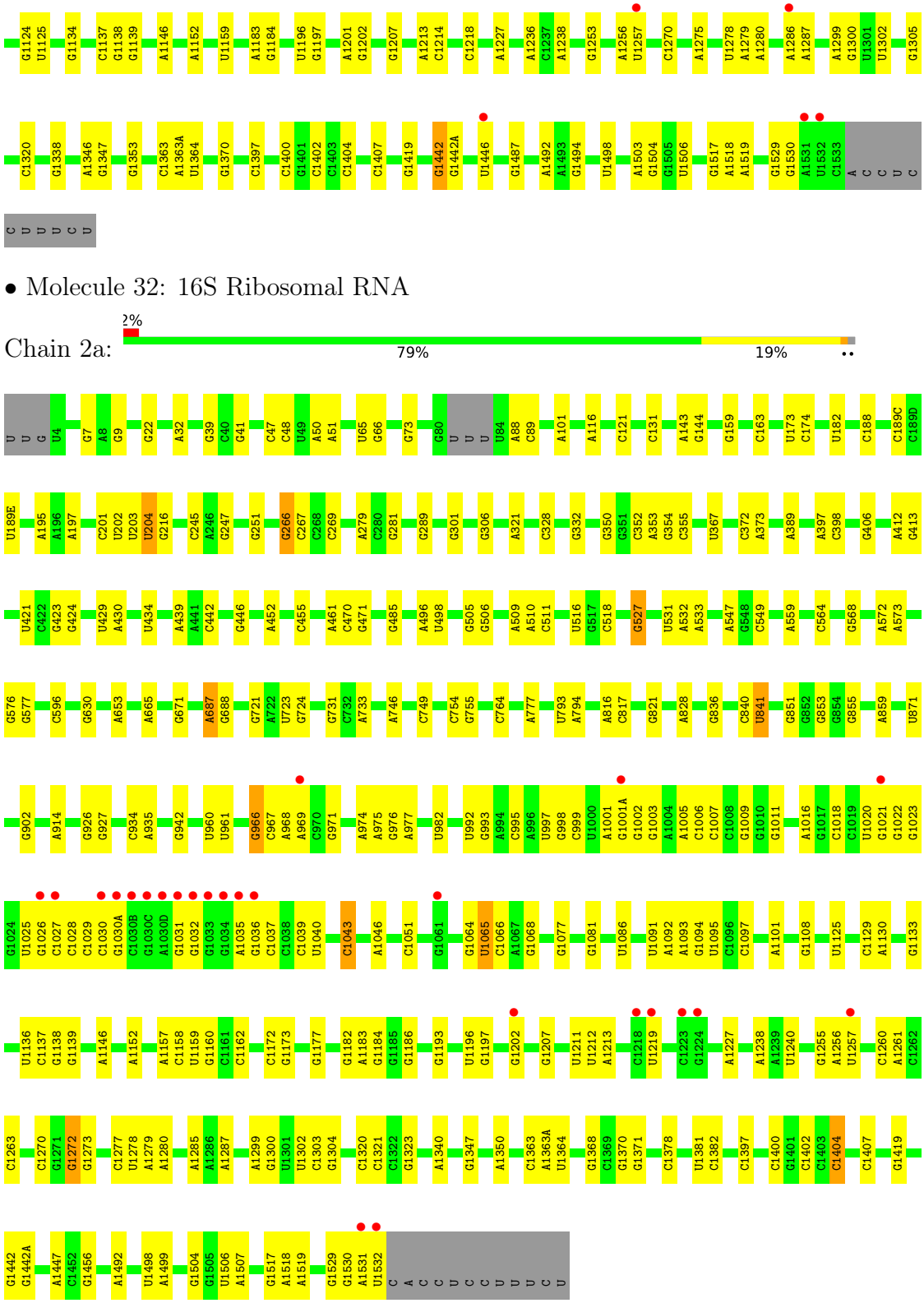
Chain 29: 16% 95% 5%



• Molecule 32: 16S Ribosomal RNA

Chain 1a: % 83% 15% ••



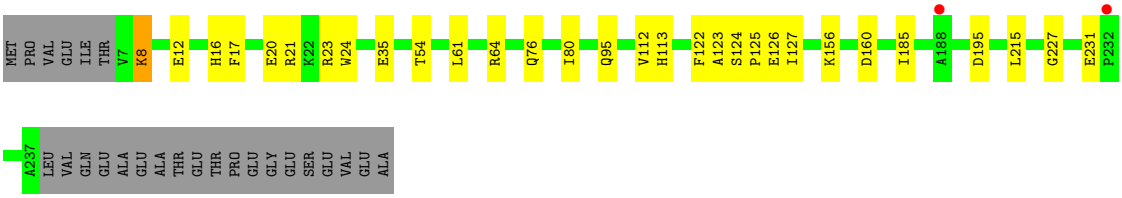


- Molecule 32: 16S Ribosomal RNA

Chain 2a: 2% 79% 19%

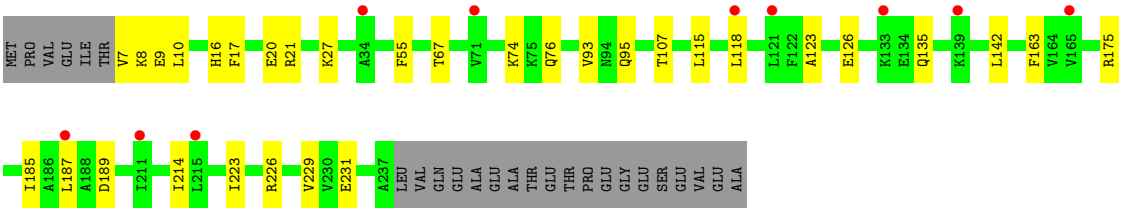
- Molecule 33: 30S ribosomal protein S2

Chain 1b: % 79% 11% 10%



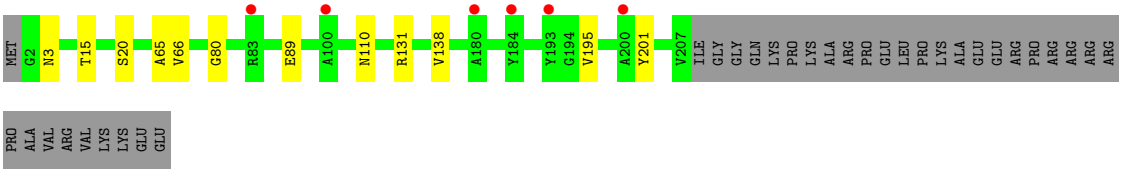
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



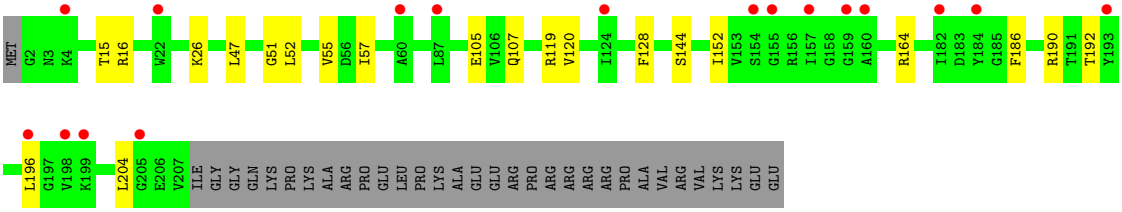
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



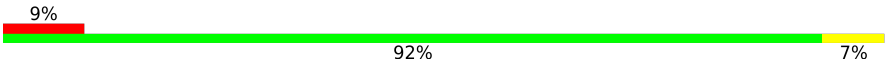
• Molecule 34: 30S ribosomal protein S3

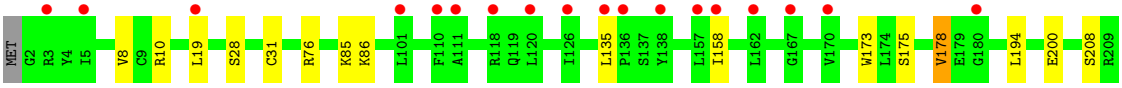
Chain 2c:



• Molecule 35: 30S ribosomal protein S4

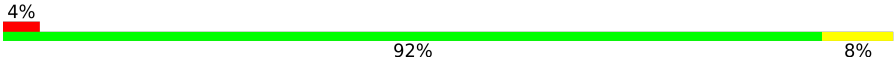
Chain 1d:

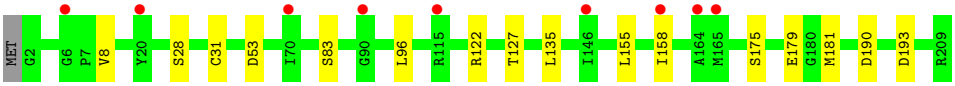




• Molecule 35: 30S ribosomal protein S4

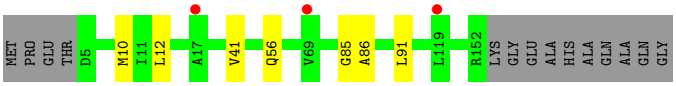
Chain 2d:





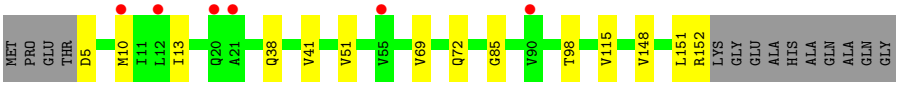
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



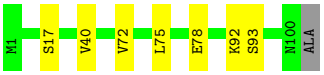
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



• Molecule 37: 30S ribosomal protein S6

Chain 1f:

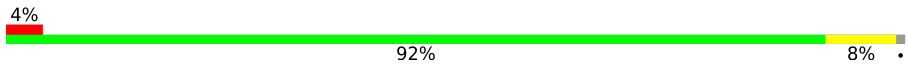


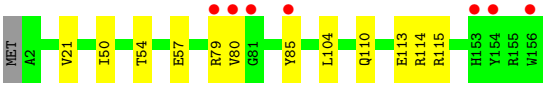
• Molecule 37: 30S ribosomal protein S6

Chain 2f:

• Molecule 38: 30S ribosomal protein S7

Chain 1g:



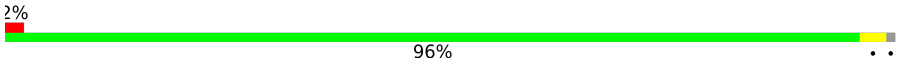


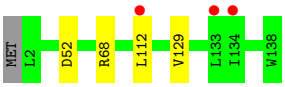
• Molecule 38: 30S ribosomal protein S7

Chain 2g:

• Molecule 39: 30S ribosomal protein S8

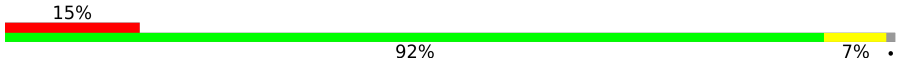
Chain 1h:

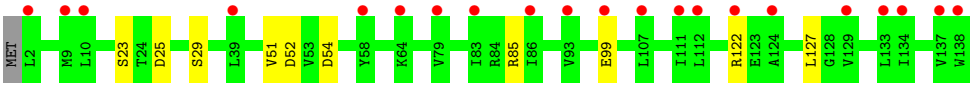




• Molecule 39: 30S ribosomal protein S8

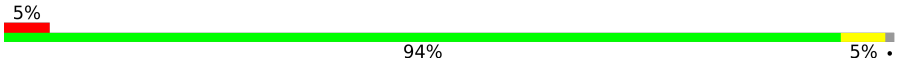
Chain 2h:

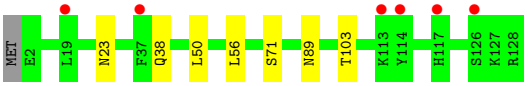




• Molecule 40: 30S ribosomal protein S9

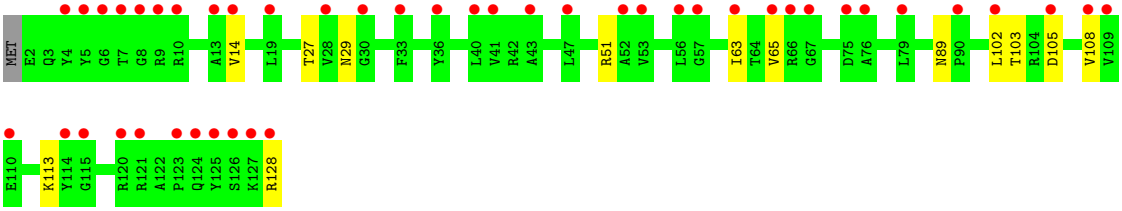
Chain 1i:





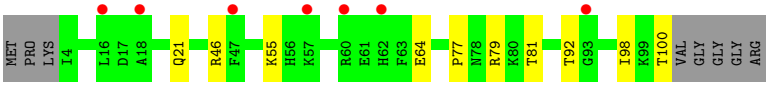
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



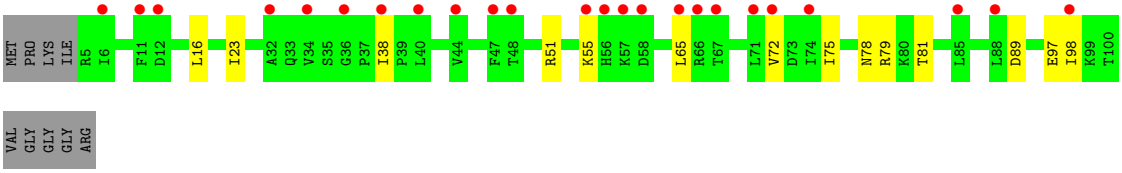
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



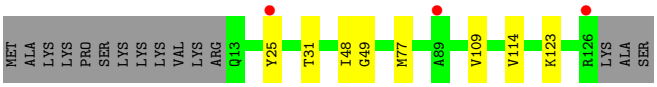
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



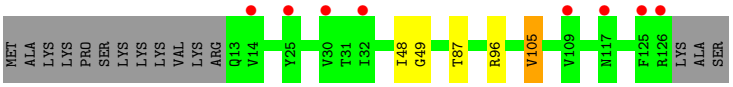
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



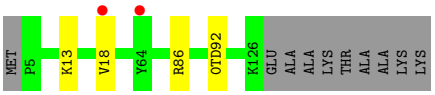
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



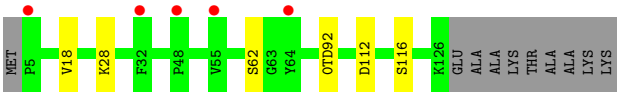
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



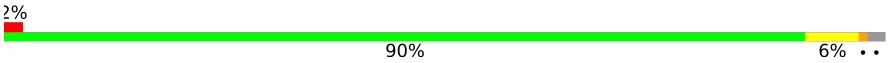
• Molecule 43: 30S ribosomal protein S12

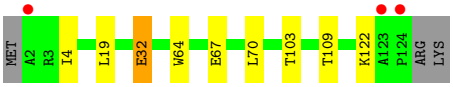
Chain 2l:



• Molecule 44: 30S ribosomal protein S13

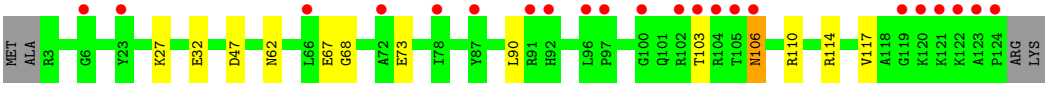
Chain 1m:





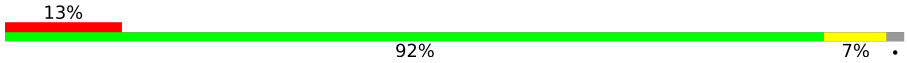
• Molecule 44: 30S ribosomal protein S13

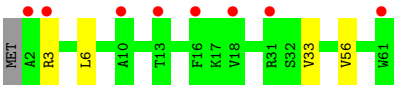
Chain 2m:



• Molecule 45: 30S ribosomal protein S14 type Z

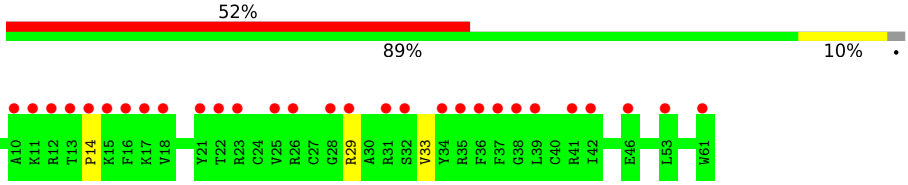
Chain 1n:





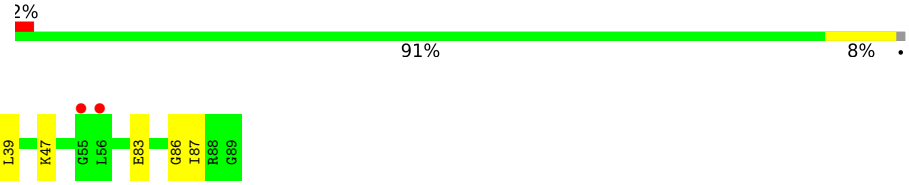
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



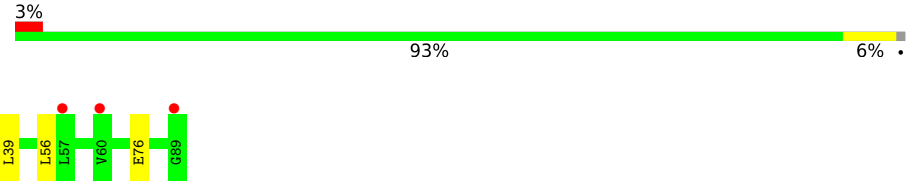
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



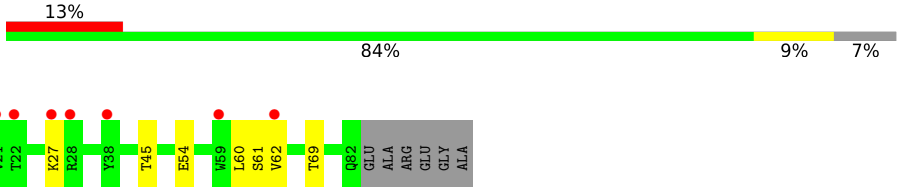
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



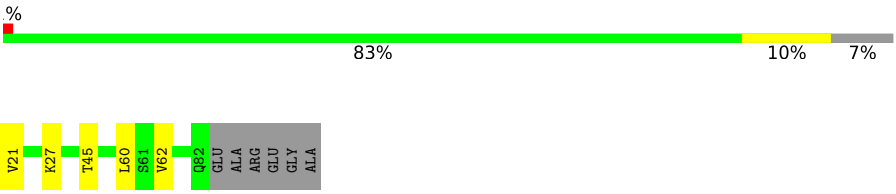
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



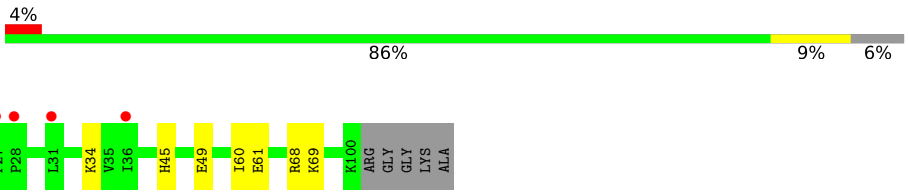
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



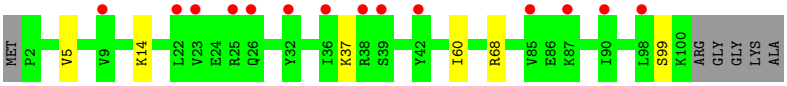
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



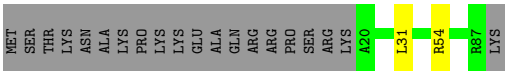
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



• Molecule 49: 30S ribosomal protein S18

Chain 1r:



• Molecule 49: 30S ribosomal protein S18

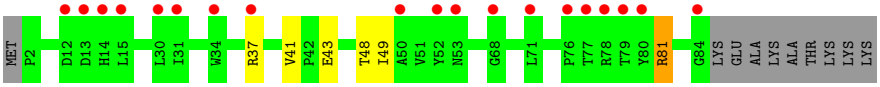
Chain 2r:

• Molecule 50: 30S ribosomal protein S19

Chain 1s:

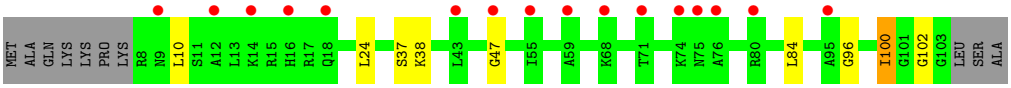
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



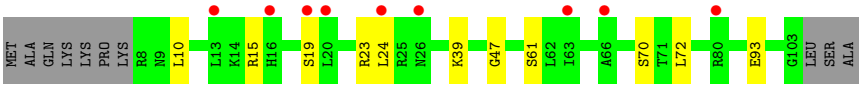
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



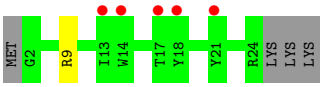
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



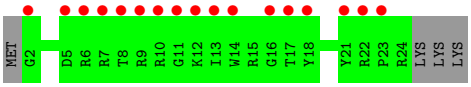
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



• Molecule 52: 30S ribosomal protein Thx

Chain 2u:

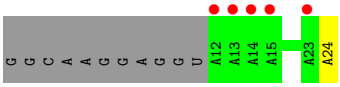


• Molecule 53: mRNA

Chain 1v:

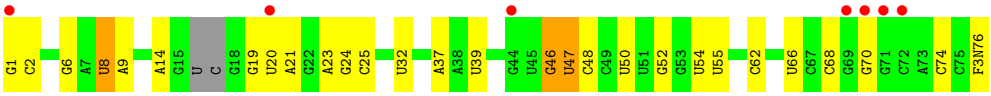
• Molecule 53: mRNA

Chain 2v:



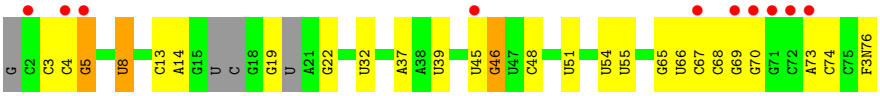
• Molecule 54: A-site tRNA

Chain 1w:



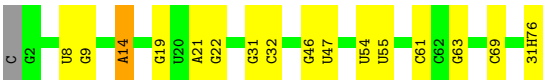
• Molecule 54: A-site tRNA

Chain 2w:



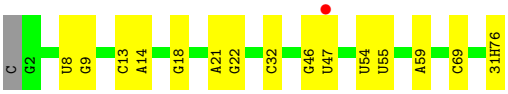
• Molecule 55: P-site tRNA

Chain 1x:



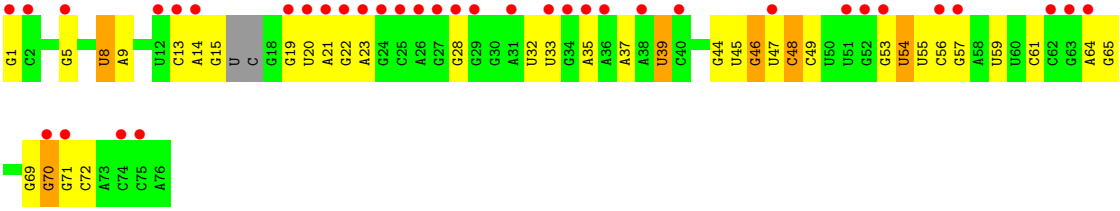
• Molecule 55: P-site tRNA

Chain 2x:



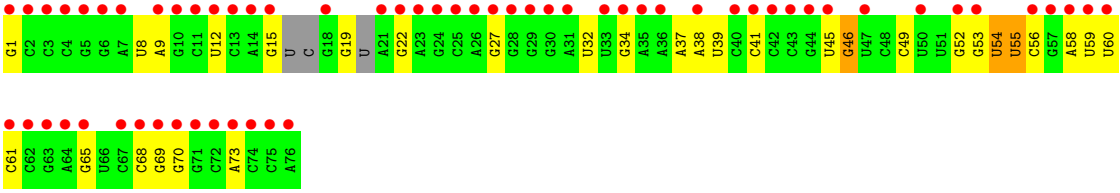
• Molecule 56: E-site tRNA

Chain 1y:



• Molecule 56: E-site tRNA

Chain 2y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.40Å 448.12Å 618.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.06 – 2.60 224.06 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (224.06-2.60) 98.4 (224.06-2.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.217 , 0.266 0.217 , 0.265	Depositor DCC
R_{free} test set	86839 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	51.3	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 53.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	299652	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, TEL, ZN, MA6, M2G, SF4, K, MG, MIA, 5MU, F3N, 7MG, 2MA, PSU, UR3, 0TD, 5MC, 31H, 4SU, OMG, 2MU, 2MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	1A	0.48	0/69009	0.95	59/107712 (0.1%)
1	2A	0.40	0/67293	0.88	44/105034 (0.0%)
2	1B	0.45	1/2882 (0.0%)	0.87	0/4494
2	2B	0.38	1/2879 (0.0%)	0.82	1/4487 (0.0%)
3	1D	0.37	0/2186	0.57	0/2944
3	2D	0.32	0/2186	0.52	0/2944
4	1E	0.32	0/1592	0.54	0/2149
4	2E	0.32	0/1592	0.51	0/2149
5	1F	0.33	0/1619	0.53	0/2193
5	2F	0.29	0/1615	0.51	0/2188
6	1G	0.31	0/1448	0.54	1/1957 (0.1%)
6	2G	0.28	0/1453	0.48	0/1963
7	1H	0.31	0/1356	0.49	0/1834
7	2H	0.28	0/1356	0.46	0/1834
8	1I	0.29	0/1112	0.50	0/1514
8	2I	0.27	0/1079	0.47	0/1475
9	1N	0.31	0/1144	0.49	0/1543
9	2N	0.28	0/1144	0.45	0/1543
10	1O	0.32	0/943	0.54	0/1269
10	2O	0.31	0/943	0.51	0/1269
11	1P	0.32	0/1152	0.58	1/1533 (0.1%)
11	2P	0.31	0/1152	0.53	0/1533
12	1Q	0.35	0/1143	0.53	0/1527
12	2Q	0.31	0/1143	0.51	0/1527
13	1R	0.32	0/982	0.53	0/1312
13	2R	0.28	0/982	0.50	0/1312
14	1S	0.30	0/883	0.51	0/1176
14	2S	0.29	0/880	0.51	0/1172
15	1T	0.33	0/1105	0.50	0/1477
15	2T	0.29	0/1097	0.49	0/1468
16	1U	0.35	0/977	0.52	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.29	0/977	0.45	0/1301
17	1V	0.33	0/782	0.53	0/1049
17	2V	0.28	0/782	0.51	0/1049
18	1W	0.32	0/897	0.52	0/1205
18	2W	0.31	0/897	0.49	0/1205
19	1X	0.38	0/764	0.57	1/1025 (0.1%)
19	2X	0.30	0/764	0.58	1/1025 (0.1%)
20	1Y	0.34	0/819	0.54	0/1095
20	2Y	0.31	0/819	0.55	0/1095
21	1Z	0.32	0/1267	0.51	0/1717
21	2Z	0.30	0/1299	0.50	0/1763
22	10	0.33	0/662	0.54	0/881
22	20	0.30	0/662	0.49	0/881
23	11	0.32	0/762	0.48	0/1014
23	21	0.31	0/762	0.49	0/1014
24	12	0.28	0/590	0.46	0/781
24	22	0.28	0/590	0.40	0/781
25	13	0.32	0/474	0.49	0/635
25	23	0.29	0/469	0.45	0/630
26	14	0.32	0/565	0.56	0/761
26	24	0.30	0/545	0.51	0/737
27	15	0.30	0/469	0.52	0/635
27	25	0.32	0/469	0.51	0/635
28	16	0.32	0/460	0.51	0/613
28	26	0.28	0/456	0.50	0/608
29	17	0.32	0/426	0.53	0/561
29	27	0.27	0/426	0.51	0/561
30	18	0.32	0/525	0.51	0/691
30	28	0.28	0/525	0.47	0/691
31	19	0.31	0/310	0.54	0/407
31	29	0.29	0/310	0.51	0/407
32	1a	0.37	0/35795	0.87	25/55864 (0.0%)
32	2a	0.36	2/35886 (0.0%)	0.90	33/56005 (0.1%)
33	1b	0.30	0/1881	0.49	0/2542
33	2b	0.29	0/1860	0.50	0/2518
34	1c	0.29	0/1572	0.47	0/2126
34	2c	0.28	0/1566	0.47	0/2119
35	1d	0.29	0/1685	0.47	0/2262
35	2d	0.28	0/1704	0.46	0/2284
36	1e	0.30	0/1145	0.52	0/1543
36	2e	0.28	0/1149	0.51	0/1548
37	1f	0.28	0/823	0.48	0/1115
37	2f	0.29	0/829	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.29	0/1250	0.44	0/1679
38	2g	0.27	0/1254	0.44	0/1683
39	1h	0.29	0/1108	0.48	0/1494
39	2h	0.27	0/1108	0.46	0/1494
40	1i	0.29	0/1002	0.51	0/1346
40	2i	0.29	0/997	0.51	0/1343
41	1j	0.28	0/722	0.48	0/982
41	2j	0.28	0/727	0.50	0/988
42	1k	0.29	0/844	0.48	0/1145
42	2k	0.30	0/848	0.46	0/1149
43	1l	0.32	0/937	0.52	0/1260
43	2l	0.28	0/937	0.48	0/1260
44	1m	0.28	0/969	0.48	0/1302
44	2m	0.27	0/961	0.48	0/1291
45	1n	0.31	0/501	0.49	0/664
45	2n	0.32	0/501	0.50	0/664
46	1o	0.27	0/739	0.43	0/985
46	2o	0.26	0/739	0.41	0/985
47	1p	0.27	0/697	0.50	0/939
47	2p	0.27	0/693	0.50	0/935
48	1q	0.29	0/836	0.48	0/1117
48	2q	0.28	0/836	0.46	0/1117
49	1r	0.29	0/560	0.50	0/746
49	2r	0.28	0/560	0.47	0/746
50	1s	0.30	0/667	0.53	0/900
50	2s	0.28	0/661	0.53	0/893
51	1t	0.28	0/730	0.45	0/965
51	2t	0.27	0/729	0.45	0/965
52	1u	0.28	0/203	0.47	0/266
52	2u	0.27	0/203	0.47	0/266
53	1v	0.43	0/310	0.89	0/480
53	2v	0.40	0/310	0.90	0/480
54	1w	0.53	1/1581 (0.1%)	1.13	4/2458 (0.2%)
54	2w	0.42	0/1531	1.05	2/2379 (0.1%)
55	1x	0.54	2/1700 (0.1%)	1.12	19/2650 (0.7%)
55	2x	0.47	0/1700	1.04	12/2650 (0.5%)
56	1y	0.57	1/1606 (0.1%)	1.16	8/2497 (0.3%)
56	2y	0.54	1/1583 (0.1%)	1.05	2/2459 (0.1%)
All	All	0.39	9/316586 (0.0%)	0.82	213/473957 (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
11	1P	0	2
11	2P	0	1
33	1b	0	3
46	1o	0	1
All	All	0	7

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2B	1	U	OP3-P	-10.47	1.48	1.61
54	1w	1	G	OP3-P	-10.28	1.48	1.61
56	1y	1	G	OP3-P	-10.18	1.49	1.61
2	1B	1	U	OP3-P	-10.17	1.49	1.61
56	2y	1	G	OP3-P	-10.01	1.49	1.61
32	2a	1272	G	N1-C2	-8.74	1.30	1.37
32	2a	1272	G	C6-N1	-8.19	1.33	1.39
55	1x	22	G	N7-C5	5.60	1.42	1.39
55	1x	14	A	C8-N7	-5.54	1.27	1.31

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1263	C	N1-C2-O2	23.86	133.21	118.90
32	2a	1272	G	N3-C2-N2	21.78	135.15	119.90
32	2a	1272	G	N1-C2-N2	-18.18	99.84	116.20
32	2a	1272	G	C5-C6-O6	16.65	138.59	128.60
32	2a	1263	C	C2-N3-C4	14.86	127.33	119.90
32	2a	1263	C	N3-C2-O2	-13.10	112.73	121.90
32	2a	1263	C	C5-C6-N1	12.28	127.14	121.00
32	2a	1272	G	C6-N1-C2	11.61	132.06	125.10
55	1x	46	G	C6-N1-C2	-11.40	118.26	125.10
1	1A	1063	G	C5-C6-O6	11.14	135.28	128.60
1	1A	1075	C	N1-C2-O2	11.01	125.50	118.90
1	1A	1075	C	C2-N3-C4	10.25	125.02	119.90
55	2x	46	G	C6-N1-C2	-9.93	119.14	125.10
32	2a	1272	G	C5-C6-N1	-9.37	106.82	111.50
32	2a	1263	C	C2-N1-C1'	9.30	129.03	118.80
55	2x	14	A	C4-C5-C6	9.15	121.57	117.00
54	1w	47	U	C2-N1-C1'	8.97	128.46	117.70
1	2A	2136	C	N1-C2-O2	8.94	124.26	118.90
55	1x	22	G	C5-N7-C8	-8.93	99.83	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	14	A	C5-N7-C8	8.90	108.35	103.90
55	1x	14	A	C4-C5-C6	8.88	121.44	117.00
32	2a	1272	G	N1-C6-O6	-8.88	114.57	119.90
1	1A	1063	G	N3-C2-N2	8.78	126.05	119.90
32	2a	1263	C	C6-N1-C2	-8.67	116.83	120.30
2	2B	80	U	O4'-C1'-N1	8.57	115.06	108.20
32	1a	1030(B)	C	C2-N1-C1'	8.48	128.13	118.80
1	1A	1776	G	O5'-P-OP2	-8.44	98.10	105.70
1	1A	624	C	O5'-P-OP1	-8.44	98.11	105.70
1	1A	2554	U	O5'-P-OP1	-8.41	98.13	105.70
55	1x	14	A	C5-N7-C8	8.35	108.08	103.90
32	2a	1263	C	C4-C5-C6	-8.25	113.28	117.40
1	1A	1063	G	C6-N1-C2	8.21	130.02	125.10
32	2a	1272	G	C4-N9-C1'	8.19	137.15	126.50
1	2A	2155	G	C6-N1-C2	8.05	129.93	125.10
32	1a	1030(B)	C	N1-C2-O2	8.03	123.72	118.90
32	2a	1272	G	C8-N9-C1'	-7.93	116.69	127.00
1	2A	2155	G	C5-C6-O6	7.87	133.32	128.60
55	1x	22	G	C4-C5-C6	-7.69	114.19	118.80
55	2x	22	G	C5-N7-C8	-7.56	100.52	104.30
1	1A	975	C	N1-C2-O2	-7.43	114.44	118.90
32	2a	841	U	C5-C6-N1	7.43	126.41	122.70
32	2a	1263	C	N1-C2-N3	-7.40	114.02	119.20
1	1A	512	G	O4'-C1'-N9	7.38	114.10	108.20
32	2a	1272	G	C2-N3-C4	-7.36	108.22	111.90
1	2A	2061	G	O5'-P-OP2	-7.34	99.10	105.70
32	1a	1030(B)	C	C6-N1-C2	-7.20	117.42	120.30
1	2A	2140	C	C2-N1-C1'	7.12	126.64	118.80
1	2A	1614	A	O5'-P-OP1	-7.06	99.35	105.70
32	1a	754	C	C2-N1-C1'	6.98	126.48	118.80
55	1x	14	A	C5-C6-N1	-6.84	114.28	117.70
55	1x	22	G	N3-C4-N9	-6.83	121.90	126.00
1	2A	645	C	N1-C2-O2	6.82	122.99	118.90
1	1A	1075	C	C5-C4-N4	6.77	124.94	120.20
1	2A	1313	U	C2-N1-C1'	6.72	125.77	117.70
32	1a	266	G	P-O3'-C3'	6.71	127.75	119.70
1	1A	999	U	O5'-P-OP2	-6.69	99.68	105.70
6	1G	21	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	1A	2689	U	P-O3'-C3'	6.66	127.69	119.70
1	1A	1992	G	P-O3'-C3'	6.56	127.58	119.70
54	1w	47	U	C6-N1-C1'	-6.55	112.02	121.20
1	2A	2430	A	O5'-P-OP2	-6.54	99.81	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1063	G	N1-C6-O6	-6.54	115.98	119.90
32	1a	1030(B)	C	N3-C2-O2	-6.52	117.33	121.90
19	2X	57	LEU	CA-CB-CG	6.52	130.30	115.30
55	2x	46	G	N3-C2-N2	-6.50	115.35	119.90
55	1x	46	G	C5-C6-N1	6.49	114.75	111.50
1	1A	1187	G	N1-C6-O6	-6.48	116.01	119.90
56	1y	48	C	N1-C2-O2	-6.48	115.01	118.90
32	1a	1442	G	N3-C4-C5	-6.44	125.38	128.60
1	1A	1380	G	O5'-P-OP2	-6.43	99.92	105.70
1	1A	845	G	O4'-C1'-N9	6.41	113.33	108.20
54	1w	47	U	N1-C2-O2	6.41	127.28	122.80
1	2A	645	C	C2-N1-C1'	6.34	125.77	118.80
1	2A	2140	C	N1-C2-O2	6.29	122.67	118.90
55	2x	22	G	C4-C5-C6	-6.29	115.03	118.80
32	1a	754	C	N1-C2-O2	6.28	122.67	118.90
32	1a	1025	U	N1-C2-O2	6.25	127.17	122.80
32	2a	754	C	C2-N1-C1'	6.23	125.65	118.80
1	1A	2682	U	O5'-P-OP2	-6.20	100.12	105.70
56	2y	22	G	N1-C6-O6	6.19	123.61	119.90
32	2a	1263	C	C5-C4-N4	6.18	124.53	120.20
55	2x	14	A	C5-C6-N1	-6.17	114.61	117.70
1	2A	512	G	O4'-C1'-N9	6.16	113.13	108.20
1	2A	847	U	C2-N1-C1'	6.15	125.08	117.70
1	2A	141	A	N7-C8-N9	6.13	116.86	113.80
55	2x	46	G	C5-C6-N1	6.12	114.56	111.50
1	1A	2167	U	C2-N1-C1'	6.12	125.05	117.70
1	2A	801	G	O5'-P-OP2	-6.11	100.20	105.70
1	1A	1644	C	C2-N1-C1'	6.09	125.50	118.80
1	2A	2151	G	C5-C6-O6	-6.05	124.97	128.60
56	1y	33	U	N1-C2-O2	6.05	127.03	122.80
55	1x	46	G	N3-C4-C5	-6.01	125.59	128.60
1	1A	1936	A	O4'-C1'-N9	5.99	113.00	108.20
1	2A	2136	C	N3-C2-O2	-5.97	117.72	121.90
1	1A	975	C	C2-N1-C1'	-5.96	112.24	118.80
1	1A	2629	A	P-O3'-C3'	5.94	126.83	119.70
55	1x	46	G	N1-C2-N3	5.94	127.47	123.90
55	1x	46	G	C5-C6-O6	-5.91	125.06	128.60
1	2A	228	A	OP1-P-O3'	5.91	118.19	105.20
55	1x	22	G	C8-N9-C1'	5.89	134.65	127.00
32	2a	1272	G	N3-C4-N9	5.87	129.52	126.00
1	1A	2848	G	O4'-C1'-N9	5.87	112.89	108.20
55	1x	22	G	N7-C8-N9	5.87	116.03	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1075	C	N3-C2-O2	-5.86	117.80	121.90
1	2A	2155	G	N3-C2-N2	5.85	124.00	119.90
1	1A	847	U	C2-N1-C1'	5.84	124.71	117.70
1	2A	746	A	O4'-C1'-N9	5.84	112.87	108.20
56	1y	64	A	N1-C6-N6	-5.81	115.12	118.60
1	2A	787	U	O5'-P-OP1	-5.80	100.48	105.70
1	1A	588	U	O5'-P-OP2	-5.79	100.48	105.70
1	1A	1080	C	N1-C2-O2	5.76	122.36	118.90
1	1A	801	G	O5'-P-OP2	-5.75	100.53	105.70
1	2A	2318	G	C4-N9-C1'	5.75	133.97	126.50
56	1y	64	A	C5-C6-N6	5.75	128.30	123.70
1	2A	2447	G	C8-N9-C4	5.74	108.70	106.40
1	2A	2447	G	C4-N9-C1'	-5.73	119.06	126.50
1	1A	2249	U	N3-C4-O4	-5.72	115.39	119.40
55	1x	22	G	N3-C4-C5	5.72	131.46	128.60
1	2A	1992	G	P-O3'-C3'	5.72	126.56	119.70
1	2A	228	A	P-O3'-C3'	5.68	126.51	119.70
1	1A	1063	G	N1-C2-N2	-5.66	111.11	116.20
32	2a	687	A	P-O3'-C3'	5.65	126.48	119.70
56	1y	33	U	C2-N1-C1'	5.64	124.47	117.70
1	2A	2140	C	C6-N1-C1'	-5.64	114.03	120.80
56	1y	33	U	N3-C2-O2	-5.63	118.26	122.20
32	2a	1263	C	C6-N1-C1'	-5.62	114.06	120.80
1	1A	2059	A	C8-N9-C4	5.61	108.04	105.80
32	1a	1030(B)	C	C5-C6-N1	5.57	123.79	121.00
1	1A	226	G	O4'-C1'-N9	5.57	112.66	108.20
1	2A	2142	C	C2-N1-C1'	5.57	124.93	118.80
32	1a	1065	U	P-O3'-C3'	5.56	126.38	119.70
32	1a	1442	G	C2-N3-C4	5.56	114.68	111.90
1	1A	2167	U	N3-C2-O2	-5.55	118.32	122.20
1	1A	1174	A	P-O3'-C3'	5.55	126.36	119.70
1	1A	881	G	N7-C8-N9	5.54	115.87	113.10
1	1A	1063	G	C5-C6-N1	-5.54	108.73	111.50
1	1A	2577	A	O5'-P-OP1	-5.54	100.71	105.70
55	1x	22	G	N1-C6-O6	-5.53	116.58	119.90
1	2A	2119	A	OP1-P-O3'	5.53	117.36	105.20
32	1a	1030	C	N1-C2-O2	5.52	122.21	118.90
1	1A	1131	G	O4'-C1'-N9	5.51	112.61	108.20
54	1w	47	U	C5-C6-N1	5.50	125.45	122.70
32	1a	841	U	C5-C6-N1	5.49	125.45	122.70
1	1A	748	G	C4-N9-C1'	-5.48	119.38	126.50
1	2A	90	U	C2-N1-C1'	5.47	124.27	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1065	U	P-O3'-C3'	5.46	126.26	119.70
56	1y	15	G	N3-C2-N2	5.45	123.72	119.90
1	1A	1686	C	C6-N1-C2	-5.44	118.12	120.30
19	1X	57	LEU	CA-CB-CG	5.43	127.79	115.30
1	2A	1698	A	O4'-C1'-N9	5.42	112.54	108.20
32	2a	1263	C	N3-C4-N4	-5.40	114.22	118.00
1	1A	2790	A	C2-N3-C4	5.40	113.30	110.60
32	2a	266	G	P-O3'-C3'	5.40	126.18	119.70
32	2a	1272	G	N9-C4-C5	-5.39	103.25	105.40
32	1a	1030(B)	C	C6-N1-C1'	-5.36	114.36	120.80
55	1x	14	A	C8-N9-C1'	-5.35	118.06	127.70
32	2a	204	U	C2-N1-C1'	5.35	124.12	117.70
32	1a	960	U	C2-N1-C1'	5.34	124.11	117.70
32	1a	754	C	N3-C2-O2	-5.33	118.17	121.90
55	2x	46	G	C4-C5-N7	-5.33	108.67	110.80
54	2w	5	G	C4-N9-C1'	-5.32	119.58	126.50
32	1a	1002	G	C4-N9-C1'	5.32	133.41	126.50
1	1A	2593	U	N3-C4-O4	-5.31	115.69	119.40
32	2a	841	U	C6-N1-C2	-5.31	117.82	121.00
1	2A	2155	G	N1-C6-O6	-5.30	116.72	119.90
56	1y	70	G	N3-C4-N9	5.30	129.18	126.00
56	2y	60	U	N3-C2-O2	-5.30	118.49	122.20
1	2A	2689	U	P-O3'-C3'	5.29	126.05	119.70
1	2A	1022	G	N3-C4-N9	-5.29	122.83	126.00
1	2A	752	A	P-O3'-C3'	5.27	126.02	119.70
55	1x	14	A	C4-N9-C1'	5.26	135.77	126.30
1	1A	805	G	N9-C4-C5	-5.26	103.30	105.40
1	2A	1298	C	O5'-P-OP2	-5.26	100.97	105.70
1	1A	372	G	O4'-C1'-N9	5.24	112.39	108.20
32	2a	754	C	N1-C2-O2	5.24	122.04	118.90
11	1P	43	GLY	C-N-CA	5.24	133.30	122.30
32	2a	1043	C	N1-C2-O2	5.24	122.04	118.90
1	2A	1313	U	N3-C2-O2	-5.23	118.54	122.20
55	1x	46	G	N3-C2-N2	-5.22	116.25	119.90
1	1A	614	U	C2-N1-C1'	5.20	123.94	117.70
1	2A	1204	A	O4'-C1'-N9	5.18	112.34	108.20
55	1x	46	G	N9-C4-C5	5.18	107.47	105.40
54	2w	5	G	C8-N9-C1'	5.17	133.72	127.00
32	1a	266	G	OP2-P-O3'	5.17	116.56	105.20
1	1A	961	C	C2-N3-C4	-5.17	117.32	119.90
32	1a	955	U	C5-C4-O4	5.16	129.00	125.90
1	2A	2318	G	O4'-C1'-N9	5.16	112.33	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2167	U	N1-C2-O2	5.15	126.41	122.80
1	1A	2347	C	N1-C2-O2	5.14	121.98	118.90
1	2A	2155	G	N1-C2-N3	-5.14	120.81	123.90
1	1A	748	G	C8-N9-C1'	5.14	133.68	127.00
32	1a	1027	C	C2-N1-C1'	-5.11	113.18	118.80
55	2x	14	A	C4-C5-N7	-5.10	108.15	110.70
1	2A	847	U	N1-C2-O2	5.09	126.36	122.80
1	1A	548	A	P-O3'-C3'	5.09	125.80	119.70
32	2a	65	U	P-O3'-C3'	5.08	125.80	119.70
1	1A	1174	A	OP1-P-O3'	5.08	116.39	105.20
1	1A	2553	G	N3-C4-N9	5.08	129.05	126.00
32	1a	532	A	O4'-C1'-N9	5.08	112.27	108.20
1	2A	1021	A	C8-N9-C4	-5.08	103.77	105.80
1	1A	784	A	P-O3'-C3'	5.08	125.79	119.70
32	1a	1027	C	C6-N1-C1'	5.07	126.88	120.80
1	2A	2318	G	N3-C4-N9	5.07	129.04	126.00
55	2x	14	A	C4-N9-C1'	5.06	135.41	126.30
1	1A	2491	U	OP1-P-O3'	5.06	116.33	105.20
32	2a	1158	C	C2-N1-C1'	5.05	124.36	118.80
1	1A	827	U	OP2-P-O3'	5.05	116.31	105.20
32	1a	1036	G	N3-C2-N2	-5.04	116.37	119.90
55	2x	14	A	C8-N9-C1'	-5.03	118.64	127.70
1	2A	2447	G	C6-C5-N7	5.02	133.41	130.40
32	1a	975	A	O4'-C1'-N9	-5.01	104.19	108.20
1	1A	1313	U	O4'-C1'-N1	5.00	112.20	108.20
1	1A	2096	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
11	1P	37	GLY	Peptide
33	1b	122	PHE	Peptide
33	1b	123	ALA	Peptide
33	1b	124	SER	Peptide
46	1o	83	GLU	Peptide
11	2P	35	HIS	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	34	57
4	1E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	29	52
4	2E	202/206 (98%)	184 (91%)	15 (7%)	3 (2%)	10	21
5	1F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	29	52
5	2F	201/210 (96%)	186 (92%)	12 (6%)	3 (2%)	10	21
6	1G	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	14	30
6	2G	179/182 (98%)	153 (86%)	19 (11%)	7 (4%)	3	4
7	1H	172/180 (96%)	162 (94%)	8 (5%)	2 (1%)	13	27
7	2H	172/180 (96%)	154 (90%)	16 (9%)	2 (1%)	13	27
8	1I	144/148 (97%)	124 (86%)	19 (13%)	1 (1%)	22	43
8	2I	144/148 (97%)	121 (84%)	21 (15%)	2 (1%)	11	22
9	1N	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	22	43
9	2N	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	22	43
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	11	22
11	2P	147/150 (98%)	132 (90%)	13 (9%)	2 (1%)	11	22
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	22	43
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	8	15
15	1T	129/146 (88%)	119 (92%)	9 (7%)	1 (1%)	19	39
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	7	14
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	32
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	3 (3%)	2 (2%)	6	12
19	2X	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	14	30
20	1Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
20	2Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	15	32
21	1Z	148/206 (72%)	136 (92%)	9 (6%)	3 (2%)	7	14
21	2Z	156/206 (76%)	136 (87%)	17 (11%)	3 (2%)	8	15
22	10	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13	27
22	20	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	13	27
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	30
23	21	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	14	30
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	8	16
26	14	67/71 (94%)	52 (78%)	8 (12%)	7 (10%)	0	0
26	24	67/71 (94%)	45 (67%)	18 (27%)	4 (6%)	1	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100

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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%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	199 (87%)	22 (10%)	8 (4%)	3	5
33	2b	229/256 (90%)	193 (84%)	27 (12%)	9 (4%)	3	4
34	1c	204/239 (85%)	186 (91%)	15 (7%)	3 (2%)	10	21
34	2c	204/239 (85%)	166 (81%)	35 (17%)	3 (2%)	10	21
35	1d	206/209 (99%)	195 (95%)	8 (4%)	3 (2%)	10	21
35	2d	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
36	1e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	11	22
36	2e	146/162 (90%)	130 (89%)	13 (9%)	3 (2%)	7	13
37	1f	98/101 (97%)	90 (92%)	7 (7%)	1 (1%)	15	32
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	12	24
38	2g	153/156 (98%)	135 (88%)	17 (11%)	1 (1%)	22	43
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	123 (91%)	12 (9%)	0	100	100
40	1i	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
40	2i	125/128 (98%)	106 (85%)	19 (15%)	0	100	100
41	1j	95/105 (90%)	80 (84%)	13 (14%)	2 (2%)	7	13
41	2j	94/105 (90%)	81 (86%)	10 (11%)	3 (3%)	4	6
42	1k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	8	16
42	2k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	8	16
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
44	1m	121/126 (96%)	106 (88%)	13 (11%)	2 (2%)	9	18
44	2m	120/126 (95%)	99 (82%)	18 (15%)	3 (2%)	5	9
45	1n	58/61 (95%)	58 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	2n	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	9	18
46	1o	86/89 (97%)	78 (91%)	6 (7%)	2 (2%)	6	11
46	2o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	13	27
47	1p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
47	2p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
48	1q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	15	32
48	2q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	15	32
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
50	1s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	13	27
50	2s	81/93 (87%)	66 (82%)	14 (17%)	1 (1%)	13	27
51	1t	94/106 (89%)	82 (87%)	8 (8%)	4 (4%)	2	3
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	13
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11370/12128 (94%)	10425 (92%)	818 (7%)	127 (1%)	14	30

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
23	11	3	LYS
26	14	53	GLU
26	14	62	ARG
33	1b	125	PRO
38	1g	80	VAL
41	1j	79	ARG
42	1k	49	GLY
44	1m	67	GLU
5	2F	130	ALA
6	2G	28	VAL
6	2G	51	ARG
11	2P	45	LEU
20	2Y	57	GLN
23	21	3	LYS
33	2b	17	PHE
38	2g	80	VAL

