



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 04:38 AM EST

PDB ID : 5J4C
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with cisplatin (soaked) and bound to mRNA and A-, P- and E-site tRNAs at 2.8Å resolution
Authors : Melnikov, S.V.; Soll, D.; Steitz, T.A.; Polikanov, Y.S.
Deposited on : 2016-03-31
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

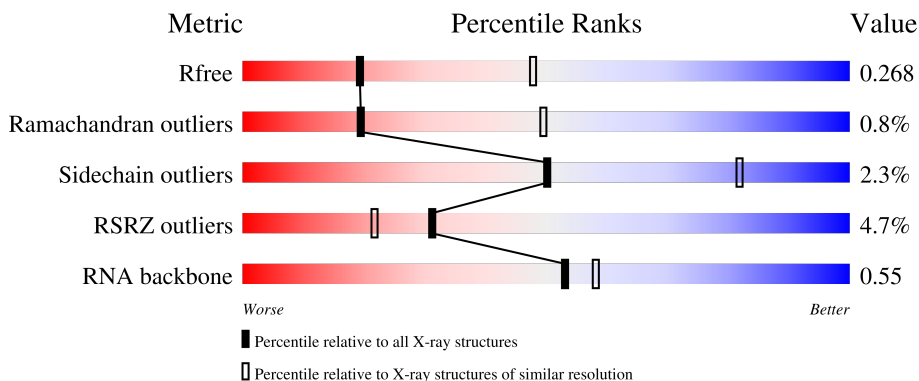
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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 $\leq 5\%$. 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% 83% 15% ..
1	2A	2915	 % 79% 16% .
2	1B	121	 % 89% 9% ..
2	2B	121	 % 79% 20% .

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Mol	Chain	Length	Quality of chain
3	1D	276	97%
3	2D	276	98%
4	1E	206	95%
4	2E	206	94%
5	1F	210	93%
5	2F	210	91%
6	1G	182	98%
6	2G	182	97%
7	1H	180	93%
7	2H	180	93%
8	1I	148	95%
8	2I	148	97%
9	1N	140	97%
9	2N	140	97%
10	1O	122	99%
10	2O	122	99%
11	1P	150	98%
11	2P	150	98%
12	1Q	141	99%
12	2Q	141	96%
13	1R	118	95%
13	2R	118	95%
14	1S	112	97%
14	2S	112	96%
15	1T	146	88%

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Mol	Chain	Length	Quality of chain
15	2T	146	3% 88% 10%
16	1U	118	% 97%
16	2U	118	2% 97%
17	1V	101	94% 5%
17	2V	101	6% 96%
18	1W	113	2% 96%
18	2W	113	% 95%
19	1X	96	99%
19	2X	96	5% 98%
20	1Y	110	% 93% 5%
20	2Y	110	3% 95%
21	1Z	206	3% 72% 25%
21	2Z	206	12% 76% 22%
22	10	85	% 98%
22	20	85	% 96%
23	11	98	3% 99%
23	21	98	4% 98%
24	12	72	97%
24	22	72	4% 97%
25	13	60	2% 97%
25	23	60	8% 97%
26	14	71	18% 87% 10%
26	24	71	21% 87% 10%
27	15	60	2% 93% 5%
27	25	60	93% 5%

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

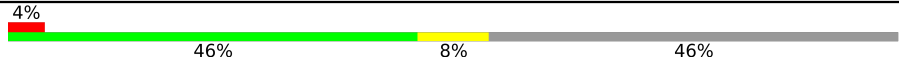
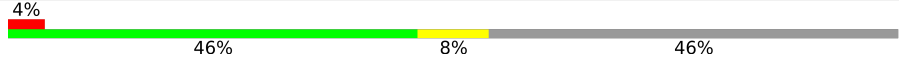
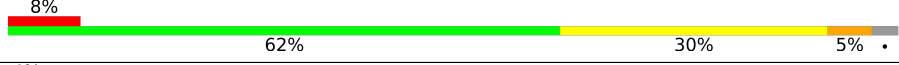

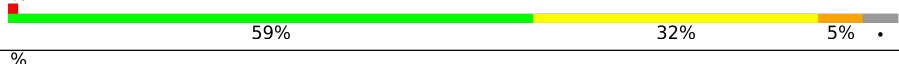
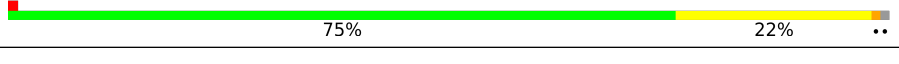

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Mol	Chain	Length	Quality of chain
40	2i	128	47% 97%
41	1j	105	10% 86% 7% 8%
41	2j	105	38% 86% 6% 9%
42	1k	129	5% 85% 12%
42	2k	129	2% 88% 12%
43	1l	132	% 91% 8%
43	2l	132	91% 8%
44	1m	126	4% 96% ..
44	2m	126	27% 94% ..
45	1n	61	3% 95% ..
45	2n	61	72% 93% 5% .
46	1o	89	6% 99% .
46	2o	89	99% .
47	1p	88	6% 92% 7%
47	2p	88	91% 7%
48	1q	105	2% 94% 6%
48	2q	105	10% 92% 6%
49	1r	88	5% 75% 23%
49	2r	88	2% 77% 23%
50	1s	93	3% 86% 11%
50	2s	93	20% 86% 11%
51	1t	106	24% 87% 9%
51	2t	106	20% 87% 9%
52	1u	27	85% 15%
52	2u	27	44% 85% 15%

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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	MG	10	102	-	-	-	X
56	MG	15	102	-	-	-	X
56	MG	16	102	-	-	-	X
56	MG	1A	3091	-	-	-	X
56	MG	1A	3112	-	-	-	X
56	MG	1A	3151	-	-	-	X
56	MG	1A	3222	-	-	-	X
56	MG	1A	3251	-	-	-	X
56	MG	1A	3312	-	-	-	X
56	MG	1A	3351	-	-	-	X
56	MG	1A	3366	-	-	-	X
56	MG	1A	3367	-	-	-	X
56	MG	1A	3369	-	-	-	X
56	MG	1A	3370	-	-	-	X
56	MG	1A	3375	-	-	-	X
56	MG	1A	3383	-	-	-	X
56	MG	1A	3392	-	-	-	X
56	MG	1A	3417	-	-	-	X
56	MG	1A	3560	-	-	-	X
56	MG	1A	3575	-	-	-	X
56	MG	1A	3688	-	-	-	X
56	MG	1A	4066	-	-	-	X
56	MG	1A	4114	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	4146	-	-	-	X
56	MG	1A	4186	-	-	-	X
56	MG	1B	227	-	-	-	X
56	MG	1a	1602	-	-	-	X
56	MG	1a	1615	-	-	-	X
56	MG	1a	1723	-	-	-	X
56	MG	1w	103	-	-	-	X
56	MG	1x	102	-	-	-	X
56	MG	23	3001	-	-	-	X
56	MG	2A	3057	-	-	-	X
56	MG	2A	3092	-	-	-	X
56	MG	2A	3195	-	-	-	X
56	MG	2A	3214	-	-	-	X
56	MG	2A	3248	-	-	-	X
56	MG	2A	3251	-	-	-	X
56	MG	2A	3270	-	-	-	X
56	MG	2A	3301	-	-	-	X
56	MG	2A	3343	-	-	-	X
56	MG	2A	3377	-	-	-	X
56	MG	2A	3382	-	-	-	X
56	MG	2A	3387	-	-	-	X
56	MG	2A	3394	-	-	-	X
56	MG	2A	3411	-	-	-	X
56	MG	2A	3456	-	-	-	X
56	MG	2A	3479	-	-	-	X
56	MG	2A	3495	-	-	-	X
56	MG	2A	3792	-	-	-	X
56	MG	2A	3823	-	-	-	X
56	MG	2B	3011	-	-	-	X
56	MG	2a	3026	-	-	-	X
56	MG	2a	3029	-	-	-	X
56	MG	2a	3031	-	-	-	X
56	MG	2a	3034	-	-	-	X
56	MG	2a	3057	-	-	-	X
56	MG	2a	3060	-	-	-	X
56	MG	2a	3064	-	-	-	X
56	MG	2a	3086	-	-	-	X
56	MG	2a	3222	-	-	-	X
56	MG	2l	3001	-	-	-	X
56	MG	2v	102	-	-	-	X
56	MG	2v	103	-	-	-	X
56	MG	2w	103	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	CPT	1a	1930	-	-	-	X

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 301288 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	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

- 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	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- 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	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	173	Total	C	N	O	S	0	0	0
			1321	839	246	235	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1321	839	246	235	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	Total 959	C 608	N 201	O 149	S 1	0	0	0
16	2U	116	Total 959	C 608	N 201	O 149	S 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	Total 771	C 495	N 140	O 135	S 1	0	0	0
17	2V	101	Total 771	C 495	N 140	O 135	S 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	Total 886	C 557	N 174	O 153	S 2	0	0	0
18	2W	112	Total 886	C 557	N 174	O 153	S 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	Total 750	C 488	N 135	O 126	S 1	0	0	0
19	2X	95	Total 750	C 488	N 135	O 126	S 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	Total 806	C 517	N 152	O 131	S 6	0	0	0
20	2Y	107	Total 806	C 517	N 152	O 131	S 6	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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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	Total 823	C 528	N 151	O 142	S 2	0	0	0
48	2q	99	Total 823	C 528	N 151	O 142	S 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	S			
49	1r	68	Total 555	C 355	N 108	O 92	S	0	0	0
49	2r	68	Total 555	C 355	N 108	O 92	S	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	Total 652	C 417	N 120	O 113	S 2	0	0	0
50	2s	83	Total 646	C 412	N 119	O 113	S 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	Total 728	C 446	N 156	O 124	S 2	0	0	0
51	2t	96	Total 727	C 446	N 155	O 124	S 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	S			
52	1u	23	Total 199	C 122	N 48	O 29	S	0	0	0
52	2u	23	Total 199	C 122	N 48	O 29	S	0	0	0

- Molecule 53 is a RNA chain called mRNA.

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

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1254	Total	Mg	0	0
			1254	1254		
56	1B	36	Total	Mg	0	0
			36	36		
56	1D	12	Total	Mg	0	0
			12	12		
56	1E	13	Total	Mg	0	0
			13	13		
56	1F	10	Total	Mg	0	0
			10	10		
56	1G	5	Total	Mg	0	0
			5	5		
56	1H	1	Total	Mg	0	0
			1	1		
56	1I	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1N	7	Total 7	Mg 7	0	0
56	1O	5	Total 5	Mg 5	0	0
56	1P	3	Total 3	Mg 3	0	0
56	1Q	5	Total 5	Mg 5	0	0
56	1R	3	Total 3	Mg 3	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1U	6	Total 6	Mg 6	0	0
56	1V	2	Total 2	Mg 2	0	0
56	1W	6	Total 6	Mg 6	0	0
56	1X	6	Total 6	Mg 6	0	0
56	1Y	2	Total 2	Mg 2	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	10	7	Total 7	Mg 7	0	0
56	11	3	Total 3	Mg 3	0	0
56	12	2	Total 2	Mg 2	0	0
56	13	2	Total 2	Mg 2	0	0
56	15	4	Total 4	Mg 4	0	0
56	16	2	Total 2	Mg 2	0	0
56	17	4	Total 4	Mg 4	0	0
56	18	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	19	2	Total Mg 2 2	0	0
56	1a	330	Total Mg 330 330	0	0
56	1b	2	Total Mg 2 2	0	0
56	1c	2	Total Mg 2 2	0	0
56	1d	1	Total Mg 1 1	0	0
56	1e	2	Total Mg 2 2	0	0
56	1f	2	Total Mg 2 2	0	0
56	1l	4	Total Mg 4 4	0	0
56	1m	1	Total Mg 1 1	0	0
56	1n	1	Total Mg 1 1	0	0
56	1s	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1v	1	Total Mg 1 1	0	0
56	1w	11	Total Mg 11 11	0	0
56	1x	18	Total Mg 18 18	0	0
56	1y	5	Total Mg 5 5	0	0
56	2A	919	Total Mg 919 919	0	0
56	2B	21	Total Mg 21 21	0	0
56	2D	3	Total Mg 3 3	0	0
56	2E	8	Total Mg 8 8	0	0
56	2F	4	Total Mg 4 4	0	0

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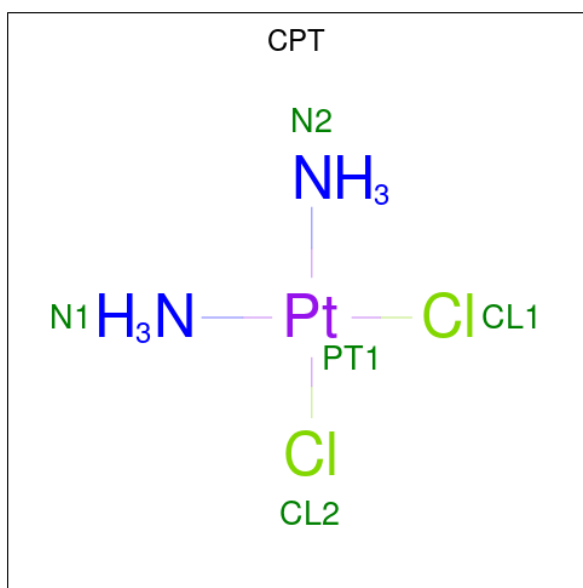
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2G	1	Total Mg 1 1	0	0
56	2N	1	Total Mg 1 1	0	0
56	2O	1	Total Mg 1 1	0	0
56	2P	2	Total Mg 2 2	0	0
56	2Q	3	Total Mg 3 3	0	0
56	2R	2	Total Mg 2 2	0	0
56	2T	1	Total Mg 1 1	0	0
56	2U	6	Total Mg 6 6	0	0
56	2V	1	Total Mg 1 1	0	0
56	2W	4	Total Mg 4 4	0	0
56	2X	2	Total Mg 2 2	0	0
56	2Z	1	Total Mg 1 1	0	0
56	20	3	Total Mg 3 3	0	0
56	23	3	Total Mg 3 3	0	0
56	25	4	Total Mg 4 4	0	0
56	27	1	Total Mg 1 1	0	0
56	28	3	Total Mg 3 3	0	0
56	2a	236	Total Mg 236 236	0	0
56	2d	1	Total Mg 1 1	0	0
56	2e	1	Total Mg 1 1	0	0
56	2f	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2g	1	Total Mg 1 1	0	0
56	2j	2	Total Mg 2 2	0	0
56	2l	4	Total Mg 4 4	0	0
56	2n	1	Total Mg 1 1	0	0
56	2p	1	Total Mg 1 1	0	0
56	2q	4	Total Mg 4 4	0	0
56	2r	1	Total Mg 1 1	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	6	Total Mg 6 6	0	0
56	2w	7	Total Mg 7 7	0	0
56	2x	6	Total Mg 6 6	0	0
56	2y	7	Total Mg 7 7	0	0

- Molecule 57 is Cisplatin (three-letter code: CPT) (formula: $\text{Cl}_2\text{H}_6\text{N}_2\text{Pt}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	1I	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	1a	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	2A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	2A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	2I	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	2a	1	Total	Cl	N	Pt	0	0
			4	1	2	1		

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

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

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

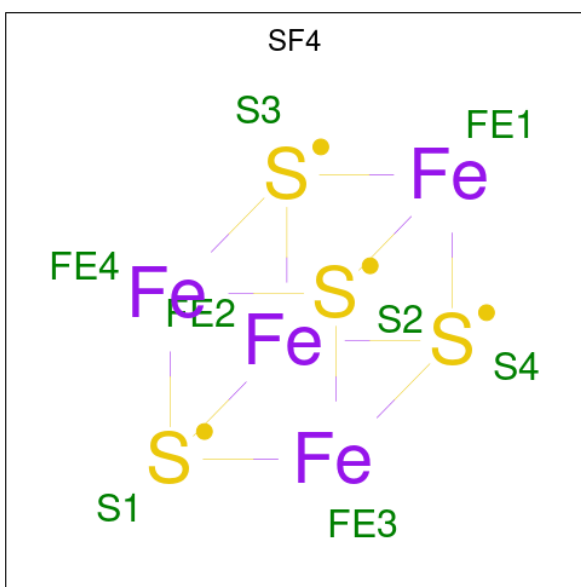
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	25	1	Total Zn 1 1	0	0
59	26	1	Total Zn 1 1	0	0
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2273	Total O 2273 2273	0	0
61	1B	70	Total O 70 70	0	0
61	1D	28	Total O 28 28	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1E	27	Total 27	O 27	0	0
61	1F	15	Total 15	O 15	0	0
61	1G	7	Total 7	O 7	0	0
61	1H	1	Total 1	O 1	0	0
61	1I	1	Total 1	O 1	0	0
61	1N	3	Total 3	O 3	0	0
61	1O	6	Total 6	O 6	0	0
61	1P	23	Total 23	O 23	0	0
61	1Q	12	Total 12	O 12	0	0
61	1R	15	Total 15	O 15	0	0
61	1S	5	Total 5	O 5	0	0
61	1T	10	Total 10	O 10	0	0
61	1U	16	Total 16	O 16	0	0
61	1V	11	Total 11	O 11	0	0
61	1W	13	Total 13	O 13	0	0
61	1X	6	Total 6	O 6	0	0
61	1Y	5	Total 5	O 5	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	12	Total 12	O 12	0	0
61	11	14	Total 14	O 14	0	0
61	12	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	5	Total 5	O 5	0	0
61	14	1	Total 1	O 1	0	0
61	15	7	Total 7	O 7	0	0
61	16	2	Total 2	O 2	0	0
61	17	7	Total 7	O 7	0	0
61	18	10	Total 10	O 10	0	0
61	1a	520	Total 520	O 520	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	2	Total 2	O 2	0	0
61	1e	1	Total 1	O 1	0	0
61	1g	2	Total 2	O 2	0	0
61	1i	1	Total 1	O 1	0	0
61	1l	10	Total 10	O 10	0	0
61	1m	2	Total 2	O 2	0	0
61	1n	1	Total 1	O 1	0	0
61	1o	2	Total 2	O 2	0	0
61	1p	2	Total 2	O 2	0	0
61	1q	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	5	Total 5	O 5	0	0
61	1w	19	Total 19	O 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1x	15	Total 15	O 15	0	0
61	1y	2	Total 2	O 2	0	0
61	2A	1393	Total 1393	O 1393	0	0
61	2B	28	Total 28	O 28	0	0
61	2D	29	Total 29	O 29	0	0
61	2E	18	Total 18	O 18	0	0
61	2F	17	Total 17	O 17	0	0
61	2I	4	Total 4	O 4	0	0
61	2N	1	Total 1	O 1	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	16	Total 16	O 16	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	7	Total 7	O 7	0	0
61	2U	3	Total 3	O 3	0	0
61	2V	2	Total 2	O 2	0	0
61	2W	4	Total 4	O 4	0	0
61	2X	2	Total 2	O 2	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	2	Total 2	O 2	0	0
61	20	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	21	11	Total O 11 11	0	0
61	22	1	Total O 1 1	0	0
61	23	1	Total O 1 1	0	0
61	25	3	Total O 3 3	0	0
61	27	3	Total O 3 3	0	0
61	28	4	Total O 4 4	0	0
61	29	1	Total O 1 1	0	0
61	2a	373	Total O 373 373	0	0
61	2d	2	Total O 2 2	0	0
61	2e	2	Total O 2 2	0	0
61	2g	1	Total O 1 1	0	0
61	2i	1	Total O 1 1	0	0
61	2j	4	Total O 4 4	0	0
61	2l	6	Total O 6 6	0	0
61	2p	1	Total O 1 1	0	0
61	2q	1	Total O 1 1	0	0
61	2r	1	Total O 1 1	0	0
61	2t	4	Total O 4 4	0	0
61	2v	2	Total O 2 2	0	0
61	2w	3	Total O 3 3	0	0
61	2x	9	Total O 9 9	0	0

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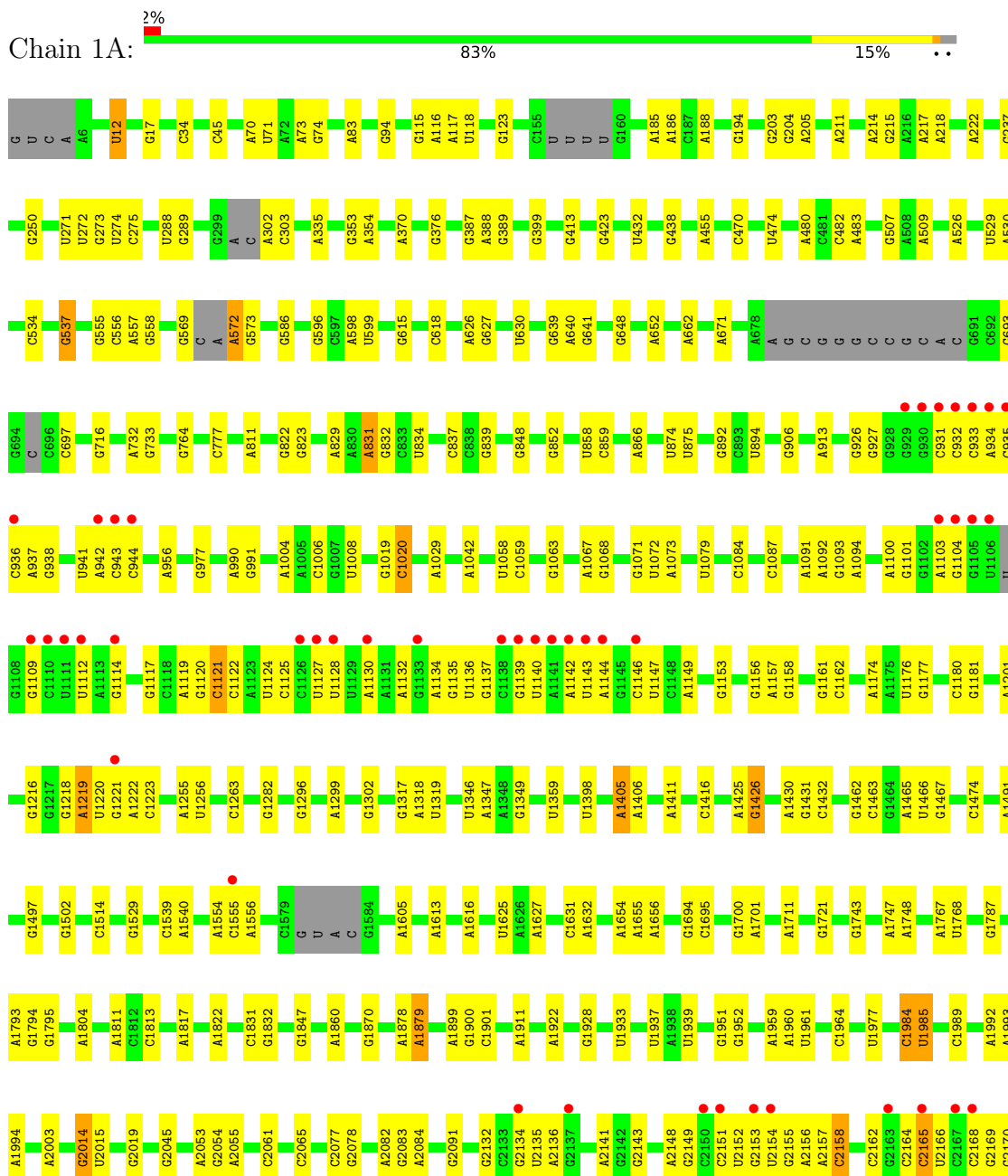
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2y	20	Total	O	0	0
			20	20		

3 Residue-property plots

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





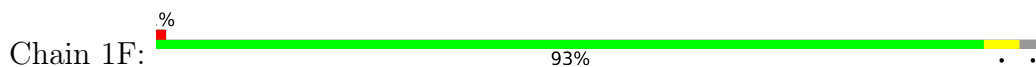
- Molecule 4: 50S ribosomal protein L3



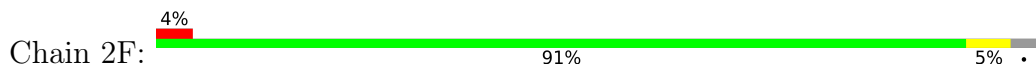
- Molecule 4: 50S ribosomal protein L3



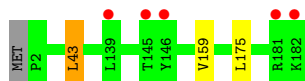
- Molecule 5: 50S ribosomal protein L4



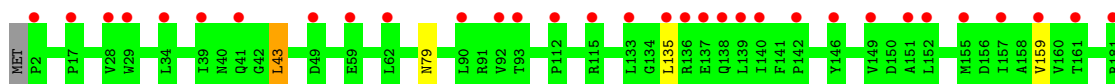
- Molecule 5: 50S ribosomal protein L4



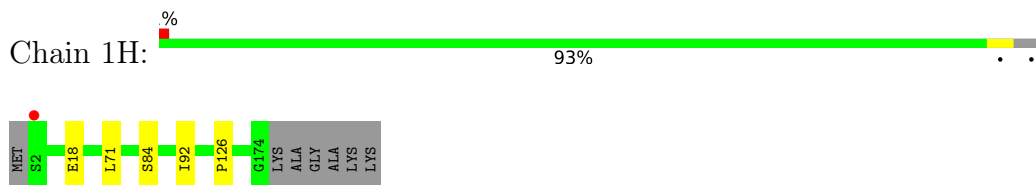
- Molecule 6: 50S ribosomal protein L5



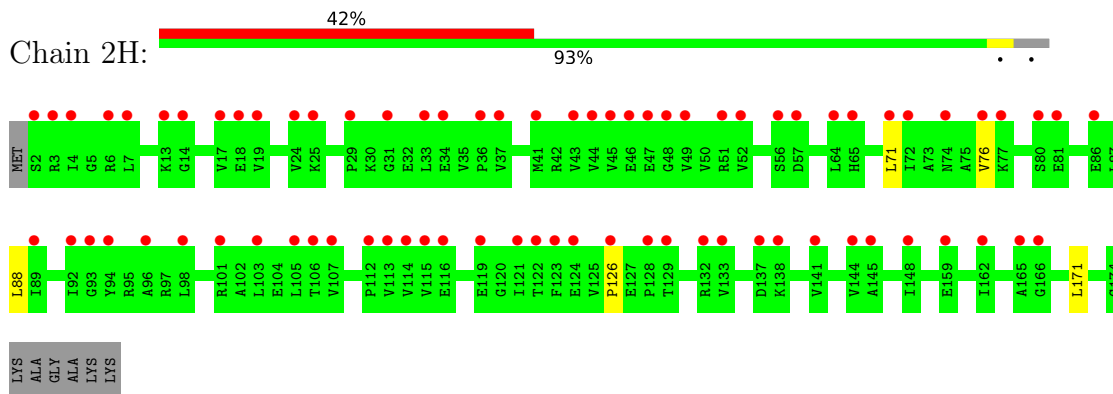
- Molecule 6: 50S ribosomal protein L5



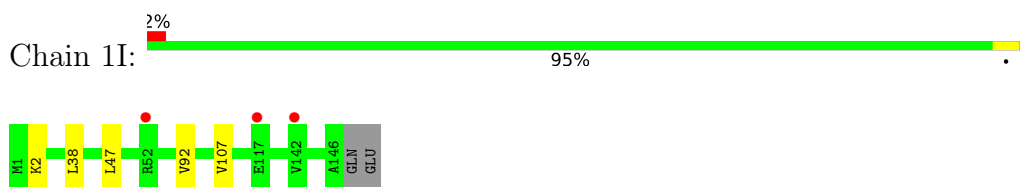
- Molecule 7: 50S ribosomal protein L6



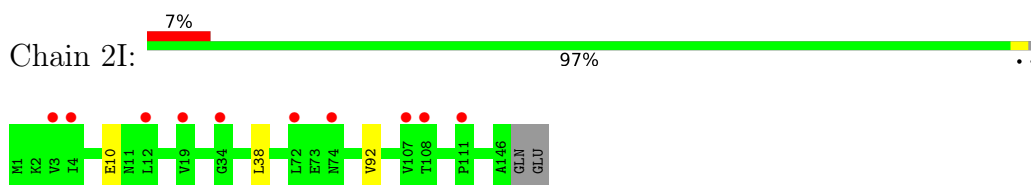
- Molecule 7: 50S ribosomal protein L6



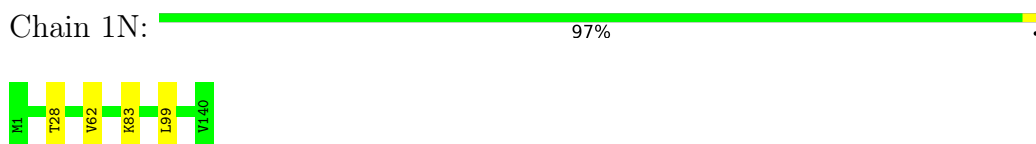
- Molecule 8: 50S ribosomal protein L9



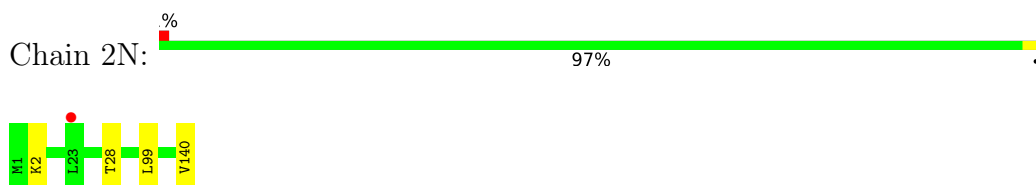
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13

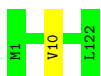


- Molecule 9: 50S ribosomal protein L13



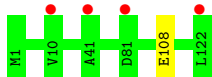
- Molecule 10: 50S ribosomal protein L14

Chain 1O:  99%



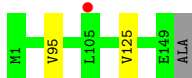
- Molecule 10: 50S ribosomal protein L14

Chain 2O:  99%



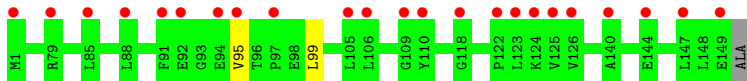
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  98%



- Molecule 11: 50S ribosomal protein L15

Chain 2P:  98%



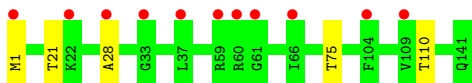
- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  99%



- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  96%

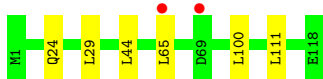


- Molecule 13: 50S ribosomal protein L17

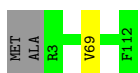
Chain 1R:  95%



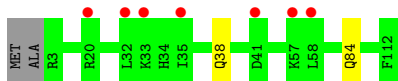
- Molecule 13: 50S ribosomal protein L17



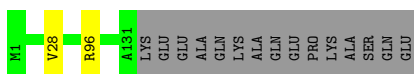
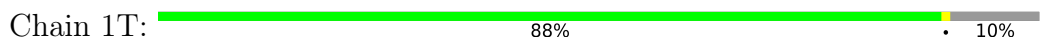
- Molecule 14: 50S ribosomal protein L18



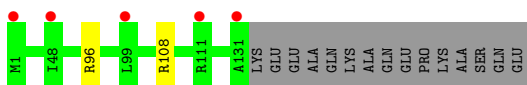
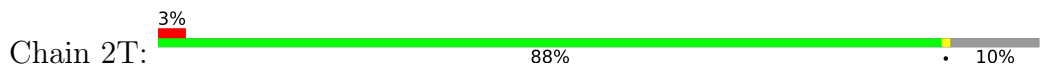
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20





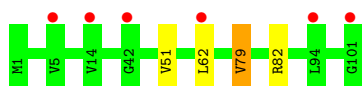
- Molecule 17: 50S ribosomal protein L21

Chain 1V: 94% 5%



- Molecule 17: 50S ribosomal protein L21

Chain 2V: 6% 96%



- Molecule 18: 50S ribosomal protein L22

Chain 1W: 2% 96%



- Molecule 18: 50S ribosomal protein L22

Chain 2W: % 95%



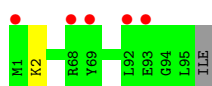
- Molecule 19: 50S ribosomal protein L23

Chain 1X: 99%

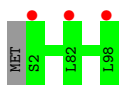


- Molecule 19: 50S ribosomal protein L23

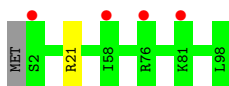
Chain 2X: 5% 98%



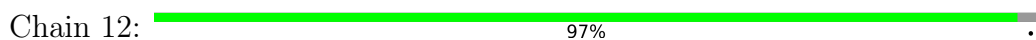
- Molecule 20: 50S ribosomal protein L24



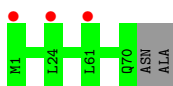
- Molecule 23: 50S ribosomal protein L28



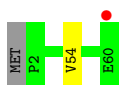
- Molecule 24: 50S ribosomal protein L29



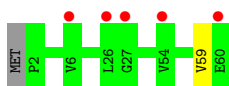
- Molecule 24: 50S ribosomal protein L29



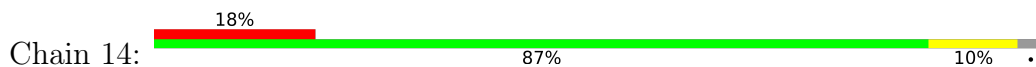
- Molecule 25: 50S ribosomal protein L30



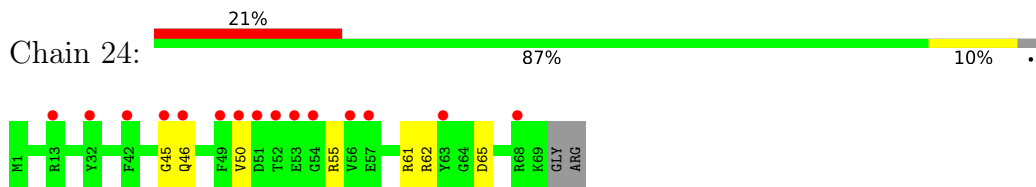
- Molecule 25: 50S ribosomal protein L30



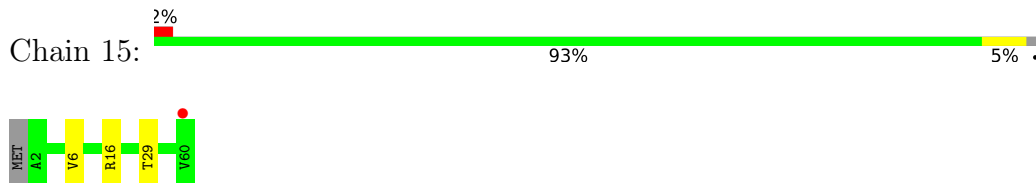
- Molecule 26: 50S ribosomal protein L31



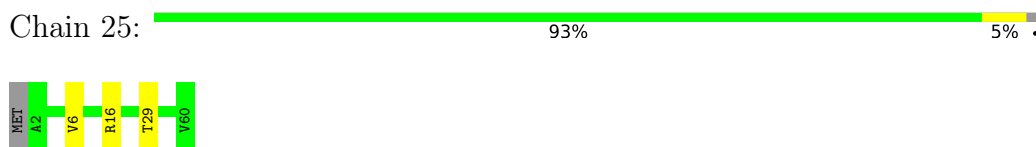
- Molecule 26: 50S ribosomal protein L31



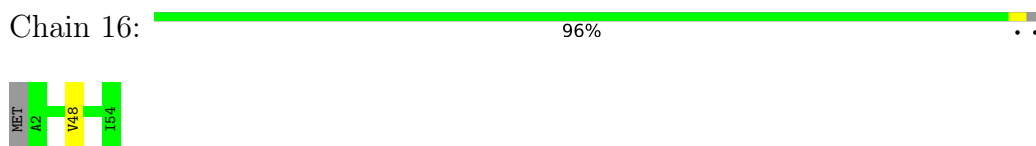
- Molecule 27: 50S ribosomal protein L32



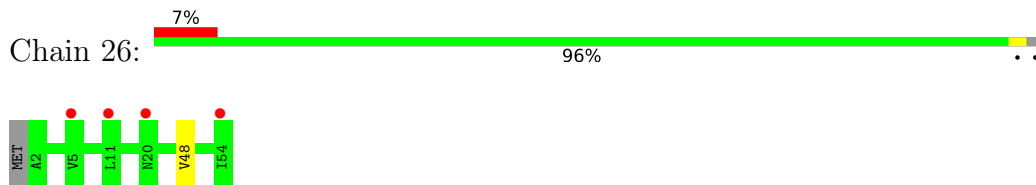
- Molecule 27: 50S ribosomal protein L32



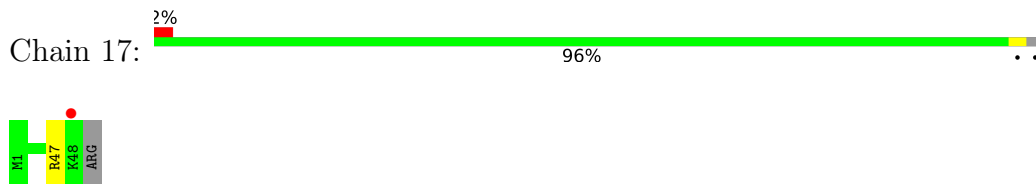
- Molecule 28: 50S ribosomal protein L33



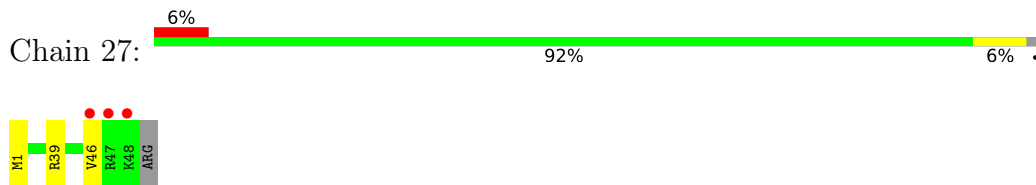
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

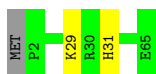


- Molecule 29: 50S ribosomal protein L34



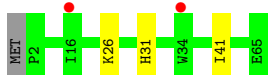
- Molecule 30: 50S ribosomal protein L35

Chain 18:  95%



- Molecule 30: 50S ribosomal protein L35

Chain 28:  94% 5%



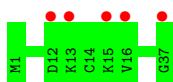
- Molecule 31: 50S ribosomal protein L36

Chain 19:  100%


There are no outlier residues recorded for this chain.