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Mol	Chain	Res	Type
7	1H	126	PRO
17	1V	100	ARG
21	1Z	52	SER
26	14	47	GLN
33	1b	8	LYS
34	1c	66	VAL
36	1e	85	GLY
42	1k	77	MET
6	2G	42	GLY
6	2G	43	LEU
8	2I	10	GLU
12	2Q	27	VAL
14	2S	84	GLN
17	2V	79	VAL
19	2X	93	GLU
21	2Z	52	SER
21	2Z	93	ASP
42	2k	49	GLY
44	2m	68	GLY
48	2q	68	ARG
50	2s	81	ARG
51	2t	10	LEU
4	1E	52	LEU
8	1I	42	SER
17	1V	79	VAL
22	10	4	LYS
26	14	49	PHE
33	1b	17	PHE
33	1b	126	GLU
48	1q	61	GLU
50	1s	27	GLU
4	2E	52	LEU
4	2E	69	LYS
6	2G	29	TRP
26	24	55	ARG
33	2b	8	LYS
33	2b	9	GLU
33	2b	20	GLU
33	2b	21	ARG
33	2b	74	LYS
33	2b	123	ALA
36	2e	85	GLY

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Mol	Chain	Res	Type
36	2e	98	THR
41	2j	78	ASN
41	2j	79	ARG
44	2m	106	ASN
51	2t	47	GLY
6	1G	150	ASP
15	1T	37	GLY
21	1Z	93	ASP
21	1Z	163	LEU
26	14	44	THR
26	14	68	ARG
33	1b	227	GLY
35	1d	173	TRP
41	1j	77	PRO
44	1m	32	GLU
46	1o	19	PRO
5	2F	21	ALA
8	2I	40	THR
9	2N	2	LYS
11	2P	140	ALA
22	20	4	LYS
26	24	29	PRO
33	2b	126	GLU
34	2c	107	GLN
41	2j	75	ILE
44	2m	67	GLU
6	1G	43	LEU
7	1H	92	ILE
11	1P	29	LYS
11	1P	38	GLN
19	1X	2	LYS
26	14	61	ARG
33	1b	16	HIS
33	1b	20	GLU
35	1d	85	LYS
36	1e	86	ALA
51	1t	47	GLY
51	1t	96	GLY
51	1t	100	ILE
3	2D	257	LEU
6	2G	110	ALA
14	2S	20	ARG

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Mol	Chain	Res	Type
26	24	47	GLN
34	2c	26	LYS
36	2e	69	VAL
42	2k	105	VAL
9	1N	2	LYS
33	1b	231	GLU
34	1c	65	ALA
34	1c	80	GLY
38	1g	54	THR
7	2H	12	PRO
37	1f	40	VAL
35	1d	178	VAL
46	1o	86	GLY
4	2E	71	GLY
25	23	59	VAL
45	2n	14	PRO
46	2o	19	PRO
19	1X	67	GLY
5	2F	207	GLY
6	2G	24	GLY
34	2c	51	GLY
51	1t	102	GLY
21	2Z	146	ILE
26	24	45	GLY
7	2H	126	PRO
33	2b	231	GLU

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	215/218 (99%)	201 (94%)	14 (6%)	17 34
3	2D	215/218 (99%)	201 (94%)	14 (6%)	17 34
4	1E	164/166 (99%)	152 (93%)	12 (7%)	14 28
4	2E	164/166 (99%)	156 (95%)	8 (5%)	25 48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11	23
5	2F	159/166 (96%)	147 (92%)	12 (8%)	13	27
6	1G	143/156 (92%)	129 (90%)	14 (10%)	8	15
6	2G	143/156 (92%)	125 (87%)	18 (13%)	4	8
7	1H	144/148 (97%)	136 (94%)	8 (6%)	21	42
7	2H	144/148 (97%)	131 (91%)	13 (9%)	9	18
8	1I	113/124 (91%)	97 (86%)	16 (14%)	3	5
8	2I	105/124 (85%)	95 (90%)	10 (10%)	8	16
9	1N	118/119 (99%)	109 (92%)	9 (8%)	13	26
9	2N	118/119 (99%)	106 (90%)	12 (10%)	7	14
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	67
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41	67
11	1P	115/116 (99%)	103 (90%)	12 (10%)	7	13
11	2P	115/116 (99%)	98 (85%)	17 (15%)	3	5
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18	36
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	35	61
13	1R	101/101 (100%)	95 (94%)	6 (6%)	19	39
13	2R	101/101 (100%)	94 (93%)	7 (7%)	15	31
14	1S	86/88 (98%)	73 (85%)	13 (15%)	3	4
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4	7
15	1T	115/127 (91%)	108 (94%)	7 (6%)	18	38
15	2T	113/127 (89%)	108 (96%)	5 (4%)	28	53
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22	44
16	2U	93/94 (99%)	85 (91%)	8 (9%)	10	20
17	1V	80/82 (98%)	74 (92%)	6 (8%)	13	27
17	2V	80/82 (98%)	71 (89%)	9 (11%)	6	10
18	1W	90/92 (98%)	82 (91%)	8 (9%)	9	19
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28	53
19	1X	77/78 (99%)	74 (96%)	3 (4%)	32	58
19	2X	77/78 (99%)	73 (95%)	4 (5%)	23	46
20	1Y	85/91 (93%)	77 (91%)	8 (9%)	8	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	14	29
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	23
21	2Z	137/179 (76%)	123 (90%)	14 (10%)	7	14
22	10	65/67 (97%)	63 (97%)	2 (3%)	40	66
22	20	65/67 (97%)	63 (97%)	2 (3%)	40	66
23	11	80/83 (96%)	78 (98%)	2 (2%)	47	73
23	21	80/83 (96%)	75 (94%)	5 (6%)	18	36
24	12	65/67 (97%)	61 (94%)	4 (6%)	18	37
24	22	65/67 (97%)	63 (97%)	2 (3%)	40	66
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	6
25	23	50/52 (96%)	46 (92%)	4 (8%)	12	24
26	14	59/63 (94%)	48 (81%)	11 (19%)	1	2
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	4
27	15	50/52 (96%)	45 (90%)	5 (10%)	7	14
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	39
28	16	51/52 (98%)	40 (78%)	11 (22%)	1	1
28	26	50/52 (96%)	46 (92%)	4 (8%)	12	24
29	17	41/42 (98%)	40 (98%)	1 (2%)	49	74
29	27	41/42 (98%)	37 (90%)	4 (10%)	8	15
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	28
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	28
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	32 (94%)	2 (6%)	19	39
33	1b	192/220 (87%)	172 (90%)	20 (10%)	7	13
33	2b	187/220 (85%)	164 (88%)	23 (12%)	4	9
34	1c	142/188 (76%)	133 (94%)	9 (6%)	18	36
34	2c	140/188 (74%)	122 (87%)	18 (13%)	4	7
35	1d	169/181 (93%)	155 (92%)	14 (8%)	11	22
35	2d	173/181 (96%)	157 (91%)	16 (9%)	9	17
36	1e	113/123 (92%)	108 (96%)	5 (4%)	28	53
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	1f	84/90 (93%)	78 (93%)	6 (7%)	14	29
37	2f	85/90 (94%)	77 (91%)	8 (9%)	8	17
38	1g	119/127 (94%)	109 (92%)	10 (8%)	11	21
38	2g	120/127 (94%)	103 (86%)	17 (14%)	3	5
39	1h	114/119 (96%)	110 (96%)	4 (4%)	36	62
39	2h	114/119 (96%)	104 (91%)	10 (9%)	10	19
40	1i	90/99 (91%)	83 (92%)	7 (8%)	12	25
40	2i	89/99 (90%)	76 (85%)	13 (15%)	3	5
41	1j	66/92 (72%)	58 (88%)	8 (12%)	5	9
41	2j	69/92 (75%)	58 (84%)	11 (16%)	2	4
42	1k	82/99 (83%)	76 (93%)	6 (7%)	14	28
42	2k	83/99 (84%)	79 (95%)	4 (5%)	25	49
43	1l	96/108 (89%)	93 (97%)	3 (3%)	40	66
43	2l	96/108 (89%)	91 (95%)	5 (5%)	23	46
44	1m	93/101 (92%)	85 (91%)	8 (9%)	10	20
44	2m	92/101 (91%)	81 (88%)	11 (12%)	5	9
45	1n	49/50 (98%)	45 (92%)	4 (8%)	11	22
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	14
46	1o	78/80 (98%)	74 (95%)	4 (5%)	24	46
46	2o	78/80 (98%)	74 (95%)	4 (5%)	24	46
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	10
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	7
48	1q	94/97 (97%)	86 (92%)	8 (8%)	10	21
48	2q	94/97 (97%)	89 (95%)	5 (5%)	22	45
49	1r	59/77 (77%)	57 (97%)	2 (3%)	37	63
49	2r	59/77 (77%)	56 (95%)	3 (5%)	24	46
50	1s	69/80 (86%)	65 (94%)	4 (6%)	20	40
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	18
51	1t	70/82 (85%)	64 (91%)	6 (9%)	10	20
51	2t	70/82 (85%)	61 (87%)	9 (13%)	4	7
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	2u	18/22 (82%)	18 (100%)	0	100 100
All	All	9303/10064 (92%)	8539 (92%)	764 (8%)	11 22

All (764) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	38	LYS
3	1D	68	LYS
3	1D	71	ASP
3	1D	106	ILE
3	1D	113	VAL
3	1D	141	VAL
3	1D	155	LEU
3	1D	157	ARG
3	1D	162	SER
3	1D	181	GLU
3	1D	190	TYR
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
4	1E	1	MET
4	1E	12	THR
4	1E	34	VAL
4	1E	41	LYS
4	1E	73	GLU
4	1E	93	VAL
4	1E	116	VAL
4	1E	170	LEU
4	1E	175	VAL
4	1E	184	VAL
4	1E	188	VAL
4	1E	195	LEU
5	1F	24	LEU
5	1F	53	THR
5	1F	70	THR
5	1F	74	ARG
5	1F	127	GLU
5	1F	132	VAL
5	1F	144	LYS
5	1F	158	THR
5	1F	162	LEU
5	1F	175	THR

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Mol	Chain	Res	Type
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	5	VAL
6	1G	7	LEU
6	1G	21	ARG
6	1G	22	ARG
6	1G	31	VAL
6	1G	43	LEU
6	1G	49	ASP
6	1G	82	LEU
6	1G	91	ARG
6	1G	133	LEU
6	1G	136	ARG
6	1G	140	ILE
6	1G	170	ARG
6	1G	175	LEU
7	1H	7	LEU
7	1H	52	VAL
7	1H	56	SER
7	1H	57	ASP
7	1H	90	LYS
7	1H	98	LEU
7	1H	114	VAL
7	1H	119	GLU
8	1I	10	GLU
8	1I	20	ASP
8	1I	40	THR
8	1I	41	GLU
8	1I	47	LEU
8	1I	50	ARG
8	1I	58	LEU
8	1I	74	ASN
8	1I	85	GLU
8	1I	92	VAL
8	1I	101	LEU
8	1I	102	SER
8	1I	108	THR
8	1I	109	ILE
8	1I	117	GLU
8	1I	121	LYS
9	1N	14	VAL

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Mol	Chain	Res	Type
9	1N	48	MET
9	1N	61	ARG
9	1N	62	VAL
9	1N	67	LEU
9	1N	87	LEU
9	1N	96	GLU
9	1N	131	GLN
9	1N	137	LYS
10	1O	28	SER
10	1O	89	ASN
10	1O	108	GLU
11	1P	2	LYS
11	1P	7	ARG
11	1P	45	LEU
11	1P	95	VAL
11	1P	98	GLU
11	1P	101	VAL
11	1P	112	LEU
11	1P	119	GLU
11	1P	125	VAL
11	1P	133	SER
11	1P	138	LEU
11	1P	148	LEU
12	1Q	16	ARG
12	1Q	60	ARG
12	1Q	75	THR
12	1Q	89	ASN
12	1Q	98	LYS
12	1Q	109	VAL
12	1Q	112	GLU
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	67	LEU
13	1R	79	LEU
13	1R	114	VAL
14	1S	3	ARG
14	1S	8	GLU
14	1S	14	VAL
14	1S	15	ARG
14	1S	17	ARG
14	1S	46	VAL

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Mol	Chain	Res	Type
14	1S	48	LEU
14	1S	49	VAL
14	1S	68	GLN
14	1S	71	ARG
14	1S	73	LEU
14	1S	78	LEU
14	1S	110	LEU
15	1T	21	GLU
15	1T	28	VAL
15	1T	51	ARG
15	1T	89	VAL
15	1T	96	ARG
15	1T	104	ASN
15	1T	128	GLU
16	1U	50	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	78	THR
16	1U	95	LEU
17	1V	32	THR
17	1V	52	VAL
17	1V	62	LEU
17	1V	73	SER
17	1V	79	VAL
17	1V	95	LEU
18	1W	4	LYS
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	49	LYS
18	1W	67	ASP
18	1W	68	ARG
19	1X	35	THR
19	1X	57	LEU
19	1X	72	LYS
20	1Y	7	VAL
20	1Y	14	LEU
20	1Y	40	GLU
20	1Y	43	ASN
20	1Y	64	GLU
20	1Y	73	ARG

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Mol	Chain	Res	Type
20	1Y	99	CYS
20	1Y	106	LEU
21	1Z	46	LYS
21	1Z	49	ARG
21	1Z	70	LEU
21	1Z	124	ILE
21	1Z	139	VAL
21	1Z	150	LEU
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	156	LYS
21	1Z	169	GLU
21	1Z	171	ILE
22	10	14	ARG
22	10	55	ARG
23	11	46	LEU
23	11	83	GLU
24	12	1	MET
24	12	3	LEU
24	12	19	VAL
24	12	38	GLN
25	13	7	LYS
25	13	23	LEU
25	13	29	ARG
25	13	37	LEU
25	13	54	VAL
25	13	55	ARG
25	13	60	GLU
26	14	1	MET
26	14	48	ARG
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	53	GLU
26	14	58	ARG
26	14	61	ARG
26	14	63	TYR
26	14	67	TYR
26	14	69	LYS
27	15	6	VAL
27	15	35	GLU
27	15	40	LYS

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Mol	Chain	Res	Type
27	15	58	LEU
27	15	59	GLU
28	16	4	GLU
28	16	5	VAL
28	16	6	ARG
28	16	9	LEU
28	16	14	THR
28	16	19	ARG
28	16	23	THR
28	16	24	GLU
28	16	29	ASN
28	16	44	ARG
28	16	47	THR
29	17	41	ARG
30	18	14	VAL
30	18	29	LYS
30	18	31	HIS
30	18	34	TRP
33	1b	8	LYS
33	1b	12	GLU
33	1b	21	ARG
33	1b	23	ARG
33	1b	24	TRP
33	1b	35	GLU
33	1b	54	THR
33	1b	61	LEU
33	1b	64	ARG
33	1b	76	GLN
33	1b	80	ILE
33	1b	95	GLN
33	1b	112	VAL
33	1b	113	HIS
33	1b	127	ILE
33	1b	156	LYS
33	1b	160	ASP
33	1b	185	ILE
33	1b	195	ASP
33	1b	215	LEU
34	1c	3	ASN
34	1c	15	THR
34	1c	20	SER
34	1c	89	GLU

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Mol	Chain	Res	Type
34	1c	110	ASN
34	1c	131	ARG
34	1c	138	VAL
34	1c	195	VAL
34	1c	201	TYR
35	1d	8	VAL
35	1d	10	ARG
35	1d	19	LEU
35	1d	28	SER
35	1d	31	CYS
35	1d	76	ARG
35	1d	86	LYS
35	1d	135	LEU
35	1d	158	ILE
35	1d	175	SER
35	1d	178	VAL
35	1d	194	LEU
35	1d	200	GLU
35	1d	208	SER
36	1e	10	MET
36	1e	12	LEU
36	1e	41	VAL
36	1e	56	GLN
36	1e	91	LEU
37	1f	17	SER
37	1f	72	VAL
37	1f	75	LEU
37	1f	78	GLU
37	1f	92	LYS
37	1f	93	SER
38	1g	21	VAL
38	1g	50	ILE
38	1g	57	GLU
38	1g	79	ARG
38	1g	85	TYR
38	1g	104	LEU
38	1g	110	GLN
38	1g	113	GLU
38	1g	114	ARG
38	1g	115	ARG
39	1h	52	ASP
39	1h	68	ARG

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Mol	Chain	Res	Type
39	1h	112	LEU
39	1h	129	VAL
40	1i	23	ASN
40	1i	38	GLN
40	1i	50	LEU
40	1i	56	LEU
40	1i	71	SER
40	1i	89	ASN
40	1i	103	THR
41	1j	21	GLN
41	1j	46	ARG
41	1j	55	LYS
41	1j	64	GLU
41	1j	81	THR
41	1j	92	THR
41	1j	98	ILE
41	1j	100	THR
42	1k	25	TYR
42	1k	31	THR
42	1k	48	ILE
42	1k	109	VAL
42	1k	114	VAL
42	1k	123	LYS
43	1l	13	LYS
43	1l	18	VAL
43	1l	86	ARG
44	1m	4	ILE
44	1m	19	LEU
44	1m	32	GLU
44	1m	64	TRP
44	1m	70	LEU
44	1m	103	THR
44	1m	109	THR
44	1m	122	LYS
45	1n	3	ARG
45	1n	6	LEU
45	1n	33	VAL
45	1n	56	VAL
46	1o	5	LYS
46	1o	39	LEU
46	1o	47	LYS
46	1o	87	ILE

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Mol	Chain	Res	Type
47	1p	20	VAL
47	1p	27	LYS
47	1p	45	THR
47	1p	54	GLU
47	1p	60	LEU
47	1p	61	SER
47	1p	62	VAL
47	1p	69	THR
48	1q	9	VAL
48	1q	14	LYS
48	1q	34	LYS
48	1q	45	HIS
48	1q	49	GLU
48	1q	60	ILE
48	1q	68	ARG
48	1q	69	LYS
49	1r	31	LEU
49	1r	54	ARG
50	1s	6	LYS
50	1s	32	LYS
50	1s	41	VAL
50	1s	51	VAL
51	1t	10	LEU
51	1t	24	LEU
51	1t	37	SER
51	1t	38	LYS
51	1t	84	LEU
51	1t	100	ILE
52	1u	9	ARG
3	2D	20	ASP
3	2D	22	SER
3	2D	37	LEU
3	2D	88	ARG
3	2D	106	ILE
3	2D	122	ASP
3	2D	138	VAL
3	2D	173	VAL
3	2D	183	ARG
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR

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Mol	Chain	Res	Type
3	2D	260	ARG
4	2E	12	THR
4	2E	38	THR
4	2E	73	GLU
4	2E	90	THR
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	175	VAL
5	2F	24	LEU
5	2F	33	LEU
5	2F	74	ARG
5	2F	95	ARG
5	2F	96	ASP
5	2F	106	ARG
5	2F	135	LYS
5	2F	137	LYS
5	2F	145	GLU
5	2F	165	ARG
5	2F	170	LEU
5	2F	192	LEU
6	2G	18	GLU
6	2G	22	ARG
6	2G	28	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	49	ASP
6	2G	53	LEU
6	2G	60	LEU
6	2G	77	ILE
6	2G	79	ASN
6	2G	91	ARG
6	2G	108	ASN
6	2G	126	ASP
6	2G	133	LEU
6	2G	137	GLU
6	2G	148	MET
6	2G	165	THR
6	2G	170	ARG
7	2H	7	LEU
7	2H	15	VAL
7	2H	23	ARG

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Mol	Chain	Res	Type
7	2H	45	VAL
7	2H	49	VAL
7	2H	57	ASP
7	2H	70	THR
7	2H	90	LYS
7	2H	95	ARG
7	2H	106	THR
7	2H	110	SER
7	2H	134	SER
7	2H	136	ILE
8	2I	38	LEU
8	2I	58	LEU
8	2I	61	ARG
8	2I	82	ARG
8	2I	92	VAL
8	2I	96	ASP
8	2I	101	LEU
8	2I	117	GLU
8	2I	127	VAL
8	2I	129	THR
9	2N	9	VAL
9	2N	10	GLU
9	2N	14	VAL
9	2N	15	LEU
9	2N	38	HIS
9	2N	58	ASP
9	2N	61	ARG
9	2N	62	VAL
9	2N	67	LEU
9	2N	73	THR
9	2N	83	LYS
9	2N	87	LEU
10	2O	28	SER
10	2O	78	ARG
10	2O	108	GLU
11	2P	3	LEU
11	2P	7	ARG
11	2P	15	ARG
11	2P	45	LEU
11	2P	83	VAL
11	2P	90	ARG
11	2P	95	VAL

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Mol	Chain	Res	Type
11	2P	96	THR
11	2P	98	GLU
11	2P	112	LEU
11	2P	117	GLU
11	2P	119	GLU
11	2P	121	LYS
11	2P	125	VAL
11	2P	135	LEU
11	2P	138	LEU
11	2P	148	LEU
12	2Q	8	LYS
12	2Q	106	VAL
12	2Q	109	VAL
12	2Q	119	ARG
13	2R	6	SER
13	2R	15	SER
13	2R	29	LEU
13	2R	33	ARG
13	2R	67	LEU
13	2R	79	LEU
13	2R	114	VAL
14	2S	5	THR
14	2S	25	ARG
14	2S	35	ILE
14	2S	36	TYR
14	2S	43	GLU
14	2S	58	LEU
14	2S	64	GLU
14	2S	68	GLN
14	2S	83	LYS
14	2S	85	VAL
14	2S	93	LYS
15	2T	9	LEU
15	2T	17	THR
15	2T	49	VAL
15	2T	96	ARG
15	2T	108	ARG
16	2U	5	LYS
16	2U	31	SER
16	2U	55	ARG
16	2U	59	ARG
16	2U	74	LEU

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Mol	Chain	Res	Type
16	2U	95	LEU
16	2U	100	VAL
16	2U	111	GLU
17	2V	7	THR
17	2V	32	THR
17	2V	51	VAL
17	2V	52	VAL
17	2V	56	SER
17	2V	62	LEU
17	2V	73	SER
17	2V	79	VAL
17	2V	85	LYS
18	2W	11	ARG
18	2W	23	LEU
18	2W	63	ASP
18	2W	67	ASP
19	2X	35	THR
19	2X	57	LEU
19	2X	72	LYS
19	2X	88	LYS
20	2Y	6	HIS
20	2Y	7	VAL
20	2Y	9	LYS
20	2Y	85	VAL
20	2Y	97	ARG
20	2Y	99	CYS
21	2Z	5	LEU
21	2Z	35	ARG
21	2Z	42	VAL
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	100	VAL
21	2Z	121	HIS
21	2Z	122	ARG
21	2Z	126	VAL
21	2Z	144	LEU
21	2Z	154	ASP
21	2Z	161	VAL
21	2Z	163	LEU
21	2Z	171	ILE
22	20	10	THR
22	20	14	ARG

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Mol	Chain	Res	Type
23	21	46	LEU
23	21	65	SER
23	21	80	LEU
23	21	91	LYS
23	21	98	LEU
24	22	8	LYS
24	22	35	LEU
25	23	5	LYS
25	23	31	LEU
25	23	54	VAL
25	23	56	VAL
26	24	26	SER
26	24	27	THR
26	24	34	GLU
26	24	49	PHE
26	24	59	PHE
26	24	62	ARG
26	24	67	TYR
26	24	68	ARG
27	25	6	VAL
27	25	35	GLU
27	25	59	GLU
28	26	6	ARG
28	26	9	LEU
28	26	14	THR
28	26	19	ARG
29	27	1	MET
29	27	29	LYS
29	27	46	VAL
29	27	47	ARG
30	28	23	VAL
30	28	31	HIS
30	28	34	TRP
30	28	49	VAL
31	29	7	VAL
31	29	17	ILE
33	2b	7	VAL
33	2b	10	LEU
33	2b	16	HIS
33	2b	27	LYS
33	2b	55	PHE
33	2b	67	THR

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Mol	Chain	Res	Type
33	2b	76	GLN
33	2b	93	VAL
33	2b	95	GLN
33	2b	107	THR
33	2b	115	LEU
33	2b	118	LEU
33	2b	135	GLN
33	2b	142	LEU
33	2b	163	PHE
33	2b	175	ARG
33	2b	185	ILE
33	2b	187	LEU
33	2b	189	ASP
33	2b	214	ILE
33	2b	223	ILE
33	2b	226	ARG
33	2b	229	VAL
34	2c	15	THR
34	2c	16	ARG
34	2c	47	LEU
34	2c	52	LEU
34	2c	55	VAL
34	2c	57	ILE
34	2c	105	GLU
34	2c	119	ARG
34	2c	120	VAL
34	2c	128	PHE
34	2c	144	SER
34	2c	152	ILE
34	2c	164	ARG
34	2c	186	PHE
34	2c	190	ARG
34	2c	192	THR
34	2c	196	LEU
34	2c	204	LEU
35	2d	8	VAL
35	2d	28	SER
35	2d	31	CYS
35	2d	53	ASP
35	2d	83	SER
35	2d	96	LEU
35	2d	122	ARG

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Mol	Chain	Res	Type
35	2d	127	THR
35	2d	135	LEU
35	2d	155	LEU
35	2d	158	ILE
35	2d	175	SER
35	2d	179	GLU
35	2d	181	MET
35	2d	190	ASP
35	2d	193	ASP
36	2e	5	ASP
36	2e	10	MET
36	2e	13	ILE
36	2e	38	GLN
36	2e	41	VAL
36	2e	51	VAL
36	2e	72	GLN
36	2e	115	VAL
36	2e	148	VAL
36	2e	151	LEU
36	2e	152	ARG
37	2f	19	LEU
37	2f	45	LEU
37	2f	63	TYR
37	2f	69	GLU
37	2f	72	VAL
37	2f	81	ILE
37	2f	83	ASP
37	2f	94	GLN
38	2g	9	VAL
38	2g	12	LEU
38	2g	15	ASP
38	2g	27	ILE
38	2g	32	ARG
38	2g	52	GLU
38	2g	53	LYS
38	2g	56	GLN
38	2g	75	VAL
38	2g	78	ARG
38	2g	79	ARG
38	2g	85	TYR
38	2g	110	GLN
38	2g	114	ARG

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Mol	Chain	Res	Type
38	2g	115	ARG
38	2g	139	GLU
38	2g	151	TYR
39	2h	23	SER
39	2h	25	ASP
39	2h	29	SER
39	2h	51	VAL
39	2h	52	ASP
39	2h	54	ASP
39	2h	85	ARG
39	2h	99	GLU
39	2h	122	ARG
39	2h	127	LEU
40	2i	14	VAL
40	2i	27	THR
40	2i	29	ASN
40	2i	51	ARG
40	2i	63	ILE
40	2i	65	VAL
40	2i	89	ASN
40	2i	102	LEU
40	2i	103	THR
40	2i	105	ASP
40	2i	108	VAL
40	2i	113	LYS
40	2i	128	ARG
41	2j	16	LEU
41	2j	23	ILE
41	2j	38	ILE
41	2j	51	ARG
41	2j	55	LYS
41	2j	65	LEU
41	2j	72	VAL
41	2j	81	THR
41	2j	89	ASP
41	2j	97	GLU
41	2j	98	ILE
42	2k	48	ILE
42	2k	87	THR
42	2k	96	ARG
42	2k	105	VAL
43	2l	18	VAL

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Mol	Chain	Res	Type
43	2l	28	LYS
43	2l	62	SER
43	2l	112	ASP
43	2l	116	SER
44	2m	27	LYS
44	2m	32	GLU
44	2m	47	ASP
44	2m	62	ASN
44	2m	73	GLU
44	2m	90	LEU
44	2m	103	THR
44	2m	106	ASN
44	2m	110	ARG
44	2m	114	ARG
44	2m	117	VAL
45	2n	3	ARG
45	2n	4	LYS
45	2n	7	ILE
45	2n	29	ARG
45	2n	33	VAL
46	2o	22	THR
46	2o	39	LEU
46	2o	56	LEU
46	2o	76	GLU
47	2p	1	MET
47	2p	4	ILE
47	2p	8	ARG
47	2p	20	VAL
47	2p	21	VAL
47	2p	27	LYS
47	2p	45	THR
47	2p	60	LEU
47	2p	62	VAL
48	2q	5	VAL
48	2q	14	LYS
48	2q	37	LYS
48	2q	60	ILE
48	2q	99	SER
49	2r	31	LEU
49	2r	37	VAL
49	2r	47	THR
50	2s	37	ARG

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Mol	Chain	Res	Type
50	2s	41	VAL
50	2s	43	GLU
50	2s	48	THR
50	2s	49	ILE
50	2s	81	ARG
51	2t	15	ARG
51	2t	19	SER
51	2t	23	ARG
51	2t	24	LEU
51	2t	39	LYS
51	2t	61	SER
51	2t	70	SER
51	2t	72	LEU
51	2t	93	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
5	1F	69	HIS
5	1F	203	GLN
8	1I	105	HIS
10	1O	3	GLN
12	1Q	12	GLN
13	1R	71	GLN
14	1S	38	GLN
14	1S	68	GLN
15	1T	58	ASN
16	1U	81	HIS
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
21	1Z	73	GLN
21	1Z	132	ASN
21	1Z	151	HIS
23	11	56	GLN
33	1b	78	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	162	GLN
34	1c	181	ASN
35	1d	116	GLN

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Mol	Chain	Res	Type
35	1d	119	GLN
35	1d	123	HIS
36	1e	20	GLN
36	1e	78	HIS
36	1e	141	GLN
37	1f	13	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
39	1h	15	ASN
40	1i	3	GLN
40	1i	23	ASN
40	1i	31	GLN
40	1i	34	ASN
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS
42	1k	117	ASN
43	1l	99	HIS
44	1m	92	HIS
47	1p	76	GLN
49	1r	63	GLN
50	1s	23	ASN
50	1s	47	HIS
50	1s	83	HIS
4	2E	48	GLN
5	2F	69	HIS
6	2G	27	ASN
6	2G	41	GLN
7	2H	143	GLN
8	2I	139	GLN
10	2O	3	GLN
10	2O	5	GLN
11	2P	27	HIS
12	2Q	12	GLN
12	2Q	57	HIS
14	2S	38	GLN
15	2T	58	ASN
16	2U	117	GLN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	43	ASN

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Mol	Chain	Res	Type
21	2Z	73	GLN
23	21	56	GLN
33	2b	40	HIS
33	2b	76	GLN
33	2b	140	HIS
34	2c	102	ASN
34	2c	139	GLN
34	2c	162	GLN
35	2d	45	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	129	ASN
36	2e	20	GLN
36	2e	73	ASN
36	2e	78	HIS
37	2f	100	ASN
38	2g	28	ASN
38	2g	68	ASN
38	2g	86	GLN
38	2g	148	ASN
40	2i	58	HIS
41	2j	13	HIS
41	2j	62	HIS
42	2k	22	HIS
42	2k	117	ASN
43	2l	99	HIS
44	2m	77	ASN
48	2q	26	GLN
49	2r	63	GLN
50	2s	83	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	425 (14%)	29 (1%)
1	2A	2788/2915 (95%)	453 (16%)	22 (0%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	118/121 (97%)	24 (20%)	0
32	1a	1494/1521 (98%)	219 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	2a	1498/1521 (98%)	284 (18%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	70/76 (92%)	21 (30%)	0
54	2w	67/76 (88%)	20 (29%)	0
55	1x	74/77 (96%)	9 (12%)	0
55	2x	74/77 (96%)	7 (9%)	0
56	1y	71/76 (93%)	30 (42%)	0
56	2y	69/76 (90%)	24 (34%)	0
All	All	9327/9620 (96%)	1529 (16%)	51 (0%)

All (1529) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	34	C
1	1A	38	A
1	1A	45	C
1	1A	55	G
1	1A	63	U
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	188	G
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G

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Mol	Chain	Res	Type
1	1A	271(A)	A
1	1A	271(C)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	449	A
1	1A	454	A
1	1A	455	C
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	528	A
1	1A	529	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G

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Mol	Chain	Res	Type
1	1A	549	G
1	1A	551	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(A)	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	726	G
1	1A	730	C
1	1A	746	A
1	1A	747	U
1	1A	762	U
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	877	U
1	1A	879	G

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Mol	Chain	Res	Type
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	894	C
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	910	A
1	1A	931	G
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1025	G
1	1A	1026	U
1	1A	1033	U
1	1A	1040	C
1	1A	1043	C
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1058	G
1	1A	1063	G
1	1A	1064	C
1	1A	1066	U

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Mol	Chain	Res	Type
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1081	U
1	1A	1087	G
1	1A	1088	A
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1096	A
1	1A	1098	A
1	1A	1099	G
1	1A	1101	U
1	1A	1102	C
1	1A	1108	U
1	1A	1109	C
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1128	A
1	1A	1135	C
1	1A	1136	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	1244	G
1	1A	1247	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1300	U
1	1A	1301	A

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Mol	Chain	Res	Type
1	1A	1303	G
1	1A	1308	A
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1466	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1539	G
1	1A	1540	U
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1647	G
1	1A	1648	C
1	1A	1664	A
1	1A	1674	G

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Mol	Chain	Res	Type
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1740	G
1	1A	1743	C
1	1A	1745(A)	C
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
1	1A	1847	A
1	1A	1877	A
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	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

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Mol	Chain	Res	Type
1	1A	2039	C
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	2098	U
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U
1	1A	2120	G
1	1A	2121	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U

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Mol	Chain	Res	Type
1	1A	2173	A
1	1A	2175	C
1	1A	2182	G
1	1A	2183	C
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2218	U
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2358	G
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C

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Mol	Chain	Res	Type
1	1A	2448	A
1	1A	2449	U
1	1A	2470	G
1	1A	2474	C
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2494	G
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2530	A
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2555	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2578	G
1	1A	2582	G
1	1A	2585	U
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2744	G

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Mol	Chain	Res	Type
1	1A	2758	A
1	1A	2760	C
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2802	G
1	1A	2803	C
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
1	1A	2895	U
2	1B	2	C
2	1B	12	C
2	1B	13	A
2	1B	15	A
2	1B	16	G
2	1B	42	C
2	1B	45	A
2	1B	56	G
2	1B	66	A
2	1B	73	A
2	1B	110	G
32	1a	9	G
32	1a	31	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	77	G
32	1a	79	G
32	1a	91	C
32	1a	93	G

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Mol	Chain	Res	Type
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	168	G
32	1a	174	C
32	1a	182	U
32	1a	189(H)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	218	C
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	344	A
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	383	A
32	1a	384	G
32	1a	392	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G

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Mol	Chain	Res	Type
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	457	C
32	1a	461	A
32	1a	470	C
32	1a	474	G
32	1a	482	A
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	524	G
32	1a	531	U
32	1a	532	A
32	1a	536	C
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	616	G
32	1a	618	C
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	671	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	717	C

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Mol	Chain	Res	Type
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	749	C
32	1a	752	G
32	1a	755	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	902	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	958	A
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	998	G
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G

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Mol	Chain	Res	Type
32	1a	1020	U
32	1a	1021	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(C)	G
32	1a	1031	G
32	1a	1032	G
32	1a	1033	G
32	1a	1039	C
32	1a	1044	A
32	1a	1066	C
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1124	G
32	1a	1125	U
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1213	A
32	1a	1214	C
32	1a	1218	C
32	1a	1227	A

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Mol	Chain	Res	Type
32	1a	1236	A
32	1a	1238	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1364	U
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
54	1w	2	C
54	1w	6	G

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Mol	Chain	Res	Type
54	1w	8	4SU
54	1w	9	A
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	25	C
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	52	G
54	1w	62	C
54	1w	66	U
54	1w	68	C
54	1w	70	G
54	1w	74	C
55	1x	9	G
55	1x	14	A
55	1x	19	G
55	1x	21	A
55	1x	31	G
55	1x	47	U
55	1x	61	C
55	1x	63	G
55	1x	69	C
56	1y	5	G
56	1y	8	4SU
56	1y	9	A
56	1y	13	C
56	1y	14	A
56	1y	19	G
56	1y	20	U
56	1y	21	A
56	1y	22	G
56	1y	23	A
56	1y	28	G
56	1y	35	A
56	1y	39	PSU
56	1y	44	G

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Mol	Chain	Res	Type
56	1y	45	U
56	1y	46	7MG
56	1y	47	U
56	1y	48	C
56	1y	49	C
56	1y	53	G
56	1y	54	5MU
56	1y	56	C
56	1y	57	G
56	1y	59	U
56	1y	61	C
56	1y	65	G
56	1y	69	G
56	1y	70	G
56	1y	71	G
56	1y	72	C
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	49	A
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	125	G
1	2A	131	G
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G

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Mol	Chain	Res	Type
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	232	G
1	2A	233	A
1	2A	248	G
1	2A	271(J)	C
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(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	317	G
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	363	G
1	2A	363(B)	G
1	2A	372	G
1	2A	386	G
1	2A	396	G
1	2A	399	G
1	2A	403	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	422	A
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A

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Mol	Chain	Res	Type
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	545	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	608	A
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	651	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	762	U
1	2A	764	A
1	2A	770	G

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Mol	Chain	Res	Type
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	832	G
1	2A	857	C
1	2A	859	G
1	2A	874	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	904	C
1	2A	910	A
1	2A	914	C
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	961	C
1	2A	974	G

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Mol	Chain	Res	Type
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	999	U
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1021	A
1	2A	1022	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1036	G
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
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	1139	G
1	2A	1142(A)	A
1	2A	1148	A
1	2A	1151	G
1	2A	1171	G
1	2A	1195	G
1	2A	1205	U
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1225	G
1	2A	1236	G
1	2A	1252	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U

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Mol	Chain	Res	Type
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1306	C
1	2A	1314	C
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1379	A
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	1427	A
1	2A	1428	C
1	2A	1435	G
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1459	G
1	2A	1460	A
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	1494	A
1	2A	1496	A
1	2A	1497	U
1	2A	1506	C
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C

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Mol	Chain	Res	Type
1	2A	1532	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1577	C
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1588	C
1	2A	1595	G
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A

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Mol	Chain	Res	Type
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	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	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2036	C
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	2074	U
1	2A	2108	C
1	2A	2110	G
1	2A	2111	C
1	2A	2116	G
1	2A	2117	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2125	G
1	2A	2126	A

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Mol	Chain	Res	Type
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2141	G
1	2A	2145	C
1	2A	2146	C
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2188	C
1	2A	2189	U
1	2A	2193	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G

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Mol	Chain	Res	Type
1	2A	2239	G
1	2A	2275	C
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2304	G
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2403	C
1	2A	2406	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	2445	G
1	2A	2448	A
1	2A	2469	A
1	2A	2476	A
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C

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Mol	Chain	Res	Type
1	2A	2525	G
1	2A	2529	G
1	2A	2536	G
1	2A	2549	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2574	G
1	2A	2585	U
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2652	C
1	2A	2654	A
1	2A	2673	G
1	2A	2679	A
1	2A	2689	U
1	2A	2690	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2751	G
1	2A	2757	A
1	2A	2760	C
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2807	G
1	2A	2820	A
1	2A	2821	A

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Mol	Chain	Res	Type
1	2A	2833	G
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2873	A
1	2A	2892	A
1	2A	2894	G
2	2B	2	C
2	2B	3	C
2	2B	8	U
2	2B	9	G
2	2B	24	G
2	2B	41	U
2	2B	42	C
2	2B	44	G
2	2B	47	C
2	2B	51	G
2	2B	53	A
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	91	C
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	114	C
2	2B	119	G
2	2B	120	A
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	41	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	66	G

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Mol	Chain	Res	Type
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	143	A
32	2a	144	G
32	2a	159	G
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	188	C
32	2a	189(C)	C
32	2a	189(E)	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	245	C
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	269	C
32	2a	279	A
32	2a	281	G
32	2a	289	G
32	2a	301	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	352	C
32	2a	353	A
32	2a	354	G

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Mol	Chain	Res	Type
32	2a	355	C
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	389	A
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	434	U
32	2a	439	A
32	2a	442	C
32	2a	446	G
32	2a	452	A
32	2a	455	C
32	2a	461	A
32	2a	470	C
32	2a	471	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	7MG
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	549	C
32	2a	559	A
32	2a	564	C
32	2a	568	G

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Mol	Chain	Res	Type
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	733	A
32	2a	746	A
32	2a	749	C
32	2a	755	G
32	2a	764	C
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	836	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	855	G
32	2a	859	A
32	2a	871	U
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	942	G

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Mol	Chain	Res	Type
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1001	A
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1007	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1018	C
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1035	A

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Mol	Chain	Res	Type
32	2a	1036	G
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U
32	2a	1043	C
32	2a	1046	A
32	2a	1051	C
32	2a	1064	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1086	U
32	2a	1091	U
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1097	C
32	2a	1101	A
32	2a	1108	G
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1162	C
32	2a	1172	C
32	2a	1173	G
32	2a	1177	G
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G

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Mol	Chain	Res	Type
32	2a	1186	G
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1219	U
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1261	A
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1285	A
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1304	G
32	2a	1320	C
32	2a	1321	C
32	2a	1323	G
32	2a	1340	A
32	2a	1347	G
32	2a	1350	A
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1364	U
32	2a	1368	G
32	2a	1370	G

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Mol	Chain	Res	Type
32	2a	1371	G
32	2a	1378	C
32	2a	1381	U
32	2a	1382	C
32	2a	1397	C
32	2a	1404	5MC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1456	G
32	2a	1492	A
32	2a	1499	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	24	A
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	8	4SU
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	45	U
54	2w	46	7MG
54	2w	48	C
54	2w	51	U
54	2w	65	G
54	2w	66	U
54	2w	67	C
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	73	A
54	2w	74	C

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Mol	Chain	Res	Type
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	21	A
55	2x	47	U
55	2x	59	A
55	2x	69	C
56	2y	9	A
56	2y	12	U
56	2y	15	G
56	2y	19	G
56	2y	27	G
56	2y	34	G
56	2y	38	A
56	2y	41	C
56	2y	45	U
56	2y	46	7MG
56	2y	49	C
56	2y	52	G
56	2y	53	G
56	2y	54	5MU
56	2y	55	PSU
56	2y	56	C
56	2y	58	A
56	2y	59	U
56	2y	61	C
56	2y	65	G
56	2y	68	C
56	2y	69	G
56	2y	70	G
56	2y	73	A

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	764	A

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Mol	Chain	Res	Type
1	1A	827	U
1	1A	974	G
1	1A	1047	G
1	1A	1065	U
1	1A	1078	U
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1700	A
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	746	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A

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Mol	Chain	Res	Type
1	2A	2126	A
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	2A	1917	1	18,21,22	1.39	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	1A	1911	1	18,21,22	1.42	2 (11%)	22,30,33	1.82	3 (13%)
32	5MC	1a	967	32	18,22,23	0.96	2 (11%)	26,32,35	1.10	3 (11%)
32	5MC	1a	1404	32	18,22,23	1.00	2 (11%)	26,32,35	1.13	3 (11%)
54	MIA	1w	37	54	24,31,32	2.19	3 (12%)	26,44,47	2.79	10 (38%)
54	4SU	2w	8	54	18,21,22	1.62	4 (22%)	26,30,33	2.38	5 (19%)
56	PSU	1y	39	56	18,21,22	1.29	1 (5%)	22,30,33	2.03	3 (13%)
1	4OC	1A	1920	1	19,22,24	0.82	0	26,31,35	0.87	1 (3%)
1	PSU	1A	1917	1	18,21,22	1.32	2 (11%)	22,30,33	2.02	3 (13%)
32	PSU	1a	516	32	18,21,22	1.36	2 (11%)	22,30,33	1.87	4 (18%)
1	2MU	2A	2552	1,57	19,22,24	1.24	3 (15%)	26,31,36	1.68	6 (23%)
54	MIA	2w	37	54	20,27,32	1.74	3 (15%)	22,39,47	2.03	7 (31%)
32	5MC	2a	1400	32	18,22,23	0.98	2 (11%)	26,32,35	1.23	4 (15%)
55	31H	1x	76	57,55	28,34,35	1.08	2 (7%)	23,47,50	1.72	5 (21%)
56	7MG	2y	46	56	22,26,27	1.47	4 (18%)	29,39,42	2.70	7 (24%)
32	MA6	1a	1518	32	19,26,27	0.86	0	18,38,41	1.49	2 (11%)
55	5MC	1x	32	55	18,22,23	1.04	2 (11%)	26,32,35	1.32	3 (11%)
32	5MC	1a	1400	32	18,22,23	0.91	2 (11%)	26,32,35	1.15	2 (7%)
1	5MC	2A	1942	1	18,22,23	0.96	2 (11%)	26,32,35	1.21	3 (11%)
32	PSU	2a	516	32	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	5MU	1A	1939	1,57	19,22,23	1.44	5 (26%)	28,32,35	2.32	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	4OC	2A	1920	1	19,22,24	0.80	0	26,31,35	0.84	0
32	MA6	2a	1519	32	19,26,27	0.80	0	18,38,41	1.49	2 (11%)
55	31H	2x	76	57,58,55	28,34,35	1.12	3 (10%)	23,47,50	1.57	5 (21%)
1	5MC	1A	1942	1	18,22,23	0.98	2 (11%)	26,32,35	1.21	3 (11%)
56	PSU	2y	55	56	18,21,22	1.32	2 (11%)	22,30,33	1.85	4 (18%)
55	5MU	1x	54	55	19,22,23	1.47	5 (26%)	28,32,35	1.86	6 (21%)
56	PSU	1y	32	56	18,21,22	1.31	2 (11%)	22,30,33	1.80	3 (13%)
43	0TD	2l	92	43	7,9,10	4.86	1 (14%)	6,11,13	5.98	3 (50%)
1	OMG	2A	2251	1,55	18,26,27	0.99	1 (5%)	19,38,41	1.11	2 (10%)
54	PSU	1w	39	54	18,21,22	1.30	2 (11%)	22,30,33	1.89	3 (13%)
1	5MU	1A	1915	1	19,22,23	1.39	6 (31%)	28,32,35	2.26	7 (25%)
32	MA6	1a	1519	32	19,26,27	0.83	0	18,38,41	1.46	2 (11%)
1	5MU	2A	1939	1,57	19,22,23	1.34	4 (21%)	28,32,35	2.22	6 (21%)
54	4SU	1w	8	54	18,21,22	1.73	6 (33%)	26,30,33	1.54	3 (11%)
54	PSU	2w	39	54	18,21,22	1.36	2 (11%)	22,30,33	1.65	4 (18%)
32	7MG	2a	527	32,57	22,26,27	1.39	4 (18%)	29,39,42	2.38	7 (24%)
32	4OC	1a	1402	32	20,23,24	0.77	0	26,32,35	1.01	1 (3%)
1	2MU	1A	2552	1	19,22,24	1.15	1 (5%)	26,31,36	1.72	6 (23%)
1	5MU	2A	1915	1	19,22,23	1.45	6 (31%)	28,32,35	2.16	7 (25%)
56	7MG	1y	46	56	22,26,27	1.41	4 (18%)	29,39,42	2.56	6 (20%)
55	PSU	2x	55	55	18,21,22	1.36	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	1A	2605	1,57	18,21,22	1.35	2 (11%)	22,30,33	1.72	3 (13%)
54	7MG	1w	46	54	22,26,27	1.44	4 (18%)	29,39,42	2.48	6 (20%)
54	5MU	1w	54	54	19,22,23	1.33	4 (21%)	28,32,35	2.02	6 (21%)
32	7MG	1a	527	32,57	22,26,27	1.47	4 (18%)	29,39,42	2.43	8 (27%)
54	F3N	2w	76	54,1	30,36,37	1.42	6 (20%)	29,51,54	1.28	2 (6%)
1	PSU	2A	2605	1	18,21,22	1.37	3 (16%)	22,30,33	1.94	4 (18%)
55	5MU	2x	54	55	19,22,23	1.38	5 (26%)	28,32,35	2.03	6 (21%)
54	PSU	1w	32	54,57	18,21,22	1.31	2 (11%)	22,30,33	1.76	3 (13%)
55	4SU	1x	8	55	18,21,22	2.16	5 (27%)	26,30,33	1.58	6 (23%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	22,30,33	1.81	3 (13%)
32	UR3	2a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.43	1 (3%)
56	PSU	1y	55	56	18,21,22	1.38	2 (11%)	22,30,33	1.92	3 (13%)
56	4SU	1y	8	56	18,21,22	1.67	4 (22%)	26,30,33	2.10	5 (19%)
54	F3N	1w	76	54,1	30,36,37	1.49	6 (20%)	29,51,54	1.31	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	5MC	2a	967	32,57	18,22,23	0.93	2 (11%)	26,32,35	1.03	2 (7%)
1	5MC	2A	1962	1,57	18,22,23	1.01	2 (11%)	26,32,35	1.13	2 (7%)
54	5MU	2w	54	54	19,22,23	1.37	4 (21%)	28,32,35	1.77	6 (21%)
56	MIA	1y	37	56	18,24,32	1.12	2 (11%)	18,35,47	1.25	2 (11%)
54	PSU	2w	55	54	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
56	PSU	2y	32	56	18,21,22	1.37	2 (11%)	22,30,33	1.83	3 (13%)
32	5MC	1a	1407	32	18,22,23	0.95	1 (5%)	26,32,35	1.13	2 (7%)
32	UR3	1a	1498	32	19,22,23	0.96	1 (5%)	26,32,35	1.45	2 (7%)
54	PSU	1w	55	54	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
32	5MC	2a	1407	32	18,22,23	0.98	2 (11%)	26,32,35	1.16	2 (7%)
43	0TD	1l	92	43	7,9,10	4.65	1 (14%)	6,11,13	3.91	2 (33%)
55	5MC	2x	32	55	18,22,23	1.00	2 (11%)	26,32,35	1.19	3 (11%)
56	4SU	2y	8	56	18,21,22	1.78	5 (27%)	26,30,33	1.91	5 (19%)
32	M2G	2a	966	32	20,27,28	1.54	3 (15%)	22,40,43	0.99	1 (4%)
32	2MG	1a	1207	32	18,26,27	0.99	1 (5%)	16,38,41	1.11	2 (12%)
1	OMG	1A	2251	1,57,55	18,26,27	0.95	1 (5%)	19,38,41	1.19	3 (15%)
56	5MU	1y	54	56	19,22,23	1.46	5 (26%)	28,32,35	1.69	5 (17%)
55	4SU	2x	8	55	18,21,22	2.00	5 (27%)	26,30,33	1.56	4 (15%)
1	5MC	1A	1962	1	18,22,23	0.94	2 (11%)	26,32,35	1.22	3 (11%)
32	M2G	1a	966	32	20,27,28	1.43	3 (15%)	22,40,43	0.95	2 (9%)
32	MA6	2a	1518	32	19,26,27	0.85	0	18,38,41	1.46	2 (11%)
56	5MU	2y	54	56	19,22,23	1.39	4 (21%)	28,32,35	1.93	5 (17%)
54	7MG	2w	46	54	22,26,27	1.29	3 (13%)	29,39,42	2.49	7 (24%)
32	5MC	2a	1404	32	18,22,23	0.97	2 (11%)	26,32,35	1.18	2 (7%)
56	PSU	2y	39	56	18,21,22	1.37	2 (11%)	22,30,33	1.64	2 (9%)
54	PSU	2w	32	54	18,21,22	1.37	2 (11%)	22,30,33	1.80	4 (18%)
1	2MA	2A	2503	1,57	17,25,26	1.05	2 (11%)	17,37,40	0.95	2 (11%)
56	MIA	2y	37	56	18,24,32	1.17	2 (11%)	18,35,47	1.32	2 (11%)
32	4OC	2a	1402	32	20,23,24	0.76	0	26,32,35	1.02	1 (3%)
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	22,30,33	1.82	3 (13%)
32	2MG	2a	1207	32	18,26,27	0.95	1 (5%)	16,38,41	1.01	1 (6%)
1	2MA	1A	2503	1,57	17,25,26	1.05	1 (5%)	17,37,40	1.02	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
1	4OC	1A	1920	1	-	0/9/27/30	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
54	MIA	2w	37	54	-	0/7/29/34	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
55	31H	1x	76	57,55	-	3/18/40/41	0/3/3/3
56	7MG	2y	46	56	-	5/7/37/38	0/3/3/3
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
55	31H	2x	76	57,58,55	-	3/18/40/41	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	2/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,57	-	3/7/37/38	0/3/3/3
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
1	2MU	1A	2552	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
56	7MG	1y	46	56	-	3/7/37/38	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	1/7/37/38	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,57	-	3/7/37/38	0/3/3/3
54	F3N	2w	76	54,1	-	3/15/37/38	0/4/4/4
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54,57	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	2/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	54,1	-	1/15/37/38	0/4/4/4
32	5MC	2a	967	32,57	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
56	MIA	1y	37	56	-	0/3/25/34	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	4/7/12/14	-
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	1/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	OMG	1A	2251	1,57,55	-	0/5/27/28	0/3/3/3
56	5MU	1y	54	56	-	2/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	2/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
56	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1404	32	-	1/7/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	1/3/25/26	0/3/3/3
56	MIA	2y	37	56	-	3/3/25/34	0/3/3/3
32	4OC	2a	1402	32	-	4/9/29/30	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	2MA	1A	2503	1,57	-	2/3/25/26	0/3/3/3

All (219) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.55	1.69	1.82
43	1l	92	0TD	CB-SB	-11.92	1.70	1.82
54	1w	37	MIA	C13-C14	7.10	1.52	1.32
54	1w	37	MIA	C2-S10	-6.76	1.70	1.75
54	2w	37	MIA	C2-S10	-6.40	1.70	1.75
32	2a	966	M2G	C2-N3	5.20	1.37	1.30
55	1x	8	4SU	C4-N3	-5.18	1.32	1.37
54	1w	76	F3N	CB-CG	-4.72	1.40	1.51
55	2x	8	4SU	C4-N3	-4.63	1.32	1.37
54	2w	76	F3N	CB-CG	-4.44	1.40	1.51
32	1a	966	M2G	C2-N3	4.38	1.36	1.30
56	2y	8	4SU	C4-S4	-4.37	1.60	1.68
54	2w	8	4SU	C4-S4	-4.29	1.60	1.68
55	2x	8	4SU	C4-S4	-4.20	1.60	1.68
55	1x	8	4SU	C2-N3	-4.14	1.30	1.38
56	1y	8	4SU	C4-S4	-4.10	1.60	1.68
32	1a	527	7MG	C4-N9	-4.09	1.33	1.37
55	1x	8	4SU	C4-S4	-4.07	1.60	1.68
54	1w	8	4SU	C4-S4	-3.93	1.60	1.68
56	1y	55	PSU	C6-C5	3.90	1.39	1.35
56	2y	32	PSU	C6-C5	3.89	1.39	1.35
32	2a	527	7MG	C4-N9	-3.89	1.33	1.37
56	1y	39	PSU	C6-C5	3.69	1.39	1.35
56	2y	39	PSU	C6-C5	3.66	1.39	1.35
54	1w	55	PSU	C6-C5	3.66	1.39	1.35
56	1y	32	PSU	C6-C5	3.59	1.39	1.35
54	2w	55	PSU	C6-C5	3.58	1.39	1.35
54	1w	8	4SU	C4-N3	-3.58	1.33	1.37
54	2w	39	PSU	C6-C5	3.55	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2605	PSU	C6-C5	3.50	1.39	1.35
32	2a	516	PSU	C6-C5	3.47	1.39	1.35
1	2A	1917	PSU	C6-C5	3.43	1.39	1.35
55	1x	55	PSU	C6-C5	3.41	1.39	1.35
54	2w	32	PSU	C6-C5	3.41	1.39	1.35
56	2y	8	4SU	C4-N3	-3.35	1.34	1.37
54	1w	76	F3N	O4'-C1'	3.35	1.45	1.41
55	1x	8	4SU	C5-C4	-3.33	1.38	1.42
54	2w	46	7MG	C4-N9	-3.33	1.33	1.37
56	2y	46	7MG	C5-C4	3.31	1.48	1.38
54	1w	39	PSU	C6-C5	3.31	1.39	1.35
1	1A	1917	PSU	C6-C5	3.29	1.39	1.35
32	1a	516	PSU	C6-C5	3.23	1.39	1.35
55	2x	55	PSU	C6-C5	3.22	1.39	1.35
56	1y	46	7MG	C5-C4	3.20	1.48	1.38
56	2y	46	7MG	C8-N9	3.20	1.47	1.46
1	2A	1911	PSU	C6-C5	3.14	1.39	1.35
54	2w	76	F3N	O4'-C1'	3.13	1.45	1.41
54	1w	46	7MG	C5-C4	3.13	1.48	1.38
55	2x	8	4SU	C2-N3	-3.12	1.32	1.38
56	2y	55	PSU	C6-C5	3.11	1.38	1.35
1	1A	1911	PSU	C6-C5	3.11	1.38	1.35
55	1x	54	5MU	C6-C5	3.10	1.39	1.34
55	2x	76	31H	C5-C4	-3.10	1.32	1.40
55	2x	8	4SU	C5-C4	-3.09	1.38	1.42
54	1w	32	PSU	C6-C5	3.07	1.38	1.35
56	1y	54	5MU	C6-C5	3.06	1.39	1.34
32	1a	527	7MG	C5-C4	3.00	1.47	1.38
55	1x	76	31H	C5-C4	-3.00	1.33	1.40
56	2y	54	5MU	C6-C5	2.99	1.39	1.34
54	1w	46	7MG	C4-N9	-2.98	1.34	1.37
32	2a	527	7MG	C5-C4	2.97	1.47	1.38
1	1A	1939	5MU	C4-N3	-2.95	1.33	1.38
32	1a	1407	5MC	C6-C5	2.95	1.39	1.34
54	2w	46	7MG	C5-C4	2.93	1.47	1.38
32	2a	1404	5MC	C6-C5	2.92	1.39	1.34
54	2w	54	5MU	C6-C5	2.91	1.39	1.34
32	2a	966	M2G	C2-N2	2.90	1.40	1.35
1	2A	1942	5MC	C6-C5	2.88	1.39	1.34
1	2A	2251	OMG	C6-N1	-2.88	1.33	1.37
56	1y	54	5MU	C4-N3	-2.87	1.33	1.38
54	1w	76	F3N	C5-C4	-2.87	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	37	MIA	C5-C4	2.86	1.48	1.40
56	1y	8	4SU	C2-N1	2.86	1.43	1.38
55	1x	54	5MU	C4-N3	-2.86	1.33	1.38
55	2x	32	5MC	C6-C5	2.84	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.83	1.33	1.38
55	1x	32	5MC	C6-C5	2.82	1.39	1.34
54	2w	76	F3N	C5-C4	-2.82	1.33	1.40
32	1a	1207	2MG	C6-N1	-2.80	1.33	1.37
54	2w	37	MIA	C5-C4	2.79	1.48	1.40
1	1A	2605	PSU	C6-C5	2.78	1.38	1.35
32	1a	1404	5MC	C6-C5	2.77	1.39	1.34
32	1a	966	M2G	C2-N2	2.76	1.40	1.35
54	1w	54	5MU	C6-C5	2.74	1.39	1.34
55	1x	76	31H	C6-C5	-2.73	1.33	1.43
32	2a	1400	5MC	C6-C5	2.73	1.39	1.34
1	1A	1939	5MU	C6-N1	-2.73	1.33	1.38
55	2x	54	5MU	C6-C5	2.72	1.39	1.34
54	1w	32	PSU	C4-N3	-2.72	1.33	1.38
1	1A	1911	PSU	C4-N3	-2.71	1.33	1.38
1	2A	1939	5MU	C6-C5	2.70	1.39	1.34
1	2A	1962	5MC	C6-N1	-2.70	1.33	1.38
56	1y	8	4SU	C4-N3	-2.70	1.34	1.37
1	2A	1911	PSU	C4-N3	-2.70	1.33	1.38
56	1y	46	7MG	C8-N9	2.69	1.47	1.46
1	1A	1942	5MC	C6-C5	2.67	1.39	1.34
1	1A	1915	5MU	C4-N3	-2.67	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.67	1.33	1.38
56	1y	37	MIA	C5-C4	2.66	1.48	1.40
1	1A	1915	5MU	C6-C5	2.66	1.39	1.34
56	2y	37	MIA	C2-N3	2.63	1.36	1.32
32	1a	967	5MC	C6-C5	2.62	1.38	1.34
1	1A	1942	5MC	C6-N1	-2.62	1.33	1.38
54	2w	32	PSU	C4-N3	-2.62	1.34	1.38
54	2w	8	4SU	C4-N3	-2.62	1.34	1.37
54	1w	46	7MG	C8-N9	2.62	1.47	1.46
54	1w	37	MIA	C5-C4	2.62	1.47	1.40
32	2a	967	5MC	C6-C5	2.61	1.38	1.34
1	2A	1915	5MU	C6-C5	2.60	1.38	1.34
56	1y	37	MIA	C2-N3	2.60	1.36	1.32
1	2A	2552	2MU	C4-N3	-2.59	1.33	1.38
56	2y	54	5MU	C2-N1	2.59	1.42	1.38
56	2y	39	PSU	C4-N3	-2.58	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1917	PSU	C4-N3	-2.58	1.34	1.38
32	2a	1407	5MC	C6-C5	2.56	1.38	1.34
1	1A	1939	5MU	C6-C5	2.56	1.38	1.34
55	2x	54	5MU	C4-N3	-2.56	1.34	1.38
1	2A	1915	5MU	C2-N1	2.56	1.42	1.38
56	2y	8	4SU	C5-C4	-2.55	1.39	1.42
1	2A	1962	5MC	C6-C5	2.55	1.38	1.34
1	2A	1915	5MU	C4-C5	2.54	1.49	1.44
56	2y	46	7MG	C6-N1	-2.54	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.54	1.34	1.37
54	2w	54	5MU	C4-N3	-2.53	1.34	1.38
32	1a	966	M2G	C6-N1	-2.53	1.34	1.37
54	2w	8	4SU	C5-C4	-2.53	1.39	1.42
1	1A	1939	5MU	C2-N3	-2.52	1.33	1.38
32	2a	516	PSU	C4-N3	-2.52	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.52	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.52	1.33	1.38
54	2w	76	F3N	C6-C5	-2.50	1.34	1.43
32	2a	1400	5MC	C6-N1	-2.49	1.33	1.38
55	1x	55	PSU	C4-N3	-2.49	1.34	1.38
55	2x	55	PSU	C4-N3	-2.48	1.34	1.38
32	1a	1400	5MC	C6-C5	2.48	1.38	1.34
54	2w	39	PSU	C4-N3	-2.48	1.34	1.38
54	1w	76	F3N	C6-C5	-2.47	1.34	1.43
56	2y	55	PSU	C4-N3	-2.47	1.34	1.38
55	1x	32	5MC	C6-N1	-2.47	1.33	1.38
54	1w	46	7MG	C6-N1	-2.45	1.34	1.38
56	1y	46	7MG	C6-N1	-2.45	1.34	1.38
54	1w	54	5MU	C4-N3	-2.44	1.34	1.38
54	1w	8	4SU	C2-N3	-2.44	1.33	1.38
54	1w	39	PSU	C4-N3	-2.44	1.34	1.38
1	1A	2552	2MU	C4-N3	-2.43	1.34	1.38
56	2y	54	5MU	C4-N3	-2.42	1.34	1.38
54	2w	55	PSU	C4-N3	-2.42	1.34	1.38
54	1w	8	4SU	C5-C4	-2.41	1.39	1.42
1	1A	2251	OMG	C6-N1	-2.40	1.34	1.37
32	2a	1407	5MC	C6-N1	-2.40	1.33	1.38
1	2A	1939	5MU	C6-N1	-2.40	1.33	1.38
1	1A	2503	2MA	C2-N3	2.40	1.36	1.31
1	1A	1962	5MC	C6-C5	2.39	1.38	1.34
32	1a	1400	5MC	C6-N1	-2.39	1.34	1.38
1	2A	1939	5MU	C4-C5	2.38	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1y	54	5MU	C4-C5	2.38	1.48	1.44
56	1y	32	PSU	C4-N3	-2.38	1.34	1.38
55	1x	54	5MU	C2-N1	2.38	1.42	1.38
56	1y	8	4SU	C5-C4	-2.37	1.39	1.42
56	2y	8	4SU	C2-N1	2.37	1.42	1.38
1	2A	2503	2MA	C2-N3	2.37	1.36	1.31
54	2w	37	MIA	C2-N3	2.36	1.37	1.34
1	2A	1939	5MU	C4-N3	-2.35	1.34	1.38
55	2x	54	5MU	C2-N1	2.35	1.42	1.38
55	1x	54	5MU	C4-C5	2.34	1.48	1.44
55	2x	76	31H	C6-C5	-2.33	1.34	1.43
32	1a	967	5MC	C6-N1	-2.33	1.34	1.38
32	1a	516	PSU	C4-N3	-2.32	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.32	1.34	1.38
56	1y	55	PSU	C4-N3	-2.30	1.34	1.38
54	1w	55	PSU	C4-N3	-2.25	1.34	1.38
55	2x	32	5MC	C6-N1	-2.25	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.24	1.34	1.38
56	2y	32	PSU	C4-N3	-2.24	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.24	1.34	1.38
1	1A	1915	5MU	C4-C5	2.23	1.48	1.44
32	2a	966	M2G	C6-N1	-2.20	1.34	1.37
32	1a	527	7MG	C6-N1	-2.20	1.34	1.38
1	1A	1915	5MU	C2-N1	2.18	1.42	1.38
54	1w	76	F3N	C2'-C3'	-2.18	1.50	1.53
56	1y	54	5MU	C2-N1	2.18	1.41	1.38
55	2x	76	31H	C5-N7	-2.16	1.31	1.39
1	2A	2552	2MU	C2-N3	-2.16	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.16	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.16	1.34	1.38
54	2w	8	4SU	C2-N1	2.15	1.41	1.38
1	2A	2552	2MU	C5-C4	2.15	1.48	1.43
55	2x	54	5MU	C4-C5	2.13	1.48	1.44
32	1a	1498	UR3	C6-C5	2.13	1.40	1.35
1	2A	2605	PSU	C2-N3	-2.13	1.33	1.37
56	2y	54	5MU	C4-C5	2.12	1.48	1.44
32	1a	527	7MG	C8-N9	2.11	1.47	1.46
54	1w	54	5MU	C4-C5	2.11	1.48	1.44
1	1A	1915	5MU	C2-N3	-2.10	1.34	1.38
54	2w	76	F3N	C5-N7	-2.10	1.32	1.39
32	2a	967	5MC	C6-N1	-2.10	1.34	1.38
54	1w	54	5MU	C2-N3	-2.09	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	76	F3N	C5-N7	-2.08	1.32	1.39
1	2A	2503	2MA	C6-N1	-2.08	1.33	1.38
32	2a	527	7MG	C6-N1	-2.08	1.35	1.38
55	1x	8	4SU	O2-C2	2.08	1.26	1.23
54	1w	8	4SU	C2-N1	2.08	1.41	1.38
56	1y	54	5MU	C2-N3	-2.08	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.07	1.34	1.38
1	2A	1915	5MU	C2-N3	-2.07	1.34	1.38
56	2y	8	4SU	C2-N3	-2.06	1.34	1.38
56	2y	46	7MG	C2-N3	2.05	1.38	1.33
32	2a	527	7MG	C5-C6	2.05	1.48	1.43
32	2a	1498	UR3	C2-N1	2.05	1.41	1.38
54	2w	46	7MG	C5-C6	2.05	1.48	1.43
1	1A	1939	5MU	C4-C5	2.05	1.48	1.44
54	2w	76	F3N	C2'-C3'	-2.05	1.50	1.53
55	2x	54	5MU	C6-N1	-2.05	1.34	1.38
56	1y	46	7MG	C5-C6	2.04	1.48	1.43
55	2x	8	4SU	O2-C2	2.04	1.26	1.23
55	1x	54	5MU	C2-N3	-2.02	1.34	1.38
54	2w	54	5MU	C2-N3	-2.02	1.34	1.38
54	2w	54	5MU	C2-N1	2.01	1.41	1.38
54	1w	8	4SU	C6-C5	2.00	1.39	1.35

All (318) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-14.00	77.12	102.44
56	2y	46	7MG	N9-C4-N3	9.98	140.40	125.47
54	1w	37	MIA	C12-C13-C14	-9.29	109.06	127.14
56	1y	46	7MG	N9-C4-N3	9.29	139.36	125.47
54	1w	46	7MG	N9-C4-N3	8.96	138.87	125.47
43	1l	92	0TD	CSB-SB-CB	8.86	118.46	102.44
32	1a	527	7MG	N9-C4-N3	8.30	137.88	125.47
54	2w	46	7MG	N9-C4-N3	8.19	137.72	125.47
32	2a	527	7MG	N9-C4-N3	7.97	137.40	125.47
54	2w	8	4SU	C4-N3-C2	-7.55	120.01	127.34
1	1A	1917	PSU	N1-C2-N3	6.29	122.25	115.13
56	1y	39	PSU	N1-C2-N3	6.20	122.16	115.13
56	1y	55	PSU	N1-C2-N3	6.19	122.14	115.13
32	1a	1498	UR3	C4-N3-C2	-6.14	118.78	124.56
54	2w	8	4SU	C5-C4-N3	6.09	120.34	114.69
1	2A	2605	PSU	N1-C2-N3	6.04	121.98	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1917	PSU	N1-C2-N3	5.99	121.92	115.13
55	2x	55	PSU	N1-C2-N3	5.93	121.85	115.13
32	2a	516	PSU	N1-C2-N3	5.87	121.78	115.13
55	1x	76	31H	N3-C2-N1	-5.87	119.51	128.68
32	2a	1498	UR3	C4-N3-C2	-5.86	119.04	124.56
56	1y	8	4SU	C4-N3-C2	-5.83	121.68	127.34
1	1A	1911	PSU	N1-C2-N3	5.82	121.73	115.13
54	1w	39	PSU	N1-C2-N3	5.79	121.69	115.13
56	2y	46	7MG	C5-C4-N3	-5.78	117.12	128.13
55	1x	55	PSU	N1-C2-N3	5.72	121.61	115.13
1	1A	1915	5MU	C4-N3-C2	-5.72	119.95	127.35
54	2w	32	PSU	N1-C2-N3	5.71	121.60	115.13
54	2w	55	PSU	N1-C2-N3	5.67	121.55	115.13
54	1w	55	PSU	N1-C2-N3	5.66	121.54	115.13
1	2A	1911	PSU	N1-C2-N3	5.65	121.54	115.13
1	1A	1939	5MU	C4-N3-C2	-5.65	120.04	127.35
56	1y	46	7MG	C5-C4-N3	-5.64	117.38	128.13
56	2y	55	PSU	N1-C2-N3	5.64	121.52	115.13
56	2y	32	PSU	N1-C2-N3	5.63	121.51	115.13
56	1y	32	PSU	N1-C2-N3	5.63	121.51	115.13
54	1w	76	F3N	N3-C2-N1	-5.62	119.90	128.68
1	1A	1939	5MU	C5-C4-N3	5.60	120.09	115.31
54	2w	76	F3N	N3-C2-N1	-5.60	119.93	128.68
55	2x	76	31H	N3-C2-N1	-5.56	119.99	128.68
54	1w	32	PSU	N1-C2-N3	5.55	121.42	115.13
1	2A	1939	5MU	C4-N3-C2	-5.54	120.18	127.35
32	1a	516	PSU	N1-C2-N3	5.52	121.38	115.13
54	2w	46	7MG	N9-C8-N7	-5.48	95.54	103.38
56	2y	8	4SU	C5-C4-N3	5.42	119.72	114.69
1	2A	1915	5MU	C4-N3-C2	-5.42	120.33	127.35
32	2a	527	7MG	N9-C8-N7	-5.42	95.62	103.38
56	2y	8	4SU	C4-N3-C2	-5.37	122.12	127.34
1	1A	1915	5MU	N3-C2-N1	5.35	121.99	114.89
56	1y	8	4SU	C5-C4-N3	5.34	119.64	114.69
56	2y	39	PSU	N1-C2-N3	5.30	121.13	115.13
32	1a	527	7MG	N9-C8-N7	-5.29	95.81	103.38
1	1A	1915	5MU	C5-C4-N3	5.27	119.81	115.31
54	1w	46	7MG	C5-C4-N3	-5.24	118.15	128.13
1	1A	2605	PSU	N1-C2-N3	5.20	121.02	115.13
1	1A	1939	5MU	C5-C6-N1	-5.15	118.04	123.34
54	2w	46	7MG	C5-C4-N3	-5.12	118.38	128.13
54	2w	39	PSU	N1-C2-N3	5.11	120.92	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	46	7MG	N9-C8-N7	-5.11	96.07	103.38
55	1x	54	5MU	N3-C2-N1	5.06	121.60	114.89
32	2a	1518	MA6	N3-C2-N1	-4.97	120.91	128.68
1	2A	1939	5MU	N3-C2-N1	4.96	121.47	114.89
1	2A	1915	5MU	N3-C2-N1	4.96	121.47	114.89
32	1a	527	7MG	C5-C4-N3	-4.96	118.68	128.13
1	2A	1915	5MU	C5-C4-N3	4.92	119.51	115.31
55	2x	54	5MU	C4-N3-C2	-4.91	121.00	127.35
55	2x	54	5MU	N3-C2-N1	4.90	121.39	114.89
54	2w	37	MIA	C12-N6-C6	-4.89	118.66	122.87
54	1w	54	5MU	C4-N3-C2	-4.83	121.10	127.35
32	2a	1519	MA6	N3-C2-N1	-4.82	121.15	128.68
32	1a	1518	MA6	N3-C2-N1	-4.82	121.15	128.68
56	1y	46	7MG	N9-C8-N7	-4.81	96.49	103.38
32	2a	527	7MG	C5-C4-N3	-4.79	118.99	128.13
1	1A	1939	5MU	O4-C4-C5	-4.79	119.35	124.90
54	1w	37	MIA	C12-N6-C6	-4.75	115.50	122.55
1	1A	2552	2MU	N3-C2-N1	4.74	121.18	114.89
32	1a	1519	MA6	N3-C2-N1	-4.68	121.37	128.68
56	2y	54	5MU	O4-C4-C5	-4.65	119.51	124.90
56	2y	54	5MU	C5-C4-N3	4.63	119.26	115.31
54	1w	54	5MU	C5-C4-N3	4.62	119.25	115.31
56	1y	46	7MG	C2-N3-C4	4.61	120.52	112.30
54	1w	54	5MU	N3-C2-N1	4.61	121.00	114.89
1	2A	1939	5MU	O4-C4-C5	-4.57	119.60	124.90
1	2A	1939	5MU	C5-C4-N3	4.57	119.21	115.31
56	2y	54	5MU	C4-N3-C2	-4.55	121.46	127.35
1	2A	2552	2MU	N3-C2-N1	4.54	120.92	114.89
56	2y	46	7MG	C2-N3-C4	4.52	120.36	112.30
56	1y	39	PSU	C4-N3-C2	-4.46	119.92	126.34
55	1x	54	5MU	C4-N3-C2	-4.44	121.61	127.35
56	2y	46	7MG	N9-C8-N7	-4.43	97.04	103.38
54	2w	8	4SU	C5-C4-S4	-4.42	118.77	124.47
1	1A	1939	5MU	N3-C2-N1	4.41	120.75	114.89
54	1w	8	4SU	C5-C4-N3	4.41	118.78	114.69
1	1A	1915	5MU	O4-C4-C5	-4.38	119.82	124.90
54	1w	54	5MU	O4-C4-C5	-4.34	119.87	124.90
54	1w	37	MIA	C2-N3-C4	4.34	121.30	115.32
54	2w	54	5MU	N3-C2-N1	4.32	120.62	114.89
54	2w	8	4SU	N3-C2-N1	4.29	120.58	114.89
54	2w	46	7MG	C2-N3-C4	4.28	119.92	112.30
56	2y	54	5MU	N3-C2-N1	4.27	120.55	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	1y	54	5MU	N3-C2-N1	4.26	120.55	114.89
55	2x	54	5MU	O4-C4-C5	-4.25	119.98	124.90
1	1A	1917	PSU	C4-N3-C2	-4.21	120.27	126.34
55	1x	32	5MC	C5-C6-N1	-4.21	119.01	123.34
1	1A	1917	PSU	O2-C2-N1	-4.18	118.19	122.79
32	2a	1404	5MC	C5-C6-N1	-4.14	119.08	123.34
54	1w	39	PSU	C4-N3-C2	-4.14	120.37	126.34
55	2x	54	5MU	C5-C4-N3	4.11	118.81	115.31
54	1w	46	7MG	C2-N3-C4	4.09	119.59	112.30
32	2a	527	7MG	C2-N3-C4	4.09	119.59	112.30
1	2A	2605	PSU	C4-N3-C2	-4.09	120.45	126.34
54	1w	37	MIA	C16-C14-C13	-4.07	110.88	122.65
54	1w	37	MIA	C15-C14-C13	-4.06	110.92	122.65
54	2w	37	MIA	C2-N3-C4	4.05	120.91	115.32
54	2w	54	5MU	C4-N3-C2	-4.05	122.11	127.35
1	1A	2552	2MU	C4-N3-C2	-4.03	121.26	126.58
1	2A	1939	5MU	C5-C6-N1	-4.02	119.20	123.34
54	1w	55	PSU	O2-C2-N1	-4.01	118.37	122.79
55	1x	8	4SU	C6-C5-C4	-4.00	116.49	119.95
54	2w	54	5MU	O4-C4-C5	-3.99	120.27	124.90
1	1A	1962	5MC	C5-C6-N1	-3.99	119.23	123.34
32	1a	527	7MG	C2-N3-C4	3.98	119.39	112.30
54	1w	8	4SU	C4-N3-C2	-3.92	123.54	127.34
32	1a	516	PSU	C4-N3-C2	-3.91	120.70	126.34
1	1A	1942	5MC	C5-C6-N1	-3.91	119.32	123.34
56	1y	54	5MU	C4-N3-C2	-3.90	122.30	127.35
56	1y	39	PSU	O2-C2-N1	-3.88	118.51	122.79
56	1y	55	PSU	O2-C2-N1	-3.88	118.52	122.79
32	2a	1400	5MC	C5-C6-N1	-3.88	119.35	123.34
55	2x	8	4SU	C1'-N1-C2	3.87	124.58	117.57
1	2A	2552	2MU	C4-N3-C2	-3.86	121.49	126.58
32	2a	516	PSU	C4-N3-C2	-3.83	120.83	126.34
56	1y	8	4SU	C5-C4-S4	-3.79	119.59	124.47
55	1x	55	PSU	C4-N3-C2	-3.78	120.89	126.34
54	2w	32	PSU	C4-N3-C2	-3.78	120.89	126.34
55	2x	32	5MC	C5-C6-N1	-3.78	119.45	123.34
1	2A	1915	5MU	O4-C4-C5	-3.77	120.54	124.90
55	2x	55	PSU	C4-N3-C2	-3.76	120.92	126.34
56	2y	55	PSU	O2-C2-N1	-3.75	118.66	122.79
32	2a	1407	5MC	C5-C6-N1	-3.74	119.49	123.34
1	2A	1939	5MU	O2-C2-N1	-3.74	117.81	122.79
55	1x	8	4SU	O2-C2-N1	3.73	127.75	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1915	5MU	C5-C6-N1	-3.72	119.51	123.34
1	2A	1911	PSU	C4-N3-C2	-3.70	121.00	126.34
54	2w	54	5MU	C5-C4-N3	3.67	118.45	115.31
54	2w	55	PSU	C4-N3-C2	-3.65	121.08	126.34
1	1A	1911	PSU	C4-N3-C2	-3.65	121.08	126.34
56	1y	54	5MU	C5-C4-N3	3.65	118.42	115.31
1	2A	1917	PSU	C4-N3-C2	-3.64	121.10	126.34
54	1w	32	PSU	C4-N3-C2	-3.63	121.10	126.34
1	2A	1942	5MC	C5-C6-N1	-3.60	119.64	123.34
55	2x	8	4SU	C5-C4-N3	3.59	118.02	114.69
32	1a	1400	5MC	C5-C6-N1	-3.58	119.65	123.34
56	1y	32	PSU	C4-N3-C2	-3.58	121.18	126.34
55	1x	54	5MU	C5-C4-N3	3.57	118.36	115.31
1	1A	2605	PSU	C4-N3-C2	-3.56	121.21	126.34
56	1y	8	4SU	N3-C2-N1	3.56	119.61	114.89
56	1y	8	4SU	C1'-N1-C2	3.54	123.98	117.57
56	2y	32	PSU	C4-N3-C2	-3.53	121.25	126.34
56	2y	32	PSU	O2-C2-N1	-3.52	118.92	122.79
32	1a	516	PSU	O2-C2-N1	-3.51	118.92	122.79
56	1y	55	PSU	C4-N3-C2	-3.51	121.28	126.34
54	2w	37	MIA	C11-S10-C2	-3.50	99.66	102.27
1	2A	1962	5MC	C5-C6-N1	-3.49	119.75	123.34
32	2a	967	5MC	C5-C6-N1	-3.47	119.77	123.34
32	1a	1404	5MC	C5-C6-N1	-3.46	119.78	123.34
56	1y	37	MIA	N3-C2-N1	-3.45	123.28	128.68
1	1A	1915	5MU	C5-C6-N1	-3.42	119.82	123.34
55	2x	54	5MU	C5-C6-N1	-3.41	119.83	123.34
54	1w	55	PSU	C4-N3-C2	-3.40	121.44	126.34
1	1A	1911	PSU	O2-C2-N1	-3.39	119.06	122.79
54	2w	37	MIA	C5-C6-N1	-3.39	118.00	120.81
56	2y	8	4SU	N3-C2-N1	3.38	119.38	114.89
32	1a	1407	5MC	C5-C6-N1	-3.38	119.86	123.34
54	1w	54	5MU	C5-C6-N1	-3.37	119.87	123.34
56	1y	32	PSU	O2-C2-N1	-3.36	119.09	122.79
56	2y	55	PSU	C4-N3-C2	-3.35	121.51	126.34
55	1x	54	5MU	C5-C6-N1	-3.32	119.92	123.34
56	2y	37	MIA	N3-C2-N1	-3.30	123.53	128.68
54	2w	55	PSU	O2-C2-N1	-3.29	119.17	122.79
43	2l	92	0TD	OD2-CG-CB	3.28	120.23	113.15
32	2a	516	PSU	O2-C2-N1	-3.28	119.18	122.79
55	2x	55	PSU	O2-C2-N1	-3.27	119.19	122.79
55	2x	8	4SU	C6-C5-C4	-3.26	117.12	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	54	5MU	O4-C4-C5	-3.25	121.13	124.90
56	2y	54	5MU	C5-C6-N1	-3.24	120.00	123.34
54	2w	39	PSU	C4-N3-C2	-3.24	121.67	126.34
1	2A	1917	PSU	O2-C2-N1	-3.23	119.23	122.79
1	2A	1911	PSU	O2-C2-N1	-3.21	119.26	122.79
56	1y	54	5MU	C5-C6-N1	-3.17	120.08	123.34
54	1w	37	MIA	C5-C6-N1	-3.17	118.18	120.81
1	1A	2552	2MU	O2-C2-N1	-3.13	118.62	122.79
56	2y	39	PSU	C4-N3-C2	-3.13	121.83	126.34
32	1a	967	5MC	C5-C6-N1	-3.12	120.13	123.34
32	1a	1519	MA6	C4-C5-N7	-3.10	106.17	109.40
32	2a	1519	MA6	C4-C5-N7	-3.07	106.20	109.40
1	2A	2552	2MU	C2'-C1'-N1	-3.03	108.33	114.22
54	1w	8	4SU	N3-C2-N1	3.03	118.91	114.89
32	1a	1518	MA6	C4-C5-N7	-3.02	106.25	109.40
54	1w	54	5MU	O2-C2-N1	-3.01	118.79	122.79
1	1A	2552	2MU	O4-C4-C5	-3.01	119.87	125.16
56	1y	54	5MU	O4-C4-C5	-3.00	121.42	124.90
1	2A	2552	2MU	O2-C2-N1	-3.00	118.80	122.79
56	2y	46	7MG	C5-C4-N9	-3.00	102.46	106.35
54	1w	32	PSU	O2-C2-N1	-2.99	119.50	122.79
54	2w	54	5MU	C5-C6-N1	-2.99	120.27	123.34
55	1x	76	31H	O4'-C1'-C2'	-2.97	102.58	106.93
55	1x	8	4SU	C5-C4-N3	2.96	117.43	114.69
54	1w	39	PSU	O2-C2-N1	-2.93	119.57	122.79
56	2y	8	4SU	C5-C4-S4	-2.92	120.71	124.47
32	2a	1518	MA6	C4-C5-N7	-2.86	106.42	109.40
32	1a	1407	5MC	C5-C4-N3	-2.85	118.60	121.67
1	1A	2605	PSU	O2-C2-N1	-2.84	119.66	122.79
1	2A	2605	PSU	O2-C2-N1	-2.84	119.67	122.79
56	2y	37	MIA	C4-C5-N7	-2.82	106.46	109.40
54	1w	37	MIA	C2-N1-C6	2.80	122.19	117.19
56	1y	37	MIA	C4-C5-N7	-2.79	106.49	109.40
1	2A	2251	OMG	C5-C6-N1	2.78	118.87	113.95
54	2w	46	7MG	C5-C6-N1	2.76	115.86	110.99
55	2x	76	31H	O2'-C2'-C3'	2.76	117.93	111.16
1	1A	1942	5MC	C5-C4-N3	-2.76	118.69	121.67
1	1A	1915	5MU	O2-C2-N1	-2.74	119.14	122.79
54	2w	76	F3N	C3'-N3'-C	-2.74	119.08	123.21
32	1a	1207	2MG	C8-N7-C5	2.73	108.19	102.99
1	2A	1942	5MC	C5-C4-N3	-2.73	118.73	121.67
55	1x	55	PSU	O2-C2-N1	-2.71	119.80	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1407	5MC	C5-C4-N3	-2.70	118.76	121.67
55	1x	32	5MC	C5-C4-N3	-2.66	118.80	121.67
43	1l	92	0TD	OD2-CG-CB	2.66	118.90	113.15
32	1a	1404	5MC	C5-C4-N3	-2.65	118.82	121.67
55	2x	8	4SU	O2-C2-N1	2.64	126.29	122.79
54	1w	46	7MG	C5-C4-N9	-2.59	102.99	106.35
54	1w	37	MIA	C4-C5-N7	-2.59	106.70	109.40
1	1A	2503	2MA	C5-C6-N1	2.58	118.47	114.02
32	1a	527	7MG	C5-C6-N1	2.56	115.50	110.99
56	2y	55	PSU	C6-C5-C4	-2.54	116.42	118.20
1	2A	2552	2MU	C5-C4-N3	2.53	118.62	114.84
54	2w	32	PSU	O2-C2-N1	-2.51	120.02	122.79
55	1x	32	5MC	O2-C2-N3	-2.50	118.26	122.33
54	2w	37	MIA	C2-N1-C6	2.49	121.65	117.19
1	1A	2251	OMG	O6-C6-C5	-2.49	119.51	124.37
32	1a	967	5MC	C5-C4-N3	-2.48	119.00	121.67
1	1A	2503	2MA	C8-N7-C5	2.45	107.67	102.99
43	2l	92	0TD	OD1-CG-CB	-2.44	117.32	122.44
32	2a	527	7MG	C5-C6-N1	2.44	115.29	110.99
32	2a	1402	4OC	C6-C5-C4	2.43	119.94	116.96
32	1a	1402	4OC	C6-C5-C4	2.42	119.93	116.96
55	1x	8	4SU	S4-C4-N3	-2.41	117.83	120.21
1	1A	2552	2MU	C5-C4-N3	2.41	118.45	114.84
32	1a	1400	5MC	C5-C4-N3	-2.41	119.07	121.67
1	2A	1915	5MU	C5M-C5-C4	2.41	121.42	118.77
55	2x	32	5MC	C5-C4-N3	-2.39	119.09	121.67
56	1y	46	7MG	C5-C6-N1	2.39	115.20	110.99
56	1y	46	7MG	C5-C4-N9	-2.38	103.26	106.35
1	1A	1939	5MU	O2-C2-N1	-2.38	119.62	122.79
55	2x	32	5MC	O2-C2-N3	-2.38	118.47	122.33
32	2a	1207	2MG	C8-N7-C5	2.37	107.51	102.99
54	2w	37	MIA	C4-C5-N7	-2.37	106.93	109.40
54	2w	8	4SU	O2-C2-N1	-2.37	119.64	122.79
1	2A	2552	2MU	O4-C4-C5	-2.35	121.02	125.16
32	2a	527	7MG	CM7-N7-C5	2.35	132.46	126.40
1	2A	2503	2MA	C5-C6-N1	2.34	118.06	114.02
1	2A	2503	2MA	C8-N7-C5	2.34	107.45	102.99
1	2A	1942	5MC	O2-C2-N3	-2.34	118.53	122.33
32	2a	1400	5MC	C5-C4-N3	-2.34	119.15	121.67
55	1x	76	31H	O2'-C2'-C3'	2.33	116.87	111.16
55	2x	54	5MU	O2-C2-N1	-2.33	119.69	122.79
1	1A	1962	5MC	C5-C4-N3	-2.32	119.17	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	8	4SU	C1'-N1-C2	2.31	121.75	117.57
1	2A	1962	5MC	C5-C4-N3	-2.31	119.18	121.67
56	2y	46	7MG	C5-C6-N1	2.31	115.06	110.99
55	1x	8	4SU	O2-C2-N3	-2.31	117.20	121.50
1	1A	2251	OMG	C5-C6-N1	2.31	118.03	113.95
54	1w	37	MIA	N3-C2-N1	-2.30	122.75	126.98
32	1a	1404	5MC	CM5-C5-C6	-2.29	119.78	122.85
54	2w	46	7MG	O6-C6-C5	-2.29	121.92	127.54
54	2w	39	PSU	O2-C2-N1	-2.29	120.27	122.79
32	1a	527	7MG	C5-C4-N9	-2.26	103.42	106.35
55	2x	76	31H	O4'-C1'-C2'	-2.25	103.63	106.93
1	1A	1915	5MU	C5M-C5-C4	2.25	121.25	118.77
1	1A	1942	5MC	CM5-C5-C6	-2.25	119.84	122.85
1	2A	2251	OMG	C8-N7-C5	2.24	107.26	102.99
32	1a	1207	2MG	CM2-N2-C2	-2.23	118.93	123.86
55	1x	76	31H	OCN-CN-N	-2.22	119.42	125.27
1	1A	2251	OMG	C8-N7-C5	2.22	107.22	102.99
32	1a	966	M2G	C8-N7-C5	2.22	107.22	102.99
54	2w	54	5MU	O2-C2-N1	-2.20	119.86	122.79
32	1a	527	7MG	O6-C6-C5	-2.20	122.14	127.54
32	2a	967	5MC	C5-C4-N3	-2.19	119.31	121.67
54	1w	37	MIA	C11-S10-C2	-2.18	100.64	102.27
54	1w	76	F3N	C3'-N3'-C	-2.17	119.94	123.21
56	2y	8	4SU	C1'-N1-C2	2.17	121.49	117.57
32	1a	1498	UR3	C3U-N3-C2	2.17	121.11	117.31
32	1a	527	7MG	CM7-N7-C5	2.16	131.99	126.40
1	2A	2605	PSU	C5-C6-N1	-2.16	118.87	122.11
32	2a	1404	5MC	C5-C4-N3	-2.15	119.36	121.67
55	1x	76	31H	CA-N-CN	-2.14	119.53	122.82
55	2x	76	31H	OCN-CN-N	-2.14	119.65	125.27
32	1a	966	M2G	C5-C6-N1	2.13	117.71	113.95
32	2a	527	7MG	C5-C4-N9	-2.12	103.60	106.35
54	2w	46	7MG	N2-C2-N3	-2.10	115.64	119.73
1	1A	1962	5MC	CM5-C5-C6	-2.09	120.05	122.85
1	1A	2552	2MU	C2'-C1'-N1	-2.09	110.16	114.22
32	2a	966	M2G	C5-C6-N1	2.09	117.64	113.95
54	1w	46	7MG	C5-C6-N1	2.09	114.66	110.99
54	2w	32	PSU	C5-C6-N1	-2.08	118.99	122.11
32	1a	516	PSU	O4'-C1'-C2'	2.08	108.07	105.14
32	2a	1400	5MC	CM5-C5-C6	-2.08	120.07	122.85
56	2y	46	7MG	O6-C6-C5	-2.06	122.49	127.54
54	2w	37	MIA	C1'-N9-C4	2.05	130.25	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2w	39	PSU	C6-C5-C4	-2.05	116.77	118.20
1	2A	1915	5MU	C5M-C5-C6	-2.04	120.12	122.85
32	2a	1400	5MC	O2-C2-N3	-2.04	119.02	122.33
55	2x	76	31H	CA-N-CN	-2.03	119.69	122.82
32	1a	967	5MC	CM5-C5-C6	-2.02	120.15	122.85
54	1w	76	F3N	O2'-C2'-C3'	-2.02	106.22	111.16
1	1A	1920	4OC	O2-C2-N3	-2.01	119.06	122.33
55	1x	54	5MU	O2-C2-N1	-2.01	120.12	122.79

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	1l	92	0TD	SB-CB-CG-OD2
54	1w	37	MIA	C12-C13-C14-C16
56	1y	46	7MG	C4'-C5'-O5'-P
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
56	2y	37	MIA	C3'-C4'-C5'-O5'
56	2y	54	5MU	C3'-C4'-C5'-O5'
56	2y	54	5MU	O4'-C4'-C5'-O5'
56	2y	55	PSU	C2'-C1'-C5-C6
55	1x	76	31H	C3'-C4'-C5'-O5'
55	2x	76	31H	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
56	1y	54	5MU	C3'-C4'-C5'-O5'
56	1y	54	5MU	O4'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
56	2y	37	MIA	O4'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
55	2x	76	31H	C4'-C5'-O5'-P
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
56	2y	46	7MG	O4'-C4'-C5'-O5'
54	2w	76	F3N	N-CA-CB-CG
54	1w	46	7MG	C4'-C5'-O5'-P
56	2y	46	7MG	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
32	2a	1402	4OC	O4'-C4'-C5'-O5'
56	2y	46	7MG	O4'-C1'-N9-C4
32	2a	1519	MA6	C4'-C5'-O5'-P
56	1y	46	7MG	C2'-C1'-N9-C8
54	2w	46	7MG	C2'-C1'-N9-C8
55	1x	76	31H	C4'-C5'-O5'-P
32	1a	527	7MG	O4'-C4'-C5'-O5'
56	2y	46	7MG	C3'-C4'-C5'-O5'
32	2a	527	7MG	C4'-C5'-O5'-P
56	2y	37	MIA	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
56	1y	55	PSU	O4'-C1'-C5-C4
32	2a	1402	4OC	C3'-C2'-O2'-CM2
43	1l	92	0TD	CA-CB-SB-CSB
54	2w	76	F3N	C-CA-CB-CG
32	1a	1400	5MC	O4'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
56	2y	46	7MG	O4'-C1'-N9-C8
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1404	5MC	C3'-C4'-C5'-O5'
56	1y	55	PSU	O4'-C1'-C5-C6
56	2y	55	PSU	O4'-C1'-C5-C6
32	1a	527	7MG	C4'-C5'-O5'-P
54	1w	76	F3N	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD1
1	1A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
54	2w	76	F3N	O4'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C1'-N9-C8
1	1A	1962	5MC	C2'-C1'-N1-C6
32	2a	1402	4OC	C2'-C1'-N1-C2
56	2y	8	4SU	C2'-C1'-N1-C2
1	1A	1962	5MC	O4'-C1'-N1-C6
56	1y	46	7MG	O4'-C1'-N9-C8

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 2693 ligands modelled in this entry, 2689 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
61	SF4	1d	302	35	0,12,12	-	-	-		
59	TEL	1A	4076	-	59,62,62	1.28	6 (10%)	77,92,92	1.56	7 (9%)
61	SF4	2d	303	35	0,12,12	-	-	-		
59	TEL	2A	3845	-	59,62,62	1.29	7 (11%)	77,92,92	1.89	13 (16%)

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
61	SF4	1d	302	35	-	-	0/6/5/5
59	TEL	1A	4076	-	-	2/73/108/108	0/4/5/5
61	SF4	2d	303	35	-	-	0/6/5/5
59	TEL	2A	3845	-	-	10/73/108/108	0/4/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	2A	3845	TEL	O5-C10	5.50	1.44	1.35
59	1A	4076	TEL	O5-C10	5.04	1.43	1.35
59	2A	3845	TEL	O9-C15	4.62	1.45	1.34
59	1A	4076	TEL	O9-C15	4.57	1.45	1.34
59	1A	4076	TEL	O5-C2	-3.05	1.43	1.47
59	2A	3845	TEL	O5-C2	-2.96	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	4076	TEL	O9-C4	-2.88	1.41	1.46
59	2A	3845	TEL	C36-N31	-2.70	1.34	1.38
59	1A	4076	TEL	C36-N31	-2.64	1.34	1.38
59	1A	4076	TEL	C30-C26	-2.57	1.48	1.52
59	2A	3845	TEL	O9-C4	-2.51	1.42	1.46
59	2A	3845	TEL	C21-C26	-2.09	1.49	1.52
59	2A	3845	TEL	C30-C26	-2.01	1.49	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	2A	3845	TEL	O9-C15-C21	7.78	118.78	110.88
59	2A	3845	TEL	C17-C11-N6	-6.94	102.59	113.31
59	1A	4076	TEL	C11-N6-C10	6.03	129.86	122.25
59	2A	3845	TEL	C11-N6-C10	5.80	129.57	122.25
59	1A	4076	TEL	C17-C11-N6	-5.68	104.54	113.31
59	1A	4076	TEL	O9-C15-C21	5.23	116.20	110.88
59	2A	3845	TEL	C8-C4-C2	-3.86	109.91	115.23
59	2A	3845	TEL	C4-O9-C15	-3.23	112.43	118.18
59	2A	3845	TEL	O9-C15-O20	-2.92	118.49	123.94
59	2A	3845	TEL	C38-O32-C28	2.91	123.61	117.55
59	2A	3845	TEL	C56-N52-C47	2.74	121.59	116.85
59	2A	3845	TEL	C55-C50-C54	-2.73	109.12	113.40
59	1A	4076	TEL	O5-C2-C1	2.61	111.53	106.93
59	2A	3845	TEL	O5-C2-C3	2.41	105.59	103.16
59	2A	3845	TEL	O5-C2-C1	2.39	111.13	106.93
59	1A	4076	TEL	C56-N52-C47	2.33	120.87	116.85
59	2A	3845	TEL	O18-C13-C19	-2.32	116.97	121.26
59	1A	4076	TEL	C8-C4-C2	-2.29	112.07	115.23
59	2A	3845	TEL	O5-C10-N6	-2.16	108.08	109.81
59	1A	4076	TEL	C33-C28-C34	2.14	113.01	109.75

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	2A	3845	TEL	C1-C2-C4-C8
59	2A	3845	TEL	C3-C2-C4-C8
59	2A	3845	TEL	O5-C2-C4-C8
59	2A	3845	TEL	O5-C2-C4-O9
59	2A	3845	TEL	C24-C28-O32-C38
59	2A	3845	TEL	C33-C28-O32-C38

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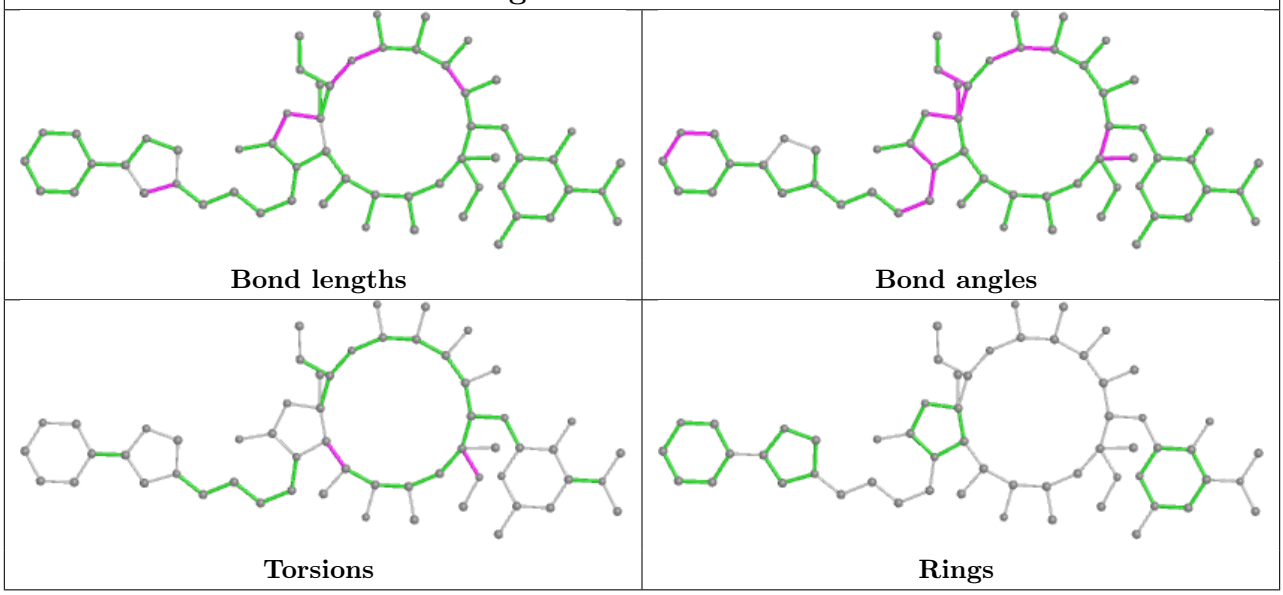
Mol	Chain	Res	Type	Atoms
59	2A	3845	TEL	C34-C28-O32-C38
59	2A	3845	TEL	C1-C2-C4-O9
59	2A	3845	TEL	C3-C2-C4-O9
59	2A	3845	TEL	O9-C4-C8-C14
59	1A	4076	TEL	N6-C3-C7-C12
59	1A	4076	TEL	C34-C28-O32-C38

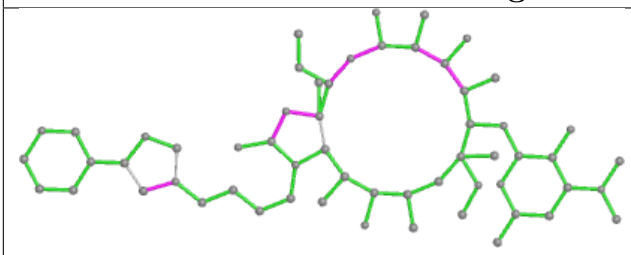
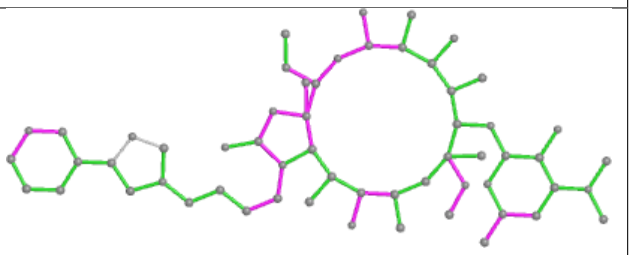
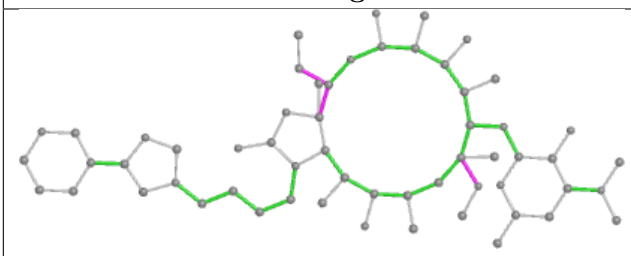
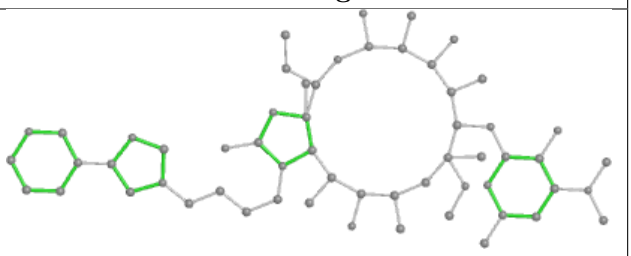
There are no ring outliers.