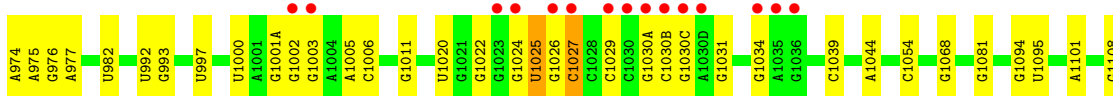
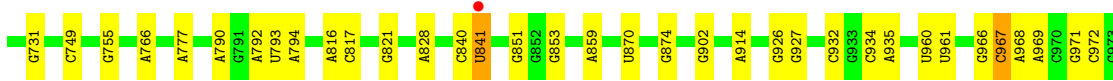
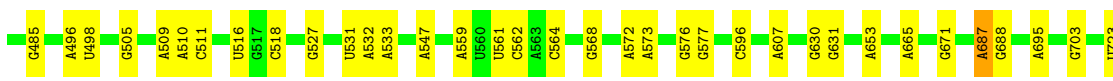
- Molecule 31: 50S ribosomal protein L36

Chain 29:  100% 14%



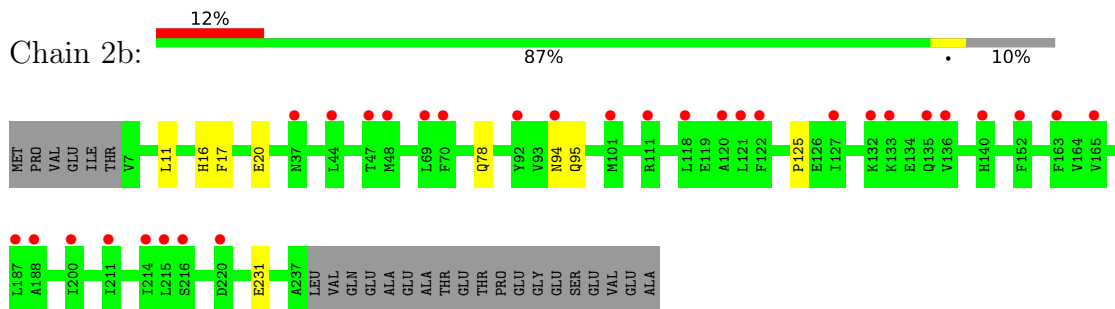
- Molecule 32: 16S ribosomal RNA

Chain 1a:  83% 15%

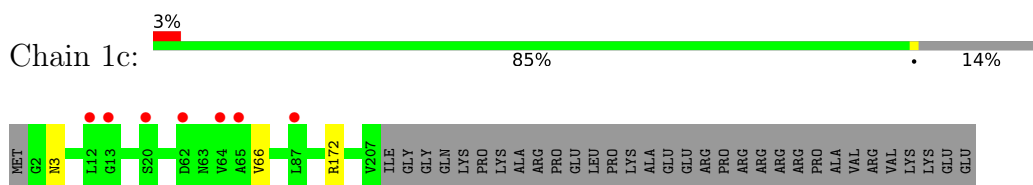


VAL
GLU
ALA

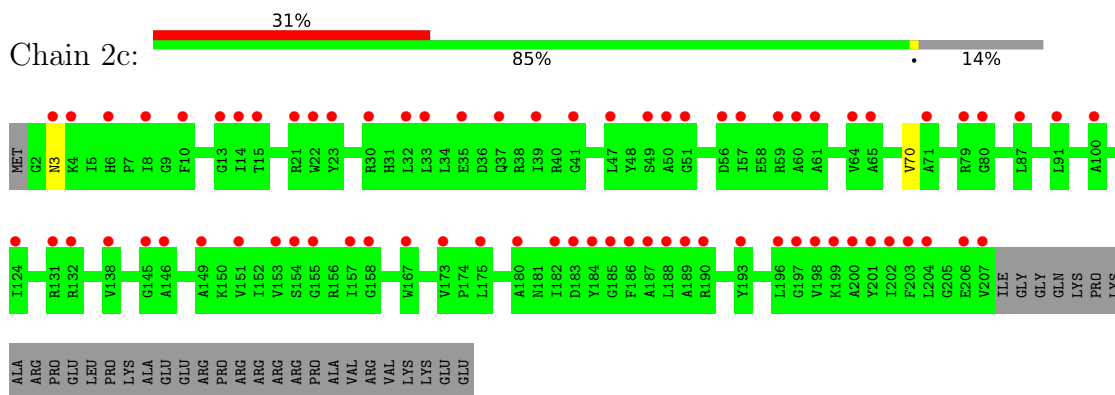
- Molecule 33: 30S ribosomal protein S2



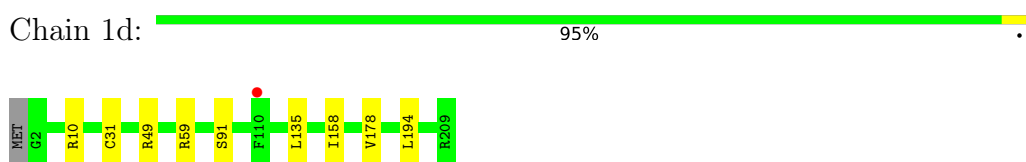
- Molecule 34: 30S ribosomal protein S3



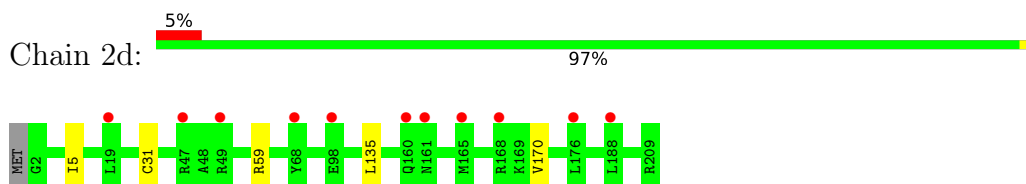
- Molecule 34: 30S ribosomal protein S3




- Molecule 35: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S4

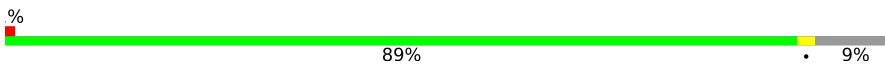


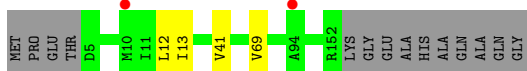
- Molecule 36: 30S ribosomal protein S5

Chain 1e:  87% 9%



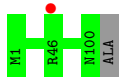
• Molecule 36: 30S ribosomal protein S5

Chain 2e:  89% 9%



• Molecule 37: 30S ribosomal protein S6

Chain 1f:  99%



• Molecule 37: 30S ribosomal protein S6

Chain 2f:  98%



• Molecule 38: 30S ribosomal protein S7

Chain 1g:  97% 10%



• Molecule 38: 30S ribosomal protein S7

Chain 2g:  97% 19%

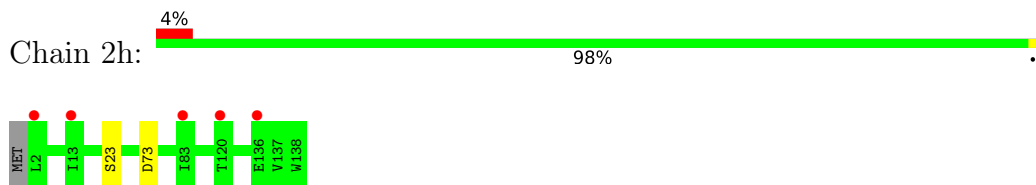


• Molecule 39: 30S ribosomal protein S8

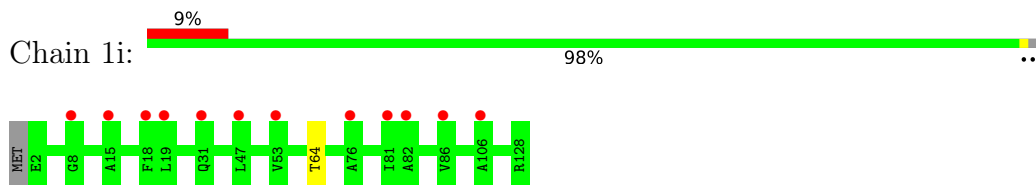
Chain 1h:  98%



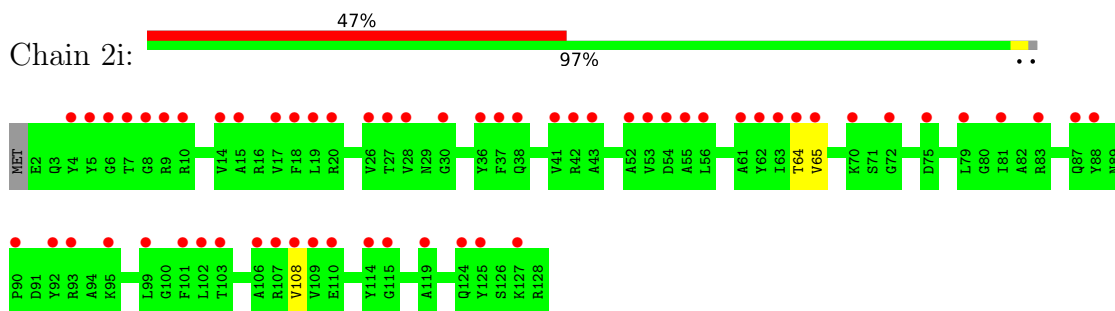
- Molecule 39: 30S ribosomal protein S8



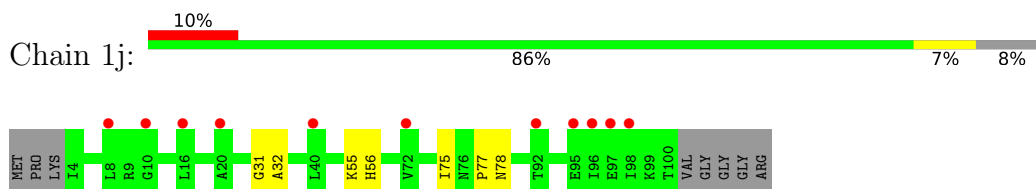
- Molecule 40: 30S ribosomal protein S9



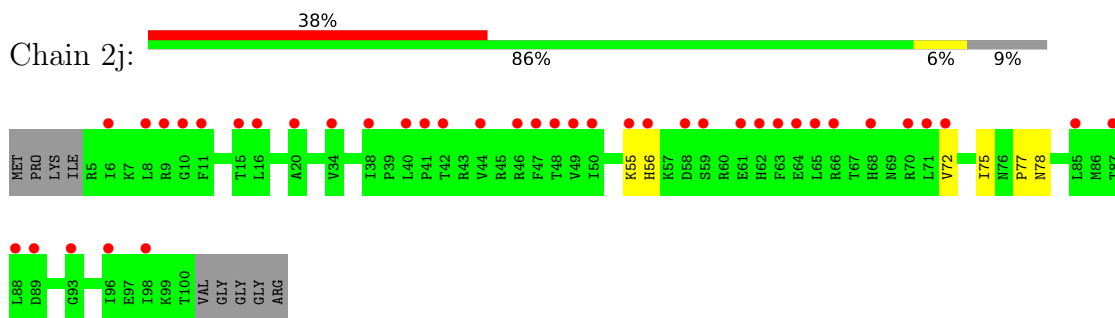
- Molecule 40: 30S ribosomal protein S9



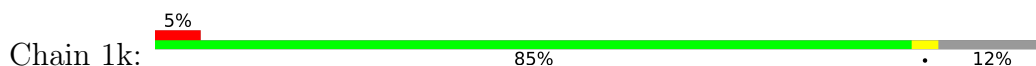
- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10

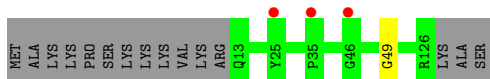
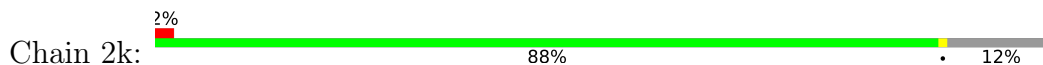


- Molecule 42: 30S ribosomal protein S11

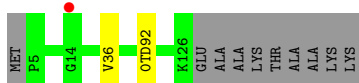
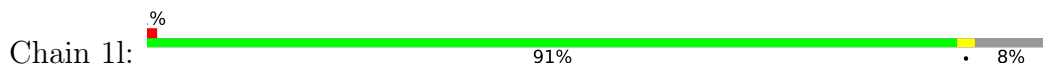




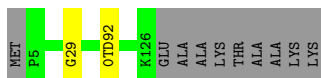
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



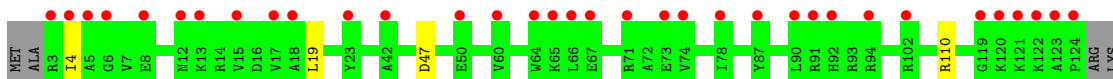
- Molecule 43: 30S ribosomal protein S12



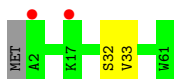
- Molecule 44: 30S ribosomal protein S13



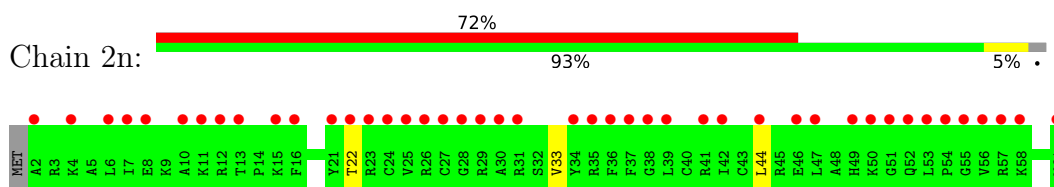
- Molecule 44: 30S ribosomal protein S13



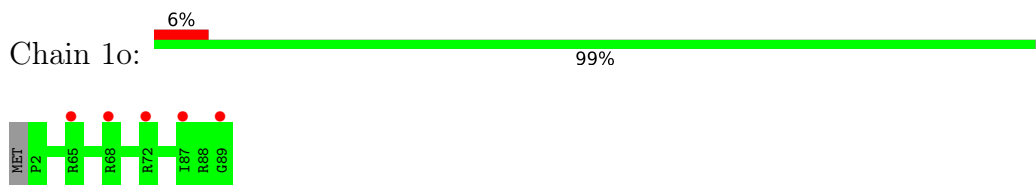
- Molecule 45: 30S ribosomal protein S14 type Z



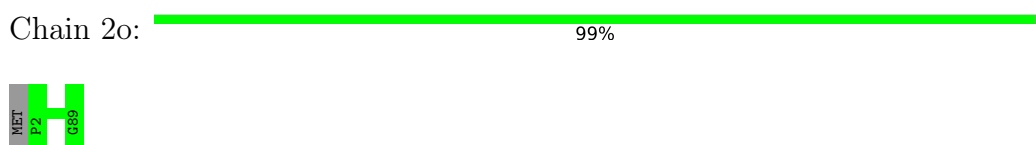
- Molecule 45: 30S ribosomal protein S14 type Z



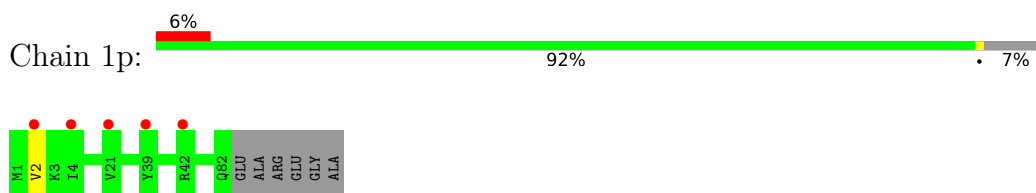
- Molecule 46: 30S ribosomal protein S15



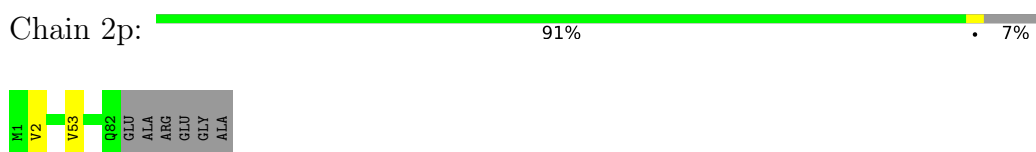
- Molecule 46: 30S ribosomal protein S15



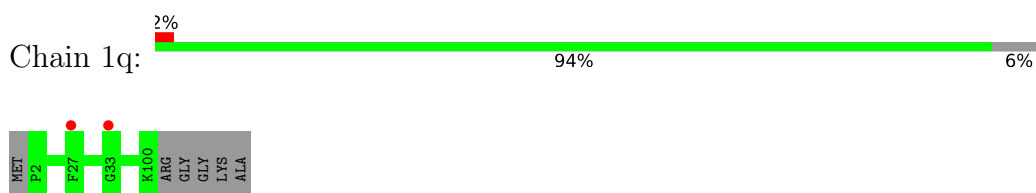
- Molecule 47: 30S ribosomal protein S16



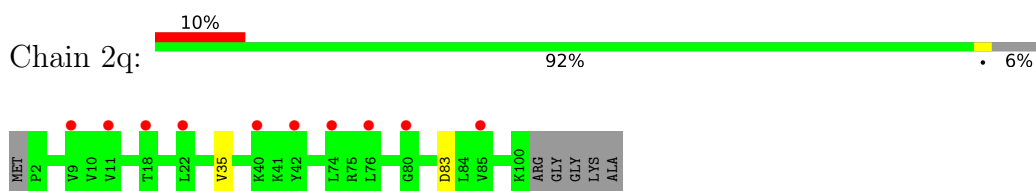
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17

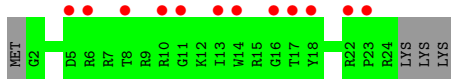
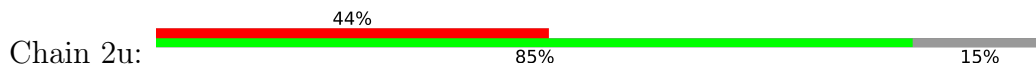


- Molecule 48: 30S ribosomal protein S17





- Molecule 52: 30S ribosomal protein Thx



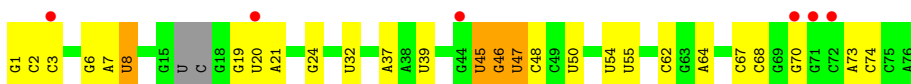
- Molecule 53: mRNA



- Molecule 53: mRNA



- Molecule 54: A-site and E-site tRNAs



- Molecule 54: A-site and E-site tRNAs

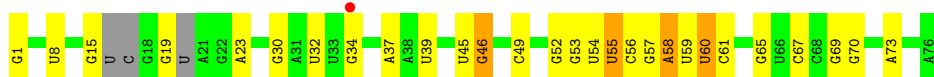


- Molecule 54: A-site and E-site tRNAs

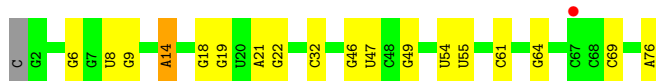
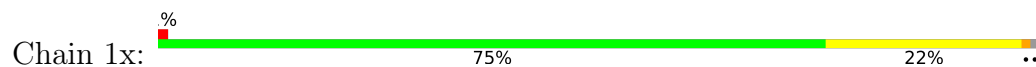


- Molecule 54: A-site and E-site tRNAs

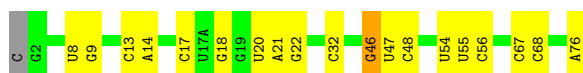
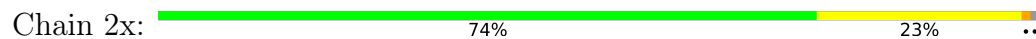




- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.98Å 446.99Å 621.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.65 – 2.80 152.64 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (152.65-2.80) 98.3 (152.64-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.82Å)	Xtrriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.219 , 0.268 0.219 , 0.268	Depositor DCC
R_{free} test set	69488 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtrriage
Anisotropy	0.259	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	301288	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: K, 5MC, MG, 0TD, 5MU, 7MG, 2MU, UR3, 4SU, 2MG, MA6, SF4, ZN, 2MA, MIA, OMG, PSU, CPT, M2G, 4OC

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	0.51	2/69009 (0.0%)	0.91	44/107712 (0.0%)
1	2A	0.41	2/67293 (0.0%)	0.90	25/105034 (0.0%)
2	1B	0.44	1/2882 (0.0%)	0.83	0/4494
2	2B	0.49	1/2879 (0.0%)	0.92	2/4487 (0.0%)
3	1D	0.38	0/2186	0.58	0/2944
3	2D	0.33	0/2186	0.58	1/2944 (0.0%)
4	1E	0.36	0/1592	0.54	0/2149
4	2E	0.33	0/1592	0.57	1/2149 (0.0%)
5	1F	0.35	0/1619	0.52	0/2193
5	2F	0.33	0/1615	0.54	0/2188
6	1G	0.30	0/1448	0.51	0/1957
6	2G	0.31	0/1453	0.54	0/1963
7	1H	0.32	0/1347	0.51	0/1823
7	2H	0.29	0/1347	0.52	1/1823 (0.1%)
8	1I	0.29	0/1112	0.52	0/1514
8	2I	0.27	0/1079	0.50	0/1475
9	1N	0.35	0/1144	0.49	0/1543
9	2N	0.31	0/1144	0.50	0/1543
10	1O	0.37	0/943	0.53	0/1269
10	2O	0.30	0/943	0.48	0/1269
11	1P	0.35	0/1152	0.56	0/1533
11	2P	0.31	0/1152	0.58	0/1533
12	1Q	0.36	0/1143	0.50	0/1527
12	2Q	0.32	0/1143	0.55	0/1527
13	1R	0.35	0/982	0.54	0/1312
13	2R	0.31	0/982	0.53	0/1312
14	1S	0.32	0/883	0.51	0/1176
14	2S	0.32	0/880	0.51	0/1172
15	1T	0.34	0/1105	0.50	0/1477
15	2T	0.31	0/1097	0.50	0/1468
16	1U	0.39	0/977	0.52	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.32	0/977	0.50	0/1301
17	1V	0.35	0/782	0.51	0/1049
17	2V	0.32	0/782	0.52	0/1049
18	1W	0.38	0/897	0.52	0/1205
18	2W	0.33	0/897	0.52	0/1205
19	1X	0.38	0/764	0.57	0/1025
19	2X	0.31	0/764	0.49	0/1025
20	1Y	0.36	0/819	0.55	0/1095
20	2Y	0.32	0/819	0.51	0/1095
21	1Z	0.30	0/1267	0.52	0/1717
21	2Z	0.31	0/1299	0.54	0/1763
22	10	0.36	0/662	0.54	0/881
22	20	0.30	0/662	0.49	0/881
23	11	0.34	0/762	0.51	0/1014
23	21	0.31	0/762	0.52	0/1014
24	12	0.34	0/590	0.51	0/781
24	22	0.31	0/590	0.43	0/781
25	13	0.35	0/474	0.52	0/635
25	23	0.29	0/469	0.48	0/630
26	14	0.36	0/565	0.64	0/761
26	24	0.32	0/545	0.50	0/737
27	15	0.33	0/469	0.52	0/635
27	25	0.31	0/469	0.50	0/635
28	16	0.35	0/460	0.48	0/613
28	26	0.33	0/456	0.48	0/608
29	17	0.36	0/426	0.52	0/561
29	27	0.33	0/426	0.58	0/561
30	18	0.36	0/525	0.53	0/691
30	28	0.31	0/525	0.51	0/691
31	19	0.39	0/310	0.53	0/407
31	29	0.29	0/310	0.49	0/407
32	1a	0.37	1/35795 (0.0%)	0.86	23/55864 (0.0%)
32	2a	0.35	3/35886 (0.0%)	0.86	30/56005 (0.1%)
33	1b	0.29	0/1881	0.53	0/2542
33	2b	0.31	0/1860	0.52	0/2518
34	1c	0.28	0/1572	0.47	0/2126
34	2c	0.30	0/1566	0.50	0/2119
35	1d	0.30	0/1685	0.50	0/2262
35	2d	0.29	0/1704	0.50	0/2284
36	1e	0.31	0/1145	0.52	0/1543
36	2e	0.31	0/1149	0.54	0/1548
37	1f	0.30	0/823	0.50	0/1115
37	2f	0.30	0/829	0.45	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.29	0/1250	0.47	0/1679
38	2g	0.28	0/1254	0.49	0/1683
39	1h	0.28	0/1108	0.49	0/1494
39	2h	0.27	0/1108	0.50	0/1494
40	1i	0.29	0/1002	0.52	0/1346
40	2i	0.28	0/997	0.50	0/1343
41	1j	0.27	0/722	0.53	0/982
41	2j	0.30	0/727	0.53	0/988
42	1k	0.28	0/844	0.49	0/1145
42	2k	0.29	0/848	0.49	0/1149
43	1l	0.32	0/937	0.53	0/1260
43	2l	0.28	0/937	0.57	1/1260 (0.1%)
44	1m	0.29	0/969	0.53	0/1302
44	2m	0.29	0/961	0.56	0/1291
45	1n	0.32	0/501	0.54	0/664
45	2n	0.29	0/501	0.52	0/664
46	1o	0.28	0/739	0.46	0/985
46	2o	0.28	0/739	0.50	0/985
47	1p	0.29	0/697	0.51	0/939
47	2p	0.29	0/693	0.50	0/935
48	1q	0.30	0/836	0.49	0/1117
48	2q	0.28	0/836	0.49	0/1117
49	1r	0.30	0/560	0.53	0/746
49	2r	0.30	0/560	0.47	0/746
50	1s	0.27	0/667	0.52	0/900
50	2s	0.32	0/661	0.61	0/893
51	1t	0.27	0/730	0.49	0/965
51	2t	0.27	0/729	0.48	0/965
52	1u	0.26	0/203	0.47	0/266
52	2u	0.26	0/203	0.49	0/266
53	1v	0.35	0/310	0.82	0/480
53	2v	0.34	0/310	0.78	0/480
54	1w	0.53	1/1606 (0.1%)	1.07	5/2497 (0.2%)
54	1y	0.48	1/1606 (0.1%)	1.02	4/2497 (0.2%)
54	2w	0.44	0/1556	1.03	0/2418
54	2y	0.51	1/1583 (0.1%)	1.06	3/2459 (0.1%)
55	1x	0.54	2/1725 (0.1%)	1.14	16/2689 (0.6%)
55	2x	0.46	0/1725	1.08	16/2689 (0.6%)
All	All	0.40	15/316668 (0.0%)	0.82	172/474091 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	1	G	OP3-P	-10.24	1.48	1.61
2	2B	1	U	OP3-P	-10.23	1.48	1.61
54	1y	1	G	OP3-P	-10.13	1.49	1.61
2	1B	1	U	OP3-P	-10.08	1.49	1.61
54	1w	1	G	OP3-P	-9.91	1.49	1.61
1	2A	1848	A	C8-N7	9.09	1.38	1.31
1	1A	1879	A	C8-N7	8.93	1.37	1.31
32	2a	790	A	C8-N7	8.69	1.37	1.31
32	1a	790	A	C8-N7	8.68	1.37	1.31
1	2A	2531	A	C8-N7	8.67	1.37	1.31
1	1A	2543	A	C8-N7	8.01	1.37	1.31
32	2a	1272	G	C6-N1	-7.94	1.33	1.39
32	2a	1272	G	N1-C2	-6.71	1.32	1.37
55	1x	22	G	N7-C5	5.51	1.42	1.39
55	1x	14	A	N7-C5	-5.03	1.36	1.39

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C5-C6-O6	16.43	138.46	128.60
32	2a	1272	G	N3-C2-N2	14.39	129.97	119.90
32	2a	1263	C	N1-C2-O2	14.28	127.47	118.90
32	2a	1272	G	N1-C2-N2	-14.21	103.41	116.20
32	2a	1272	G	N1-C6-O6	-12.06	112.66	119.90
2	2B	80	U	O4'-C1'-N1	10.54	116.63	108.20
32	2a	1263	C	N3-C2-O2	-10.00	114.90	121.90
1	1A	1121	C	N1-C2-O2	9.97	124.88	118.90
55	1x	46	G	C6-N1-C2	-9.16	119.60	125.10
32	2a	1263	C	C2-N3-C4	9.15	124.48	119.90
1	1A	1121	C	C2-N3-C4	9.15	124.47	119.90
55	1x	14	A	C4-C5-C6	8.98	121.49	117.00
55	2x	46	G	C6-N1-C2	-8.83	119.80	125.10
32	1a	1027	C	C5-C4-N4	8.69	126.29	120.20
32	1a	1027	C	N3-C4-C5	-8.51	118.50	121.90
55	1x	14	A	C5-N7-C8	8.34	108.07	103.90
32	1a	1027	C	N3-C2-O2	-8.34	116.06	121.90
1	1A	2189	U	C2-N1-C1'	8.27	127.62	117.70
32	2a	1272	G	C4-N9-C1'	8.11	137.05	126.50
1	1A	1109	G	C5-C6-O6	8.09	133.46	128.60
54	1y	33	U	C2-N1-C1'	8.08	127.40	117.70
1	2A	2473	U	C2-N1-C1'	7.91	127.19	117.70
32	1a	1027	C	C6-N1-C2	-7.79	117.19	120.30
32	2a	1272	G	C8-N9-C1'	-7.50	117.25	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2189	U	N1-C2-O2	7.44	128.01	122.80
1	1A	12	U	C2-N1-C1'	7.43	126.62	117.70
1	2A	2140	C	N1-C2-O2	7.31	123.29	118.90
1	1A	848	G	O5'-P-OP2	-7.30	99.13	105.70
1	1A	1109	G	C6-N1-C2	7.29	129.47	125.10
1	2A	2167	U	C2-N1-C1'	7.28	126.43	117.70
32	1a	1030(B)	C	C2-N1-C1'	7.26	126.78	118.80
1	2A	787	U	O5'-P-OP1	-7.25	99.18	105.70
32	1a	1030(B)	C	N1-C2-O2	7.24	123.25	118.90
1	1A	1985	U	C2-N1-C1'	7.20	126.34	117.70
1	1A	1359	U	C2-N1-C1'	7.20	126.34	117.70
32	2a	1263	C	C6-N1-C2	-7.08	117.47	120.30
1	1A	537	G	O4'-C1'-N9	7.05	113.84	108.20
55	2x	17	C	N1-C2-O2	7.03	123.12	118.90
55	2x	17	C	N3-C2-O2	-6.96	117.03	121.90
1	2A	2167	U	N1-C2-O2	6.96	127.67	122.80
55	1x	14	A	C5-C6-N1	-6.89	114.26	117.70
1	2A	2248	C	O5'-P-OP2	-6.87	99.52	105.70
55	2x	22	G	C5-N7-C8	-6.84	100.88	104.30
1	1A	2189	U	N3-C2-O2	-6.83	117.42	122.20
1	2A	2167	U	N3-C2-O2	-6.78	117.45	122.20
55	2x	46	G	N3-C2-N2	-6.78	115.16	119.90
32	1a	254	G	O5'-P-OP1	-6.73	99.64	105.70
1	1A	1985	U	N1-C2-O2	6.72	127.50	122.80
54	1w	47	U	C2-N1-C1'	6.71	125.76	117.70
1	1A	831	A	O4'-C1'-N9	6.68	113.54	108.20
55	1x	22	G	C4-C5-C6	-6.67	114.80	118.80
55	1x	22	G	N1-C6-O6	-6.63	115.92	119.90
1	1A	2701	U	P-O3'-C3'	6.60	127.62	119.70
32	1a	1030(B)	C	C6-N1-C2	-6.53	117.69	120.30
32	2a	1025	U	N1-C2-O2	6.51	127.36	122.80
1	1A	1426	G	O5'-P-OP2	-6.46	99.88	105.70
32	2a	1001(A)	G	N3-C4-N9	6.46	129.88	126.00
1	1A	215	G	O4'-C1'-N9	6.44	113.35	108.20
1	1A	1109	G	N3-C2-N2	6.26	124.28	119.90
1	2A	2128	C	C2-N3-C4	6.26	123.03	119.90
1	1A	1020	C	N1-C2-O2	-6.23	115.16	118.90
32	2a	1263	C	C5-C4-N4	6.20	124.54	120.20
55	1x	22	G	C5-N7-C8	-6.19	101.20	104.30
32	1a	1034	G	N3-C2-N2	6.19	124.23	119.90
1	2A	1992	G	P-O3'-C3'	6.15	127.08	119.70
55	2x	14	A	C5-N7-C8	6.09	106.95	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1034	G	N9-C4-C5	-6.09	102.96	105.40
1	1A	1128	U	C2-N1-C1'	6.06	124.98	117.70
55	2x	22	G	C4-C5-C6	-6.05	115.17	118.80
55	2x	17	C	C2-N1-C1'	6.04	125.44	118.80
1	2A	2061	G	O5'-P-OP2	-6.00	100.30	105.70
32	1a	1030(B)	C	N3-C2-O2	-5.97	117.72	121.90
1	1A	894	U	C2-N1-C1'	5.95	124.84	117.70
1	2A	801	G	O5'-P-OP2	-5.93	100.36	105.70
1	1A	2158	C	C5-C6-N1	5.92	123.96	121.00
32	1a	1027	C	N1-C2-O2	5.90	122.44	118.90
1	1A	2014	G	P-O3'-C3'	5.90	126.78	119.70
1	1A	834	U	O5'-P-OP1	-5.87	100.41	105.70
1	1A	2641	A	P-O3'-C3'	5.84	126.70	119.70
32	1a	266	G	P-O3'-C3'	5.83	126.69	119.70
54	1y	33	U	C6-N1-C1'	-5.82	113.06	121.20
54	1y	33	U	N1-C2-O2	5.81	126.87	122.80
32	2a	1025	U	C2-N1-C1'	5.79	124.65	117.70
32	2a	1003	G	C8-N9-C4	-5.79	104.08	106.40
1	2A	2130	U	C5-C6-N1	5.78	125.59	122.70
3	2D	94	LEU	CA-CB-CG	5.78	128.59	115.30
32	2a	1003	G	N7-C8-N9	5.74	115.97	113.10
55	1x	46	G	N9-C4-C5	5.74	107.69	105.40
55	2x	17	C	C6-N1-C2	-5.74	118.01	120.30
32	1a	1158	C	N1-C2-O2	5.72	122.33	118.90
55	1x	22	G	N3-C4-N9	-5.72	122.57	126.00
55	1x	22	G	C8-N9-C1'	5.71	134.42	127.00
32	2a	1263	C	C5-C6-N1	5.68	123.84	121.00
1	1A	2189	U	C5-C6-N1	5.67	125.54	122.70
32	2a	754	C	C2-N1-C1'	5.65	125.01	118.80
54	2y	58	A	OP1-P-O3'	5.64	117.61	105.20
1	2A	2689	U	P-O3'-C3'	5.62	126.45	119.70
55	2x	14	A	C4-C5-C6	5.60	119.80	117.00
1	1A	1219	A	OP1-P-O3'	5.59	117.51	105.20
54	1w	45	U	C2-N1-C1'	5.59	124.40	117.70
1	1A	1121	C	C5-C4-N4	5.58	124.11	120.20
32	1a	1158	C	C2-N1-C1'	5.56	124.92	118.80
32	2a	1001(A)	G	C4-N9-C1'	5.55	133.72	126.50
1	2A	748	G	C8-N9-C1'	5.55	134.21	127.00
1	2A	576	U	O5'-P-OP1	-5.54	100.71	105.70
32	2a	266	G	P-O3'-C3'	5.54	126.34	119.70
32	2a	1029	C	N1-C2-O2	5.53	122.22	118.90
32	1a	1025	U	N1-C2-O2	5.52	126.67	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	46	G	C5-C6-N1	5.52	114.26	111.50
32	2a	1272	G	C6-N1-C2	5.51	128.41	125.10
1	1A	1219	A	P-O3'-C3'	5.50	126.30	119.70
1	1A	892	G	O4'-C1'-N9	5.49	112.59	108.20
32	2a	754	C	N1-C2-O2	5.49	122.19	118.90
54	1w	45	U	N1-C2-O2	5.47	126.63	122.80
1	2A	2140	C	C2-N1-C1'	5.46	124.80	118.80
55	2x	22	G	N1-C6-O6	-5.45	116.63	119.90
1	2A	748	G	C4-N9-C1'	-5.44	119.43	126.50
55	2x	14	A	C5-C6-N1	-5.43	114.98	117.70
55	1x	22	G	C6-C5-N7	5.40	133.64	130.40
54	1y	33	U	C5-C6-N1	5.39	125.40	122.70
55	1x	46	G	C4-C5-N7	-5.36	108.66	110.80
32	2a	1272	G	C2-N3-C4	-5.36	109.22	111.90
55	2x	22	G	C8-N9-C1'	5.36	133.96	127.00
1	1A	2802	C	C2-N1-C1'	-5.34	112.92	118.80
32	1a	1027	C	C2-N3-C4	5.33	122.56	119.90
1	1A	1405	A	N1-C2-N3	5.32	131.96	129.30
55	1x	46	G	C5-C6-N1	5.31	114.16	111.50
55	2x	22	G	C5-C6-N1	5.30	114.15	111.50
4	2E	119	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	1A	572	A	P-O3'-C3'	5.27	126.02	119.70
1	1A	2165	C	C2-N3-C4	5.27	122.53	119.90
1	1A	1121	C	N3-C2-O2	-5.26	118.22	121.90
1	1A	599	U	O5'-P-OP1	-5.26	100.96	105.70
32	2a	1272	G	C5-C6-N1	-5.25	108.88	111.50
32	2a	65	U	P-O3'-C3'	5.24	125.99	119.70
54	1w	47	U	N1-C2-O2	5.24	126.47	122.80
1	2A	528	A	OP1-P-O3'	5.23	116.70	105.20
54	1w	47	U	C5-C6-N1	5.23	125.31	122.70
32	1a	1002	G	C4-N9-C1'	5.22	133.28	126.50
1	1A	1901	C	C6-N1-C2	-5.21	118.22	120.30
32	2a	266	G	N3-C4-C5	-5.20	126.00	128.60
32	1a	687	A	P-O3'-C3'	5.20	125.94	119.70
1	2A	2345	G	C8-N9-C4	-5.20	104.32	106.40
1	2A	2473	U	C6-N1-C1'	-5.19	113.93	121.20
2	2B	1	U	C2-N1-C1'	5.18	123.92	117.70
55	1x	14	A	C4-N9-C1'	5.17	135.61	126.30
32	2a	913	A	P-O3'-C3'	5.17	125.90	119.70
55	1x	14	A	C8-N9-C1'	-5.16	118.41	127.70
1	1A	12	U	N1-C2-O2	5.15	126.40	122.80
54	2y	58	A	P-O3'-C3'	5.15	125.88	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1027	C	C6-N1-C1'	5.13	126.96	120.80
1	2A	228	A	P-O3'-C3'	5.13	125.86	119.70
1	1A	12	U	N3-C2-O2	-5.12	118.62	122.20
32	1a	841	U	C5-C6-N1	5.12	125.26	122.70
32	1a	1034	G	C6-N1-C2	5.12	128.17	125.10
1	1A	1177	G	O4'-C1'-N9	5.11	112.28	108.20
1	1A	2189	U	C6-N1-C1'	-5.09	114.07	121.20
32	2a	1025	U	C6-N1-C1'	-5.09	114.07	121.20
1	1A	2621	U	N1-C2-O2	-5.09	119.23	122.80
54	2y	60	U	N3-C2-O2	-5.09	118.64	122.20
43	2l	29	GLY	N-CA-C	-5.08	100.39	113.10
55	1x	22	G	C5-C6-N1	5.08	114.04	111.50
1	2A	897	C	C5-C6-N1	5.08	123.54	121.00
1	2A	1779	U	O4'-C1'-N1	5.07	112.26	108.20
1	1A	2701	U	N3-C2-O2	-5.07	118.65	122.20
7	2H	171	LEU	CA-CB-CG	5.05	126.93	115.30
1	2A	1204	A	O4'-C1'-N9	5.05	112.24	108.20
55	2x	46	G	N9-C4-C5	5.05	107.42	105.40
1	2A	2174	C	N1-C2-O2	5.05	121.93	118.90
32	1a	1030(B)	C	C5-C6-N1	5.04	123.52	121.00
1	1A	1985	U	N3-C2-O2	-5.03	118.68	122.20
32	2a	563	A	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

There are no planarity outliers.

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%)	263 (96%)	10 (4%)	0	100	100
3	2D	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	34	66
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	61
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	61
5	1F	201/210 (96%)	198 (98%)	2 (1%)	1 (0%)	29	61
5	2F	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	15	44
6	1G	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	25	56
6	2G	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	25	56
7	1H	171/180 (95%)	161 (94%)	8 (5%)	2 (1%)	13	39
7	2H	171/180 (95%)	162 (95%)	8 (5%)	1 (1%)	25	56
8	1I	144/148 (97%)	136 (94%)	8 (6%)	0	100	100
8	2I	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	22	53
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	22	53
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	140 (95%)	7 (5%)	0	100	100
11	2P	147/150 (98%)	136 (92%)	11 (8%)	0	100	100
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
12	2Q	139/141 (99%)	132 (95%)	6 (4%)	1 (1%)	22	53
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
14	2S	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	17	46
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	44
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	44
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	41
20	1Y	105/110 (96%)	100 (95%)	3 (3%)	2 (2%)	8	26
20	2Y	105/110 (96%)	101 (96%)	3 (3%)	1 (1%)	15	44
21	1Z	148/206 (72%)	134 (90%)	14 (10%)	0	100	100
21	2Z	156/206 (76%)	139 (89%)	16 (10%)	1 (1%)	25	56
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	13	39
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	68 (100%)	0	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	28
26	14	67/71 (94%)	55 (82%)	7 (10%)	5 (8%)	1	2
26	24	67/71 (94%)	53 (79%)	8 (12%)	6 (9%)	1	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	51 (100%)	0	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	6	22
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	201 (88%)	20 (9%)	8 (4%)	3	12
33	2b	229/256 (90%)	202 (88%)	20 (9%)	7 (3%)	4	14
34	1c	204/239 (85%)	189 (93%)	13 (6%)	2 (1%)	15	44
34	2c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	29	61
35	1d	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	29	61
36	1e	146/162 (90%)	141 (97%)	2 (1%)	3 (2%)	7	23
36	2e	146/162 (90%)	139 (95%)	6 (4%)	1 (1%)	22	53
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	145 (95%)	6 (4%)	2 (1%)	12	36
38	2g	153/156 (98%)	142 (93%)	8 (5%)	3 (2%)	7	24
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	22	53
40	1i	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
40	2i	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
41	1j	95/105 (90%)	82 (86%)	6 (6%)	7 (7%)	1	2
41	2j	94/105 (90%)	84 (89%)	5 (5%)	5 (5%)	2	6
42	1k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	8	28
42	2k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	17	46
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	113 (93%)	7 (6%)	1 (1%)	19	49
44	2m	120/126 (95%)	112 (93%)	7 (6%)	1 (1%)	19	49
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
47	1p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	12	36
48	1q	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
48	2q	97/105 (92%)	96 (99%)	1 (1%)	0	100	100
49	1r	66/88 (75%)	66 (100%)	0	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	73 (90%)	7 (9%)	1 (1%)	13	39
50	2s	81/93 (87%)	72 (89%)	7 (9%)	2 (2%)	5	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	8
51	2t	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	2	8
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11368/12128 (94%)	10766 (95%)	507 (4%)	95 (1%)	19	49

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
26	14	53	GLU
26	14	61	ARG
33	1b	17	PHE
38	1g	79	ARG
41	1j	32	ALA
50	1s	81	ARG
5	2F	21	ALA
5	2F	130	ALA
7	2H	126	PRO
8	2I	10	GLU
12	2Q	28	ALA
26	24	55	ARG
26	24	61	ARG
29	27	46	VAL
33	2b	16	HIS
33	2b	17	PHE
38	2g	79	ARG
50	2s	81	ARG
6	1G	43	LEU
7	1H	126	PRO
17	1V	79	VAL
26	14	45	GLY
26	14	57	GLU
41	1j	55	LYS
41	1j	56	HIS
41	1j	75	ILE
42	1k	49	GLY
51	1t	47	GLY
51	1t	96	GLY
51	1t	100	ILE
4	2E	52	LEU

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Mol	Chain	Res	Type
9	2N	2	LYS
17	2V	79	VAL
26	24	45	GLY
33	2b	78	GLN
41	2j	56	HIS
41	2j	75	ILE
51	2t	47	GLY
51	2t	100	ILE
4	1E	52	LEU
20	1Y	78	ALA
26	14	44	THR
33	1b	20	GLU
33	1b	21	ARG
33	1b	231	GLU
41	1j	78	ASN
3	2D	3	VAL
6	2G	43	LEU
14	2S	84	GLN
26	24	46	GLN
26	24	62	ARG
33	2b	231	GLU
38	2g	7	ALA
41	2j	55	LYS
41	2j	78	ASN
42	2k	49	GLY
44	2m	4	ILE
50	2s	29	ARG
51	2t	95	ALA
20	1Y	54	LYS
33	1b	78	GLN
33	1b	125	PRO
34	1c	3	ASN
35	1d	178	VAL
36	1e	86	ALA
41	1j	31	GLY
41	1j	77	PRO
19	2X	2	LYS
20	2Y	78	ALA
21	2Z	146	ILE
22	20	4	LYS
33	2b	125	PRO
34	2c	3	ASN

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Mol	Chain	Res	Type
36	2e	69	VAL
38	2g	80	VAL
39	2h	73	ASP
33	1b	16	HIS
33	1b	37	ASN
34	1c	66	VAL
38	1g	80	VAL
26	24	65	ASP
33	2b	20	GLU
36	1e	69	VAL
33	2b	95	GLN
41	2j	77	PRO
44	1m	6	GLY
47	2p	53	VAL
7	1H	92	ILE
42	1k	105	VAL
51	1t	102	GLY
36	1e	85	GLY
25	23	59	VAL
35	2d	5	ILE
51	2t	102	GLY

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%)	209 (97%)	6 (3%)	43 77
3	2D	215/218 (99%)	211 (98%)	4 (2%)	57 85
4	1E	164/166 (99%)	156 (95%)	8 (5%)	25 57
4	2E	164/166 (99%)	153 (93%)	11 (7%)	16 43
5	1F	160/166 (96%)	153 (96%)	7 (4%)	28 61
5	2F	159/166 (96%)	150 (94%)	9 (6%)	20 50
6	1G	143/156 (92%)	140 (98%)	3 (2%)	53 84
6	2G	143/156 (92%)	139 (97%)	4 (3%)	43 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	1H	143/148 (97%)	140 (98%)	3 (2%)	53	84
7	2H	143/148 (97%)	140 (98%)	3 (2%)	53	84
8	1I	113/124 (91%)	108 (96%)	5 (4%)	28	61
8	2I	105/124 (85%)	103 (98%)	2 (2%)	57	85
9	1N	118/119 (99%)	114 (97%)	4 (3%)	37	71
9	2N	118/119 (99%)	115 (98%)	3 (2%)	47	80
10	1O	100/100 (100%)	99 (99%)	1 (1%)	76	93
10	2O	100/100 (100%)	99 (99%)	1 (1%)	76	93
11	1P	115/116 (99%)	113 (98%)	2 (2%)	60	87
11	2P	115/116 (99%)	113 (98%)	2 (2%)	60	87
12	1Q	111/111 (100%)	110 (99%)	1 (1%)	78	94
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	35	69
13	1R	101/101 (100%)	95 (94%)	6 (6%)	19	49
13	2R	101/101 (100%)	95 (94%)	6 (6%)	19	49
14	1S	86/88 (98%)	85 (99%)	1 (1%)	71	92
14	2S	85/88 (97%)	84 (99%)	1 (1%)	71	92
15	1T	115/127 (91%)	113 (98%)	2 (2%)	60	87
15	2T	113/127 (89%)	111 (98%)	2 (2%)	59	86
16	1U	93/94 (99%)	91 (98%)	2 (2%)	52	83
16	2U	93/94 (99%)	91 (98%)	2 (2%)	52	83
17	1V	80/82 (98%)	74 (92%)	6 (8%)	13	37
17	2V	80/82 (98%)	76 (95%)	4 (5%)	24	56
18	1W	90/92 (98%)	87 (97%)	3 (3%)	38	72
18	2W	90/92 (98%)	85 (94%)	5 (6%)	21	51
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	77 (100%)	0	100	100
20	1Y	85/91 (93%)	82 (96%)	3 (4%)	36	70
20	2Y	85/91 (93%)	83 (98%)	2 (2%)	49	81
21	1Z	135/179 (75%)	130 (96%)	5 (4%)	34	68
21	2Z	137/179 (76%)	134 (98%)	3 (2%)	52	83
22	10	65/67 (97%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	20	65/67 (97%)	65 (100%)	0	100	100
23	11	80/83 (96%)	80 (100%)	0	100	100
23	21	80/83 (96%)	79 (99%)	1 (1%)	69	91
24	12	65/67 (97%)	65 (100%)	0	100	100
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	50 (98%)	1 (2%)	55	84
25	23	50/52 (96%)	50 (100%)	0	100	100
26	14	59/63 (94%)	57 (97%)	2 (3%)	37	71
26	24	53/63 (84%)	52 (98%)	1 (2%)	57	85
27	15	50/52 (96%)	47 (94%)	3 (6%)	19	48
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	48
28	16	51/52 (98%)	50 (98%)	1 (2%)	55	84
28	26	50/52 (96%)	49 (98%)	1 (2%)	55	84
29	17	41/42 (98%)	40 (98%)	1 (2%)	49	81
29	27	41/42 (98%)	39 (95%)	2 (5%)	25	57
30	18	54/55 (98%)	52 (96%)	2 (4%)	34	68
30	28	54/55 (98%)	51 (94%)	3 (6%)	21	51
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	190 (99%)	2 (1%)	76	93
33	2b	187/220 (85%)	185 (99%)	2 (1%)	73	92
34	1c	142/188 (76%)	141 (99%)	1 (1%)	84	95
34	2c	140/188 (74%)	139 (99%)	1 (1%)	84	95
35	1d	169/181 (93%)	161 (95%)	8 (5%)	26	59
35	2d	173/181 (96%)	169 (98%)	4 (2%)	50	82
36	1e	113/123 (92%)	109 (96%)	4 (4%)	36	70
36	2e	114/123 (93%)	111 (97%)	3 (3%)	46	79
37	1f	84/90 (93%)	84 (100%)	0	100	100
37	2f	85/90 (94%)	84 (99%)	1 (1%)	71	92
38	1g	119/127 (94%)	118 (99%)	1 (1%)	81	94
38	2g	120/127 (94%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	1h	114/119 (96%)	112 (98%)	2 (2%)	59	86
39	2h	114/119 (96%)	113 (99%)	1 (1%)	78	94
40	1i	90/99 (91%)	89 (99%)	1 (1%)	73	92
40	2i	89/99 (90%)	86 (97%)	3 (3%)	37	71
41	1j	66/92 (72%)	66 (100%)	0	100	100
41	2j	69/92 (75%)	68 (99%)	1 (1%)	67	90
42	1k	82/99 (83%)	80 (98%)	2 (2%)	49	81
42	2k	83/99 (84%)	83 (100%)	0	100	100
43	1l	96/108 (89%)	95 (99%)	1 (1%)	76	93
43	2l	96/108 (89%)	96 (100%)	0	100	100
44	1m	93/101 (92%)	92 (99%)	1 (1%)	73	92
44	2m	92/101 (91%)	89 (97%)	3 (3%)	38	72
45	1n	49/50 (98%)	47 (96%)	2 (4%)	30	64
45	2n	49/50 (98%)	46 (94%)	3 (6%)	18	48
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	78 (100%)	0	100	100
47	1p	69/74 (93%)	68 (99%)	1 (1%)	67	90
47	2p	68/74 (92%)	67 (98%)	1 (2%)	65	89
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	92 (98%)	2 (2%)	53	84
49	1r	59/77 (77%)	57 (97%)	2 (3%)	37	71
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	67 (97%)	2 (3%)	42	76
50	2s	67/80 (84%)	66 (98%)	1 (2%)	65	89
51	1t	70/82 (85%)	70 (100%)	0	100	100
51	2t	70/82 (85%)	70 (100%)	0	100	100
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9301/10064 (92%)	9088 (98%)	213 (2%)	50	82