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 TEL 1A 4076



Ligand TEL 2A 3845	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1A	2860/2915 (98%)	0.36	66 (2%)	60	54	18, 34, 91, 102	0
1	2A	2789/2915 (95%)	0.27	90 (3%)	47	40	27, 51, 88, 101	0
2	1B	120/121 (99%)	0.04	0	100	100	29, 46, 60, 87	0
2	2B	120/121 (99%)	-0.22	0	100	100	55, 68, 78, 87	0
3	1D	275/276 (99%)	0.44	0	100	100	19, 34, 47, 70	0
3	2D	275/276 (99%)	0.63	7 (2%)	57	51	26, 45, 58, 78	0
4	1E	204/206 (99%)	0.34	0	100	100	19, 38, 57, 67	0
4	2E	204/206 (99%)	0.42	7 (3%)	45	38	30, 53, 66, 78	0
5	1F	203/210 (96%)	0.26	0	100	100	19, 40, 62, 79	0
5	2F	203/210 (96%)	0.33	3 (1%)	73	70	30, 61, 73, 80	0
6	1G	181/182 (99%)	0.15	1 (0%)	89	88	35, 54, 70, 76	0
6	2G	181/182 (99%)	0.61	13 (7%)	15	11	56, 71, 78, 82	0
7	1H	174/180 (96%)	0.17	0	100	100	35, 52, 64, 68	0
7	2H	174/180 (96%)	0.96	26 (14%)	2	1	59, 76, 82, 90	0
8	1I	146/148 (98%)	-0.13	0	100	100	39, 66, 75, 81	0
8	2I	146/148 (98%)	0.39	10 (6%)	17	12	53, 67, 77, 80	0
9	1N	140/140 (100%)	0.33	0	100	100	23, 38, 59, 67	0
9	2N	140/140 (100%)	0.50	6 (4%)	35	28	38, 56, 70, 80	0
10	1O	122/122 (100%)	0.27	0	100	100	27, 38, 54, 59	0
10	2O	122/122 (100%)	0.48	2 (1%)	72	68	38, 50, 65, 72	0
11	1P	149/150 (99%)	0.32	0	100	100	20, 42, 64, 69	0
11	2P	149/150 (99%)	0.66	6 (4%)	38	31	34, 60, 75, 87	0
12	1Q	141/141 (100%)	0.34	1 (0%)	87	86	23, 39, 55, 67	0
12	2Q	141/141 (100%)	0.77	12 (8%)	10	7	38, 57, 68, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.31	0	100	100	25, 34, 47, 57	0
13	2R	118/118 (100%)	0.43	1 (0%)	86	84	34, 47, 56, 61	0
14	1S	110/112 (98%)	0.15	0	100	100	37, 46, 57, 66	0
14	2S	110/112 (98%)	0.19	0	100	100	55, 64, 71, 75	0
15	1T	131/146 (89%)	0.29	0	100	100	30, 42, 64, 73	0
15	2T	131/146 (89%)	0.32	1 (0%)	86	84	43, 55, 68, 74	0
16	1U	116/118 (98%)	0.41	0	100	100	19, 30, 47, 60	0
16	2U	116/118 (98%)	0.46	3 (2%)	56	50	39, 53, 67, 74	0
17	1V	101/101 (100%)	0.19	0	100	100	22, 39, 54, 63	0
17	2V	101/101 (100%)	0.29	0	100	100	38, 63, 70, 80	0
18	1W	112/113 (99%)	0.33	0	100	100	22, 31, 47, 74	0
18	2W	112/113 (99%)	0.56	2 (1%)	68	64	33, 45, 61, 78	0
19	1X	95/96 (98%)	0.27	0	100	100	24, 35, 55, 69	0
19	2X	95/96 (98%)	0.51	4 (4%)	36	29	39, 53, 68, 76	0
20	1Y	107/110 (97%)	0.16	0	100	100	34, 46, 61, 75	0
20	2Y	107/110 (97%)	0.66	7 (6%)	18	14	54, 65, 76, 85	0
21	1Z	154/206 (74%)	0.20	3 (1%)	66	62	41, 61, 78, 84	0
21	2Z	160/206 (77%)	0.44	12 (7%)	14	10	55, 73, 84, 88	0
22	10	83/85 (97%)	0.38	0	100	100	26, 35, 47, 60	0
22	20	83/85 (97%)	0.64	1 (1%)	79	76	36, 54, 63, 68	0
23	11	97/98 (98%)	0.42	2 (2%)	63	58	26, 42, 64, 72	0
23	21	97/98 (98%)	0.82	7 (7%)	15	11	38, 54, 70, 73	0
24	12	70/72 (97%)	0.19	0	100	100	32, 45, 57, 65	0
24	22	70/72 (97%)	0.30	1 (1%)	75	71	53, 63, 72, 85	0
25	13	59/60 (98%)	0.20	0	100	100	22, 35, 56, 67	0
25	23	59/60 (98%)	1.00	7 (11%)	4	3	44, 57, 72, 81	0
26	14	69/71 (97%)	0.06	0	100	100	49, 71, 81, 84	0
26	24	69/71 (97%)	0.77	7 (10%)	7	4	72, 80, 88, 90	0
27	15	59/60 (98%)	0.33	1 (1%)	70	66	21, 33, 52, 57	0
27	25	59/60 (98%)	0.32	1 (1%)	70	66	30, 46, 62, 74	0
28	16	53/54 (98%)	0.24	0	100	100	32, 42, 52, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.57	3 (5%)	23	18	45, 55, 63, 65	0
29	17	48/49 (97%)	0.67	3 (6%)	20	15	21, 26, 49, 58	0
29	27	48/49 (97%)	0.93	4 (8%)	11	8	30, 38, 56, 64	0
30	18	64/65 (98%)	0.41	0	100	100	25, 32, 40, 48	0
30	28	64/65 (98%)	0.97	3 (4%)	31	25	40, 49, 55, 61	0
31	19	37/37 (100%)	0.57	0	100	100	26, 37, 53, 60	0
31	29	37/37 (100%)	1.11	6 (16%)	1	1	49, 59, 69, 72	0
32	1a	1488/1521 (97%)	0.09	15 (1%)	82	80	31, 58, 86, 99	0
32	2a	1491/1521 (98%)	0.12	25 (1%)	70	66	43, 70, 88, 101	0
33	1b	231/256 (90%)	0.03	2 (0%)	84	82	56, 71, 81, 88	0
33	2b	231/256 (90%)	0.39	10 (4%)	35	28	65, 76, 82, 85	0
34	1c	206/239 (86%)	0.38	6 (2%)	51	45	52, 63, 75, 81	0
34	2c	206/239 (86%)	0.64	17 (8%)	11	8	64, 75, 82, 87	0
35	1d	208/209 (99%)	0.72	18 (8%)	10	7	46, 61, 70, 74	0
35	2d	208/209 (99%)	0.49	9 (4%)	35	28	55, 68, 75, 79	0
36	1e	148/162 (91%)	0.47	3 (2%)	65	60	45, 57, 67, 75	0
36	2e	148/162 (91%)	0.65	6 (4%)	37	30	60, 69, 76, 81	0
37	1f	100/101 (99%)	0.06	0	100	100	46, 57, 66, 69	0
37	2f	100/101 (99%)	0.11	0	100	100	51, 63, 69, 76	0
38	1g	155/156 (99%)	0.27	7 (4%)	33	26	55, 65, 78, 86	0
38	2g	155/156 (99%)	1.03	24 (15%)	2	1	63, 73, 80, 86	0
39	1h	137/138 (99%)	0.35	3 (2%)	62	56	51, 60, 67, 76	0
39	2h	137/138 (99%)	0.86	21 (15%)	2	1	61, 69, 75, 82	0
40	1i	127/128 (99%)	0.33	6 (4%)	31	25	49, 69, 76, 80	0
40	2i	127/128 (99%)	1.66	45 (35%)	0	0	66, 77, 83, 87	0
41	1j	97/105 (92%)	0.33	7 (7%)	15	11	51, 69, 79, 82	0
41	2j	96/105 (91%)	1.37	24 (25%)	0	0	65, 78, 84, 86	0
42	1k	114/129 (88%)	0.37	3 (2%)	56	50	39, 62, 71, 73	0
42	2k	114/129 (88%)	0.62	8 (7%)	16	12	50, 66, 74, 79	0
43	1l	121/132 (91%)	0.33	2 (1%)	70	66	36, 45, 59, 68	0
43	2l	121/132 (91%)	0.61	5 (4%)	37	30	48, 59, 67, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.21	3 (2%) 59 53	45, 64, 72, 81	0
44	2m	122/126 (96%)	1.17	22 (18%) 1 0	63, 75, 81, 84	0
45	1n	60/61 (98%)	1.07	8 (13%) 3 2	51, 59, 66, 72	0
45	2n	60/61 (98%)	2.34	32 (53%) 0 0	68, 76, 81, 82	0
46	1o	88/89 (98%)	0.36	2 (2%) 60 54	41, 58, 68, 71	0
46	2o	88/89 (98%)	0.46	3 (3%) 45 38	54, 65, 74, 76	0
47	1p	82/88 (93%)	0.97	11 (13%) 3 2	53, 62, 69, 75	0
47	2p	82/88 (93%)	0.51	1 (1%) 79 76	51, 63, 71, 77	0
48	1q	99/105 (94%)	0.57	4 (4%) 38 31	46, 61, 70, 75	0
48	2q	99/105 (94%)	0.98	14 (14%) 2 1	56, 66, 74, 77	0
49	1r	68/88 (77%)	0.45	0 100 100	49, 59, 69, 74	0
49	2r	68/88 (77%)	0.42	2 (2%) 51 45	56, 65, 75, 79	0
50	1s	83/93 (89%)	-0.04	1 (1%) 79 76	56, 65, 75, 78	0
50	2s	83/93 (89%)	1.14	19 (22%) 0 0	72, 77, 83, 85	0
51	1t	96/106 (90%)	0.80	16 (16%) 1 1	53, 63, 73, 79	0
51	2t	96/106 (90%)	0.77	9 (9%) 8 5	51, 64, 76, 78	0
52	1u	23/27 (85%)	1.39	5 (21%) 0 0	56, 62, 67, 72	0
52	2u	23/27 (85%)	2.32	17 (73%) 0 0	68, 76, 78, 80	0
53	1v	13/24 (54%)	1.21	2 (15%) 2 1	40, 46, 87, 94	0
53	2v	13/24 (54%)	2.15	5 (38%) 0 0	57, 65, 89, 102	0
54	1w	66/76 (86%)	0.57	7 (10%) 6 4	23, 78, 90, 96	0
54	2w	64/76 (84%)	1.06	10 (15%) 2 1	38, 84, 91, 98	0
55	1x	71/77 (92%)	0.14	0 100 100	21, 54, 76, 83	0
55	2x	71/77 (92%)	0.01	1 (1%) 75 71	34, 67, 81, 91	0
56	1y	67/76 (88%)	2.41	37 (55%) 0 0	58, 93, 98, 99	0
56	2y	66/76 (86%)	3.87	61 (92%) 0 0	68, 95, 99, 102	0
All	All	20871/21748 (95%)	0.40	887 (4%) 36 29	18, 57, 82, 102	0

All (887) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	18.6
44	2m	123	ALA	17.5

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Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	11.0
56	2y	36	A	9.8
54	2w	71	G	9.4
53	2v	12	A	9.4
38	2g	80	VAL	9.1
38	2g	154	TYR	9.1
56	2y	35	A	8.9
56	2y	34	G	8.5
54	1w	70	G	8.3
1	2A	2146	C	7.5
44	2m	122	LYS	7.4
38	2g	81	GLY	7.3
40	2i	109	VAL	7.3
54	2w	70	G	7.3
56	1y	36	A	7.1
38	2g	82	GLY	7.0
56	1y	34	G	6.9
32	2a	1030(B)	C	6.8
56	2y	73	A	6.6
1	2A	2145	C	6.6
45	2n	25	VAL	6.6
1	2A	2111	C	6.5
56	2y	74	C	6.5
56	1y	35	A	6.4
56	2y	1	G	6.3
21	2Z	144	LEU	6.2
1	2A	2147	G	6.2
38	1g	80	VAL	6.2
44	1m	123	ALA	6.1
38	2g	79	ARG	6.0
45	2n	38	GLY	5.9
23	11	2	SER	5.8
1	2A	2128	C	5.8
1	1A	2130	U	5.8
3	2D	2	ALA	5.7
56	2y	15	G	5.7
1	2A	883	G	5.7
54	2w	72	C	5.7
1	2A	2144	U	5.6
40	2i	36	TYR	5.6
1	2A	2129	C	5.6
32	2a	1030(A)	G	5.5

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Mol	Chain	Res	Type	RSRZ
56	2y	14	A	5.5
42	2k	25	TYR	5.5
56	2y	29	G	5.4
31	29	37	GLY	5.4
1	2A	2155	G	5.4
1	1A	2803	C	5.3
1	2A	2174	C	5.3
1	1A	2129	C	5.3
56	2y	72	C	5.2
45	2n	2	ALA	5.2
44	2m	120	LYS	5.2
54	2w	73	A	5.2
1	1A	2132	U	5.2
45	2n	22	THR	5.1
56	2y	71	G	5.1
45	2n	42	ILE	5.1
1	2A	2802	G	5.1
56	2y	12	U	5.1
41	2j	38	ILE	5.0
32	2a	1532	U	5.0
32	1a	1036	G	5.0
1	1A	2141	G	4.9
1	2A	2143	C	4.9
29	27	47	ARG	4.9
56	2y	2	C	4.9
1	2A	2127	G	4.9
40	2i	125	TYR	4.9
56	1y	5	G	4.9
41	2j	65	LEU	4.9
23	21	2	SER	4.9
1	1A	884	C	4.8
29	27	1	MET	4.8
44	2m	102	ARG	4.8
44	2m	121	LYS	4.8
26	24	50	VAL	4.7
56	2y	6	G	4.7
56	2y	62	C	4.7
38	2g	156	TRP	4.7
1	2A	2112	G	4.7
1	1A	2115	G	4.7
45	2n	29	ARG	4.7
1	1A	2146	C	4.7

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Mol	Chain	Res	Type	RSRZ
56	1y	20	U	4.7
56	2y	76	A	4.7
56	2y	22	G	4.6
1	2A	2154	G	4.6
1	2A	888	C	4.6
45	2n	34	TYR	4.6
45	2n	39	LEU	4.6
1	2A	884	C	4.6
56	2y	44	G	4.5
56	2y	65	G	4.5
45	1n	2	ALA	4.5
1	1A	2145	C	4.5
21	1Z	1	MET	4.5
1	2A	2123	G	4.5
56	2y	75	C	4.5
40	2i	9	ARG	4.5
56	2y	33	U	4.5
1	2A	2142	C	4.5
52	2u	11	GLY	4.5
52	2u	16	GLY	4.5
1	2A	2113	U	4.4
26	24	51	ASP	4.4
34	2c	184	TYR	4.4
1	2A	885	C	4.4
50	2s	84	GLY	4.4
52	2u	17	THR	4.4
56	2y	25	C	4.4
1	1A	2112	G	4.4
56	2y	28	G	4.4
45	2n	35	ARG	4.4
53	2v	14	A	4.4
1	2A	2100	G	4.4
44	2m	23	TYR	4.4
32	2a	1257	U	4.3
56	2y	70	G	4.3
38	2g	78	ARG	4.3
56	1y	24	G	4.3
56	2y	53	G	4.3
41	2j	85	LEU	4.3
1	1A	2131	G	4.3
1	2A	2133	G	4.3
56	2y	26	A	4.3

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Mol	Chain	Res	Type	RSRZ
1	2A	2160	G	4.3
56	2y	31	A	4.2
40	2i	128	ARG	4.2
1	1A	896	A	4.2
1	1A	2160	G	4.2
43	2l	64	TYR	4.2
1	1A	2181	G	4.2
1	2A	2166	G	4.2
1	2A	2167	U	4.2
54	1w	71	G	4.2
41	2j	66	ARG	4.2
32	1a	1257	U	4.2
1	1A	2143	C	4.2
1	2A	2181	G	4.1
21	2Z	155	LEU	4.1
41	2j	71	LEU	4.1
33	2b	165	VAL	4.1
1	2A	2803	C	4.1
1	1A	2161	C	4.1
1	2A	2159	G	4.1
56	2y	57	G	4.1
56	2y	24	G	4.1
1	2A	2115	G	4.1
1	2A	2141	G	4.1
34	2c	154	SER	4.1
26	24	49	PHE	4.1
20	2Y	1	MET	4.1
1	1A	2140	C	4.1
1	2A	2175	C	4.1
56	2y	52	G	4.1
41	2j	88	LEU	4.0
56	2y	10	G	4.0
50	2s	80	TYR	4.0
54	2w	4	C	4.0
40	2i	7	THR	4.0
56	2y	45	U	4.0
46	2o	60	VAL	4.0
1	2A	2117	A	4.0
1	2A	2109	U	4.0
56	2y	38	A	3.9
47	1p	19	ILE	3.9
1	2A	2168	G	3.9

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Mol	Chain	Res	Type	RSRZ
1	1A	885	C	3.9
34	2c	157	ILE	3.9
1	1A	2108	C	3.9
45	2n	31	ARG	3.9
1	1A	2159	G	3.9
56	1y	75	C	3.9
45	2n	12	ARG	3.9
53	1v	12	A	3.9
40	2i	115	GLY	3.8
53	1v	13	A	3.8
3	2D	38	LYS	3.8
29	17	48	LYS	3.8
32	2a	1030(C)	G	3.8
56	2y	23	A	3.8
38	2g	83	ALA	3.7
56	1y	1	G	3.7
40	2i	66	ARG	3.7
7	2H	105	LEU	3.7
33	2b	215	LEU	3.7
7	2H	6	ARG	3.7
48	1q	36	ILE	3.7
1	2A	2116	G	3.7
40	2i	40	LEU	3.7
1	2A	2162	G	3.7
1	2A	2182	G	3.7
32	1a	1030(A)	G	3.7
51	1t	18	GLN	3.7
56	2y	27	G	3.7
35	1d	120	LEU	3.6
38	2g	32	ARG	3.6
1	2A	2110	G	3.6
53	2v	13	A	3.6
21	2Z	149	SER	3.6
38	1g	79	ARG	3.6
7	2H	169	VAL	3.6
41	2j	72	VAL	3.6
1	1A	2109	U	3.6
1	2A	2101	G	3.6
56	1y	57	G	3.6
40	2i	102	LEU	3.6
1	2A	1026	U	3.6
52	2u	21	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
54	1w	72	C	3.6
19	2X	92	LEU	3.5
1	1A	2111	C	3.5
32	2a	1034	G	3.5
38	2g	40	ALA	3.5
1	2A	2173	A	3.5
1	1A	2174	C	3.5
40	2i	90	PRO	3.5
40	2i	19	LEU	3.5
41	2j	40	LEU	3.5
47	1p	1	MET	3.5
35	1d	111	ALA	3.5
56	1y	47	U	3.5
40	2i	121	ARG	3.5
34	2c	159	GLY	3.5
50	2s	12	ASP	3.5
32	2a	1031	G	3.5
56	2y	61	C	3.5
26	24	57	GLU	3.5
35	1d	138	TYR	3.5
48	2q	22	LEU	3.5
56	2y	64	A	3.4
1	2A	2104	G	3.4
45	2n	6	LEU	3.4
45	2n	37	PHE	3.4
40	1i	114	TYR	3.4
21	2Z	126	VAL	3.4
40	2i	127	LYS	3.4
41	2j	44	VAL	3.4
56	1y	56	C	3.4
52	2u	22	ARG	3.4
16	2U	2	PRO	3.4
1	1A	2135	A	3.4
32	2a	1531	A	3.4
21	2Z	96	VAL	3.4
26	24	55	ARG	3.4
7	2H	35	VAL	3.4
40	2i	30	GLY	3.4
44	2m	91	ARG	3.4
56	1y	38	A	3.4
39	2h	134	ILE	3.3
48	2q	90	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
39	2h	93	VAL	3.3
56	2y	5	G	3.3
32	1a	1030(B)	C	3.3
39	2h	2	LEU	3.3
51	2t	13	LEU	3.3
12	2Q	6	ARG	3.3
35	2d	115	ARG	3.3
42	1k	126	ARG	3.3
12	2Q	47	ILE	3.3
29	27	48	LYS	3.3
50	2s	30	LEU	3.3
38	2g	85	TYR	3.3
45	2n	7	ILE	3.3
1	1A	2138	C	3.2
56	2y	68	C	3.2
40	2i	4	TYR	3.2
41	2j	74	ILE	3.2
51	1t	55	ILE	3.2
52	2u	13	ILE	3.2
44	2m	66	LEU	3.2
39	2h	58	TYR	3.2
54	1w	44	G	3.2
7	2H	115	VAL	3.2
8	2I	18	VAL	3.2
43	2l	32	PHE	3.2
56	2y	13	C	3.2
38	2g	22	LEU	3.2
50	2s	15	LEU	3.2
1	2A	2120	G	3.2
8	2I	1	MET	3.2
56	1y	13	C	3.2
7	2H	145	ALA	3.2
19	2X	69	TYR	3.2
6	2G	29	TRP	3.1
39	2h	112	LEU	3.1
40	2i	124	GLN	3.1
50	2s	71	LEU	3.1
56	1y	33	U	3.1
50	2s	68	GLY	3.1
9	2N	116	LEU	3.1
7	2H	123	PHE	3.1
1	2A	2130	U	3.1

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Mol	Chain	Res	Type	RSRZ
32	1a	1532	U	3.1
32	2a	1202	G	3.1
31	29	17	ILE	3.1
52	2u	12	LYS	3.1
50	2s	50	ALA	3.1
45	2n	23	ARG	3.1
41	2j	58	ASP	3.1
52	2u	23	PRO	3.1
1	2A	882	G	3.1
40	2i	41	VAL	3.1
7	2H	103	LEU	3.1
35	1d	3	ARG	3.1
39	2h	83	ILE	3.1
1	2A	2165	G	3.0
23	21	98	LEU	3.0
35	1d	157	LEU	3.0
40	2i	43	ALA	3.0
1	2A	2108	C	3.0
1	2A	2138	C	3.0
40	2i	28	VAL	3.0
35	1d	101	LEU	3.0
1	2A	881	G	3.0
35	1d	158	ILE	3.0
56	1y	22	G	3.0
1	1A	1096	A	3.0
1	1A	2144	U	3.0
7	2H	107	VAL	3.0
52	2u	9	ARG	3.0
48	2q	39	SER	3.0
35	2d	164	ALA	3.0
38	1g	85	TYR	3.0
1	2A	2139	C	3.0
34	2c	196	LEU	3.0
56	1y	12	U	3.0
41	2j	32	ALA	3.0
12	2Q	33	GLY	3.0
23	21	28	GLY	3.0
40	2i	114	TYR	3.0
39	2h	9	MET	3.0
56	2y	30	G	3.0
40	2i	108	VAL	3.0
1	1A	1064	C	3.0

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Mol	Chain	Res	Type	RSRZ
1	1A	2142	C	3.0
1	2A	2148	G	3.0
1	2A	2804	C	3.0
21	1Z	51	ALA	3.0
11	2P	15	ARG	3.0
1	2A	896	A	3.0
50	2s	79	THR	3.0
7	2H	113	VAL	3.0
25	23	29	ARG	3.0
1	2A	2793	G	2.9
4	2E	134	ILE	2.9
56	2y	3	C	2.9
34	2c	193	TYR	2.9
54	1w	69	G	2.9
56	2y	21	A	2.9
50	2s	76	PRO	2.9
56	1y	19	G	2.9
50	2s	53	ASN	2.9
12	2Q	104	PHE	2.9
40	2i	56	LEU	2.9
40	2i	76	ALA	2.9
51	1t	43	LEU	2.9
6	2G	146	TYR	2.9
36	2e	10	MET	2.9
40	2i	65	VAL	2.9
41	2j	34	VAL	2.9
29	17	45	ALA	2.9
40	2i	13	ALA	2.9
40	2i	75	ASP	2.9
45	2n	11	LYS	2.9
8	2I	117	GLU	2.9
1	1A	2158	A	2.9
41	2j	55	LYS	2.9
47	1p	21	VAL	2.9
45	2n	26	ARG	2.9
45	2n	53	LEU	2.9
38	2g	5	ARG	2.9
40	2i	14	VAL	2.9
40	2i	120	ARG	2.9
56	1y	29	G	2.9
1	2A	2158	A	2.8
1	2A	886	C	2.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2161	C	2.8
47	1p	2	VAL	2.8
56	1y	71	G	2.8
32	1a	1286	A	2.8
38	2g	41	ARG	2.8
39	2h	107	LEU	2.8
45	2n	41	ARG	2.8
1	1A	897	C	2.8
7	2H	102	ALA	2.8
52	2u	6	ARG	2.8
1	1A	2162	G	2.8
33	2b	121	LEU	2.8
54	2w	5	G	2.8
56	1y	53	G	2.8
51	1t	9	ASN	2.8
56	1y	62	C	2.8
33	2b	187	LEU	2.8
35	1d	135	LEU	2.8
54	1w	20	U	2.8
56	2y	47	U	2.8
1	1A	2133	G	2.8
8	2I	13	GLY	2.8
25	23	51	ALA	2.8
32	1a	1531	A	2.8
32	2a	1061	G	2.8
45	1n	10	ALA	2.8
56	1y	74	C	2.8
42	2k	109	VAL	2.8
1	2A	898	C	2.8
1	2A	2164	C	2.8
1	2A	2183	C	2.8
41	2j	36	GLY	2.8
1	2A	2118	U	2.8
38	1g	156	TRP	2.8
1	1A	2182	G	2.8
32	2a	1036	G	2.8
44	2m	87	TYR	2.7
16	2U	20	LEU	2.7
25	23	53	LEU	2.7
33	2b	139	LYS	2.7
41	2j	47	PHE	2.7
40	2i	63	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
46	2o	89	GLY	2.7
41	1j	60	ARG	2.7
1	2A	2119	A	2.7
1	1A	2180	U	2.7
11	2P	51	PHE	2.7
39	2h	122	ARG	2.7
40	2i	6	GLY	2.7
40	2i	57	GLY	2.7
36	2e	21	ALA	2.7
56	2y	42	C	2.7
52	1u	13	ILE	2.7
47	1p	7	ALA	2.7
1	1A	2136	C	2.7
56	2y	4	C	2.7
56	1y	27	G	2.7
56	1y	63	G	2.7
1	2A	2179	C	2.7
56	1y	25	C	2.7
1	1A	2114	A	2.7
51	2t	63	ILE	2.7
56	2y	63	G	2.7
47	1p	27	LYS	2.7
35	2d	70	ILE	2.7
1	1A	2178	C	2.7
1	2A	2114	A	2.7
56	1y	23	A	2.7
7	2H	48	GLY	2.7
51	2t	26	ASN	2.7
4	2E	52	LEU	2.7
7	2H	46	GLU	2.7
48	2q	32	TYR	2.7
1	1A	1094	U	2.6
27	15	60	VAL	2.6
44	2m	92	HIS	2.6
20	2Y	5	MET	2.6
6	2G	152	LEU	2.6
32	2a	1224	G	2.6
20	2Y	55	TYR	2.6
31	29	26	ILE	2.6
52	2u	18	TYR	2.6
35	2d	90	GLY	2.6
36	1e	69	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
51	1t	16	HIS	2.6
56	2y	40	C	2.6
35	1d	162	LEU	2.6
1	2A	2169	A	2.6
56	1y	21	A	2.6
21	2Z	93	ASP	2.6
30	28	16	ILE	2.6
32	1a	1003	G	2.6
32	2a	1021	G	2.6
33	2b	211	ILE	2.6
50	2s	31	ILE	2.6
52	1u	17	THR	2.6
44	2m	96	LEU	2.6
48	2q	98	LEU	2.6
56	2y	11	C	2.6
41	2j	6	ILE	2.6
53	2v	15	A	2.6
12	2Q	121	ALA	2.6
1	2A	2156	G	2.6
32	1a	1030(C)	G	2.6
56	2y	18	G	2.6
45	2n	36	PHE	2.6
45	2n	61	TRP	2.6
1	1A	2117	A	2.6
12	2Q	5	ARG	2.6
28	26	20	ASN	2.6
29	17	47	ARG	2.6
42	2k	117	ASN	2.6
40	2i	53	VAL	2.6
25	23	23	LEU	2.6
46	2o	57	LEU	2.6
45	1n	16	PHE	2.6
54	2w	69	G	2.6
20	2Y	54	LYS	2.6
7	2H	47	GLU	2.6
56	1y	51	U	2.6
1	2A	2896	C	2.6
10	2O	65	THR	2.6
44	2m	103	THR	2.6
34	2c	198	VAL	2.6
1	2A	2801(A)	A	2.6
41	2j	57	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
45	2n	46	GLU	2.6
32	1a	204	U	2.6
6	2G	39	ILE	2.6
7	2H	36	PRO	2.6
1	1A	2804	C	2.6
11	2P	149	GLU	2.6
1	2A	2126	A	2.6
6	2G	2	PRO	2.5
48	2q	26	GLN	2.5
34	2c	160	ALA	2.5
1	2A	2121	G	2.5
36	2e	12	LEU	2.5
1	2A	1509	C	2.5
34	2c	205	GLY	2.5
38	2g	155	ARG	2.5
48	1q	27	PHE	2.5
49	2r	87	ARG	2.5
33	1b	188	ALA	2.5
39	2h	124	ALA	2.5
23	21	71	TYR	2.5
7	2H	49	VAL	2.5
38	2g	4	ARG	2.5
12	2Q	1	MET	2.5
40	1i	117	HIS	2.5
21	2Z	125	LEU	2.5
38	1g	81	GLY	2.5
34	1c	100	ALA	2.5
34	2c	4	LYS	2.5
38	2g	7	ALA	2.5
38	2g	10	ARG	2.5
47	1p	59	TRP	2.5
21	1Z	165	VAL	2.5
39	2h	79	VAL	2.5
48	2q	42	TYR	2.5
1	1A	1026	U	2.5
1	1A	2801(A)	A	2.5
1	2A	2170	A	2.5
32	2a	1030(D)	A	2.5
1	2A	2125	G	2.5
7	2H	72	ILE	2.5
32	1a	1001(A)	G	2.5
40	2i	52	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
51	1t	76	ALA	2.5
56	1y	2	C	2.5
39	2h	133	LEU	2.5
1	1A	2189	U	2.5
32	1a	1000	U	2.5
32	2a	1219	U	2.5
48	2q	87	LYS	2.5
1	1A	2170	A	2.5
7	2H	128	PRO	2.5
45	1n	18	VAL	2.5
1	1A	2793	G	2.5
7	2H	148	ILE	2.5
51	2t	20	LEU	2.5
56	2y	58	A	2.5
1	1A	888	C	2.5
22	20	54	GLY	2.4
40	2i	8	GLY	2.4
56	2y	50	U	2.4
34	2c	199	LYS	2.4
44	2m	105	THR	2.4
40	1i	19	LEU	2.4
33	2b	71	VAL	2.4
35	1d	110	PHE	2.4
51	2t	80	ARG	2.4
1	1A	2137	C	2.4
51	1t	47	GLY	2.4
33	2b	133	LYS	2.4
34	1c	200	ALA	2.4
51	2t	16	HIS	2.4
6	2G	43	LEU	2.4
6	2G	151	ALA	2.4
3	2D	155	LEU	2.4
9	2N	112	LEU	2.4
36	1e	119	LEU	2.4
39	2h	111	ILE	2.4
54	2w	45	U	2.4
40	2i	126	SER	2.4
8	2I	3	VAL	2.4
36	2e	55	VAL	2.4
39	2h	64	LYS	2.4
45	2n	15	LYS	2.4
50	2s	34	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
35	2d	165	MET	2.4
1	2A	2134	A	2.4
1	2A	2135	A	2.4
11	2P	31	ALA	2.4
23	11	98	LEU	2.4
27	25	2	ALA	2.4
34	2c	87	LEU	2.4
48	2q	36	ILE	2.4
43	1l	64	TYR	2.4
52	1u	18	TYR	2.4
44	2m	97	PRO	2.4
41	1j	57	LYS	2.4
34	2c	124	ILE	2.4
51	2t	19	SER	2.4
40	2i	105	ASP	2.4
1	1A	2128	C	2.4
23	21	30	VAL	2.4
6	2G	136	ARG	2.4
12	1Q	59	ARG	2.4
19	2X	68	ARG	2.4
40	2i	5	TYR	2.4
50	2s	52	TYR	2.4
8	2I	4	ILE	2.4
16	2U	43	GLY	2.4
41	1j	47	PHE	2.4
52	1u	14	TRP	2.4
7	2H	51	ARG	2.4
40	2i	110	GLU	2.4
54	2w	2	C	2.4
7	2H	157	TYR	2.4
11	2P	45	LEU	2.4
34	2c	60	ALA	2.4
1	1A	2110	G	2.4
1	2A	2149	G	2.4
3	2D	270	ILE	2.4
10	2O	1	MET	2.3
32	2a	1223	C	2.3
47	1p	38	TYR	2.3
39	1h	112	LEU	2.3
52	2u	5	ASP	2.3
30	28	29	LYS	2.3
35	2d	158	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
56	2y	69	G	2.3
1	1A	2167	U	2.3
3	2D	276	LYS	2.3
38	2g	153	HIS	2.3
46	1o	56	LEU	2.3
51	1t	95	ALA	2.3
56	2y	43	C	2.3
56	2y	67	C	2.3
6	2G	3	LEU	2.3
7	2H	71	LEU	2.3
44	2m	72	ALA	2.3
51	2t	24	LEU	2.3
52	2u	2	GLY	2.3
34	2c	22	TRP	2.3
44	2m	6	GLY	2.3
45	2n	21	TYR	2.3
56	2y	60	U	2.3
32	2a	1026	G	2.3
32	2a	1033	G	2.3
56	1y	70	G	2.3
1	1A	898	C	2.3
8	2I	21	VAL	2.3
32	2a	1030	C	2.3
48	2q	23	VAL	2.3
1	2A	229	A	2.3
32	2a	1035	A	2.3
41	2j	48	THR	2.3
41	2j	67	THR	2.3
40	2i	10	ARG	2.3
56	1y	28	G	2.3
56	2y	56	C	2.3
7	2H	98	LEU	2.3
36	2e	20	GLN	2.3
1	2A	2150	U	2.3
23	21	13	ILE	2.3
42	2k	32	ILE	2.3
42	2k	125	PHE	2.3
29	27	46	VAL	2.3
47	1p	62	VAL	2.3
47	2p	2	VAL	2.3
55	2x	47	U	2.3
1	2A	2124	G	2.3