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	106	ILE
3	1D	122	ASP
3	1D	229	VAL
3	1D	242	ARG
3	1D	257	LEU
4	1E	9	VAL
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	34	VAL
4	1E	75	VAL
4	1E	116	VAL
4	1E	181	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	106	ARG
5	1F	183	VAL
5	1F	192	LEU
6	1G	43	LEU
6	1G	159	VAL
6	1G	175	LEU
7	1H	18	GLU
7	1H	71	LEU
7	1H	84	SER
8	1I	2	LYS
8	1I	38	LEU
8	1I	47	LEU
8	1I	92	VAL
8	1I	107	VAL
9	1N	28	THR
9	1N	62	VAL
9	1N	83	LYS
9	1N	99	LEU
10	1O	10	VAL
11	1P	95	VAL
11	1P	125	VAL
12	1Q	75	THR
13	1R	6	SER
13	1R	24	GLN
13	1R	29	LEU

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Mol	Chain	Res	Type
13	1R	44	LEU
13	1R	100	LEU
13	1R	111	LEU
14	1S	69	VAL
15	1T	28	VAL
15	1T	96	ARG
16	1U	74	LEU
16	1U	95	LEU
17	1V	46	VAL
17	1V	52	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
17	1V	82	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	107	LEU
20	1Y	11	ASP
20	1Y	43	ASN
20	1Y	90	LEU
21	1Z	33	LEU
21	1Z	42	VAL
21	1Z	86	VAL
21	1Z	154	ASP
21	1Z	170	THR
25	13	54	VAL
26	14	50	VAL
26	14	56	VAL
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
28	16	48	VAL
29	17	47	ARG
30	18	29	LYS
30	18	31	HIS
33	1b	112	VAL
33	1b	223	ILE
34	1c	172	ARG
35	1d	10	ARG
35	1d	31	CYS
35	1d	49	ARG
35	1d	59	ARG

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Mol	Chain	Res	Type
35	1d	91	SER
35	1d	135	LEU
35	1d	158	ILE
35	1d	194	LEU
36	1e	12	LEU
36	1e	31	LEU
36	1e	41	VAL
36	1e	149	GLU
38	1g	50	ILE
39	1h	69	ARG
39	1h	112	LEU
40	1i	64	THR
42	1k	31	THR
42	1k	114	VAL
43	1l	36	VAL
44	1m	19	LEU
45	1n	32	SER
45	1n	33	VAL
47	1p	2	VAL
49	1r	31	LEU
49	1r	54	ARG
50	1s	5	LEU
50	1s	41	VAL
3	2D	94	LEU
3	2D	106	ILE
3	2D	142	VAL
3	2D	242	ARG
4	2E	9	VAL
4	2E	12	THR
4	2E	24	THR
4	2E	34	VAL
4	2E	52	LEU
4	2E	75	VAL
4	2E	116	VAL
4	2E	119	ARG
4	2E	170	LEU
4	2E	181	LEU
4	2E	195	LEU
5	2F	33	LEU
5	2F	70	THR
5	2F	74	ARG
5	2F	88	VAL

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Mol	Chain	Res	Type
5	2F	106	ARG
5	2F	120	GLU
5	2F	158	THR
5	2F	183	VAL
5	2F	192	LEU
6	2G	43	LEU
6	2G	79	ASN
6	2G	135	LEU
6	2G	159	VAL
7	2H	71	LEU
7	2H	76	VAL
7	2H	88	LEU
8	2I	38	LEU
8	2I	92	VAL
9	2N	28	THR
9	2N	99	LEU
9	2N	140	VAL
10	2O	108	GLU
11	2P	95	VAL
11	2P	99	LEU
12	2Q	1	MET
12	2Q	21	THR
12	2Q	75	THR
12	2Q	110	THR
13	2R	24	GLN
13	2R	29	LEU
13	2R	44	LEU
13	2R	65	LEU
13	2R	100	LEU
13	2R	111	LEU
14	2S	38	GLN
15	2T	96	ARG
15	2T	108	ARG
16	2U	74	LEU
16	2U	95	LEU
17	2V	51	VAL
17	2V	62	LEU
17	2V	79	VAL
17	2V	82	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	67	ASP

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Mol	Chain	Res	Type
18	2W	100	THR
18	2W	107	LEU
20	2Y	72	VAL
20	2Y	97	ARG
21	2Z	42	VAL
21	2Z	144	LEU
21	2Z	154	ASP
23	21	21	ARG
26	24	50	VAL
27	25	6	VAL
27	25	16	ARG
27	25	29	THR
28	26	48	VAL
29	27	1	MET
29	27	39	ARG
30	28	26	LYS
30	28	31	HIS
30	28	41	ILE
33	2b	11	LEU
33	2b	94	ASN
34	2c	70	VAL
35	2d	31	CYS
35	2d	59	ARG
35	2d	135	LEU
35	2d	170	VAL
36	2e	12	LEU
36	2e	13	ILE
36	2e	41	VAL
37	2f	81	ILE
39	2h	23	SER
40	2i	64	THR
40	2i	65	VAL
40	2i	108	VAL
41	2j	72	VAL
44	2m	19	LEU
44	2m	47	ASP
44	2m	110	ARG
45	2n	22	THR
45	2n	33	VAL
45	2n	44	LEU
47	2p	2	VAL
48	2q	35	VAL

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Mol	Chain	Res	Type
48	2q	83	ASP
50	2s	12	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	166	GLN
4	1E	48	GLN
4	1E	143	ASN
5	1F	69	HIS
6	1G	79	ASN
10	1O	3	GLN
13	1R	24	GLN
13	1R	91	GLN
16	1U	81	HIS
18	1W	60	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	32	HIS
21	1Z	73	GLN
23	11	56	GLN
30	18	35	GLN
33	1b	40	HIS
33	1b	212	GLN
34	1c	6	HIS
34	1c	102	ASN
34	1c	162	GLN
34	1c	176	HIS
35	1d	77	ASN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	78	HIS
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
39	1h	82	HIS
40	1i	3	GLN
40	1i	58	HIS
40	1i	89	ASN

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Mol	Chain	Res	Type
40	1i	124	GLN
43	1l	99	HIS
47	1p	13	HIS
48	1q	26	GLN
49	1r	63	GLN
50	1s	69	HIS
50	1s	83	HIS
51	1t	16	HIS
51	1t	42	GLN
5	2F	69	HIS
8	2I	11	ASN
8	2I	105	HIS
11	2P	27	HIS
12	2Q	12	GLN
12	2Q	57	HIS
12	2Q	123	HIS
14	2S	38	GLN
17	2V	64	HIS
18	2W	60	ASN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
21	2Z	55	HIS
21	2Z	73	GLN
23	2l	56	GLN
30	28	35	GLN
33	2b	19	HIS
33	2b	40	HIS
33	2b	140	HIS
33	2b	212	GLN
34	2c	98	ASN
35	2d	77	ASN
35	2d	116	GLN
35	2d	125	HIS
36	2e	78	HIS
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	148	ASN
39	2h	82	HIS
40	2i	3	GLN
40	2i	58	HIS

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Mol	Chain	Res	Type
40	2i	89	ASN
40	2i	124	GLN
42	2k	22	HIS
43	2l	99	HIS
46	2o	28	GLN
49	2r	63	GLN
50	2s	47	HIS
50	2s	69	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	427 (14%)	30 (1%)
1	2A	2788/2915 (95%)	455 (16%)	22 (0%)
2	1B	120/121 (99%)	11 (9%)	1 (0%)
2	2B	118/121 (97%)	22 (18%)	0
32	1a	1494/1521 (98%)	217 (14%)	0
32	2a	1498/1521 (98%)	239 (15%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	71/76 (93%)	21 (29%)	0
54	1y	71/76 (93%)	20 (28%)	0
54	2w	68/76 (89%)	18 (26%)	0
54	2y	69/76 (90%)	22 (31%)	0
55	1x	75/77 (97%)	12 (16%)	0
55	2x	75/77 (97%)	12 (16%)	0
All	All	9332/9620 (97%)	1480 (15%)	53 (0%)

All (1480) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	17	G
1	1A	34	C
1	1A	45	C
1	1A	70	A
1	1A	71	U
1	1A	73	A
1	1A	74	G
1	1A	83	A
1	1A	94	G

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Mol	Chain	Res	Type
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	123	G
1	1A	185	A
1	1A	186	A
1	1A	188	A
1	1A	194	G
1	1A	203	G
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	214	A
1	1A	217	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	250	G
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	274	U
1	1A	275	C
1	1A	288	U
1	1A	289	G
1	1A	303	C
1	1A	335	A
1	1A	353	G
1	1A	354	A
1	1A	370	A
1	1A	376	G
1	1A	387	G
1	1A	388	A
1	1A	389	G
1	1A	399	G
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	455	A
1	1A	470	C
1	1A	474	U

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Mol	Chain	Res	Type
1	1A	480	A
1	1A	482	C
1	1A	483	A
1	1A	507	G
1	1A	526	A
1	1A	529	U
1	1A	530	A
1	1A	534	C
1	1A	537	G
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	615	G
1	1A	618	C
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	639	G
1	1A	640	A
1	1A	641	G
1	1A	648	G
1	1A	652	A
1	1A	662	A
1	1A	671	A
1	1A	693	G
1	1A	697	C
1	1A	716	G
1	1A	733	G
1	1A	764	G
1	1A	777	C
1	1A	811	A
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	831	A
1	1A	832	G

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Mol	Chain	Res	Type
1	1A	837	C
1	1A	839	G
1	1A	852	G
1	1A	858	U
1	1A	859	C
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	913	A
1	1A	926	G
1	1A	927	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	938	G
1	1A	941	U
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	956	A
1	1A	977	G
1	1A	990	A
1	1A	991	G
1	1A	1004	A
1	1A	1006	C
1	1A	1008	U
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1058	U
1	1A	1059	C
1	1A	1063	G
1	1A	1068	G
1	1A	1071	G
1	1A	1072	U
1	1A	1073	A

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Mol	Chain	Res	Type
1	1A	1079	U
1	1A	1084	C
1	1A	1087	C
1	1A	1091	A
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1101	G
1	1A	1103	A
1	1A	1104	G
1	1A	1112	U
1	1A	1114	G
1	1A	1117	G
1	1A	1119	A
1	1A	1120	G
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1125	C
1	1A	1127	U
1	1A	1130	A
1	1A	1132	A
1	1A	1134	A
1	1A	1135	G
1	1A	1136	U
1	1A	1137	G
1	1A	1139	G
1	1A	1140	U
1	1A	1142	A
1	1A	1144	A
1	1A	1146	C
1	1A	1147	U
1	1A	1149	A
1	1A	1153	G
1	1A	1156	G
1	1A	1157	A
1	1A	1158	G
1	1A	1161	G
1	1A	1162	C
1	1A	1174	A
1	1A	1176	U

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Mol	Chain	Res	Type
1	1A	1180	C
1	1A	1181	G
1	1A	1201	A
1	1A	1216	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1223	C
1	1A	1256	U
1	1A	1263	C
1	1A	1282	G
1	1A	1296	G
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1416	C
1	1A	1426	G
1	1A	1430	A
1	1A	1431	G
1	1A	1432	C
1	1A	1462	G
1	1A	1463	C
1	1A	1465	A
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1514	C
1	1A	1529	G

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Mol	Chain	Res	Type
1	1A	1539	C
1	1A	1540	A
1	1A	1555	C
1	1A	1556	A
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1627	A
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1656	A
1	1A	1694	G
1	1A	1695	C
1	1A	1701	A
1	1A	1711	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1748	A
1	1A	1767	A
1	1A	1768	U
1	1A	1787	G
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1817	A
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1870	G
1	1A	1878	A
1	1A	1879	A
1	1A	1899	A
1	1A	1900	G

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Mol	Chain	Res	Type
1	1A	1911	A
1	1A	1922	A
1	1A	1928	G
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1984	5MC
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2003	A
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2045	G
1	1A	2053	A
1	1A	2054	G
1	1A	2055	A
1	1A	2061	C
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G
1	1A	2132	G
1	1A	2134	G
1	1A	2135	U
1	1A	2136	A
1	1A	2141	A
1	1A	2143	G
1	1A	2148	A
1	1A	2149	G
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U

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Mol	Chain	Res	Type
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2158	C
1	1A	2162	C
1	1A	2164	C
1	1A	2165	C
1	1A	2166	U
1	1A	2168	C
1	1A	2169	G
1	1A	2170	G
1	1A	2172	U
1	1A	2173	G
1	1A	2177	G
1	1A	2178	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G
1	1A	2184	G
1	1A	2187	G
1	1A	2188	G
1	1A	2190	G
1	1A	2193	A
1	1A	2194	U
1	1A	2200	C
1	1A	2203	G
1	1A	2204	G
1	1A	2206	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2230	U
1	1A	2237	A
1	1A	2247	G
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2285	A
1	1A	2292	G

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Mol	Chain	Res	Type
1	1A	2295	C
1	1A	2299	A
1	1A	2317	A
1	1A	2320	G
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2366	G
1	1A	2373	A
1	1A	2395	G
1	1A	2397	C
1	1A	2418	U
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A
1	1A	2443	U
1	1A	2446	A
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2486	C
1	1A	2488	A
1	1A	2490	A
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2541	G
1	1A	2547	G
1	1A	2561	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2586	G
1	1A	2594	G
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U

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Mol	Chain	Res	Type
1	1A	2624	C
1	1A	2641	A
1	1A	2642	G
1	1A	2666	A
1	1A	2691	A
1	1A	2701	U
1	1A	2702	C
1	1A	2703	C
1	1A	2714	U
1	1A	2715	C
1	1A	2719	G
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2745	G
1	1A	2746	A
1	1A	2757	G
1	1A	2770	A
1	1A	2771	A
1	1A	2777	A
1	1A	2778	A
1	1A	2779	G
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C
1	1A	2806	G
1	1A	2813	G
1	1A	2814	C
1	1A	2818	U
1	1A	2830	A
1	1A	2831	A
1	1A	2843	G
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
1	1A	2904	U
2	1B	2	C
2	1B	9	G
2	1B	13	A

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Mol	Chain	Res	Type
2	1B	30	C
2	1B	35	U
2	1B	42	C
2	1B	52	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	65	U
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	189(G)	G
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	247	G
32	1a	251	G
32	1a	258	G

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Mol	Chain	Res	Type
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
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	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	421	U
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	564	C

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Mol	Chain	Res	Type
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	607	A
32	1a	630	G
32	1a	631	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	703	G
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	766	A
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	853	G
32	1a	859	A
32	1a	870	U
32	1a	874	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	932	C
32	1a	934	C

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Mol	Chain	Res	Type
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	967	5MC
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1011	G
32	1a	1020	U
32	1a	1022	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1029	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1039	C
32	1a	1044	A
32	1a	1054	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A

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Mol	Chain	Res	Type
32	1a	1125	U
32	1a	1133	G
32	1a	1134	G
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1172	C
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	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	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G

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Mol	Chain	Res	Type
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
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
32	1a	1532	U
53	1v	13	A
53	1v	14	A
54	1w	2	C
54	1w	3	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	64	A
54	1w	67	C
54	1w	68	C
54	1w	70	G
54	1w	73	A
54	1w	74	C
55	1x	6	G
55	1x	9	G
55	1x	14	A
55	1x	18	G

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Mol	Chain	Res	Type
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	49	G
55	1x	61	C
55	1x	64	G
55	1x	69	C
55	1x	76	A
54	1y	5	G
54	1y	6	G
54	1y	8	4SU
54	1y	13	C
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	54	5MU
54	1y	56	C
54	1y	59	U
54	1y	61	C
54	1y	64	A
54	1y	65	G
54	1y	70	G
1	2A	11	G
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	78	A
1	2A	84	A
1	2A	90	U
1	2A	95	G

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Mol	Chain	Res	Type
1	2A	100	G
1	2A	102	G
1	2A	104	U
1	2A	118	A
1	2A	120	U
1	2A	154(A)	C
1	2A	157	U
1	2A	172	C
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	204	A
1	2A	205	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	233	A
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	266	G
1	2A	267	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	279	C
1	2A	294	A
1	2A	311	A
1	2A	312	G
1	2A	317	G
1	2A	323	G
1	2A	329	G
1	2A	330	A
1	2A	338	G

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Mol	Chain	Res	Type
1	2A	342	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	422	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	498	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	551	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A

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Mol	Chain	Res	Type
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	783	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	828	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	874	G
1	2A	877	U
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	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A

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Mol	Chain	Res	Type
1	2A	901	A
1	2A	910	A
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	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1113	U
1	2A	1116	C
1	2A	1119	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1143	A
1	2A	1144	G
1	2A	1152	C
1	2A	1169	G
1	2A	1171	G
1	2A	1210	A

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Mol	Chain	Res	Type
1	2A	1211	U
1	2A	1220	A
1	2A	1237	A
1	2A	1247	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1313	U
1	2A	1314	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	1373	A
1	2A	1378	A
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1411	C
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	1436	G
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A

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Mol	Chain	Res	Type
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1514	U
1	2A	1531	C
1	2A	1532	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1582	C
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1722	A
1	2A	1746	G
1	2A	1756	G
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A

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Mol	Chain	Res	Type
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	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	1955	U
1	2A	1963	U
1	2A	1965	C
1	2A	1966	A
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
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	2096	U
1	2A	2099	U
1	2A	2107	C
1	2A	2108	C
1	2A	2110	G
1	2A	2111	C
1	2A	2116	G

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Mol	Chain	Res	Type
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2141	G
1	2A	2143	C
1	2A	2146	C
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2162	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2174	C
1	2A	2178	C
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
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	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2312	U
1	2A	2320	A
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2346	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	2402	C
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2424	C
1	2A	2425	A
1	2A	2428	G
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2478	A
1	2A	2490	G

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Mol	Chain	Res	Type
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2555	U
1	2A	2562	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2582	G
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2638	G
1	2A	2646	C
1	2A	2654	A
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2703	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	2739	U
1	2A	2750	A
1	2A	2751	G
1	2A	2757	A
1	2A	2758	A
1	2A	2759	G
1	2A	2761	G

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Mol	Chain	Res	Type
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
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	2808	U
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2879	C
1	2A	2880	C
1	2A	2889	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	12	C
2	2B	13	A
2	2B	19	G
2	2B	20	C
2	2B	24	G
2	2B	34	U
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	66	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

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Mol	Chain	Res	Type
2	2B	120	A
32	2a	7	G
32	2a	8	A
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	66	G
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(J)	G
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	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	301	G
32	2a	316	G
32	2a	321	A
32	2a	328	C
32	2a	332	G

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Mol	Chain	Res	Type
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	424	G
32	2a	429	U
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	574	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

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Mol	Chain	Res	Type
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	703	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	787	A
32	2a	790	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	873	A
32	2a	885	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	932	C
32	2a	934	C
32	2a	935	A
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

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Mol	Chain	Res	Type
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	997	U
32	2a	999	C
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
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	1029	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1033	G
32	2a	1035	A
32	2a	1036	G
32	2a	1039	C
32	2a	1040	U
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C

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Mol	Chain	Res	Type
32	2a	1131	G
32	2a	1132	C
32	2a	1133	G
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1172	C
32	2a	1173	G
32	2a	1174	G
32	2a	1182	G
32	2a	1184	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	1214	C
32	2a	1226	C
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1246	C
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1275	A
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1299	A

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Mol	Chain	Res	Type
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1320	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1370	G
32	2a	1379	G
32	2a	1398	A
32	2a	1400	5MC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1492	A
32	2a	1494	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1532	U
53	2v	13	A
53	2v	14	A
54	2w	3	C
54	2w	4	C
54	2w	7	A
54	2w	8	4SU
54	2w	13	C
54	2w	19	G
54	2w	22	G
54	2w	25	C
54	2w	34	G
54	2w	46	7MG

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Mol	Chain	Res	Type
54	2w	48	C
54	2w	59	U
54	2w	62	C
54	2w	64	A
54	2w	65	G
54	2w	68	C
54	2w	69	G
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	20	U
55	2x	21	A
55	2x	46	G
55	2x	47	U
55	2x	48	C
55	2x	56	C
55	2x	67	C
55	2x	68	C
55	2x	76	A
54	2y	15	G
54	2y	19	G
54	2y	23	A
54	2y	30	G
54	2y	34	G
54	2y	45	U
54	2y	46	7MG
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	55	PSU
54	2y	56	C
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	60	U
54	2y	61	C
54	2y	65	G
54	2y	67	C
54	2y	69	G
54	2y	70	G
54	2y	73	A

All (53) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	185	A
1	1A	271	U
1	1A	302	A
1	1A	509	A
1	1A	572	A
1	1A	732	A
1	1A	811	A
1	1A	913	A
1	1A	941	U
1	1A	1067	A
1	1A	1093	G
1	1A	1136	U
1	1A	1143	U
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1425	A
1	1A	1554	A
1	1A	1700	G
1	1A	2014	G
1	1A	2156	A
1	1A	2203	G
1	1A	2205	C
1	1A	2442	A
1	1A	2641	A
1	1A	2701	U
1	1A	2769	U
2	1B	1	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	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A

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Mol	Chain	Res	Type
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
1	2A	2126	A
1	2A	2406	U
1	2A	2689	U
1	2A	2756	U

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

84 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$
55	5MC	2x	32	55	18,22,23	1.00	2 (11%)	26,32,35	1.13	3 (11%)
1	2MA	2A	2503	1,56	17,25,26	0.99	1 (5%)	17,37,40	1.03	2 (11%)
1	PSU	1A	2617	1,56	18,21,22	1.43	4 (22%)	22,30,33	1.92	4 (18%)
1	PSU	2A	1917	1	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)
1	5MC	2A	1942	1	18,22,23	0.97	2 (11%)	26,32,35	1.15	3 (11%)
32	4OC	2a	1402	32	20,23,24	0.76	0	26,32,35	1.10	2 (7%)
32	5MC	2a	1404	32	18,22,23	0.98	2 (11%)	26,32,35	1.19	2 (7%)
32	MA6	1a	1519	32	19,26,27	1.04	1 (5%)	18,38,41	1.63	4 (22%)
43	0TD	2l	92	43	7,9,10	4.85	1 (14%)	6,11,13	4.44	3 (50%)
55	5MU	1x	54	55	19,22,23	1.43	6 (31%)	28,32,35	1.94	6 (21%)
43	0TD	1l	92	43	7,9,10	4.95	1 (14%)	6,11,13	2.42	2 (33%)
1	PSU	1A	1939	1	18,21,22	1.36	2 (11%)	22,30,33	1.93	4 (18%)
1	PSU	2A	1911	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
32	7MG	1a	527	32	22,26,27	1.39	3 (13%)	29,39,42	2.43	8 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	1407	32,56	18,22,23	1.00	2 (11%)	26,32,35	1.18	2 (7%)
54	MIA	1y	37	54	18,24,32	1.14	2 (11%)	18,35,47	1.26	2 (11%)
1	PSU	2A	2605	1	18,21,22	1.42	3 (16%)	22,30,33	1.92	4 (18%)
54	7MG	1w	46	54	22,26,27	1.36	3 (13%)	29,39,42	2.43	6 (20%)
54	PSU	2w	39	54	18,21,22	1.41	2 (11%)	22,30,33	1.58	3 (13%)
54	PSU	2y	39	54	18,21,22	1.35	2 (11%)	22,30,33	1.68	3 (13%)
32	5MC	1a	1404	32	18,22,23	1.03	2 (11%)	26,32,35	1.19	3 (11%)
1	5MU	2A	1939	1,56	19,22,23	1.32	4 (21%)	28,32,35	2.19	6 (21%)
32	UR3	2a	1498	32	19,22,23	1.04	1 (5%)	26,32,35	1.48	2 (7%)
1	4OC	1A	1942	1	19,22,24	0.85	0	26,31,35	0.91	0
32	PSU	1a	516	32	18,21,22	1.38	2 (11%)	22,30,33	1.95	4 (18%)
32	5MC	2a	1400	32	18,22,23	0.96	2 (11%)	26,32,35	1.16	2 (7%)
1	PSU	1A	1933	1	18,21,22	1.34	2 (11%)	22,30,33	1.87	4 (18%)
1	5MC	1A	1964	1	18,22,23	0.98	2 (11%)	26,32,35	1.23	3 (11%)
55	5MC	1x	32	55	18,22,23	1.01	2 (11%)	26,32,35	1.12	3 (11%)
32	PSU	2a	516	32	18,21,22	1.32	2 (11%)	22,30,33	1.80	4 (18%)
1	2MU	2A	2552	1,56	19,22,24	1.28	3 (15%)	26,31,36	1.68	7 (26%)
55	4SU	1x	8	55	18,21,22	2.15	5 (27%)	26,30,33	1.50	6 (23%)
32	5MC	1a	1407	32	18,22,23	0.88	2 (11%)	26,32,35	1.16	2 (7%)
1	OMG	1A	2263	1,55,56	18,26,27	0.98	1 (5%)	19,38,41	1.06	2 (10%)
1	4OC	2A	1920	1	19,22,24	0.82	0	26,31,35	0.79	0
54	7MG	2w	46	54	22,26,27	1.33	3 (13%)	29,39,42	2.52	7 (24%)
32	UR3	1a	1498	32	19,22,23	0.98	1 (5%)	26,32,35	1.54	2 (7%)
32	2MG	1a	1207	32	18,26,27	1.01	1 (5%)	16,38,41	1.13	2 (12%)
1	OMG	2A	2251	1,55,56	18,26,27	0.98	1 (5%)	19,38,41	1.11	3 (15%)
1	5MU	1A	1937	1	19,22,23	1.42	5 (26%)	28,32,35	2.17	7 (25%)
1	5MU	2A	1915	1	19,22,23	1.44	6 (31%)	28,32,35	2.04	5 (17%)
54	PSU	1y	39	54	18,21,22	1.36	2 (11%)	22,30,33	1.70	3 (13%)
54	MIA	1w	37	54	24,31,32	2.27	3 (12%)	26,44,47	2.50	9 (34%)
54	PSU	2w	32	54	18,21,22	1.34	3 (16%)	22,30,33	1.75	4 (18%)
32	4OC	1a	1402	32	20,23,24	0.75	0	26,32,35	1.09	2 (7%)
54	PSU	1w	55	54	18,21,22	1.38	2 (11%)	22,30,33	1.87	4 (18%)
32	2MG	2a	1207	32,56	18,26,27	0.91	1 (5%)	16,38,41	1.07	3 (18%)
32	M2G	2a	966	32	20,27,28	1.43	3 (15%)	22,40,43	1.07	2 (9%)
55	PSU	2x	55	55	18,21,22	1.32	2 (11%)	22,30,33	1.88	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	2w	55	54	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
1	5MC	2A	1962	1,56	18,22,23	0.97	2 (11%)	26,32,35	1.30	4 (15%)
54	5MU	1y	54	54	19,22,23	1.59	5 (26%)	28,32,35	1.85	7 (25%)
32	5MC	1a	967	32	18,22,23	0.91	2 (11%)	26,32,35	1.23	4 (15%)
32	M2G	1a	966	32	20,27,28	1.46	3 (15%)	22,40,43	0.95	2 (9%)
32	MA6	2a	1519	32	19,26,27	0.98	1 (5%)	18,38,41	1.60	4 (22%)
54	MIA	2y	37	54	18,24,32	1.16	2 (11%)	18,35,47	1.36	3 (16%)
54	5MU	2y	54	54	19,22,23	1.44	4 (21%)	28,32,35	2.20	7 (25%)
54	PSU	1w	32	54	18,21,22	1.34	2 (11%)	22,30,33	1.73	3 (13%)
55	5MU	2x	54	55	19,22,23	1.37	4 (21%)	28,32,35	2.20	6 (21%)
1	2MA	1A	2515	1,56	17,25,26	0.93	0	17,37,40	1.01	2 (11%)
54	4SU	1y	8	54	18,21,22	1.63	4 (22%)	26,30,33	1.82	5 (19%)
54	PSU	1y	55	54	18,21,22	1.36	2 (11%)	22,30,33	1.80	3 (13%)
54	PSU	1y	32	54	18,21,22	1.29	2 (11%)	22,30,33	1.78	3 (13%)
32	MA6	1a	1518	32	19,26,27	1.02	1 (5%)	18,38,41	1.67	5 (27%)
54	PSU	1w	39	54	18,21,22	1.32	2 (11%)	22,30,33	1.99	3 (13%)
54	5MU	1w	54	54	19,22,23	1.36	5 (26%)	28,32,35	1.94	7 (25%)
54	MIA	2w	37	54	20,27,32	1.78	3 (15%)	22,39,47	1.86	7 (31%)
54	4SU	2y	8	54	18,21,22	1.69	4 (22%)	26,30,33	2.41	5 (19%)
54	7MG	2y	46	54	22,26,27	1.38	3 (13%)	29,39,42	2.60	6 (20%)
1	5MC	1A	1984	1	18,22,23	0.96	2 (11%)	26,32,35	1.09	2 (7%)
54	7MG	1y	46	54	22,26,27	1.39	3 (13%)	29,39,42	2.57	6 (20%)
32	5MC	2a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.13	2 (7%)
54	4SU	2w	8	54	18,21,22	1.61	4 (22%)	26,30,33	2.43	6 (23%)
54	5MU	2w	54	54	19,22,23	1.37	4 (21%)	28,32,35	2.00	7 (25%)
54	4SU	1w	8	54	18,21,22	1.77	5 (27%)	26,30,33	2.05	4 (15%)
54	PSU	2y	55	54	18,21,22	1.35	2 (11%)	22,30,33	1.85	4 (18%)
55	4SU	2x	8	55,56	18,21,22	1.97	5 (27%)	26,30,33	1.69	6 (23%)
55	PSU	1x	55	55,56	18,21,22	1.33	2 (11%)	22,30,33	1.77	3 (13%)
1	2MU	1A	2564	1,56	19,22,24	1.28	3 (15%)	26,31,36	1.89	6 (23%)
1	5MU	1A	1961	1,56	19,22,23	1.36	4 (21%)	28,32,35	2.18	6 (21%)
54	PSU	2y	32	54	18,21,22	1.32	2 (11%)	22,30,33	1.78	3 (13%)
32	MA6	2a	1518	32	19,26,27	1.02	1 (5%)	18,38,41	1.65	4 (22%)
32	5MC	1a	1400	32	18,22,23	0.98	2 (11%)	26,32,35	1.17	3 (11%)
32	7MG	2a	527	32,56	22,26,27	1.33	3 (13%)	29,39,42	2.51	7 (24%)

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
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32	-	3/7/37/38	0/3/3/3
32	5MC	2a	1407	32,56	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1	-	1/9/27/30	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	1/9/27/28	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	1,55,56	-	0/5/27/28	0/3/3/3
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
54	7MG	2w	46	54	-	4/7/37/38	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	OMG	2A	2251	1,55,56	-	0/5/27/28	0/3/3/3
1	5MU	1A	1937	1	-	2/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	0/5/27/28	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
54	MIA	2y	37	54	-	2/3/25/34	0/3/3/3
54	5MU	2y	54	54	-	2/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	1,56	-	1/3/25/26	0/3/3/3
54	4SU	1y	8	54	-	4/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	1/7/29/30	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	1/7/29/34	0/3/3/3
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
1	5MC	1A	1984	1	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	4/7/37/38	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	2/7/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
1	2MU	1A	2564	1,56	-	0/9/27/28	0/2/2/2
1	5MU	1A	1961	1,56	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	3/7/37/38	0/3/3/3

All (203) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.75	1.69	1.82
43	2l	92	0TD	CB-SB	-12.51	1.69	1.82
54	1w	37	MIA	C13-C14	7.28	1.53	1.32
54	1w	37	MIA	C2-S10	-6.91	1.69	1.75
54	2w	37	MIA	C2-S10	-6.61	1.70	1.75
55	1x	8	4SU	C4-N3	-5.32	1.31	1.37
32	2a	966	M2G	C2-N3	4.80	1.36	1.30
32	1a	966	M2G	C2-N3	4.64	1.36	1.30
54	2y	8	4SU	C4-S4	-4.54	1.59	1.68
54	1w	8	4SU	C4-S4	-4.53	1.59	1.68
55	2x	8	4SU	C4-S4	-4.48	1.59	1.68
55	2x	8	4SU	C4-N3	-4.22	1.33	1.37
54	2w	8	4SU	C4-S4	-4.21	1.60	1.68
55	1x	8	4SU	C4-S4	-4.07	1.60	1.68
55	1x	8	4SU	C2-N3	-3.91	1.31	1.38
54	1y	8	4SU	C4-S4	-3.88	1.61	1.68
54	2w	39	PSU	C6-C5	3.83	1.39	1.35
54	1w	55	PSU	C6-C5	3.80	1.39	1.35
54	2w	55	PSU	C6-C5	3.69	1.39	1.35
54	2y	32	PSU	C6-C5	3.69	1.39	1.35
54	2y	39	PSU	C6-C5	3.63	1.39	1.35
54	1y	39	PSU	C6-C5	3.61	1.39	1.35
54	1y	55	PSU	C6-C5	3.58	1.39	1.35
1	1A	1939	PSU	C6-C5	3.54	1.39	1.35
54	2w	32	PSU	C6-C5	3.48	1.39	1.35
32	1a	527	7MG	C4-N9	-3.47	1.33	1.37
1	2A	2605	PSU	C6-C5	3.45	1.39	1.35
32	2a	516	PSU	C6-C5	3.43	1.39	1.35
55	2x	55	PSU	C6-C5	3.38	1.39	1.35
54	1y	46	7MG	C5-C4	3.34	1.49	1.38
54	1y	32	PSU	C6-C5	3.32	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	39	PSU	C6-C5	3.32	1.39	1.35
54	1w	32	PSU	C6-C5	3.32	1.39	1.35
54	2w	46	7MG	C4-N9	-3.25	1.33	1.37
54	1w	46	7MG	C4-N9	-3.23	1.34	1.37
54	1w	8	4SU	C4-N3	-3.22	1.34	1.37
54	2y	46	7MG	C5-C4	3.21	1.48	1.38
55	1x	55	PSU	C6-C5	3.21	1.39	1.35
54	1y	54	5MU	C6-C5	3.16	1.39	1.34
55	1x	8	4SU	C5-C4	-3.11	1.38	1.42
32	2a	527	7MG	C4-N9	-3.09	1.34	1.37
1	2A	1917	PSU	C6-C5	3.06	1.38	1.35
55	2x	8	4SU	C2-N3	-3.05	1.32	1.38
1	1A	1933	PSU	C6-C5	3.05	1.38	1.35
54	1w	46	7MG	C5-C4	3.04	1.48	1.38
1	1A	2617	PSU	C4-N3	-3.04	1.33	1.38
32	1a	1404	5MC	C6-C5	3.03	1.39	1.34
54	2w	46	7MG	C5-C4	3.02	1.48	1.38
54	2y	54	5MU	C2-N1	3.02	1.43	1.38
32	1a	527	7MG	C5-C4	3.01	1.47	1.38
54	1y	54	5MU	C4-C5	2.99	1.49	1.44
54	2y	55	PSU	C6-C5	2.97	1.38	1.35
32	1a	966	M2G	C2-N2	2.96	1.40	1.35
55	1x	32	5MC	C6-C5	2.94	1.39	1.34
1	1A	2564	2MU	C4-N3	-2.93	1.33	1.38
54	2w	54	5MU	C6-C5	2.91	1.39	1.34
54	1y	54	5MU	C2-N1	2.91	1.43	1.38
55	2x	8	4SU	C5-C4	-2.91	1.38	1.42
1	2A	1911	PSU	C4-N3	-2.90	1.33	1.38
55	2x	32	5MC	C6-C5	2.90	1.39	1.34
1	2A	1915	5MU	C6-C5	2.87	1.39	1.34
1	1A	1984	5MC	C6-C5	2.86	1.39	1.34
32	2a	527	7MG	C5-C4	2.85	1.47	1.38
55	2x	54	5MU	C6-C5	2.85	1.39	1.34
54	2y	54	5MU	C6-C5	2.84	1.39	1.34
1	1A	1937	5MU	C6-C5	2.83	1.39	1.34
1	2A	1911	PSU	C6-C5	2.82	1.38	1.35
54	1y	8	4SU	C4-N3	-2.80	1.34	1.37
32	1a	1400	5MC	C6-C5	2.80	1.39	1.34
1	2A	2605	PSU	C4-N3	-2.80	1.33	1.38
1	1A	1961	5MU	C6-C5	2.79	1.39	1.34
32	1a	516	PSU	C4-N3	-2.79	1.33	1.38
54	2y	37	MIA	C5-C4	2.79	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1961	5MU	C4-N3	-2.78	1.33	1.38
54	1w	54	5MU	C6-C5	2.78	1.39	1.34
1	2A	1939	5MU	C6-C5	2.76	1.39	1.34
1	2A	1915	5MU	C2-N1	2.74	1.42	1.38
54	2y	8	4SU	C5-C4	-2.74	1.39	1.42
1	1A	1964	5MC	C6-C5	2.72	1.39	1.34
32	2a	1518	MA6	C5-C4	2.72	1.48	1.40
54	2y	37	MIA	C2-N3	2.71	1.36	1.32
1	2A	1942	5MC	C6-C5	2.71	1.39	1.34
32	1a	1207	2MG	C6-N1	-2.70	1.33	1.37
54	2w	8	4SU	C4-N3	-2.70	1.34	1.37
54	1y	37	MIA	C5-C4	2.69	1.48	1.40
32	2a	967	5MC	C6-C5	2.69	1.39	1.34
1	1A	2617	PSU	C6-C5	2.68	1.38	1.35
1	2A	2251	OMG	C6-N1	-2.68	1.33	1.37
1	2A	1917	PSU	C4-N3	-2.67	1.33	1.38
54	1y	37	MIA	C2-N3	2.67	1.36	1.32
55	1x	54	5MU	C6-C5	2.67	1.39	1.34
32	2a	1404	5MC	C6-C5	2.66	1.39	1.34
54	2y	46	7MG	C8-N9	2.66	1.47	1.46
54	2w	39	PSU	C4-N3	-2.66	1.33	1.38
32	2a	1400	5MC	C6-C5	2.64	1.38	1.34
55	1x	54	5MU	C4-N3	-2.64	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.64	1.33	1.38
1	1A	2263	OMG	C6-N1	-2.64	1.33	1.37
32	2a	1407	5MC	C6-C5	2.63	1.38	1.34
54	2y	55	PSU	C4-N3	-2.62	1.34	1.38
32	1a	516	PSU	C6-C5	2.61	1.38	1.35
54	1w	8	4SU	C5-C4	-2.60	1.39	1.42
54	1y	54	5MU	C4-N3	-2.59	1.34	1.38
1	2A	1962	5MC	C6-C5	2.59	1.38	1.34
54	2w	37	MIA	C5-C4	2.58	1.47	1.40
1	2A	1962	5MC	C6-N1	-2.57	1.33	1.38
32	2a	1519	MA6	C5-C4	2.57	1.47	1.40
1	2A	1939	5MU	C4-N3	-2.56	1.34	1.38
32	1a	1518	MA6	C5-C4	2.55	1.47	1.40
54	2w	54	5MU	C4-C5	2.55	1.49	1.44
54	1y	46	7MG	C8-N9	2.54	1.47	1.46
54	1w	37	MIA	C5-C4	2.54	1.47	1.40
32	2a	516	PSU	C4-N3	-2.53	1.34	1.38
54	1y	8	4SU	C2-N1	2.51	1.42	1.38
54	2w	55	PSU	C4-N3	-2.51	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	966	M2G	C2-N2	2.51	1.39	1.35
32	1a	1519	MA6	C5-C4	2.50	1.47	1.40
54	1w	32	PSU	C4-N3	-2.49	1.34	1.38
1	2A	2552	2MU	C5-C4	2.49	1.49	1.43
1	1A	1937	5MU	C4-N3	-2.49	1.34	1.38
32	1a	1407	5MC	C6-C5	2.48	1.38	1.34
54	2y	8	4SU	C4-N3	-2.47	1.35	1.37
54	2y	54	5MU	C4-C5	2.47	1.48	1.44
1	1A	1937	5MU	C4-C5	2.46	1.48	1.44
1	1A	2564	2MU	C2-N3	-2.46	1.33	1.38
1	1A	1939	PSU	C4-N3	-2.46	1.34	1.38
54	2y	39	PSU	C4-N3	-2.45	1.34	1.38
55	2x	55	PSU	C4-N3	-2.45	1.34	1.38
1	1A	1933	PSU	C4-N3	-2.45	1.34	1.38
54	2w	8	4SU	C2-N1	2.43	1.42	1.38
55	2x	54	5MU	C4-N3	-2.43	1.34	1.38
54	1w	54	5MU	C4-N3	-2.42	1.34	1.38
55	1x	55	PSU	C4-N3	-2.42	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.41	1.34	1.37
54	1y	39	PSU	C4-N3	-2.41	1.34	1.38
32	1a	967	5MC	C6-N1	-2.40	1.33	1.38
1	1A	1937	5MU	C2-N1	2.40	1.42	1.38
55	1x	54	5MU	C4-C5	2.40	1.48	1.44
54	2y	46	7MG	C6-N1	-2.40	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.39	1.34	1.38
54	1w	46	7MG	C6-N1	-2.39	1.34	1.38
54	2y	8	4SU	C2-N1	2.38	1.42	1.38
1	1A	1961	5MU	C6-N1	-2.38	1.34	1.38
54	1w	39	PSU	C4-N3	-2.38	1.34	1.38
54	1y	46	7MG	C6-N1	-2.37	1.34	1.38
54	2y	54	5MU	C4-N3	-2.37	1.34	1.38
55	2x	54	5MU	C4-C5	2.37	1.48	1.44
1	2A	1939	5MU	C6-N1	-2.36	1.34	1.38
1	2A	2552	2MU	C4-N3	-2.33	1.34	1.38
32	1a	967	5MC	C6-C5	2.33	1.38	1.34
32	2a	527	7MG	C6-N1	-2.32	1.34	1.38
54	1y	8	4SU	C5-C4	-2.32	1.39	1.42
54	1w	54	5MU	C4-C5	2.30	1.48	1.44
54	2w	32	PSU	C4-N3	-2.29	1.34	1.38
32	1a	966	M2G	C6-N1	-2.29	1.34	1.37
1	1A	1964	5MC	C6-N1	-2.29	1.34	1.38
54	1y	32	PSU	C4-N3	-2.27	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	32	5MC	C6-N1	-2.27	1.34	1.38
54	2y	32	PSU	C4-N3	-2.26	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.26	1.34	1.38
54	1w	55	PSU	C4-N3	-2.26	1.34	1.38
1	1A	2617	PSU	C2-N3	-2.25	1.33	1.37
32	1a	1404	5MC	C6-N1	-2.25	1.34	1.38
54	1y	55	PSU	C4-N3	-2.25	1.34	1.38
55	1x	54	5MU	C2-N1	2.24	1.42	1.38
1	1A	1984	5MC	C6-N1	-2.24	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.24	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.23	1.33	1.37
32	1a	527	7MG	C6-N1	-2.22	1.34	1.38
54	1w	8	4SU	C2-N1	2.22	1.42	1.38
54	1w	8	4SU	C2-N3	-2.22	1.34	1.38
1	2A	2503	2MA	C2-N3	2.22	1.35	1.31
54	1y	54	5MU	C2-N3	-2.21	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.20	1.34	1.38
54	2w	54	5MU	C4-N3	-2.19	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.19	1.34	1.38
32	2a	967	5MC	C6-N1	-2.19	1.34	1.38
1	2A	1939	5MU	C4-C5	2.19	1.48	1.44
32	2a	966	M2G	C6-N1	-2.18	1.34	1.37
55	2x	8	4SU	C2-N1	2.16	1.41	1.38
54	2w	8	4SU	C5-C4	-2.16	1.39	1.42
1	1A	2564	2MU	C5-C4	2.16	1.48	1.43
32	2a	1400	5MC	C6-N1	-2.15	1.34	1.38
55	2x	54	5MU	C2-N1	2.13	1.41	1.38
54	2w	54	5MU	C2-N1	2.11	1.41	1.38
55	1x	8	4SU	O2-C2	2.10	1.26	1.23
1	1A	1961	5MU	C2-N3	-2.10	1.34	1.38
1	1A	1937	5MU	C6-N1	-2.09	1.34	1.38
55	1x	54	5MU	C6-N1	-2.09	1.34	1.38
55	1x	54	5MU	C2-N3	-2.08	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.07	1.34	1.38
32	2a	1498	UR3	C2-N1	2.07	1.41	1.38
1	2A	1915	5MU	C4-C5	2.06	1.48	1.44
54	1w	54	5MU	C6-N1	-2.05	1.34	1.38
54	2w	46	7MG	C6-N1	-2.04	1.35	1.38
54	1w	54	5MU	C2-N3	-2.04	1.34	1.38
32	1a	1498	UR3	C6-C5	2.03	1.39	1.35
1	2A	1915	5MU	C2-N3	-2.03	1.34	1.38
54	2w	32	PSU	C4-C5	2.02	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	2MU	C6-C5	2.01	1.39	1.35
54	2w	37	MIA	C6-N1	2.01	1.35	1.32
1	1A	2617	PSU	C2-N1	-2.00	1.34	1.36
55	2x	32	5MC	C6-N1	-2.00	1.34	1.38

All (332) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-9.96	84.42	102.44
54	1y	46	7MG	N9-C4-N3	9.56	139.76	125.47
54	2y	46	7MG	N9-C4-N3	9.46	139.61	125.47
54	2w	46	7MG	N9-C4-N3	8.65	138.40	125.47
32	2a	527	7MG	N9-C4-N3	8.62	138.37	125.47
54	1w	46	7MG	N9-C4-N3	8.60	138.34	125.47
32	1a	527	7MG	N9-C4-N3	8.42	138.07	125.47
54	1w	37	MIA	C12-C13-C14	-8.22	111.14	127.14
54	2w	8	4SU	C4-N3-C2	-7.78	119.78	127.34
54	2y	8	4SU	C4-N3-C2	-6.96	120.58	127.34
54	1w	39	PSU	N1-C2-N3	6.21	122.17	115.13
1	2A	2605	PSU	N1-C2-N3	6.20	122.15	115.13
54	2y	8	4SU	C5-C4-N3	6.16	120.40	114.69
32	2a	1498	UR3	C4-N3-C2	-6.12	118.80	124.56
1	1A	2617	PSU	N1-C2-N3	6.11	122.05	115.13
32	1a	516	PSU	N1-C2-N3	6.09	122.03	115.13
32	1a	1498	UR3	C4-N3-C2	-6.06	118.85	124.56
54	1w	8	4SU	C5-C4-N3	6.02	120.28	114.69
1	2A	1911	PSU	N1-C2-N3	6.00	121.92	115.13
54	2w	8	4SU	C5-C4-N3	5.98	120.24	114.69
1	1A	1939	PSU	N1-C2-N3	5.94	121.86	115.13
1	2A	1917	PSU	N1-C2-N3	5.92	121.84	115.13
54	1w	8	4SU	C4-N3-C2	-5.92	121.59	127.34
54	2w	55	PSU	N1-C2-N3	5.92	121.84	115.13
55	2x	55	PSU	N1-C2-N3	5.91	121.82	115.13
54	2y	46	7MG	C5-C4-N3	-5.82	117.04	128.13
54	1w	55	PSU	N1-C2-N3	5.71	121.61	115.13
54	2y	55	PSU	N1-C2-N3	5.70	121.59	115.13
54	1y	55	PSU	N1-C2-N3	5.66	121.54	115.13
54	1y	46	7MG	C5-C4-N3	-5.62	117.41	128.13
32	2a	516	PSU	N1-C2-N3	5.62	121.49	115.13
1	1A	2564	2MU	N3-C2-N1	5.58	122.29	114.89
55	2x	54	5MU	C4-N3-C2	-5.56	120.16	127.35
54	2y	32	PSU	N1-C2-N3	5.55	121.42	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	46	7MG	N9-C8-N7	-5.54	95.45	103.38
54	1y	32	PSU	N1-C2-N3	5.50	121.37	115.13
32	2a	527	7MG	N9-C8-N7	-5.50	95.51	103.38
54	1w	32	PSU	N1-C2-N3	5.49	121.35	115.13
1	1A	1933	PSU	N1-C2-N3	5.42	121.27	115.13
55	1x	55	PSU	N1-C2-N3	5.39	121.23	115.13
1	2A	1939	5MU	C4-N3-C2	-5.38	120.38	127.35
54	2w	32	PSU	N1-C2-N3	5.38	121.23	115.13
1	1A	1937	5MU	C4-N3-C2	-5.36	120.41	127.35
54	1y	39	PSU	N1-C2-N3	5.35	121.19	115.13
54	2y	54	5MU	C4-N3-C2	-5.34	120.44	127.35
55	2x	54	5MU	N3-C2-N1	5.30	121.93	114.89
1	1A	1961	5MU	C4-N3-C2	-5.29	120.51	127.35
54	1w	46	7MG	N9-C8-N7	-5.27	95.85	103.38
32	2a	527	7MG	C5-C4-N3	-5.24	118.14	128.13
54	2y	54	5MU	C5-C4-N3	5.24	119.78	115.31
54	1y	8	4SU	C4-N3-C2	-5.23	122.26	127.34
54	2y	39	PSU	N1-C2-N3	5.23	121.05	115.13
1	1A	1937	5MU	C5-C4-N3	5.21	119.75	115.31
32	1a	527	7MG	N9-C8-N7	-5.18	95.96	103.38
54	2y	8	4SU	C5-C4-S4	-5.18	117.80	124.47
32	1a	527	7MG	C5-C4-N3	-5.17	118.28	128.13
54	2w	46	7MG	C5-C4-N3	-5.11	118.40	128.13
54	1w	46	7MG	C5-C4-N3	-5.02	118.56	128.13
1	1A	1961	5MU	C5-C4-N3	5.02	119.60	115.31
1	2A	1915	5MU	C4-N3-C2	-4.99	120.89	127.35
1	2A	1939	5MU	N3-C2-N1	4.93	121.43	114.89
54	2w	39	PSU	N1-C2-N3	4.92	120.71	115.13
1	1A	1961	5MU	O4-C4-C5	-4.86	119.27	124.90
54	2w	54	5MU	C4-N3-C2	-4.86	121.06	127.35
1	1A	1937	5MU	N3-C2-N1	4.82	121.29	114.89
1	2A	1915	5MU	N3-C2-N1	4.82	121.28	114.89
54	1w	37	MIA	C5-C6-N1	-4.80	116.82	120.81
54	2y	46	7MG	C2-N3-C4	4.75	120.77	112.30
54	2y	54	5MU	O4-C4-C5	-4.74	119.41	124.90
55	1x	54	5MU	N3-C2-N1	4.74	121.18	114.89
54	2w	54	5MU	C5-C4-N3	4.72	119.34	115.31
54	1w	54	5MU	C4-N3-C2	-4.65	121.33	127.35
54	2y	54	5MU	N3-C2-N1	4.65	121.06	114.89
1	2A	2552	2MU	N3-C2-N1	4.64	121.04	114.89
55	1x	54	5MU	C4-N3-C2	-4.62	121.38	127.35
1	2A	1915	5MU	C5-C4-N3	4.60	119.24	115.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	54	5MU	C5-C4-N3	4.60	119.24	115.31
54	2y	46	7MG	N9-C8-N7	-4.60	96.81	103.38
54	1y	46	7MG	N9-C8-N7	-4.58	96.83	103.38
54	1w	54	5MU	N3-C2-N1	4.56	120.94	114.89
1	1A	1961	5MU	N3-C2-N1	4.55	120.93	114.89
1	1A	2564	2MU	C4-N3-C2	-4.55	120.58	126.58
1	1A	1937	5MU	O4-C4-C5	-4.50	119.68	124.90
1	2A	1939	5MU	C5-C6-N1	-4.50	118.71	123.34
54	1y	8	4SU	C5-C4-N3	4.49	118.86	114.69
54	2w	8	4SU	N3-C2-N1	4.49	120.85	114.89
1	2A	1915	5MU	O4-C4-C5	-4.47	119.72	124.90
54	1y	54	5MU	N3-C2-N1	4.47	120.82	114.89
54	1y	46	7MG	C2-N3-C4	4.46	120.24	112.30
43	1l	92	0TD	CSB-SB-CB	4.41	110.41	102.44
54	2w	54	5MU	N3-C2-N1	4.37	120.70	114.89
1	1A	1961	5MU	C5-C6-N1	-4.36	118.86	123.34
32	2a	527	7MG	C2-N3-C4	4.35	120.05	112.30
54	1w	39	PSU	C4-N3-C2	-4.32	120.11	126.34
55	2x	54	5MU	O4-C4-C5	-4.30	119.92	124.90
55	2x	8	4SU	C5-C4-N3	4.29	118.67	114.69
54	1y	54	5MU	C4-N3-C2	-4.28	121.81	127.35
54	2w	54	5MU	O4-C4-C5	-4.24	119.99	124.90
1	1A	2617	PSU	C4-N3-C2	-4.22	120.26	126.34
54	2w	37	MIA	C2-N3-C4	4.22	121.14	115.32
1	2A	1939	5MU	C5-C4-N3	4.21	118.91	115.31
54	1w	54	5MU	C5-C4-N3	4.20	118.90	115.31
54	2w	46	7MG	C2-N3-C4	4.19	119.76	112.30
1	1A	1964	5MC	C5-C6-N1	-4.18	119.04	123.34
32	1a	527	7MG	C2-N3-C4	4.09	119.59	112.30
1	2A	1939	5MU	O4-C4-C5	-4.08	120.17	124.90
54	2w	8	4SU	C5-C4-S4	-4.08	119.21	124.47
32	1a	516	PSU	C4-N3-C2	-4.07	120.48	126.34
54	1w	37	MIA	C15-C14-C13	-4.05	110.93	122.65
54	1y	54	5MU	C5-C4-N3	4.04	118.76	115.31
1	2A	1939	5MU	O2-C2-N1	-4.02	117.44	122.79
1	1A	1939	PSU	C4-N3-C2	-4.00	120.58	126.34
1	2A	2552	2MU	C4-N3-C2	-3.97	121.35	126.58
1	2A	1917	PSU	C4-N3-C2	-3.97	120.62	126.34
54	1w	46	7MG	C2-N3-C4	3.96	119.35	112.30
55	2x	8	4SU	C1'-N1-C2	3.95	124.73	117.57
55	1x	54	5MU	C5-C4-N3	3.95	118.68	115.31
55	2x	55	PSU	C4-N3-C2	-3.94	120.66	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	54	5MU	O4-C4-C5	-3.86	120.42	124.90
1	2A	2605	PSU	C4-N3-C2	-3.84	120.81	126.34
54	2y	55	PSU	C4-N3-C2	-3.83	120.83	126.34
54	2w	55	PSU	C4-N3-C2	-3.82	120.83	126.34
1	2A	1911	PSU	C4-N3-C2	-3.82	120.84	126.34
32	2a	516	PSU	C4-N3-C2	-3.81	120.85	126.34
54	2y	8	4SU	N3-C2-N1	3.81	119.94	114.89
1	1A	1933	PSU	C4-N3-C2	-3.79	120.88	126.34
55	2x	54	5MU	C5-C6-N1	-3.79	119.44	123.34
32	1a	516	PSU	O2-C2-N1	-3.71	118.70	122.79
54	2y	37	MIA	N3-C2-N1	-3.69	122.91	128.68
54	2w	37	MIA	C5-C6-N1	-3.68	117.76	120.81
32	2a	1404	5MC	C5-C6-N1	-3.66	119.57	123.34
32	1a	1407	5MC	C5-C6-N1	-3.66	119.57	123.34
1	1A	2564	2MU	O2-C2-N1	-3.66	117.92	122.79
32	2a	1518	MA6	C4-C5-N7	-3.64	105.60	109.40
54	1y	55	PSU	O2-C2-N1	-3.64	118.78	122.79
32	2a	1407	5MC	C5-C6-N1	-3.64	119.59	123.34
1	2A	1911	PSU	O2-C2-N1	-3.64	118.79	122.79
32	2a	967	5MC	C5-C6-N1	-3.62	119.61	123.34
54	1w	37	MIA	C2-N3-C4	3.62	120.31	115.32
55	1x	8	4SU	C6-C5-C4	-3.60	116.83	119.95
54	1y	37	MIA	N3-C2-N1	-3.60	123.05	128.68
55	1x	55	PSU	C4-N3-C2	-3.59	121.16	126.34
54	1w	37	MIA	C16-C14-C13	-3.57	112.34	122.65
32	1a	1404	5MC	C5-C6-N1	-3.56	119.68	123.34
54	1y	32	PSU	C4-N3-C2	-3.55	121.22	126.34
32	2a	1518	MA6	C9-N6-C6	-3.51	108.88	119.51
54	1y	8	4SU	N3-C2-N1	3.51	119.55	114.89
55	1x	54	5MU	O4-C4-C5	-3.51	120.84	124.90
54	1w	55	PSU	C4-N3-C2	-3.49	121.30	126.34
54	2y	32	PSU	C4-N3-C2	-3.49	121.31	126.34
1	1A	1933	PSU	O2-C2-N1	-3.49	118.95	122.79
54	1w	55	PSU	O2-C2-N1	-3.48	118.95	122.79
54	2w	32	PSU	C4-N3-C2	-3.48	121.32	126.34
1	2A	1917	PSU	O2-C2-N1	-3.47	118.97	122.79
1	2A	1962	5MC	C5-C6-N1	-3.47	119.77	123.34
54	1w	8	4SU	C5-C4-S4	-3.46	120.01	124.47
54	1y	32	PSU	O2-C2-N1	-3.46	118.98	122.79
32	1a	1518	MA6	N3-C2-N1	-3.44	123.30	128.68
32	1a	1518	MA6	C4-C5-N7	-3.44	105.81	109.40
1	1A	1984	5MC	C5-C6-N1	-3.44	119.80	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	55	PSU	C4-N3-C2	-3.44	121.38	126.34
54	1w	32	PSU	C4-N3-C2	-3.44	121.39	126.34
55	1x	32	5MC	C5-C6-N1	-3.43	119.81	123.34
1	2A	1915	5MU	C5-C6-N1	-3.42	119.82	123.34
55	2x	54	5MU	O2-C2-N1	-3.40	118.27	122.79
54	1w	39	PSU	O2-C2-N1	-3.40	119.05	122.79
54	2w	55	PSU	O2-C2-N1	-3.40	119.05	122.79
54	2y	55	PSU	O2-C2-N1	-3.39	119.06	122.79
54	1y	39	PSU	C4-N3-C2	-3.37	121.48	126.34
32	1a	1519	MA6	N3-C2-N1	-3.37	123.41	128.68
54	1w	8	4SU	N3-C2-N1	3.35	119.34	114.89
54	1y	54	5MU	C5-C6-N1	-3.34	119.91	123.34
55	1x	55	PSU	O2-C2-N1	-3.33	119.12	122.79
32	2a	1400	5MC	C5-C6-N1	-3.33	119.91	123.34
43	2l	92	0TD	OD2-CG-CB	3.33	120.33	113.15
55	1x	8	4SU	O2-C2-N1	3.30	127.18	122.79
32	2a	1518	MA6	N3-C2-N1	-3.28	123.56	128.68
32	2a	1519	MA6	C9-N6-C6	-3.27	109.62	119.51
54	2w	54	5MU	C5-C6-N1	-3.26	119.98	123.34
32	1a	1400	5MC	C5-C6-N1	-3.25	119.99	123.34
1	1A	1939	PSU	O2-C2-N1	-3.25	119.21	122.79
1	1A	1937	5MU	C5-C6-N1	-3.25	120.00	123.34
55	2x	55	PSU	O2-C2-N1	-3.25	119.22	122.79
32	2a	1519	MA6	C4-C5-N7	-3.22	106.04	109.40
54	2y	39	PSU	C4-N3-C2	-3.22	121.70	126.34
54	2y	32	PSU	O2-C2-N1	-3.22	119.25	122.79
55	2x	32	5MC	C5-C6-N1	-3.21	120.03	123.34
54	2y	54	5MU	C5-C6-N1	-3.18	120.07	123.34
54	1w	54	5MU	C5-C6-N1	-3.17	120.08	123.34
55	1x	54	5MU	C5-C6-N1	-3.17	120.08	123.34
32	1a	967	5MC	C5-C6-N1	-3.16	120.09	123.34
32	1a	1519	MA6	N1-C6-N6	3.15	120.37	117.06
32	1a	1519	MA6	C9-N6-C6	-3.14	109.99	119.51
54	2w	32	PSU	O2-C2-N1	-3.12	119.35	122.79
55	1x	8	4SU	C5-C4-N3	3.09	117.56	114.69
54	1y	8	4SU	C5-C4-S4	-3.08	120.50	124.47
32	1a	1518	MA6	C9-N6-C6	-3.05	110.28	119.51
54	1w	37	MIA	C2-N1-C6	3.05	122.65	117.19
54	2w	37	MIA	C12-N6-C6	-3.03	120.26	122.87
55	1x	32	5MC	C5-C4-N3	-3.03	118.41	121.67
43	1l	92	0TD	OD2-CG-CB	3.00	119.64	113.15
32	2a	1519	MA6	N3-C2-N1	-2.99	124.00	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1404	5MC	C5-C4-N3	-2.98	118.46	121.67
54	1w	32	PSU	O2-C2-N1	-2.95	119.54	122.79
54	1w	54	5MU	O2-C2-N1	-2.94	118.87	122.79
54	2w	37	MIA	C4-C5-N7	-2.94	106.33	109.40
54	2w	39	PSU	C4-N3-C2	-2.88	122.18	126.34
1	2A	1942	5MC	C5-C6-N1	-2.88	120.37	123.34
55	2x	8	4SU	C6-C5-C4	-2.85	117.48	119.95
1	2A	1962	5MC	C5-C4-N3	-2.81	118.65	121.67
1	1A	2617	PSU	O2-C2-N1	-2.80	119.70	122.79
1	1A	1961	5MU	O2-C2-N1	-2.79	119.08	122.79
1	1A	1933	PSU	C6-C5-C4	-2.78	116.25	118.20
32	1a	1519	MA6	C4-C5-N7	-2.78	106.50	109.40
32	2a	527	7MG	C5-C6-N1	2.76	115.85	110.99
54	2w	37	MIA	C2-N1-C6	2.76	122.13	117.19
32	2a	1404	5MC	C5-C4-N3	-2.74	118.72	121.67
1	2A	2552	2MU	O2-C2-N1	-2.73	119.15	122.79
54	2w	54	5MU	O2-C2-N1	-2.73	119.15	122.79
54	1y	37	MIA	C4-C5-N7	-2.73	106.55	109.40
32	2a	516	PSU	O2-C2-N1	-2.73	119.78	122.79
54	1y	39	PSU	O2-C2-N1	-2.73	119.79	122.79
32	1a	1402	4OC	C6-C5-C4	2.73	120.30	116.96
54	1y	54	5MU	O4-C4-C5	-2.73	121.74	124.90
1	2A	2503	2MA	C5-C6-N1	2.72	118.71	114.02
54	1y	46	7MG	C5-C4-N9	-2.72	102.82	106.35
55	2x	8	4SU	O2-C2-N1	2.71	126.39	122.79
1	2A	1942	5MC	C5-C4-N3	-2.71	118.75	121.67
54	2y	37	MIA	C4-C5-N7	-2.70	106.59	109.40
54	2w	46	7MG	C5-C6-N1	2.69	115.74	110.99
32	1a	1207	2MG	C8-N7-C5	2.69	108.11	102.99
54	2w	8	4SU	O2-C2-N1	-2.68	119.22	122.79
32	2a	1407	5MC	C5-C4-N3	-2.68	118.78	121.67
32	1a	1400	5MC	C5-C4-N3	-2.67	118.80	121.67
1	1A	2564	2MU	C5-C4-N3	2.61	118.74	114.84
1	2A	2552	2MU	C5-C4-N3	2.61	118.74	114.84
54	1y	8	4SU	C1'-N1-C2	2.60	122.27	117.57
32	1a	1404	5MC	O2-C2-N3	-2.60	118.11	122.33
55	2x	8	4SU	O2-C2-N3	-2.59	116.67	121.50
1	2A	2251	OMG	C5-C6-N1	2.59	118.52	113.95
54	2y	8	4SU	C1'-N1-C2	2.56	122.21	117.57
55	1x	8	4SU	C1'-N1-C2	2.55	122.19	117.57
1	1A	2515	2MA	C8-N7-C5	2.54	107.84	102.99
55	1x	8	4SU	S4-C4-N3	-2.53	117.72	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1984	5MC	C5-C4-N3	-2.52	118.95	121.67
54	2y	39	PSU	O2-C2-N1	-2.50	120.03	122.79
54	2y	54	5MU	C1'-N1-C2	2.50	122.10	117.57
32	1a	527	7MG	C5-C6-N1	2.50	115.40	110.99
54	1w	46	7MG	C5-C4-N9	-2.50	103.11	106.35
32	2a	1402	4OC	C6-C5-C4	2.48	120.00	116.96
55	2x	32	5MC	C5-C4-N3	-2.48	119.00	121.67
32	1a	967	5MC	C1'-N1-C6	-2.45	117.04	121.12
54	2w	46	7MG	C5-C4-N9	-2.44	103.18	106.35
54	1w	37	MIA	C4-C5-N7	-2.44	106.86	109.40
54	2w	37	MIA	C11-S10-C2	-2.43	100.45	102.27
1	1A	1964	5MC	O2-C2-N3	-2.42	118.39	122.33
32	2a	1207	2MG	C8-N7-C5	2.41	107.58	102.99
32	1a	1498	UR3	C1'-N1-C2	2.37	120.99	116.99
32	1a	966	M2G	C5-C6-N1	2.37	118.14	113.95
32	1a	1407	5MC	C5-C4-N3	-2.36	119.13	121.67
1	1A	2564	2MU	O4-C4-C5	-2.35	121.03	125.16
1	2A	2605	PSU	O2-C2-N1	-2.35	120.20	122.79
32	2a	1402	4OC	O2-C2-N3	-2.35	118.52	122.33
32	2a	966	M2G	C5-C6-N1	2.34	118.09	113.95
54	1y	54	5MU	C5M-C5-C4	2.34	121.34	118.77
1	1A	2263	OMG	C5-C6-N1	2.34	118.08	113.95
54	2w	32	PSU	C6-C5-C4	-2.32	116.57	118.20
1	1A	2263	OMG	C8-N7-C5	2.32	107.42	102.99
54	2y	46	7MG	C5-C4-N9	-2.32	103.33	106.35
1	1A	1964	5MC	C5-C4-N3	-2.32	119.17	121.67
55	1x	54	5MU	C5M-C5-C4	2.32	121.32	118.77
1	1A	1937	5MU	O2-C2-N1	-2.32	119.71	122.79
54	2w	37	MIA	N3-C2-N1	-2.31	122.73	126.98
32	2a	1519	MA6	N1-C6-N6	2.31	119.49	117.06
1	2A	2251	OMG	C8-N7-C5	2.29	107.35	102.99
32	2a	1518	MA6	C10-N6-C9	-2.28	108.79	116.12
43	2l	92	0TD	OD1-CG-CB	-2.27	117.68	122.44
32	1a	967	5MC	C5-C4-N3	-2.27	119.23	121.67
32	2a	1400	5MC	C5-C4-N3	-2.27	119.23	121.67
32	1a	1207	2MG	CM2-N2-C2	-2.27	118.85	123.86
1	1A	2564	2MU	C2'-C1'-N1	-2.26	109.84	114.22
1	1A	2515	2MA	C5-C6-N1	2.26	117.92	114.02
54	2y	46	7MG	C5-C6-N1	2.26	114.96	110.99
54	2y	54	5MU	C1'-N1-C6	-2.25	117.38	121.12
1	2A	2503	2MA	C8-N7-C5	2.24	107.26	102.99
1	2A	1962	5MC	C1'-N1-C6	-2.24	117.40	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	54	5MU	O2-C2-N3	-2.23	117.34	121.50
32	1a	966	M2G	C8-N7-C5	2.21	107.20	102.99
54	1w	46	7MG	C5-C6-N1	2.21	114.89	110.99
1	2A	2605	PSU	O2-C2-N3	-2.21	117.65	121.82
32	2a	527	7MG	C5-C4-N9	-2.21	103.48	106.35
55	2x	32	5MC	O2-C2-N3	-2.20	118.75	122.33
32	2a	966	M2G	C8-N7-C5	2.18	107.15	102.99
1	1A	1937	5MU	C5M-C5-C4	2.17	121.16	118.77
54	2w	54	5MU	C5M-C5-C4	2.17	121.16	118.77
54	1y	46	7MG	C5-C6-N1	2.17	114.81	110.99
32	2a	967	5MC	C5-C4-N3	-2.17	119.33	121.67
55	1x	8	4SU	O2-C2-N3	-2.17	117.46	121.50
32	1a	516	PSU	O4'-C1'-C2'	2.17	108.20	105.14
32	2a	1207	2MG	CM2-N2-C2	-2.16	119.09	123.86
54	1w	37	MIA	N3-C2-N1	-2.15	123.03	126.98
1	2A	2552	2MU	O4-C4-C5	-2.15	121.39	125.16
32	1a	967	5MC	O2-C2-N3	-2.15	118.84	122.33
1	2A	2552	2MU	C2'-C1'-N1	-2.14	110.08	114.22
1	1A	2617	PSU	C5-C6-N1	-2.13	118.92	122.11
55	2x	55	PSU	C5-C6-N1	-2.12	118.93	122.11
32	1a	1518	MA6	C10-N6-C9	-2.11	109.32	116.12
54	2w	46	7MG	O6-C6-C5	-2.11	122.37	127.54
32	2a	1498	UR3	C3U-N3-C4	2.11	120.90	117.89
32	1a	527	7MG	C5-C4-N9	-2.09	103.64	106.35
1	2A	1942	5MC	O2-C2-N3	-2.09	118.94	122.33
54	1w	54	5MU	C5M-C5-C4	2.09	121.06	118.77
1	2A	1962	5MC	O2-C2-N3	-2.08	118.95	122.33
55	1x	32	5MC	O2-C2-N3	-2.07	118.96	122.33
32	1a	527	7MG	O6-C6-C5	-2.06	122.47	127.54
32	1a	527	7MG	CM7-N7-C5	2.06	131.71	126.40
32	1a	1400	5MC	O2-C2-N3	-2.05	118.99	122.33
1	2A	2552	2MU	O5'-C5'-C4'	-2.05	102.02	108.99
55	2x	8	4SU	C1'-N1-C6	-2.05	116.38	120.84
32	2a	516	PSU	O4'-C1'-C2'	2.04	108.03	105.14
54	2w	8	4SU	C1'-N1-C2	2.04	121.26	117.57
54	1w	37	MIA	C12-N6-C6	-2.04	119.53	122.55
32	1a	1402	4OC	C5-C6-N1	-2.04	118.40	121.81
54	1w	55	PSU	C6-C5-C4	-2.04	116.77	118.20
1	1A	1939	PSU	C6-C5-C4	-2.04	116.78	118.20
54	2w	39	PSU	C6-C5-C4	-2.03	116.78	118.20
54	2y	55	PSU	O4'-C1'-C2'	2.03	108.01	105.14
32	1a	1518	MA6	N1-C6-N6	2.02	119.18	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	CM7-N7-C5	2.01	131.59	126.40
54	2y	37	MIA	C2-N1-C6	2.01	122.19	118.75
32	2a	1207	2MG	C5-C6-N1	2.01	117.50	113.95
1	2A	2251	OMG	O6-C6-C5	-2.00	120.46	124.37

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	967	5MC	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
54	1y	8	4SU	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
54	2w	37	MIA	N1-C6-N6-C12
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	1y	46	7MG	C4'-C5'-O5'-P
54	1y	54	5MU	C3'-C4'-C5'-O5'
54	1y	54	5MU	O4'-C4'-C5'-O5'
54	2y	55	PSU	C3'-C4'-C5'-O5'
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
54	2y	55	PSU	O4'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C4'-C5'-O5'
32	2a	1518	MA6	N1-C6-N6-C9
54	2y	37	MIA	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
54	2w	46	7MG	C3'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C10
32	2a	527	7MG	C3'-C4'-C5'-O5'
54	2y	46	7MG	O4'-C1'-N9-C4
1	1A	1937	5MU	O4'-C4'-C5'-O5'
54	2y	46	7MG	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	C4'-C5'-O5'-P
43	2l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CA-CB-CG-OD2
32	1a	1519	MA6	C5-C6-N6-C10
54	1y	46	7MG	C2'-C1'-N9-C8
32	2a	527	7MG	C4'-C5'-O5'-P
54	1y	8	4SU	C4'-C5'-O5'-P
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	1a	527	7MG	C4'-C5'-O5'-P
54	1w	46	7MG	C4'-C5'-O5'-P
54	1w	46	7MG	C2'-C1'-N9-C8
43	1l	92	0TD	CA-CB-SB-CSB
1	1A	2515	2MA	O4'-C4'-C5'-O5'
1	2A	2552	2MU	O4'-C4'-C5'-O5'
54	2y	46	7MG	O4'-C1'-N9-C8
54	2w	46	7MG	C2'-C1'-N9-C8
54	2y	54	5MU	C3'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C1'-N9-C8
54	2y	54	5MU	C2'-C1'-N1-C2
1	1A	1937	5MU	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	1y	46	7MG	C3'-C4'-C5'-O5'
54	1y	8	4SU	C2'-C1'-N1-C2
32	2a	1402	4OC	C2'-C1'-N1-C2
54	2w	46	7MG	C4'-C5'-O5'-P
1	1A	1942	4OC	C2'-C1'-N1-C2

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 3095 ligands modelled in this entry, 3085 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	SF4	2d	501	35	0,12,12	-	-	-		
57	CPT	1a	1930	32	0,3,4	-	-	-		
60	SF4	1d	501	35	0,12,12	-	-	-		
57	CPT	1A	4209	1	0,3,4	-	-	-		
57	CPT	2A	3904	1	0,3,4	-	-	-		
57	CPT	2I	201	8	0,3,4	-	-	-		
57	CPT	1A	4210	1	0,3,4	-	-	-		
57	CPT	2a	3235	32	0,3,4	-	-	-		
57	CPT	1I	3002	8	0,3,4	-	-	-		
57	CPT	2A	3903	1	0,3,4	-	-	-		

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	1d	501	35	-	-	0/6/5/5
60	SF4	2d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

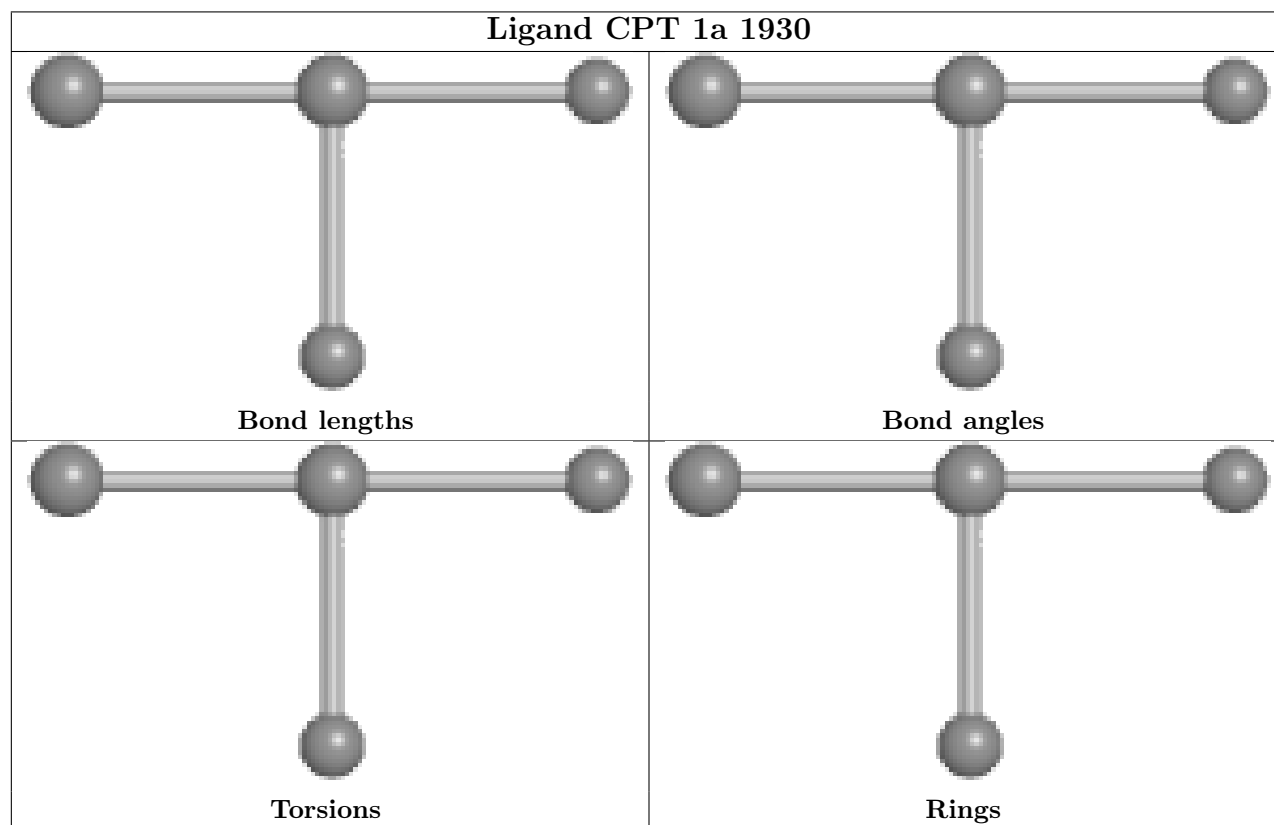
There are no torsion outliers.

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 than 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.



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%)	0.29	49 (1%) 70 63	24, 45, 94, 107	0
1	2A	2789/2915 (95%)	-0.12	33 (1%) 79 73	27, 48, 92, 107	0
2	1B	120/121 (99%)	-0.05	0 100 100	40, 60, 72, 93	0
2	2B	120/121 (99%)	-0.23	1 (0%) 86 81	46, 65, 75, 93	0
3	1D	275/276 (99%)	0.21	2 (0%) 87 84	23, 43, 59, 79	0
3	2D	275/276 (99%)	0.01	0 100 100	24, 44, 61, 79	0
4	1E	204/206 (99%)	0.20	0 100 100	25, 50, 66, 82	0
4	2E	204/206 (99%)	0.29	4 (1%) 65 56	27, 52, 68, 85	0
5	1F	203/210 (96%)	0.24	2 (0%) 82 77	26, 54, 77, 90	0
5	2F	203/210 (96%)	0.34	9 (4%) 34 24	28, 57, 79, 89	0
6	1G	181/182 (99%)	0.32	5 (2%) 53 43	49, 69, 80, 95	0
6	2G	181/182 (99%)	0.90	33 (18%) 1 1	52, 72, 83, 98	0
7	1H	173/180 (96%)	0.04	1 (0%) 89 86	54, 68, 77, 85	0
7	2H	173/180 (96%)	1.91	76 (43%) 0 0	57, 72, 81, 86	0
8	1I	146/148 (98%)	0.33	3 (2%) 63 54	51, 75, 85, 90	0
8	2I	146/148 (98%)	0.26	10 (6%) 17 10	53, 74, 86, 92	0
9	1N	140/140 (100%)	0.16	0 100 100	34, 51, 73, 78	0
9	2N	140/140 (100%)	0.24	1 (0%) 87 84	37, 55, 75, 81	0
10	1O	122/122 (100%)	-0.12	0 100 100	25, 41, 58, 68	0
10	2O	122/122 (100%)	0.48	4 (3%) 46 36	45, 62, 74, 80	0
11	1P	149/150 (99%)	0.22	1 (0%) 87 84	27, 57, 78, 87	0
11	2P	149/150 (99%)	0.87	23 (15%) 2 1	29, 60, 79, 88	0
12	1Q	141/141 (100%)	0.37	2 (1%) 75 70	36, 53, 69, 84	0
12	2Q	141/141 (100%)	0.50	11 (7%) 13 7	38, 57, 73, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.05	0 100 100	32, 42, 57, 67	0
13	2R	118/118 (100%)	0.19	2 (1%) 70 63	35, 45, 58, 69	0
14	1S	110/112 (98%)	0.12	0 100 100	45, 60, 73, 77	0
14	2S	110/112 (98%)	0.58	7 (6%) 19 12	49, 64, 76, 79	0
15	1T	131/146 (89%)	0.15	0 100 100	42, 54, 76, 86	0
15	2T	131/146 (89%)	0.55	5 (3%) 40 30	46, 57, 76, 86	0
16	1U	116/118 (98%)	0.29	1 (0%) 84 80	28, 45, 61, 75	0
16	2U	116/118 (98%)	0.09	2 (1%) 70 63	34, 49, 65, 77	0
17	1V	101/101 (100%)	0.13	0 100 100	31, 54, 70, 82	0
17	2V	101/101 (100%)	0.57	6 (5%) 22 14	34, 58, 73, 81	0
18	1W	112/113 (99%)	0.17	2 (1%) 68 61	30, 40, 64, 88	0
18	2W	112/113 (99%)	-0.05	1 (0%) 84 80	33, 42, 65, 90	0
19	1X	95/96 (98%)	-0.21	0 100 100	24, 38, 64, 78	0
19	2X	95/96 (98%)	0.63	5 (5%) 26 17	43, 61, 75, 87	0
20	1Y	107/110 (97%)	0.12	1 (0%) 84 80	47, 61, 74, 84	0
20	2Y	107/110 (97%)	0.37	3 (2%) 53 43	51, 64, 76, 86	0
21	1Z	154/206 (74%)	0.49	6 (3%) 39 29	55, 73, 89, 97	0
21	2Z	160/206 (77%)	1.09	25 (15%) 2 1	58, 76, 91, 98	0
22	10	83/85 (97%)	0.27	1 (1%) 79 73	23, 40, 62, 71	0
22	20	83/85 (97%)	0.41	1 (1%) 79 73	46, 65, 76, 84	0
23	11	97/98 (98%)	0.19	3 (3%) 49 39	27, 45, 72, 79	0
23	21	97/98 (98%)	0.45	4 (4%) 37 27	41, 56, 79, 88	0
24	12	70/72 (97%)	0.05	0 100 100	43, 58, 71, 82	0
24	22	70/72 (97%)	0.64	3 (4%) 35 25	46, 61, 75, 82	0
25	13	59/60 (98%)	0.29	1 (1%) 70 63	36, 50, 70, 83	0
25	23	59/60 (98%)	0.62	5 (8%) 10 5	41, 53, 74, 84	0
26	14	69/71 (97%)	0.79	13 (18%) 1 1	68, 82, 92, 96	0
26	24	69/71 (97%)	1.13	15 (21%) 0 0	72, 83, 92, 95	0
27	15	59/60 (98%)	0.05	1 (1%) 70 63	27, 41, 66, 71	0
27	25	59/60 (98%)	-0.08	0 100 100	29, 45, 67, 71	0
28	16	53/54 (98%)	0.18	0 100 100	41, 50, 65, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.34	4 (7%) 14 8	42, 53, 67, 73	0
29	17	48/49 (97%)	0.21	1 (2%) 63 54	26, 32, 62, 71	0
29	27	48/49 (97%)	0.08	3 (6%) 20 12	28, 34, 62, 70	0
30	18	64/65 (98%)	0.20	0 100 100	35, 44, 55, 68	0
30	28	64/65 (98%)	0.46	2 (3%) 49 39	38, 47, 58, 67	0
31	19	37/37 (100%)	0.11	0 100 100	31, 40, 58, 65	0
31	29	37/37 (100%)	0.97	5 (13%) 3 1	52, 71, 80, 81	0
32	1a	1488/1521 (97%)	0.03	22 (1%) 73 68	35, 63, 92, 109	0
32	2a	1491/1521 (98%)	0.11	31 (2%) 63 54	47, 77, 96, 107	0
33	1b	231/256 (90%)	0.29	11 (4%) 30 21	65, 82, 89, 96	0
33	2b	231/256 (90%)	0.88	31 (13%) 3 1	68, 83, 90, 98	0
34	1c	206/239 (86%)	0.32	7 (3%) 45 35	63, 76, 84, 91	0
34	2c	206/239 (86%)	1.63	73 (35%) 0 0	67, 78, 86, 91	0
35	1d	208/209 (99%)	0.14	1 (0%) 91 88	59, 71, 82, 87	0
35	2d	208/209 (99%)	0.61	11 (5%) 26 17	60, 72, 83, 88	0
36	1e	148/162 (91%)	0.17	0 100 100	57, 70, 79, 87	0
36	2e	148/162 (91%)	0.37	2 (1%) 75 70	60, 72, 81, 88	0
37	1f	100/101 (99%)	0.00	1 (1%) 82 77	48, 65, 77, 82	0
37	2f	100/101 (99%)	-0.05	1 (1%) 82 77	53, 70, 79, 86	0
38	1g	155/156 (99%)	0.60	15 (9%) 7 4	63, 72, 83, 95	0
38	2g	155/156 (99%)	1.09	29 (18%) 1 1	64, 74, 84, 95	0
39	1h	137/138 (99%)	0.19	2 (1%) 73 68	59, 72, 79, 88	0
39	2h	137/138 (99%)	0.70	5 (3%) 42 32	63, 74, 81, 88	0
40	1i	127/128 (99%)	0.66	12 (9%) 8 4	49, 73, 85, 91	0
40	2i	127/128 (99%)	2.02	60 (47%) 0 0	69, 83, 91, 93	0
41	1j	97/105 (92%)	0.65	11 (11%) 5 3	60, 80, 90, 93	0
41	2j	96/105 (91%)	2.08	40 (41%) 0 0	63, 81, 91, 97	0
42	1k	114/129 (88%)	0.66	7 (6%) 21 13	53, 68, 78, 85	0
42	2k	114/129 (88%)	0.24	3 (2%) 56 46	53, 69, 79, 85	0
43	1l	121/132 (91%)	0.04	1 (0%) 86 81	45, 58, 70, 84	0
43	2l	121/132 (91%)	0.02	0 100 100	46, 61, 72, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.30	5 (4%) 37 27	50, 67, 80, 88	0
44	2m	122/126 (96%)	1.28	34 (27%) 0 0	67, 83, 89, 93	0
45	1n	60/61 (98%)	0.44	2 (3%) 46 36	62, 71, 76, 81	0
45	2n	60/61 (98%)	2.76	44 (73%) 0 0	67, 74, 80, 85	0
46	1o	88/89 (98%)	0.49	5 (5%) 23 15	55, 68, 79, 83	0
46	2o	88/89 (98%)	0.20	0 100 100	58, 70, 80, 83	0
47	1p	82/88 (93%)	0.69	5 (6%) 21 13	57, 68, 79, 81	0
47	2p	82/88 (93%)	0.38	0 100 100	60, 68, 78, 84	0
48	1q	99/105 (94%)	0.56	2 (2%) 65 56	57, 70, 79, 83	0
48	2q	99/105 (94%)	0.97	10 (10%) 7 4	58, 70, 81, 84	0
49	1r	68/88 (77%)	0.68	4 (5%) 22 14	58, 68, 80, 83	0
49	2r	68/88 (77%)	0.01	2 (2%) 51 41	59, 69, 80, 85	0
50	1s	83/93 (89%)	0.52	3 (3%) 42 32	67, 76, 85, 92	0
50	2s	83/93 (89%)	1.20	19 (22%) 0 0	71, 79, 86, 93	0
51	1t	96/106 (90%)	1.40	25 (26%) 0 0	59, 70, 82, 89	0
51	2t	96/106 (90%)	1.32	21 (21%) 0 0	59, 70, 82, 89	0
52	1u	23/27 (85%)	0.63	0 100 100	64, 71, 77, 82	0
52	2u	23/27 (85%)	2.00	12 (52%) 0 0	67, 73, 79, 83	0
53	1v	13/24 (54%)	0.39	1 (7%) 13 7	43, 51, 74, 97	0
53	2v	13/24 (54%)	0.48	1 (7%) 13 7	63, 82, 98, 100	0
54	1w	67/76 (88%)	0.38	6 (8%) 9 5	49, 84, 99, 106	0
54	1y	67/76 (88%)	0.46	3 (4%) 33 23	39, 91, 99, 103	0
54	2w	65/76 (85%)	0.41	6 (9%) 9 5	62, 95, 102, 105	0
54	2y	66/76 (86%)	0.61	1 (1%) 73 68	49, 97, 101, 102	0
55	1x	72/77 (93%)	0.07	1 (1%) 75 70	33, 66, 82, 91	0
55	2x	72/77 (93%)	-0.01	0 100 100	50, 79, 88, 95	0
All	All	20873/21748 (95%)	0.31	986 (4%) 31 22	23, 63, 89, 109	0