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Mol	Chain	Res	Type	RSRZ
25	23	26	LEU	2.3
41	1j	62	HIS	2.3
45	2n	14	PRO	2.3
45	2n	32	SER	2.3
45	1n	13	THR	2.3
50	2s	77	THR	2.3
56	1y	14	A	2.3
28	26	28	ARG	2.3
4	2E	77	ILE	2.3
21	2Z	141	VAL	2.3
45	2n	18	VAL	2.3
45	2n	28	GLY	2.2
46	1o	55	GLY	2.2
8	2I	75	LEU	2.2
18	2W	14	PRO	2.2
1	2A	2105	C	2.2
34	1c	193	TYR	2.2
12	2Q	66	ILE	2.2
34	2c	182	ILE	2.2
41	2j	12	ASP	2.2
44	2m	78	ILE	2.2
1	2A	2132	U	2.2
1	2A	2897	U	2.2
48	1q	28	PRO	2.2
24	22	8	LYS	2.2
30	28	25	MET	2.2
33	2b	34	ALA	2.2
45	1n	31	ARG	2.2
1	1A	2166	G	2.2
56	1y	52	G	2.2
38	2g	36	LYS	2.2
40	1i	126	SER	2.2
1	2A	1847	A	2.2
6	1G	139	LEU	2.2
32	2a	969	A	2.2
51	1t	75	ASN	2.2
50	1s	71	LEU	2.2
56	1y	31	A	2.2
8	2I	82	ARG	2.2
38	2g	8	GLU	2.2
12	2Q	2	LEU	2.2
38	2g	115	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
39	2h	138	TRP	2.2
51	1t	12	ALA	2.2
20	2Y	29	GLU	2.2
39	2h	99	GLU	2.2
9	2N	140	VAL	2.2
39	1h	134	ILE	2.2
42	2k	126	ARG	2.2
18	2W	82	LEU	2.2
21	2Z	156	LYS	2.2
56	1y	64	A	2.2
6	2G	157	ILE	2.2
9	2N	9	VAL	2.2
39	2h	86	ILE	2.2
35	1d	19	LEU	2.2
41	1j	16	LEU	2.2
7	2H	96	ALA	2.2
42	1k	89	ALA	2.2
32	1a	1446	U	2.2
56	2y	59	U	2.2
1	1A	2101	G	2.2
1	2A	614(B)	G	2.2
32	2a	1032	G	2.2
34	1c	184	TYR	2.2
5	2F	37	VAL	2.2
7	2H	141	VAL	2.2
12	2Q	109	VAL	2.2
39	2h	137	VAL	2.2
1	2A	887	A	2.2
39	1h	133	LEU	2.2
41	2j	56	HIS	2.2
43	2l	5	PRO	2.2
21	2Z	152	ALA	2.2
41	1j	18	ALA	2.2
48	2q	38	ARG	2.2
50	2s	78	ARG	2.2
1	1A	1075	C	2.2
1	1A	1509	C	2.2
26	24	63	TYR	2.1
40	1i	113	LYS	2.1
20	2Y	106	LEU	2.1
26	24	54	GLY	2.1
31	29	12	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
51	2t	66	ALA	2.1
44	2m	106	ASN	2.1
1	2A	897	C	2.1
1	2A	2188	C	2.1
12	2Q	102	VAL	2.1
35	1d	126	ILE	2.1
52	1u	21	TYR	2.1
7	2H	171	LEU	2.1
20	2Y	31	LEU	2.1
38	2g	16	LEU	2.1
48	1q	31	LEU	2.1
35	1d	167	GLY	2.1
48	2q	25	ARG	2.1
1	1A	1095	A	2.1
40	1i	37	PHE	2.1
25	23	50	VAL	2.1
52	2u	8	THR	2.1
1	1A	2792	G	2.1
4	2E	158	GLY	2.1
8	2I	29	TYR	2.1
35	1d	5	ILE	2.1
35	2d	6	GLY	2.1
35	2d	146	ILE	2.1
41	2j	98	ILE	2.1
43	1l	18	VAL	2.1
51	1t	74	LYS	2.1
52	2u	10	ARG	2.1
1	1A	2179	C	2.1
21	2Z	170	THR	2.1
45	1n	61	TRP	2.1
52	2u	14	TRP	2.1
41	2j	11	PHE	2.1
6	2G	160	VAL	2.1
34	2c	155	GLY	2.1
1	1A	2147	G	2.1
35	2d	20	TYR	2.1
39	2h	10	LEU	2.1
3	2D	153	ALA	2.1
5	2F	80	ALA	2.1
56	1y	40	C	2.1
15	2T	111	ARG	2.1
34	1c	83	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
35	1d	118	ARG	2.1
38	2g	76	ARG	2.1
40	2i	33	PHE	2.1
50	2s	13	ASP	2.1
4	2E	4	ILE	2.1
35	1d	170	VAL	2.1
39	2h	129	VAL	2.1
43	2l	55	VAL	2.1
43	2l	48	PRO	2.1
1	2A	2191	G	2.1
12	2Q	114	ALA	2.1
32	1a	1030(D)	A	2.1
32	2a	1001(A)	G	2.1
45	2n	10	ALA	2.1
1	1A	2113	U	2.1
44	2m	104	ARG	2.1
45	1n	3	ARG	2.1
47	1p	28	ARG	2.1
35	1d	180	GLY	2.1
25	23	47	VAL	2.1
33	2b	118	LEU	2.1
45	2n	17	LYS	2.1
45	2n	13	THR	2.1
1	1A	2165	G	2.0
1	2A	2190	G	2.0
44	2m	119	GLY	2.1
54	1w	1	G	2.0
56	1y	26	A	2.1
56	2y	7	A	2.1
1	1A	2188	C	2.0
6	2G	41	GLN	2.0
11	2P	39	LYS	2.0
28	26	11	LEU	2.0
31	29	25	VAL	2.0
32	2a	1218	C	2.0
39	2h	39	LEU	2.0
36	2e	90	VAL	2.0
38	1g	153	HIS	2.0
49	2r	84	LYS	2.0
33	1b	232	PRO	2.0
42	2k	14	VAL	2.0
3	2D	247	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
34	1c	180	ALA	2.0
44	1m	2	ALA	2.0
51	1t	59	ALA	2.0
51	1t	80	ARG	2.0
31	29	1	MET	2.0
41	1j	93	GLY	2.0
47	1p	22	THR	2.0
51	1t	14	LYS	2.0
1	1A	2897	U	2.0
32	1a	841	U	2.0
21	2Z	139	VAL	2.0
42	2k	30	VAL	2.0
50	2s	14	HIS	2.0
9	2N	85	ILE	2.0
32	2a	1027	C	2.0
50	2s	37	ARG	2.0
52	2u	7	ARG	2.0
38	1g	154	TYR	2.0
42	1k	25	TYR	2.0
36	1e	17	ALA	2.0
45	2n	16	PHE	2.0
40	2i	47	LEU	2.0
9	2N	44	PRO	2.0
13	2R	66	VAL	2.0
40	2i	123	PRO	2.0
1	1A	2169	A	2.0
53	2v	23	A	2.0
56	2y	9	A	2.0
1	1A	883	G	2.0
4	2E	157	ALA	2.0
5	2F	49	ALA	2.0
23	21	84	GLY	2.0
40	2i	67	GLY	2.0
44	2m	100	GLY	2.0
54	2w	67	C	2.0
56	2y	41	C	2.0
51	1t	71	THR	2.0
4	2E	51	PHE	2.0
6	2G	155	MET	2.0
19	2X	60	ARG	2.0
40	2i	79	LEU	2.0
35	1d	136	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
48	2q	9	VAL	2.0
48	2q	85	VAL	2.0
51	1t	68	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	4SU	2y	8	20/21	0.62	0.28	95,101,112,124	0
56	7MG	2y	46	24/25	0.71	0.31	88,94,102,113	0
56	7MG	1y	46	24/25	0.73	0.20	84,91,98,114	0
56	PSU	1y	55	20/21	0.73	0.35	87,94,104,113	0
56	5MU	2y	54	21/22	0.73	0.41	87,95,102,121	0
56	MIA	2y	37	22/30	0.78	0.50	75,92,102,116	0
56	PSU	2y	32	20/21	0.79	0.46	82,91,98,103	0
56	PSU	1y	32	20/21	0.79	0.35	80,89,98,105	0
54	7MG	2w	46	24/25	0.80	0.21	74,84,101,121	0
56	PSU	1y	39	20/21	0.80	0.39	79,88,95,97	0
56	5MU	1y	54	21/22	0.81	0.32	85,91,97,114	0
56	4SU	1y	8	20/21	0.81	0.21	88,94,102,115	0
54	7MG	1w	46	24/25	0.82	0.15	73,80,98,118	0
56	PSU	2y	39	20/21	0.83	0.36	86,91,98,108	0
56	PSU	2y	55	20/21	0.83	0.36	89,93,100,109	0
56	MIA	1y	37	22/30	0.85	0.32	76,87,98,106	0
54	4SU	2w	8	20/21	0.86	0.20	75,83,98,102	0
32	2MG	2a	1207	24/25	0.90	0.17	69,74,79,81	0
54	4SU	1w	8	20/21	0.90	0.17	72,78,86,90	0
54	PSU	2w	55	20/21	0.91	0.19	71,78,85,90	0
32	M2G	2a	966	25/26	0.92	0.25	54,61,73,79	0
54	PSU	2w	32	20/21	0.93	0.27	68,72,77,83	0
55	4SU	2x	8	20/21	0.93	0.16	62,67,73,74	0
55	5MU	2x	54	21/22	0.93	0.23	70,75,82,86	0
54	MIA	2w	37	25/30	0.93	0.31	51,66,73,93	0
54	PSU	1w	55	20/21	0.93	0.18	60,67,74,77	0
32	PSU	2a	516	20/21	0.94	0.15	61,68,72,72	0
54	PSU	2w	39	20/21	0.94	0.25	63,69,76,79	0
55	PSU	2x	55	20/21	0.94	0.17	63,70,78,81	0
54	PSU	1w	32	20/21	0.94	0.18	52,60,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	5MC	2a	967	21/22	0.94	0.23	53,63,70,77	0
43	0TD	2l	92	10/11	0.95	0.21	50,56,58,65	0
54	MIA	1w	37	29/30	0.95	0.23	32,44,61,88	0
1	PSU	2A	1917	20/21	0.95	0.17	48,57,60,62	0
55	4SU	1x	8	20/21	0.95	0.20	43,55,66,66	0
55	5MU	1x	54	21/22	0.95	0.17	56,63,66,73	0
55	PSU	1x	55	20/21	0.95	0.17	54,59,69,70	0
54	5MU	2w	54	21/22	0.95	0.18	62,69,74,76	0
32	PSU	1a	516	20/21	0.95	0.17	44,50,54,56	0
32	5MC	2a	1400	21/22	0.95	0.26	58,62,68,70	0
43	0TD	1l	92	10/11	0.96	0.20	38,44,47,48	0
54	5MU	1w	54	21/22	0.96	0.18	43,57,64,68	0
55	5MC	2x	32	21/22	0.96	0.22	63,67,73,75	0
32	5MC	2a	1404	21/22	0.96	0.21	43,52,56,60	0
32	5MC	2a	1407	21/22	0.96	0.23	43,48,51,54	0
1	5MU	2A	1915	21/22	0.96	0.20	50,60,66,71	0
1	5MU	1A	1915	21/22	0.96	0.20	35,43,49,52	0
1	4OC	2A	1920	21/23	0.96	0.18	43,52,56,58	0
32	7MG	1a	527	24/25	0.96	0.15	35,43,51,56	0
32	7MG	2a	527	24/25	0.96	0.20	49,58,64,71	0
55	5MC	1x	32	21/22	0.96	0.21	42,46,52,55	0
32	2MG	1a	1207	24/25	0.96	0.17	52,56,60,63	0
32	5MC	1a	1400	21/22	0.97	0.17	36,42,46,48	0
32	4OC	2a	1402	22/23	0.97	0.19	37,57,59,62	0
32	4OC	1a	1402	22/23	0.97	0.17	35,40,47,51	0
1	PSU	1A	1917	20/21	0.97	0.16	33,40,43,43	0
32	UR3	2a	1498	21/22	0.97	0.23	38,51,56,59	0
32	MA6	2a	1518	24/25	0.97	0.24	46,53,59,60	0
32	MA6	2a	1519	24/25	0.97	0.28	46,54,57,58	0
1	5MC	2A	1962	21/22	0.97	0.21	39,43,51,66	0
32	M2G	1a	966	25/26	0.97	0.19	36,47,53,60	0
32	5MC	1a	967	21/22	0.97	0.20	42,51,56,59	0
1	PSU	1A	1911	20/21	0.97	0.20	37,38,40,45	0
54	PSU	1w	39	20/21	0.97	0.22	46,54,65,69	0
1	PSU	2A	1911	20/21	0.97	0.22	45,58,61,61	0
54	F3N	2w	76	33/34	0.97	0.24	29,35,38,41	0
55	31H	1x	76	32/33	0.97	0.22	13,22,28,29	10
55	31H	2x	76	32/33	0.97	0.21	28,34,37,39	0
1	PSU	1A	2605	20/21	0.98	0.21	18,21,29,30	0
1	4OC	1A	1920	21/23	0.98	0.21	29,35,39,42	0
1	5MU	1A	1939	21/22	0.98	0.23	19,24,29,30	0
1	5MC	1A	1942	21/22	0.98	0.20	29,35,42,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MC	1A	1962	21/22	0.98	0.20	28,34,38,44	0
1	OMG	1A	2251	24/25	0.98	0.21	19,23,26,30	0
1	2MA	1A	2503	23/24	0.98	0.21	16,20,23,28	0
1	2MU	1A	2552	21/23	0.98	0.21	21,26,29,32	0
32	5MC	1a	1404	21/22	0.98	0.20	29,37,39,40	0
32	5MC	1a	1407	21/22	0.98	0.19	29,34,39,42	0
32	MA6	1a	1518	24/25	0.98	0.22	32,37,41,48	0
1	5MU	2A	1939	21/22	0.98	0.19	28,34,37,38	0
1	5MC	2A	1942	21/22	0.98	0.20	42,51,55,62	0
32	MA6	1a	1519	24/25	0.98	0.21	35,39,43,44	0
54	F3N	1w	76	33/34	0.98	0.22	16,20,24,25	0
1	OMG	2A	2251	24/25	0.98	0.21	30,33,40,41	0
1	2MU	2A	2552	21/23	0.98	0.20	33,37,43,45	0
1	PSU	2A	2605	20/21	0.98	0.18	29,32,37,37	0
1	2MA	2A	2503	23/24	0.99	0.22	26,30,34,35	0
32	UR3	1a	1498	21/22	0.99	0.20	31,36,38,43	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2w	108	1/1	0.36	0.17	77,77,77,77	0
57	MG	1w	101	1/1	0.37	0.26	73,73,73,73	0
57	MG	2A	3797	1/1	0.38	0.11	62,62,62,62	0
57	MG	2A	3560	1/1	0.51	0.21	70,70,70,70	0
57	MG	1A	3866	1/1	0.52	0.20	54,54,54,54	0
57	MG	2A	3759	1/1	0.53	0.31	65,65,65,65	0
57	MG	2r	101	1/1	0.54	0.13	65,65,65,65	0
57	MG	2a	1791	1/1	0.54	0.14	64,64,64,64	0
57	MG	1a	1691	1/1	0.55	0.27	59,59,59,59	0
57	MG	1A	3904	1/1	0.55	0.14	57,57,57,57	0
57	MG	1E	309	1/1	0.56	0.30	71,71,71,71	0
57	MG	2A	3052	1/1	0.56	0.32	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	ZN	14	102	1/1	0.58	0.16	136,136,136,136	0
57	MG	1A	3961	1/1	0.59	0.12	65,65,65,65	0
57	MG	2a	1620	1/1	0.59	0.24	72,72,72,72	0
57	MG	2A	3321	1/1	0.60	0.24	67,67,67,67	0
57	MG	2a	1687	1/1	0.60	0.14	64,64,64,64	0
57	MG	1A	3444	1/1	0.60	0.17	59,59,59,59	0
57	MG	1A	3584	1/1	0.63	0.18	62,62,62,62	0
57	MG	1A	4041	1/1	0.63	0.16	57,57,57,57	0
57	MG	2a	1770	1/1	0.64	0.14	71,71,71,71	0
57	MG	2A	3279	1/1	0.64	0.15	64,64,64,64	0
57	MG	2A	3293	1/1	0.64	0.17	69,69,69,69	0
57	MG	1A	3002	1/1	0.64	0.19	58,58,58,58	0
57	MG	1A	3348	1/1	0.64	0.24	54,54,54,54	0
57	MG	2A	3682	1/1	0.65	0.07	60,60,60,60	0
57	MG	2a	1632	1/1	0.65	0.15	71,71,71,71	0
57	MG	1A	3723	1/1	0.66	0.19	46,46,46,46	0
57	MG	1A	4006	1/1	0.66	0.22	51,51,51,51	0
57	MG	2a	1633	1/1	0.66	0.15	54,54,54,54	0
57	MG	1A	4037	1/1	0.66	0.20	53,53,53,53	0
57	MG	2a	1755	1/1	0.66	0.08	83,83,83,83	0
57	MG	1A	3933	1/1	0.67	0.17	59,59,59,59	0
57	MG	2a	1734	1/1	0.67	0.17	67,67,67,67	0
57	MG	2A	3777	1/1	0.67	0.28	60,60,60,60	0
57	MG	2a	1652	1/1	0.67	0.26	60,60,60,60	0
57	MG	1A	4049	1/1	0.68	0.18	55,55,55,55	0
57	MG	2A	3149	1/1	0.68	0.32	56,56,56,56	0
57	MG	2w	107	1/1	0.68	0.19	62,62,62,62	0
57	MG	1A	3929	1/1	0.68	0.13	62,62,62,62	0
57	MG	2A	3587	1/1	0.68	0.17	62,62,62,62	0
57	MG	1A	3362	1/1	0.69	0.23	43,43,43,43	0
57	MG	1A	4021	1/1	0.69	0.14	35,35,35,35	0
57	MG	2A	3033	1/1	0.69	0.58	61,61,61,61	0
57	MG	2n	101	1/1	0.69	0.27	69,69,69,69	0
57	MG	1a	1677	1/1	0.69	0.10	69,69,69,69	0
57	MG	2A	3483	1/1	0.69	0.08	68,68,68,68	0
57	MG	2a	1710	1/1	0.69	0.21	48,48,48,48	0
57	MG	2A	3534	1/1	0.69	0.25	71,71,71,71	0
57	MG	1A	4020	1/1	0.70	0.12	47,47,47,47	0
57	MG	1A	3381	1/1	0.70	0.63	44,44,44,44	0
57	MG	2A	3228	1/1	0.70	0.30	61,61,61,61	0
57	MG	2A	3402	1/1	0.70	0.17	57,57,57,57	0
57	MG	2A	3641	1/1	0.70	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1646	1/1	0.70	0.36	59,59,59,59	0
57	MG	2A	3448	1/1	0.70	0.22	67,67,67,67	0
57	MG	2A	3454	1/1	0.70	0.22	73,73,73,73	0
57	MG	2A	3763	1/1	0.70	0.25	73,73,73,73	0
57	MG	2A	3174	1/1	0.71	0.13	65,65,65,65	0
57	MG	2g	201	1/1	0.71	0.29	72,72,72,72	0
57	MG	1x	103	1/1	0.71	0.29	55,55,55,55	0
57	MG	2a	1724	1/1	0.71	0.34	60,60,60,60	0
57	MG	2A	3769	1/1	0.71	0.19	51,51,51,51	0
57	MG	2A	3335	1/1	0.71	0.21	56,56,56,56	0
57	MG	1A	3463	1/1	0.71	0.39	65,65,65,65	0
57	MG	1A	3763	1/1	0.72	0.12	61,61,61,61	0
57	MG	2a	1744	1/1	0.72	0.11	62,62,62,62	0
57	MG	2A	3581	1/1	0.72	0.13	35,35,35,35	0
57	MG	2A	3340	1/1	0.72	0.16	54,54,54,54	0
57	MG	2A	3593	1/1	0.72	0.14	30,30,30,30	0
57	MG	1A	3247	1/1	0.72	0.17	59,59,59,59	0
57	MG	1A	3203	1/1	0.72	0.13	50,50,50,50	0
57	MG	2A	3757	1/1	0.72	0.14	58,58,58,58	0
57	MG	2A	3317	1/1	0.72	0.19	59,59,59,59	0
57	MG	1A	4028	1/1	0.72	0.08	49,49,49,49	0
57	MG	2A	3325	1/1	0.72	0.14	69,69,69,69	0
57	MG	1A	3277	1/1	0.73	0.32	42,42,42,42	0
57	MG	2a	1773	1/1	0.73	0.15	71,71,71,71	0
57	MG	2a	1658	1/1	0.73	0.18	63,63,63,63	0
57	MG	2a	1806	1/1	0.73	0.23	66,66,66,66	0
57	MG	1b	302	1/1	0.73	0.09	75,75,75,75	0
57	MG	2a	1613	1/1	0.73	0.18	57,57,57,57	0
57	MG	2A	3371	1/1	0.73	0.21	60,60,60,60	0
57	MG	1B	227	1/1	0.73	0.25	77,77,77,77	0
57	MG	2A	3078	1/1	0.73	0.28	62,62,62,62	0
57	MG	2A	3327	1/1	0.73	0.39	58,58,58,58	0
57	MG	1A	3308	1/1	0.74	0.19	52,52,52,52	0
57	MG	2A	3326	1/1	0.74	0.15	69,69,69,69	0
57	MG	1A	3630	1/1	0.74	0.13	60,60,60,60	0
57	MG	2A	3332	1/1	0.74	0.26	75,75,75,75	0
57	MG	1a	1756	1/1	0.74	0.16	70,70,70,70	0
57	MG	2A	3167	1/1	0.74	0.16	73,73,73,73	0
57	MG	2A	3368	1/1	0.74	0.14	59,59,59,59	0
57	MG	1a	1794	1/1	0.74	0.13	61,61,61,61	0
57	MG	2A	3204	1/1	0.74	0.28	58,58,58,58	0
57	MG	2A	3773	1/1	0.74	0.23	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1780	1/1	0.74	0.19	71,71,71,71	0
57	MG	1A	3396	1/1	0.74	0.18	67,67,67,67	0
57	MG	1A	3925	1/1	0.74	0.17	57,57,57,57	0
57	MG	2A	3459	1/1	0.74	0.22	55,55,55,55	0
57	MG	13	103	1/1	0.74	0.26	51,51,51,51	0
57	MG	2a	1630	1/1	0.74	0.19	55,55,55,55	0
57	MG	2A	3512	1/1	0.74	0.18	53,53,53,53	0
57	MG	1x	110	1/1	0.74	0.23	62,62,62,62	0
57	MG	1a	1660	1/1	0.74	0.15	73,73,73,73	0
57	MG	2A	3025	1/1	0.75	0.17	60,60,60,60	0
57	MG	1A	3307	1/1	0.75	0.24	38,38,38,38	0
57	MG	2A	3267	1/1	0.75	0.28	62,62,62,62	0
57	MG	1A	3889	1/1	0.75	0.14	47,47,47,47	0
57	MG	2a	1636	1/1	0.75	0.11	54,54,54,54	0
57	MG	1A	3432	1/1	0.75	0.18	63,63,63,63	0
57	MG	2A	3341	1/1	0.75	0.23	62,62,62,62	0
57	MG	1A	3788	1/1	0.75	0.12	56,56,56,56	0
57	MG	1A	3831	1/1	0.75	0.10	52,52,52,52	0
57	MG	2a	1694	1/1	0.75	0.37	70,70,70,70	0
57	MG	2w	102	1/1	0.75	0.11	75,75,75,75	0
57	MG	2A	3383	1/1	0.75	0.21	62,62,62,62	0
57	MG	2G	201	1/1	0.75	0.12	58,58,58,58	0
57	MG	1a	1710	1/1	0.75	0.21	59,59,59,59	0
57	MG	1A	3349	1/1	0.76	0.29	51,51,51,51	0
57	MG	2a	1623	1/1	0.76	0.19	56,56,56,56	0
57	MG	2A	3706	1/1	0.76	0.10	57,57,57,57	0
57	MG	1A	3240	1/1	0.76	0.19	47,47,47,47	0
57	MG	2A	3278	1/1	0.76	0.28	67,67,67,67	0
57	MG	1A	3885	1/1	0.76	0.10	46,46,46,46	0
57	MG	2A	3292	1/1	0.76	0.19	60,60,60,60	0
57	MG	1a	1729	1/1	0.76	0.17	48,48,48,48	0
57	MG	1a	1637	1/1	0.76	0.13	43,43,43,43	0
57	MG	2A	3196	1/1	0.76	0.20	52,52,52,52	0
57	MG	1A	3223	1/1	0.76	0.27	50,50,50,50	0
57	MG	23	102	1/1	0.76	0.52	63,63,63,63	0
57	MG	2A	3220	1/1	0.76	0.25	68,68,68,68	0
57	MG	2a	1618	1/1	0.76	0.17	63,63,63,63	0
57	MG	1A	3585	1/1	0.77	0.22	56,56,56,56	0
57	MG	2A	3832	1/1	0.77	0.16	63,63,63,63	0
57	MG	1B	232	1/1	0.77	0.33	70,70,70,70	0
57	MG	1A	3825	1/1	0.77	0.10	35,35,35,35	0
57	MG	2A	3338	1/1	0.77	0.27	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3071	1/1	0.77	0.15	59,59,59,59	0
57	MG	1A	3616	1/1	0.77	0.10	31,31,31,31	0
57	MG	2A	3365	1/1	0.77	0.15	60,60,60,60	0
57	MG	2A	3084	1/1	0.77	0.19	38,38,38,38	0
57	MG	2A	3370	1/1	0.77	0.11	61,61,61,61	0
57	MG	1a	1611	1/1	0.77	0.15	61,61,61,61	0
57	MG	2A	3304	1/1	0.77	0.20	47,47,47,47	0
57	MG	1A	3323	1/1	0.77	0.23	53,53,53,53	0
57	MG	2v	101	1/1	0.77	0.11	52,52,52,52	0
57	MG	2A	3403	1/1	0.77	0.18	57,57,57,57	0
57	MG	1a	1643	1/1	0.77	0.14	56,56,56,56	0
57	MG	1A	3581	1/1	0.77	0.20	60,60,60,60	0
57	MG	1A	3320	1/1	0.77	0.26	45,45,45,45	0
57	MG	1a	1674	1/1	0.78	0.15	52,52,52,52	0
57	MG	2a	1661	1/1	0.78	0.20	70,70,70,70	0
57	MG	1A	4016	1/1	0.78	0.16	48,48,48,48	0
57	MG	2a	1690	1/1	0.78	0.47	59,59,59,59	0
57	MG	1A	3354	1/1	0.78	0.57	53,53,53,53	0
57	MG	1A	3345	1/1	0.78	0.14	61,61,61,61	0
57	MG	1A	3764	1/1	0.78	0.14	41,41,41,41	0
57	MG	1A	3260	1/1	0.78	0.23	45,45,45,45	0
57	MG	2a	1741	1/1	0.78	0.22	56,56,56,56	0
57	MG	2A	3842	1/1	0.78	0.32	54,54,54,54	0
57	MG	2a	1748	1/1	0.78	0.12	43,43,43,43	0
57	MG	2A	3080	1/1	0.78	0.10	62,62,62,62	0
57	MG	2A	3282	1/1	0.78	0.13	56,56,56,56	0
57	MG	2a	1602	1/1	0.78	0.11	58,58,58,58	0
57	MG	2A	3346	1/1	0.78	0.29	57,57,57,57	0
57	MG	2a	1790	1/1	0.78	0.14	65,65,65,65	0
57	MG	1A	3983	1/1	0.78	0.17	36,36,36,36	0
57	MG	2A	3104	1/1	0.78	0.18	49,49,49,49	0
57	MG	1a	1640	1/1	0.78	0.22	56,56,56,56	0
57	MG	2A	3314	1/1	0.78	0.52	55,55,55,55	0
57	MG	2A	3698	1/1	0.78	0.12	33,33,33,33	0
57	MG	1A	3341	1/1	0.78	0.28	61,61,61,61	0
57	MG	2A	3732	1/1	0.78	0.16	45,45,45,45	0
57	MG	2a	1644	1/1	0.78	0.15	70,70,70,70	0
57	MG	2A	3398	1/1	0.78	0.59	61,61,61,61	0
57	MG	2y	104	1/1	0.78	0.12	68,68,68,68	0
57	MG	1B	204	1/1	0.78	0.33	57,57,57,57	0
57	MG	2A	3374	1/1	0.79	0.15	74,74,74,74	0
57	MG	2A	3197	1/1	0.79	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3855	1/1	0.79	0.07	35,35,35,35	0
57	MG	2A	3208	1/1	0.79	0.61	49,49,49,49	0
57	MG	1A	3436	1/1	0.79	0.39	48,48,48,48	0
57	MG	1t	201	1/1	0.79	0.12	49,49,49,49	0
57	MG	1S	201	1/1	0.79	0.68	49,49,49,49	0
57	MG	2A	3768	1/1	0.79	0.17	43,43,43,43	0
57	MG	1A	3694	1/1	0.79	0.14	28,28,28,28	0
57	MG	2a	1804	1/1	0.79	0.21	56,56,56,56	0
57	MG	2A	3467	1/1	0.79	0.11	62,62,62,62	0
57	MG	2A	3110	1/1	0.79	0.25	58,58,58,58	0
57	MG	1A	3464	1/1	0.79	0.28	49,49,49,49	0
57	MG	2a	1668	1/1	0.79	0.12	56,56,56,56	0
57	MG	1a	1622	1/1	0.79	0.20	66,66,66,66	0
57	MG	1B	226	1/1	0.79	0.19	64,64,64,64	0
57	MG	2A	3294	1/1	0.79	0.44	66,66,66,66	0
57	MG	2A	3297	1/1	0.79	0.25	54,54,54,54	0
57	MG	2x	103	1/1	0.79	0.12	65,65,65,65	0
57	MG	2A	3177	1/1	0.79	0.22	46,46,46,46	0
57	MG	1A	3382	1/1	0.79	0.30	49,49,49,49	0
57	MG	1x	104	1/1	0.80	0.19	69,69,69,69	0
57	MG	1F	309	1/1	0.80	0.22	47,47,47,47	0
57	MG	1A	3645	1/1	0.80	0.17	52,52,52,52	0
57	MG	2A	3300	1/1	0.80	0.35	59,59,59,59	0
57	MG	2A	3181	1/1	0.80	0.15	63,63,63,63	0
57	MG	2A	3195	1/1	0.80	0.18	58,58,58,58	0
57	MG	2a	1696	1/1	0.80	0.17	61,61,61,61	0
57	MG	2a	1700	1/1	0.80	0.16	59,59,59,59	0
57	MG	2A	3436	1/1	0.80	0.54	59,59,59,59	0
57	MG	1A	3380	1/1	0.80	0.49	41,41,41,41	0
57	MG	1A	3810	1/1	0.80	0.15	33,33,33,33	0
57	MG	1A	3821	1/1	0.80	0.16	50,50,50,50	0
57	MG	2A	3834	1/1	0.80	0.14	60,60,60,60	0
57	MG	2A	3077	1/1	0.80	0.26	52,52,52,52	0
57	MG	2A	3843	1/1	0.80	0.10	47,47,47,47	0
57	MG	2A	3844	1/1	0.80	0.24	60,60,60,60	0
57	MG	2B	202	1/1	0.80	0.44	57,57,57,57	0
57	MG	2B	216	1/1	0.80	0.09	64,64,64,64	0
57	MG	1a	1782	1/1	0.80	0.11	51,51,51,51	0
57	MG	2A	3330	1/1	0.80	0.22	58,58,58,58	0
57	MG	1A	3897	1/1	0.80	0.15	27,27,27,27	0
57	MG	2A	3262	1/1	0.80	0.15	55,55,55,55	0
57	MG	1A	4007	1/1	0.80	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3276	1/1	0.80	0.15	55,55,55,55	0
57	MG	2A	3088	1/1	0.80	0.12	71,71,71,71	0
57	MG	2A	3625	1/1	0.80	0.13	51,51,51,51	0
57	MG	2A	3634	1/1	0.80	0.12	79,79,79,79	0
57	MG	1A	3422	1/1	0.80	0.23	46,46,46,46	0
57	MG	1A	3922	1/1	0.80	0.21	53,53,53,53	0
57	MG	2A	3287	1/1	0.80	0.26	69,69,69,69	0
57	MG	1A	3392	1/1	0.80	0.31	41,41,41,41	0
57	MG	2A	3718	1/1	0.80	0.18	71,71,71,71	0
57	MG	1A	3528	1/1	0.81	0.27	48,48,48,48	0
57	MG	2a	1647	1/1	0.81	0.15	59,59,59,59	0
57	MG	2a	1651	1/1	0.81	0.24	69,69,69,69	0
57	MG	2A	3129	1/1	0.81	0.16	45,45,45,45	0
57	MG	2a	1653	1/1	0.81	0.23	65,65,65,65	0
57	MG	1A	3742	1/1	0.81	0.15	28,28,28,28	0
57	MG	2A	3726	1/1	0.81	0.09	45,45,45,45	0
57	MG	2A	3382	1/1	0.81	0.12	67,67,67,67	0
57	MG	1A	3754	1/1	0.81	0.20	28,28,28,28	0
57	MG	1A	3292	1/1	0.81	0.17	39,39,39,39	0
57	MG	1A	3907	1/1	0.81	0.13	58,58,58,58	0
57	MG	1A	3058	1/1	0.81	0.20	34,34,34,34	0
57	MG	2A	3407	1/1	0.81	0.17	62,62,62,62	0
57	MG	2A	3193	1/1	0.81	0.10	62,62,62,62	0
57	MG	2a	1712	1/1	0.81	0.10	61,61,61,61	0
57	MG	2A	3437	1/1	0.81	0.18	47,47,47,47	0
57	MG	1A	3330	1/1	0.81	0.20	57,57,57,57	0
57	MG	2a	1736	1/1	0.81	0.14	58,58,58,58	0
57	MG	2A	3818	1/1	0.81	0.11	33,33,33,33	0
57	MG	1A	3072	1/1	0.81	0.23	60,60,60,60	0
57	MG	1A	3318	1/1	0.81	0.15	50,50,50,50	0
57	MG	2A	3038	1/1	0.81	0.12	59,59,59,59	0
57	MG	1A	3513	1/1	0.81	0.12	49,49,49,49	0
57	MG	2A	3494	1/1	0.81	0.11	61,61,61,61	0
57	MG	2A	3498	1/1	0.81	0.20	58,58,58,58	0
57	MG	2A	3216	1/1	0.81	0.51	63,63,63,63	0
57	MG	1A	3657	1/1	0.81	0.16	26,26,26,26	0
57	MG	2a	1801	1/1	0.81	0.20	73,73,73,73	0
57	MG	2Q	204	1/1	0.81	0.28	45,45,45,45	0
57	MG	1A	3674	1/1	0.81	0.25	67,67,67,67	0
57	MG	1a	1711	1/1	0.81	0.17	57,57,57,57	0
57	MG	2A	3264	1/1	0.81	0.23	63,63,63,63	0
57	MG	1A	3519	1/1	0.81	0.22	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3273	1/1	0.81	0.19	48,48,48,48	0
57	MG	2A	3630	1/1	0.81	0.30	58,58,58,58	0
57	MG	2w	104	1/1	0.81	0.34	79,79,79,79	0
57	MG	1F	312	1/1	0.81	0.18	45,45,45,45	0
57	MG	1a	1762	1/1	0.81	0.10	62,62,62,62	0
57	MG	2A	3655	1/1	0.81	0.08	50,50,50,50	0
57	MG	2A	3657	1/1	0.81	0.15	57,57,57,57	0
57	MG	1H	201	1/1	0.81	0.30	41,41,41,41	0
57	MG	1A	3214	1/1	0.82	0.21	41,41,41,41	0
57	MG	2A	3136	1/1	0.82	0.23	41,41,41,41	0
57	MG	1A	3976	1/1	0.82	0.12	55,55,55,55	0
57	MG	2A	3295	1/1	0.82	0.55	66,66,66,66	0
57	MG	2a	1666	1/1	0.82	0.18	67,67,67,67	0
57	MG	1A	3321	1/1	0.82	0.31	53,53,53,53	0
57	MG	2a	1678	1/1	0.82	0.27	55,55,55,55	0
57	MG	1A	3092	1/1	0.82	0.15	54,54,54,54	0
57	MG	1d	301	1/1	0.82	0.18	59,59,59,59	0
57	MG	2A	3179	1/1	0.82	0.14	59,59,59,59	0
57	MG	2A	3810	1/1	0.82	0.31	65,65,65,65	0
57	MG	1A	3837	1/1	0.82	0.18	47,47,47,47	0
57	MG	1A	3587	1/1	0.82	0.25	68,68,68,68	0
57	MG	2A	3322	1/1	0.82	0.14	67,67,67,67	0
57	MG	1A	3751	1/1	0.82	0.15	22,22,22,22	0
57	MG	1a	1614	1/1	0.82	0.17	59,59,59,59	0
57	MG	1A	3506	1/1	0.82	0.24	51,51,51,51	0
57	MG	1A	3758	1/1	0.82	0.14	25,25,25,25	0
57	MG	1A	3626	1/1	0.82	0.14	38,38,38,38	0
57	MG	2A	3036	1/1	0.82	0.10	59,59,59,59	0
57	MG	1A	3168	1/1	0.82	0.17	50,50,50,50	0
57	MG	2T	202	1/1	0.82	0.12	63,63,63,63	0
57	MG	2A	3224	1/1	0.82	0.69	44,44,44,44	0
57	MG	25	3101	1/1	0.82	0.18	47,47,47,47	0
57	MG	27	102	1/1	0.82	0.49	47,47,47,47	0
57	MG	1A	4046	1/1	0.82	0.08	53,53,53,53	0
57	MG	1a	1663	1/1	0.82	0.22	53,53,53,53	0
57	MG	1A	3784	1/1	0.82	0.20	20,20,20,20	0
57	MG	2A	3646	1/1	0.82	0.18	42,42,42,42	0
57	MG	1A	4068	1/1	0.82	0.18	70,70,70,70	0
57	MG	2a	1625	1/1	0.82	0.17	57,57,57,57	0
57	MG	1B	202	1/1	0.82	0.30	49,49,49,49	0
57	MG	1A	3184	1/1	0.82	0.21	36,36,36,36	0
57	MG	2A	3086	1/1	0.82	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3796	1/1	0.82	0.12	39,39,39,39	0
57	MG	2a	1643	1/1	0.82	0.36	57,57,57,57	0
57	MG	2A	3716	1/1	0.82	0.15	50,50,50,50	0
57	MG	1A	3799	1/1	0.82	0.12	50,50,50,50	0
57	MG	2A	3389	1/1	0.82	0.27	49,49,49,49	0
57	MG	1A	3078	1/1	0.82	0.26	40,40,40,40	0
57	MG	1A	3568	1/1	0.83	0.17	30,30,30,30	0
57	MG	2A	3169	1/1	0.83	0.67	55,55,55,55	0
57	MG	2A	3421	1/1	0.83	0.15	50,50,50,50	0
57	MG	2A	3424	1/1	0.83	0.12	58,58,58,58	0
57	MG	1a	1601	1/1	0.83	0.10	47,47,47,47	0
57	MG	1A	3683	1/1	0.83	0.14	39,39,39,39	0
57	MG	1A	4039	1/1	0.83	0.15	56,56,56,56	0
57	MG	1A	3130	1/1	0.83	0.20	38,38,38,38	0
57	MG	2a	1669	1/1	0.83	0.27	59,59,59,59	0
57	MG	2A	3792	1/1	0.83	0.15	38,38,38,38	0
57	MG	1a	1634	1/1	0.83	0.18	51,51,51,51	0
57	MG	2A	3465	1/1	0.83	0.29	60,60,60,60	0
57	MG	1A	3221	1/1	0.83	0.32	46,46,46,46	0
57	MG	2A	3468	1/1	0.83	0.24	58,58,58,58	0
57	MG	1A	3359	1/1	0.83	0.23	50,50,50,50	0
57	MG	2A	3031	1/1	0.83	0.34	50,50,50,50	0
57	MG	1A	3499	1/1	0.83	0.37	51,51,51,51	0
57	MG	2a	1714	1/1	0.83	0.14	50,50,50,50	0
57	MG	1A	3832	1/1	0.83	0.10	58,58,58,58	0
57	MG	2a	1727	1/1	0.83	0.27	63,63,63,63	0
57	MG	2A	3209	1/1	0.83	0.11	55,55,55,55	0
57	MG	2B	203	1/1	0.83	0.13	53,53,53,53	0
57	MG	2a	1740	1/1	0.83	0.25	60,60,60,60	0
57	MG	2B	204	1/1	0.83	0.18	60,60,60,60	0
57	MG	2B	214	1/1	0.83	0.19	59,59,59,59	0
57	MG	2A	3543	1/1	0.83	0.10	38,38,38,38	0
57	MG	1A	3974	1/1	0.83	0.12	29,29,29,29	0
57	MG	2A	3044	1/1	0.83	0.18	54,54,54,54	0
57	MG	1a	1670	1/1	0.83	0.22	57,57,57,57	0
57	MG	1B	217	1/1	0.83	0.18	64,64,64,64	0
57	MG	2A	3259	1/1	0.83	0.23	65,65,65,65	0
57	MG	1A	3593	1/1	0.83	0.18	26,26,26,26	0
57	MG	2A	3360	1/1	0.83	0.14	62,62,62,62	0
57	MG	2a	1611	1/1	0.83	0.18	64,64,64,64	0
57	MG	1A	3404	1/1	0.83	0.13	42,42,42,42	0
57	MG	1a	1708	1/1	0.83	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3319	1/1	0.83	0.24	53,53,53,53	0
57	MG	1A	3295	1/1	0.83	0.23	54,54,54,54	0
57	MG	2A	3659	1/1	0.83	0.12	54,54,54,54	0
57	MG	1A	4012	1/1	0.83	0.16	73,73,73,73	0
57	MG	1A	3524	1/1	0.83	0.18	59,59,59,59	0
57	MG	1A	3893	1/1	0.83	0.28	39,39,39,39	0
57	MG	1A	3056	1/1	0.83	0.17	41,41,41,41	0
57	MG	2A	3717	1/1	0.83	0.20	41,41,41,41	0
57	MG	1a	1783	1/1	0.83	0.09	64,64,64,64	0
57	MG	1U	205	1/1	0.83	0.31	39,39,39,39	0
57	MG	2A	3554	1/1	0.84	0.15	30,30,30,30	0
57	MG	1a	1657	1/1	0.84	0.12	64,64,64,64	0
57	MG	1A	3274	1/1	0.84	0.23	46,46,46,46	0
57	MG	2A	3584	1/1	0.84	0.19	53,53,53,53	0
57	MG	2a	1626	1/1	0.84	0.10	68,68,68,68	0
57	MG	2a	1627	1/1	0.84	0.16	57,57,57,57	0
57	MG	2A	3107	1/1	0.84	0.17	61,61,61,61	0
57	MG	1A	3753	1/1	0.84	0.15	28,28,28,28	0
57	MG	2A	3594	1/1	0.84	0.21	48,48,48,48	0
57	MG	1A	3360	1/1	0.84	0.24	56,56,56,56	0
57	MG	1A	3361	1/1	0.84	0.12	57,57,57,57	0
57	MG	1A	3179	1/1	0.84	0.14	58,58,58,58	0
57	MG	2a	1645	1/1	0.84	0.09	68,68,68,68	0
57	MG	1A	4061	1/1	0.84	0.16	47,47,47,47	0
57	MG	1a	1698	1/1	0.84	0.13	57,57,57,57	0
57	MG	1A	3291	1/1	0.84	0.13	31,31,31,31	0
57	MG	1A	3910	1/1	0.84	0.18	28,28,28,28	0
57	MG	1B	203	1/1	0.84	0.14	37,37,37,37	0
57	MG	1a	1720	1/1	0.84	0.08	75,75,75,75	0
57	MG	2A	3350	1/1	0.84	0.22	65,65,65,65	0
57	MG	1A	3469	1/1	0.84	0.18	55,55,55,55	0
57	MG	2A	3711	1/1	0.84	0.12	53,53,53,53	0
57	MG	2A	3363	1/1	0.84	0.14	43,43,43,43	0
57	MG	1a	1750	1/1	0.84	0.16	49,49,49,49	0
57	MG	1A	3099	1/1	0.84	0.13	59,59,59,59	0
57	MG	2A	3369	1/1	0.84	0.13	64,64,64,64	0
57	MG	1a	1759	1/1	0.84	0.14	43,43,43,43	0
57	MG	1B	220	1/1	0.84	0.17	57,57,57,57	0
57	MG	1A	3928	1/1	0.84	0.15	29,29,29,29	0
57	MG	1A	3633	1/1	0.84	0.16	32,32,32,32	0
57	MG	1A	3798	1/1	0.84	0.11	59,59,59,59	0
57	MG	1A	3953	1/1	0.84	0.18	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1715	1/1	0.84	0.23	68,68,68,68	0
57	MG	1A	3083	1/1	0.84	0.53	30,30,30,30	0
57	MG	2A	3775	1/1	0.84	0.16	48,48,48,48	0
57	MG	2A	3400	1/1	0.84	0.21	44,44,44,44	0
57	MG	1A	3651	1/1	0.84	0.18	58,58,58,58	0
57	MG	1A	3241	1/1	0.84	0.19	59,59,59,59	0
57	MG	1w	104	1/1	0.84	0.16	58,58,58,58	0
57	MG	2A	3419	1/1	0.84	0.19	53,53,53,53	0
57	MG	1R	205	1/1	0.84	0.27	42,42,42,42	0
57	MG	2a	1749	1/1	0.84	0.19	58,58,58,58	0
57	MG	1A	3977	1/1	0.84	0.23	55,55,55,55	0
57	MG	2a	1764	1/1	0.84	0.17	59,59,59,59	0
57	MG	1A	3981	1/1	0.84	0.13	45,45,45,45	0
57	MG	10	102	1/1	0.84	0.32	44,44,44,44	0
57	MG	2A	3443	1/1	0.84	0.15	51,51,51,51	0
57	MG	1A	3672	1/1	0.84	0.12	44,44,44,44	0
57	MG	16	101	1/1	0.84	0.32	55,55,55,55	0
57	MG	2a	1797	1/1	0.84	0.20	64,64,64,64	0
57	MG	1A	3988	1/1	0.84	0.07	69,69,69,69	0
57	MG	1A	3395	1/1	0.84	0.23	60,60,60,60	0
57	MG	1A	3028	1/1	0.84	0.15	33,33,33,33	0
57	MG	2F	302	1/1	0.84	0.18	39,39,39,39	0
57	MG	2j	201	1/1	0.84	0.15	66,66,66,66	0
57	MG	2j	202	1/1	0.84	0.17	72,72,72,72	0
57	MG	1a	1617	1/1	0.84	0.15	43,43,43,43	0
57	MG	2A	3475	1/1	0.84	0.17	65,65,65,65	0
57	MG	1A	3400	1/1	0.84	0.17	56,56,56,56	0
57	MG	1a	1627	1/1	0.84	0.15	57,57,57,57	0
57	MG	1A	3838	1/1	0.84	0.10	66,66,66,66	0
57	MG	25	3103	1/1	0.84	0.33	50,50,50,50	0
57	MG	2A	3508	1/1	0.84	0.11	37,37,37,37	0
57	MG	1A	3844	1/1	0.84	0.62	39,39,39,39	0
57	MG	1A	3259	1/1	0.84	0.15	47,47,47,47	0
57	MG	1A	3219	1/1	0.84	0.36	37,37,37,37	0
57	MG	1a	1724	1/1	0.85	0.19	49,49,49,49	0
57	MG	2A	3738	1/1	0.85	0.11	61,61,61,61	0
57	MG	1W	208	1/1	0.85	0.30	44,44,44,44	0
57	MG	2A	3097	1/1	0.85	0.14	59,59,59,59	0
57	MG	2a	1654	1/1	0.85	0.14	67,67,67,67	0
57	MG	1a	1738	1/1	0.85	0.22	47,47,47,47	0
57	MG	1a	1739	1/1	0.85	0.32	62,62,62,62	0
57	MG	1A	3279	1/1	0.85	0.17	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3111	1/1	0.85	0.32	33,33,33,33	0
57	MG	14	101	1/1	0.85	0.19	67,67,67,67	0
57	MG	1A	4047	1/1	0.85	0.28	55,55,55,55	0
57	MG	2a	1686	1/1	0.85	0.11	67,67,67,67	0
57	MG	2A	3462	1/1	0.85	0.13	50,50,50,50	0
57	MG	2A	3165	1/1	0.85	0.08	62,62,62,62	0
57	MG	2A	3166	1/1	0.85	0.31	56,56,56,56	0
57	MG	2A	3815	1/1	0.85	0.08	49,49,49,49	0
57	MG	1A	3248	1/1	0.85	0.17	19,19,19,19	0
57	MG	2A	3470	1/1	0.85	0.24	54,54,54,54	0
57	MG	1A	3459	1/1	0.85	0.19	42,42,42,42	0
57	MG	1A	3843	1/1	0.85	0.16	51,51,51,51	0
57	MG	1A	3401	1/1	0.85	0.21	46,46,46,46	0
57	MG	2a	1720	1/1	0.85	0.15	58,58,58,58	0
57	MG	1A	3637	1/1	0.85	0.12	55,55,55,55	0
57	MG	1A	3372	1/1	0.85	0.14	30,30,30,30	0
57	MG	2A	3185	1/1	0.85	0.09	62,62,62,62	0
57	MG	2a	1735	1/1	0.85	0.14	51,51,51,51	0
57	MG	2A	3188	1/1	0.85	0.17	40,40,40,40	0
57	MG	1B	211	1/1	0.85	0.12	51,51,51,51	0
57	MG	1A	3466	1/1	0.85	0.22	37,37,37,37	0
57	MG	2A	3339	1/1	0.85	0.26	65,65,65,65	0
57	MG	1A	3767	1/1	0.85	0.19	33,33,33,33	0
57	MG	2Q	201	1/1	0.85	0.11	61,61,61,61	0
57	MG	1A	4000	1/1	0.85	0.12	46,46,46,46	0
57	MG	1A	3652	1/1	0.85	0.16	34,34,34,34	0
57	MG	1A	3580	1/1	0.85	0.22	36,36,36,36	0
57	MG	1A	3393	1/1	0.85	0.18	43,43,43,43	0
57	MG	1A	3482	1/1	0.85	0.11	53,53,53,53	0
57	MG	2a	1788	1/1	0.85	0.18	56,56,56,56	0
57	MG	2A	3626	1/1	0.85	0.66	51,51,51,51	0
57	MG	1a	1671	1/1	0.85	0.15	61,61,61,61	0
57	MG	2a	1605	1/1	0.85	0.20	61,61,61,61	0
57	MG	2A	3223	1/1	0.85	0.23	46,46,46,46	0
57	MG	2a	1802	1/1	0.85	0.23	61,61,61,61	0
57	MG	1A	3679	1/1	0.85	0.16	28,28,28,28	0
57	MG	1G	203	1/1	0.85	0.16	68,68,68,68	0
57	MG	2d	301	1/1	0.85	0.21	59,59,59,59	0
57	MG	2e	202	1/1	0.85	0.36	58,58,58,58	0
57	MG	2A	3247	1/1	0.85	0.15	50,50,50,50	0
57	MG	2A	3258	1/1	0.85	0.21	62,62,62,62	0
57	MG	2A	3381	1/1	0.85	0.31	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2l	201	1/1	0.85	0.12	64,64,64,64	0
57	MG	1A	3914	1/1	0.85	0.14	40,40,40,40	0
57	MG	2A	3261	1/1	0.85	0.36	71,71,71,71	0
57	MG	2A	3062	1/1	0.85	0.10	55,55,55,55	0
57	MG	2v	102	1/1	0.85	0.12	66,66,66,66	0
57	MG	2A	3710	1/1	0.85	0.11	59,59,59,59	0
57	MG	1A	3488	1/1	0.85	0.25	67,67,67,67	0
57	MG	2A	3713	1/1	0.85	0.09	38,38,38,38	0
57	MG	1R	206	1/1	0.85	0.22	43,43,43,43	0
57	MG	1A	3495	1/1	0.85	0.24	30,30,30,30	0
57	MG	1A	3696	1/1	0.85	0.11	40,40,40,40	0
57	MG	1V	206	1/1	0.85	0.19	58,58,58,58	0
57	MG	2A	3336	1/1	0.86	0.38	56,56,56,56	0
57	MG	1A	3730	1/1	0.86	0.21	21,21,21,21	0
57	MG	1A	4052	1/1	0.86	0.13	47,47,47,47	0
57	MG	1A	3734	1/1	0.86	0.26	74,74,74,74	0
57	MG	18	105	1/1	0.86	0.56	52,52,52,52	0
57	MG	2A	3645	1/1	0.86	0.10	27,27,27,27	0
57	MG	1a	1793	1/1	0.86	0.06	52,52,52,52	0
57	MG	2A	3653	1/1	0.86	0.13	48,48,48,48	0
57	MG	2A	3191	1/1	0.86	0.18	55,55,55,55	0
57	MG	1A	3425	1/1	0.86	0.24	38,38,38,38	0
57	MG	1A	3971	1/1	0.86	0.18	29,29,29,29	0
57	MG	2A	3662	1/1	0.86	0.12	68,68,68,68	0
57	MG	2A	3676	1/1	0.86	0.23	63,63,63,63	0
57	MG	1A	3504	1/1	0.86	0.18	43,43,43,43	0
57	MG	2A	3685	1/1	0.86	0.10	71,71,71,71	0
57	MG	2A	3687	1/1	0.86	0.09	64,64,64,64	0
57	MG	2A	3366	1/1	0.86	0.52	52,52,52,52	0
57	MG	2A	3705	1/1	0.86	0.14	53,53,53,53	0
57	MG	1A	3204	1/1	0.86	0.19	33,33,33,33	0
57	MG	1B	209	1/1	0.86	0.25	50,50,50,50	0
57	MG	1A	3435	1/1	0.86	0.14	57,57,57,57	0
57	MG	1A	3864	1/1	0.86	0.13	43,43,43,43	0
57	MG	1A	3206	1/1	0.86	0.13	61,61,61,61	0
57	MG	2A	3380	1/1	0.86	0.65	47,47,47,47	0
57	MG	1A	3871	1/1	0.86	0.20	42,42,42,42	0
57	MG	1A	3438	1/1	0.86	0.16	56,56,56,56	0
57	MG	2A	3027	1/1	0.86	0.20	56,56,56,56	0
57	MG	2A	3227	1/1	0.86	0.74	56,56,56,56	0
57	MG	2A	3753	1/1	0.86	0.10	37,37,37,37	0
57	MG	1B	228	1/1	0.86	0.24	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3032	1/1	0.86	0.15	42,42,42,42	0
57	MG	2A	3761	1/1	0.86	0.07	36,36,36,36	0
57	MG	2A	3250	1/1	0.86	0.18	57,57,57,57	0
57	MG	2A	3765	1/1	0.86	0.09	76,76,76,76	0
57	MG	1A	3020	1/1	0.86	0.31	44,44,44,44	0
57	MG	1a	1662	1/1	0.86	0.14	56,56,56,56	0
57	MG	1A	3322	1/1	0.86	0.17	56,56,56,56	0
57	MG	1a	1668	1/1	0.86	0.18	51,51,51,51	0
57	MG	1A	3394	1/1	0.86	0.64	41,41,41,41	0
57	MG	1A	3141	1/1	0.86	0.13	46,46,46,46	0
57	MG	2A	3063	1/1	0.86	0.16	54,54,54,54	0
57	MG	1a	1673	1/1	0.86	0.36	61,61,61,61	0
57	MG	2a	1743	1/1	0.86	0.20	60,60,60,60	0
57	MG	1A	3906	1/1	0.86	0.18	37,37,37,37	0
57	MG	1a	1675	1/1	0.86	0.21	71,71,71,71	0
57	MG	1A	3325	1/1	0.86	0.30	59,59,59,59	0
57	MG	2A	3286	1/1	0.86	0.55	60,60,60,60	0
57	MG	1O	202	1/1	0.86	0.24	51,51,51,51	0
57	MG	1a	1694	1/1	0.86	0.12	52,52,52,52	0
57	MG	1a	1695	1/1	0.86	0.15	60,60,60,60	0
57	MG	2B	201	1/1	0.86	0.22	60,60,60,60	0
57	MG	1P	205	1/1	0.86	0.18	41,41,41,41	0
57	MG	2A	3100	1/1	0.86	0.07	68,68,68,68	0
57	MG	1A	4026	1/1	0.86	0.15	46,46,46,46	0
57	MG	2B	209	1/1	0.86	0.13	58,58,58,58	0
57	MG	2B	212	1/1	0.86	0.23	53,53,53,53	0
57	MG	2B	213	1/1	0.86	0.14	62,62,62,62	0
57	MG	1A	3188	1/1	0.86	0.27	28,28,28,28	0
57	MG	1A	3371	1/1	0.86	0.13	47,47,47,47	0
57	MG	2B	219	1/1	0.86	0.11	61,61,61,61	0
57	MG	2A	3504	1/1	0.86	0.15	56,56,56,56	0
57	MG	2A	3308	1/1	0.86	0.18	63,63,63,63	0
57	MG	2A	3116	1/1	0.86	0.10	50,50,50,50	0
57	MG	1a	1717	1/1	0.86	0.23	64,64,64,64	0
57	MG	2A	3537	1/1	0.86	0.17	38,38,38,38	0
57	MG	1A	3196	1/1	0.86	0.13	31,31,31,31	0
57	MG	2A	3550	1/1	0.86	0.10	49,49,49,49	0
57	MG	2A	3140	1/1	0.86	0.14	50,50,50,50	0
57	MG	1V	203	1/1	0.86	0.26	49,49,49,49	0
57	MG	28	104	1/1	0.86	0.07	67,67,67,67	0
57	MG	1A	3704	1/1	0.86	0.23	60,60,60,60	0
57	MG	1A	3711	1/1	0.86	0.15	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1607	1/1	0.86	0.12	61,61,61,61	0
57	MG	1Z	301	1/1	0.86	0.21	59,59,59,59	0
57	MG	1A	3006	1/1	0.86	0.16	49,49,49,49	0
57	MG	11	101	1/1	0.86	0.69	35,35,35,35	0
57	MG	2R	201	1/1	0.87	0.22	55,55,55,55	0
57	MG	2A	3111	1/1	0.87	0.17	44,44,44,44	0
57	MG	2X	102	1/1	0.87	0.18	43,43,43,43	0
57	MG	1A	3586	1/1	0.87	0.17	54,54,54,54	0
57	MG	2A	3539	1/1	0.87	0.13	30,30,30,30	0
57	MG	2A	3542	1/1	0.87	0.08	45,45,45,45	0
57	MG	2A	3126	1/1	0.87	0.23	58,58,58,58	0
57	MG	1A	3416	1/1	0.87	0.23	46,46,46,46	0
57	MG	10	108	1/1	0.87	0.18	53,53,53,53	0
57	MG	2A	3558	1/1	0.87	0.13	42,42,42,42	0
57	MG	2A	3320	1/1	0.87	0.11	64,64,64,64	0
57	MG	1A	3727	1/1	0.87	0.16	52,52,52,52	0
57	MG	2A	3146	1/1	0.87	0.23	52,52,52,52	0
57	MG	2a	1615	1/1	0.87	0.12	54,54,54,54	0
57	MG	1A	4063	1/1	0.87	0.20	38,38,38,38	0
57	MG	2A	3154	1/1	0.87	0.31	62,62,62,62	0
57	MG	1A	3350	1/1	0.87	0.13	53,53,53,53	0
57	MG	2A	3602	1/1	0.87	0.10	35,35,35,35	0
57	MG	2A	3607	1/1	0.87	0.18	66,66,66,66	0
57	MG	2A	3619	1/1	0.87	0.25	46,46,46,46	0
57	MG	1A	3489	1/1	0.87	0.11	50,50,50,50	0
57	MG	1a	1771	1/1	0.87	0.11	63,63,63,63	0
57	MG	1A	3740	1/1	0.87	0.22	45,45,45,45	0
57	MG	1A	3050	1/1	0.87	0.18	44,44,44,44	0
57	MG	1B	207	1/1	0.87	0.23	60,60,60,60	0
57	MG	1A	3391	1/1	0.87	0.13	44,44,44,44	0
57	MG	1a	1806	1/1	0.87	0.08	74,74,74,74	0
57	MG	2A	3183	1/1	0.87	0.17	61,61,61,61	0
57	MG	2A	3343	1/1	0.87	0.15	60,60,60,60	0
57	MG	2A	3656	1/1	0.87	0.19	66,66,66,66	0
57	MG	2A	3345	1/1	0.87	0.11	59,59,59,59	0
57	MG	1A	3982	1/1	0.87	0.14	48,48,48,48	0
57	MG	2A	3348	1/1	0.87	0.34	67,67,67,67	0
57	MG	1A	3303	1/1	0.87	0.24	47,47,47,47	0
57	MG	1A	3229	1/1	0.87	0.13	40,40,40,40	0
57	MG	1a	1628	1/1	0.87	0.10	41,41,41,41	0
57	MG	2A	3364	1/1	0.87	0.12	57,57,57,57	0
57	MG	1A	3989	1/1	0.87	0.05	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1671	1/1	0.87	0.24	53,53,53,53	0
57	MG	1A	3998	1/1	0.87	0.09	37,37,37,37	0
57	MG	1A	3877	1/1	0.87	0.18	33,33,33,33	0
57	MG	1x	109	1/1	0.87	0.13	56,56,56,56	0
57	MG	1A	3507	1/1	0.87	0.11	49,49,49,49	0
57	MG	2A	3003	1/1	0.87	0.24	48,48,48,48	0
57	MG	2A	3715	1/1	0.87	0.09	53,53,53,53	0
57	MG	2A	3214	1/1	0.87	0.16	47,47,47,47	0
57	MG	1a	1652	1/1	0.87	0.08	38,38,38,38	0
57	MG	1E	305	1/1	0.87	0.19	30,30,30,30	0
57	MG	2A	3719	1/1	0.87	0.10	58,58,58,58	0
57	MG	2A	3222	1/1	0.87	0.33	52,52,52,52	0
57	MG	1A	3231	1/1	0.87	0.18	57,57,57,57	0
57	MG	1F	308	1/1	0.87	0.14	45,45,45,45	0
57	MG	2a	1725	1/1	0.87	0.29	68,68,68,68	0
57	MG	1A	4011	1/1	0.87	0.11	41,41,41,41	0
57	MG	2a	1730	1/1	0.87	0.14	67,67,67,67	0
57	MG	1A	3209	1/1	0.87	0.73	42,42,42,42	0
57	MG	2A	3236	1/1	0.87	0.12	51,51,51,51	0
57	MG	2A	3242	1/1	0.87	0.12	65,65,65,65	0
57	MG	2A	3404	1/1	0.87	0.25	54,54,54,54	0
57	MG	2A	3244	1/1	0.87	0.11	66,66,66,66	0
57	MG	1A	3520	1/1	0.87	0.18	60,60,60,60	0
57	MG	1G	204	1/1	0.87	0.16	57,57,57,57	0
57	MG	1A	3367	1/1	0.87	0.15	52,52,52,52	0
57	MG	2A	3427	1/1	0.87	0.48	60,60,60,60	0
57	MG	2A	3430	1/1	0.87	0.46	40,40,40,40	0
57	MG	1I	201	1/1	0.87	0.18	49,49,49,49	0
57	MG	1N	202	1/1	0.87	0.25	48,48,48,48	0
57	MG	2A	3805	1/1	0.87	0.14	43,43,43,43	0
57	MG	2A	3441	1/1	0.87	0.27	52,52,52,52	0
57	MG	1A	3114	1/1	0.87	0.34	37,37,37,37	0
57	MG	1a	1682	1/1	0.87	0.17	58,58,58,58	0
57	MG	1O	204	1/1	0.87	0.24	62,62,62,62	0
57	MG	1A	4023	1/1	0.87	0.17	50,50,50,50	0
57	MG	2A	3836	1/1	0.87	0.19	70,70,70,70	0
57	MG	2A	3841	1/1	0.87	0.31	52,52,52,52	0
57	MG	2A	3460	1/1	0.87	0.11	61,61,61,61	0
57	MG	1A	3121	1/1	0.87	0.26	56,56,56,56	0
57	MG	1A	3016	1/1	0.87	0.22	52,52,52,52	0
57	MG	1A	3413	1/1	0.87	0.30	54,54,54,54	0
57	MG	2f	202	1/1	0.87	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3094	1/1	0.87	0.12	67,67,67,67	0
57	MG	1A	3470	1/1	0.87	0.20	56,56,56,56	0
57	MG	1A	3480	1/1	0.87	0.13	55,55,55,55	0
57	MG	2A	3101	1/1	0.87	0.12	70,70,70,70	0
57	MG	2B	210	1/1	0.87	0.18	69,69,69,69	0
57	MG	2B	211	1/1	0.87	0.31	59,59,59,59	0
57	MG	2A	3491	1/1	0.87	0.22	61,61,61,61	0
57	MG	2A	3492	1/1	0.87	0.13	32,32,32,32	0
57	MG	1V	205	1/1	0.87	0.39	55,55,55,55	0
57	MG	1A	3823	1/1	0.87	0.18	49,49,49,49	0
57	MG	2A	3108	1/1	0.87	0.17	62,62,62,62	0
57	MG	1A	3706	1/1	0.87	0.12	52,52,52,52	0
57	MG	2A	3298	1/1	0.87	0.37	54,54,54,54	0
57	MG	2y	102	1/1	0.87	0.09	79,79,79,79	0
57	MG	2A	3528	1/1	0.87	0.08	41,41,41,41	0
57	MG	2A	3530	1/1	0.87	0.14	47,47,47,47	0
57	MG	2a	1617	1/1	0.88	0.43	60,60,60,60	0
57	MG	1A	3789	1/1	0.88	0.10	28,28,28,28	0
57	MG	2A	3394	1/1	0.88	0.16	54,54,54,54	0
57	MG	2A	3246	1/1	0.88	0.16	48,48,48,48	0
57	MG	1A	3297	1/1	0.88	0.14	45,45,45,45	0
57	MG	1A	3047	1/1	0.88	0.22	42,42,42,42	0
57	MG	1a	1696	1/1	0.88	0.19	56,56,56,56	0
57	MG	1A	3415	1/1	0.88	0.10	48,48,48,48	0
57	MG	2a	1631	1/1	0.88	0.16	66,66,66,66	0
57	MG	1a	1699	1/1	0.88	0.13	39,39,39,39	0
57	MG	1a	1707	1/1	0.88	0.20	57,57,57,57	0
57	MG	1A	3930	1/1	0.88	0.18	56,56,56,56	0
57	MG	2A	3266	1/1	0.88	0.54	64,64,64,64	0
57	MG	1A	3531	1/1	0.88	0.17	57,57,57,57	0
57	MG	1A	3938	1/1	0.88	0.32	61,61,61,61	0
57	MG	2A	3095	1/1	0.88	0.15	39,39,39,39	0
57	MG	1A	3949	1/1	0.88	0.17	26,26,26,26	0
57	MG	1Y	203	1/1	0.88	0.09	67,67,67,67	0
57	MG	1A	4064	1/1	0.88	0.12	31,31,31,31	0
57	MG	2A	3447	1/1	0.88	0.51	58,58,58,58	0
57	MG	1A	3557	1/1	0.88	0.23	36,36,36,36	0
57	MG	2A	3106	1/1	0.88	0.17	39,39,39,39	0
57	MG	2a	1660	1/1	0.88	0.13	49,49,49,49	0
57	MG	1a	1730	1/1	0.88	0.14	58,58,58,58	0
57	MG	2a	1665	1/1	0.88	0.13	59,59,59,59	0
57	MG	2A	3747	1/1	0.88	0.12	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3748	1/1	0.88	0.61	62,62,62,62	0
57	MG	1a	1735	1/1	0.88	0.21	65,65,65,65	0
57	MG	1A	4075	1/1	0.88	0.26	42,42,42,42	0
57	MG	1A	3562	1/1	0.88	0.12	43,43,43,43	0
57	MG	2a	1684	1/1	0.88	0.23	52,52,52,52	0
57	MG	2a	1685	1/1	0.88	0.18	58,58,58,58	0
57	MG	1A	3057	1/1	0.88	0.18	42,42,42,42	0
57	MG	1A	3417	1/1	0.88	0.46	43,43,43,43	0
57	MG	1A	3475	1/1	0.88	0.13	57,57,57,57	0
57	MG	1A	3717	1/1	0.88	0.14	59,59,59,59	0
57	MG	1A	3356	1/1	0.88	0.70	49,49,49,49	0
57	MG	1a	1781	1/1	0.88	0.24	47,47,47,47	0
57	MG	2a	1704	1/1	0.88	0.23	68,68,68,68	0
57	MG	1A	3281	1/1	0.88	0.13	55,55,55,55	0
57	MG	2a	1711	1/1	0.88	0.25	70,70,70,70	0
57	MG	1A	3728	1/1	0.88	0.19	59,59,59,59	0
57	MG	2A	3496	1/1	0.88	0.18	58,58,58,58	0
57	MG	1A	3485	1/1	0.88	0.13	50,50,50,50	0
57	MG	2a	1717	1/1	0.88	0.35	76,76,76,76	0
57	MG	1A	3486	1/1	0.88	0.25	37,37,37,37	0
57	MG	1a	1805	1/1	0.88	0.09	62,62,62,62	0
57	MG	1A	3326	1/1	0.88	0.12	56,56,56,56	0
57	MG	2A	3517	1/1	0.88	0.13	45,45,45,45	0
57	MG	2A	3825	1/1	0.88	0.22	65,65,65,65	0
57	MG	2a	1733	1/1	0.88	0.09	60,60,60,60	0
57	MG	2A	3518	1/1	0.88	0.07	56,56,56,56	0
57	MG	2A	3172	1/1	0.88	0.18	45,45,45,45	0
57	MG	1A	3603	1/1	0.88	0.14	31,31,31,31	0
57	MG	2A	3533	1/1	0.88	0.19	44,44,44,44	0
57	MG	1A	3315	1/1	0.88	0.17	49,49,49,49	0
57	MG	1A	3883	1/1	0.88	0.10	53,53,53,53	0
57	MG	1F	304	1/1	0.88	0.14	33,33,33,33	0
57	MG	1A	3494	1/1	0.88	0.25	61,61,61,61	0
57	MG	1A	3339	1/1	0.88	0.29	59,59,59,59	0
57	MG	1a	1655	1/1	0.88	0.12	47,47,47,47	0
57	MG	2a	1761	1/1	0.88	0.13	44,44,44,44	0
57	MG	2A	3553	1/1	0.88	0.11	69,69,69,69	0
57	MG	2a	1769	1/1	0.88	0.15	54,54,54,54	0
57	MG	1x	107	1/1	0.88	0.26	64,64,64,64	0
57	MG	2A	3342	1/1	0.88	0.10	53,53,53,53	0
57	MG	1F	310	1/1	0.88	0.15	30,30,30,30	0
57	MG	2A	3579	1/1	0.88	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3215	1/1	0.88	0.39	41,41,41,41	0
57	MG	1A	4019	1/1	0.88	0.32	60,60,60,60	0
57	MG	2A	3004	1/1	0.88	0.12	57,57,57,57	0
57	MG	2A	3198	1/1	0.88	0.15	59,59,59,59	0
57	MG	2A	3008	1/1	0.88	0.25	49,49,49,49	0
57	MG	1A	3439	1/1	0.88	0.12	56,56,56,56	0
57	MG	2A	3606	1/1	0.88	0.16	33,33,33,33	0
57	MG	1A	3025	1/1	0.88	0.26	42,42,42,42	0
57	MG	1A	3445	1/1	0.88	0.26	56,56,56,56	0
57	MG	2A	3623	1/1	0.88	0.42	57,57,57,57	0
57	MG	1N	201	1/1	0.88	0.20	45,45,45,45	0
57	MG	23	101	1/1	0.88	0.22	62,62,62,62	0
57	MG	1A	4024	1/1	0.88	0.27	38,38,38,38	0
57	MG	2A	3629	1/1	0.88	0.20	39,39,39,39	0
57	MG	1A	3777	1/1	0.88	0.12	83,83,83,83	0
57	MG	1A	3454	1/1	0.88	0.16	68,68,68,68	0
57	MG	1P	203	1/1	0.88	0.38	30,30,30,30	0
57	MG	2A	3047	1/1	0.88	0.55	41,41,41,41	0
57	MG	2a	1604	1/1	0.88	0.12	68,68,68,68	0
57	MG	1A	3113	1/1	0.88	0.26	34,34,34,34	0
57	MG	2A	3649	1/1	0.88	0.21	72,72,72,72	0
57	MG	2a	1608	1/1	0.88	0.10	57,57,57,57	0
57	MG	2a	1610	1/1	0.88	0.20	65,65,65,65	0
57	MG	2A	3235	1/1	0.88	0.24	56,56,56,56	0
57	MG	2y	103	1/1	0.88	0.10	78,78,78,78	0
57	MG	2A	3054	1/1	0.88	0.11	56,56,56,56	0
57	MG	2A	3056	1/1	0.88	0.13	71,71,71,71	0
57	MG	1A	3591	1/1	0.89	0.16	29,29,29,29	0
57	MG	1w	105	1/1	0.89	0.13	69,69,69,69	0
57	MG	1w	106	1/1	0.89	0.13	61,61,61,61	0
57	MG	1A	3129	1/1	0.89	0.08	71,71,71,71	0
57	MG	1A	3051	1/1	0.89	0.11	48,48,48,48	0
57	MG	2A	3643	1/1	0.89	0.14	59,59,59,59	0
57	MG	1A	3614	1/1	0.89	0.15	25,25,25,25	0
57	MG	1a	1639	1/1	0.89	0.10	46,46,46,46	0
57	MG	2A	3207	1/1	0.89	0.29	61,61,61,61	0
57	MG	2A	3650	1/1	0.89	0.23	75,75,75,75	0
57	MG	1A	3084	1/1	0.89	0.34	29,29,29,29	0
57	MG	1A	3622	1/1	0.89	0.12	29,29,29,29	0
57	MG	2A	3376	1/1	0.89	0.16	61,61,61,61	0
57	MG	2A	3378	1/1	0.89	0.22	52,52,52,52	0
57	MG	1A	3377	1/1	0.89	0.29	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3660	1/1	0.89	0.12	41,41,41,41	0
57	MG	1A	3944	1/1	0.89	0.10	50,50,50,50	0
57	MG	2a	1634	1/1	0.89	0.32	64,64,64,64	0
57	MG	2a	1635	1/1	0.89	0.09	59,59,59,59	0
57	MG	2A	3674	1/1	0.89	0.13	68,68,68,68	0
57	MG	1a	1656	1/1	0.89	0.21	60,60,60,60	0
57	MG	1A	3775	1/1	0.89	0.10	44,44,44,44	0
57	MG	2A	3028	1/1	0.89	0.19	55,55,55,55	0
57	MG	1A	3503	1/1	0.89	0.17	56,56,56,56	0
57	MG	2A	3691	1/1	0.89	0.12	37,37,37,37	0
57	MG	1A	3957	1/1	0.89	0.10	54,54,54,54	0
57	MG	2A	3702	1/1	0.89	0.14	41,41,41,41	0
57	MG	1A	3287	1/1	0.89	0.35	31,31,31,31	0
57	MG	2A	3230	1/1	0.89	0.12	57,57,57,57	0
57	MG	1A	3289	1/1	0.89	0.23	43,43,43,43	0
57	MG	1a	1669	1/1	0.89	0.13	61,61,61,61	0
57	MG	2A	3241	1/1	0.89	0.17	54,54,54,54	0
57	MG	2A	3714	1/1	0.89	0.13	60,60,60,60	0
57	MG	1A	3198	1/1	0.89	0.24	37,37,37,37	0
57	MG	1F	306	1/1	0.89	0.43	34,34,34,34	0
57	MG	2A	3423	1/1	0.89	0.11	58,58,58,58	0
57	MG	1A	3794	1/1	0.89	0.22	40,40,40,40	0
57	MG	1A	3383	1/1	0.89	0.34	62,62,62,62	0
57	MG	1A	3515	1/1	0.89	0.28	45,45,45,45	0
57	MG	2A	3252	1/1	0.89	0.10	50,50,50,50	0
57	MG	1A	3143	1/1	0.89	0.23	40,40,40,40	0
57	MG	1A	3658	1/1	0.89	0.15	27,27,27,27	0
57	MG	2A	3065	1/1	0.89	0.13	55,55,55,55	0
57	MG	2A	3751	1/1	0.89	0.19	70,70,70,70	0
57	MG	1A	3663	1/1	0.89	0.16	24,24,24,24	0
57	MG	1A	3822	1/1	0.89	0.16	60,60,60,60	0
57	MG	2a	1701	1/1	0.89	0.06	68,68,68,68	0
57	MG	2A	3265	1/1	0.89	0.17	51,51,51,51	0
57	MG	1A	3670	1/1	0.89	0.20	55,55,55,55	0
57	MG	1A	3147	1/1	0.89	0.20	42,42,42,42	0
57	MG	1A	3828	1/1	0.89	0.08	62,62,62,62	0
57	MG	2a	1713	1/1	0.89	0.18	66,66,66,66	0
57	MG	1A	3830	1/1	0.89	0.19	45,45,45,45	0
57	MG	2A	3466	1/1	0.89	0.10	55,55,55,55	0
57	MG	1A	3244	1/1	0.89	0.17	44,44,44,44	0
57	MG	1A	3164	1/1	0.89	0.31	32,32,32,32	0
57	MG	2A	3776	1/1	0.89	0.13	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3681	1/1	0.89	0.16	62,62,62,62	0
57	MG	2A	3283	1/1	0.89	0.18	53,53,53,53	0
57	MG	2A	3795	1/1	0.89	0.12	37,37,37,37	0
57	MG	2a	1732	1/1	0.89	0.29	56,56,56,56	0
57	MG	1R	204	1/1	0.89	0.27	31,31,31,31	0
57	MG	2A	3801	1/1	0.89	0.10	64,64,64,64	0
57	MG	2A	3487	1/1	0.89	0.23	51,51,51,51	0
57	MG	1A	3167	1/1	0.89	0.47	39,39,39,39	0
57	MG	1A	3692	1/1	0.89	0.15	47,47,47,47	0
57	MG	1a	1721	1/1	0.89	0.14	48,48,48,48	0
57	MG	2A	3819	1/1	0.89	0.10	48,48,48,48	0
57	MG	1A	3533	1/1	0.89	0.11	55,55,55,55	0
57	MG	1A	3542	1/1	0.89	0.27	37,37,37,37	0
57	MG	1A	3702	1/1	0.89	0.27	61,61,61,61	0
57	MG	2a	1753	1/1	0.89	0.13	60,60,60,60	0
57	MG	1A	3258	1/1	0.89	0.17	59,59,59,59	0
57	MG	1A	3867	1/1	0.89	0.28	31,31,31,31	0
57	MG	2A	3302	1/1	0.89	0.29	47,47,47,47	0
57	MG	2a	1768	1/1	0.89	0.07	60,60,60,60	0
57	MG	1A	3399	1/1	0.89	0.19	36,36,36,36	0
57	MG	2A	3118	1/1	0.89	0.14	47,47,47,47	0
57	MG	2a	1771	1/1	0.89	0.14	64,64,64,64	0
57	MG	2A	3310	1/1	0.89	0.59	55,55,55,55	0
57	MG	1A	3564	1/1	0.89	0.30	54,54,54,54	0
57	MG	1A	3351	1/1	0.89	0.17	49,49,49,49	0
57	MG	1A	3312	1/1	0.89	0.14	59,59,59,59	0
57	MG	2A	3538	1/1	0.89	0.11	45,45,45,45	0
57	MG	1A	3726	1/1	0.89	0.12	46,46,46,46	0
57	MG	2A	3540	1/1	0.89	0.11	37,37,37,37	0
57	MG	1a	1769	1/1	0.89	0.15	49,49,49,49	0
57	MG	1A	3314	1/1	0.89	0.13	39,39,39,39	0
57	MG	2A	3153	1/1	0.89	0.30	51,51,51,51	0
57	MG	1a	1772	1/1	0.89	0.13	52,52,52,52	0
57	MG	2A	3156	1/1	0.89	0.23	56,56,56,56	0
57	MG	2A	3157	1/1	0.89	0.21	54,54,54,54	0
57	MG	2F	306	1/1	0.89	0.15	52,52,52,52	0
57	MG	2i	201	1/1	0.89	0.10	62,62,62,62	0
57	MG	1l	103	1/1	0.89	0.11	41,41,41,41	0
57	MG	1A	3583	1/1	0.89	0.18	53,53,53,53	0
57	MG	2Q	202	1/1	0.89	0.16	40,40,40,40	0
57	MG	2l	205	1/1	0.89	0.15	63,63,63,63	0
57	MG	1A	3903	1/1	0.89	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1787	1/1	0.89	0.11	40,40,40,40	0
57	MG	1A	4062	1/1	0.89	0.21	32,32,32,32	0
57	MG	1A	3019	1/1	0.89	0.21	41,41,41,41	0
57	MG	1A	3044	1/1	0.89	0.20	28,28,28,28	0
57	MG	1a	1606	1/1	0.89	0.17	57,57,57,57	0
57	MG	2A	3605	1/1	0.89	0.09	62,62,62,62	0
57	MG	1A	3182	1/1	0.89	0.15	65,65,65,65	0
57	MG	1A	4070	1/1	0.89	0.15	34,34,34,34	0
57	MG	1A	3275	1/1	0.89	0.14	58,58,58,58	0
57	MG	2A	3621	1/1	0.89	0.16	39,39,39,39	0
57	MG	1A	3749	1/1	0.89	0.20	18,18,18,18	0
57	MG	2A	3352	1/1	0.89	0.21	52,52,52,52	0
57	MG	1E	306	1/1	0.90	0.13	28,28,28,28	0
57	MG	2A	3355	1/1	0.90	0.24	53,53,53,53	0
57	MG	2A	3357	1/1	0.90	0.10	61,61,61,61	0
57	MG	1a	1649	1/1	0.90	0.17	55,55,55,55	0
57	MG	2A	3639	1/1	0.90	0.10	49,49,49,49	0
57	MG	1A	3991	1/1	0.90	0.12	30,30,30,30	0
57	MG	1w	108	1/1	0.90	0.12	59,59,59,59	0
57	MG	1A	3759	1/1	0.90	0.07	51,51,51,51	0
57	MG	1A	3186	1/1	0.90	0.15	50,50,50,50	0
57	MG	1A	3347	1/1	0.90	0.16	50,50,50,50	0
57	MG	1x	108	1/1	0.90	0.14	56,56,56,56	0
57	MG	1A	3765	1/1	0.90	0.12	33,33,33,33	0
57	MG	2a	1624	1/1	0.90	0.35	52,52,52,52	0
57	MG	1A	3526	1/1	0.90	0.29	62,62,62,62	0
57	MG	2A	3206	1/1	0.90	0.15	61,61,61,61	0
57	MG	1x	115	1/1	0.90	0.20	55,55,55,55	0
57	MG	1A	3592	1/1	0.90	0.16	40,40,40,40	0
57	MG	1A	3112	1/1	0.90	0.10	41,41,41,41	0
57	MG	1A	3300	1/1	0.90	0.23	48,48,48,48	0
57	MG	2A	3015	1/1	0.90	0.17	35,35,35,35	0
57	MG	1A	3443	1/1	0.90	0.24	59,59,59,59	0
57	MG	1A	3541	1/1	0.90	0.24	34,34,34,34	0
57	MG	2A	3391	1/1	0.90	0.23	31,31,31,31	0
57	MG	1a	1672	1/1	0.90	0.21	73,73,73,73	0
57	MG	1A	3617	1/1	0.90	0.13	41,41,41,41	0
57	MG	2A	3695	1/1	0.90	0.20	52,52,52,52	0
57	MG	1A	3909	1/1	0.90	0.12	51,51,51,51	0
57	MG	1N	204	1/1	0.90	0.52	52,52,52,52	0
57	MG	2A	3703	1/1	0.90	0.14	61,61,61,61	0
57	MG	1A	3473	1/1	0.90	0.16	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3231	1/1	0.90	0.28	49,49,49,49	0
57	MG	2A	3405	1/1	0.90	0.20	57,57,57,57	0
57	MG	2A	3037	1/1	0.90	0.27	47,47,47,47	0
57	MG	2A	3414	1/1	0.90	0.10	59,59,59,59	0
57	MG	2A	3415	1/1	0.90	0.14	45,45,45,45	0
57	MG	1O	203	1/1	0.90	0.12	61,61,61,61	0
57	MG	2A	3239	1/1	0.90	0.18	63,63,63,63	0
57	MG	2A	3422	1/1	0.90	0.17	47,47,47,47	0
57	MG	2A	3043	1/1	0.90	0.13	47,47,47,47	0
57	MG	1A	3543	1/1	0.90	0.16	66,66,66,66	0
57	MG	2A	3722	1/1	0.90	0.10	42,42,42,42	0
57	MG	1A	4032	1/1	0.90	0.13	40,40,40,40	0
57	MG	2A	3730	1/1	0.90	0.27	50,50,50,50	0
57	MG	2A	3049	1/1	0.90	0.10	58,58,58,58	0
57	MG	2A	3734	1/1	0.90	0.12	55,55,55,55	0
57	MG	1P	204	1/1	0.90	0.49	32,32,32,32	0
57	MG	2A	3249	1/1	0.90	0.21	41,41,41,41	0
57	MG	2A	3053	1/1	0.90	0.14	40,40,40,40	0
57	MG	2a	1698	1/1	0.90	0.13	63,63,63,63	0
57	MG	2A	3749	1/1	0.90	0.11	44,44,44,44	0
57	MG	2A	3750	1/1	0.90	0.12	49,49,49,49	0
57	MG	1A	3721	1/1	0.90	0.08	63,63,63,63	0
57	MG	2a	1705	1/1	0.90	0.11	51,51,51,51	0
57	MG	2a	1708	1/1	0.90	0.20	61,61,61,61	0
57	MG	2A	3055	1/1	0.90	0.14	55,55,55,55	0
57	MG	1A	3802	1/1	0.90	0.15	55,55,55,55	0
57	MG	2A	3452	1/1	0.90	0.32	35,35,35,35	0
57	MG	1A	3547	1/1	0.90	0.17	46,46,46,46	0
57	MG	1a	1701	1/1	0.90	0.18	51,51,51,51	0
57	MG	1A	3550	1/1	0.90	0.22	22,22,22,22	0
57	MG	1A	3474	1/1	0.90	0.46	44,44,44,44	0
57	MG	2a	1718	1/1	0.90	0.21	58,58,58,58	0
57	MG	1U	201	1/1	0.90	0.34	35,35,35,35	0
57	MG	2a	1723	1/1	0.90	0.13	52,52,52,52	0
57	MG	1A	3418	1/1	0.90	0.13	44,44,44,44	0
57	MG	1A	3505	1/1	0.90	0.13	68,68,68,68	0
57	MG	1A	4055	1/1	0.90	0.11	70,70,70,70	0
57	MG	2A	3277	1/1	0.90	0.14	49,49,49,49	0
57	MG	1A	3476	1/1	0.90	0.18	59,59,59,59	0
57	MG	1W	201	1/1	0.90	0.28	34,34,34,34	0
57	MG	2A	3280	1/1	0.90	0.14	53,53,53,53	0
57	MG	1a	1728	1/1	0.90	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
57	MG	1A	3735	1/1	0.90	0.17	54,54,54,54	0
57	MG	1A	3737	1/1	0.90	0.19	34,34,34,34	0
57	MG	2A	3812	1/1	0.90	0.08	50,50,50,50	0
57	MG	1a	1732	1/1	0.90	0.21	49,49,49,49	0
57	MG	1A	3954	1/1	0.90	0.19	58,58,58,58	0
57	MG	2A	3502	1/1	0.90	0.10	53,53,53,53	0
57	MG	1A	4066	1/1	0.90	0.13	47,47,47,47	0
57	MG	2A	3105	1/1	0.90	0.11	52,52,52,52	0
57	MG	2A	3510	1/1	0.90	0.15	40,40,40,40	0
57	MG	10	105	1/1	0.90	0.30	55,55,55,55	0
57	MG	2A	3838	1/1	0.90	0.07	74,74,74,74	0
57	MG	2A	3296	1/1	0.90	0.31	55,55,55,55	0
57	MG	1a	1746	1/1	0.90	0.13	47,47,47,47	0
57	MG	1A	3738	1/1	0.90	0.12	61,61,61,61	0
57	MG	1A	3960	1/1	0.90	0.08	64,64,64,64	0
57	MG	1a	1757	1/1	0.90	0.16	42,42,42,42	0
57	MG	2a	1775	1/1	0.90	0.15	66,66,66,66	0
57	MG	2a	1776	1/1	0.90	0.20	74,74,74,74	0
57	MG	2A	3113	1/1	0.90	0.15	61,61,61,61	0
57	MG	2a	1784	1/1	0.90	0.12	52,52,52,52	0
57	MG	1A	4074	1/1	0.90	0.12	38,38,38,38	0
57	MG	2A	3117	1/1	0.90	0.08	67,67,67,67	0
57	MG	1A	3655	1/1	0.90	0.13	33,33,33,33	0
57	MG	2A	3121	1/1	0.90	0.17	39,39,39,39	0
57	MG	2a	1799	1/1	0.90	0.18	65,65,65,65	0
57	MG	1a	1766	1/1	0.90	0.22	59,59,59,59	0
57	MG	1A	3963	1/1	0.90	0.28	71,71,71,71	0
57	MG	1A	3970	1/1	0.90	0.15	26,26,26,26	0
57	MG	2a	1805	1/1	0.90	0.10	71,71,71,71	0
57	MG	2A	3551	1/1	0.90	0.10	67,67,67,67	0
57	MG	2A	3323	1/1	0.90	0.27	47,47,47,47	0
57	MG	2B	218	1/1	0.90	0.11	67,67,67,67	0
57	MG	1A	3091	1/1	0.90	0.16	49,49,49,49	0
57	MG	2D	304	1/1	0.90	0.56	49,49,49,49	0
57	MG	2E	304	1/1	0.90	0.13	44,44,44,44	0
57	MG	2A	3144	1/1	0.90	0.23	43,43,43,43	0
57	MG	1A	3747	1/1	0.90	0.18	45,45,45,45	0
57	MG	1B	208	1/1	0.90	0.16	43,43,43,43	0
57	MG	2l	203	1/1	0.90	0.39	58,58,58,58	0
57	MG	1A	3511	1/1	0.90	0.56	37,37,37,37	0
57	MG	1A	3582	1/1	0.90	0.16	48,48,48,48	0
57	MG	2Q	203	1/1	0.90	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1792	1/1	0.90	0.12	45,45,45,45	0
57	MG	1A	3978	1/1	0.90	0.06	46,46,46,46	0
57	MG	2v	103	1/1	0.90	0.15	75,75,75,75	0
57	MG	1A	3856	1/1	0.90	0.50	40,40,40,40	0
57	MG	1B	221	1/1	0.90	0.16	56,56,56,56	0
57	MG	1A	3863	1/1	0.90	0.14	52,52,52,52	0
57	MG	1a	1814	1/1	0.90	0.21	53,53,53,53	0
57	MG	1A	3403	1/1	0.90	0.10	41,41,41,41	0
57	MG	2y	101	1/1	0.90	0.37	81,81,81,81	0
57	MG	1A	3483	1/1	0.90	0.14	45,45,45,45	0
57	MG	1e	201	1/1	0.90	0.11	55,55,55,55	0
57	MG	1A	3059	1/1	0.90	0.11	48,48,48,48	0
57	MG	1A	3990	1/1	0.90	0.13	45,45,45,45	0
57	MG	1A	3610	1/1	0.91	0.15	32,32,32,32	0
57	MG	2A	3591	1/1	0.91	0.16	46,46,46,46	0
57	MG	1a	1623	1/1	0.91	0.12	57,57,57,57	0
57	MG	1B	214	1/1	0.91	0.12	38,38,38,38	0
57	MG	1f	201	1/1	0.91	0.22	36,36,36,36	0
57	MG	1l	201	1/1	0.91	0.11	60,60,60,60	0
57	MG	1A	3973	1/1	0.91	0.17	29,29,29,29	0
57	MG	1a	1632	1/1	0.91	0.19	39,39,39,39	0
57	MG	2A	3610	1/1	0.91	0.10	31,31,31,31	0
57	MG	2A	3612	1/1	0.91	0.17	53,53,53,53	0
57	MG	1w	102	1/1	0.91	0.14	41,41,41,41	0
57	MG	2A	3349	1/1	0.91	0.33	47,47,47,47	0
57	MG	2A	3622	1/1	0.91	0.15	45,45,45,45	0
57	MG	1A	3834	1/1	0.91	0.10	58,58,58,58	0
57	MG	1a	1635	1/1	0.91	0.29	60,60,60,60	0
57	MG	1a	1636	1/1	0.91	0.15	60,60,60,60	0
57	MG	1A	3975	1/1	0.91	0.14	82,82,82,82	0
57	MG	2A	3187	1/1	0.91	0.12	60,60,60,60	0
57	MG	2A	3631	1/1	0.91	0.17	58,58,58,58	0
57	MG	1A	3613	1/1	0.91	0.14	55,55,55,55	0
57	MG	2A	3189	1/1	0.91	0.17	53,53,53,53	0
57	MG	1A	3334	1/1	0.91	0.16	47,47,47,47	0
57	MG	1A	3104	1/1	0.91	0.17	27,27,27,27	0
57	MG	1A	3472	1/1	0.91	0.46	43,43,43,43	0
57	MG	1D	304	1/1	0.91	0.26	32,32,32,32	0
57	MG	1E	302	1/1	0.91	0.36	36,36,36,36	0
57	MG	1x	113	1/1	0.91	0.24	57,57,57,57	0
57	MG	2A	3201	1/1	0.91	0.16	43,43,43,43	0
57	MG	1A	3845	1/1	0.91	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3001	1/1	0.91	0.21	48,48,48,48	0
57	MG	1A	3848	1/1	0.91	0.12	49,49,49,49	0
57	MG	1E	307	1/1	0.91	0.14	21,21,21,21	0
57	MG	2A	3005	1/1	0.91	0.16	55,55,55,55	0
57	MG	1A	3379	1/1	0.91	0.12	47,47,47,47	0
57	MG	2A	3665	1/1	0.91	0.11	64,64,64,64	0
57	MG	1A	3530	1/1	0.91	0.14	57,57,57,57	0
57	MG	2A	3218	1/1	0.91	0.40	33,33,33,33	0
57	MG	2A	3393	1/1	0.91	0.27	40,40,40,40	0
57	MG	1A	3183	1/1	0.91	0.18	32,32,32,32	0
57	MG	2A	3686	1/1	0.91	0.09	63,63,63,63	0
57	MG	1A	3309	1/1	0.91	0.23	48,48,48,48	0
57	MG	1A	3997	1/1	0.91	0.17	39,39,39,39	0
57	MG	1A	3540	1/1	0.91	0.49	44,44,44,44	0
57	MG	2A	3697	1/1	0.91	0.10	58,58,58,58	0
57	MG	1A	3097	1/1	0.91	0.20	53,53,53,53	0
57	MG	1G	202	1/1	0.91	0.25	55,55,55,55	0
57	MG	1A	3280	1/1	0.91	0.19	35,35,35,35	0
57	MG	2A	3406	1/1	0.91	0.15	53,53,53,53	0
57	MG	1A	3876	1/1	0.91	0.13	22,22,22,22	0
57	MG	2a	1672	1/1	0.91	0.12	57,57,57,57	0
57	MG	2A	3707	1/1	0.91	0.10	47,47,47,47	0
57	MG	2a	1682	1/1	0.91	0.25	69,69,69,69	0
57	MG	2A	3708	1/1	0.91	0.19	65,65,65,65	0
57	MG	1A	3428	1/1	0.91	0.50	37,37,37,37	0
57	MG	1A	3205	1/1	0.91	0.12	43,43,43,43	0
57	MG	2A	3416	1/1	0.91	0.08	38,38,38,38	0
57	MG	1a	1685	1/1	0.91	0.25	58,58,58,58	0
57	MG	2a	1692	1/1	0.91	0.13	61,61,61,61	0
57	MG	1A	3252	1/1	0.91	0.21	43,43,43,43	0
57	MG	1A	3888	1/1	0.91	0.15	53,53,53,53	0
57	MG	1A	3555	1/1	0.91	0.50	34,34,34,34	0
57	MG	1A	3254	1/1	0.91	0.18	36,36,36,36	0
57	MG	2A	3426	1/1	0.91	0.22	58,58,58,58	0
57	MG	1A	3118	1/1	0.91	0.19	36,36,36,36	0
57	MG	1A	3142	1/1	0.91	0.16	53,53,53,53	0
57	MG	1A	3493	1/1	0.91	0.15	45,45,45,45	0
57	MG	2A	3060	1/1	0.91	0.18	51,51,51,51	0
57	MG	2A	3438	1/1	0.91	0.11	50,50,50,50	0
57	MG	1A	3773	1/1	0.91	0.14	25,25,25,25	0
57	MG	1A	4031	1/1	0.91	0.17	26,26,26,26	0
57	MG	2A	3445	1/1	0.91	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1R	203	1/1	0.91	0.17	42,42,42,42	0
57	MG	2A	3070	1/1	0.91	0.16	32,32,32,32	0
57	MG	1A	3570	1/1	0.91	0.17	39,39,39,39	0
57	MG	1a	1713	1/1	0.91	0.16	34,34,34,34	0
57	MG	2A	3458	1/1	0.91	0.10	41,41,41,41	0
57	MG	1A	4034	1/1	0.91	0.10	43,43,43,43	0
57	MG	2A	3760	1/1	0.91	0.10	59,59,59,59	0
57	MG	1A	3575	1/1	0.91	0.18	36,36,36,36	0
57	MG	2A	3762	1/1	0.91	0.11	54,54,54,54	0
57	MG	1A	3778	1/1	0.91	0.16	52,52,52,52	0
57	MG	1A	3442	1/1	0.91	0.44	36,36,36,36	0
57	MG	1A	3915	1/1	0.91	0.07	48,48,48,48	0
57	MG	2A	3093	1/1	0.91	0.20	55,55,55,55	0
57	MG	1A	3786	1/1	0.91	0.18	40,40,40,40	0
57	MG	2a	1737	1/1	0.91	0.18	72,72,72,72	0
57	MG	2a	1739	1/1	0.91	0.19	55,55,55,55	0
57	MG	2A	3469	1/1	0.91	0.13	56,56,56,56	0
57	MG	1A	3923	1/1	0.91	0.18	36,36,36,36	0
57	MG	1A	3685	1/1	0.91	0.15	21,21,21,21	0
57	MG	2A	3783	1/1	0.91	0.09	62,62,62,62	0
57	MG	2A	3478	1/1	0.91	0.19	38,38,38,38	0
57	MG	2A	3480	1/1	0.91	0.16	54,54,54,54	0
57	MG	2A	3098	1/1	0.91	0.09	55,55,55,55	0
57	MG	2a	1754	1/1	0.91	0.08	57,57,57,57	0
57	MG	2A	3485	1/1	0.91	0.20	60,60,60,60	0
57	MG	1A	3233	1/1	0.91	0.21	36,36,36,36	0
57	MG	1A	3266	1/1	0.91	0.28	35,35,35,35	0
57	MG	1Y	201	1/1	0.91	0.32	49,49,49,49	0
57	MG	2A	3814	1/1	0.91	0.10	64,64,64,64	0
57	MG	1A	3270	1/1	0.91	0.65	39,39,39,39	0
57	MG	2A	3817	1/1	0.91	0.12	53,53,53,53	0
57	MG	2a	1772	1/1	0.91	0.08	71,71,71,71	0
57	MG	1A	3449	1/1	0.91	0.22	47,47,47,47	0
57	MG	2a	1774	1/1	0.91	0.14	62,62,62,62	0
57	MG	1A	3453	1/1	0.91	0.18	42,42,42,42	0
57	MG	2A	3824	1/1	0.91	0.07	40,40,40,40	0
57	MG	10	104	1/1	0.91	0.45	36,36,36,36	0
57	MG	1A	4065	1/1	0.91	0.17	47,47,47,47	0
57	MG	10	106	1/1	0.91	0.12	42,42,42,42	0
57	MG	1A	3301	1/1	0.91	0.16	43,43,43,43	0
57	MG	2A	3301	1/1	0.91	0.75	61,61,61,61	0
57	MG	2A	3514	1/1	0.91	0.17	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3709	1/1	0.91	0.20	30,30,30,30	0
57	MG	1A	3951	1/1	0.91	0.14	36,36,36,36	0
57	MG	2A	3524	1/1	0.91	0.17	37,37,37,37	0
57	MG	1A	4071	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3120	1/1	0.91	0.14	65,65,65,65	0
57	MG	2A	3531	1/1	0.91	0.10	26,26,26,26	0
57	MG	2a	1807	1/1	0.91	0.14	58,58,58,58	0
57	MG	1a	1775	1/1	0.91	0.09	51,51,51,51	0
57	MG	2d	302	1/1	0.91	0.19	68,68,68,68	0
57	MG	2A	3316	1/1	0.91	0.22	53,53,53,53	0
57	MG	1A	3329	1/1	0.91	0.06	55,55,55,55	0
57	MG	2A	3128	1/1	0.91	0.19	35,35,35,35	0
57	MG	1A	3461	1/1	0.91	0.38	38,38,38,38	0
57	MG	17	101	1/1	0.91	0.13	35,35,35,35	0
57	MG	2A	3138	1/1	0.91	0.17	42,42,42,42	0
57	MG	2B	215	1/1	0.91	0.14	58,58,58,58	0
57	MG	2A	3324	1/1	0.91	0.26	60,60,60,60	0
57	MG	18	101	1/1	0.91	0.38	54,54,54,54	0
57	MG	2A	3143	1/1	0.91	0.18	48,48,48,48	0
57	MG	2D	303	1/1	0.91	0.73	40,40,40,40	0
57	MG	2t	201	1/1	0.91	0.14	49,49,49,49	0
57	MG	1A	3080	1/1	0.91	0.34	29,29,29,29	0
57	MG	2A	3329	1/1	0.91	0.14	53,53,53,53	0
57	MG	2F	301	1/1	0.91	0.14	55,55,55,55	0
57	MG	1A	3958	1/1	0.91	0.28	69,69,69,69	0
57	MG	2F	303	1/1	0.91	0.18	54,54,54,54	0
57	MG	2A	3559	1/1	0.91	0.07	61,61,61,61	0
57	MG	1A	3722	1/1	0.91	0.12	49,49,49,49	0
57	MG	2N	201	1/1	0.91	0.17	60,60,60,60	0
57	MG	2A	3563	1/1	0.91	0.18	56,56,56,56	0
57	MG	1A	3407	1/1	0.91	0.12	42,42,42,42	0
57	MG	1A	3725	1/1	0.91	0.13	51,51,51,51	0
57	MG	1A	3408	1/1	0.91	0.16	45,45,45,45	0
57	MG	2A	3586	1/1	0.91	0.20	56,56,56,56	0
57	MG	1E	301	1/1	0.92	0.37	38,38,38,38	0
57	MG	1A	3964	1/1	0.92	0.13	67,67,67,67	0
57	MG	2A	3515	1/1	0.92	0.08	60,60,60,60	0
57	MG	1A	3452	1/1	0.92	0.11	49,49,49,49	0
57	MG	1A	3324	1/1	0.92	0.17	41,41,41,41	0
57	MG	2A	3521	1/1	0.92	0.17	48,48,48,48	0
57	MG	1A	3001	1/1	0.92	0.10	36,36,36,36	0
57	MG	2A	3284	1/1	0.92	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3026	1/1	0.92	0.15	48,48,48,48	0
57	MG	1F	303	1/1	0.92	0.38	34,34,34,34	0
57	MG	2D	305	1/1	0.92	0.26	35,35,35,35	0
57	MG	1A	3081	1/1	0.92	0.16	29,29,29,29	0
57	MG	1A	3812	1/1	0.92	0.15	40,40,40,40	0
57	MG	1A	3669	1/1	0.92	0.14	26,26,26,26	0
57	MG	2A	3073	1/1	0.92	0.26	41,41,41,41	0
57	MG	2A	3074	1/1	0.92	0.35	37,37,37,37	0
57	MG	2A	3075	1/1	0.92	0.14	36,36,36,36	0
57	MG	1A	3082	1/1	0.92	0.21	29,29,29,29	0
57	MG	2P	202	1/1	0.92	0.15	63,63,63,63	0
57	MG	1a	1689	1/1	0.92	0.22	65,65,65,65	0
57	MG	2A	3544	1/1	0.92	0.10	54,54,54,54	0
57	MG	1A	3018	1/1	0.92	0.14	23,23,23,23	0
57	MG	1A	3238	1/1	0.92	0.19	41,41,41,41	0
57	MG	1A	3677	1/1	0.92	0.16	32,32,32,32	0
57	MG	2A	3305	1/1	0.92	0.43	63,63,63,63	0
57	MG	2A	3557	1/1	0.92	0.13	32,32,32,32	0
57	MG	1A	3467	1/1	0.92	0.14	55,55,55,55	0
57	MG	2A	3089	1/1	0.92	0.07	51,51,51,51	0
57	MG	1A	3544	1/1	0.92	0.14	61,61,61,61	0
57	MG	1A	3034	1/1	0.92	0.09	33,33,33,33	0
57	MG	2A	3575	1/1	0.92	0.17	54,54,54,54	0
57	MG	28	102	1/1	0.92	0.14	42,42,42,42	0
57	MG	1A	3187	1/1	0.92	0.27	37,37,37,37	0
57	MG	1a	1702	1/1	0.92	0.10	51,51,51,51	0
57	MG	1a	1704	1/1	0.92	0.15	45,45,45,45	0
57	MG	1A	3994	1/1	0.92	0.19	34,34,34,34	0
57	MG	2a	1606	1/1	0.92	0.09	65,65,65,65	0
57	MG	1A	3296	1/1	0.92	0.26	40,40,40,40	0
57	MG	1A	3556	1/1	0.92	0.56	53,53,53,53	0
57	MG	2a	1609	1/1	0.92	0.10	43,43,43,43	0
57	MG	1A	3243	1/1	0.92	0.42	30,30,30,30	0
57	MG	1A	3698	1/1	0.92	0.14	50,50,50,50	0
57	MG	1A	3558	1/1	0.92	0.42	41,41,41,41	0
57	MG	2a	1614	1/1	0.92	0.10	53,53,53,53	0
57	MG	1a	1719	1/1	0.92	0.12	55,55,55,55	0
57	MG	1A	4010	1/1	0.92	0.13	57,57,57,57	0
57	MG	1A	3846	1/1	0.92	0.07	33,33,33,33	0
57	MG	2A	3608	1/1	0.92	0.17	44,44,44,44	0
57	MG	2a	1621	1/1	0.92	0.33	56,56,56,56	0
57	MG	2A	3333	1/1	0.92	0.09	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3334	1/1	0.92	0.58	56,56,56,56	0
57	MG	2A	3616	1/1	0.92	0.12	38,38,38,38	0
57	MG	2A	3617	1/1	0.92	0.15	37,37,37,37	0
57	MG	1a	1722	1/1	0.92	0.14	59,59,59,59	0
57	MG	2A	3620	1/1	0.92	0.17	35,35,35,35	0
57	MG	2A	3114	1/1	0.92	0.13	31,31,31,31	0
57	MG	2A	3337	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3298	1/1	0.92	0.17	57,57,57,57	0
57	MG	1Q	204	1/1	0.92	0.23	46,46,46,46	0
57	MG	1A	3122	1/1	0.92	0.24	28,28,28,28	0
57	MG	1A	3190	1/1	0.92	0.14	43,43,43,43	0
57	MG	2a	1642	1/1	0.92	0.16	69,69,69,69	0
57	MG	1A	3411	1/1	0.92	0.15	37,37,37,37	0
57	MG	1A	3716	1/1	0.92	0.17	62,62,62,62	0
57	MG	1a	1737	1/1	0.92	0.20	56,56,56,56	0
57	MG	1A	3571	1/1	0.92	0.34	63,63,63,63	0
57	MG	2A	3132	1/1	0.92	0.23	35,35,35,35	0
57	MG	2A	3642	1/1	0.92	0.10	73,73,73,73	0
57	MG	1T	3603	1/1	0.92	0.23	45,45,45,45	0
57	MG	1a	1740	1/1	0.92	0.20	44,44,44,44	0
57	MG	1A	3089	1/1	0.92	0.07	49,49,49,49	0
57	MG	1A	3576	1/1	0.92	0.14	60,60,60,60	0
57	MG	1A	3875	1/1	0.92	0.17	38,38,38,38	0
57	MG	2A	3145	1/1	0.92	0.14	61,61,61,61	0
57	MG	1A	3579	1/1	0.92	0.20	50,50,50,50	0
57	MG	1A	3724	1/1	0.92	0.09	47,47,47,47	0
57	MG	1A	3305	1/1	0.92	0.28	31,31,31,31	0
57	MG	1W	203	1/1	0.92	0.14	37,37,37,37	0
57	MG	2A	3367	1/1	0.92	0.21	53,53,53,53	0
57	MG	2A	3661	1/1	0.92	0.19	66,66,66,66	0
57	MG	2a	1676	1/1	0.92	0.16	50,50,50,50	0
57	MG	1W	207	1/1	0.92	0.21	27,27,27,27	0
57	MG	1A	4036	1/1	0.92	0.17	22,22,22,22	0
57	MG	2A	3668	1/1	0.92	0.08	60,60,60,60	0
57	MG	2A	3669	1/1	0.92	0.19	46,46,46,46	0
57	MG	2A	3671	1/1	0.92	0.23	52,52,52,52	0
57	MG	1A	3251	1/1	0.92	0.20	35,35,35,35	0
57	MG	1A	3038	1/1	0.92	0.15	54,54,54,54	0
57	MG	2A	3372	1/1	0.92	0.20	47,47,47,47	0
57	MG	2A	3373	1/1	0.92	0.14	59,59,59,59	0
57	MG	1a	1777	1/1	0.92	0.11	61,61,61,61	0
57	MG	1A	3136	1/1	0.92	0.42	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3690	1/1	0.92	0.16	33,33,33,33	0
57	MG	1A	3891	1/1	0.92	0.15	47,47,47,47	0
57	MG	2A	3694	1/1	0.92	0.38	46,46,46,46	0
57	MG	1A	3042	1/1	0.92	0.12	34,34,34,34	0
57	MG	2a	1706	1/1	0.92	0.10	64,64,64,64	0
57	MG	2A	3175	1/1	0.92	0.23	52,52,52,52	0
57	MG	1A	3491	1/1	0.92	0.09	45,45,45,45	0
57	MG	1A	3898	1/1	0.92	0.24	38,38,38,38	0
57	MG	2A	3388	1/1	0.92	0.23	44,44,44,44	0
57	MG	2A	3704	1/1	0.92	0.10	38,38,38,38	0
57	MG	2A	3180	1/1	0.92	0.17	51,51,51,51	0
57	MG	1A	3096	1/1	0.92	0.11	43,43,43,43	0
57	MG	1A	4056	1/1	0.92	0.11	38,38,38,38	0
57	MG	1a	1802	1/1	0.92	0.10	61,61,61,61	0
57	MG	2A	3709	1/1	0.92	0.11	64,64,64,64	0
57	MG	2a	1721	1/1	0.92	0.08	57,57,57,57	0
57	MG	11	102	1/1	0.92	0.26	62,62,62,62	0
57	MG	1A	4058	1/1	0.92	0.21	52,52,52,52	0
57	MG	1A	4060	1/1	0.92	0.26	51,51,51,51	0
57	MG	2A	3190	1/1	0.92	0.15	65,65,65,65	0
57	MG	2a	1728	1/1	0.92	0.15	56,56,56,56	0
57	MG	13	104	1/1	0.92	0.15	39,39,39,39	0
57	MG	1A	3427	1/1	0.92	0.29	33,33,33,33	0
57	MG	15	105	1/1	0.92	0.09	48,48,48,48	0
57	MG	1A	3905	1/1	0.92	0.23	28,28,28,28	0
57	MG	2A	3409	1/1	0.92	0.22	45,45,45,45	0
57	MG	1k	201	1/1	0.92	0.16	48,48,48,48	0
57	MG	2A	3724	1/1	0.92	0.29	66,66,66,66	0
57	MG	1A	3588	1/1	0.92	0.17	47,47,47,47	0
57	MG	17	103	1/1	0.92	0.17	34,34,34,34	0
57	MG	1A	3368	1/1	0.92	0.29	35,35,35,35	0
57	MG	1A	3369	1/1	0.92	0.28	19,19,19,19	0
57	MG	1A	3370	1/1	0.92	0.48	33,33,33,33	0
57	MG	2a	1747	1/1	0.92	0.14	67,67,67,67	0
57	MG	2A	3743	1/1	0.92	0.14	32,32,32,32	0
57	MG	1A	3596	1/1	0.92	0.19	52,52,52,52	0
57	MG	2a	1752	1/1	0.92	0.12	63,63,63,63	0
57	MG	1A	3024	1/1	0.92	0.14	38,38,38,38	0
57	MG	2A	3210	1/1	0.92	0.18	51,51,51,51	0
57	MG	1a	1612	1/1	0.92	0.09	62,62,62,62	0
57	MG	2A	3428	1/1	0.92	0.50	43,43,43,43	0
57	MG	2A	3215	1/1	0.92	0.08	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1765	1/1	0.92	0.11	73,73,73,73	0
57	MG	2a	1766	1/1	0.92	0.20	56,56,56,56	0
57	MG	2A	3755	1/1	0.92	0.09	63,63,63,63	0
57	MG	1A	3262	1/1	0.92	0.23	28,28,28,28	0
57	MG	1a	1615	1/1	0.92	0.09	46,46,46,46	0
57	MG	1A	4073	1/1	0.92	0.13	40,40,40,40	0
57	MG	1a	1619	1/1	0.92	0.27	55,55,55,55	0
57	MG	1a	1620	1/1	0.92	0.12	41,41,41,41	0
57	MG	1A	3374	1/1	0.92	0.23	57,57,57,57	0
57	MG	1x	112	1/1	0.92	0.25	48,48,48,48	0
57	MG	1A	3756	1/1	0.92	0.17	32,32,32,32	0
57	MG	1A	3046	1/1	0.92	0.13	16,16,16,16	0
57	MG	1A	3509	1/1	0.92	0.18	54,54,54,54	0
57	MG	2A	3457	1/1	0.92	0.20	70,70,70,70	0
57	MG	1a	1630	1/1	0.92	0.33	59,59,59,59	0
57	MG	1a	1631	1/1	0.92	0.17	46,46,46,46	0
57	MG	2A	3780	1/1	0.92	0.07	48,48,48,48	0
57	MG	1A	3151	1/1	0.92	0.28	37,37,37,37	0
57	MG	1A	3512	1/1	0.92	0.39	36,36,36,36	0
57	MG	2A	3794	1/1	0.92	0.07	44,44,44,44	0
57	MG	2A	3463	1/1	0.92	0.15	58,58,58,58	0
57	MG	1A	3100	1/1	0.92	0.13	33,33,33,33	0
57	MG	2A	3799	1/1	0.92	0.25	55,55,55,55	0
57	MG	1A	3943	1/1	0.92	0.13	39,39,39,39	0
57	MG	1A	3073	1/1	0.92	0.17	26,26,26,26	0
57	MG	1a	1638	1/1	0.92	0.23	49,49,49,49	0
57	MG	2A	3029	1/1	0.92	0.10	54,54,54,54	0
57	MG	1A	3447	1/1	0.92	0.31	39,39,39,39	0
57	MG	2A	3472	1/1	0.92	0.24	48,48,48,48	0
57	MG	2A	3251	1/1	0.92	0.14	51,51,51,51	0
57	MG	2A	3477	1/1	0.92	0.25	39,39,39,39	0
57	MG	1A	3635	1/1	0.92	0.16	25,25,25,25	0
57	MG	2A	3254	1/1	0.92	0.18	62,62,62,62	0
57	MG	2A	3481	1/1	0.92	0.18	59,59,59,59	0
57	MG	2A	3830	1/1	0.92	0.15	36,36,36,36	0
57	MG	1A	3220	1/1	0.92	0.22	42,42,42,42	0
57	MG	2A	3833	1/1	0.92	0.18	65,65,65,65	0
57	MG	1A	3640	1/1	0.92	0.14	37,37,37,37	0
57	MG	1B	222	1/1	0.92	0.20	53,53,53,53	0
57	MG	1A	3643	1/1	0.92	0.19	41,41,41,41	0
57	MG	2A	3263	1/1	0.92	0.15	65,65,65,65	0
57	MG	2A	3041	1/1	0.92	0.23	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2w	103	1/1	0.92	0.16	66,66,66,66	0
57	MG	1A	3450	1/1	0.92	0.19	43,43,43,43	0
57	MG	2w	105	1/1	0.92	0.33	44,44,44,44	0
57	MG	1A	3648	1/1	0.92	0.18	24,24,24,24	0
57	MG	2A	3500	1/1	0.92	0.12	36,36,36,36	0
57	MG	1B	230	1/1	0.92	0.11	60,60,60,60	0
57	MG	2A	3048	1/1	0.92	0.22	51,51,51,51	0
57	MG	1A	3650	1/1	0.92	0.15	20,20,20,20	0
57	MG	2B	208	1/1	0.92	0.14	51,51,51,51	0
57	MG	2A	3509	1/1	0.92	0.07	40,40,40,40	0
57	MG	1A	3525	1/1	0.92	0.13	50,50,50,50	0
60	ZN	2Y	501	1/1	0.92	0.18	89,89,89,89	0
57	MG	2A	3026	1/1	0.93	0.11	42,42,42,42	0
57	MG	1A	3757	1/1	0.93	0.13	33,33,33,33	0
57	MG	1A	3918	1/1	0.93	0.10	50,50,50,50	0
57	MG	1A	3919	1/1	0.93	0.13	30,30,30,30	0
57	MG	1A	3920	1/1	0.93	0.13	27,27,27,27	0
57	MG	1A	3423	1/1	0.93	0.42	44,44,44,44	0
57	MG	1A	3249	1/1	0.93	0.30	43,43,43,43	0
57	MG	1A	3479	1/1	0.93	0.35	30,30,30,30	0
57	MG	1A	3926	1/1	0.93	0.06	30,30,30,30	0
57	MG	1A	3927	1/1	0.93	0.10	25,25,25,25	0
57	MG	2A	3275	1/1	0.93	0.35	70,70,70,70	0
57	MG	1A	3644	1/1	0.93	0.17	37,37,37,37	0
57	MG	1B	218	1/1	0.93	0.19	49,49,49,49	0
57	MG	1A	3545	1/1	0.93	0.32	49,49,49,49	0
57	MG	1A	3646	1/1	0.93	0.16	36,36,36,36	0
57	MG	1A	3932	1/1	0.93	0.15	47,47,47,47	0
57	MG	1a	1651	1/1	0.93	0.10	38,38,38,38	0
57	MG	1A	3771	1/1	0.93	0.15	56,56,56,56	0
57	MG	1a	1653	1/1	0.93	0.09	48,48,48,48	0
57	MG	1A	3936	1/1	0.93	0.17	47,47,47,47	0
57	MG	1A	3250	1/1	0.93	0.18	38,38,38,38	0
57	MG	2A	3291	1/1	0.93	0.09	46,46,46,46	0
57	MG	1A	3774	1/1	0.93	0.08	42,42,42,42	0
57	MG	2A	3547	1/1	0.93	0.10	34,34,34,34	0
57	MG	2O	202	1/1	0.93	0.12	55,55,55,55	0
57	MG	1A	3649	1/1	0.93	0.18	19,19,19,19	0
57	MG	2A	3061	1/1	0.93	0.21	49,49,49,49	0
57	MG	1D	302	1/1	0.93	0.15	36,36,36,36	0
57	MG	1A	3548	1/1	0.93	0.15	66,66,66,66	0
57	MG	1a	1664	1/1	0.93	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3067	1/1	0.93	0.11	28,28,28,28	0
57	MG	2A	3299	1/1	0.93	0.11	72,72,72,72	0
57	MG	2X	101	1/1	0.93	0.15	61,61,61,61	0
57	MG	1a	1665	1/1	0.93	0.20	44,44,44,44	0
57	MG	21	101	1/1	0.93	0.47	50,50,50,50	0
57	MG	2A	3562	1/1	0.93	0.10	58,58,58,58	0
57	MG	1D	308	1/1	0.93	0.28	30,30,30,30	0
57	MG	2A	3568	1/1	0.93	0.17	69,69,69,69	0
57	MG	2A	3571	1/1	0.93	0.11	50,50,50,50	0
57	MG	2A	3072	1/1	0.93	0.14	56,56,56,56	0
57	MG	27	103	1/1	0.93	0.14	47,47,47,47	0
57	MG	2A	3577	1/1	0.93	0.17	60,60,60,60	0
57	MG	1D	313	1/1	0.93	0.24	36,36,36,36	0
57	MG	1A	3950	1/1	0.93	0.20	38,38,38,38	0
57	MG	2a	1603	1/1	0.93	0.08	65,65,65,65	0
57	MG	2A	3582	1/1	0.93	0.08	69,69,69,69	0
57	MG	2A	3306	1/1	0.93	0.12	34,34,34,34	0
57	MG	1A	3133	1/1	0.93	0.14	29,29,29,29	0
57	MG	2A	3309	1/1	0.93	0.55	72,72,72,72	0
57	MG	1A	3779	1/1	0.93	0.12	44,44,44,44	0
57	MG	1A	3553	1/1	0.93	0.16	54,54,54,54	0
57	MG	2A	3315	1/1	0.93	0.36	41,41,41,41	0
57	MG	1A	3654	1/1	0.93	0.17	27,27,27,27	0
57	MG	2a	1612	1/1	0.93	0.12	63,63,63,63	0
57	MG	2A	3603	1/1	0.93	0.10	29,29,29,29	0
57	MG	2A	3082	1/1	0.93	0.39	48,48,48,48	0
57	MG	1A	3429	1/1	0.93	0.26	35,35,35,35	0
57	MG	1A	3484	1/1	0.93	0.18	38,38,38,38	0
57	MG	1A	3218	1/1	0.93	0.25	39,39,39,39	0
57	MG	2a	1619	1/1	0.93	0.10	66,66,66,66	0
57	MG	1a	1683	1/1	0.93	0.18	65,65,65,65	0
57	MG	2A	3611	1/1	0.93	0.20	45,45,45,45	0
57	MG	2A	3091	1/1	0.93	0.41	41,41,41,41	0
57	MG	1F	305	1/1	0.93	0.07	42,42,42,42	0
57	MG	1a	1687	1/1	0.93	0.27	46,46,46,46	0
57	MG	1A	3433	1/1	0.93	0.25	50,50,50,50	0
57	MG	1A	3665	1/1	0.93	0.11	22,22,22,22	0
57	MG	2a	1628	1/1	0.93	0.14	42,42,42,42	0
57	MG	1A	3968	1/1	0.93	0.08	45,45,45,45	0
57	MG	2A	3099	1/1	0.93	0.13	29,29,29,29	0
57	MG	1A	3667	1/1	0.93	0.09	43,43,43,43	0
57	MG	1A	3487	1/1	0.93	0.57	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1G	201	1/1	0.93	0.17	38,38,38,38	0
57	MG	1A	3805	1/1	0.93	0.12	20,20,20,20	0
57	MG	1A	3563	1/1	0.93	0.17	37,37,37,37	0
57	MG	1A	3253	1/1	0.93	0.24	55,55,55,55	0
57	MG	1a	1703	1/1	0.93	0.07	56,56,56,56	0
57	MG	2A	3109	1/1	0.93	0.15	61,61,61,61	0
57	MG	1A	3816	1/1	0.93	0.15	48,48,48,48	0
57	MG	1A	3817	1/1	0.93	0.15	41,41,41,41	0
57	MG	1A	3565	1/1	0.93	0.31	51,51,51,51	0
57	MG	2A	3644	1/1	0.93	0.10	61,61,61,61	0
57	MG	2A	3344	1/1	0.93	0.23	52,52,52,52	0
57	MG	1A	3165	1/1	0.93	0.24	38,38,38,38	0
57	MG	2A	3648	1/1	0.93	0.14	60,60,60,60	0
57	MG	1A	3194	1/1	0.93	0.17	39,39,39,39	0
57	MG	1A	3102	1/1	0.93	0.17	47,47,47,47	0
57	MG	2A	3651	1/1	0.93	0.12	42,42,42,42	0
57	MG	1A	3573	1/1	0.93	0.19	43,43,43,43	0
57	MG	2A	3654	1/1	0.93	0.12	44,44,44,44	0
57	MG	1A	3829	1/1	0.93	0.12	56,56,56,56	0
57	MG	2A	3351	1/1	0.93	0.09	59,59,59,59	0
57	MG	1A	3441	1/1	0.93	0.14	43,43,43,43	0
57	MG	2A	3124	1/1	0.93	0.27	45,45,45,45	0
57	MG	2A	3356	1/1	0.93	0.23	50,50,50,50	0
57	MG	1A	3138	1/1	0.93	0.21	40,40,40,40	0
57	MG	2A	3127	1/1	0.93	0.09	40,40,40,40	0
57	MG	1A	3577	1/1	0.93	0.46	37,37,37,37	0
57	MG	1Q	201	1/1	0.93	0.49	36,36,36,36	0
57	MG	1a	1726	1/1	0.93	0.11	63,63,63,63	0
57	MG	2A	3133	1/1	0.93	0.12	68,68,68,68	0
57	MG	2A	3134	1/1	0.93	0.17	34,34,34,34	0
57	MG	2A	3675	1/1	0.93	0.17	58,58,58,58	0
57	MG	1A	3498	1/1	0.93	0.43	41,41,41,41	0
57	MG	2A	3679	1/1	0.93	0.16	68,68,68,68	0
57	MG	1R	201	1/1	0.93	0.21	31,31,31,31	0
57	MG	2a	1699	1/1	0.93	0.06	65,65,65,65	0
57	MG	2A	3683	1/1	0.93	0.21	62,62,62,62	0
57	MG	1A	3836	1/1	0.93	0.16	16,16,16,16	0
57	MG	1A	3304	1/1	0.93	0.23	46,46,46,46	0
57	MG	1A	3700	1/1	0.93	0.23	49,49,49,49	0
57	MG	2A	3688	1/1	0.93	0.23	40,40,40,40	0
57	MG	1A	3840	1/1	0.93	0.18	16,16,16,16	0
57	MG	2a	1709	1/1	0.93	0.19	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4008	1/1	0.93	0.15	54,54,54,54	0
57	MG	2A	3692	1/1	0.93	0.35	55,55,55,55	0
57	MG	2A	3693	1/1	0.93	0.15	55,55,55,55	0
57	MG	1S	203	1/1	0.93	0.19	50,50,50,50	0
57	MG	2A	3377	1/1	0.93	0.16	55,55,55,55	0
57	MG	2A	3150	1/1	0.93	0.37	40,40,40,40	0
57	MG	2a	1716	1/1	0.93	0.21	52,52,52,52	0
57	MG	2A	3379	1/1	0.93	0.10	51,51,51,51	0
57	MG	2A	3152	1/1	0.93	0.10	64,64,64,64	0
57	MG	2a	1719	1/1	0.93	0.26	62,62,62,62	0
57	MG	1A	3261	1/1	0.93	0.44	45,45,45,45	0
57	MG	1A	3199	1/1	0.93	0.16	31,31,31,31	0
57	MG	1A	3200	1/1	0.93	0.08	44,44,44,44	0
57	MG	1U	206	1/1	0.93	0.23	28,28,28,28	0
57	MG	1A	3448	1/1	0.93	0.16	38,38,38,38	0
57	MG	1A	3352	1/1	0.93	0.30	31,31,31,31	0
57	MG	1A	3854	1/1	0.93	0.60	37,37,37,37	0
57	MG	2a	1729	1/1	0.93	0.37	69,69,69,69	0
57	MG	1A	3713	1/1	0.93	0.12	56,56,56,56	0
57	MG	2A	3170	1/1	0.93	0.20	48,48,48,48	0
57	MG	2A	3399	1/1	0.93	0.22	55,55,55,55	0
57	MG	1A	3353	1/1	0.93	1.02	56,56,56,56	0
57	MG	2A	3173	1/1	0.93	0.19	61,61,61,61	0
57	MG	1A	3860	1/1	0.93	0.25	50,50,50,50	0
57	MG	1A	3088	1/1	0.93	0.12	47,47,47,47	0
57	MG	1X	101	1/1	0.93	0.11	54,54,54,54	0
57	MG	1X	106	1/1	0.93	0.19	48,48,48,48	0
57	MG	1a	1778	1/1	0.93	0.11	55,55,55,55	0
57	MG	2A	3408	1/1	0.93	0.18	49,49,49,49	0
57	MG	1A	4027	1/1	0.93	0.14	45,45,45,45	0
57	MG	2A	3411	1/1	0.93	0.13	53,53,53,53	0
57	MG	1Y	202	1/1	0.93	0.26	52,52,52,52	0
57	MG	1A	3106	1/1	0.93	0.44	30,30,30,30	0
57	MG	1A	3357	1/1	0.93	0.41	35,35,35,35	0
57	MG	1a	1791	1/1	0.93	0.09	41,41,41,41	0
57	MG	2A	3745	1/1	0.93	0.11	61,61,61,61	0
57	MG	1A	3358	1/1	0.93	0.33	43,43,43,43	0
57	MG	1A	3460	1/1	0.93	0.70	48,48,48,48	0
57	MG	1A	3872	1/1	0.93	0.13	39,39,39,39	0
57	MG	1A	3004	1/1	0.93	0.16	24,24,24,24	0
57	MG	1A	3599	1/1	0.93	0.14	33,33,33,33	0
57	MG	1A	4040	1/1	0.93	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1807	1/1	0.93	0.14	64,64,64,64	0
57	MG	1A	3600	1/1	0.93	0.19	37,37,37,37	0
57	MG	1A	3879	1/1	0.93	0.09	68,68,68,68	0
57	MG	12	102	1/1	0.93	0.16	38,38,38,38	0
57	MG	1A	3521	1/1	0.93	0.26	44,44,44,44	0
57	MG	1A	4048	1/1	0.93	0.09	42,42,42,42	0
57	MG	1A	3061	1/1	0.93	0.24	41,41,41,41	0
57	MG	2A	3764	1/1	0.93	0.10	57,57,57,57	0
57	MG	2A	3444	1/1	0.93	0.40	34,34,34,34	0
57	MG	2a	1782	1/1	0.93	0.12	67,67,67,67	0
57	MG	15	102	1/1	0.93	0.17	31,31,31,31	0
57	MG	1n	101	1/1	0.93	0.24	50,50,50,50	0
57	MG	15	103	1/1	0.93	0.23	38,38,38,38	0
57	MG	2A	3449	1/1	0.93	0.11	21,21,21,21	0
57	MG	2a	1794	1/1	0.93	0.33	66,66,66,66	0
57	MG	2a	1796	1/1	0.93	0.11	57,57,57,57	0
57	MG	1A	3731	1/1	0.93	0.13	20,20,20,20	0
57	MG	1A	3409	1/1	0.93	0.28	53,53,53,53	0
57	MG	2a	1800	1/1	0.93	0.15	70,70,70,70	0
57	MG	2A	3217	1/1	0.93	0.10	53,53,53,53	0
57	MG	2A	3781	1/1	0.93	0.12	49,49,49,49	0
57	MG	2a	1803	1/1	0.93	0.11	64,64,64,64	0
57	MG	1A	3208	1/1	0.93	0.41	49,49,49,49	0
57	MG	2A	3784	1/1	0.93	0.13	39,39,39,39	0
57	MG	2A	3786	1/1	0.93	0.06	56,56,56,56	0
57	MG	2A	3788	1/1	0.93	0.13	49,49,49,49	0
57	MG	1A	4057	1/1	0.93	0.13	63,63,63,63	0
57	MG	17	104	1/1	0.93	0.10	40,40,40,40	0
57	MG	2A	3461	1/1	0.93	0.20	47,47,47,47	0
57	MG	1A	3148	1/1	0.93	0.25	32,32,32,32	0
57	MG	1A	3894	1/1	0.93	0.22	35,35,35,35	0
57	MG	2A	3225	1/1	0.93	0.45	40,40,40,40	0
57	MG	2A	3804	1/1	0.93	0.14	47,47,47,47	0
57	MG	1A	3245	1/1	0.93	0.19	57,57,57,57	0
57	MG	2A	3809	1/1	0.93	0.09	46,46,46,46	0
57	MG	1a	1603	1/1	0.93	0.08	62,62,62,62	0
57	MG	1a	1605	1/1	0.93	0.10	53,53,53,53	0
57	MG	1A	3620	1/1	0.93	0.16	20,20,20,20	0
57	MG	1a	1609	1/1	0.93	0.19	48,48,48,48	0
57	MG	1A	3902	1/1	0.93	0.19	59,59,59,59	0
57	MG	2A	3237	1/1	0.93	0.16	58,58,58,58	0
57	MG	2A	3238	1/1	0.93	0.16	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3621	1/1	0.93	0.13	52,52,52,52	0
57	MG	2w	101	1/1	0.93	0.12	50,50,50,50	0
57	MG	1A	3746	1/1	0.93	0.18	13,13,13,13	0
57	MG	1A	3283	1/1	0.93	0.12	40,40,40,40	0
57	MG	2A	3831	1/1	0.93	0.09	47,47,47,47	0
57	MG	2A	3243	1/1	0.93	0.11	62,62,62,62	0
57	MG	1A	3286	1/1	0.93	0.44	60,60,60,60	0
57	MG	1A	3536	1/1	0.93	0.25	47,47,47,47	0
57	MG	1A	3211	1/1	0.93	0.20	48,48,48,48	0
57	MG	2x	105	1/1	0.93	0.24	69,69,69,69	0
57	MG	1a	1621	1/1	0.93	0.36	64,64,64,64	0
57	MG	1A	3086	1/1	0.93	0.26	46,46,46,46	0
57	MG	2A	3018	1/1	0.93	0.13	47,47,47,47	0
57	MG	2A	3022	1/1	0.93	0.22	39,39,39,39	0
57	MG	1A	3636	1/1	0.93	0.13	30,30,30,30	0
57	MG	2A	3257	1/1	0.93	0.10	65,65,65,65	0
60	ZN	24	501	1/1	0.93	0.06	124,124,124,124	0
57	MG	2A	3194	1/1	0.94	0.17	43,43,43,43	0
57	MG	1A	3851	1/1	0.94	0.13	24,24,24,24	0
57	MG	1A	4022	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3481	1/1	0.94	0.27	36,36,36,36	0
57	MG	1A	3293	1/1	0.94	0.21	44,44,44,44	0
57	MG	1a	1788	1/1	0.94	0.17	40,40,40,40	0
57	MG	2A	3822	1/1	0.94	0.15	45,45,45,45	0
57	MG	2A	3202	1/1	0.94	0.19	63,63,63,63	0
57	MG	1Z	302	1/1	0.94	0.23	47,47,47,47	0
57	MG	2A	3826	1/1	0.94	0.11	47,47,47,47	0
57	MG	2A	3828	1/1	0.94	0.12	50,50,50,50	0
57	MG	2A	3829	1/1	0.94	0.12	48,48,48,48	0
57	MG	2A	3205	1/1	0.94	0.21	63,63,63,63	0
57	MG	1A	3705	1/1	0.94	0.16	35,35,35,35	0
57	MG	10	103	1/1	0.94	0.29	39,39,39,39	0
57	MG	1A	3054	1/1	0.94	0.15	40,40,40,40	0
57	MG	1a	1797	1/1	0.94	0.13	56,56,56,56	0
57	MG	1a	1800	1/1	0.94	0.17	54,54,54,54	0
57	MG	2A	3213	1/1	0.94	0.17	46,46,46,46	0
57	MG	2A	3839	1/1	0.94	0.15	54,54,54,54	0
57	MG	2A	3840	1/1	0.94	0.16	41,41,41,41	0
57	MG	2A	3476	1/1	0.94	0.09	49,49,49,49	0
57	MG	1A	3412	1/1	0.94	0.10	36,36,36,36	0
57	MG	1A	3178	1/1	0.94	0.48	34,34,34,34	0
57	MG	1A	3414	1/1	0.94	0.29	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3109	1/1	0.94	0.34	30,30,30,30	0
57	MG	2A	3482	1/1	0.94	0.15	52,52,52,52	0
57	MG	1a	1808	1/1	0.94	0.21	59,59,59,59	0
57	MG	1a	1812	1/1	0.94	0.13	51,51,51,51	0
57	MG	2B	205	1/1	0.94	0.16	58,58,58,58	0
57	MG	1a	1813	1/1	0.94	0.26	52,52,52,52	0
57	MG	2A	3489	1/1	0.94	0.14	56,56,56,56	0
57	MG	2A	3490	1/1	0.94	0.09	53,53,53,53	0
57	MG	1A	3007	1/1	0.94	0.28	39,39,39,39	0
57	MG	1A	3212	1/1	0.94	0.17	33,33,33,33	0
57	MG	1A	3874	1/1	0.94	0.20	19,19,19,19	0
57	MG	1A	3022	1/1	0.94	0.12	37,37,37,37	0
57	MG	2A	3497	1/1	0.94	0.11	18,18,18,18	0
57	MG	1A	3492	1/1	0.94	0.20	45,45,45,45	0
57	MG	2B	217	1/1	0.94	0.24	67,67,67,67	0
57	MG	1f	202	1/1	0.94	0.23	48,48,48,48	0
57	MG	1A	3419	1/1	0.94	0.33	27,27,27,27	0
57	MG	2A	3503	1/1	0.94	0.08	55,55,55,55	0
57	MG	1A	3027	1/1	0.94	0.21	56,56,56,56	0
57	MG	1m	3001	1/1	0.94	0.13	57,57,57,57	0
57	MG	1A	3880	1/1	0.94	0.24	34,34,34,34	0
57	MG	15	104	1/1	0.94	0.18	26,26,26,26	0
57	MG	1A	3257	1/1	0.94	0.51	46,46,46,46	0
57	MG	2A	3240	1/1	0.94	0.33	63,63,63,63	0
57	MG	1A	3589	1/1	0.94	0.14	38,38,38,38	0
57	MG	1A	4054	1/1	0.94	0.21	48,48,48,48	0
57	MG	1A	3590	1/1	0.94	0.16	26,26,26,26	0
57	MG	1A	3729	1/1	0.94	0.14	49,49,49,49	0
57	MG	2A	3245	1/1	0.94	0.30	54,54,54,54	0
57	MG	2A	3527	1/1	0.94	0.14	31,31,31,31	0
57	MG	17	105	1/1	0.94	0.20	41,41,41,41	0
57	MG	2A	3529	1/1	0.94	0.12	33,33,33,33	0
57	MG	1x	101	1/1	0.94	0.14	17,17,17,17	0
57	MG	1A	3890	1/1	0.94	0.17	43,43,43,43	0
57	MG	1A	3185	1/1	0.94	0.46	35,35,35,35	0
57	MG	2V	201	1/1	0.94	0.20	63,63,63,63	0
57	MG	18	106	1/1	0.94	0.11	38,38,38,38	0
57	MG	2A	3535	1/1	0.94	0.14	35,35,35,35	0
57	MG	18	108	1/1	0.94	0.20	39,39,39,39	0
57	MG	1A	3017	1/1	0.94	0.16	50,50,50,50	0
57	MG	1A	3501	1/1	0.94	0.17	43,43,43,43	0
57	MG	23	104	1/1	0.94	0.21	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1x	111	1/1	0.94	0.10	68,68,68,68	0
57	MG	2A	3541	1/1	0.94	0.24	59,59,59,59	0
57	MG	1a	1604	1/1	0.94	0.14	47,47,47,47	0
57	MG	2A	3260	1/1	0.94	0.11	53,53,53,53	0
57	MG	28	101	1/1	0.94	0.25	57,57,57,57	0
57	MG	1A	3895	1/1	0.94	0.16	20,20,20,20	0
57	MG	28	103	1/1	0.94	0.15	55,55,55,55	0
57	MG	2A	3546	1/1	0.94	0.14	36,36,36,36	0
57	MG	1x	114	1/1	0.94	0.14	66,66,66,66	0
57	MG	1A	3595	1/1	0.94	0.17	22,22,22,22	0
57	MG	1A	3502	1/1	0.94	0.25	66,66,66,66	0
57	MG	1A	3900	1/1	0.94	0.12	56,56,56,56	0
57	MG	1A	3597	1/1	0.94	0.12	30,30,30,30	0
57	MG	1A	3598	1/1	0.94	0.16	42,42,42,42	0
57	MG	2A	3268	1/1	0.94	0.34	54,54,54,54	0
57	MG	2A	3006	1/1	0.94	0.24	47,47,47,47	0
57	MG	1A	4069	1/1	0.94	0.08	68,68,68,68	0
57	MG	2A	3011	1/1	0.94	0.09	47,47,47,47	0
57	MG	1A	3145	1/1	0.94	0.28	26,26,26,26	0
57	MG	2A	3565	1/1	0.94	0.15	50,50,50,50	0
57	MG	1A	3146	1/1	0.94	0.14	30,30,30,30	0
57	MG	2A	3569	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	4072	1/1	0.94	0.10	56,56,56,56	0
57	MG	1A	3431	1/1	0.94	0.26	33,33,33,33	0
57	MG	1A	3605	1/1	0.94	0.23	31,31,31,31	0
57	MG	1A	3908	1/1	0.94	0.10	55,55,55,55	0
57	MG	1a	1624	1/1	0.94	0.20	48,48,48,48	0
57	MG	2A	3285	1/1	0.94	0.15	50,50,50,50	0
57	MG	1A	3310	1/1	0.94	0.29	52,52,52,52	0
57	MG	2A	3030	1/1	0.94	0.16	37,37,37,37	0
57	MG	2A	3288	1/1	0.94	0.08	52,52,52,52	0
57	MG	2A	3289	1/1	0.94	0.23	60,60,60,60	0
57	MG	2A	3592	1/1	0.94	0.14	22,22,22,22	0
57	MG	1A	3366	1/1	0.94	0.17	38,38,38,38	0
57	MG	1a	1629	1/1	0.94	0.15	46,46,46,46	0
57	MG	2A	3598	1/1	0.94	0.14	37,37,37,37	0
57	MG	1A	3913	1/1	0.94	0.06	48,48,48,48	0
57	MG	1B	206	1/1	0.94	0.29	43,43,43,43	0
57	MG	1A	3189	1/1	0.94	0.32	34,34,34,34	0
57	MG	1A	3755	1/1	0.94	0.18	38,38,38,38	0
57	MG	2a	1638	1/1	0.94	0.18	71,71,71,71	0
57	MG	2a	1640	1/1	0.94	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3040	1/1	0.94	0.20	57,57,57,57	0
57	MG	1A	3313	1/1	0.94	0.27	46,46,46,46	0
57	MG	1B	210	1/1	0.94	0.21	37,37,37,37	0
57	MG	1A	3437	1/1	0.94	0.31	45,45,45,45	0
57	MG	2A	3045	1/1	0.94	0.10	48,48,48,48	0
57	MG	1A	3263	1/1	0.94	0.11	44,44,44,44	0
57	MG	2a	1648	1/1	0.94	0.10	69,69,69,69	0
57	MG	2a	1649	1/1	0.94	0.06	64,64,64,64	0
57	MG	1B	216	1/1	0.94	0.18	34,34,34,34	0
57	MG	1A	3227	1/1	0.94	0.09	37,37,37,37	0
57	MG	2A	3051	1/1	0.94	0.17	48,48,48,48	0
57	MG	1a	1642	1/1	0.94	0.18	47,47,47,47	0
57	MG	1A	3518	1/1	0.94	0.15	46,46,46,46	0
57	MG	1a	1645	1/1	0.94	0.17	48,48,48,48	0
57	MG	2A	3313	1/1	0.94	0.07	50,50,50,50	0
57	MG	2a	1663	1/1	0.94	0.15	49,49,49,49	0
57	MG	2a	1664	1/1	0.94	0.07	48,48,48,48	0
57	MG	1a	1648	1/1	0.94	0.17	46,46,46,46	0
57	MG	1A	3117	1/1	0.94	0.33	35,35,35,35	0
57	MG	2a	1667	1/1	0.94	0.10	61,61,61,61	0
57	MG	2A	3058	1/1	0.94	0.09	53,53,53,53	0
57	MG	1A	3273	1/1	0.94	0.10	51,51,51,51	0
57	MG	2a	1670	1/1	0.94	0.11	58,58,58,58	0
57	MG	1A	3060	1/1	0.94	0.18	46,46,46,46	0
57	MG	1B	224	1/1	0.94	0.16	36,36,36,36	0
57	MG	1a	1654	1/1	0.94	0.10	42,42,42,42	0
57	MG	1A	3768	1/1	0.94	0.10	45,45,45,45	0
57	MG	2a	1679	1/1	0.94	0.09	67,67,67,67	0
57	MG	1A	3769	1/1	0.94	0.18	46,46,46,46	0
57	MG	1A	3375	1/1	0.94	0.47	50,50,50,50	0
57	MG	1a	1659	1/1	0.94	0.18	41,41,41,41	0
57	MG	1A	3195	1/1	0.94	0.24	28,28,28,28	0
57	MG	2A	3647	1/1	0.94	0.20	58,58,58,58	0
57	MG	2a	1688	1/1	0.94	0.14	50,50,50,50	0
57	MG	1a	1661	1/1	0.94	0.16	47,47,47,47	0
57	MG	2a	1691	1/1	0.94	0.11	52,52,52,52	0
57	MG	1A	3237	1/1	0.94	0.39	35,35,35,35	0
57	MG	2A	3331	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	3935	1/1	0.94	0.10	55,55,55,55	0
57	MG	2a	1697	1/1	0.94	0.13	59,59,59,59	0
57	MG	1A	3150	1/1	0.94	0.28	31,31,31,31	0
57	MG	1A	3641	1/1	0.94	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3529	1/1	0.94	0.27	40,40,40,40	0
57	MG	1A	3239	1/1	0.94	0.20	37,37,37,37	0
57	MG	1A	3945	1/1	0.94	0.12	23,23,23,23	0
57	MG	2A	3658	1/1	0.94	0.08	71,71,71,71	0
57	MG	2A	3085	1/1	0.94	0.23	49,49,49,49	0
57	MG	2a	1707	1/1	0.94	0.15	48,48,48,48	0
57	MG	1A	3946	1/1	0.94	0.11	43,43,43,43	0
57	MG	1A	3947	1/1	0.94	0.13	43,43,43,43	0
57	MG	1A	3052	1/1	0.94	0.20	38,38,38,38	0
57	MG	2A	3664	1/1	0.94	0.16	41,41,41,41	0
57	MG	1A	3158	1/1	0.94	0.14	29,29,29,29	0
57	MG	1A	3385	1/1	0.94	0.10	32,32,32,32	0
57	MG	1A	3386	1/1	0.94	0.29	31,31,31,31	0
57	MG	2A	3670	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3793	1/1	0.94	0.41	27,27,27,27	0
57	MG	1A	3455	1/1	0.94	0.26	40,40,40,40	0
57	MG	1A	3456	1/1	0.94	0.21	42,42,42,42	0
57	MG	1A	3959	1/1	0.94	0.15	41,41,41,41	0
57	MG	1A	3457	1/1	0.94	0.12	47,47,47,47	0
57	MG	2A	3681	1/1	0.94	0.09	70,70,70,70	0
57	MG	1A	3327	1/1	0.94	0.38	39,39,39,39	0
57	MG	2A	3102	1/1	0.94	0.07	50,50,50,50	0
57	MG	2A	3684	1/1	0.94	0.09	27,27,27,27	0
57	MG	1A	3801	1/1	0.94	0.14	27,27,27,27	0
57	MG	1A	3328	1/1	0.94	0.16	42,42,42,42	0
57	MG	1A	3966	1/1	0.94	0.14	64,64,64,64	0
57	MG	1A	3656	1/1	0.94	0.15	19,19,19,19	0
57	MG	2A	3362	1/1	0.94	0.09	58,58,58,58	0
57	MG	1A	3969	1/1	0.94	0.20	18,18,18,18	0
57	MG	1A	3807	1/1	0.94	0.13	21,21,21,21	0
57	MG	1A	3284	1/1	0.94	0.15	30,30,30,30	0
57	MG	1A	3285	1/1	0.94	0.26	44,44,44,44	0
57	MG	2A	3112	1/1	0.94	0.34	47,47,47,47	0
57	MG	1A	3814	1/1	0.94	0.14	38,38,38,38	0
57	MG	1N	205	1/1	0.94	0.26	43,43,43,43	0
57	MG	1A	3160	1/1	0.94	0.40	27,27,27,27	0
57	MG	2a	1742	1/1	0.94	0.10	69,69,69,69	0
57	MG	1A	3551	1/1	0.94	0.13	42,42,42,42	0
57	MG	1A	3336	1/1	0.94	0.29	41,41,41,41	0
57	MG	2a	1746	1/1	0.94	0.08	60,60,60,60	0
57	MG	1P	201	1/1	0.94	0.31	32,32,32,32	0
57	MG	1a	1714	1/1	0.94	0.09	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3375	1/1	0.94	0.08	58,58,58,58	0
57	MG	2a	1751	1/1	0.94	0.16	69,69,69,69	0
57	MG	2A	3122	1/1	0.94	0.52	62,62,62,62	0
57	MG	1P	202	1/1	0.94	0.25	30,30,30,30	0
57	MG	2A	3125	1/1	0.94	0.10	55,55,55,55	0
57	MG	1a	1718	1/1	0.94	0.35	41,41,41,41	0
57	MG	2a	1757	1/1	0.94	0.06	60,60,60,60	0
57	MG	1A	3398	1/1	0.94	0.16	38,38,38,38	0
57	MG	1A	3101	1/1	0.94	0.19	32,32,32,32	0
57	MG	1A	3340	1/1	0.94	0.22	57,57,57,57	0
57	MG	1A	3063	1/1	0.94	0.15	51,51,51,51	0
57	MG	2A	3384	1/1	0.94	0.20	39,39,39,39	0
57	MG	1a	1723	1/1	0.94	0.08	52,52,52,52	0
57	MG	1A	3559	1/1	0.94	0.56	32,32,32,32	0
57	MG	2A	3135	1/1	0.94	0.09	49,49,49,49	0
57	MG	2A	3723	1/1	0.94	0.31	63,63,63,63	0
57	MG	1a	1725	1/1	0.94	0.11	57,57,57,57	0
57	MG	1A	3678	1/1	0.94	0.17	20,20,20,20	0
57	MG	2A	3397	1/1	0.94	0.11	39,39,39,39	0
57	MG	2A	3731	1/1	0.94	0.55	42,42,42,42	0
57	MG	2a	1778	1/1	0.94	0.20	57,57,57,57	0
57	MG	2A	3139	1/1	0.94	0.19	51,51,51,51	0
57	MG	2A	3733	1/1	0.94	0.11	45,45,45,45	0
57	MG	2a	1783	1/1	0.94	0.10	57,57,57,57	0
57	MG	1a	1727	1/1	0.94	0.34	55,55,55,55	0
57	MG	2a	1785	1/1	0.94	0.09	66,66,66,66	0
57	MG	2a	1786	1/1	0.94	0.13	63,63,63,63	0
57	MG	2a	1787	1/1	0.94	0.08	64,64,64,64	0
57	MG	1A	3402	1/1	0.94	0.13	47,47,47,47	0
57	MG	2a	1789	1/1	0.94	0.16	61,61,61,61	0
57	MG	2A	3742	1/1	0.94	0.09	28,28,28,28	0
57	MG	1A	3343	1/1	0.94	0.26	34,34,34,34	0
57	MG	2a	1793	1/1	0.94	0.21	55,55,55,55	0
57	MG	2A	3744	1/1	0.94	0.14	51,51,51,51	0
57	MG	2a	1795	1/1	0.94	0.21	53,53,53,53	0
57	MG	1A	3992	1/1	0.94	0.16	25,25,25,25	0
57	MG	2A	3746	1/1	0.94	0.07	47,47,47,47	0
57	MG	2a	1798	1/1	0.94	0.09	71,71,71,71	0
57	MG	1a	1731	1/1	0.94	0.27	41,41,41,41	0
57	MG	1A	3993	1/1	0.94	0.08	31,31,31,31	0
57	MG	1a	1733	1/1	0.94	0.20	48,48,48,48	0
57	MG	1a	1734	1/1	0.94	0.19	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3246	1/1	0.94	0.40	42,42,42,42	0
57	MG	1A	3684	1/1	0.94	0.07	33,33,33,33	0
57	MG	1T	3601	1/1	0.94	0.29	50,50,50,50	0
57	MG	2A	3413	1/1	0.94	0.17	53,53,53,53	0
57	MG	1A	3406	1/1	0.94	0.09	60,60,60,60	0
57	MG	2a	1808	1/1	0.94	0.22	57,57,57,57	0
57	MG	2A	3159	1/1	0.94	0.26	62,62,62,62	0
57	MG	1A	3686	1/1	0.94	0.19	30,30,30,30	0
57	MG	2e	201	1/1	0.94	0.10	59,59,59,59	0
57	MG	1U	203	1/1	0.94	0.17	51,51,51,51	0
57	MG	1a	1747	1/1	0.94	0.17	27,27,27,27	0
57	MG	2A	3168	1/1	0.94	0.15	45,45,45,45	0
57	MG	1U	204	1/1	0.94	0.32	35,35,35,35	0
57	MG	1a	1751	1/1	0.94	0.17	47,47,47,47	0
57	MG	1a	1752	1/1	0.94	0.16	78,78,78,78	0
57	MG	2A	3770	1/1	0.94	0.12	41,41,41,41	0
57	MG	2l	202	1/1	0.94	0.24	55,55,55,55	0
57	MG	1a	1755	1/1	0.94	0.10	43,43,43,43	0
57	MG	1A	3689	1/1	0.94	0.19	23,23,23,23	0
57	MG	1A	3842	1/1	0.94	0.14	40,40,40,40	0
57	MG	1A	3567	1/1	0.94	0.45	37,37,37,37	0
57	MG	2A	3779	1/1	0.94	0.12	58,58,58,58	0
57	MG	1A	3478	1/1	0.94	0.29	31,31,31,31	0
57	MG	1A	3569	1/1	0.94	0.15	26,26,26,26	0
57	MG	2A	3439	1/1	0.94	0.17	62,62,62,62	0
57	MG	2A	3440	1/1	0.94	0.12	48,48,48,48	0
57	MG	1a	1767	1/1	0.94	0.12	55,55,55,55	0
57	MG	1A	3346	1/1	0.94	0.26	48,48,48,48	0
57	MG	1A	4013	1/1	0.94	0.28	45,45,45,45	0
57	MG	2A	3793	1/1	0.94	0.09	29,29,29,29	0
57	MG	1A	3847	1/1	0.94	0.24	42,42,42,42	0
57	MG	2A	3446	1/1	0.94	0.84	44,44,44,44	0
57	MG	1a	1774	1/1	0.94	0.11	43,43,43,43	0
57	MG	2x	104	1/1	0.94	0.12	50,50,50,50	0
57	MG	1A	4018	1/1	0.94	0.11	45,45,45,45	0
57	MG	2x	106	1/1	0.94	0.16	54,54,54,54	0
57	MG	1A	3053	1/1	0.94	0.20	29,29,29,29	0
57	MG	2A	3803	1/1	0.94	0.14	45,45,45,45	0
57	MG	1A	3850	1/1	0.94	0.22	60,60,60,60	0
57	MG	2A	3453	1/1	0.94	0.10	41,41,41,41	0
57	MG	1a	1780	1/1	0.94	0.11	58,58,58,58	0
57	MG	2A	3455	1/1	0.94	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3811	1/1	0.94	0.07	47,47,47,47	0
57	MG	1A	3166	1/1	0.95	0.16	32,32,32,32	0
57	MG	2A	3203	1/1	0.95	0.10	51,51,51,51	0
57	MG	2A	3635	1/1	0.95	0.25	46,46,46,46	0
57	MG	2A	3637	1/1	0.95	0.36	66,66,66,66	0
57	MG	27	101	1/1	0.95	0.11	55,55,55,55	0
57	MG	2A	3638	1/1	0.95	0.17	64,64,64,64	0
57	MG	1a	1686	1/1	0.95	0.18	35,35,35,35	0
57	MG	2A	3392	1/1	0.95	0.21	42,42,42,42	0
57	MG	1A	3710	1/1	0.95	0.22	23,23,23,23	0
57	MG	1A	3316	1/1	0.95	0.17	56,56,56,56	0
57	MG	1U	208	1/1	0.95	0.19	30,30,30,30	0
57	MG	1U	209	1/1	0.95	0.30	38,38,38,38	0
57	MG	1A	4059	1/1	0.95	0.12	24,24,24,24	0
57	MG	1A	3317	1/1	0.95	0.11	57,57,57,57	0
57	MG	1A	3714	1/1	0.95	0.11	65,65,65,65	0
57	MG	1A	3937	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3715	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3108	1/1	0.95	0.09	40,40,40,40	0
57	MG	1A	3618	1/1	0.95	0.10	21,21,21,21	0
57	MG	1A	3365	1/1	0.95	0.34	34,34,34,34	0
57	MG	1A	4067	1/1	0.95	0.11	61,61,61,61	0
57	MG	2A	3039	1/1	0.95	0.15	52,52,52,52	0
57	MG	2A	3410	1/1	0.95	0.16	50,50,50,50	0
57	MG	1A	3278	1/1	0.95	0.19	25,25,25,25	0
57	MG	1A	3201	1/1	0.95	0.14	24,24,24,24	0
57	MG	2a	1616	1/1	0.95	0.11	50,50,50,50	0
57	MG	1A	3029	1/1	0.95	0.23	26,26,26,26	0
57	MG	2A	3226	1/1	0.95	0.54	39,39,39,39	0
57	MG	1A	3242	1/1	0.95	0.18	28,28,28,28	0
57	MG	1A	3631	1/1	0.95	0.17	62,62,62,62	0
57	MG	2A	3046	1/1	0.95	0.13	24,24,24,24	0
57	MG	2a	1622	1/1	0.95	0.10	45,45,45,45	0
57	MG	1A	3952	1/1	0.95	0.24	44,44,44,44	0
57	MG	2A	3234	1/1	0.95	0.29	41,41,41,41	0
57	MG	1A	3552	1/1	0.95	0.22	26,26,26,26	0
57	MG	1A	3169	1/1	0.95	0.19	14,14,14,14	0
57	MG	1A	3171	1/1	0.95	0.38	38,38,38,38	0
57	MG	1A	3426	1/1	0.95	0.30	33,33,33,33	0
57	MG	2A	3429	1/1	0.95	0.15	51,51,51,51	0
57	MG	1A	3639	1/1	0.95	0.09	35,35,35,35	0
57	MG	1A	3094	1/1	0.95	0.11	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3207	1/1	0.95	0.16	31,31,31,31	0
57	MG	1A	3013	1/1	0.95	0.20	25,25,25,25	0
57	MG	12	101	1/1	0.95	0.18	39,39,39,39	0
57	MG	2A	3059	1/1	0.95	0.09	33,33,33,33	0
57	MG	2a	1637	1/1	0.95	0.15	48,48,48,48	0
57	MG	1A	3430	1/1	0.95	0.11	40,40,40,40	0
57	MG	2a	1639	1/1	0.95	0.13	53,53,53,53	0
57	MG	13	101	1/1	0.95	0.13	29,29,29,29	0
57	MG	1A	3376	1/1	0.95	0.51	25,25,25,25	0
57	MG	2A	3689	1/1	0.95	0.12	25,25,25,25	0
57	MG	1A	3852	1/1	0.95	0.13	40,40,40,40	0
57	MG	1A	3180	1/1	0.95	0.20	51,51,51,51	0
57	MG	2A	3066	1/1	0.95	0.12	47,47,47,47	0
57	MG	15	101	1/1	0.95	0.59	34,34,34,34	0
57	MG	1A	3009	1/1	0.95	0.10	25,25,25,25	0
57	MG	2A	3450	1/1	0.95	0.14	36,36,36,36	0
57	MG	2A	3696	1/1	0.95	0.08	35,35,35,35	0
57	MG	1A	3144	1/1	0.95	0.39	35,35,35,35	0
57	MG	1A	3331	1/1	0.95	0.16	35,35,35,35	0
57	MG	1A	3497	1/1	0.95	0.31	34,34,34,34	0
57	MG	2a	1656	1/1	0.95	0.12	56,56,56,56	0
57	MG	1A	3332	1/1	0.95	0.66	35,35,35,35	0
57	MG	2a	1659	1/1	0.95	0.11	59,59,59,59	0
57	MG	2A	3456	1/1	0.95	0.35	57,57,57,57	0
57	MG	1A	3865	1/1	0.95	0.09	48,48,48,48	0
57	MG	2A	3076	1/1	0.95	0.17	22,22,22,22	0
57	MG	1B	223	1/1	0.95	0.18	53,53,53,53	0
57	MG	1a	1741	1/1	0.95	0.19	54,54,54,54	0
57	MG	2A	3079	1/1	0.95	0.19	40,40,40,40	0
57	MG	1A	3653	1/1	0.95	0.17	34,34,34,34	0
57	MG	1A	3055	1/1	0.95	0.16	26,26,26,26	0
57	MG	2A	3464	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3083	1/1	0.95	0.32	48,48,48,48	0
57	MG	2A	3270	1/1	0.95	0.51	48,48,48,48	0
57	MG	2A	3272	1/1	0.95	0.28	38,38,38,38	0
57	MG	2a	1673	1/1	0.95	0.09	62,62,62,62	0
57	MG	1a	1748	1/1	0.95	0.15	33,33,33,33	0
57	MG	1a	1749	1/1	0.95	0.10	30,30,30,30	0
57	MG	1A	3980	1/1	0.95	0.11	51,51,51,51	0
57	MG	2a	1681	1/1	0.95	0.24	56,56,56,56	0
57	MG	2A	3087	1/1	0.95	0.39	42,42,42,42	0
57	MG	2A	3473	1/1	0.95	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3474	1/1	0.95	0.11	48,48,48,48	0
57	MG	1A	3572	1/1	0.95	0.10	51,51,51,51	0
57	MG	2A	3729	1/1	0.95	0.11	37,37,37,37	0
57	MG	1B	229	1/1	0.95	0.12	57,57,57,57	0
57	MG	2A	3090	1/1	0.95	0.27	33,33,33,33	0
57	MG	2A	3281	1/1	0.95	0.07	58,58,58,58	0
57	MG	2A	3479	1/1	0.95	0.20	53,53,53,53	0
57	MG	2a	1693	1/1	0.95	0.08	58,58,58,58	0
57	MG	1A	3384	1/1	0.95	0.29	29,29,29,29	0
57	MG	2A	3737	1/1	0.95	0.09	51,51,51,51	0
57	MG	1B	231	1/1	0.95	0.09	44,44,44,44	0
57	MG	2A	3741	1/1	0.95	0.09	51,51,51,51	0
57	MG	1A	3873	1/1	0.95	0.10	44,44,44,44	0
57	MG	1B	233	1/1	0.95	0.21	65,65,65,65	0
57	MG	2A	3484	1/1	0.95	0.15	66,66,66,66	0
57	MG	2a	1703	1/1	0.95	0.15	50,50,50,50	0
57	MG	2A	3096	1/1	0.95	0.25	52,52,52,52	0
57	MG	2A	3486	1/1	0.95	0.10	49,49,49,49	0
57	MG	1D	301	1/1	0.95	0.18	25,25,25,25	0
57	MG	1A	3986	1/1	0.95	0.15	19,19,19,19	0
57	MG	1A	3066	1/1	0.95	0.25	42,42,42,42	0
57	MG	1a	1610	1/1	0.95	0.11	27,27,27,27	0
57	MG	1a	1770	1/1	0.95	0.38	64,64,64,64	0
57	MG	1A	3338	1/1	0.95	0.22	50,50,50,50	0
57	MG	2A	3754	1/1	0.95	0.15	47,47,47,47	0
57	MG	1D	309	1/1	0.95	0.20	34,34,34,34	0
57	MG	1D	312	1/1	0.95	0.22	39,39,39,39	0
57	MG	2A	3758	1/1	0.95	0.18	56,56,56,56	0
57	MG	1A	3760	1/1	0.95	0.31	33,33,33,33	0
57	MG	2A	3499	1/1	0.95	0.14	35,35,35,35	0
57	MG	1A	3761	1/1	0.95	0.12	23,23,23,23	0
57	MG	1a	1618	1/1	0.95	0.23	47,47,47,47	0
57	MG	1a	1779	1/1	0.95	0.15	60,60,60,60	0
57	MG	1A	3660	1/1	0.95	0.16	20,20,20,20	0
57	MG	2a	1722	1/1	0.95	0.20	61,61,61,61	0
57	MG	2A	3507	1/1	0.95	0.12	48,48,48,48	0
57	MG	1A	3661	1/1	0.95	0.15	22,22,22,22	0
57	MG	1A	3387	1/1	0.95	0.20	33,33,33,33	0
57	MG	2A	3303	1/1	0.95	0.22	50,50,50,50	0
57	MG	2A	3772	1/1	0.95	0.12	46,46,46,46	0
57	MG	1A	3884	1/1	0.95	0.15	51,51,51,51	0
57	MG	2A	3774	1/1	0.95	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
57	MG	1a	1785	1/1	0.95	0.10	52,52,52,52	0
57	MG	2A	3115	1/1	0.95	0.43	46,46,46,46	0
57	MG	2A	3307	1/1	0.95	0.08	52,52,52,52	0
57	MG	2A	3778	1/1	0.95	0.17	35,35,35,35	0
57	MG	1a	1786	1/1	0.95	0.16	51,51,51,51	0
57	MG	2A	3520	1/1	0.95	0.18	42,42,42,42	0
57	MG	1A	3388	1/1	0.95	0.25	42,42,42,42	0
57	MG	1E	310	1/1	0.95	0.23	40,40,40,40	0
57	MG	2A	3525	1/1	0.95	0.09	48,48,48,48	0
57	MG	2A	3526	1/1	0.95	0.10	38,38,38,38	0
57	MG	1a	1789	1/1	0.95	0.16	71,71,71,71	0
57	MG	1E	312	1/1	0.95	0.13	43,43,43,43	0
57	MG	2a	1745	1/1	0.95	0.15	75,75,75,75	0
57	MG	1A	3999	1/1	0.95	0.18	30,30,30,30	0
57	MG	1A	3389	1/1	0.95	0.29	40,40,40,40	0
57	MG	1A	3390	1/1	0.95	0.31	42,42,42,42	0
57	MG	2A	3532	1/1	0.95	0.17	31,31,31,31	0
57	MG	2A	3798	1/1	0.95	0.09	37,37,37,37	0
57	MG	2A	3319	1/1	0.95	0.28	51,51,51,51	0
57	MG	1A	3068	1/1	0.95	0.16	12,12,12,12	0
57	MG	1a	1798	1/1	0.95	0.12	47,47,47,47	0
57	MG	2A	3536	1/1	0.95	0.09	37,37,37,37	0
57	MG	1A	3049	1/1	0.95	0.25	30,30,30,30	0
57	MG	2a	1758	1/1	0.95	0.16	60,60,60,60	0
57	MG	2A	3806	1/1	0.95	0.17	22,22,22,22	0
57	MG	2a	1762	1/1	0.95	0.09	42,42,42,42	0
57	MG	2a	1763	1/1	0.95	0.15	44,44,44,44	0
57	MG	1A	3255	1/1	0.95	0.18	51,51,51,51	0
57	MG	1A	3256	1/1	0.95	0.35	42,42,42,42	0
57	MG	1A	3344	1/1	0.95	0.13	43,43,43,43	0
57	MG	1A	3041	1/1	0.95	0.30	30,30,30,30	0
57	MG	1A	3397	1/1	0.95	0.18	37,37,37,37	0
57	MG	1a	1810	1/1	0.95	0.18	57,57,57,57	0
57	MG	2A	3816	1/1	0.95	0.13	32,32,32,32	0
57	MG	1A	4017	1/1	0.95	0.13	19,19,19,19	0
57	MG	1A	3899	1/1	0.95	0.29	32,32,32,32	0
57	MG	1A	3780	1/1	0.95	0.10	45,45,45,45	0
57	MG	2A	3820	1/1	0.95	0.14	36,36,36,36	0
57	MG	1b	301	1/1	0.95	0.10	79,79,79,79	0
57	MG	2a	1777	1/1	0.95	0.11	59,59,59,59	0
57	MG	2A	3823	1/1	0.95	0.19	56,56,56,56	0
57	MG	1A	3781	1/1	0.95	0.19	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1781	1/1	0.95	0.27	66,66,66,66	0
57	MG	2A	3552	1/1	0.95	0.09	40,40,40,40	0
57	MG	1a	1644	1/1	0.95	0.12	57,57,57,57	0
57	MG	1A	3124	1/1	0.95	0.52	34,34,34,34	0
57	MG	2A	3555	1/1	0.95	0.14	36,36,36,36	0
57	MG	2A	3148	1/1	0.95	0.10	58,58,58,58	0
57	MG	1a	1646	1/1	0.95	0.08	42,42,42,42	0
57	MG	1a	1647	1/1	0.95	0.16	42,42,42,42	0
57	MG	1A	3222	1/1	0.95	0.29	46,46,46,46	0
57	MG	1A	3787	1/1	0.95	0.10	42,42,42,42	0
57	MG	1l	202	1/1	0.95	0.16	57,57,57,57	0
57	MG	2A	3837	1/1	0.95	0.07	58,58,58,58	0
57	MG	1A	3522	1/1	0.95	0.23	24,24,24,24	0
57	MG	2A	3566	1/1	0.95	0.09	38,38,38,38	0
57	MG	2A	3567	1/1	0.95	0.10	26,26,26,26	0
57	MG	1A	3154	1/1	0.95	0.17	39,39,39,39	0
57	MG	1n	102	1/1	0.95	0.10	40,40,40,40	0
57	MG	2A	3160	1/1	0.95	0.19	45,45,45,45	0
57	MG	2A	3572	1/1	0.95	0.22	58,58,58,58	0
57	MG	2A	3161	1/1	0.95	0.14	32,32,32,32	0
57	MG	2A	3162	1/1	0.95	0.08	54,54,54,54	0
57	MG	2A	3163	1/1	0.95	0.27	74,74,74,74	0
57	MG	1A	3306	1/1	0.95	0.38	26,26,26,26	0
57	MG	1A	3226	1/1	0.95	0.46	31,31,31,31	0
57	MG	2B	207	1/1	0.95	0.13	61,61,61,61	0
57	MG	1A	3192	1/1	0.95	0.30	24,24,24,24	0
57	MG	1A	3695	1/1	0.95	0.23	30,30,30,30	0
57	MG	1A	4033	1/1	0.95	0.16	35,35,35,35	0
57	MG	2A	3589	1/1	0.95	0.12	55,55,55,55	0
57	MG	2A	3590	1/1	0.95	0.23	52,52,52,52	0
57	MG	1A	3128	1/1	0.95	0.17	32,32,32,32	0
57	MG	2f	201	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3697	1/1	0.95	0.14	37,37,37,37	0
57	MG	1A	3105	1/1	0.95	0.20	33,33,33,33	0
57	MG	1Q	202	1/1	0.95	0.17	32,32,32,32	0
57	MG	2A	3596	1/1	0.95	0.13	37,37,37,37	0
57	MG	1A	3804	1/1	0.95	0.19	40,40,40,40	0
57	MG	2A	3600	1/1	0.95	0.11	42,42,42,42	0
57	MG	2D	301	1/1	0.95	0.34	32,32,32,32	0
57	MG	1x	106	1/1	0.95	0.19	58,58,58,58	0
57	MG	1A	3311	1/1	0.95	0.16	34,34,34,34	0
57	MG	2A	3604	1/1	0.95	0.13	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1R	202	1/1	0.95	0.18	40,40,40,40	0
57	MG	1a	1666	1/1	0.95	0.14	57,57,57,57	0
57	MG	1a	1667	1/1	0.95	0.23	60,60,60,60	0
57	MG	1A	3701	1/1	0.95	0.08	63,63,63,63	0
57	MG	1A	4042	1/1	0.95	0.30	40,40,40,40	0
57	MG	1A	3808	1/1	0.95	0.22	32,32,32,32	0
57	MG	1A	3924	1/1	0.95	0.17	46,46,46,46	0
57	MG	1A	3232	1/1	0.95	0.15	24,24,24,24	0
57	MG	1A	3534	1/1	0.95	0.27	28,28,28,28	0
57	MG	2A	3618	1/1	0.95	0.10	43,43,43,43	0
57	MG	2w	106	1/1	0.95	0.36	49,49,49,49	0
57	MG	2A	3192	1/1	0.95	0.13	52,52,52,52	0
57	MG	1A	3010	1/1	0.95	0.15	32,32,32,32	0
57	MG	1T	3602	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	4053	1/1	0.95	0.15	22,22,22,22	0
57	MG	2T	201	1/1	0.95	0.12	47,47,47,47	0
57	MG	1a	1681	1/1	0.95	0.12	58,58,58,58	0
57	MG	1A	3815	1/1	0.95	0.15	55,55,55,55	0
57	MG	2V	202	1/1	0.95	0.56	56,56,56,56	0
57	MG	1A	3107	1/1	0.95	0.34	35,35,35,35	0
57	MG	2A	3627	1/1	0.95	0.08	52,52,52,52	0
58	K	2x	101	1/1	0.95	0.11	46,46,46,46	0
60	ZN	1Y	205	1/1	0.95	0.16	59,59,59,59	0
57	MG	20	101	1/1	0.95	0.15	54,54,54,54	0
57	MG	2A	3014	1/1	0.95	0.15	36,36,36,36	0
57	MG	2A	3386	1/1	0.95	0.23	40,40,40,40	0
60	ZN	2n	102	1/1	0.95	0.11	83,83,83,83	0
57	MG	10	107	1/1	0.96	0.17	42,42,42,42	0
57	MG	1A	3163	1/1	0.96	0.14	49,49,49,49	0
57	MG	2A	3119	1/1	0.96	0.11	42,42,42,42	0
57	MG	1A	3795	1/1	0.96	0.16	38,38,38,38	0
57	MG	2A	3599	1/1	0.96	0.12	56,56,56,56	0
57	MG	1a	1760	1/1	0.96	0.14	49,49,49,49	0
57	MG	1A	3032	1/1	0.96	0.34	29,29,29,29	0
57	MG	1a	1765	1/1	0.96	0.15	44,44,44,44	0
57	MG	2A	3347	1/1	0.96	0.53	48,48,48,48	0
57	MG	2T	203	1/1	0.96	0.13	39,39,39,39	0
57	MG	1A	3079	1/1	0.96	0.26	32,32,32,32	0
57	MG	1A	3510	1/1	0.96	0.26	32,32,32,32	0
57	MG	2V	203	1/1	0.96	0.72	46,46,46,46	0
57	MG	1a	1768	1/1	0.96	0.18	41,41,41,41	0
57	MG	1A	3299	1/1	0.96	0.20	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3688	1/1	0.96	0.11	49,49,49,49	0
57	MG	2A	3131	1/1	0.96	0.39	36,36,36,36	0
57	MG	1A	3131	1/1	0.96	0.20	32,32,32,32	0
57	MG	2A	3614	1/1	0.96	0.17	42,42,42,42	0
57	MG	1A	3690	1/1	0.96	0.15	18,18,18,18	0
57	MG	2A	3359	1/1	0.96	0.29	53,53,53,53	0
57	MG	1A	3451	1/1	0.96	0.24	59,59,59,59	0
57	MG	2A	3361	1/1	0.96	0.10	51,51,51,51	0
57	MG	1A	3132	1/1	0.96	0.13	35,35,35,35	0
57	MG	1A	3809	1/1	0.96	0.16	34,34,34,34	0
57	MG	1A	3302	1/1	0.96	0.09	37,37,37,37	0
57	MG	1A	3008	1/1	0.96	0.12	25,25,25,25	0
57	MG	1A	3940	1/1	0.96	0.18	42,42,42,42	0
57	MG	2A	3141	1/1	0.96	0.23	35,35,35,35	0
57	MG	2a	1601	1/1	0.96	0.16	52,52,52,52	0
57	MG	1A	3941	1/1	0.96	0.18	53,53,53,53	0
57	MG	1B	205	1/1	0.96	0.15	49,49,49,49	0
57	MG	1A	3942	1/1	0.96	0.10	33,33,33,33	0
57	MG	1A	3134	1/1	0.96	0.09	41,41,41,41	0
57	MG	2A	3147	1/1	0.96	0.14	37,37,37,37	0
57	MG	1A	3170	1/1	0.96	0.14	39,39,39,39	0
57	MG	2A	3636	1/1	0.96	0.07	56,56,56,56	0
57	MG	1A	3699	1/1	0.96	0.16	44,44,44,44	0
57	MG	1A	3135	1/1	0.96	0.23	24,24,24,24	0
57	MG	2A	3151	1/1	0.96	0.20	46,46,46,46	0
57	MG	2A	3640	1/1	0.96	0.14	61,61,61,61	0
57	MG	1A	3819	1/1	0.96	0.20	48,48,48,48	0
57	MG	1B	212	1/1	0.96	0.12	57,57,57,57	0
57	MG	1B	213	1/1	0.96	0.22	42,42,42,42	0
57	MG	1a	1602	1/1	0.96	0.14	59,59,59,59	0
57	MG	1A	3948	1/1	0.96	0.15	39,39,39,39	0
57	MG	1a	1796	1/1	0.96	0.17	72,72,72,72	0
57	MG	1B	215	1/1	0.96	0.23	44,44,44,44	0
57	MG	1A	3523	1/1	0.96	0.25	46,46,46,46	0
57	MG	2A	3385	1/1	0.96	0.21	55,55,55,55	0
57	MG	1a	1799	1/1	0.96	0.12	54,54,54,54	0
57	MG	1A	3458	1/1	0.96	0.13	43,43,43,43	0
57	MG	2A	3164	1/1	0.96	0.07	53,53,53,53	0
57	MG	1a	1608	1/1	0.96	0.18	42,42,42,42	0
57	MG	1a	1804	1/1	0.96	0.12	46,46,46,46	0
57	MG	1A	3703	1/1	0.96	0.10	13,13,13,13	0
57	MG	1A	3824	1/1	0.96	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3395	1/1	0.96	0.29	53,53,53,53	0
57	MG	1A	3213	1/1	0.96	0.37	37,37,37,37	0
57	MG	1A	3826	1/1	0.96	0.25	52,52,52,52	0
57	MG	1a	1613	1/1	0.96	0.23	46,46,46,46	0
57	MG	1a	1811	1/1	0.96	0.16	42,42,42,42	0
57	MG	2A	3663	1/1	0.96	0.16	67,67,67,67	0
57	MG	2A	3401	1/1	0.96	0.23	54,54,54,54	0
57	MG	1A	3955	1/1	0.96	0.14	48,48,48,48	0
57	MG	2A	3666	1/1	0.96	0.11	56,56,56,56	0
57	MG	2A	3667	1/1	0.96	0.06	57,57,57,57	0
57	MG	1A	3956	1/1	0.96	0.07	49,49,49,49	0
57	MG	2a	1641	1/1	0.96	0.14	62,62,62,62	0
57	MG	2A	3176	1/1	0.96	0.20	64,64,64,64	0
57	MG	1a	1616	1/1	0.96	0.11	42,42,42,42	0
57	MG	1B	225	1/1	0.96	0.15	32,32,32,32	0
57	MG	2A	3672	1/1	0.96	0.14	52,52,52,52	0
57	MG	1A	3601	1/1	0.96	0.12	41,41,41,41	0
57	MG	1A	3602	1/1	0.96	0.14	15,15,15,15	0
57	MG	1A	3707	1/1	0.96	0.17	40,40,40,40	0
57	MG	2A	3677	1/1	0.96	0.12	42,42,42,42	0
57	MG	2A	3678	1/1	0.96	0.10	65,65,65,65	0
57	MG	1A	3175	1/1	0.96	0.15	20,20,20,20	0
57	MG	2A	3680	1/1	0.96	0.07	60,60,60,60	0
57	MG	2A	3186	1/1	0.96	0.15	48,48,48,48	0
57	MG	2A	3412	1/1	0.96	0.29	42,42,42,42	0
57	MG	1A	3405	1/1	0.96	0.11	35,35,35,35	0
57	MG	1A	3962	1/1	0.96	0.12	35,35,35,35	0
57	MG	1A	3833	1/1	0.96	0.11	42,42,42,42	0
57	MG	1a	1626	1/1	0.96	0.15	49,49,49,49	0
57	MG	2a	1662	1/1	0.96	0.10	35,35,35,35	0
57	MG	2A	3417	1/1	0.96	0.13	46,46,46,46	0
57	MG	1A	3609	1/1	0.96	0.14	24,24,24,24	0
57	MG	1B	234	1/1	0.96	0.06	42,42,42,42	0
57	MG	1B	235	1/1	0.96	0.15	37,37,37,37	0
57	MG	1A	3965	1/1	0.96	0.09	55,55,55,55	0
57	MG	1A	3462	1/1	0.96	0.15	36,36,36,36	0
57	MG	1A	3611	1/1	0.96	0.18	36,36,36,36	0
57	MG	1D	305	1/1	0.96	0.14	20,20,20,20	0
57	MG	1D	306	1/1	0.96	0.17	35,35,35,35	0
57	MG	1A	3612	1/1	0.96	0.15	46,46,46,46	0
57	MG	1A	3177	1/1	0.96	0.14	28,28,28,28	0
57	MG	2a	1674	1/1	0.96	0.17	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3432	1/1	0.96	0.27	41,41,41,41	0
57	MG	2A	3699	1/1	0.96	0.14	42,42,42,42	0
57	MG	2A	3700	1/1	0.96	0.11	62,62,62,62	0
57	MG	2A	3701	1/1	0.96	0.25	36,36,36,36	0
57	MG	2A	3434	1/1	0.96	0.35	42,42,42,42	0
57	MG	1D	311	1/1	0.96	0.49	32,32,32,32	0
57	MG	1A	3110	1/1	0.96	0.19	35,35,35,35	0
57	MG	1A	3615	1/1	0.96	0.13	51,51,51,51	0
57	MG	1x	105	1/1	0.96	0.17	44,44,44,44	0
57	MG	1a	1641	1/1	0.96	0.09	55,55,55,55	0
57	MG	2a	1689	1/1	0.96	0.16	57,57,57,57	0
57	MG	1A	3532	1/1	0.96	0.14	51,51,51,51	0
57	MG	1A	3035	1/1	0.96	0.20	35,35,35,35	0
57	MG	1A	3140	1/1	0.96	0.23	15,15,15,15	0
57	MG	2A	3211	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	3468	1/1	0.96	0.15	35,35,35,35	0
57	MG	2a	1695	1/1	0.96	0.28	55,55,55,55	0
57	MG	1A	3538	1/1	0.96	0.34	27,27,27,27	0
57	MG	1A	3849	1/1	0.96	0.14	37,37,37,37	0
57	MG	1A	3181	1/1	0.96	0.23	51,51,51,51	0
57	MG	1A	3624	1/1	0.96	0.07	41,41,41,41	0
57	MG	2A	3451	1/1	0.96	0.06	54,54,54,54	0
57	MG	1A	3625	1/1	0.96	0.14	35,35,35,35	0
57	MG	2a	1702	1/1	0.96	0.10	52,52,52,52	0
57	MG	1A	3853	1/1	0.96	0.24	29,29,29,29	0
57	MG	2A	3002	1/1	0.96	0.25	52,52,52,52	0
57	MG	1A	3987	1/1	0.96	0.16	27,27,27,27	0
57	MG	1A	3264	1/1	0.96	0.21	22,22,22,22	0
57	MG	1F	307	1/1	0.96	0.23	26,26,26,26	0
57	MG	1A	3471	1/1	0.96	0.18	39,39,39,39	0
57	MG	1A	3363	1/1	0.96	0.70	43,43,43,43	0
57	MG	2A	3010	1/1	0.96	0.13	38,38,38,38	0
57	MG	1a	1658	1/1	0.96	0.13	45,45,45,45	0
57	MG	2A	3013	1/1	0.96	0.24	48,48,48,48	0
57	MG	2A	3736	1/1	0.96	0.13	45,45,45,45	0
57	MG	2A	3232	1/1	0.96	0.24	42,42,42,42	0
57	MG	1A	3364	1/1	0.96	0.15	36,36,36,36	0
57	MG	2A	3739	1/1	0.96	0.09	44,44,44,44	0
57	MG	1A	3634	1/1	0.96	0.15	28,28,28,28	0
57	MG	2A	3016	1/1	0.96	0.09	63,63,63,63	0
57	MG	2A	3017	1/1	0.96	0.12	44,44,44,44	0
57	MG	1A	3023	1/1	0.96	0.15	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3267	1/1	0.96	0.42	34,34,34,34	0
57	MG	2A	3024	1/1	0.96	0.47	48,48,48,48	0
57	MG	2A	3471	1/1	0.96	0.22	35,35,35,35	0
57	MG	1A	3269	1/1	0.96	0.34	35,35,35,35	0
57	MG	1A	3638	1/1	0.96	0.19	36,36,36,36	0
57	MG	2a	1726	1/1	0.96	0.23	33,33,33,33	0
57	MG	1A	3869	1/1	0.96	0.14	28,28,28,28	0
57	MG	1A	3870	1/1	0.96	0.19	19,19,19,19	0
57	MG	1A	4001	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	4003	1/1	0.96	0.10	54,54,54,54	0
57	MG	1N	203	1/1	0.96	0.18	40,40,40,40	0
57	MG	2A	3756	1/1	0.96	0.11	40,40,40,40	0
57	MG	1A	4004	1/1	0.96	0.07	56,56,56,56	0
57	MG	1A	3549	1/1	0.96	0.30	24,24,24,24	0
57	MG	2A	3034	1/1	0.96	0.25	39,39,39,39	0
57	MG	1A	3477	1/1	0.96	0.23	37,37,37,37	0
57	MG	1A	3098	1/1	0.96	0.13	34,34,34,34	0
57	MG	2A	3255	1/1	0.96	0.23	45,45,45,45	0
57	MG	2A	3256	1/1	0.96	0.24	50,50,50,50	0
57	MG	1A	3271	1/1	0.96	0.15	36,36,36,36	0
57	MG	1A	3069	1/1	0.96	0.28	28,28,28,28	0
57	MG	1a	1676	1/1	0.96	0.23	56,56,56,56	0
57	MG	1A	3115	1/1	0.96	0.18	20,20,20,20	0
57	MG	2A	3042	1/1	0.96	0.06	72,72,72,72	0
57	MG	1a	1678	1/1	0.96	0.13	48,48,48,48	0
57	MG	1A	3424	1/1	0.96	0.48	37,37,37,37	0
57	MG	1A	4015	1/1	0.96	0.10	55,55,55,55	0
57	MG	2a	1750	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3070	1/1	0.96	0.49	35,35,35,35	0
57	MG	1A	3276	1/1	0.96	0.15	47,47,47,47	0
57	MG	1A	3881	1/1	0.96	0.15	35,35,35,35	0
57	MG	1A	3882	1/1	0.96	0.10	30,30,30,30	0
57	MG	1Q	205	1/1	0.96	0.34	41,41,41,41	0
57	MG	1a	1690	1/1	0.96	0.26	44,44,44,44	0
57	MG	1Q	206	1/1	0.96	0.19	33,33,33,33	0
57	MG	2a	1759	1/1	0.96	0.15	57,57,57,57	0
57	MG	2A	3506	1/1	0.96	0.08	31,31,31,31	0
57	MG	2A	3274	1/1	0.96	0.10	47,47,47,47	0
57	MG	2A	3785	1/1	0.96	0.06	33,33,33,33	0
57	MG	1a	1693	1/1	0.96	0.09	40,40,40,40	0
57	MG	2A	3787	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3085	1/1	0.96	0.21	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3789	1/1	0.96	0.16	37,37,37,37	0
57	MG	1A	3561	1/1	0.96	0.14	36,36,36,36	0
57	MG	2A	3511	1/1	0.96	0.16	53,53,53,53	0
57	MG	1A	3040	1/1	0.96	0.22	25,25,25,25	0
57	MG	1a	1697	1/1	0.96	0.16	47,47,47,47	0
57	MG	1A	3887	1/1	0.96	0.17	40,40,40,40	0
57	MG	1A	3762	1/1	0.96	0.12	36,36,36,36	0
57	MG	1A	3087	1/1	0.96	0.21	30,30,30,30	0
57	MG	1A	3236	1/1	0.96	0.20	25,25,25,25	0
57	MG	2A	3802	1/1	0.96	0.33	44,44,44,44	0
57	MG	1S	202	1/1	0.96	0.13	45,45,45,45	0
57	MG	2A	3522	1/1	0.96	0.14	30,30,30,30	0
57	MG	1A	3149	1/1	0.96	0.47	31,31,31,31	0
57	MG	1a	1705	1/1	0.96	0.14	41,41,41,41	0
57	MG	2A	3808	1/1	0.96	0.09	60,60,60,60	0
57	MG	2A	3068	1/1	0.96	0.29	41,41,41,41	0
57	MG	1A	4030	1/1	0.96	0.22	29,29,29,29	0
57	MG	1A	3892	1/1	0.96	0.15	33,33,33,33	0
57	MG	2A	3290	1/1	0.96	0.15	50,50,50,50	0
57	MG	2A	3813	1/1	0.96	0.19	21,21,21,21	0
57	MG	1a	1709	1/1	0.96	0.20	40,40,40,40	0
57	MG	1A	3191	1/1	0.96	0.23	29,29,29,29	0
57	MG	1A	3123	1/1	0.96	0.28	36,36,36,36	0
57	MG	1a	1712	1/1	0.96	0.14	37,37,37,37	0
57	MG	1A	3434	1/1	0.96	0.26	36,36,36,36	0
57	MG	1A	4035	1/1	0.96	0.14	38,38,38,38	0
57	MG	1A	3193	1/1	0.96	0.22	30,30,30,30	0
57	MG	1A	3772	1/1	0.96	0.12	37,37,37,37	0
57	MG	1U	207	1/1	0.96	0.47	40,40,40,40	0
57	MG	2A	3081	1/1	0.96	0.13	44,44,44,44	0
57	MG	1A	3048	1/1	0.96	0.19	24,24,24,24	0
57	MG	1A	3662	1/1	0.96	0.19	18,18,18,18	0
57	MG	1A	3496	1/1	0.96	0.21	30,30,30,30	0
57	MG	1V	204	1/1	0.96	0.10	32,32,32,32	0
57	MG	1A	3776	1/1	0.96	0.18	24,24,24,24	0
57	MG	1A	4043	1/1	0.96	0.18	26,26,26,26	0
57	MG	1A	4044	1/1	0.96	0.09	34,34,34,34	0
57	MG	2A	3548	1/1	0.96	0.11	38,38,38,38	0
57	MG	2A	3549	1/1	0.96	0.13	35,35,35,35	0
57	MG	1W	202	1/1	0.96	0.28	37,37,37,37	0
57	MG	1A	3126	1/1	0.96	0.30	33,33,33,33	0
57	MG	1W	205	1/1	0.96	0.30	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3311	1/1	0.96	0.41	58,58,58,58	0
57	MG	2A	3092	1/1	0.96	0.13	35,35,35,35	0
57	MG	1W	206	1/1	0.96	0.20	36,36,36,36	0
57	MG	1A	3155	1/1	0.96	0.46	34,34,34,34	0
57	MG	1A	3668	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3156	1/1	0.96	0.13	29,29,29,29	0
57	MG	2A	3318	1/1	0.96	0.43	41,41,41,41	0
57	MG	2A	3561	1/1	0.96	0.14	22,22,22,22	0
57	MG	1X	103	1/1	0.96	0.20	31,31,31,31	0
57	MG	1X	104	1/1	0.96	0.29	43,43,43,43	0
57	MG	2A	3564	1/1	0.96	0.11	49,49,49,49	0
57	MG	1X	105	1/1	0.96	0.27	36,36,36,36	0
57	MG	1A	3500	1/1	0.96	0.36	29,29,29,29	0
57	MG	1A	3783	1/1	0.96	0.15	19,19,19,19	0
57	MG	1A	3671	1/1	0.96	0.18	19,19,19,19	0
57	MG	2A	3103	1/1	0.96	0.23	41,41,41,41	0
57	MG	2A	3570	1/1	0.96	0.07	52,52,52,52	0
57	MG	1A	3785	1/1	0.96	0.15	35,35,35,35	0
57	MG	1a	1742	1/1	0.96	0.11	59,59,59,59	0
57	MG	2A	3574	1/1	0.96	0.10	31,31,31,31	0
57	MG	2A	3328	1/1	0.96	0.13	49,49,49,49	0
57	MG	2A	3576	1/1	0.96	0.56	52,52,52,52	0
57	MG	1a	1743	1/1	0.96	0.12	59,59,59,59	0
57	MG	1A	3440	1/1	0.96	0.23	39,39,39,39	0
57	MG	2A	3580	1/1	0.96	0.12	62,62,62,62	0
57	MG	2x	102	1/1	0.96	0.10	51,51,51,51	0
57	MG	1A	3127	1/1	0.96	0.23	41,41,41,41	0
57	MG	10	101	1/1	0.96	0.20	32,32,32,32	0
57	MG	1A	3917	1/1	0.96	0.22	47,47,47,47	0
57	MG	2E	301	1/1	0.96	0.33	50,50,50,50	0
57	MG	2A	3585	1/1	0.96	0.08	63,63,63,63	0
57	MG	2E	306	1/1	0.96	0.06	44,44,44,44	0
57	MG	2E	307	1/1	0.96	0.18	37,37,37,37	0
57	MG	1A	3075	1/1	0.96	0.16	38,38,38,38	0
57	MG	1A	3162	1/1	0.96	0.18	35,35,35,35	0
57	MG	1A	3791	1/1	0.96	0.10	36,36,36,36	0
57	MG	2F	304	1/1	0.96	0.60	40,40,40,40	0
57	MG	1a	1753	1/1	0.96	0.16	45,45,45,45	0
57	MG	1a	1754	1/1	0.96	0.20	40,40,40,40	0
57	MG	1A	3342	1/1	0.96	0.19	46,46,46,46	0
57	MG	1A	3743	1/1	0.97	0.16	56,56,56,56	0
57	MG	2A	3433	1/1	0.97	0.06	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3744	1/1	0.97	0.23	43,43,43,43	0
57	MG	2A	3123	1/1	0.97	0.19	45,45,45,45	0
57	MG	1w	107	1/1	0.97	0.21	73,73,73,73	0
57	MG	1E	311	1/1	0.97	0.20	51,51,51,51	0
57	MG	2A	3790	1/1	0.97	0.12	32,32,32,32	0
57	MG	1A	3745	1/1	0.97	0.23	41,41,41,41	0
57	MG	1x	102	1/1	0.97	0.32	44,44,44,44	0
57	MG	2A	3613	1/1	0.97	0.14	33,33,33,33	0
57	MG	1F	302	1/1	0.97	0.14	24,24,24,24	0
57	MG	2A	3796	1/1	0.97	0.10	33,33,33,33	0
57	MG	1A	3153	1/1	0.97	0.35	35,35,35,35	0
57	MG	1A	3230	1/1	0.97	0.26	41,41,41,41	0
57	MG	1A	3021	1/1	0.97	0.18	24,24,24,24	0
57	MG	18	102	1/1	0.97	0.44	44,44,44,44	0
57	MG	2a	1675	1/1	0.97	0.14	53,53,53,53	0
57	MG	18	103	1/1	0.97	0.40	37,37,37,37	0
57	MG	2a	1677	1/1	0.97	0.14	45,45,45,45	0
57	MG	18	104	1/1	0.97	0.25	36,36,36,36	0
57	MG	1A	3835	1/1	0.97	0.20	33,33,33,33	0
57	MG	1a	1715	1/1	0.97	0.17	54,54,54,54	0
57	MG	1a	1716	1/1	0.97	0.17	47,47,47,47	0
57	MG	1A	3410	1/1	0.97	0.25	36,36,36,36	0
57	MG	1A	3934	1/1	0.97	0.11	51,51,51,51	0
57	MG	2A	3628	1/1	0.97	0.33	41,41,41,41	0
57	MG	1A	3752	1/1	0.97	0.17	38,38,38,38	0
57	MG	1A	3373	1/1	0.97	0.15	42,42,42,42	0
57	MG	1A	4038	1/1	0.97	0.19	14,14,14,14	0
57	MG	2A	3632	1/1	0.97	0.07	44,44,44,44	0
57	MG	2A	3633	1/1	0.97	0.12	58,58,58,58	0
57	MG	1A	3839	1/1	0.97	0.10	58,58,58,58	0
57	MG	1A	3033	1/1	0.97	0.30	34,34,34,34	0
57	MG	1A	3939	1/1	0.97	0.09	46,46,46,46	0
57	MG	1a	1607	1/1	0.97	0.17	46,46,46,46	0
57	MG	2A	3007	1/1	0.97	0.14	49,49,49,49	0
57	MG	1A	3841	1/1	0.97	0.23	26,26,26,26	0
57	MG	2A	3009	1/1	0.97	0.18	31,31,31,31	0
57	MG	1A	3137	1/1	0.97	0.15	36,36,36,36	0
57	MG	1A	3606	1/1	0.97	0.21	29,29,29,29	0
57	MG	1A	4045	1/1	0.97	0.11	19,19,19,19	0
57	MG	1A	3676	1/1	0.97	0.19	22,22,22,22	0
57	MG	1A	3608	1/1	0.97	0.19	30,30,30,30	0
57	MG	1A	3265	1/1	0.97	0.31	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3234	1/1	0.97	0.16	28,28,28,28	0
57	MG	1O	201	1/1	0.97	0.46	51,51,51,51	0
57	MG	2A	3019	1/1	0.97	0.16	30,30,30,30	0
57	MG	2A	3020	1/1	0.97	0.24	59,59,59,59	0
57	MG	2A	3835	1/1	0.97	0.21	40,40,40,40	0
57	MG	2A	3021	1/1	0.97	0.09	25,25,25,25	0
57	MG	2A	3652	1/1	0.97	0.12	52,52,52,52	0
57	MG	1A	3378	1/1	0.97	0.21	25,25,25,25	0
57	MG	2A	3023	1/1	0.97	0.18	38,38,38,38	0
57	MG	1a	1736	1/1	0.97	0.17	47,47,47,47	0
57	MG	1A	3235	1/1	0.97	0.17	41,41,41,41	0
57	MG	1A	3074	1/1	0.97	0.16	28,28,28,28	0
57	MG	2A	3171	1/1	0.97	0.14	33,33,33,33	0
57	MG	1A	3015	1/1	0.97	0.22	28,28,28,28	0
57	MG	1A	3420	1/1	0.97	0.12	41,41,41,41	0
57	MG	1A	3421	1/1	0.97	0.19	38,38,38,38	0
57	MG	1A	3090	1/1	0.97	0.14	21,21,21,21	0
57	MG	1A	3560	1/1	0.97	0.09	31,31,31,31	0
57	MG	1a	1744	1/1	0.97	0.08	46,46,46,46	0
57	MG	2B	206	1/1	0.97	0.17	67,67,67,67	0
57	MG	1A	3770	1/1	0.97	0.17	20,20,20,20	0
57	MG	1A	3619	1/1	0.97	0.11	33,33,33,33	0
57	MG	1A	3862	1/1	0.97	0.27	30,30,30,30	0
57	MG	2A	3182	1/1	0.97	0.19	51,51,51,51	0
57	MG	1A	3693	1/1	0.97	0.21	31,31,31,31	0
57	MG	2A	3493	1/1	0.97	0.11	55,55,55,55	0
57	MG	1A	3125	1/1	0.97	0.28	34,34,34,34	0
57	MG	1A	3465	1/1	0.97	0.09	47,47,47,47	0
57	MG	1A	3077	1/1	0.97	0.20	32,32,32,32	0
57	MG	1a	1633	1/1	0.97	0.24	22,22,22,22	0
57	MG	1A	3623	1/1	0.97	0.12	16,16,16,16	0
57	MG	1A	3210	1/1	0.97	0.19	39,39,39,39	0
57	MG	2a	1738	1/1	0.97	0.34	42,42,42,42	0
57	MG	1A	3005	1/1	0.97	0.14	32,32,32,32	0
57	MG	1A	3566	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3628	1/1	0.97	0.13	18,18,18,18	0
57	MG	2A	3505	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3967	1/1	0.97	0.06	56,56,56,56	0
57	MG	1A	3064	1/1	0.97	0.16	35,35,35,35	0
57	MG	2E	302	1/1	0.97	0.13	52,52,52,52	0
57	MG	1a	1763	1/1	0.97	0.20	38,38,38,38	0
57	MG	2E	305	1/1	0.97	0.14	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1764	1/1	0.97	0.19	47,47,47,47	0
57	MG	1A	3782	1/1	0.97	0.20	21,21,21,21	0
57	MG	2A	3199	1/1	0.97	0.08	40,40,40,40	0
57	MG	1A	3514	1/1	0.97	0.21	37,37,37,37	0
57	MG	2A	3513	1/1	0.97	0.16	28,28,28,28	0
57	MG	1A	3065	1/1	0.97	0.13	27,27,27,27	0
57	MG	1A	3972	1/1	0.97	0.15	18,18,18,18	0
57	MG	2A	3353	1/1	0.97	0.07	62,62,62,62	0
57	MG	1A	3516	1/1	0.97	0.26	47,47,47,47	0
57	MG	2O	201	1/1	0.97	0.12	67,67,67,67	0
57	MG	1A	3878	1/1	0.97	0.14	21,21,21,21	0
57	MG	2P	201	1/1	0.97	0.23	47,47,47,47	0
57	MG	1A	3037	1/1	0.97	0.43	30,30,30,30	0
57	MG	2A	3358	1/1	0.97	0.27	44,44,44,44	0
57	MG	2A	3523	1/1	0.97	0.12	42,42,42,42	0
57	MG	1A	3030	1/1	0.97	0.24	25,25,25,25	0
57	MG	1a	1773	1/1	0.97	0.12	41,41,41,41	0
57	MG	2a	1767	1/1	0.97	0.12	58,58,58,58	0
57	MG	1A	3216	1/1	0.97	0.23	38,38,38,38	0
57	MG	1A	3355	1/1	0.97	0.32	31,31,31,31	0
57	MG	2A	3064	1/1	0.97	0.10	50,50,50,50	0
57	MG	2A	3212	1/1	0.97	0.19	50,50,50,50	0
57	MG	2T	204	1/1	0.97	0.19	42,42,42,42	0
57	MG	1a	1776	1/1	0.97	0.24	56,56,56,56	0
57	MG	1A	3790	1/1	0.97	0.20	21,21,21,21	0
57	MG	1U	210	1/1	0.97	0.40	35,35,35,35	0
57	MG	1A	3282	1/1	0.97	0.15	46,46,46,46	0
57	MG	2A	3069	1/1	0.97	0.13	40,40,40,40	0
57	MG	1A	3792	1/1	0.97	0.18	20,20,20,20	0
57	MG	2a	1779	1/1	0.97	0.19	57,57,57,57	0
57	MG	1A	3886	1/1	0.97	0.26	31,31,31,31	0
57	MG	2A	3221	1/1	0.97	0.34	33,33,33,33	0
57	MG	1A	3985	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3217	1/1	0.97	0.16	36,36,36,36	0
57	MG	1a	1784	1/1	0.97	0.14	40,40,40,40	0
57	MG	25	3102	1/1	0.97	0.23	42,42,42,42	0
57	MG	1A	3578	1/1	0.97	0.26	47,47,47,47	0
57	MG	1A	3642	1/1	0.97	0.17	21,21,21,21	0
57	MG	1A	3039	1/1	0.97	0.11	28,28,28,28	0
57	MG	1A	3797	1/1	0.97	0.18	38,38,38,38	0
57	MG	2A	3720	1/1	0.97	0.41	40,40,40,40	0
57	MG	2A	3721	1/1	0.97	0.07	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3229	1/1	0.97	0.32	49,49,49,49	0
57	MG	1A	3031	1/1	0.97	0.17	23,23,23,23	0
57	MG	1a	1790	1/1	0.97	0.11	35,35,35,35	0
57	MG	1A	3718	1/1	0.97	0.10	49,49,49,49	0
57	MG	2A	3727	1/1	0.97	0.10	49,49,49,49	0
57	MG	2A	3728	1/1	0.97	0.40	51,51,51,51	0
57	MG	1A	3800	1/1	0.97	0.12	66,66,66,66	0
57	MG	1A	3720	1/1	0.97	0.15	18,18,18,18	0
57	MG	1A	3995	1/1	0.97	0.12	23,23,23,23	0
57	MG	1A	3173	1/1	0.97	0.26	28,28,28,28	0
57	MG	1A	3527	1/1	0.97	0.19	51,51,51,51	0
57	MG	1A	3174	1/1	0.97	0.17	30,30,30,30	0
57	MG	1A	3288	1/1	0.97	0.36	42,42,42,42	0
57	MG	1A	3071	1/1	0.97	0.17	14,14,14,14	0
57	MG	1A	3197	1/1	0.97	0.24	21,21,21,21	0
57	MG	1a	1803	1/1	0.97	0.17	60,60,60,60	0
57	MG	2A	3740	1/1	0.97	0.17	57,57,57,57	0
57	MG	2A	3396	1/1	0.97	0.12	31,31,31,31	0
57	MG	1A	3224	1/1	0.97	0.12	19,19,19,19	0
57	MG	1A	3811	1/1	0.97	0.11	29,29,29,29	0
57	MG	1A	3225	1/1	0.97	0.18	24,24,24,24	0
57	MG	1A	3813	1/1	0.97	0.21	44,44,44,44	0
57	MG	1A	4009	1/1	0.97	0.15	41,41,41,41	0
57	MG	1a	1809	1/1	0.97	0.23	41,41,41,41	0
57	MG	1a	1679	1/1	0.97	0.10	50,50,50,50	0
57	MG	1A	3176	1/1	0.97	0.15	18,18,18,18	0
57	MG	2A	3253	1/1	0.97	0.20	45,45,45,45	0
57	MG	1D	303	1/1	0.97	0.32	34,34,34,34	0
57	MG	1A	3535	1/1	0.97	0.19	25,25,25,25	0
57	MG	1A	3152	1/1	0.97	0.10	26,26,26,26	0
57	MG	1A	3732	1/1	0.97	0.21	19,19,19,19	0
57	MG	2q	201	1/1	0.97	0.07	69,69,69,69	0
57	MG	1A	3818	1/1	0.97	0.26	51,51,51,51	0
57	MG	1a	1688	1/1	0.97	0.26	45,45,45,45	0
57	MG	1A	3733	1/1	0.97	0.17	19,19,19,19	0
57	MG	1e	202	1/1	0.97	0.42	48,48,48,48	0
57	MG	1D	310	1/1	0.97	0.13	36,36,36,36	0
57	MG	2v	104	1/1	0.97	0.14	51,51,51,51	0
57	MG	1A	3537	1/1	0.97	0.20	31,31,31,31	0
57	MG	1a	1692	1/1	0.97	0.21	39,39,39,39	0
57	MG	1A	3446	1/1	0.97	0.18	36,36,36,36	0
57	MG	2A	3418	1/1	0.97	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
57	MG	13	102	1/1	0.97	0.39	43,43,43,43	0
57	MG	2A	3767	1/1	0.97	0.11	60,60,60,60	0
57	MG	2A	3420	1/1	0.97	0.16	34,34,34,34	0
57	MG	1A	3594	1/1	0.97	0.13	32,32,32,32	0
57	MG	1A	3539	1/1	0.97	0.20	32,32,32,32	0
57	MG	2A	3269	1/1	0.97	0.11	52,52,52,52	0
57	MG	1A	3921	1/1	0.97	0.12	26,26,26,26	0
57	MG	2A	3425	1/1	0.97	0.29	44,44,44,44	0
57	MG	2A	3595	1/1	0.97	0.11	33,33,33,33	0
57	MG	1A	3228	1/1	0.97	0.15	38,38,38,38	0
57	MG	2a	1650	1/1	0.97	0.10	58,58,58,58	0
57	MG	1A	3741	1/1	0.97	0.14	23,23,23,23	0
57	MG	1a	1700	1/1	0.97	0.43	49,49,49,49	0
57	MG	1w	103	1/1	0.97	0.11	73,73,73,73	0
59	TEL	1A	4076	58/58	0.97	0.25	13,24,29,32	0
59	TEL	2A	3845	58/58	0.97	0.30	24,32,38,40	0
57	MG	2A	3601	1/1	0.97	0.18	47,47,47,47	0
57	MG	2a	1655	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3490	1/1	0.97	0.23	23,23,23,23	0
57	MG	2a	1657	1/1	0.97	0.10	46,46,46,46	0
60	ZN	29	501	1/1	0.97	0.10	63,63,63,63	0
57	MG	2A	3431	1/1	0.97	0.13	54,54,54,54	0
57	MG	23	103	1/1	0.98	0.27	53,53,53,53	0
57	MG	1A	3675	1/1	0.98	0.15	23,23,23,23	0
57	MG	1A	3861	1/1	0.98	0.12	20,20,20,20	0
57	MG	1A	3979	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	3554	1/1	0.98	0.20	34,34,34,34	0
57	MG	1A	3268	1/1	0.98	0.32	33,33,33,33	0
57	MG	1D	307	1/1	0.98	0.18	26,26,26,26	0
57	MG	2A	3219	1/1	0.98	0.12	55,55,55,55	0
57	MG	1A	3012	1/1	0.98	0.14	23,23,23,23	0
57	MG	1A	4050	1/1	0.98	0.18	14,14,14,14	0
57	MG	2a	1731	1/1	0.98	0.16	39,39,39,39	0
57	MG	1A	3119	1/1	0.98	0.19	27,27,27,27	0
57	MG	1a	1706	1/1	0.98	0.10	40,40,40,40	0
57	MG	1V	201	1/1	0.98	0.34	22,22,22,22	0
57	MG	1a	1795	1/1	0.98	0.23	43,43,43,43	0
57	MG	1A	3766	1/1	0.98	0.14	20,20,20,20	0
57	MG	2A	3545	1/1	0.98	0.15	32,32,32,32	0
57	MG	2A	3791	1/1	0.98	0.13	47,47,47,47	0
57	MG	2A	3435	1/1	0.98	0.20	15,15,15,15	0
57	MG	2A	3035	1/1	0.98	0.16	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3680	1/1	0.98	0.12	19,19,19,19	0
57	MG	1A	3868	1/1	0.98	0.13	27,27,27,27	0
57	MG	2A	3130	1/1	0.98	0.20	44,44,44,44	0
57	MG	1a	1625	1/1	0.98	0.18	58,58,58,58	0
57	MG	1A	3508	1/1	0.98	0.19	39,39,39,39	0
57	MG	2A	3673	1/1	0.98	0.13	30,30,30,30	0
57	MG	2A	3800	1/1	0.98	0.15	38,38,38,38	0
57	MG	2A	3442	1/1	0.98	0.50	34,34,34,34	0
57	MG	2A	3233	1/1	0.98	0.19	54,54,54,54	0
57	MG	1a	1801	1/1	0.98	0.08	51,51,51,51	0
57	MG	1A	3682	1/1	0.98	0.20	23,23,23,23	0
57	MG	1E	303	1/1	0.98	0.27	28,28,28,28	0
57	MG	1E	304	1/1	0.98	0.41	29,29,29,29	0
57	MG	2A	3137	1/1	0.98	0.15	35,35,35,35	0
57	MG	1W	204	1/1	0.98	0.45	31,31,31,31	0
57	MG	2a	1756	1/1	0.98	0.11	62,62,62,62	0
57	MG	1A	3290	1/1	0.98	0.17	26,26,26,26	0
57	MG	1A	3202	1/1	0.98	0.15	26,26,26,26	0
57	MG	1A	3931	1/1	0.98	0.14	39,39,39,39	0
57	MG	2a	1760	1/1	0.98	0.09	60,60,60,60	0
57	MG	1E	308	1/1	0.98	0.17	23,23,23,23	0
57	MG	1A	3333	1/1	0.98	0.27	33,33,33,33	0
57	MG	1X	102	1/1	0.98	0.25	33,33,33,33	0
57	MG	2a	1629	1/1	0.98	0.22	45,45,45,45	0
57	MG	1A	3820	1/1	0.98	0.10	33,33,33,33	0
57	MG	1A	3647	1/1	0.98	0.14	27,27,27,27	0
57	MG	2A	3248	1/1	0.98	0.10	47,47,47,47	0
57	MG	1A	3687	1/1	0.98	0.23	31,31,31,31	0
57	MG	1F	301	1/1	0.98	0.31	28,28,28,28	0
57	MG	2A	3821	1/1	0.98	0.30	42,42,42,42	0
57	MG	2A	3573	1/1	0.98	0.11	30,30,30,30	0
57	MG	1A	3272	1/1	0.98	0.12	43,43,43,43	0
57	MG	2A	3057	1/1	0.98	0.14	51,51,51,51	0
57	MG	1A	3335	1/1	0.98	0.26	32,32,32,32	0
57	MG	1A	3120	1/1	0.98	0.19	28,28,28,28	0
57	MG	2A	3827	1/1	0.98	0.18	45,45,45,45	0
57	MG	1A	3003	1/1	0.98	0.14	23,23,23,23	0
57	MG	2A	3155	1/1	0.98	0.45	36,36,36,36	0
57	MG	1A	4002	1/1	0.98	0.10	61,61,61,61	0
57	MG	1A	3827	1/1	0.98	0.14	29,29,29,29	0
57	MG	2A	3583	1/1	0.98	0.09	47,47,47,47	0
57	MG	2A	3158	1/1	0.98	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3172	1/1	0.98	0.19	26,26,26,26	0
57	MG	1A	4005	1/1	0.98	0.10	44,44,44,44	0
57	MG	1A	3517	1/1	0.98	0.26	31,31,31,31	0
57	MG	2A	3588	1/1	0.98	0.17	32,32,32,32	0
57	MG	1F	311	1/1	0.98	0.09	34,34,34,34	0
57	MG	1A	3736	1/1	0.98	0.22	33,33,33,33	0
57	MG	1A	3157	1/1	0.98	0.14	51,51,51,51	0
57	MG	1B	201	1/1	0.98	0.23	44,44,44,44	0
57	MG	2A	3712	1/1	0.98	0.12	52,52,52,52	0
57	MG	2a	1792	1/1	0.98	0.20	56,56,56,56	0
57	MG	1A	3043	1/1	0.98	0.21	30,30,30,30	0
57	MG	1A	3739	1/1	0.98	0.12	35,35,35,35	0
57	MG	1G	205	1/1	0.98	0.16	54,54,54,54	0
57	MG	1A	3159	1/1	0.98	0.21	22,22,22,22	0
57	MG	2A	3597	1/1	0.98	0.13	33,33,33,33	0
57	MG	1A	3062	1/1	0.98	0.21	30,30,30,30	0
57	MG	1a	1745	1/1	0.98	0.14	48,48,48,48	0
57	MG	1A	3161	1/1	0.98	0.55	30,30,30,30	0
57	MG	1A	4014	1/1	0.98	0.18	35,35,35,35	0
57	MG	1A	3627	1/1	0.98	0.15	51,51,51,51	0
57	MG	1A	3093	1/1	0.98	0.27	29,29,29,29	0
57	MG	1A	3629	1/1	0.98	0.15	15,15,15,15	0
57	MG	2A	3488	1/1	0.98	0.13	29,29,29,29	0
57	MG	1A	3574	1/1	0.98	0.33	26,26,26,26	0
57	MG	2A	3178	1/1	0.98	0.17	30,30,30,30	0
57	MG	1A	3664	1/1	0.98	0.12	24,24,24,24	0
57	MG	2A	3609	1/1	0.98	0.16	57,57,57,57	0
57	MG	1A	3896	1/1	0.98	0.10	27,27,27,27	0
57	MG	1A	3748	1/1	0.98	0.17	35,35,35,35	0
57	MG	2A	3387	1/1	0.98	0.16	36,36,36,36	0
57	MG	2A	3495	1/1	0.98	0.12	24,24,24,24	0
57	MG	2A	3735	1/1	0.98	0.11	56,56,56,56	0
57	MG	2D	302	1/1	0.98	0.09	21,21,21,21	0
57	MG	2a	1680	1/1	0.98	0.14	50,50,50,50	0
57	MG	1O	205	1/1	0.98	0.18	70,70,70,70	0
57	MG	2A	3615	1/1	0.98	0.10	37,37,37,37	0
57	MG	2a	1683	1/1	0.98	0.15	31,31,31,31	0
57	MG	1A	3014	1/1	0.98	0.16	24,24,24,24	0
57	MG	2A	3184	1/1	0.98	0.08	56,56,56,56	0
57	MG	2l	204	1/1	0.98	0.19	63,63,63,63	0
57	MG	1A	3750	1/1	0.98	0.14	35,35,35,35	0
57	MG	17	102	1/1	0.98	0.17	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3501	1/1	0.98	0.10	53,53,53,53	0
57	MG	1A	3632	1/1	0.98	0.24	20,20,20,20	0
57	MG	1a	1761	1/1	0.98	0.15	48,48,48,48	0
57	MG	1A	3901	1/1	0.98	0.16	32,32,32,32	0
57	MG	1B	219	1/1	0.98	0.26	58,58,58,58	0
57	MG	1A	3095	1/1	0.98	0.19	15,15,15,15	0
57	MG	1A	3708	1/1	0.98	0.13	32,32,32,32	0
57	MG	2F	305	1/1	0.98	0.83	49,49,49,49	0
57	MG	1Q	203	1/1	0.98	0.19	37,37,37,37	0
57	MG	1A	4029	1/1	0.98	0.20	31,31,31,31	0
57	MG	1A	3045	1/1	0.98	0.18	27,27,27,27	0
57	MG	2A	3752	1/1	0.98	0.12	34,34,34,34	0
57	MG	1A	3604	1/1	0.98	0.17	13,13,13,13	0
57	MG	18	107	1/1	0.98	0.21	38,38,38,38	0
57	MG	1a	1684	1/1	0.98	0.25	41,41,41,41	0
57	MG	1A	3139	1/1	0.98	0.19	25,25,25,25	0
57	MG	2A	3200	1/1	0.98	0.05	59,59,59,59	0
57	MG	2A	3516	1/1	0.98	0.17	31,31,31,31	0
57	MG	1A	3712	1/1	0.98	0.14	27,27,27,27	0
57	MG	1A	3803	1/1	0.98	0.21	29,29,29,29	0
57	MG	2A	3519	1/1	0.98	0.10	36,36,36,36	0
57	MG	2A	3012	1/1	0.98	0.09	36,36,36,36	0
57	MG	1A	3036	1/1	0.98	0.15	22,22,22,22	0
57	MG	1A	3673	1/1	0.98	0.13	25,25,25,25	0
58	K	1A	3546	1/1	0.98	0.13	26,26,26,26	0
57	MG	1A	3911	1/1	0.98	0.14	29,29,29,29	0
57	MG	1A	3912	1/1	0.98	0.14	38,38,38,38	0
57	MG	1A	3806	1/1	0.98	0.14	18,18,18,18	0
57	MG	1A	3607	1/1	0.98	0.11	52,52,52,52	0
57	MG	2A	3312	1/1	0.98	0.15	51,51,51,51	0
60	ZN	1n	103	1/1	0.98	0.17	56,56,56,56	0
57	MG	2A	3771	1/1	0.98	0.07	64,64,64,64	0
57	MG	1A	3858	1/1	0.98	0.26	30,30,30,30	0
60	ZN	25	3104	1/1	0.98	0.17	65,65,65,65	0
60	ZN	26	501	1/1	0.98	0.17	62,62,62,62	0
57	MG	1A	3916	1/1	0.98	0.13	23,23,23,23	0
57	MG	1A	3859	1/1	0.98	0.39	37,37,37,37	0
57	MG	2A	3050	1/1	0.99	0.15	54,54,54,54	0
57	MG	1A	3691	1/1	0.99	0.10	12,12,12,12	0
57	MG	1A	3116	1/1	0.99	0.17	28,28,28,28	0
57	MG	2A	3766	1/1	0.99	0.17	42,42,42,42	0
57	MG	2A	3556	1/1	0.99	0.11	32,32,32,32	0