All (986) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	10.0
41	2j	47	PHE	8.1

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Mol	Chain	Res	Type	RSRZ
38	1g	82	GLY	7.8
38	2g	82	GLY	7.6
21	2Z	144	LEU	7.3
33	2b	165	VAL	7.2
45	2n	39	LEU	7.1
1	2A	883	G	6.7
44	2m	123	ALA	6.6
32	2a	1030(B)	C	6.6
1	1A	931	C	6.5
45	2n	2	ALA	6.3
45	2n	25	VAL	6.3
34	2c	198	VAL	6.1
38	2g	80	VAL	6.1
51	2t	24	LEU	6.0
38	1g	79	ARG	5.9
54	1w	70	G	5.8
38	1g	83	ALA	5.8
34	2c	13	GLY	5.6
45	2n	34	TYR	5.6
41	2j	40	LEU	5.5
11	2P	1	MET	5.5
38	1g	80	VAL	5.5
7	2H	45	VAL	5.4
34	2c	182	ILE	5.4
41	2j	10	GLY	5.4
26	14	54	GLY	5.3
1	1A	942	A	5.2
32	1a	1030(B)	C	5.1
34	2c	33	LEU	5.1
40	2i	19	LEU	5.0
38	2g	156	TRP	5.0
1	1A	932	C	5.0
38	2g	16	LEU	4.9
7	2H	2	SER	4.9
45	2n	10	ALA	4.9
33	2b	215	LEU	4.8
6	2G	137	GLU	4.8
40	2i	7	THR	4.8
34	2c	204	LEU	4.8
26	24	51	ASP	4.7
6	2G	146	TYR	4.7
40	2i	109	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
26	24	49	PHE	4.6
38	2g	85	TYR	4.6
51	1t	95	ALA	4.6
44	2m	102	ARG	4.6
44	2m	6	GLY	4.6
32	2a	1034	G	4.5
1	2A	2146	C	4.5
33	2b	121	LEU	4.5
48	2q	80	GLY	4.5
41	2j	64	GLU	4.5
32	1a	1036	G	4.5
6	2G	140	ILE	4.5
21	1Z	149	SER	4.5
12	2Q	104	PHE	4.4
41	2j	55	LYS	4.4
21	2Z	155	LEU	4.4
34	2c	189	ALA	4.4
41	2j	63	PHE	4.4
5	2F	21	ALA	4.4
54	2w	71	G	4.4
50	2s	71	LEU	4.4
41	2j	44	VAL	4.4
1	2A	885	C	4.4
1	2A	884	C	4.3
44	2m	90	LEU	4.3
1	2A	2131	G	4.3
7	2H	115	VAL	4.3
1	1A	1555	C	4.3
1	2A	896	A	4.3
44	2m	15	VAL	4.3
44	2m	3	ARG	4.3
34	2c	14	ILE	4.3
45	2n	37	PHE	4.3
6	2G	139	LEU	4.3
54	1w	71	G	4.3
7	2H	98	LEU	4.2
51	2t	26	ASN	4.2
17	2V	101	GLY	4.2
7	2H	123	PHE	4.2
34	2c	155	GLY	4.1
7	2H	159	GLU	4.1
34	2c	158	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
40	2i	115	GLY	4.1
41	2j	62	HIS	4.1
7	2H	93	GLY	4.1
34	2c	188	LEU	4.1
40	2i	17	VAL	4.1
26	24	50	VAL	4.1
23	11	2	SER	4.1
51	1t	55	ILE	4.0
32	1a	1030(A)	G	4.0
41	2j	72	VAL	4.0
1	2A	1509	C	4.0
40	2i	26	VAL	4.0
6	1G	146	TYR	4.0
7	2H	166	GLY	4.0
38	1g	156	TRP	4.0
33	2b	122	PHE	4.0
41	2j	48	THR	4.0
45	2n	23	ARG	4.0
32	2a	1030(C)	G	4.0
7	2H	37	VAL	4.0
26	14	57	GLU	4.0
35	2d	47	ARG	4.0
51	2t	21	LYS	4.0
23	21	2	SER	4.0
1	1A	2167	C	3.9
32	1a	1030(C)	G	3.9
33	2b	48	MET	3.9
32	1a	204	U	3.9
7	2H	148	ILE	3.9
34	2c	21	ARG	3.9
34	2c	60	ALA	3.9
11	2P	123	LEU	3.9
38	2g	79	ARG	3.9
45	2n	35	ARG	3.9
34	2c	186	PHE	3.9
7	2H	145	ALA	3.9
26	14	4	GLY	3.9
40	2i	9	ARG	3.9
41	2j	46	ARG	3.9
16	1U	117	GLN	3.9
41	2j	66	ARG	3.8
21	2Z	156	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
34	2c	41	GLY	3.8
1	2A	882	G	3.8
34	2c	185	GLY	3.8
33	2b	118	LEU	3.8
45	2n	53	LEU	3.8
7	2H	24	VAL	3.8
34	2c	206	GLU	3.8
21	2Z	149	SER	3.8
34	2c	201	TYR	3.8
34	1c	13	GLY	3.8
45	2n	22	THR	3.8
6	2G	142	PRO	3.8
6	2G	152	LEU	3.7
45	2n	50	LYS	3.7
33	2b	135	GLN	3.7
17	2V	14	VAL	3.7
32	2a	1257	U	3.7
44	2m	73	GLU	3.7
50	2s	80	TYR	3.7
6	2G	133	LEU	3.7
7	2H	72	ILE	3.7
40	2i	125	TYR	3.7
38	2g	83	ALA	3.7
26	24	56	VAL	3.7
33	1b	215	LEU	3.7
35	2d	176	LEU	3.7
25	23	60	GLU	3.7
7	2H	43	VAL	3.7
52	2u	14	TRP	3.7
7	2H	46	GLU	3.7
34	2c	65	ALA	3.7
41	2j	11	PHE	3.7
41	1j	98	ILE	3.7
31	29	12	ASP	3.6
41	2j	87	THR	3.7
41	1j	95	GLU	3.6
25	23	26	LEU	3.6
51	2t	23	ARG	3.6
20	2Y	91	GLU	3.6
40	2i	110	GLU	3.6
40	2i	15	ALA	3.6
44	2m	66	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
35	2d	160	GLN	3.6
40	2i	81	ILE	3.6
34	2c	184	TYR	3.6
34	2c	132	ARG	3.6
52	2u	17	THR	3.6
26	24	54	GLY	3.6
40	2i	90	PRO	3.6
51	2t	80	ARG	3.6
7	2H	76	VAL	3.6
52	2u	10	ARG	3.6
32	2a	1030(A)	G	3.6
7	2H	34	GLU	3.6
26	14	66	SER	3.6
50	2s	79	THR	3.6
40	2i	65	VAL	3.5
45	2n	11	LYS	3.5
50	2s	30	LEU	3.5
51	1t	80	ARG	3.5
45	2n	61	TRP	3.5
34	2c	6	HIS	3.5
45	2n	24	CYS	3.5
19	2X	92	LEU	3.5
45	2n	6	LEU	3.5
11	2P	94	GLU	3.5
32	2a	1026	G	3.5
33	2b	92	TYR	3.5
41	2j	20	ALA	3.5
1	1A	1127	U	3.5
1	1A	930	G	3.5
1	1A	1105	G	3.5
34	2c	157	ILE	3.5
50	1s	40	ILE	3.5
39	2h	83	ILE	3.5
34	2c	8	ILE	3.5
44	2m	60	VAL	3.5
40	2i	30	GLY	3.4
41	2j	59	SER	3.4
45	2n	38	GLY	3.4
26	24	45	GLY	3.4
38	2g	7	ALA	3.4
7	2H	144	VAL	3.4
7	2H	47	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
42	1k	92	GLU	3.4
21	2Z	50	GLN	3.4
40	2i	52	ALA	3.4
41	2j	96	ILE	3.4
50	2s	12	ASP	3.4
40	2i	114	TYR	3.4
32	2a	80	G	3.4
7	2H	113	VAL	3.4
20	2Y	106	LEU	3.4
32	1a	1030	C	3.4
1	2A	2158	A	3.4
39	2h	2	LEU	3.4
40	2i	4	TYR	3.4
7	2H	48	GLY	3.3
15	2T	1	MET	3.3
40	2i	61	ALA	3.3
1	2A	2896	C	3.3
33	2b	187	LEU	3.3
48	2q	11	VAL	3.3
32	2a	1035	A	3.3
44	1m	124	PRO	3.3
29	27	47	ARG	3.3
35	2d	168	ARG	3.3
5	2F	7	TYR	3.3
28	26	20	ASN	3.3
51	2t	9	ASN	3.3
7	2H	105	LEU	3.3
40	2i	27	THR	3.3
7	2H	52	VAL	3.3
33	2b	133	LYS	3.3
7	2H	44	VAL	3.3
38	2g	140	ASP	3.3
1	1A	1104	G	3.3
14	2S	57	LYS	3.3
34	2c	50	ALA	3.3
40	2i	18	PHE	3.3
1	1A	2163	G	3.3
32	2a	1036	G	3.3
40	2i	75	ASP	3.3
7	1H	2	SER	3.3
34	2c	196	LEU	3.3
1	2A	2132	U	3.3

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Mol	Chain	Res	Type	RSRZ
7	2H	13	LYS	3.3
45	2n	12	ARG	3.3
11	2P	125	VAL	3.2
31	29	13	LYS	3.2
50	2s	83	HIS	3.2
54	2w	45	U	3.2
1	1A	1103	A	3.2
1	2A	229	A	3.2
34	2c	190	ARG	3.2
6	2G	155	MET	3.2
6	2G	136	ARG	3.2
21	2Z	137	ILE	3.2
54	1y	20	U	3.2
21	2Z	170	THR	3.2
1	2A	2145	C	3.2
5	2F	23	ASP	3.2
40	2i	119	ALA	3.2
42	1k	14	VAL	3.2
52	2u	23	PRO	3.2
13	2R	69	ASP	3.2
34	2c	124	ILE	3.2
1	2A	888	C	3.2
41	2j	65	LEU	3.2
6	2G	157	ILE	3.2
32	1a	1446	U	3.2
44	2m	13	LYS	3.2
6	2G	49	ASP	3.2
41	1j	20	ALA	3.2
52	2u	6	ARG	3.2
51	2t	20	LEU	3.2
45	2n	4	LYS	3.1
26	24	32	TYR	3.1
45	2n	29	ARG	3.1
45	2n	57	ARG	3.1
7	2H	165	ALA	3.1
11	2P	140	ALA	3.1
34	2c	37	GLN	3.1
7	2H	94	TYR	3.1
7	2H	41	MET	3.1
40	2i	54	ASP	3.1
11	2P	124	LYS	3.1
1	1A	936	C	3.1

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Mol	Chain	Res	Type	RSRZ
21	2Z	121	HIS	3.1
34	2c	87	LEU	3.1
32	1a	1447	A	3.1
31	29	37	GLY	3.1
40	2i	108	VAL	3.1
11	2P	126	VAL	3.1
29	27	48	LYS	3.1
41	2j	56	HIS	3.1
41	2j	50	ILE	3.1
40	2i	14	VAL	3.1
19	2X	1	MET	3.1
45	2n	31	ARG	3.1
1	1A	1141	A	3.1
20	1Y	1	MET	3.1
40	2i	5	TYR	3.1
7	2H	89	ILE	3.1
45	2n	42	ILE	3.1
44	2m	120	LYS	3.1
12	2Q	61	GLY	3.1
21	1Z	100	VAL	3.0
34	2c	180	ALA	3.0
1	1A	935	C	3.0
35	2d	98	GLU	3.0
38	1g	85	TYR	3.0
33	2b	136	VAL	3.0
45	1n	2	ALA	3.0
1	1A	934	A	3.0
1	1A	2168	C	3.0
3	1D	275	LYS	3.0
33	2b	127	ILE	3.0
40	2i	70	LYS	3.0
7	2H	122	THR	3.0
11	2P	109	GLY	3.0
41	1j	10	GLY	3.0
50	2s	68	GLY	3.0
6	2G	39	ILE	3.0
10	2O	10	VAL	3.0
32	2a	1033	G	3.0
32	2a	1202	G	3.0
39	2h	13	ILE	3.0
7	2H	49	VAL	3.0
7	2H	133	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
26	24	63	TYR	3.0
21	2Z	96	VAL	3.0
41	2j	49	VAL	3.0
1	1A	1144	A	3.0
7	2H	71	LEU	3.0
24	22	1	MET	3.0
1	1A	929	G	3.0
6	2G	59	GLU	3.0
32	1a	1257	U	3.0
41	2j	88	LEU	3.0
32	1a	1030(D)	A	3.0
32	2a	1030(D)	A	3.0
26	14	55	ARG	3.0
45	2n	54	PRO	3.0
1	1A	1139	G	3.0
7	2H	6	ARG	3.0
51	1t	47	GLY	3.0
46	1o	87	ILE	3.0
21	2Z	70	LEU	2.9
40	2i	92	TYR	2.9
44	2m	65	LYS	2.9
33	2b	152	PHE	2.9
34	2c	71	ALA	2.9
45	2n	55	GLY	2.9
11	2P	149	GLU	2.9
32	2a	1030	C	2.9
45	2n	26	ARG	2.9
51	2t	22	ARG	2.9
34	2c	187	ALA	2.9
6	2G	41	GLN	2.9
34	2c	4	LYS	2.9
51	2t	63	ILE	2.9
12	2Q	109	VAL	2.9
34	2c	200	ALA	2.9
48	2q	22	LEU	2.9
54	1w	44	G	2.9
54	1y	47	U	2.9
7	2H	74	ASN	2.9
38	1g	78	ARG	2.9
45	2n	41	ARG	2.9
41	1j	96	ILE	2.9
51	1t	69	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	1A	2153	G	2.9
32	2a	1031	G	2.9
7	2H	162	ILE	2.9
6	2G	159	VAL	2.9
29	17	48	LYS	2.9
40	2i	64	THR	2.9
41	2j	71	LEU	2.9
1	1A	2154	U	2.9
32	1a	1024	G	2.9
40	2i	36	TYR	2.9
11	2P	144	GLU	2.9
21	2Z	145	GLU	2.9
5	2F	208	GLY	2.9
33	1b	163	PHE	2.9
1	2A	2127	G	2.9
7	2H	51	ARG	2.9
37	1f	46	ARG	2.9
38	1g	81	GLY	2.9
24	22	61	LEU	2.9
38	1g	153	HIS	2.8
11	2P	118	GLY	2.8
51	2t	83	ARG	2.8
41	2j	85	LEU	2.8
51	2t	29	LYS	2.8
50	2s	69	HIS	2.8
33	2b	220	ASP	2.8
44	2m	71	ARG	2.8
40	2i	101	PHE	2.8
47	1p	21	VAL	2.8
6	1G	182	LYS	2.8
33	2b	132	LYS	2.8
1	2A	2173	A	2.8
6	2G	161	THR	2.8
41	2j	70	ARG	2.8
40	2i	38	GLN	2.8
1	1A	1140	U	2.8
34	2c	79	ARG	2.8
51	1t	86	ARG	2.8
45	2n	7	ILE	2.8
32	2a	1001(A)	G	2.8
42	1k	81	ASP	2.8
51	1t	74	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
50	2s	52	TYR	2.8
11	1P	105	LEU	2.8
7	2H	36	PRO	2.8
11	2P	97	PRO	2.8
18	1W	111	HIS	2.8
34	2c	57	ILE	2.8
41	2j	98	ILE	2.8
6	2G	34	LEU	2.8
40	2i	28	VAL	2.8
21	2Z	122	ARG	2.8
1	1A	1128	U	2.8
44	2m	4	ILE	2.8
8	1I	117	GLU	2.8
19	2X	93	GLU	2.8
34	2c	32	LEU	2.8
31	29	15	LYS	2.8
40	2i	87	GLN	2.8
17	2V	42	GLY	2.8
33	2b	216	SER	2.8
26	14	58	ARG	2.8
38	1g	16	LEU	2.8
1	1A	933	C	2.8
1	1A	2176	G	2.8
32	2a	1021	G	2.8
54	2w	70	G	2.8
7	2H	126	PRO	2.8
35	2d	49	ARG	2.8
38	2g	78	ARG	2.8
6	2G	182	LYS	2.8
6	1G	145	THR	2.8
33	2b	37	ASN	2.7
28	26	54	ILE	2.7
40	2i	63	ILE	2.7
11	2P	105	LEU	2.7
17	2V	94	LEU	2.7
45	2n	47	LEU	2.7
38	2g	147	ALA	2.7
54	1w	3	C	2.7
7	2H	7	LEU	2.7
26	14	50	VAL	2.7
54	2w	44	G	2.7
40	1i	106	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
34	2c	145	GLY	2.7
51	1t	83	ARG	2.7
41	2j	38	ILE	2.7
34	2c	138	VAL	2.7
40	2i	56	LEU	2.7
1	1A	943	C	2.7
7	2H	19	VAL	2.7
7	2H	128	PRO	2.7
26	14	56	VAL	2.7
33	2b	188	ALA	2.7
36	2e	94	ALA	2.7
38	2g	40	ALA	2.7
40	2i	62	TYR	2.7
12	2Q	66	ILE	2.7
33	2b	70	PHE	2.7
6	2G	92	VAL	2.7
5	2F	131	GLY	2.7
35	2d	165	MET	2.7
38	1g	154	TYR	2.7
21	2Z	69	THR	2.7
35	1d	110	PHE	2.7
1	1A	1133	G	2.7
6	2G	17	PRO	2.7
6	2G	28	VAL	2.7
51	2t	13	LEU	2.7
21	2Z	138	GLU	2.7
49	2r	46	GLU	2.7
12	1Q	33	GLY	2.7
1	1A	2134	G	2.7
40	1i	15	ALA	2.7
40	1i	76	ALA	2.7
51	2t	30	LYS	2.7
44	2m	87	TYR	2.7
54	1w	20	U	2.7
38	2g	84	ASN	2.7
6	2G	2	PRO	2.7
34	2c	199	LYS	2.7
34	2c	149	ALA	2.7
7	2H	56	SER	2.6
32	1a	1531	A	2.6
26	24	53	GLU	2.6
34	2c	175	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
40	2i	102	LEU	2.6
4	2E	115	GLY	2.6
45	2n	28	GLY	2.6
1	2A	886	C	2.6
1	2A	2128	C	2.6
32	2a	1117	G	2.6
34	2c	39	ILE	2.6
40	2i	88	TYR	2.6
11	2P	122	PRO	2.6
40	2i	10	ARG	2.6
40	2i	107	ARG	2.6
52	2u	13	ILE	2.6
8	2I	12	LEU	2.6
32	1a	1003	G	2.6
32	1a	1034	G	2.6
44	1m	87	TYR	2.6
1	1A	1142	A	2.6
40	2i	53	VAL	2.6
10	2O	41	ALA	2.6
38	2g	8	GLU	2.6
6	2G	62	LEU	2.6
11	2P	88	LEU	2.6
38	2g	77	SER	2.6
34	2c	173	VAL	2.6
40	2i	6	GLY	2.6
1	1A	1114	G	2.6
1	2A	2155	G	2.6
33	2b	211	ILE	2.6
7	2H	80	SER	2.6
12	2Q	28	ALA	2.6
40	2i	106	ALA	2.6
41	2j	41	PRO	2.6
38	2g	33	ASP	2.6
7	2H	18	GLU	2.6
44	2m	5	ALA	2.6
7	2H	101	ARG	2.6
1	2A	652(B)	A	2.6
11	2P	106	LEU	2.6
8	2I	3	VAL	2.6
48	2q	42	TYR	2.6
51	1t	71	THR	2.6
1	1A	2174	G	2.6

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Mol	Chain	Res	Type	RSRZ
7	2H	124	GLU	2.6
32	2a	204	U	2.6
41	2j	68	HIS	2.6
51	1t	24	LEU	2.6
32	2a	1024	G	2.6
11	2P	95	VAL	2.6
31	29	16	VAL	2.6
7	2H	3	ARG	2.6
38	2g	62	PHE	2.6
45	2n	30	ALA	2.6
49	1r	25	THR	2.5
51	1t	84	LEU	2.5
52	2u	8	THR	2.5
1	1A	2165	C	2.5
12	2Q	60	ARG	2.5
14	2S	20	ARG	2.5
25	23	6	VAL	2.5
40	2i	95	LYS	2.5
51	2t	34	LYS	2.5
54	1y	56	C	2.5
52	2u	18	TYR	2.5
34	2c	203	PHE	2.5
34	2c	51	GLY	2.5
19	2X	68	ARG	2.5
46	1o	68	ARG	2.5
44	1m	2	ALA	2.5
40	2i	124	GLN	2.5
44	2m	122	LYS	2.5
32	1a	1035	A	2.5
7	2H	119	GLU	2.5
34	2c	202	ILE	2.5
51	2t	25	ARG	2.5
34	2c	91	LEU	2.5
21	2Z	173	ALA	2.5
25	13	60	GLU	2.5
6	2G	181	ARG	2.5
26	24	68	ARG	2.5
51	1t	70	SER	2.5
38	1g	42	ILE	2.5
40	2i	41	VAL	2.5
34	2c	146	ALA	2.5
1	2A	2174	C	2.5

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Mol	Chain	Res	Type	RSRZ
32	2a	1116	C	2.5
14	2S	35	ILE	2.5
40	1i	81	ILE	2.5
33	2b	69	LEU	2.5
45	2n	58	LYS	2.5
7	2H	81	GLU	2.5
33	2b	140	HIS	2.5
45	2n	8	GLU	2.5
50	2s	14	HIS	2.5
8	2I	19	VAL	2.5
34	2c	64	VAL	2.5
42	1k	91	ARG	2.5
41	1j	92	THR	2.5
54	2y	34	G	2.5
40	2i	127	LYS	2.5
40	2i	79	LEU	2.5
50	2s	35	SER	2.5
41	1j	97	GLU	2.5
44	2m	8	GLU	2.5
33	2b	163	PHE	2.5
7	2H	77	LYS	2.5
38	2g	51	GLN	2.5
52	2u	16	GLY	2.5
7	2H	106	THR	2.5
11	2P	110	TYR	2.5
33	1b	61	LEU	2.5
41	2j	34	VAL	2.4
21	2Z	51	ALA	2.4
33	2b	47	THR	2.4
34	2c	193	TYR	2.4
1	1A	2151	C	2.4
45	2n	36	PHE	2.4
50	2s	32	LYS	2.4
50	2s	82	GLY	2.4
53	1v	12	A	2.4
21	1Z	168	GLU	2.4
51	1t	53	LEU	2.4
34	2c	80	GLY	2.4
6	2G	151	ALA	2.4
46	1o	65	ARG	2.4
21	1Z	169	GLU	2.4
7	2H	64	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
16	2U	88	ILE	2.4
48	2q	74	LEU	2.4
41	2j	15	THR	2.4
44	1m	23	TYR	2.4
7	2H	57	ASP	2.4
18	2W	112	GLY	2.4
33	2b	101	MET	2.4
33	1b	78	GLN	2.4
40	2i	42	ARG	2.4
51	1t	18	GLN	2.4
24	22	24	LEU	2.4
38	2g	154	TYR	2.4
7	2H	31	GLY	2.4
38	1g	77	SER	2.4
5	2F	24	LEU	2.4
7	2H	107	VAL	2.4
21	2Z	147	GLY	2.4
27	15	60	VAL	2.4
40	2i	93	ARG	2.4
44	2m	23	TYR	2.4
7	2H	138	LYS	2.4
45	2n	51	GLY	2.4
26	24	57	GLU	2.4
52	2u	5	ASP	2.4
26	24	13	ARG	2.4
44	2m	94	ARG	2.4
44	2m	121	LYS	2.4
38	2g	129	GLU	2.4
21	2Z	148	ASP	2.4
32	2a	1004	A	2.4
32	2a	1005	A	2.4
34	1c	62	ASP	2.4
34	2c	154	SER	2.4
44	2m	42	ALA	2.4
49	1r	87	ARG	2.4
12	2Q	33	GLY	2.4
51	2t	98	PRO	2.4
1	1A	2137	G	2.4
34	2c	15	THR	2.4
39	2h	120	THR	2.4
9	2N	23	LEU	2.4
51	1t	100	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
26	14	68	ARG	2.3
32	2a	1220	G	2.3
33	2b	120	ALA	2.3
50	2s	81	ARG	2.3
52	2u	22	ARG	2.3
8	2I	34	GLY	2.3
1	1A	1106	U	2.3
48	2q	40	LYS	2.3
34	2c	131	ARG	2.3
50	1s	39	THR	2.3
33	2b	44	LEU	2.3
33	2b	200	ILE	2.3
35	2d	19	LEU	2.3
51	2t	36	LEU	2.3
11	2P	91	PHE	2.3
34	2c	197	GLY	2.3
1	1A	1110	C	2.3
1	2A	652(T)	C	2.3
4	2E	175	VAL	2.3
21	2Z	139	VAL	2.3
32	1a	1029	C	2.3
41	1j	72	VAL	2.3
54	2w	4	C	2.3
6	2G	115	ARG	2.3
33	2b	94	ASN	2.3
26	14	59	PHE	2.3
44	2m	64	TRP	2.3
1	1A	1130	A	2.3
26	24	46	GLN	2.3
44	2m	17	VAL	2.3
45	2n	56	VAL	2.3
1	1A	1138	C	2.3
34	2c	183	ASP	2.3
50	2s	13	ASP	2.3
51	1t	32	ALA	2.3
41	2j	8	LEU	2.3
6	2G	29	TRP	2.3
40	1i	31	GLN	2.3
7	2H	65	HIS	2.3
32	1a	1532	U	2.3
32	2a	89	C	2.3
41	2j	58	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
50	2s	50	ALA	2.3
51	2t	55	ILE	2.3
6	2G	93	THR	2.3
42	2k	46	GLY	2.3
38	1g	17	VAL	2.3
1	1A	2183	C	2.3
42	2k	35	PRO	2.3
45	2n	15	LYS	2.3
11	2P	147	LEU	2.3
34	2c	61	ALA	2.3
11	2P	79	ARG	2.3
40	2i	72	GLY	2.3
47	1p	42	ARG	2.3
45	2n	52	GLN	2.3
7	2H	17	VAL	2.3
8	1I	142	VAL	2.3
1	2A	2111	C	2.3
15	2T	99	LEU	2.3
22	10	7	LEU	2.3
7	2H	14	GLY	2.3
32	2a	983	A	2.3
38	2g	19	GLY	2.3
22	20	69	PHE	2.3
4	2E	184	VAL	2.3
7	2H	129	THR	2.3
33	1b	133	LYS	2.3
48	2q	9	VAL	2.3
1	1A	1143	U	2.3
41	2j	9	ARG	2.3
51	1t	64	ASP	2.3
5	2F	12	LEU	2.3
33	1b	77	ALA	2.3
8	2I	4	ILE	2.3
40	2i	37	PHE	2.3
54	2w	73	A	2.3
7	2H	33	LEU	2.2
8	2I	111	PRO	2.2
26	14	69	LYS	2.2
40	2i	43	ALA	2.2
44	2m	18	ALA	2.2
51	2t	91	LEU	2.2
32	2a	1039	C	2.2

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Mol	Chain	Res	Type	RSRZ
54	1w	72	C	2.2
34	2c	3	ASN	2.2
44	2m	91	ARG	2.2
8	2I	108	THR	2.2
34	1c	87	LEU	2.2
33	2b	214	ILE	2.2
7	2H	116	GLU	2.2
1	1A	1126	C	2.2
21	2Z	126	VAL	2.2
46	1o	72	ARG	2.2
48	2q	18	THR	2.2
6	2G	90	LEU	2.2
17	2V	62	LEU	2.2
34	1c	12	LEU	2.2
50	1s	47	HIS	2.2
48	1q	27	PHE	2.2
42	1k	25	TYR	2.2
51	2t	17	ARG	2.2
1	1A	1146	C	2.2
45	1n	17	LYS	2.2
21	1Z	170	THR	2.2
21	2Z	76	LEU	2.2
23	1l	98	LEU	2.2
35	2d	188	LEU	2.2
48	2q	76	LEU	2.2
33	1b	222	ILE	2.2
1	2A	652(U)	G	2.2
1	2A	2802	G	2.2
6	2G	138	GLN	2.2
32	1a	1026	G	2.2
34	2c	30	ARG	2.2
34	2c	59	ARG	2.2
42	2k	25	TYR	2.2
34	1c	64	VAL	2.2
41	1j	8	LEU	2.2
23	2l	76	ARG	2.2
12	2Q	1	MET	2.2
1	2A	2133	G	2.2
47	1p	39	TYR	2.2
17	2V	5	VAL	2.2
44	2m	119	GLY	2.2
52	2u	11	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
7	2H	103	LEU	2.2
8	1I	52	ARG	2.2
11	2P	85	LEU	2.2
41	2j	89	ASP	2.2
40	2i	55	ALA	2.2
41	2j	42	THR	2.2
45	2n	49	HIS	2.2
23	2l	81	LYS	2.2
26	14	62	ARG	2.2
38	2g	76	ARG	2.2
46	1o	89	GLY	2.2
32	1a	1027	C	2.2
38	2g	99	LEU	2.2
41	1j	16	LEU	2.2
45	2n	44	LEU	2.2
7	2H	96	ALA	2.2
34	2c	49	SER	2.2
44	2m	92	HIS	2.2
3	1D	276	LYS	2.2
6	2G	149	VAL	2.2
7	2H	86	GLU	2.2
8	2I	107	VAL	2.2
37	2f	59	TYR	2.2
42	1k	75	TYR	2.2
10	2O	122	LEU	2.2
1	1A	1111	U	2.2
1	2A	894	C	2.2
40	1i	19	LEU	2.2
41	1j	40	LEU	2.2
49	1r	40	LEU	2.2
51	1t	62	LEU	2.2
34	2c	100	ALA	2.2
50	2s	49	ILE	2.2
7	2H	112	PRO	2.2
33	2b	111	ARG	2.2
51	1t	68	LYS	2.2
1	2A	1508	A	2.2
19	2X	69	TYR	2.2
44	2m	74	VAL	2.2
40	1i	8	GLY	2.1
14	2S	58	LEU	2.1
7	2H	4	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
51	1t	59	ALA	2.1
6	2G	112	PRO	2.1
32	1a	1002	G	2.1
32	1a	1023	G	2.1
44	2m	67	GLU	2.1
40	2i	103	THR	2.1
45	2n	27	CYS	2.1
32	2a	1447	A	2.1
40	1i	18	PHE	2.1
45	2n	16	PHE	2.1
30	28	16	ILE	2.1
34	2c	167	TRP	2.1
11	2P	92	GLU	2.1
39	2h	136	GLU	2.1
41	2j	61	GLU	2.1
45	2n	46	GLU	2.1
1	2A	2154	G	2.1
40	2i	8	GLY	2.1
48	1q	33	GLY	2.1
34	2c	10	PHE	2.1
49	2r	85	LEU	2.1
51	1t	29	LYS	2.1
51	1t	39	LYS	2.1
44	2m	50	GLU	2.1
36	2e	10	MET	2.1
55	1x	67	C	2.1
40	1i	53	VAL	2.1
42	1k	80	VAL	2.1
48	2q	85	VAL	2.1
1	1A	2173	G	2.1
26	24	52	THR	2.1
8	2I	72	LEU	2.1
26	14	32	TYR	2.1
35	2d	68	TYR	2.1
7	2H	132	ARG	2.1
14	2S	41	ASP	2.1
1	1A	944	C	2.1
30	28	34	TRP	2.1
21	2Z	129	SER	2.1
34	2c	207	VAL	2.1
12	2Q	37	LEU	2.1
38	2g	4	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
34	2c	35	GLU	2.1
34	2c	47	LEU	2.1
39	1h	133	LEU	2.1
10	2O	81	ASP	2.1
50	2s	43	GLU	2.1
16	2U	104	GLN	2.1
23	2I	58	ILE	2.1
40	1i	82	ALA	2.1
38	1g	84	ASN	2.1
5	2F	172	TRP	2.1
21	1Z	141	VAL	2.1
34	2c	22	TRP	2.1
51	1t	89	ARG	2.1
41	2j	16	LEU	2.1
51	2t	71	THR	2.1
32	2a	78	G	2.1
43	1l	14	GLY	2.1
6	1G	181	ARG	2.1
29	27	46	VAL	2.1
38	2g	32	ARG	2.1
40	2i	20	ARG	2.1
7	2H	25	LYS	2.1
7	2H	137	ASP	2.1
38	2g	13	GLN	2.1
45	2n	13	THR	2.1
1	1A	1112	U	2.1
50	2s	40	ILE	2.1
18	1W	112	GLY	2.1
15	2T	111	ARG	2.1
7	2H	29	PRO	2.1
7	2H	114	VAL	2.1
32	2a	1003	G	2.1
38	2g	155	ARG	2.1
34	2c	153	VAL	2.1
13	2R	65	LEU	2.1
15	2T	48	ILE	2.1
34	2c	56	ASP	2.1
1	2A	2144	U	2.1
15	2T	131	ALA	2.1
34	1c	65	ALA	2.1
44	1m	18	ALA	2.1
47	1p	4	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
32	1a	841	U	2.1
12	2Q	59	ARG	2.1
7	2H	141	VAL	2.1
8	2I	74	ASN	2.1
14	2S	33	LYS	2.1
33	1b	165	VAL	2.1
44	2m	12	ASN	2.1
6	1G	139	LEU	2.0
40	2i	99	LEU	2.0
1	1A	2150	C	2.0
34	1c	20	SER	2.0
7	2H	92	ILE	2.0
7	2H	121	ILE	2.0
41	2j	6	ILE	2.0
44	2m	78	ILE	2.0
49	1r	73	ALA	2.0
5	1F	89	VAL	2.0
47	1p	2	VAL	2.0
14	2S	32	LEU	2.0
28	26	11	LEU	2.0
38	2g	22	LEU	2.0
32	2a	79	G	2.0
32	2a	1131	G	2.0
53	2v	24	A	2.0
1	2A	1026	U	2.0
39	1h	3	THR	2.0
20	2Y	3	VAL	2.0
26	24	42	PHE	2.0
33	1b	94	ASN	2.0
33	1b	98	LEU	2.0
51	1t	20	LEU	2.0
12	1Q	59	ARG	2.0
4	2E	18	ASP	2.0
41	2j	93	GLY	2.0
1	2A	887	A	2.0
2	2B	119	G	2.0
21	2Z	42	VAL	2.0
28	26	5	VAL	2.0
34	2c	151	VAL	2.0
38	2g	9	VAL	2.0
40	1i	86	VAL	2.0
21	2Z	5	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
35	2d	161	ASN	2.0
12	2Q	22	LYS	2.0
25	23	27	GLY	2.0
51	1t	31	SER	2.0
1	2A	277	C	2.0
34	2c	23	TYR	2.0
45	2n	21	TYR	2.0
1	1A	1109	G	2.0
1	1A	1221	G	2.0
5	2F	6	VAL	2.0
25	23	54	VAL	2.0
40	2i	83	ARG	2.0
5	1F	41	LEU	2.0
6	2G	135	LEU	2.0
21	2Z	68	PRO	2.0
23	11	82	LEU	2.0
33	1b	76	GLN	2.0
40	1i	47	LEU	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
54	PSU	2y	55	20/21	0.73	0.29	92,98,114,119	0
54	5MU	1y	54	21/22	0.78	0.22	73,89,102,120	0
54	PSU	1y	55	20/21	0.79	0.26	86,98,106,123	0
54	7MG	2w	46	24/25	0.79	0.23	86,100,114,145	0
54	4SU	1y	8	20/21	0.81	0.18	87,98,107,113	0
54	7MG	2y	46	24/25	0.82	0.18	93,98,105,125	0
54	5MU	2y	54	21/22	0.83	0.25	82,92,106,130	0
54	4SU	2w	8	20/21	0.84	0.17	84,95,110,123	0
54	4SU	2y	8	20/21	0.84	0.13	89,98,109,120	0
54	PSU	2y	32	20/21	0.85	0.20	74,90,101,111	0
54	MIA	2y	37	22/30	0.85	0.20	71,86,96,112	0
54	4SU	1w	8	20/21	0.87	0.15	75,82,99,108	0
54	7MG	1w	46	24/25	0.87	0.15	74,87,111,126	0
54	7MG	1y	46	24/25	0.87	0.21	83,94,107,126	0
54	PSU	2w	55	20/21	0.88	0.18	66,88,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	PSU	2y	39	20/21	0.90	0.20	74,86,97,100	0
54	PSU	1y	39	20/21	0.90	0.19	69,80,87,89	0
54	PSU	1w	55	20/21	0.91	0.15	67,77,89,95	0
54	MIA	1y	37	22/30	0.91	0.12	65,81,88,93	0
55	4SU	2x	8	20/21	0.91	0.19	66,79,93,93	0
55	PSU	1x	55	20/21	0.91	0.17	62,72,91,96	0
54	PSU	2w	39	20/21	0.92	0.18	61,81,86,87	0
54	PSU	1y	32	20/21	0.92	0.18	68,86,94,94	0
55	PSU	2x	55	20/21	0.92	0.15	73,79,92,97	0
55	5MU	2x	54	21/22	0.93	0.17	74,83,90,105	0
54	PSU	2w	32	20/21	0.93	0.19	67,83,98,106	0
54	5MU	2w	54	21/22	0.93	0.14	62,80,88,92	0
32	2MG	2a	1207	24/25	0.94	0.13	70,80,89,102	0
32	4OC	2a	1402	22/23	0.94	0.17	52,64,71,74	0
55	5MU	1x	54	21/22	0.94	0.15	56,73,78,85	0
43	0TD	2l	92	10/11	0.94	0.19	53,60,64,85	0
32	M2G	2a	966	25/26	0.94	0.21	53,67,78,82	0
32	5MC	2a	967	21/22	0.94	0.17	57,71,78,79	0
32	7MG	2a	527	24/25	0.95	0.16	52,64,75,87	0
1	PSU	1A	1939	20/21	0.95	0.20	50,57,64,65	0
43	0TD	1l	92	10/11	0.95	0.22	47,57,60,73	0
1	PSU	2A	1911	20/21	0.95	0.17	42,57,65,65	0
55	4SU	1x	8	20/21	0.95	0.18	50,61,71,83	0
1	5MU	2A	1915	21/22	0.95	0.14	52,64,68,68	0
55	5MC	2x	32	21/22	0.95	0.21	65,72,77,83	0
1	PSU	2A	1917	20/21	0.95	0.15	52,62,66,70	0
54	MIA	2w	37	25/30	0.95	0.16	66,79,88,95	0
1	5MC	2A	1962	21/22	0.95	0.22	37,42,53,60	0
32	PSU	2a	516	20/21	0.95	0.16	54,68,81,87	0
32	5MC	2a	1400	21/22	0.96	0.20	50,68,78,89	0
1	5MU	1A	1937	21/22	0.96	0.19	49,62,65,68	0
54	PSU	1w	32	20/21	0.96	0.13	58,66,79,81	0
32	5MC	2a	1404	21/22	0.96	0.17	47,56,60,67	0
32	5MC	2a	1407	21/22	0.96	0.20	40,55,59,68	0
32	MA6	2a	1518	24/25	0.96	0.18	50,65,75,80	0
32	MA6	2a	1519	24/25	0.96	0.20	44,61,71,73	0
1	5MC	2A	1942	21/22	0.96	0.19	42,53,59,66	0
32	7MG	1a	527	24/25	0.96	0.16	37,48,54,61	0
32	2MG	1a	1207	24/25	0.96	0.14	56,65,69,76	0
1	2MU	1A	2564	21/23	0.97	0.22	29,36,42,46	0
32	PSU	1a	516	20/21	0.97	0.15	39,51,60,64	0
1	PSU	1A	1933	20/21	0.97	0.19	38,55,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	PSU	1w	39	20/21	0.97	0.15	35,56,64,66	0
1	5MC	1A	1984	21/22	0.97	0.22	33,39,46,58	0
1	4OC	2A	1920	21/23	0.97	0.15	43,52,58,61	0
32	5MC	1a	1400	21/22	0.97	0.17	31,45,56,63	0
32	5MC	1a	1404	21/22	0.97	0.19	30,36,44,47	0
55	5MC	1x	32	21/22	0.97	0.18	42,47,58,59	0
1	PSU	2A	2605	20/21	0.97	0.18	25,32,38,38	0
32	UR3	2a	1498	21/22	0.97	0.17	49,56,60,69	0
32	5MC	1a	1407	21/22	0.97	0.19	31,42,48,51	0
54	5MU	1w	54	21/22	0.97	0.17	48,62,67,73	0
54	MIA	1w	37	29/30	0.97	0.17	31,47,60,67	0
1	5MU	2A	1939	21/22	0.98	0.19	28,34,38,40	0
32	4OC	1a	1402	22/23	0.98	0.18	34,43,56,68	0
1	PSU	1A	2617	20/21	0.98	0.20	25,30,34,35	0
1	OMG	2A	2251	24/25	0.98	0.17	29,36,40,41	0
1	2MA	2A	2503	23/24	0.98	0.18	22,28,37,40	0
1	2MU	2A	2552	21/23	0.98	0.15	29,38,45,51	0
1	5MC	1A	1964	21/22	0.98	0.20	39,51,57,64	0
32	MA6	1a	1518	24/25	0.98	0.19	30,41,47,50	0
32	MA6	1a	1519	24/25	0.98	0.20	35,39,47,51	0
1	4OC	1A	1942	21/23	0.98	0.21	37,48,53,57	0
32	M2G	1a	966	25/26	0.98	0.18	46,54,60,69	0
32	5MC	1a	967	21/22	0.98	0.16	45,53,65,65	0
1	OMG	1A	2263	24/25	0.98	0.19	24,33,37,37	0
1	5MU	1A	1961	21/22	0.98	0.21	25,31,36,41	0
32	UR3	1a	1498	21/22	0.99	0.19	29,37,45,49	0
1	2MA	1A	2515	23/24	0.99	0.19	20,27,33,37	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
56	MG	2B	3011	1/1	0.01	0.58	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4085	1/1	0.16	0.27	99,99,99,99	0
56	MG	1a	1871	1/1	0.26	0.18	79,79,79,79	0
56	MG	2a	3146	1/1	0.27	0.13	114,114,114,114	0
56	MG	2a	3031	1/1	0.28	0.55	76,76,76,76	0
56	MG	2l	3001	1/1	0.28	0.69	62,62,62,62	0
56	MG	2A	3792	1/1	0.32	0.44	61,61,61,61	0
56	MG	1A	4054	1/1	0.33	0.26	73,73,73,73	0
56	MG	2a	3109	1/1	0.35	0.38	89,89,89,89	0
56	MG	2a	3173	1/1	0.37	0.29	104,104,104,104	0
56	MG	1A	4048	1/1	0.41	0.11	68,68,68,68	0
56	MG	2v	102	1/1	0.41	0.49	93,93,93,93	0
56	MG	2y	3006	1/1	0.41	0.10	106,106,106,106	0
56	MG	1w	103	1/1	0.42	0.57	80,80,80,80	0
56	MG	1B	227	1/1	0.42	0.63	106,106,106,106	0
56	MG	2a	3131	1/1	0.44	0.18	90,90,90,90	0
56	MG	2a	3064	1/1	0.44	0.48	83,83,83,83	0
56	MG	2A	3360	1/1	0.44	0.14	70,70,70,70	0
56	MG	2a	3056	1/1	0.45	0.21	71,71,71,71	0
56	MG	2a	3162	1/1	0.45	0.24	100,100,100,100	0
56	MG	1A	3351	1/1	0.45	0.55	72,72,72,72	0
56	MG	1l	203	1/1	0.46	0.11	75,75,75,75	0
56	MG	1A	4068	1/1	0.47	0.28	83,83,83,83	0
56	MG	2a	3029	1/1	0.48	1.16	90,90,90,90	0
56	MG	1x	110	1/1	0.49	0.20	75,75,75,75	0
56	MG	2A	3665	1/1	0.50	0.25	53,53,53,53	0
56	MG	1A	4083	1/1	0.50	0.15	63,63,63,63	0
56	MG	2A	3816	1/1	0.50	0.32	75,75,75,75	0
56	MG	1A	4141	1/1	0.50	0.11	63,63,63,63	0
56	MG	1A	3357	1/1	0.51	0.30	69,69,69,69	0
56	MG	1A	3366	1/1	0.53	0.78	60,60,60,60	0
56	MG	2A	3411	1/1	0.53	0.75	52,52,52,52	0
56	MG	1a	1615	1/1	0.53	0.53	87,87,87,87	0
56	MG	2a	3003	1/1	0.54	0.20	75,75,75,75	0
56	MG	1a	1710	1/1	0.55	0.22	79,79,79,79	0
56	MG	2A	3382	1/1	0.55	0.43	55,55,55,55	0
56	MG	1A	4116	1/1	0.56	0.35	85,85,85,85	0
56	MG	2a	3026	1/1	0.56	1.04	88,88,88,88	0
56	MG	2a	3140	1/1	0.56	0.21	95,95,95,95	0
56	MG	1A	3417	1/1	0.57	0.76	67,67,67,67	0
56	MG	2A	3798	1/1	0.57	0.21	75,75,75,75	0
56	MG	10	102	1/1	0.57	0.59	77,77,77,77	0
56	MG	2A	3872	1/1	0.57	0.33	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3182	1/1	0.58	0.16	74,74,74,74	0
56	MG	1A	4180	1/1	0.58	0.39	62,62,62,62	0
56	MG	1A	3369	1/1	0.58	1.00	66,66,66,66	0
56	MG	1A	4166	1/1	0.58	0.18	70,70,70,70	0
56	MG	1A	3260	1/1	0.59	0.33	57,57,57,57	0
56	MG	1A	4014	1/1	0.59	0.08	81,81,81,81	0
56	MG	2a	3222	1/1	0.60	0.43	94,94,94,94	0
56	MG	2A	3831	1/1	0.61	0.10	57,57,57,57	0
56	MG	1A	4099	1/1	0.61	0.10	82,82,82,82	0
56	MG	2A	3059	1/1	0.61	0.24	57,57,57,57	0
56	MG	1x	102	1/1	0.61	0.55	74,74,74,74	0
56	MG	2A	3284	1/1	0.62	0.23	56,56,56,56	0
56	MG	1A	3646	1/1	0.63	0.29	49,49,49,49	0
56	MG	2A	3864	1/1	0.63	0.12	73,73,73,73	0
56	MG	1a	1725	1/1	0.63	0.12	62,62,62,62	0
56	MG	1B	228	1/1	0.63	0.32	80,80,80,80	0
56	MG	1A	3222	1/1	0.63	0.60	71,71,71,71	0
56	MG	2A	3343	1/1	0.63	1.04	63,63,63,63	0
56	MG	1A	3540	1/1	0.63	0.34	60,60,60,60	0
56	MG	2A	3410	1/1	0.64	0.36	71,71,71,71	0
56	MG	1A	4009	1/1	0.64	0.14	81,81,81,81	0
56	MG	2A	3332	1/1	0.64	0.38	53,53,53,53	0
56	MG	2a	3204	1/1	0.64	0.18	90,90,90,90	0
56	MG	2A	3683	1/1	0.64	0.18	49,49,49,49	0
56	MG	1A	3756	1/1	0.64	0.15	67,67,67,67	0
56	MG	1a	1914	1/1	0.64	0.13	84,84,84,84	0
56	MG	1G	3002	1/1	0.64	0.17	63,63,63,63	0
56	MG	2A	3832	1/1	0.65	0.20	69,69,69,69	0
56	MG	2A	3837	1/1	0.65	0.17	48,48,48,48	0
56	MG	1x	113	1/1	0.65	0.24	48,48,48,48	0
56	MG	1A	3915	1/1	0.65	0.20	51,51,51,51	0
56	MG	2A	3894	1/1	0.65	0.24	60,60,60,60	0
56	MG	1A	4050	1/1	0.65	0.08	57,57,57,57	0
56	MG	2A	3823	1/1	0.66	0.49	79,79,79,79	0
56	MG	1A	3386	1/1	0.66	0.20	63,63,63,63	0
56	MG	1a	1658	1/1	0.66	0.25	84,84,84,84	0
56	MG	2a	3116	1/1	0.66	0.17	73,73,73,73	0
56	MG	1A	4162	1/1	0.66	0.16	68,68,68,68	0
56	MG	2a	3054	1/1	0.67	0.20	61,61,61,61	0
56	MG	2a	3169	1/1	0.67	0.14	80,80,80,80	0
56	MG	2A	3874	1/1	0.67	0.12	74,74,74,74	0
56	MG	1a	1915	1/1	0.67	0.07	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1881	1/1	0.67	0.09	73,73,73,73	0
56	MG	2A	3527	1/1	0.67	0.13	38,38,38,38	0
56	MG	2A	3617	1/1	0.67	0.20	47,47,47,47	0
56	MG	2A	3868	1/1	0.67	0.23	71,71,71,71	0
56	MG	1A	3600	1/1	0.67	0.14	64,64,64,64	0
56	MG	1A	4146	1/1	0.68	0.88	80,80,80,80	0
56	MG	2a	3066	1/1	0.68	0.30	77,77,77,77	0
56	MG	2A	3388	1/1	0.68	0.18	65,65,65,65	0
56	MG	1w	108	1/1	0.68	0.20	63,63,63,63	0
56	MG	1A	4087	1/1	0.68	0.36	79,79,79,79	0
56	MG	1a	1751	1/1	0.68	0.12	78,78,78,78	0
56	MG	1A	3007	1/1	0.68	0.35	52,52,52,52	0
56	MG	1a	1874	1/1	0.68	0.11	82,82,82,82	0
56	MG	2A	3090	1/1	0.68	0.10	71,71,71,71	0
56	MG	2A	3734	1/1	0.68	0.27	67,67,67,67	0
56	MG	1l	102	1/1	0.68	0.35	58,58,58,58	0
56	MG	1a	1607	1/1	0.68	0.14	71,71,71,71	0
56	MG	1A	3383	1/1	0.68	0.53	72,72,72,72	0
56	MG	2a	3034	1/1	0.68	0.40	64,64,64,64	0
56	MG	1A	3890	1/1	0.68	0.12	65,65,65,65	0
56	MG	2A	3362	1/1	0.68	0.29	61,61,61,61	0
56	MG	1A	3358	1/1	0.69	0.35	64,64,64,64	0
56	MG	2A	3068	1/1	0.69	0.19	56,56,56,56	0
56	MG	1A	4123	1/1	0.69	0.17	78,78,78,78	0
56	MG	1A	3987	1/1	0.69	0.09	71,71,71,71	0
56	MG	2a	3007	1/1	0.69	0.16	70,70,70,70	0
56	MG	2A	3713	1/1	0.69	0.12	63,63,63,63	0
56	MG	1a	1861	1/1	0.69	0.31	102,102,102,102	0
56	MG	1a	1693	1/1	0.69	0.16	66,66,66,66	0
56	MG	2A	3495	1/1	0.69	0.58	66,66,66,66	0
56	MG	1l	3001	1/1	0.70	0.34	76,76,76,76	0
56	MG	1A	4111	1/1	0.70	0.21	92,92,92,92	0
56	MG	1A	4038	1/1	0.70	0.15	71,71,71,71	0
56	MG	2a	3086	1/1	0.70	0.60	81,81,81,81	0
56	MG	1A	3112	1/1	0.70	0.48	54,54,54,54	0
56	MG	1A	3464	1/1	0.70	0.19	50,50,50,50	0
56	MG	1A	3370	1/1	0.70	0.84	55,55,55,55	0
56	MG	1A	4151	1/1	0.70	0.28	59,59,59,59	0
56	MG	1A	4063	1/1	0.70	0.38	63,63,63,63	0
56	MG	1A	3981	1/1	0.70	0.17	41,41,41,41	0
56	MG	1A	3265	1/1	0.70	0.19	64,64,64,64	0
56	MG	2a	3170	1/1	0.70	0.13	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	4207	1/1	0.70	0.28	60,60,60,60	0
56	MG	2A	3265	1/1	0.70	0.34	61,61,61,61	0
56	MG	1A	3634	1/1	0.70	0.21	68,68,68,68	0
56	MG	1A	3091	1/1	0.70	0.57	72,72,72,72	0
56	MG	1A	4015	1/1	0.70	0.22	73,73,73,73	0
56	MG	2a	3044	1/1	0.70	0.17	70,70,70,70	0
56	MG	1a	1887	1/1	0.70	0.16	57,57,57,57	0
56	MG	2A	3326	1/1	0.71	0.27	57,57,57,57	0
56	MG	1A	3255	1/1	0.71	0.24	60,60,60,60	0
56	MG	2A	3058	1/1	0.71	0.37	68,68,68,68	0
56	MG	1A	3312	1/1	0.71	0.41	67,67,67,67	0
56	MG	1A	3730	1/1	0.71	0.18	44,44,44,44	0
56	MG	2A	3380	1/1	0.71	0.14	67,67,67,67	0
56	MG	2a	3174	1/1	0.71	0.12	88,88,88,88	0
56	MG	2A	3888	1/1	0.71	0.13	42,42,42,42	0
56	MG	1a	1750	1/1	0.71	0.11	75,75,75,75	0
56	MG	2A	3113	1/1	0.71	0.23	71,71,71,71	0
56	MG	1A	4135	1/1	0.71	0.11	67,67,67,67	0
56	MG	2A	3271	1/1	0.71	0.21	59,59,59,59	0
56	MG	1a	1814	1/1	0.71	0.15	71,71,71,71	0
56	MG	1a	1723	1/1	0.72	0.71	69,69,69,69	0
56	MG	2A	3672	1/1	0.72	0.12	68,68,68,68	0
56	MG	1A	3934	1/1	0.72	0.12	64,64,64,64	0
56	MG	1a	1649	1/1	0.72	0.09	62,62,62,62	0
56	MG	1A	3227	1/1	0.72	0.29	65,65,65,65	0
56	MG	2a	3047	1/1	0.72	0.15	72,72,72,72	0
56	MG	2A	3757	1/1	0.72	0.19	54,54,54,54	0
56	MG	2A	3476	1/1	0.72	0.22	63,63,63,63	0
56	MG	2a	3060	1/1	0.72	0.51	82,82,82,82	0
56	MG	1A	3397	1/1	0.72	0.36	44,44,44,44	0
56	MG	2B	3009	1/1	0.72	0.14	61,61,61,61	0
56	MG	1A	4024	1/1	0.72	0.10	48,48,48,48	0
56	MG	2A	3593	1/1	0.72	0.30	71,71,71,71	0
56	MG	2A	3057	1/1	0.72	0.40	68,68,68,68	0
57	CPT	1a	1930	4/5	0.72	0.45	60,62,73,353	0
56	MG	1A	4138	1/1	0.73	0.20	76,76,76,76	0
56	MG	1A	3406	1/1	0.73	0.25	54,54,54,54	0
56	MG	1A	3352	1/1	0.73	0.27	66,66,66,66	0
56	MG	2A	3688	1/1	0.73	0.24	68,68,68,68	0
56	MG	2A	3377	1/1	0.73	0.75	64,64,64,64	0
56	MG	1A	4066	1/1	0.73	0.44	82,82,82,82	0
56	MG	2a	3143	1/1	0.73	0.16	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4008	1/1	0.73	0.07	84,84,84,84	0
56	MG	1A	4121	1/1	0.73	0.14	91,91,91,91	0
56	MG	2a	3020	1/1	0.73	0.27	61,61,61,61	0
56	MG	2A	3797	1/1	0.73	0.26	50,50,50,50	0
56	MG	1A	4179	1/1	0.73	0.22	51,51,51,51	0
56	MG	1t	3001	1/1	0.73	0.35	65,65,65,65	0
56	MG	1a	1754	1/1	0.73	0.18	63,63,63,63	0
56	MG	2A	3479	1/1	0.73	0.57	58,58,58,58	0
56	MG	1A	3246	1/1	0.73	0.19	54,54,54,54	0
56	MG	2a	3234	1/1	0.73	0.15	76,76,76,76	0
56	MG	2A	3835	1/1	0.73	0.13	32,32,32,32	0
56	MG	1A	3274	1/1	0.73	0.38	71,71,71,71	0
56	MG	2x	103	1/1	0.73	0.33	83,83,83,83	0
56	MG	2A	3329	1/1	0.73	0.21	58,58,58,58	0
56	MG	1a	1867	1/1	0.73	0.11	83,83,83,83	0
56	MG	1A	4053	1/1	0.74	0.17	41,41,41,41	0
56	MG	2A	3725	1/1	0.74	0.12	52,52,52,52	0
56	MG	2A	3387	1/1	0.74	0.58	64,64,64,64	0
56	MG	2A	3756	1/1	0.74	0.18	40,40,40,40	0
56	MG	1A	3575	1/1	0.74	0.43	54,54,54,54	0
56	MG	20	101	1/1	0.74	0.21	60,60,60,60	0
56	MG	2A	3769	1/1	0.74	0.14	54,54,54,54	0
56	MG	2a	3148	1/1	0.74	0.10	75,75,75,75	0
56	MG	2a	3152	1/1	0.74	0.20	69,69,69,69	0
56	MG	2A	3261	1/1	0.74	0.31	65,65,65,65	0
56	MG	1A	4153	1/1	0.74	0.15	90,90,90,90	0
56	MG	1A	3215	1/1	0.74	0.20	56,56,56,56	0
56	MG	2A	3810	1/1	0.74	0.10	59,59,59,59	0
56	MG	1a	1602	1/1	0.74	0.44	83,83,83,83	0
56	MG	1A	3151	1/1	0.74	0.86	54,54,54,54	0
56	MG	2a	3191	1/1	0.74	0.19	65,65,65,65	0
56	MG	1A	3960	1/1	0.74	0.13	50,50,50,50	0
56	MG	1A	4124	1/1	0.74	0.07	67,67,67,67	0
56	MG	1A	3251	1/1	0.74	0.66	57,57,57,57	0
56	MG	1a	1679	1/1	0.74	0.14	75,75,75,75	0
56	MG	2a	3057	1/1	0.74	0.79	97,97,97,97	0
56	MG	1A	3403	1/1	0.74	0.39	53,53,53,53	0
56	MG	1A	3560	1/1	0.74	0.44	55,55,55,55	0
56	MG	1a	1899	1/1	0.74	0.20	86,86,86,86	0
56	MG	1A	3392	1/1	0.75	0.59	55,55,55,55	0
56	MG	2a	3100	1/1	0.75	0.12	67,67,67,67	0
56	MG	2A	3334	1/1	0.75	0.34	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3297	1/1	0.75	0.26	67,67,67,67	0
56	MG	1A	3375	1/1	0.75	0.94	60,60,60,60	0
56	MG	2A	3719	1/1	0.75	0.25	55,55,55,55	0
56	MG	1a	1878	1/1	0.75	0.07	70,70,70,70	0
56	MG	2A	3373	1/1	0.75	0.17	72,72,72,72	0
56	MG	1A	3059	1/1	0.75	0.24	63,63,63,63	0
56	MG	1G	3003	1/1	0.75	0.28	67,67,67,67	0
56	MG	1A	3384	1/1	0.75	0.24	51,51,51,51	0
56	MG	2a	3025	1/1	0.75	0.17	68,68,68,68	0
56	MG	2A	3092	1/1	0.75	0.58	34,34,34,34	0
56	MG	1Z	302	1/1	0.75	0.23	64,64,64,64	0
56	MG	2A	3394	1/1	0.75	0.59	61,61,61,61	0
56	MG	2A	3165	1/1	0.75	0.19	72,72,72,72	0
56	MG	1A	4037	1/1	0.75	0.11	64,64,64,64	0
56	MG	2a	3192	1/1	0.75	0.10	74,74,74,74	0
56	MG	1A	3460	1/1	0.75	0.24	62,62,62,62	0
56	MG	1A	4125	1/1	0.75	0.09	77,77,77,77	0
56	MG	2a	3055	1/1	0.75	0.30	67,67,67,67	0
56	MG	1a	1781	1/1	0.75	0.22	58,58,58,58	0
56	MG	2A	3297	1/1	0.75	0.18	54,54,54,54	0
56	MG	2w	103	1/1	0.75	0.52	83,83,83,83	0
56	MG	2A	3303	1/1	0.75	0.24	45,45,45,45	0
56	MG	1A	3331	1/1	0.75	0.17	67,67,67,67	0
56	MG	1A	4186	1/1	0.75	0.47	66,66,66,66	0
56	MG	1A	3468	1/1	0.76	0.25	68,68,68,68	0
56	MG	1A	3496	1/1	0.76	0.33	57,57,57,57	0
56	MG	2A	3188	1/1	0.76	0.13	57,57,57,57	0
56	MG	2A	3671	1/1	0.76	0.34	57,57,57,57	0
56	MG	2A	3214	1/1	0.76	0.64	64,64,64,64	0
56	MG	1A	3002	1/1	0.76	0.31	59,59,59,59	0
56	MG	1A	3367	1/1	0.76	0.51	56,56,56,56	0
56	MG	1Q	204	1/1	0.76	0.10	33,33,33,33	0
56	MG	2A	3274	1/1	0.76	0.25	52,52,52,52	0
56	MG	1A	3978	1/1	0.76	0.21	35,35,35,35	0
56	MG	2A	3288	1/1	0.76	0.20	56,56,56,56	0
56	MG	2A	3296	1/1	0.76	0.34	55,55,55,55	0
56	MG	1A	3192	1/1	0.76	0.18	57,57,57,57	0
56	MG	2A	3301	1/1	0.76	0.43	64,64,64,64	0
56	MG	10	105	1/1	0.76	0.16	66,66,66,66	0
56	MG	1A	3270	1/1	0.76	0.14	64,64,64,64	0
56	MG	15	102	1/1	0.76	0.51	42,42,42,42	0
56	MG	1A	4002	1/1	0.76	0.26	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	4072	1/1	0.76	0.37	95,95,95,95	0
56	MG	1A	3633	1/1	0.76	0.29	55,55,55,55	0
56	MG	1A	4154	1/1	0.76	0.23	88,88,88,88	0
56	MG	1A	3372	1/1	0.76	0.37	74,74,74,74	0
56	MG	1a	1659	1/1	0.76	0.09	68,68,68,68	0
56	MG	1a	1673	1/1	0.76	0.29	69,69,69,69	0
56	MG	1A	3639	1/1	0.76	0.22	56,56,56,56	0
56	MG	1a	1690	1/1	0.76	0.26	71,71,71,71	0
56	MG	1A	3212	1/1	0.76	0.26	53,53,53,53	0
56	MG	1A	3296	1/1	0.76	0.17	53,53,53,53	0
56	MG	2A	3029	1/1	0.76	0.12	51,51,51,51	0
56	MG	2A	3408	1/1	0.76	0.24	60,60,60,60	0
56	MG	1A	4113	1/1	0.76	0.11	60,60,60,60	0
56	MG	1A	4114	1/1	0.76	0.50	87,87,87,87	0
56	MG	2A	3460	1/1	0.76	0.27	66,66,66,66	0
56	MG	23	3001	1/1	0.76	0.69	56,56,56,56	0
56	MG	1a	1726	1/1	0.76	0.15	85,85,85,85	0
56	MG	2v	103	1/1	0.76	0.41	67,67,67,67	0
56	MG	1a	1732	1/1	0.76	0.18	57,57,57,57	0
56	MG	1a	1742	1/1	0.76	0.16	73,73,73,73	0
56	MG	1A	3256	1/1	0.76	0.15	73,73,73,73	0
56	MG	2A	3548	1/1	0.76	0.13	49,49,49,49	0
56	MG	2A	3200	1/1	0.77	0.38	73,73,73,73	0
56	MG	2A	3201	1/1	0.77	0.17	61,61,61,61	0
56	MG	1A	3363	1/1	0.77	0.34	58,58,58,58	0
56	MG	2A	3393	1/1	0.77	0.15	67,67,67,67	0
56	MG	2A	3251	1/1	0.77	0.44	68,68,68,68	0
56	MG	2A	3400	1/1	0.77	0.22	77,77,77,77	0
56	MG	2A	3255	1/1	0.77	0.24	60,60,60,60	0
56	MG	1A	3601	1/1	0.77	0.12	70,70,70,70	0
56	MG	1A	4199	1/1	0.77	0.22	36,36,36,36	0
56	MG	1A	3688	1/1	0.77	0.45	53,53,53,53	0
56	MG	1a	1872	1/1	0.77	0.10	85,85,85,85	0
56	MG	2A	3858	1/1	0.77	0.24	52,52,52,52	0
56	MG	1x	118	1/1	0.77	0.35	66,66,66,66	0
56	MG	1A	4208	1/1	0.77	0.30	79,79,79,79	0
56	MG	2A	3516	1/1	0.77	0.06	57,57,57,57	0
56	MG	2A	3521	1/1	0.77	0.09	53,53,53,53	0
56	MG	2A	3875	1/1	0.77	0.25	48,48,48,48	0
56	MG	2A	3879	1/1	0.77	0.08	91,91,91,91	0
56	MG	1A	3467	1/1	0.77	0.26	65,65,65,65	0
56	MG	1A	3745	1/1	0.77	0.28	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3550	1/1	0.77	0.15	41,41,41,41	0
56	MG	1A	4119	1/1	0.77	0.29	73,73,73,73	0
56	MG	2E	303	1/1	0.77	0.14	51,51,51,51	0
56	MG	2A	3064	1/1	0.77	0.09	64,64,64,64	0
56	MG	2A	3312	1/1	0.77	0.24	60,60,60,60	0
56	MG	1A	3506	1/1	0.77	0.34	55,55,55,55	0
56	MG	2A	3073	1/1	0.77	0.24	43,43,43,43	0
56	MG	2A	3089	1/1	0.77	0.17	60,60,60,60	0
56	MG	1A	3984	1/1	0.77	0.27	49,49,49,49	0
56	MG	1A	3817	1/1	0.77	0.15	67,67,67,67	0
56	MG	1a	1917	1/1	0.77	0.17	55,55,55,55	0
56	MG	2A	3152	1/1	0.77	0.16	53,53,53,53	0
56	MG	1a	1755	1/1	0.77	0.13	62,62,62,62	0
56	MG	2A	3173	1/1	0.77	0.08	61,61,61,61	0
56	MG	1A	3862	1/1	0.77	0.24	31,31,31,31	0
56	MG	1a	1798	1/1	0.78	0.15	66,66,66,66	0
56	MG	2A	3195	1/1	0.78	0.45	53,53,53,53	0
56	MG	1a	1805	1/1	0.78	0.17	63,63,63,63	0
56	MG	1A	3888	1/1	0.78	0.19	54,54,54,54	0
56	MG	2B	3020	1/1	0.78	0.14	75,75,75,75	0
56	MG	2A	3456	1/1	0.78	0.56	52,52,52,52	0
56	MG	2A	3210	1/1	0.78	0.38	61,61,61,61	0
56	MG	1a	1851	1/1	0.78	0.16	76,76,76,76	0
56	MG	2A	3243	1/1	0.78	0.40	60,60,60,60	0
56	MG	1B	204	1/1	0.78	0.27	61,61,61,61	0
56	MG	2A	3355	1/1	0.78	0.35	73,73,73,73	0
56	MG	2A	3803	1/1	0.78	0.15	64,64,64,64	0
56	MG	2A	3358	1/1	0.78	0.18	78,78,78,78	0
56	MG	1A	3457	1/1	0.78	0.25	63,63,63,63	0
56	MG	1A	3519	1/1	0.78	0.11	71,71,71,71	0
56	MG	1A	3409	1/1	0.78	0.21	64,64,64,64	0
56	MG	2A	3582	1/1	0.78	0.10	76,76,76,76	0
56	MG	2A	3589	1/1	0.78	0.20	65,65,65,65	0
56	MG	2A	3270	1/1	0.78	0.46	65,65,65,65	0
56	MG	1A	4065	1/1	0.78	0.09	64,64,64,64	0
56	MG	1A	3024	1/1	0.78	0.18	53,53,53,53	0
56	MG	2p	3001	1/1	0.78	0.22	63,63,63,63	0
56	MG	1a	1880	1/1	0.78	0.17	51,51,51,51	0
56	MG	1a	1612	1/1	0.78	0.18	62,62,62,62	0
56	MG	1A	3720	1/1	0.78	0.15	37,37,37,37	0
56	MG	2A	3687	1/1	0.78	0.16	53,53,53,53	0
56	MG	2a	3073	1/1	0.78	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3177	1/1	0.78	0.31	46,46,46,46	0
56	MG	1a	1793	1/1	0.79	0.26	65,65,65,65	0
56	MG	1A	4013	1/1	0.79	0.09	50,50,50,50	0
56	MG	2B	3015	1/1	0.79	0.19	62,62,62,62	0
56	MG	1A	3649	1/1	0.79	0.39	79,79,79,79	0
56	MG	1a	1919	1/1	0.79	0.10	54,54,54,54	0
56	MG	2a	3137	1/1	0.79	0.06	87,87,87,87	0
56	MG	2a	3139	1/1	0.79	0.19	85,85,85,85	0
56	MG	2F	303	1/1	0.79	0.31	52,52,52,52	0
56	MG	2a	3142	1/1	0.79	0.14	86,86,86,86	0
56	MG	1A	4255	1/1	0.79	0.19	48,48,48,48	0
56	MG	2A	3800	1/1	0.79	0.15	67,67,67,67	0
56	MG	2A	3551	1/1	0.79	0.14	44,44,44,44	0
56	MG	2a	3004	1/1	0.79	0.12	68,68,68,68	0
56	MG	1A	3425	1/1	0.79	0.20	54,54,54,54	0
56	MG	2a	3167	1/1	0.79	0.08	75,75,75,75	0
56	MG	16	102	1/1	0.79	0.62	68,68,68,68	0
56	MG	2a	3023	1/1	0.79	0.28	72,72,72,72	0
56	MG	1A	3695	1/1	0.79	0.16	37,37,37,37	0
56	MG	2A	3604	1/1	0.79	0.22	34,34,34,34	0
56	MG	1A	3321	1/1	0.79	0.21	57,57,57,57	0
56	MG	1B	234	1/1	0.79	0.27	78,78,78,78	0
56	MG	1A	3484	1/1	0.79	0.23	58,58,58,58	0
56	MG	1x	117	1/1	0.79	0.17	78,78,78,78	0
56	MG	1A	3359	1/1	0.79	0.22	53,53,53,53	0
56	MG	1A	3327	1/1	0.79	0.33	56,56,56,56	0
56	MG	1A	4147	1/1	0.79	0.13	79,79,79,79	0
56	MG	1A	4201	1/1	0.79	0.19	51,51,51,51	0
56	MG	2A	3222	1/1	0.79	0.27	72,72,72,72	0
56	MG	2a	3059	1/1	0.79	0.17	61,61,61,61	0
56	MG	2v	105	1/1	0.79	0.17	76,76,76,76	0
56	MG	2A	3342	1/1	0.79	0.37	53,53,53,53	0
56	MG	1a	1677	1/1	0.79	0.27	70,70,70,70	0
56	MG	2y	3002	1/1	0.79	0.20	58,58,58,58	0
56	MG	1a	1902	1/1	0.79	0.10	77,77,77,77	0
56	MG	2B	3002	1/1	0.79	0.30	60,60,60,60	0
56	MG	1A	3512	1/1	0.80	0.43	59,59,59,59	0
56	MG	1A	4168	1/1	0.80	0.11	66,66,66,66	0
56	MG	2A	3824	1/1	0.80	0.21	80,80,80,80	0
56	MG	1A	4011	1/1	0.80	0.20	73,73,73,73	0
56	MG	2A	3290	1/1	0.80	0.28	62,62,62,62	0
56	MG	1a	1694	1/1	0.80	0.40	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1a	1709	1/1	0.80	0.07	73,73,73,73	0
56	MG	2a	3078	1/1	0.80	0.15	50,50,50,50	0
56	MG	2A	3853	1/1	0.80	0.13	63,63,63,63	0
56	MG	1A	3517	1/1	0.80	0.38	53,53,53,53	0
56	MG	2a	3107	1/1	0.80	0.30	75,75,75,75	0
56	MG	1A	3615	1/1	0.80	0.18	33,33,33,33	0
56	MG	1A	4193	1/1	0.80	0.15	49,49,49,49	0
56	MG	1a	1891	1/1	0.80	0.13	91,91,91,91	0
56	MG	2a	3133	1/1	0.80	0.15	94,94,94,94	0
56	MG	2a	3134	1/1	0.80	0.15	74,74,74,74	0
56	MG	2A	3146	1/1	0.80	0.21	56,56,56,56	0
56	MG	1A	3941	1/1	0.80	0.23	29,29,29,29	0
56	MG	1a	1728	1/1	0.80	0.09	62,62,62,62	0
56	MG	2A	3339	1/1	0.80	0.24	56,56,56,56	0
56	MG	1A	3472	1/1	0.80	0.20	59,59,59,59	0
56	MG	1A	4205	1/1	0.80	0.18	46,46,46,46	0
56	MG	2A	3352	1/1	0.80	0.25	47,47,47,47	0
56	MG	1A	3049	1/1	0.80	0.29	45,45,45,45	0
56	MG	2a	3157	1/1	0.80	0.09	79,79,79,79	0
56	MG	1A	3374	1/1	0.80	0.29	53,53,53,53	0
56	MG	1A	4240	1/1	0.80	0.25	51,51,51,51	0
56	MG	1A	3797	1/1	0.80	0.20	49,49,49,49	0
56	MG	1a	1776	1/1	0.80	0.42	69,69,69,69	0
56	MG	1A	3308	1/1	0.80	0.79	62,62,62,62	0
56	MG	1w	111	1/1	0.80	0.29	84,84,84,84	0
56	MG	1a	1620	1/1	0.80	0.13	54,54,54,54	0
56	MG	2a	3188	1/1	0.80	0.19	78,78,78,78	0
56	MG	2A	3726	1/1	0.80	0.09	64,64,64,64	0
56	MG	2a	3006	1/1	0.80	0.17	65,65,65,65	0
56	MG	2A	3727	1/1	0.80	0.15	53,53,53,53	0
56	MG	2a	3214	1/1	0.80	0.14	63,63,63,63	0
56	MG	2a	3216	1/1	0.80	0.18	66,66,66,66	0
56	MG	2A	3247	1/1	0.80	0.47	56,56,56,56	0
56	MG	2A	3248	1/1	0.80	0.41	66,66,66,66	0
56	MG	1A	3995	1/1	0.80	0.20	51,51,51,51	0
56	MG	2l	3002	1/1	0.80	0.17	62,62,62,62	0
56	MG	1A	3595	1/1	0.80	0.26	49,49,49,49	0
56	MG	1A	3684	1/1	0.80	0.24	67,67,67,67	0
56	MG	1E	309	1/1	0.80	0.14	54,54,54,54	0
56	MG	1F	308	1/1	0.80	0.11	45,45,45,45	0
56	MG	2v	106	1/1	0.80	0.22	68,68,68,68	0
56	MG	1a	1864	1/1	0.80	0.10	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3422	1/1	0.80	0.20	56,56,56,56	0
56	MG	2a	3048	1/1	0.80	0.11	58,58,58,58	0
56	MG	2A	3809	1/1	0.80	0.23	67,67,67,67	0
56	MG	2A	3431	1/1	0.80	0.24	58,58,58,58	0
56	MG	2A	3414	1/1	0.81	0.32	52,52,52,52	0
56	MG	1A	4100	1/1	0.81	0.08	95,95,95,95	0
56	MG	1A	3757	1/1	0.81	0.14	51,51,51,51	0
56	MG	1A	3431	1/1	0.81	0.46	47,47,47,47	0
56	MG	1A	4046	1/1	0.81	0.17	69,69,69,69	0
56	MG	1y	3005	1/1	0.81	0.44	83,83,83,83	0
56	MG	2A	3287	1/1	0.81	0.25	60,60,60,60	0
56	MG	2A	3489	1/1	0.81	0.51	82,82,82,82	0
56	MG	2A	3005	1/1	0.81	0.15	56,56,56,56	0
56	MG	1A	4115	1/1	0.81	0.13	86,86,86,86	0
56	MG	1A	3800	1/1	0.81	0.13	57,57,57,57	0
56	MG	1A	4118	1/1	0.81	0.09	66,66,66,66	0
56	MG	2A	3540	1/1	0.81	0.10	54,54,54,54	0
56	MG	1A	3801	1/1	0.81	0.15	60,60,60,60	0
56	MG	1a	1832	1/1	0.81	0.15	59,59,59,59	0
56	MG	1A	4051	1/1	0.81	0.15	55,55,55,55	0
56	MG	2A	3885	1/1	0.81	0.26	50,50,50,50	0
56	MG	2A	3313	1/1	0.81	0.42	71,71,71,71	0
56	MG	1A	3662	1/1	0.81	0.27	59,59,59,59	0
56	MG	1a	1641	1/1	0.81	0.17	73,73,73,73	0
56	MG	1A	3315	1/1	0.81	0.23	51,51,51,51	0
56	MG	1A	4007	1/1	0.81	0.13	51,51,51,51	0
56	MG	2A	3645	1/1	0.81	0.19	40,40,40,40	0
56	MG	1A	3626	1/1	0.81	0.11	64,64,64,64	0
56	MG	2A	3340	1/1	0.81	0.47	75,75,75,75	0
56	MG	1B	210	1/1	0.81	0.92	62,62,62,62	0
56	MG	2N	8001	1/1	0.81	0.14	53,53,53,53	0