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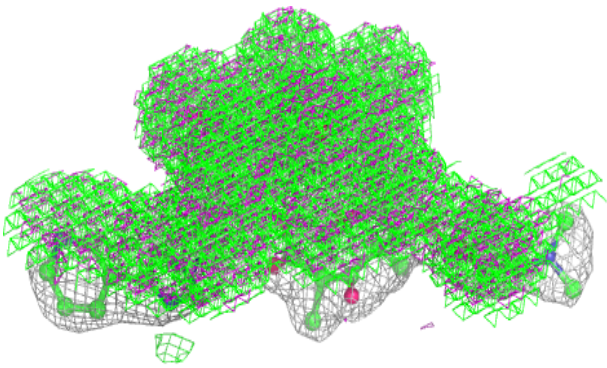
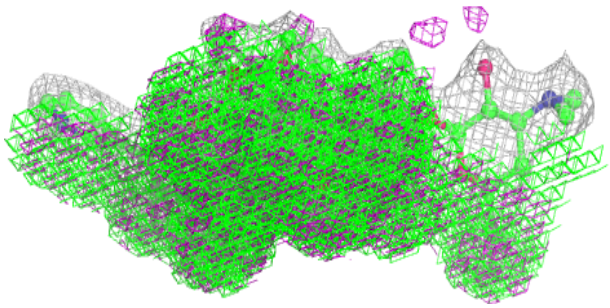
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3076	1/1	0.99	0.09	33,33,33,33	0
57	MG	1A	3857	1/1	0.99	0.22	39,39,39,39	0
57	MG	2E	303	1/1	0.99	0.11	26,26,26,26	0
57	MG	1A	3666	1/1	0.99	0.13	28,28,28,28	0
57	MG	1A	3011	1/1	0.99	0.14	23,23,23,23	0
57	MG	1A	4051	1/1	0.99	0.16	21,21,21,21	0
57	MG	2A	3271	1/1	0.99	0.15	37,37,37,37	0
57	MG	2A	3807	1/1	0.99	0.09	50,50,50,50	0
57	MG	1a	1650	1/1	0.99	0.14	39,39,39,39	0
57	MG	1A	3659	1/1	0.99	0.14	33,33,33,33	0
57	MG	1A	3294	1/1	0.99	0.14	18,18,18,18	0
57	MG	2A	3624	1/1	0.99	0.14	36,36,36,36	0
57	MG	1V	202	1/1	0.99	0.27	22,22,22,22	0
57	MG	1a	1758	1/1	0.99	0.12	48,48,48,48	0
57	MG	1A	3337	1/1	0.99	0.20	26,26,26,26	0
57	MG	1A	3996	1/1	0.99	0.07	31,31,31,31	0
57	MG	2A	3782	1/1	0.99	0.12	49,49,49,49	0
57	MG	2A	3354	1/1	0.99	0.15	35,35,35,35	0
57	MG	1A	4025	1/1	0.99	0.17	22,22,22,22	0
57	MG	1Y	204	1/1	0.99	0.32	46,46,46,46	0
57	MG	1A	3719	1/1	0.99	0.16	24,24,24,24	0
57	MG	1A	3984	1/1	0.99	0.13	15,15,15,15	0
57	MG	1a	1680	1/1	0.99	0.12	51,51,51,51	0
60	ZN	15	106	1/1	0.99	0.21	43,43,43,43	0
60	ZN	16	102	1/1	0.99	0.20	46,46,46,46	0
60	ZN	19	501	1/1	0.99	0.21	44,44,44,44	0
57	MG	2A	3725	1/1	0.99	0.09	48,48,48,48	0
57	MG	1A	3067	1/1	0.99	0.20	22,22,22,22	0
57	MG	1A	3103	1/1	0.99	0.23	36,36,36,36	0
57	MG	2A	3578	1/1	0.99	0.34	52,52,52,52	0
57	MG	1U	202	1/1	0.99	0.38	37,37,37,37	0
57	MG	2A	3142	1/1	0.99	0.10	29,29,29,29	0
57	MG	2A	3390	1/1	0.99	0.26	38,38,38,38	0
61	SF4	1d	302	8/8	0.99	0.16	48,56,60,67	0
61	SF4	2d	303	8/8	0.99	0.13	63,70,79,83	0