56	MG	1B	215	1/1	0.81	0.09	45,45,45,45	0
56	MG	1A	3152	1/1	0.81	0.24	51,51,51,51	0
56	MG	1A	3904	1/1	0.81	0.11	57,57,57,57	0
56	MG	1A	3480	1/1	0.81	0.24	53,53,53,53	0
56	MG	1E	302	1/1	0.81	0.19	51,51,51,51	0
56	MG	1a	1705	1/1	0.81	0.15	65,65,65,65	0
56	MG	2a	3196	1/1	0.81	0.24	71,71,71,71	0
56	MG	2a	3018	1/1	0.81	0.17	62,62,62,62	0
56	MG	1A	4078	1/1	0.81	0.19	24,24,24,24	0
56	MG	1A	3599	1/1	0.81	0.25	64,64,64,64	0
56	MG	2a	3221	1/1	0.81	0.10	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2a	3024	1/1	0.81	0.17	65,65,65,65	0
56	MG	1a	1713	1/1	0.81	0.61	79,79,79,79	0
56	MG	2f	3002	1/1	0.81	0.22	63,63,63,63	0
56	MG	1A	3643	1/1	0.81	0.14	51,51,51,51	0
56	MG	1A	3354	1/1	0.81	0.24	55,55,55,55	0
56	MG	2A	3761	1/1	0.81	0.51	47,47,47,47	0
56	MG	2A	3229	1/1	0.81	0.27	55,55,55,55	0
56	MG	2A	3783	1/1	0.81	0.15	42,42,42,42	0
56	MG	1G	3005	1/1	0.81	0.11	65,65,65,65	0
56	MG	1A	4091	1/1	0.81	0.14	75,75,75,75	0
56	MG	1A	4165	1/1	0.81	0.09	45,45,45,45	0
56	MG	1W	3002	1/1	0.81	0.21	51,51,51,51	0
56	MG	1X	106	1/1	0.81	0.24	56,56,56,56	0
56	MG	1A	4034	1/1	0.81	0.16	24,24,24,24	0
56	MG	2a	3058	1/1	0.81	0.54	76,76,76,76	0
56	MG	1a	1618	1/1	0.82	0.16	51,51,51,51	0
56	MG	1A	3364	1/1	0.82	0.21	52,52,52,52	0
56	MG	1a	1759	1/1	0.82	0.19	53,53,53,53	0
56	MG	2A	3618	1/1	0.82	0.12	46,46,46,46	0
56	MG	2a	3113	1/1	0.82	0.55	73,73,73,73	0
56	MG	1A	3690	1/1	0.82	0.14	52,52,52,52	0
56	MG	2A	3354	1/1	0.82	0.10	69,69,69,69	0
56	MG	2A	3202	1/1	0.82	0.16	53,53,53,53	0
56	MG	1D	312	1/1	0.82	0.21	63,63,63,63	0
56	MG	2A	3359	1/1	0.82	0.15	73,73,73,73	0
56	MG	1a	1784	1/1	0.82	0.11	59,59,59,59	0
56	MG	1A	3692	1/1	0.82	0.27	73,73,73,73	0
56	MG	1A	3611	1/1	0.82	0.20	59,59,59,59	0
56	MG	1a	1665	1/1	0.82	0.12	67,67,67,67	0
56	MG	2U	203	1/1	0.82	0.63	57,57,57,57	0
56	MG	1a	1809	1/1	0.82	0.13	64,64,64,64	0
56	MG	1A	3947	1/1	0.82	0.11	47,47,47,47	0
56	MG	2a	3156	1/1	0.82	0.10	77,77,77,77	0
56	MG	1A	3081	1/1	0.82	0.31	44,44,44,44	0
56	MG	1A	4171	1/1	0.82	0.17	74,74,74,74	0
56	MG	2A	3258	1/1	0.82	0.20	55,55,55,55	0
56	MG	2A	3001	1/1	0.82	0.35	49,49,49,49	0
56	MG	2A	3262	1/1	0.82	0.36	55,55,55,55	0
56	MG	1A	3518	1/1	0.82	0.11	81,81,81,81	0
56	MG	1A	3149	1/1	0.82	0.55	42,42,42,42	0
56	MG	2A	3050	1/1	0.82	0.46	47,47,47,47	0
56	MG	2a	3187	1/1	0.82	0.22	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3538	1/1	0.82	0.20	50,50,50,50	0
56	MG	2A	3420	1/1	0.82	0.16	61,61,61,61	0
56	MG	2a	3027	1/1	0.82	0.20	69,69,69,69	0
56	MG	1A	3469	1/1	0.82	0.19	60,60,60,60	0
56	MG	1A	3225	1/1	0.82	0.41	53,53,53,53	0
56	MG	1A	3430	1/1	0.82	0.15	50,50,50,50	0
56	MG	2A	3066	1/1	0.82	0.17	55,55,55,55	0
56	MG	1a	1875	1/1	0.82	0.13	55,55,55,55	0
56	MG	1a	1876	1/1	0.82	0.12	65,65,65,65	0
56	MG	2a	3052	1/1	0.82	0.31	65,65,65,65	0
56	MG	2A	3298	1/1	0.82	0.16	67,67,67,67	0
56	MG	1A	3648	1/1	0.82	0.23	53,53,53,53	0
56	MG	1A	3804	1/1	0.82	0.14	66,66,66,66	0
56	MG	2A	3309	1/1	0.82	0.15	66,66,66,66	0
56	MG	1A	3330	1/1	0.82	0.15	67,67,67,67	0
56	MG	1A	3269	1/1	0.82	0.28	57,57,57,57	0
56	MG	1A	3879	1/1	0.82	0.10	57,57,57,57	0
56	MG	1A	4145	1/1	0.82	0.23	35,35,35,35	0
56	MG	1A	4084	1/1	0.82	0.21	78,78,78,78	0
56	MG	2a	3068	1/1	0.82	0.13	71,71,71,71	0
56	MG	1A	3677	1/1	0.82	0.22	57,57,57,57	0
56	MG	2a	3075	1/1	0.82	0.20	70,70,70,70	0
56	MG	1A	3226	1/1	0.82	0.40	51,51,51,51	0
56	MG	2A	3376	1/1	0.83	0.20	59,59,59,59	0
56	MG	2A	3765	1/1	0.83	0.18	62,62,62,62	0
56	MG	1A	4017	1/1	0.83	0.20	29,29,29,29	0
56	MG	2A	3771	1/1	0.83	0.14	47,47,47,47	0
56	MG	2A	3204	1/1	0.83	0.14	58,58,58,58	0
56	MG	1A	3029	1/1	0.83	0.20	41,41,41,41	0
56	MG	1A	3185	1/1	0.83	0.18	41,41,41,41	0
56	MG	1A	4184	1/1	0.83	0.21	33,33,33,33	0
56	MG	1l	202	1/1	0.83	0.23	63,63,63,63	0
56	MG	1A	3189	1/1	0.83	0.20	43,43,43,43	0
56	MG	1A	3631	1/1	0.83	0.20	57,57,57,57	0
56	MG	1A	3713	1/1	0.83	0.14	50,50,50,50	0
56	MG	2A	3815	1/1	0.83	0.13	69,69,69,69	0
56	MG	1w	104	1/1	0.83	0.13	54,54,54,54	0
56	MG	2A	3820	1/1	0.83	0.23	75,75,75,75	0
56	MG	1A	3373	1/1	0.83	0.15	61,61,61,61	0
56	MG	1A	3026	1/1	0.83	0.23	56,56,56,56	0
56	MG	1A	3952	1/1	0.83	0.22	52,52,52,52	0
56	MG	1a	1782	1/1	0.83	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3053	1/1	0.83	0.12	62,62,62,62	0
56	MG	2A	3454	1/1	0.83	0.19	48,48,48,48	0
56	MG	2A	3266	1/1	0.83	0.20	62,62,62,62	0
56	MG	2a	3127	1/1	0.83	0.25	67,67,67,67	0
56	MG	1a	1792	1/1	0.83	0.21	51,51,51,51	0
56	MG	1A	3299	1/1	0.83	0.22	54,54,54,54	0
56	MG	2A	3865	1/1	0.83	0.16	57,57,57,57	0
56	MG	1A	3577	1/1	0.83	0.17	69,69,69,69	0
56	MG	1A	4137	1/1	0.83	0.20	72,72,72,72	0
56	MG	1B	208	1/1	0.83	0.13	71,71,71,71	0
56	MG	2A	3026	1/1	0.83	0.92	56,56,56,56	0
56	MG	1a	1811	1/1	0.83	0.33	68,68,68,68	0
56	MG	1B	209	1/1	0.83	0.46	73,73,73,73	0
56	MG	1A	3791	1/1	0.83	0.34	61,61,61,61	0
56	MG	1A	4139	1/1	0.83	0.13	34,34,34,34	0
56	MG	2a	3155	1/1	0.83	0.11	91,91,91,91	0
56	MG	2A	3900	1/1	0.83	0.29	53,53,53,53	0
56	MG	2A	3920	1/1	0.83	0.72	60,60,60,60	0
56	MG	2B	3001	1/1	0.83	0.15	66,66,66,66	0
56	MG	1a	1859	1/1	0.83	0.21	77,77,77,77	0
56	MG	1A	3793	1/1	0.83	0.17	36,36,36,36	0
56	MG	1A	3336	1/1	0.83	0.29	59,59,59,59	0
56	MG	1A	3997	1/1	0.83	0.18	68,68,68,68	0
56	MG	1a	1868	1/1	0.83	0.17	75,75,75,75	0
56	MG	2A	3321	1/1	0.83	0.32	62,62,62,62	0
56	MG	2E	304	1/1	0.83	0.18	55,55,55,55	0
56	MG	2A	3085	1/1	0.83	0.25	55,55,55,55	0
56	MG	1A	3343	1/1	0.83	0.39	60,60,60,60	0
56	MG	2Q	3003	1/1	0.83	0.15	41,41,41,41	0
56	MG	2A	3644	1/1	0.83	0.17	46,46,46,46	0
56	MG	2a	3200	1/1	0.83	0.14	71,71,71,71	0
56	MG	1a	1691	1/1	0.83	0.29	79,79,79,79	0
56	MG	1A	3244	1/1	0.83	0.19	55,55,55,55	0
56	MG	1A	3515	1/1	0.83	0.50	55,55,55,55	0
56	MG	1A	3805	1/1	0.83	0.23	62,62,62,62	0
56	MG	2A	3676	1/1	0.83	0.22	55,55,55,55	0
56	MG	1a	1707	1/1	0.83	0.24	59,59,59,59	0
56	MG	2a	3013	1/1	0.83	0.20	66,66,66,66	0
56	MG	2g	8001	1/1	0.83	0.08	61,61,61,61	0
56	MG	2A	3158	1/1	0.83	0.32	58,58,58,58	0
56	MG	1A	4157	1/1	0.83	0.11	61,61,61,61	0
56	MG	1A	4159	1/1	0.83	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3678	1/1	0.83	0.30	50,50,50,50	0
56	MG	2A	3722	1/1	0.83	0.17	48,48,48,48	0
56	MG	1A	3683	1/1	0.83	0.15	76,76,76,76	0
56	MG	1A	3867	1/1	0.83	0.10	62,62,62,62	0
56	MG	2A	3198	1/1	0.83	0.26	48,48,48,48	0
56	MG	2x	102	1/1	0.83	0.55	71,71,71,71	0
56	MG	1A	3605	1/1	0.83	0.16	48,48,48,48	0
56	MG	2A	3363	1/1	0.83	0.27	65,65,65,65	0
56	MG	2a	3036	1/1	0.83	0.30	60,60,60,60	0
56	MG	1a	1909	1/1	0.83	0.07	64,64,64,64	0
56	MG	1a	1639	1/1	0.84	0.07	56,56,56,56	0
56	MG	1B	230	1/1	0.84	0.10	82,82,82,82	0
56	MG	1x	107	1/1	0.84	0.14	66,66,66,66	0
56	MG	1a	1644	1/1	0.84	0.23	79,79,79,79	0
56	MG	1A	3247	1/1	0.84	1.13	71,71,71,71	0
56	MG	1x	116	1/1	0.84	0.13	65,65,65,65	0
56	MG	2A	3423	1/1	0.84	0.13	61,61,61,61	0
56	MG	1A	3318	1/1	0.84	0.31	57,57,57,57	0
56	MG	2A	3447	1/1	0.84	0.34	51,51,51,51	0
56	MG	2A	3452	1/1	0.84	0.20	60,60,60,60	0
56	MG	1A	3865	1/1	0.84	0.20	29,29,29,29	0
56	MG	2a	3080	1/1	0.84	0.42	62,62,62,62	0
56	MG	2a	3083	1/1	0.84	0.13	62,62,62,62	0
56	MG	1a	1663	1/1	0.84	0.10	73,73,73,73	0
56	MG	2A	3854	1/1	0.84	0.28	42,42,42,42	0
56	MG	1A	4059	1/1	0.84	0.15	65,65,65,65	0
56	MG	1F	302	1/1	0.84	0.58	66,66,66,66	0
56	MG	1A	3320	1/1	0.84	0.12	55,55,55,55	0
56	MG	2A	3866	1/1	0.84	0.11	63,63,63,63	0
56	MG	2a	3121	1/1	0.84	0.07	78,78,78,78	0
56	MG	1a	1834	1/1	0.84	0.25	60,60,60,60	0
56	MG	2A	3870	1/1	0.84	0.11	45,45,45,45	0
56	MG	2a	3132	1/1	0.84	0.10	59,59,59,59	0
56	MG	1A	3113	1/1	0.84	0.15	61,61,61,61	0
56	MG	2A	3514	1/1	0.84	0.16	48,48,48,48	0
56	MG	1a	1854	1/1	0.84	0.25	68,68,68,68	0
56	MG	1a	1683	1/1	0.84	0.14	80,80,80,80	0
56	MG	1a	1688	1/1	0.84	0.29	71,71,71,71	0
56	MG	1A	3132	1/1	0.84	0.36	58,58,58,58	0
56	MG	2A	3892	1/1	0.84	0.45	52,52,52,52	0
56	MG	1A	3557	1/1	0.84	0.20	59,59,59,59	0
56	MG	1A	3475	1/1	0.84	0.33	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1O	3001	1/1	0.84	0.48	82,82,82,82	0
56	MG	1A	4128	1/1	0.84	0.17	57,57,57,57	0
56	MG	2A	3086	1/1	0.84	0.13	51,51,51,51	0
56	MG	2A	3311	1/1	0.84	0.58	59,59,59,59	0
56	MG	1A	4074	1/1	0.84	0.12	58,58,58,58	0
56	MG	1A	3052	1/1	0.84	0.39	59,59,59,59	0
56	MG	2a	3168	1/1	0.84	0.09	68,68,68,68	0
56	MG	1A	3644	1/1	0.84	0.19	44,44,44,44	0
56	MG	2A	3109	1/1	0.84	0.09	58,58,58,58	0
56	MG	2A	3112	1/1	0.84	0.11	60,60,60,60	0
56	MG	1a	1711	1/1	0.84	0.11	54,54,54,54	0
56	MG	2a	3177	1/1	0.84	0.13	69,69,69,69	0
56	MG	1A	3102	1/1	0.84	0.20	42,42,42,42	0
56	MG	1a	1714	1/1	0.84	0.34	75,75,75,75	0
56	MG	10	104	1/1	0.84	0.74	53,53,53,53	0
56	MG	2A	3682	1/1	0.84	0.18	56,56,56,56	0
56	MG	1A	4140	1/1	0.84	0.31	74,74,74,74	0
56	MG	2a	3194	1/1	0.84	0.12	77,77,77,77	0
56	MG	28	103	1/1	0.84	0.24	63,63,63,63	0
56	MG	2A	3169	1/1	0.84	0.15	49,49,49,49	0
56	MG	2A	3172	1/1	0.84	0.40	55,55,55,55	0
56	MG	1A	3580	1/1	0.84	0.14	57,57,57,57	0
56	MG	1A	3489	1/1	0.84	0.42	52,52,52,52	0
56	MG	2A	3179	1/1	0.84	0.26	55,55,55,55	0
56	MG	1A	4088	1/1	0.84	0.14	62,62,62,62	0
56	MG	2a	3225	1/1	0.84	0.17	68,68,68,68	0
56	MG	1A	3598	1/1	0.84	0.22	54,54,54,54	0
56	MG	1a	1749	1/1	0.84	0.19	62,62,62,62	0
56	MG	1a	1604	1/1	0.84	0.37	63,63,63,63	0
56	MG	2A	3753	1/1	0.84	0.13	66,66,66,66	0
56	MG	1a	1605	1/1	0.84	0.49	72,72,72,72	0
56	MG	2A	3375	1/1	0.84	0.44	59,59,59,59	0
56	MG	1A	4098	1/1	0.84	0.09	81,81,81,81	0
56	MG	1A	3082	1/1	0.84	0.61	50,50,50,50	0
56	MG	2A	3206	1/1	0.84	0.18	59,59,59,59	0
56	MG	1A	3455	1/1	0.84	0.41	41,41,41,41	0
56	MG	2A	3383	1/1	0.84	0.37	59,59,59,59	0
56	MG	1a	1763	1/1	0.84	0.37	65,65,65,65	0
56	MG	1A	3338	1/1	0.84	0.21	50,50,50,50	0
56	MG	2A	3227	1/1	0.84	0.20	62,62,62,62	0
56	MG	2y	3003	1/1	0.84	0.30	71,71,71,71	0
56	MG	1A	3220	1/1	0.84	0.18	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3241	1/1	0.84	0.76	44,44,44,44	0
56	MG	1S	3002	1/1	0.85	0.58	63,63,63,63	0
56	MG	1A	3231	1/1	0.85	0.16	54,54,54,54	0
56	MG	2A	3361	1/1	0.85	0.12	57,57,57,57	0
56	MG	1a	1900	1/1	0.85	0.08	62,62,62,62	0
56	MG	1a	1715	1/1	0.85	0.25	62,62,62,62	0
56	MG	1A	3881	1/1	0.85	0.09	78,78,78,78	0
56	MG	1A	3340	1/1	0.85	0.16	65,65,65,65	0
56	MG	1A	3034	1/1	0.85	0.78	51,51,51,51	0
56	MG	1A	4117	1/1	0.85	0.09	83,83,83,83	0
56	MG	2A	3793	1/1	0.85	0.19	56,56,56,56	0
56	MG	1A	4195	1/1	0.85	0.73	59,59,59,59	0
56	MG	2A	3203	1/1	0.85	0.21	48,48,48,48	0
56	MG	1a	1734	1/1	0.85	0.16	67,67,67,67	0
56	MG	2A	3384	1/1	0.85	0.30	70,70,70,70	0
56	MG	10	106	1/1	0.85	0.13	70,70,70,70	0
56	MG	2A	3207	1/1	0.85	0.12	38,38,38,38	0
56	MG	1A	3899	1/1	0.85	0.17	35,35,35,35	0
56	MG	1A	3208	1/1	0.85	0.28	52,52,52,52	0
56	MG	2A	3395	1/1	0.85	0.08	61,61,61,61	0
56	MG	1A	3399	1/1	0.85	0.36	72,72,72,72	0
56	MG	2A	3404	1/1	0.85	0.25	55,55,55,55	0
56	MG	1A	3930	1/1	0.85	0.14	44,44,44,44	0
56	MG	2A	3409	1/1	0.85	0.37	51,51,51,51	0
56	MG	2a	3120	1/1	0.85	0.11	77,77,77,77	0
56	MG	1A	3273	1/1	0.85	0.41	45,45,45,45	0
56	MG	2a	3123	1/1	0.85	0.09	61,61,61,61	0
56	MG	2A	3230	1/1	0.85	0.33	58,58,58,58	0
56	MG	1A	4220	1/1	0.85	0.28	48,48,48,48	0
56	MG	1A	4222	1/1	0.85	0.31	45,45,45,45	0
56	MG	2A	3855	1/1	0.85	0.17	47,47,47,47	0
56	MG	2A	3244	1/1	0.85	0.25	46,46,46,46	0
56	MG	2A	3246	1/1	0.85	0.28	59,59,59,59	0
56	MG	1a	1611	1/1	0.85	0.17	63,63,63,63	0
56	MG	1x	111	1/1	0.85	0.10	61,61,61,61	0
56	MG	1A	4232	1/1	0.85	1.31	62,62,62,62	0
56	MG	1A	3371	1/1	0.85	0.34	56,56,56,56	0
56	MG	1A	3079	1/1	0.85	0.17	46,46,46,46	0
56	MG	1B	202	1/1	0.85	0.26	56,56,56,56	0
56	MG	2A	3470	1/1	0.85	0.50	60,60,60,60	0
56	MG	1y	3003	1/1	0.85	0.18	85,85,85,85	0
56	MG	1A	4133	1/1	0.85	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1B	205	1/1	0.85	0.19	48,48,48,48	0
56	MG	2A	3002	1/1	0.85	0.41	61,61,61,61	0
56	MG	2A	3503	1/1	0.85	0.10	45,45,45,45	0
56	MG	1a	1802	1/1	0.85	0.10	63,63,63,63	0
56	MG	2A	3902	1/1	0.85	0.30	61,61,61,61	0
56	MG	1a	1804	1/1	0.85	0.16	67,67,67,67	0
56	MG	1B	207	1/1	0.85	0.11	65,65,65,65	0
56	MG	1A	3413	1/1	0.85	0.20	54,54,54,54	0
56	MG	1A	3958	1/1	0.85	0.18	48,48,48,48	0
56	MG	1A	3776	1/1	0.85	0.20	43,43,43,43	0
56	MG	2A	3549	1/1	0.85	0.14	52,52,52,52	0
56	MG	1a	1818	1/1	0.85	0.42	45,45,45,45	0
56	MG	1A	3974	1/1	0.85	0.20	35,35,35,35	0
56	MG	1A	3783	1/1	0.85	0.22	37,37,37,37	0
56	MG	1A	3573	1/1	0.85	0.27	51,51,51,51	0
56	MG	1A	3292	1/1	0.85	0.23	62,62,62,62	0
56	MG	2A	3077	1/1	0.85	0.16	46,46,46,46	0
56	MG	1A	3647	1/1	0.85	0.20	40,40,40,40	0
56	MG	1A	3988	1/1	0.85	0.14	58,58,58,58	0
56	MG	1A	3483	1/1	0.85	0.15	43,43,43,43	0
56	MG	2a	3219	1/1	0.85	0.19	81,81,81,81	0
56	MG	25	101	1/1	0.85	0.34	57,57,57,57	0
56	MG	1A	3333	1/1	0.85	0.13	55,55,55,55	0
56	MG	2A	3091	1/1	0.85	0.26	55,55,55,55	0
56	MG	2A	3328	1/1	0.85	0.48	58,58,58,58	0
56	MG	2a	3237	1/1	0.85	0.18	61,61,61,61	0
56	MG	1A	3587	1/1	0.85	0.16	54,54,54,54	0
56	MG	1A	3316	1/1	0.85	0.17	51,51,51,51	0
56	MG	1A	3492	1/1	0.85	0.29	47,47,47,47	0
56	MG	2A	3335	1/1	0.85	0.10	52,52,52,52	0
56	MG	2A	3685	1/1	0.85	0.11	44,44,44,44	0
56	MG	1a	1700	1/1	0.85	0.16	55,55,55,55	0
56	MG	1a	1704	1/1	0.85	0.41	67,67,67,67	0
56	MG	1A	3826	1/1	0.85	0.21	61,61,61,61	0
56	MG	2A	3714	1/1	0.85	0.16	58,58,58,58	0
56	MG	2A	3154	1/1	0.85	0.17	50,50,50,50	0
56	MG	2w	104	1/1	0.85	0.17	81,81,81,81	0
56	MG	2A	3344	1/1	0.85	1.10	71,71,71,71	0
56	MG	1A	4010	1/1	0.85	0.45	85,85,85,85	0
56	MG	1A	3337	1/1	0.85	0.26	48,48,48,48	0
56	MG	1A	3501	1/1	0.85	0.35	62,62,62,62	0
56	MG	1A	3441	1/1	0.85	0.26	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3746	1/1	0.85	0.11	76,76,76,76	0
56	MG	2A	3427	1/1	0.86	0.36	58,58,58,58	0
56	MG	2A	3429	1/1	0.86	0.19	55,55,55,55	0
56	MG	2A	3819	1/1	0.86	0.07	64,64,64,64	0
56	MG	1A	3544	1/1	0.86	0.17	65,65,65,65	0
56	MG	1A	4093	1/1	0.86	0.21	39,39,39,39	0
56	MG	1a	1729	1/1	0.86	0.16	47,47,47,47	0
56	MG	2a	3069	1/1	0.86	0.23	65,65,65,65	0
56	MG	1A	3555	1/1	0.86	0.21	72,72,72,72	0
56	MG	1A	3288	1/1	0.86	0.23	54,54,54,54	0
56	MG	1B	229	1/1	0.86	0.20	66,66,66,66	0
56	MG	2A	3294	1/1	0.86	0.70	59,59,59,59	0
56	MG	1a	1743	1/1	0.86	0.23	66,66,66,66	0
56	MG	1A	3931	1/1	0.86	0.31	59,59,59,59	0
56	MG	2a	3090	1/1	0.86	0.13	64,64,64,64	0
56	MG	2A	3100	1/1	0.86	0.10	72,72,72,72	0
56	MG	2a	3105	1/1	0.86	0.09	57,57,57,57	0
56	MG	2A	3104	1/1	0.86	0.17	60,60,60,60	0
56	MG	2A	3106	1/1	0.86	0.09	52,52,52,52	0
56	MG	2a	3112	1/1	0.86	0.18	70,70,70,70	0
56	MG	1a	1897	1/1	0.86	0.31	95,95,95,95	0
56	MG	1A	3604	1/1	0.86	0.13	42,42,42,42	0
56	MG	1D	305	1/1	0.86	0.24	48,48,48,48	0
56	MG	2A	3126	1/1	0.86	0.09	50,50,50,50	0
56	MG	2A	3127	1/1	0.86	0.10	48,48,48,48	0
56	MG	2A	3324	1/1	0.86	0.35	57,57,57,57	0
56	MG	2A	3132	1/1	0.86	0.08	53,53,53,53	0
56	MG	1a	1901	1/1	0.86	0.10	70,70,70,70	0
56	MG	1A	3248	1/1	0.86	0.13	67,67,67,67	0
56	MG	1a	1654	1/1	0.86	0.23	52,52,52,52	0
56	MG	1A	3660	1/1	0.86	0.29	61,61,61,61	0
56	MG	2A	3159	1/1	0.86	0.38	44,44,44,44	0
56	MG	1a	1762	1/1	0.86	0.23	60,60,60,60	0
56	MG	1a	1916	1/1	0.86	0.12	79,79,79,79	0
56	MG	2A	3913	1/1	0.86	0.76	46,46,46,46	0
56	MG	1A	3565	1/1	0.86	0.16	67,67,67,67	0
56	MG	2A	3642	1/1	0.86	0.27	44,44,44,44	0
56	MG	1A	3463	1/1	0.86	0.31	59,59,59,59	0
56	MG	1A	3618	1/1	0.86	0.33	53,53,53,53	0
56	MG	1a	1667	1/1	0.86	0.12	59,59,59,59	0
56	MG	1m	201	1/1	0.86	0.14	59,59,59,59	0
56	MG	2B	3017	1/1	0.86	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3971	1/1	0.86	0.16	31,31,31,31	0
56	MG	1A	3680	1/1	0.86	0.14	64,64,64,64	0
56	MG	2A	3677	1/1	0.86	0.13	44,44,44,44	0
56	MG	1A	3624	1/1	0.86	0.25	60,60,60,60	0
56	MG	1a	1682	1/1	0.86	0.14	69,69,69,69	0
56	MG	1A	3243	1/1	0.86	0.58	47,47,47,47	0
56	MG	2T	3001	1/1	0.86	0.70	74,74,74,74	0
56	MG	1A	4197	1/1	0.86	0.33	59,59,59,59	0
56	MG	2W	202	1/1	0.86	0.39	66,66,66,66	0
56	MG	2W	203	1/1	0.86	0.11	49,49,49,49	0
56	MG	2W	204	1/1	0.86	0.43	51,51,51,51	0
56	MG	1A	3140	1/1	0.86	0.33	37,37,37,37	0
56	MG	1A	3632	1/1	0.86	0.35	60,60,60,60	0
56	MG	1A	3849	1/1	0.86	0.16	55,55,55,55	0
56	MG	1a	1813	1/1	0.86	0.13	76,76,76,76	0
56	MG	1A	3860	1/1	0.86	0.21	36,36,36,36	0
56	MG	1a	1817	1/1	0.86	0.31	56,56,56,56	0
56	MG	1A	3169	1/1	0.86	0.18	59,59,59,59	0
56	MG	1A	3535	1/1	0.86	0.28	56,56,56,56	0
56	MG	1A	3442	1/1	0.86	0.55	40,40,40,40	0
56	MG	2A	3385	1/1	0.86	0.23	55,55,55,55	0
56	MG	2A	3240	1/1	0.86	0.38	41,41,41,41	0
56	MG	2A	3755	1/1	0.86	0.21	47,47,47,47	0
56	MG	1a	1842	1/1	0.86	0.19	61,61,61,61	0
56	MG	1A	4081	1/1	0.86	0.18	99,99,99,99	0
56	MG	1A	3640	1/1	0.86	0.20	40,40,40,40	0
56	MG	1a	1858	1/1	0.86	0.15	74,74,74,74	0
56	MG	1A	3721	1/1	0.86	0.12	37,37,37,37	0
56	MG	1A	3726	1/1	0.86	0.19	30,30,30,30	0
56	MG	2a	3032	1/1	0.86	0.42	65,65,65,65	0
56	MG	2A	3055	1/1	0.86	0.18	55,55,55,55	0
56	MG	2A	3785	1/1	0.86	0.37	57,57,57,57	0
56	MG	2a	3038	1/1	0.86	0.28	58,58,58,58	0
56	MG	2A	3056	1/1	0.86	0.41	46,46,46,46	0
56	MG	1A	3728	1/1	0.86	0.10	60,60,60,60	0
56	MG	1a	1866	1/1	0.86	0.09	62,62,62,62	0
56	MG	1A	3237	1/1	0.86	0.60	39,39,39,39	0
56	MG	1A	4149	1/1	0.86	0.10	61,61,61,61	0
56	MG	1A	4150	1/1	0.86	0.13	36,36,36,36	0
56	MG	1A	4090	1/1	0.86	0.18	54,54,54,54	0
56	MG	2A	3424	1/1	0.86	0.12	65,65,65,65	0
56	MG	1A	3491	1/1	0.87	0.51	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	3975	1/1	0.87	0.27	48,48,48,48	0
56	MG	2A	3621	1/1	0.87	0.19	32,32,32,32	0
56	MG	1A	3069	1/1	0.87	0.14	45,45,45,45	0
56	MG	1A	3402	1/1	0.87	0.30	53,53,53,53	0
56	MG	2A	3080	1/1	0.87	0.22	57,57,57,57	0
56	MG	1N	3005	1/1	0.87	0.19	69,69,69,69	0
56	MG	1A	3576	1/1	0.87	0.23	54,54,54,54	0
56	MG	2A	3087	1/1	0.87	0.39	57,57,57,57	0
56	MG	1A	3295	1/1	0.87	0.18	55,55,55,55	0
56	MG	2A	3317	1/1	0.87	0.17	53,53,53,53	0
56	MG	1A	3504	1/1	0.87	0.31	51,51,51,51	0
56	MG	1A	3582	1/1	0.87	0.21	37,37,37,37	0
56	MG	1A	3802	1/1	0.87	0.15	58,58,58,58	0
56	MG	1Z	301	1/1	0.87	0.19	50,50,50,50	0
56	MG	1a	1722	1/1	0.87	0.28	58,58,58,58	0
56	MG	2A	3692	1/1	0.87	0.36	65,65,65,65	0
56	MG	2a	3039	1/1	0.87	0.17	45,45,45,45	0
56	MG	1A	3586	1/1	0.87	0.19	44,44,44,44	0
56	MG	1a	1724	1/1	0.87	0.24	52,52,52,52	0
56	MG	1A	3405	1/1	0.87	0.27	51,51,51,51	0
56	MG	1A	3812	1/1	0.87	0.15	39,39,39,39	0
56	MG	2A	3724	1/1	0.87	0.10	48,48,48,48	0
56	MG	1A	3205	1/1	0.87	0.24	27,27,27,27	0
56	MG	1A	3671	1/1	0.87	0.22	49,49,49,49	0
56	MG	1A	3837	1/1	0.87	0.18	29,29,29,29	0
56	MG	1A	3172	1/1	0.87	0.18	60,60,60,60	0
56	MG	2A	3346	1/1	0.87	0.34	55,55,55,55	0
56	MG	2A	3350	1/1	0.87	0.11	44,44,44,44	0
56	MG	2a	3061	1/1	0.87	0.10	69,69,69,69	0
56	MG	1A	3858	1/1	0.87	0.22	34,34,34,34	0
56	MG	2A	3153	1/1	0.87	0.07	63,63,63,63	0
56	MG	1A	3342	1/1	0.87	0.20	54,54,54,54	0
56	MG	2A	3357	1/1	0.87	0.39	66,66,66,66	0
56	MG	1a	1906	1/1	0.87	0.13	50,50,50,50	0
56	MG	1a	1907	1/1	0.87	0.14	58,58,58,58	0
56	MG	1A	3380	1/1	0.87	0.22	50,50,50,50	0
56	MG	2A	3773	1/1	0.87	0.20	67,67,67,67	0
56	MG	1A	3365	1/1	0.87	0.60	53,53,53,53	0
56	MG	1A	3520	1/1	0.87	0.21	52,52,52,52	0
56	MG	1A	3686	1/1	0.87	0.25	52,52,52,52	0
56	MG	2A	3366	1/1	0.87	0.46	52,52,52,52	0
56	MG	2A	3176	1/1	0.87	0.09	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3374	1/1	0.87	0.15	76,76,76,76	0
56	MG	1A	3533	1/1	0.87	0.42	53,53,53,53	0
56	MG	1A	4132	1/1	0.87	0.14	54,54,54,54	0
56	MG	2A	3181	1/1	0.87	0.17	49,49,49,49	0
56	MG	1a	1921	1/1	0.87	0.33	55,55,55,55	0
56	MG	2A	3813	1/1	0.87	0.25	39,39,39,39	0
56	MG	2A	3189	1/1	0.87	0.19	51,51,51,51	0
56	MG	2A	3194	1/1	0.87	0.20	63,63,63,63	0
56	MG	2A	3817	1/1	0.87	0.18	63,63,63,63	0
56	MG	2a	3128	1/1	0.87	0.15	60,60,60,60	0
56	MG	2a	3129	1/1	0.87	0.30	65,65,65,65	0
56	MG	1a	1927	1/1	0.87	0.07	71,71,71,71	0
56	MG	1A	3252	1/1	0.87	0.17	66,66,66,66	0
56	MG	1A	3889	1/1	0.87	0.17	49,49,49,49	0
56	MG	1a	1774	1/1	0.87	0.13	51,51,51,51	0
56	MG	2A	3825	1/1	0.87	0.18	58,58,58,58	0
56	MG	1a	1633	1/1	0.87	0.23	62,62,62,62	0
56	MG	1a	1778	1/1	0.87	0.45	65,65,65,65	0
56	MG	1A	3253	1/1	0.87	0.26	48,48,48,48	0
56	MG	1w	107	1/1	0.87	0.27	70,70,70,70	0
56	MG	2a	3144	1/1	0.87	0.08	88,88,88,88	0
56	MG	2A	3848	1/1	0.87	0.12	79,79,79,79	0
56	MG	1A	3616	1/1	0.87	0.41	69,69,69,69	0
56	MG	2a	3149	1/1	0.87	0.11	86,86,86,86	0
56	MG	1A	3707	1/1	0.87	0.20	43,43,43,43	0
56	MG	2A	3213	1/1	0.87	0.27	54,54,54,54	0
56	MG	1A	3539	1/1	0.87	0.12	57,57,57,57	0
56	MG	2A	3861	1/1	0.87	0.09	67,67,67,67	0
56	MG	2A	3863	1/1	0.87	0.26	68,68,68,68	0
56	MG	2A	3218	1/1	0.87	0.12	63,63,63,63	0
56	MG	1x	103	1/1	0.87	0.24	59,59,59,59	0
56	MG	2A	3223	1/1	0.87	0.21	50,50,50,50	0
56	MG	1x	104	1/1	0.87	0.26	68,68,68,68	0
56	MG	1B	226	1/1	0.87	0.10	54,54,54,54	0
56	MG	1a	1795	1/1	0.87	0.18	67,67,67,67	0
56	MG	2A	3232	1/1	0.87	0.20	52,52,52,52	0
56	MG	1A	4058	1/1	0.87	0.57	65,65,65,65	0
56	MG	1a	1800	1/1	0.87	0.19	56,56,56,56	0
56	MG	2A	3442	1/1	0.87	0.35	48,48,48,48	0
56	MG	2A	3446	1/1	0.87	0.19	49,49,49,49	0
56	MG	1A	3040	1/1	0.87	0.20	43,43,43,43	0
56	MG	2A	3449	1/1	0.87	0.39	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3084	1/1	0.87	0.23	42,42,42,42	0
56	MG	2A	3245	1/1	0.87	0.29	51,51,51,51	0
56	MG	1A	3629	1/1	0.87	0.26	62,62,62,62	0
56	MG	2A	3457	1/1	0.87	0.41	66,66,66,66	0
56	MG	1A	3553	1/1	0.87	0.26	76,76,76,76	0
56	MG	2A	3466	1/1	0.87	0.26	50,50,50,50	0
56	MG	1a	1671	1/1	0.87	0.23	53,53,53,53	0
56	MG	1a	1812	1/1	0.87	0.14	58,58,58,58	0
56	MG	2A	3253	1/1	0.87	0.23	57,57,57,57	0
56	MG	1A	3486	1/1	0.87	0.17	52,52,52,52	0
56	MG	1A	3487	1/1	0.87	0.36	62,62,62,62	0
56	MG	2A	3499	1/1	0.87	0.32	41,41,41,41	0
56	MG	2A	3024	1/1	0.87	0.12	42,42,42,42	0
56	MG	2j	8001	1/1	0.87	0.12	80,80,80,80	0
56	MG	2j	8002	1/1	0.87	0.43	79,79,79,79	0
56	MG	1A	3448	1/1	0.87	0.24	59,59,59,59	0
56	MG	2A	3263	1/1	0.87	0.20	58,58,58,58	0
56	MG	1E	307	1/1	0.87	0.16	67,67,67,67	0
56	MG	2A	3033	1/1	0.87	0.13	53,53,53,53	0
56	MG	2A	3040	1/1	0.87	0.35	42,42,42,42	0
56	MG	1A	3636	1/1	0.87	0.18	66,66,66,66	0
56	MG	1E	313	1/1	0.87	0.29	47,47,47,47	0
56	MG	1a	1840	1/1	0.87	0.17	50,50,50,50	0
56	MG	1A	3967	1/1	0.87	0.40	61,61,61,61	0
56	MG	1a	1849	1/1	0.87	0.09	54,54,54,54	0
56	MG	1A	3759	1/1	0.87	0.24	34,34,34,34	0
56	MG	25	103	1/1	0.87	0.31	61,61,61,61	0
56	MG	28	101	1/1	0.87	0.15	75,75,75,75	0
56	MG	2A	3293	1/1	0.87	1.25	64,64,64,64	0
56	MG	1F	309	1/1	0.87	0.16	62,62,62,62	0
56	MG	2a	3008	1/1	0.88	0.13	67,67,67,67	0
56	MG	1A	3920	1/1	0.88	0.17	60,60,60,60	0
56	MG	1A	3921	1/1	0.88	0.12	53,53,53,53	0
56	MG	1a	1624	1/1	0.88	0.08	60,60,60,60	0
56	MG	1a	1780	1/1	0.88	0.22	70,70,70,70	0
56	MG	1A	3073	1/1	0.88	0.31	52,52,52,52	0
56	MG	2A	3696	1/1	0.88	0.16	50,50,50,50	0
56	MG	2A	3706	1/1	0.88	0.19	60,60,60,60	0
56	MG	1B	221	1/1	0.88	0.16	65,65,65,65	0
56	MG	1B	223	1/1	0.88	0.12	75,75,75,75	0
56	MG	1a	1787	1/1	0.88	0.10	61,61,61,61	0
56	MG	2A	3721	1/1	0.88	0.19	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4057	1/1	0.88	0.23	47,47,47,47	0
56	MG	1a	1646	1/1	0.88	0.09	59,59,59,59	0
56	MG	2a	3037	1/1	0.88	0.55	92,92,92,92	0
56	MG	1A	3532	1/1	0.88	0.21	51,51,51,51	0
56	MG	1A	3768	1/1	0.88	0.21	28,28,28,28	0
56	MG	2a	3043	1/1	0.88	0.23	61,61,61,61	0
56	MG	1A	3314	1/1	0.88	0.26	53,53,53,53	0
56	MG	2A	3733	1/1	0.88	0.15	38,38,38,38	0
56	MG	1A	3778	1/1	0.88	0.09	66,66,66,66	0
56	MG	1A	3437	1/1	0.88	0.47	59,59,59,59	0
56	MG	2A	3748	1/1	0.88	0.08	61,61,61,61	0
56	MG	2A	3367	1/1	0.88	0.09	59,59,59,59	0
56	MG	2A	3370	1/1	0.88	0.52	62,62,62,62	0
56	MG	1a	1664	1/1	0.88	0.09	62,62,62,62	0
56	MG	2A	3205	1/1	0.88	0.18	45,45,45,45	0
56	MG	1a	1806	1/1	0.88	0.20	53,53,53,53	0
56	MG	1A	3957	1/1	0.88	0.10	57,57,57,57	0
56	MG	2A	3208	1/1	0.88	0.29	50,50,50,50	0
56	MG	2A	3379	1/1	0.88	0.31	58,58,58,58	0
56	MG	1a	1810	1/1	0.88	0.10	64,64,64,64	0
56	MG	2A	3775	1/1	0.88	0.18	40,40,40,40	0
56	MG	2A	3211	1/1	0.88	0.37	56,56,56,56	0
56	MG	1A	3106	1/1	0.88	0.52	47,47,47,47	0
56	MG	1A	3663	1/1	0.88	0.17	39,39,39,39	0
56	MG	1a	1672	1/1	0.88	0.19	61,61,61,61	0
56	MG	2A	3796	1/1	0.88	0.14	64,64,64,64	0
56	MG	2a	3082	1/1	0.88	0.12	64,64,64,64	0
56	MG	1E	303	1/1	0.88	0.45	46,46,46,46	0
56	MG	2a	3085	1/1	0.88	0.31	57,57,57,57	0
56	MG	1A	3085	1/1	0.88	0.30	48,48,48,48	0
56	MG	2A	3226	1/1	0.88	0.39	51,51,51,51	0
56	MG	2a	3099	1/1	0.88	0.10	60,60,60,60	0
56	MG	2A	3014	1/1	0.88	0.35	40,40,40,40	0
56	MG	2A	3807	1/1	0.88	0.09	50,50,50,50	0
56	MG	2A	3228	1/1	0.88	0.64	53,53,53,53	0
56	MG	1A	4156	1/1	0.88	0.08	54,54,54,54	0
56	MG	2A	3403	1/1	0.88	0.20	54,54,54,54	0
56	MG	2A	3814	1/1	0.88	0.28	56,56,56,56	0
56	MG	1A	3317	1/1	0.88	0.16	53,53,53,53	0
56	MG	2A	3405	1/1	0.88	0.10	72,72,72,72	0
56	MG	1A	3188	1/1	0.88	0.18	61,61,61,61	0
56	MG	1a	1839	1/1	0.88	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3124	1/1	0.88	0.11	81,81,81,81	0
56	MG	1A	3679	1/1	0.88	0.15	44,44,44,44	0
56	MG	2A	3042	1/1	0.88	0.20	59,59,59,59	0
56	MG	1A	3545	1/1	0.88	0.14	62,62,62,62	0
56	MG	2A	3416	1/1	0.88	0.27	52,52,52,52	0
56	MG	1A	3681	1/1	0.88	0.21	73,73,73,73	0
56	MG	1A	3548	1/1	0.88	0.31	37,37,37,37	0
56	MG	1A	3067	1/1	0.88	0.15	44,44,44,44	0
56	MG	1A	3554	1/1	0.88	0.16	53,53,53,53	0
56	MG	2A	3841	1/1	0.88	0.14	66,66,66,66	0
56	MG	2A	3426	1/1	0.88	0.07	47,47,47,47	0
56	MG	1A	3458	1/1	0.88	0.33	55,55,55,55	0
56	MG	1N	3007	1/1	0.88	0.57	56,56,56,56	0
56	MG	2A	3065	1/1	0.88	0.10	59,59,59,59	0
56	MG	2a	3145	1/1	0.88	0.13	71,71,71,71	0
56	MG	1A	3500	1/1	0.88	0.62	50,50,50,50	0
56	MG	1O	3003	1/1	0.88	0.21	50,50,50,50	0
56	MG	1A	3853	1/1	0.88	0.20	24,24,24,24	0
56	MG	2A	3076	1/1	0.88	0.33	39,39,39,39	0
56	MG	2A	3264	1/1	0.88	0.16	60,60,60,60	0
56	MG	1A	3121	1/1	0.88	0.47	54,54,54,54	0
56	MG	1U	206	1/1	0.88	0.45	41,41,41,41	0
56	MG	1A	4104	1/1	0.88	0.07	32,32,32,32	0
56	MG	2a	3164	1/1	0.88	0.06	88,88,88,88	0
56	MG	2a	3166	1/1	0.88	0.06	81,81,81,81	0
56	MG	1A	3263	1/1	0.88	0.21	61,61,61,61	0
56	MG	1a	1716	1/1	0.88	0.39	53,53,53,53	0
56	MG	2A	3276	1/1	0.88	0.29	49,49,49,49	0
56	MG	2A	3878	1/1	0.88	0.17	64,64,64,64	0
56	MG	2A	3279	1/1	0.88	0.14	60,60,60,60	0
56	MG	2A	3883	1/1	0.88	0.41	44,44,44,44	0
56	MG	1A	3356	1/1	0.88	0.34	76,76,76,76	0
56	MG	1A	3574	1/1	0.88	0.26	49,49,49,49	0
56	MG	1A	3196	1/1	0.88	0.57	44,44,44,44	0
56	MG	1A	3874	1/1	0.88	0.20	29,29,29,29	0
56	MG	2A	3897	1/1	0.88	0.31	71,71,71,71	0
56	MG	2A	3292	1/1	0.88	0.16	55,55,55,55	0
56	MG	2A	3097	1/1	0.88	0.12	64,64,64,64	0
56	MG	2a	3195	1/1	0.88	0.28	85,85,85,85	0
56	MG	1A	3875	1/1	0.88	0.06	69,69,69,69	0
56	MG	2A	3101	1/1	0.88	0.14	51,51,51,51	0
56	MG	1A	3513	1/1	0.88	0.60	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3537	1/1	0.88	0.09	50,50,50,50	0
56	MG	11	101	1/1	0.88	0.16	44,44,44,44	0
56	MG	2A	3545	1/1	0.88	0.19	30,30,30,30	0
56	MG	1A	3725	1/1	0.88	0.09	53,53,53,53	0
56	MG	12	3001	1/1	0.88	0.24	56,56,56,56	0
56	MG	2a	3224	1/1	0.88	0.17	67,67,67,67	0
56	MG	2A	3304	1/1	0.88	0.12	52,52,52,52	0
56	MG	2D	303	1/1	0.88	1.02	51,51,51,51	0
56	MG	1A	3267	1/1	0.88	0.23	57,57,57,57	0
56	MG	2A	3560	1/1	0.88	0.21	41,41,41,41	0
56	MG	1A	3378	1/1	0.88	0.17	63,63,63,63	0
56	MG	1A	4248	1/1	0.88	0.29	53,53,53,53	0
56	MG	2A	3128	1/1	0.88	0.18	56,56,56,56	0
56	MG	1A	3423	1/1	0.88	0.47	61,61,61,61	0
56	MG	2A	3318	1/1	0.88	0.35	61,61,61,61	0
56	MG	2A	3138	1/1	0.88	0.38	40,40,40,40	0
56	MG	2A	3139	1/1	0.88	0.26	45,45,45,45	0
56	MG	2A	3628	1/1	0.88	0.15	53,53,53,53	0
56	MG	1A	3735	1/1	0.88	0.16	61,61,61,61	0
56	MG	1a	1753	1/1	0.88	0.15	74,74,74,74	0
56	MG	1A	4045	1/1	0.88	0.06	57,57,57,57	0
56	MG	2A	3657	1/1	0.88	0.12	65,65,65,65	0
56	MG	2w	107	1/1	0.88	0.11	63,63,63,63	0
56	MG	1a	1609	1/1	0.88	0.09	64,64,64,64	0
56	MG	1a	1757	1/1	0.88	0.17	71,71,71,71	0
56	MG	2x	105	1/1	0.88	0.38	59,59,59,59	0
56	MG	1A	3583	1/1	0.88	0.24	51,51,51,51	0
56	MG	2A	3160	1/1	0.88	0.26	42,42,42,42	0
56	MG	1A	3909	1/1	0.88	0.10	50,50,50,50	0
56	MG	1A	3204	1/1	0.88	0.18	48,48,48,48	0
59	ZN	29	501	1/1	0.88	0.06	79,79,79,79	0
56	MG	1A	3401	1/1	0.89	0.20	46,46,46,46	0
56	MG	1A	3956	1/1	0.89	0.20	55,55,55,55	0
56	MG	1A	3239	1/1	0.89	0.15	55,55,55,55	0
56	MG	2W	201	1/1	0.89	0.11	61,61,61,61	0
56	MG	1A	3348	1/1	0.89	0.26	53,53,53,53	0
56	MG	2A	3552	1/1	0.89	0.20	34,34,34,34	0
56	MG	2A	3553	1/1	0.89	0.11	42,42,42,42	0
56	MG	2A	3555	1/1	0.89	0.14	36,36,36,36	0
56	MG	20	102	1/1	0.89	0.19	56,56,56,56	0
56	MG	2A	3557	1/1	0.89	0.08	51,51,51,51	0
56	MG	1A	3542	1/1	0.89	0.28	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3571	1/1	0.89	0.16	36,36,36,36	0