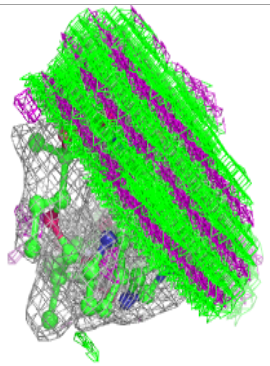
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TEL 1A 4076:

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

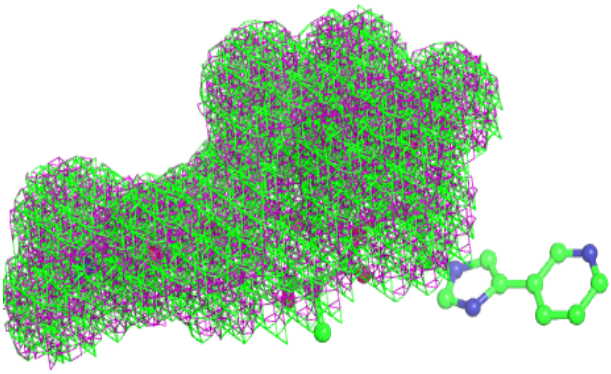


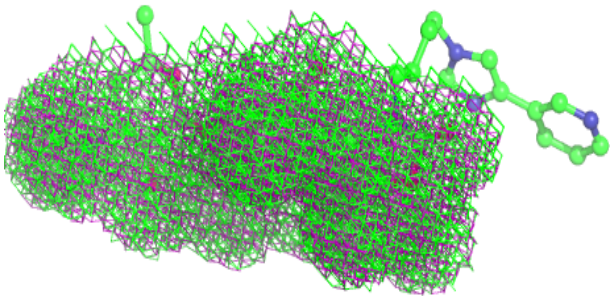


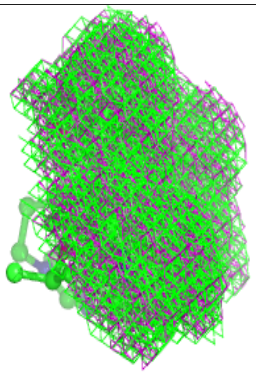


Electron density around TEL 2A 3845:

$2mF_o$-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.