56	MG	2A	3579	1/1	0.89	0.14	39,39,39,39	0
56	MG	2A	3580	1/1	0.89	0.14	47,47,47,47	0
56	MG	1A	4108	1/1	0.89	0.07	44,44,44,44	0
56	MG	2A	3583	1/1	0.89	0.07	56,56,56,56	0
56	MG	2A	3585	1/1	0.89	0.13	49,49,49,49	0
56	MG	1a	1662	1/1	0.89	0.14	47,47,47,47	0
56	MG	2A	3592	1/1	0.89	0.14	52,52,52,52	0
56	MG	2a	3011	1/1	0.89	0.06	69,69,69,69	0
56	MG	1A	3635	1/1	0.89	0.25	59,59,59,59	0
56	MG	2a	3017	1/1	0.89	0.07	71,71,71,71	0
56	MG	2A	3300	1/1	0.89	0.30	63,63,63,63	0
56	MG	1A	3774	1/1	0.89	0.19	75,75,75,75	0
56	MG	2a	3022	1/1	0.89	0.32	67,67,67,67	0
56	MG	1A	3322	1/1	0.89	0.36	50,50,50,50	0
56	MG	1A	3325	1/1	0.89	0.33	47,47,47,47	0
56	MG	1a	1670	1/1	0.89	0.34	56,56,56,56	0
56	MG	1a	1852	1/1	0.89	0.13	66,66,66,66	0
56	MG	2A	3093	1/1	0.89	0.70	48,48,48,48	0
56	MG	1A	3353	1/1	0.89	0.12	69,69,69,69	0
56	MG	2A	3098	1/1	0.89	0.15	51,51,51,51	0
56	MG	1A	3979	1/1	0.89	0.18	46,46,46,46	0
56	MG	2A	3668	1/1	0.89	0.12	41,41,41,41	0
56	MG	1A	3980	1/1	0.89	0.21	33,33,33,33	0
56	MG	1A	3788	1/1	0.89	0.15	27,27,27,27	0
56	MG	1A	3642	1/1	0.89	0.28	53,53,53,53	0
56	MG	1B	236	1/1	0.89	0.12	33,33,33,33	0
56	MG	1A	3474	1/1	0.89	0.17	51,51,51,51	0
56	MG	2A	3330	1/1	0.89	0.21	69,69,69,69	0
56	MG	1A	3412	1/1	0.89	0.27	56,56,56,56	0
56	MG	1A	3645	1/1	0.89	0.25	59,59,59,59	0
56	MG	1A	3302	1/1	0.89	0.32	33,33,33,33	0
56	MG	1a	1873	1/1	0.89	0.05	90,90,90,90	0
56	MG	2A	3131	1/1	0.89	0.20	56,56,56,56	0
56	MG	2A	3701	1/1	0.89	0.17	66,66,66,66	0
56	MG	1A	3180	1/1	0.89	0.33	52,52,52,52	0
56	MG	1A	4004	1/1	0.89	0.21	56,56,56,56	0
56	MG	1A	4006	1/1	0.89	0.22	57,57,57,57	0
56	MG	2A	3717	1/1	0.89	0.46	55,55,55,55	0
56	MG	2A	3345	1/1	0.89	0.36	58,58,58,58	0
56	MG	1A	4136	1/1	0.89	0.10	59,59,59,59	0
56	MG	1a	1879	1/1	0.89	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1F	303	1/1	0.89	0.15	57,57,57,57	0
56	MG	1F	304	1/1	0.89	0.12	44,44,44,44	0
56	MG	1a	1708	1/1	0.89	0.18	48,48,48,48	0
56	MG	1F	307	1/1	0.89	0.12	35,35,35,35	0
56	MG	2a	3077	1/1	0.89	0.15	59,59,59,59	0
56	MG	1a	1892	1/1	0.89	0.09	66,66,66,66	0
56	MG	1a	1894	1/1	0.89	0.05	71,71,71,71	0
56	MG	2A	3739	1/1	0.89	0.13	52,52,52,52	0
56	MG	2A	3744	1/1	0.89	0.13	71,71,71,71	0
56	MG	1A	3422	1/1	0.89	0.25	56,56,56,56	0
56	MG	1A	3485	1/1	0.89	0.11	51,51,51,51	0
56	MG	2a	3089	1/1	0.89	0.20	70,70,70,70	0
56	MG	1A	3650	1/1	0.89	0.25	45,45,45,45	0
56	MG	1A	3224	1/1	0.89	0.22	50,50,50,50	0
56	MG	1A	3285	1/1	0.89	0.93	43,43,43,43	0
56	MG	2a	3103	1/1	0.89	0.08	65,65,65,65	0
56	MG	1A	3828	1/1	0.89	0.08	47,47,47,47	0
56	MG	2A	3759	1/1	0.89	0.17	37,37,37,37	0
56	MG	1a	1718	1/1	0.89	0.11	57,57,57,57	0
56	MG	2A	3185	1/1	0.89	0.27	60,60,60,60	0
56	MG	2A	3768	1/1	0.89	0.25	66,66,66,66	0
56	MG	2a	3115	1/1	0.89	0.22	61,61,61,61	0
56	MG	1N	3002	1/1	0.89	0.13	46,46,46,46	0
56	MG	1A	3830	1/1	0.89	0.15	53,53,53,53	0
56	MG	2A	3772	1/1	0.89	0.10	59,59,59,59	0
56	MG	2A	3192	1/1	0.89	0.46	52,52,52,52	0
56	MG	1A	3209	1/1	0.89	0.18	57,57,57,57	0
56	MG	2A	3779	1/1	0.89	0.14	73,73,73,73	0
56	MG	1A	3382	1/1	0.89	0.32	53,53,53,53	0
56	MG	1A	3850	1/1	0.89	0.23	25,25,25,25	0
56	MG	2A	3381	1/1	0.89	0.12	53,53,53,53	0
56	MG	1O	3005	1/1	0.89	0.35	68,68,68,68	0
56	MG	1Q	203	1/1	0.89	0.16	53,53,53,53	0
56	MG	1A	3672	1/1	0.89	0.17	40,40,40,40	0
56	MG	1c	301	1/1	0.89	0.19	66,66,66,66	0
56	MG	1A	3433	1/1	0.89	0.26	57,57,57,57	0
56	MG	1a	1740	1/1	0.89	0.09	53,53,53,53	0
56	MG	2a	3141	1/1	0.89	0.14	57,57,57,57	0
56	MG	2A	3805	1/1	0.89	0.12	64,64,64,64	0
56	MG	1A	3495	1/1	0.89	0.44	48,48,48,48	0
56	MG	1s	3001	1/1	0.89	0.09	61,61,61,61	0
56	MG	1A	4043	1/1	0.89	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1745	1/1	0.89	0.36	58,58,58,58	0
56	MG	1a	1748	1/1	0.89	0.05	53,53,53,53	0
56	MG	2A	3212	1/1	0.89	0.19	58,58,58,58	0
56	MG	1A	3436	1/1	0.89	0.37	47,47,47,47	0
56	MG	1A	3498	1/1	0.89	0.22	64,64,64,64	0
56	MG	2A	3217	1/1	0.89	0.16	59,59,59,59	0
56	MG	1A	3360	1/1	0.89	0.31	54,54,54,54	0
56	MG	2a	3159	1/1	0.89	0.13	62,62,62,62	0
56	MG	1A	3361	1/1	0.89	0.27	63,63,63,63	0
56	MG	1A	3592	1/1	0.89	0.15	41,41,41,41	0
56	MG	2A	3415	1/1	0.89	0.24	59,59,59,59	0
56	MG	1A	3147	1/1	0.89	0.21	45,45,45,45	0
56	MG	2A	3417	1/1	0.89	0.16	60,60,60,60	0
56	MG	1a	1756	1/1	0.89	0.17	66,66,66,66	0
56	MG	1A	3444	1/1	0.89	0.24	45,45,45,45	0
56	MG	1A	3445	1/1	0.89	0.37	59,59,59,59	0
56	MG	2A	3842	1/1	0.89	0.18	35,35,35,35	0
56	MG	1A	3446	1/1	0.89	0.12	55,55,55,55	0
56	MG	2a	3181	1/1	0.89	0.19	62,62,62,62	0
56	MG	1x	115	1/1	0.89	0.28	49,49,49,49	0
56	MG	1A	3514	1/1	0.89	0.18	51,51,51,51	0
56	MG	1a	1766	1/1	0.89	0.37	62,62,62,62	0
56	MG	1A	3704	1/1	0.89	0.19	38,38,38,38	0
56	MG	2A	3860	1/1	0.89	0.08	70,70,70,70	0
56	MG	2A	3436	1/1	0.89	0.19	54,54,54,54	0
56	MG	1A	3011	1/1	0.89	0.19	42,42,42,42	0
56	MG	17	102	1/1	0.89	0.33	62,62,62,62	0
56	MG	18	101	1/1	0.89	0.37	77,77,77,77	0
56	MG	1A	3451	1/1	0.89	0.26	63,63,63,63	0
56	MG	1A	3913	1/1	0.89	0.24	45,45,45,45	0
56	MG	1A	3393	1/1	0.89	0.31	67,67,67,67	0
56	MG	1A	3456	1/1	0.89	0.23	57,57,57,57	0
56	MG	1A	3394	1/1	0.89	0.24	63,63,63,63	0
56	MG	2A	3458	1/1	0.89	0.44	57,57,57,57	0
56	MG	1A	3926	1/1	0.89	0.20	62,62,62,62	0
56	MG	2A	3030	1/1	0.89	0.12	35,35,35,35	0
56	MG	2a	3229	1/1	0.89	0.23	81,81,81,81	0
56	MG	2A	3882	1/1	0.89	0.27	51,51,51,51	0
56	MG	1A	4082	1/1	0.89	0.14	90,90,90,90	0
56	MG	2A	3471	1/1	0.89	0.33	59,59,59,59	0
56	MG	2A	3475	1/1	0.89	0.24	49,49,49,49	0
56	MG	1a	1797	1/1	0.89	0.24	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3928	1/1	0.89	0.14	47,47,47,47	0
56	MG	2A	3482	1/1	0.89	0.67	48,48,48,48	0
56	MG	2A	3487	1/1	0.89	0.19	45,45,45,45	0
56	MG	1A	3526	1/1	0.89	0.25	46,46,46,46	0
56	MG	1A	3219	1/1	0.89	0.10	51,51,51,51	0
56	MG	2A	3918	1/1	0.89	0.95	52,52,52,52	0
56	MG	2A	3498	1/1	0.89	0.16	62,62,62,62	0
56	MG	1A	3459	1/1	0.89	0.35	53,53,53,53	0
56	MG	1a	1632	1/1	0.89	0.22	62,62,62,62	0
56	MG	2A	3506	1/1	0.89	0.11	38,38,38,38	0
56	MG	2A	3512	1/1	0.89	0.14	53,53,53,53	0
56	MG	1A	3065	1/1	0.89	0.20	61,61,61,61	0
56	MG	1a	1636	1/1	0.89	0.12	66,66,66,66	0
56	MG	2A	3061	1/1	0.89	0.15	51,51,51,51	0
56	MG	2A	3280	1/1	0.89	0.48	59,59,59,59	0
56	MG	2A	3529	1/1	0.89	0.16	35,35,35,35	0
56	MG	2A	3281	1/1	0.89	0.22	34,34,34,34	0
56	MG	1A	3945	1/1	0.89	0.20	35,35,35,35	0
56	MG	1A	3741	1/1	0.89	0.07	58,58,58,58	0
56	MG	1A	4257	1/1	0.90	0.16	41,41,41,41	0
56	MG	2E	307	1/1	0.90	0.07	61,61,61,61	0
56	MG	2F	302	1/1	0.90	0.21	63,63,63,63	0
56	MG	1A	3164	1/1	0.90	0.30	66,66,66,66	0
56	MG	2A	3062	1/1	0.90	0.09	54,54,54,54	0
56	MG	1A	3018	1/1	0.90	0.30	50,50,50,50	0
56	MG	1a	1816	1/1	0.90	0.54	59,59,59,59	0
56	MG	1A	3613	1/1	0.90	0.16	55,55,55,55	0
56	MG	2A	3561	1/1	0.90	0.07	37,37,37,37	0
56	MG	1A	3814	1/1	0.90	0.16	64,64,64,64	0
56	MG	2A	3069	1/1	0.90	0.13	38,38,38,38	0
56	MG	2A	3072	1/1	0.90	0.15	47,47,47,47	0
56	MG	1a	1822	1/1	0.90	0.17	45,45,45,45	0
56	MG	1a	1824	1/1	0.90	0.13	67,67,67,67	0
56	MG	1a	1825	1/1	0.90	0.21	57,57,57,57	0
56	MG	1a	1826	1/1	0.90	0.14	68,68,68,68	0
56	MG	2A	3308	1/1	0.90	0.11	56,56,56,56	0
56	MG	25	104	1/1	0.90	0.17	51,51,51,51	0
56	MG	1a	1650	1/1	0.90	0.22	54,54,54,54	0
56	MG	2A	3603	1/1	0.90	0.06	44,44,44,44	0
56	MG	2A	3310	1/1	0.90	0.20	49,49,49,49	0
56	MG	2A	3609	1/1	0.90	0.20	60,60,60,60	0
56	MG	2A	3610	1/1	0.90	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3345	1/1	0.90	0.28	57,57,57,57	0
56	MG	1A	4105	1/1	0.90	0.15	33,33,33,33	0
56	MG	1A	3685	1/1	0.90	0.20	69,69,69,69	0
56	MG	2A	3622	1/1	0.90	0.15	47,47,47,47	0
56	MG	2A	3627	1/1	0.90	0.23	43,43,43,43	0
56	MG	1B	211	1/1	0.90	0.20	62,62,62,62	0
56	MG	1a	1844	1/1	0.90	0.14	52,52,52,52	0
56	MG	1a	1845	1/1	0.90	0.13	75,75,75,75	0
56	MG	1A	3493	1/1	0.90	0.31	33,33,33,33	0
56	MG	2A	3652	1/1	0.90	0.55	45,45,45,45	0
56	MG	1A	3617	1/1	0.90	0.18	48,48,48,48	0
56	MG	1A	3385	1/1	0.90	0.18	63,63,63,63	0
56	MG	1a	1853	1/1	0.90	0.09	48,48,48,48	0
56	MG	1B	225	1/1	0.90	0.12	42,42,42,42	0
56	MG	2A	3102	1/1	0.90	0.11	55,55,55,55	0
56	MG	2A	3675	1/1	0.90	0.22	42,42,42,42	0
56	MG	1a	1856	1/1	0.90	0.13	38,38,38,38	0
56	MG	1A	3841	1/1	0.90	0.19	42,42,42,42	0
56	MG	1A	3996	1/1	0.90	0.14	48,48,48,48	0
56	MG	1A	3846	1/1	0.90	0.12	47,47,47,47	0
56	MG	1A	3620	1/1	0.90	0.60	59,59,59,59	0
56	MG	2A	3121	1/1	0.90	0.25	53,53,53,53	0
56	MG	1A	3693	1/1	0.90	0.22	57,57,57,57	0
56	MG	1A	3421	1/1	0.90	0.25	46,46,46,46	0
56	MG	1A	3856	1/1	0.90	0.37	56,56,56,56	0
56	MG	2a	3050	1/1	0.90	0.09	69,69,69,69	0
56	MG	1A	3857	1/1	0.90	0.21	29,29,29,29	0
56	MG	2a	3053	1/1	0.90	0.27	82,82,82,82	0
56	MG	2A	3703	1/1	0.90	0.08	64,64,64,64	0
56	MG	1a	1684	1/1	0.90	0.22	55,55,55,55	0
56	MG	1A	3703	1/1	0.90	0.26	47,47,47,47	0
56	MG	1A	3497	1/1	0.90	0.14	59,59,59,59	0
56	MG	1A	4129	1/1	0.90	0.07	56,56,56,56	0
56	MG	1A	3706	1/1	0.90	0.16	23,23,23,23	0
56	MG	1a	1877	1/1	0.90	0.07	72,72,72,72	0
56	MG	1A	3324	1/1	0.90	0.18	62,62,62,62	0
56	MG	1E	312	1/1	0.90	0.11	62,62,62,62	0
56	MG	1A	3499	1/1	0.90	0.20	62,62,62,62	0
56	MG	1A	3387	1/1	0.90	0.41	63,63,63,63	0
56	MG	2A	3365	1/1	0.90	0.18	58,58,58,58	0
56	MG	1a	1885	1/1	0.90	0.12	78,78,78,78	0
56	MG	2a	3074	1/1	0.90	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3562	1/1	0.90	0.15	45,45,45,45	0
56	MG	1A	4019	1/1	0.90	0.11	47,47,47,47	0
56	MG	2A	3740	1/1	0.90	0.18	73,73,73,73	0
56	MG	2A	3371	1/1	0.90	0.15	53,53,53,53	0
56	MG	1A	4021	1/1	0.90	0.14	36,36,36,36	0
56	MG	1A	3723	1/1	0.90	0.16	37,37,37,37	0
56	MG	1A	3233	1/1	0.90	0.27	65,65,65,65	0
56	MG	1A	3884	1/1	0.90	0.23	63,63,63,63	0
56	MG	1A	3567	1/1	0.90	0.18	38,38,38,38	0
56	MG	1A	4040	1/1	0.90	0.12	74,74,74,74	0
56	MG	2a	3093	1/1	0.90	0.14	55,55,55,55	0
56	MG	2A	3186	1/1	0.90	0.29	54,54,54,54	0
56	MG	1A	3502	1/1	0.90	0.19	55,55,55,55	0
56	MG	2A	3762	1/1	0.90	0.16	54,54,54,54	0
56	MG	2a	3104	1/1	0.90	0.18	81,81,81,81	0
56	MG	1A	3427	1/1	0.90	0.19	44,44,44,44	0
56	MG	2A	3766	1/1	0.90	0.16	51,51,51,51	0
56	MG	2A	3191	1/1	0.90	0.27	52,52,52,52	0
56	MG	2a	3110	1/1	0.90	0.36	53,53,53,53	0
56	MG	1N	3003	1/1	0.90	0.17	53,53,53,53	0
56	MG	1A	3893	1/1	0.90	0.15	33,33,33,33	0
56	MG	1A	3898	1/1	0.90	0.13	54,54,54,54	0
56	MG	1A	3465	1/1	0.90	0.46	53,53,53,53	0
56	MG	2a	3117	1/1	0.90	0.15	63,63,63,63	0
56	MG	1A	3737	1/1	0.90	0.13	35,35,35,35	0
56	MG	1A	3466	1/1	0.90	0.25	58,58,58,58	0
56	MG	2A	3782	1/1	0.90	0.10	44,44,44,44	0
56	MG	1A	3429	1/1	0.90	0.35	48,48,48,48	0
56	MG	1A	3094	1/1	0.90	0.09	52,52,52,52	0
56	MG	1Q	205	1/1	0.90	0.16	41,41,41,41	0
56	MG	1A	3202	1/1	0.90	0.15	46,46,46,46	0
56	MG	1f	3001	1/1	0.90	0.15	44,44,44,44	0
56	MG	1f	3002	1/1	0.90	0.27	61,61,61,61	0
56	MG	1T	202	1/1	0.90	0.50	59,59,59,59	0
56	MG	1A	3471	1/1	0.90	0.50	65,65,65,65	0
56	MG	2A	3801	1/1	0.90	0.14	59,59,59,59	0
56	MG	1A	3766	1/1	0.90	0.26	26,26,26,26	0
56	MG	1a	1747	1/1	0.90	0.07	60,60,60,60	0
56	MG	1A	4169	1/1	0.90	0.13	77,77,77,77	0
56	MG	1A	3585	1/1	0.90	0.28	49,49,49,49	0
56	MG	2A	3215	1/1	0.90	0.20	61,61,61,61	0
56	MG	2A	3811	1/1	0.90	0.11	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3216	1/1	0.90	0.24	54,54,54,54	0
56	MG	1A	4172	1/1	0.90	0.18	46,46,46,46	0
56	MG	1A	4174	1/1	0.90	0.12	83,83,83,83	0
56	MG	2A	3219	1/1	0.90	0.26	56,56,56,56	0
56	MG	2A	3425	1/1	0.90	0.41	73,73,73,73	0
56	MG	2A	3220	1/1	0.90	0.21	46,46,46,46	0
56	MG	1A	3396	1/1	0.90	0.42	43,43,43,43	0
56	MG	2A	3822	1/1	0.90	0.06	78,78,78,78	0
56	MG	1A	3278	1/1	0.90	0.22	55,55,55,55	0
56	MG	1A	4071	1/1	0.90	0.20	71,71,71,71	0
56	MG	2A	3433	1/1	0.90	0.19	46,46,46,46	0
56	MG	1A	3588	1/1	0.90	0.13	50,50,50,50	0
56	MG	1A	3782	1/1	0.90	0.24	26,26,26,26	0
56	MG	1A	4076	1/1	0.90	0.19	30,30,30,30	0
56	MG	1x	109	1/1	0.90	0.30	74,74,74,74	0
56	MG	2A	3840	1/1	0.90	0.10	49,49,49,49	0
56	MG	2A	3448	1/1	0.90	0.33	61,61,61,61	0
56	MG	12	3002	1/1	0.90	0.42	48,48,48,48	0
56	MG	2A	3450	1/1	0.90	0.18	56,56,56,56	0
56	MG	2A	3235	1/1	0.90	0.21	52,52,52,52	0
56	MG	2A	3237	1/1	0.90	0.22	48,48,48,48	0
56	MG	2A	3455	1/1	0.90	0.29	44,44,44,44	0
56	MG	1A	3115	1/1	0.90	0.25	44,44,44,44	0
56	MG	2a	3189	1/1	0.90	0.12	54,54,54,54	0
56	MG	1A	4079	1/1	0.90	0.17	36,36,36,36	0
56	MG	1a	1767	1/1	0.90	0.16	51,51,51,51	0
56	MG	1A	3257	1/1	0.90	0.26	49,49,49,49	0
56	MG	1A	4204	1/1	0.90	0.23	50,50,50,50	0
56	MG	2A	3469	1/1	0.90	0.41	61,61,61,61	0
56	MG	1A	3181	1/1	0.90	0.23	53,53,53,53	0
56	MG	2a	3201	1/1	0.90	0.06	70,70,70,70	0
56	MG	1a	1603	1/1	0.90	0.18	87,87,87,87	0
56	MG	2a	3208	1/1	0.90	0.17	70,70,70,70	0
56	MG	2a	3209	1/1	0.90	0.12	61,61,61,61	0
56	MG	2a	3212	1/1	0.90	0.12	71,71,71,71	0
56	MG	2A	3474	1/1	0.90	0.36	53,53,53,53	0
56	MG	1A	3056	1/1	0.90	0.21	50,50,50,50	0
56	MG	1A	3339	1/1	0.90	0.15	53,53,53,53	0
56	MG	1A	4211	1/1	0.90	0.23	61,61,61,61	0
56	MG	2A	3877	1/1	0.90	0.07	71,71,71,71	0
56	MG	2A	3481	1/1	0.90	0.16	55,55,55,55	0
56	MG	2A	3004	1/1	0.90	0.38	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4218	1/1	0.90	0.17	36,36,36,36	0
56	MG	1A	4219	1/1	0.90	0.20	41,41,41,41	0
56	MG	2A	3019	1/1	0.90	0.14	40,40,40,40	0
56	MG	1A	3016	1/1	0.90	0.15	50,50,50,50	0
56	MG	1A	4221	1/1	0.90	0.23	35,35,35,35	0
56	MG	1A	4086	1/1	0.90	0.33	57,57,57,57	0
56	MG	1a	1619	1/1	0.90	0.08	55,55,55,55	0
56	MG	2A	3899	1/1	0.90	0.38	61,61,61,61	0
56	MG	2A	3268	1/1	0.90	0.13	59,59,59,59	0
56	MG	1A	3603	1/1	0.90	0.14	51,51,51,51	0
56	MG	2q	204	1/1	0.90	0.10	68,68,68,68	0
56	MG	2r	3001	1/1	0.90	0.27	75,75,75,75	0
56	MG	2A	3908	1/1	0.90	0.23	43,43,43,43	0
56	MG	1A	3961	1/1	0.90	0.52	60,60,60,60	0
56	MG	2A	3273	1/1	0.90	0.17	58,58,58,58	0
56	MG	1a	1627	1/1	0.90	0.09	46,46,46,46	0
56	MG	2w	102	1/1	0.90	0.28	60,60,60,60	0
56	MG	2A	3921	1/1	0.90	0.28	65,65,65,65	0
56	MG	1a	1629	1/1	0.90	0.10	43,43,43,43	0
56	MG	2w	106	1/1	0.90	0.10	71,71,71,71	0
56	MG	2A	3530	1/1	0.90	0.11	45,45,45,45	0
56	MG	2x	101	1/1	0.90	0.10	48,48,48,48	0
56	MG	2B	3004	1/1	0.90	0.08	79,79,79,79	0
56	MG	2A	3536	1/1	0.90	0.12	60,60,60,60	0
56	MG	1a	1630	1/1	0.90	0.16	57,57,57,57	0
56	MG	1A	4244	1/1	0.90	0.15	39,39,39,39	0
56	MG	1A	3408	1/1	0.90	0.30	48,48,48,48	0
56	MG	2A	3282	1/1	0.90	0.34	64,64,64,64	0
56	MG	2A	3283	1/1	0.90	0.09	53,53,53,53	0
59	ZN	2Y	501	1/1	0.90	0.07	101,101,101,101	0
56	MG	1A	3803	1/1	0.90	0.27	48,48,48,48	0
56	MG	1a	1865	1/1	0.91	0.11	51,51,51,51	0
56	MG	2A	3319	1/1	0.91	0.39	57,57,57,57	0
56	MG	1A	3906	1/1	0.91	0.11	55,55,55,55	0
56	MG	2A	3322	1/1	0.91	0.11	58,58,58,58	0
56	MG	2A	3616	1/1	0.91	0.26	31,31,31,31	0
56	MG	2A	3323	1/1	0.91	0.10	48,48,48,48	0
56	MG	1A	4163	1/1	0.91	0.13	70,70,70,70	0
56	MG	2A	3325	1/1	0.91	0.58	47,47,47,47	0
56	MG	1a	1706	1/1	0.91	0.12	54,54,54,54	0
56	MG	1a	1869	1/1	0.91	0.34	101,101,101,101	0
56	MG	2A	3108	1/1	0.91	0.20	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4164	1/1	0.91	0.11	55,55,55,55	0
56	MG	1A	3490	1/1	0.91	0.16	50,50,50,50	0
56	MG	2a	3005	1/1	0.91	0.18	54,54,54,54	0
56	MG	1A	3390	1/1	0.91	0.41	55,55,55,55	0
56	MG	2A	3118	1/1	0.91	0.17	52,52,52,52	0
56	MG	1A	3440	1/1	0.91	0.38	38,38,38,38	0
56	MG	2A	3659	1/1	0.91	0.08	45,45,45,45	0
56	MG	2A	3123	1/1	0.91	0.21	50,50,50,50	0
56	MG	2a	3016	1/1	0.91	0.16	55,55,55,55	0
56	MG	1A	4064	1/1	0.91	0.16	39,39,39,39	0
56	MG	2A	3670	1/1	0.91	0.18	42,42,42,42	0
56	MG	2a	3019	1/1	0.91	0.16	48,48,48,48	0
56	MG	1A	3391	1/1	0.91	0.50	71,71,71,71	0
56	MG	2a	3021	1/1	0.91	0.12	72,72,72,72	0
56	MG	1A	3570	1/1	0.91	0.23	54,54,54,54	0
56	MG	1A	4067	1/1	0.91	0.06	53,53,53,53	0
56	MG	1A	3109	1/1	0.91	0.16	50,50,50,50	0
56	MG	2A	3348	1/1	0.91	0.14	55,55,55,55	0
56	MG	2A	3134	1/1	0.91	0.10	39,39,39,39	0
56	MG	2A	3135	1/1	0.91	0.54	51,51,51,51	0
56	MG	1R	201	1/1	0.91	0.18	54,54,54,54	0
56	MG	2a	3030	1/1	0.91	0.14	52,52,52,52	0
56	MG	1a	1720	1/1	0.91	0.20	62,62,62,62	0
56	MG	1a	1883	1/1	0.91	0.15	47,47,47,47	0
56	MG	1A	3777	1/1	0.91	0.17	33,33,33,33	0
56	MG	1A	3004	1/1	0.91	0.26	35,35,35,35	0
56	MG	2A	3697	1/1	0.91	0.05	42,42,42,42	0
56	MG	1a	1889	1/1	0.91	0.08	77,77,77,77	0
56	MG	1U	201	1/1	0.91	0.45	53,53,53,53	0
56	MG	1A	3779	1/1	0.91	0.22	31,31,31,31	0
56	MG	1A	4075	1/1	0.91	0.19	21,21,21,21	0
56	MG	2A	3162	1/1	0.91	0.15	56,56,56,56	0
56	MG	1a	1896	1/1	0.91	0.07	77,77,77,77	0
56	MG	2A	3168	1/1	0.91	0.19	50,50,50,50	0
56	MG	1X	102	1/1	0.91	0.23	45,45,45,45	0
56	MG	1A	4194	1/1	0.91	0.20	55,55,55,55	0
56	MG	1a	1730	1/1	0.91	0.11	57,57,57,57	0
56	MG	2A	3174	1/1	0.91	0.11	66,66,66,66	0
56	MG	1A	3148	1/1	0.91	0.39	40,40,40,40	0
56	MG	1A	3937	1/1	0.91	0.33	56,56,56,56	0
56	MG	2A	3178	1/1	0.91	0.31	49,49,49,49	0
56	MG	2A	3378	1/1	0.91	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1739	1/1	0.91	0.11	49,49,49,49	0
56	MG	1A	3184	1/1	0.91	0.10	61,61,61,61	0
56	MG	2a	3063	1/1	0.91	0.30	64,64,64,64	0
56	MG	2A	3743	1/1	0.91	0.10	79,79,79,79	0
56	MG	2a	3065	1/1	0.91	0.45	47,47,47,47	0
56	MG	1A	3275	1/1	0.91	0.59	45,45,45,45	0
56	MG	1a	1912	1/1	0.91	0.15	69,69,69,69	0
56	MG	1a	1913	1/1	0.91	0.09	80,80,80,80	0
56	MG	2a	3071	1/1	0.91	0.09	71,71,71,71	0
56	MG	2a	3072	1/1	0.91	0.17	49,49,49,49	0
56	MG	1A	3651	1/1	0.91	0.12	47,47,47,47	0
56	MG	2A	3754	1/1	0.91	0.12	71,71,71,71	0
56	MG	1A	3276	1/1	0.91	0.19	55,55,55,55	0
56	MG	2a	3076	1/1	0.91	0.10	64,64,64,64	0
56	MG	1a	1746	1/1	0.91	0.07	66,66,66,66	0
56	MG	1A	4206	1/1	0.91	0.42	45,45,45,45	0
56	MG	2A	3389	1/1	0.91	0.22	52,52,52,52	0
56	MG	2A	3760	1/1	0.91	0.18	64,64,64,64	0
56	MG	1A	3795	1/1	0.91	0.14	43,43,43,43	0
56	MG	1A	3400	1/1	0.91	0.17	56,56,56,56	0
56	MG	2A	3764	1/1	0.91	0.11	51,51,51,51	0
56	MG	1A	3218	1/1	0.91	0.44	55,55,55,55	0
56	MG	1a	1928	1/1	0.91	0.12	57,57,57,57	0
56	MG	2A	3401	1/1	0.91	0.17	50,50,50,50	0
56	MG	2a	3096	1/1	0.91	0.06	70,70,70,70	0
56	MG	1A	4215	1/1	0.91	0.48	73,73,73,73	0
56	MG	1A	3503	1/1	0.91	0.36	56,56,56,56	0
56	MG	1A	3279	1/1	0.91	0.21	40,40,40,40	0
56	MG	1A	3966	1/1	0.91	0.81	45,45,45,45	0
56	MG	2A	3774	1/1	0.91	0.07	57,57,57,57	0
56	MG	18	103	1/1	0.91	0.45	57,57,57,57	0
56	MG	19	101	1/1	0.91	0.11	49,49,49,49	0
56	MG	1A	3505	1/1	0.91	0.40	44,44,44,44	0
56	MG	2A	3209	1/1	0.91	0.12	61,61,61,61	0
56	MG	1A	3329	1/1	0.91	0.19	54,54,54,54	0
56	MG	1A	3404	1/1	0.91	0.56	69,69,69,69	0
56	MG	1A	4234	1/1	0.91	0.69	46,46,46,46	0
56	MG	2A	3795	1/1	0.91	0.23	63,63,63,63	0
56	MG	1A	3807	1/1	0.91	0.14	44,44,44,44	0
56	MG	1a	1771	1/1	0.91	0.26	51,51,51,51	0
56	MG	1a	1773	1/1	0.91	0.15	53,53,53,53	0
56	MG	1A	4243	1/1	0.91	0.59	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3282	1/1	0.91	0.61	51,51,51,51	0
56	MG	2A	3802	1/1	0.91	0.18	43,43,43,43	0
56	MG	1a	1777	1/1	0.91	0.38	51,51,51,51	0
56	MG	1A	3051	1/1	0.91	0.30	43,43,43,43	0
56	MG	1a	1614	1/1	0.91	0.19	63,63,63,63	0
56	MG	1A	3044	1/1	0.91	0.45	48,48,48,48	0
56	MG	1A	4106	1/1	0.91	0.15	28,28,28,28	0
56	MG	1a	1783	1/1	0.91	0.06	88,88,88,88	0
56	MG	1x	114	1/1	0.91	0.20	59,59,59,59	0
56	MG	1A	3516	1/1	0.91	0.14	48,48,48,48	0
56	MG	1A	3291	1/1	0.91	0.14	49,49,49,49	0
56	MG	1a	1789	1/1	0.91	0.20	69,69,69,69	0
56	MG	1a	1791	1/1	0.91	0.29	71,71,71,71	0
56	MG	1a	1621	1/1	0.91	0.25	59,59,59,59	0
56	MG	1y	3004	1/1	0.91	0.26	78,78,78,78	0
56	MG	2A	3821	1/1	0.91	0.09	76,76,76,76	0
56	MG	1A	3411	1/1	0.91	0.22	58,58,58,58	0
56	MG	1A	3831	1/1	0.91	0.11	46,46,46,46	0
56	MG	1A	3834	1/1	0.91	0.25	28,28,28,28	0
56	MG	1A	3117	1/1	0.91	0.36	46,46,46,46	0
56	MG	1A	3190	1/1	0.91	0.30	40,40,40,40	0
56	MG	1A	3998	1/1	0.91	0.42	48,48,48,48	0
56	MG	2A	3461	1/1	0.91	0.33	47,47,47,47	0
56	MG	2A	3463	1/1	0.91	0.18	59,59,59,59	0
56	MG	2A	3018	1/1	0.91	0.17	56,56,56,56	0
56	MG	1A	3609	1/1	0.91	0.16	50,50,50,50	0
56	MG	1A	3610	1/1	0.91	0.29	61,61,61,61	0
56	MG	2A	3025	1/1	0.91	1.40	55,55,55,55	0
56	MG	1A	3155	1/1	0.91	0.32	47,47,47,47	0
56	MG	1a	1642	1/1	0.91	0.18	51,51,51,51	0
56	MG	1A	3418	1/1	0.91	0.25	49,49,49,49	0
56	MG	2A	3032	1/1	0.91	0.20	57,57,57,57	0
56	MG	2a	3175	1/1	0.91	0.09	58,58,58,58	0
56	MG	2a	3176	1/1	0.91	0.09	74,74,74,74	0
56	MG	1A	3854	1/1	0.91	0.15	49,49,49,49	0
56	MG	2A	3036	1/1	0.91	0.14	50,50,50,50	0
56	MG	2A	3862	1/1	0.91	0.08	62,62,62,62	0
56	MG	2a	3183	1/1	0.91	0.21	39,39,39,39	0
56	MG	2a	3185	1/1	0.91	0.13	87,87,87,87	0
56	MG	2A	3486	1/1	0.91	0.47	46,46,46,46	0
56	MG	1a	1648	1/1	0.91	0.08	53,53,53,53	0
56	MG	1A	3159	1/1	0.91	0.36	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3047	1/1	0.91	0.10	44,44,44,44	0
56	MG	1A	3473	1/1	0.91	0.15	59,59,59,59	0
56	MG	2a	3193	1/1	0.91	0.22	63,63,63,63	0
56	MG	2A	3869	1/1	0.91	0.07	54,54,54,54	0
56	MG	2A	3053	1/1	0.91	0.10	55,55,55,55	0
56	MG	2A	3502	1/1	0.91	0.10	54,54,54,54	0
56	MG	1a	1815	1/1	0.91	0.17	57,57,57,57	0
56	MG	1A	4130	1/1	0.91	0.10	49,49,49,49	0
56	MG	2A	3507	1/1	0.91	0.12	49,49,49,49	0
56	MG	2a	3206	1/1	0.91	0.10	58,58,58,58	0
56	MG	1A	3536	1/1	0.91	0.26	56,56,56,56	0
56	MG	1A	3859	1/1	0.91	0.18	37,37,37,37	0
56	MG	1a	1821	1/1	0.91	0.15	66,66,66,66	0
56	MG	2a	3213	1/1	0.91	0.20	60,60,60,60	0
56	MG	1A	3198	1/1	0.91	0.15	67,67,67,67	0
56	MG	2A	3522	1/1	0.91	0.07	63,63,63,63	0
56	MG	1A	3300	1/1	0.91	0.28	52,52,52,52	0
56	MG	1A	3479	1/1	0.91	0.32	57,57,57,57	0
56	MG	1A	3722	1/1	0.91	0.16	21,21,21,21	0
56	MG	2A	3285	1/1	0.91	0.32	55,55,55,55	0
56	MG	2A	3286	1/1	0.91	0.28	52,52,52,52	0
56	MG	2a	3227	1/1	0.91	0.15	68,68,68,68	0
56	MG	1A	3870	1/1	0.91	0.23	35,35,35,35	0
56	MG	2a	3231	1/1	0.91	0.07	77,77,77,77	0
56	MG	2A	3901	1/1	0.91	0.20	77,77,77,77	0
56	MG	2A	3067	1/1	0.91	0.37	56,56,56,56	0
56	MG	1A	3344	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3910	1/1	0.91	0.65	58,58,58,58	0
56	MG	2A	3911	1/1	0.91	0.19	43,43,43,43	0
56	MG	2A	3291	1/1	0.91	0.12	61,61,61,61	0
56	MG	1E	308	1/1	0.91	0.19	34,34,34,34	0
56	MG	1A	3627	1/1	0.91	0.26	55,55,55,55	0
56	MG	1A	3878	1/1	0.91	0.05	63,63,63,63	0
56	MG	2q	202	1/1	0.91	0.28	74,74,74,74	0
56	MG	1A	3481	1/1	0.91	0.35	52,52,52,52	0
56	MG	1A	3258	1/1	0.91	0.11	53,53,53,53	0
56	MG	1a	1846	1/1	0.91	0.26	56,56,56,56	0
56	MG	2A	3081	1/1	0.91	0.29	51,51,51,51	0
56	MG	2v	104	1/1	0.91	0.13	61,61,61,61	0
56	MG	1A	3259	1/1	0.91	0.23	61,61,61,61	0
56	MG	2A	3567	1/1	0.91	0.16	33,33,33,33	0
56	MG	2A	3569	1/1	0.91	0.13	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3105	1/1	0.91	0.12	31,31,31,31	0
56	MG	2D	301	1/1	0.91	0.27	51,51,51,51	0
56	MG	2w	105	1/1	0.91	0.32	71,71,71,71	0
56	MG	2A	3573	1/1	0.91	0.17	49,49,49,49	0
56	MG	2A	3574	1/1	0.91	0.13	32,32,32,32	0
56	MG	1A	3232	1/1	0.91	0.40	55,55,55,55	0
56	MG	1a	1687	1/1	0.91	0.20	73,73,73,73	0
56	MG	1A	3739	1/1	0.91	0.16	30,30,30,30	0
56	MG	2x	104	1/1	0.91	0.26	58,58,58,58	0
56	MG	1A	3088	1/1	0.91	0.30	54,54,54,54	0
56	MG	2x	106	1/1	0.91	0.23	57,57,57,57	0
56	MG	1A	3170	1/1	0.91	0.22	47,47,47,47	0
56	MG	1A	3751	1/1	0.91	0.14	40,40,40,40	0
56	MG	2y	3004	1/1	0.91	0.18	69,69,69,69	0
56	MG	2y	3005	1/1	0.91	0.13	79,79,79,79	0
56	MG	1A	3559	1/1	0.91	0.50	35,35,35,35	0
57	CPT	1A	4210	4/5	0.91	0.10	77,103,121,207	0
56	MG	2U	201	1/1	0.91	0.28	56,56,56,56	0
56	MG	1H	201	1/1	0.91	0.10	46,46,46,46	0
59	ZN	24	501	1/1	0.91	0.04	114,114,114,114	0
56	MG	2A	3599	1/1	0.91	0.22	55,55,55,55	0
56	MG	2a	3014	1/1	0.92	0.21	70,70,70,70	0
56	MG	1A	3543	1/1	0.92	0.20	71,71,71,71	0
56	MG	1a	1827	1/1	0.92	0.10	66,66,66,66	0
56	MG	1A	3781	1/1	0.92	0.20	26,26,26,26	0
56	MG	2A	3715	1/1	0.92	0.15	57,57,57,57	0
56	MG	1A	3326	1/1	0.92	0.14	53,53,53,53	0
56	MG	2A	3031	1/1	0.92	0.15	46,46,46,46	0
56	MG	1A	3900	1/1	0.92	0.08	64,64,64,64	0
56	MG	2A	3413	1/1	0.92	0.28	61,61,61,61	0
56	MG	1A	3903	1/1	0.92	0.09	51,51,51,51	0
56	MG	1A	3355	1/1	0.92	0.22	60,60,60,60	0
56	MG	2A	3239	1/1	0.92	0.82	54,54,54,54	0
56	MG	1a	1692	1/1	0.92	0.10	55,55,55,55	0
56	MG	2A	3730	1/1	0.92	0.14	40,40,40,40	0
56	MG	2A	3419	1/1	0.92	0.10	46,46,46,46	0
56	MG	1A	3785	1/1	0.92	0.23	33,33,33,33	0
56	MG	2A	3735	1/1	0.92	0.09	49,49,49,49	0
56	MG	2A	3421	1/1	0.92	0.23	60,60,60,60	0
56	MG	2a	3035	1/1	0.92	0.13	81,81,81,81	0
56	MG	2A	3045	1/1	0.92	0.09	48,48,48,48	0
56	MG	1A	3214	1/1	0.92	0.24	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1847	1/1	0.92	0.13	51,51,51,51	0
56	MG	1a	1848	1/1	0.92	0.29	44,44,44,44	0
56	MG	1a	1695	1/1	0.92	0.20	65,65,65,65	0
56	MG	2A	3751	1/1	0.92	0.15	46,46,46,46	0
56	MG	1A	3912	1/1	0.92	0.14	44,44,44,44	0
56	MG	2A	3249	1/1	0.92	0.34	64,64,64,64	0
56	MG	1A	4052	1/1	0.92	0.10	67,67,67,67	0
56	MG	1A	3552	1/1	0.92	0.21	34,34,34,34	0
56	MG	1A	3792	1/1	0.92	0.18	30,30,30,30	0
56	MG	2A	3758	1/1	0.92	0.17	53,53,53,53	0
56	MG	2A	3439	1/1	0.92	0.26	38,38,38,38	0
56	MG	2A	3257	1/1	0.92	0.28	70,70,70,70	0
56	MG	2A	3445	1/1	0.92	0.15	52,52,52,52	0
56	MG	1A	3416	1/1	0.92	0.24	65,65,65,65	0
56	MG	1A	3240	1/1	0.92	0.29	39,39,39,39	0
56	MG	2A	3063	1/1	0.92	0.14	46,46,46,46	0
56	MG	1A	3074	1/1	0.92	0.11	35,35,35,35	0
56	MG	2a	3062	1/1	0.92	0.20	85,85,85,85	0
56	MG	1A	4062	1/1	0.92	0.08	76,76,76,76	0
56	MG	1A	3420	1/1	0.92	0.31	50,50,50,50	0
56	MG	1A	4177	1/1	0.92	0.12	36,36,36,36	0
56	MG	1A	3929	1/1	0.92	0.16	62,62,62,62	0
56	MG	1T	201	1/1	0.92	0.14	57,57,57,57	0
56	MG	1A	3558	1/1	0.92	0.18	48,48,48,48	0
56	MG	1A	3217	1/1	0.92	0.34	59,59,59,59	0
56	MG	2A	3459	1/1	0.92	0.30	46,46,46,46	0
56	MG	2A	3781	1/1	0.92	0.10	47,47,47,47	0
56	MG	1a	1870	1/1	0.92	0.35	81,81,81,81	0
56	MG	1A	3933	1/1	0.92	0.14	81,81,81,81	0
56	MG	2A	3784	1/1	0.92	0.23	48,48,48,48	0
56	MG	1A	4188	1/1	0.92	0.18	37,37,37,37	0
56	MG	2A	3790	1/1	0.92	0.19	61,61,61,61	0
56	MG	2A	3465	1/1	0.92	0.22	52,52,52,52	0
56	MG	1A	3245	1/1	0.92	0.16	60,60,60,60	0
56	MG	1A	3334	1/1	0.92	0.32	54,54,54,54	0
56	MG	1A	3625	1/1	0.92	0.27	66,66,66,66	0
56	MG	1A	3943	1/1	0.92	0.10	68,68,68,68	0
56	MG	1A	3944	1/1	0.92	0.09	69,69,69,69	0
56	MG	2A	3799	1/1	0.92	0.06	58,58,58,58	0
56	MG	2a	3091	1/1	0.92	0.12	62,62,62,62	0
56	MG	1A	3699	1/1	0.92	0.18	24,24,24,24	0
56	MG	1A	4202	1/1	0.92	0.20	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4077	1/1	0.92	0.24	26,26,26,26	0
56	MG	1A	3946	1/1	0.92	0.16	34,34,34,34	0
56	MG	1a	1882	1/1	0.92	0.15	52,52,52,52	0
56	MG	2A	3484	1/1	0.92	0.13	57,57,57,57	0
56	MG	1A	3811	1/1	0.92	0.14	45,45,45,45	0
56	MG	1A	3950	1/1	0.92	0.15	68,68,68,68	0
56	MG	2a	3108	1/1	0.92	0.05	57,57,57,57	0
56	MG	1A	3424	1/1	0.92	0.21	75,75,75,75	0
56	MG	13	101	1/1	0.92	0.32	50,50,50,50	0
56	MG	13	102	1/1	0.92	0.17	46,46,46,46	0
56	MG	1A	3955	1/1	0.92	0.26	37,37,37,37	0
56	MG	1A	4213	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	3160	1/1	0.92	0.64	49,49,49,49	0
56	MG	2A	3505	1/1	0.92	0.20	58,58,58,58	0
56	MG	17	103	1/1	0.92	0.18	48,48,48,48	0
56	MG	1A	3568	1/1	0.92	0.14	46,46,46,46	0
56	MG	2A	3509	1/1	0.92	0.16	55,55,55,55	0
56	MG	1A	3143	1/1	0.92	0.13	44,44,44,44	0
56	MG	1A	3428	1/1	0.92	0.21	46,46,46,46	0
56	MG	2A	3122	1/1	0.92	0.19	47,47,47,47	0
56	MG	2A	3827	1/1	0.92	0.20	64,64,64,64	0
56	MG	2A	3828	1/1	0.92	0.09	64,64,64,64	0
56	MG	2A	3519	1/1	0.92	0.24	57,57,57,57	0
56	MG	2A	3520	1/1	0.92	0.18	55,55,55,55	0
56	MG	1A	3829	1/1	0.92	0.08	54,54,54,54	0
56	MG	1A	3717	1/1	0.92	0.17	49,49,49,49	0
56	MG	1A	4227	1/1	0.92	0.37	38,38,38,38	0
56	MG	1A	3036	1/1	0.92	0.32	43,43,43,43	0
56	MG	1a	1758	1/1	0.92	0.18	49,49,49,49	0
56	MG	2A	3843	1/1	0.92	0.13	27,27,27,27	0
56	MG	2A	3533	1/1	0.92	0.09	44,44,44,44	0
56	MG	2A	3851	1/1	0.92	0.09	51,51,51,51	0
56	MG	1A	3968	1/1	0.92	0.08	63,63,63,63	0
56	MG	2A	3133	1/1	0.92	0.16	63,63,63,63	0
56	MG	1A	3395	1/1	0.92	0.89	46,46,46,46	0
56	MG	2A	3543	1/1	0.92	0.14	56,56,56,56	0
56	MG	2a	3150	1/1	0.92	0.09	61,61,61,61	0
56	MG	2a	3151	1/1	0.92	0.09	74,74,74,74	0
56	MG	2A	3544	1/1	0.92	0.10	41,41,41,41	0
56	MG	1A	3063	1/1	0.92	0.29	51,51,51,51	0
56	MG	1a	1765	1/1	0.92	0.34	53,53,53,53	0
56	MG	1A	3838	1/1	0.92	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3158	1/1	0.92	0.09	47,47,47,47	0
56	MG	2A	3145	1/1	0.92	0.29	49,49,49,49	0
56	MG	1A	4103	1/1	0.92	0.15	26,26,26,26	0
56	MG	1a	1920	1/1	0.92	0.25	59,59,59,59	0
56	MG	1A	3199	1/1	0.92	0.74	56,56,56,56	0
56	MG	1a	1926	1/1	0.92	0.16	55,55,55,55	0
56	MG	1A	3844	1/1	0.92	0.15	40,40,40,40	0
56	MG	2A	3558	1/1	0.92	0.14	38,38,38,38	0
56	MG	2A	3873	1/1	0.92	0.23	57,57,57,57	0
56	MG	2A	3559	1/1	0.92	0.20	38,38,38,38	0
56	MG	1A	3579	1/1	0.92	0.13	45,45,45,45	0
56	MG	1a	1929	1/1	0.92	0.08	57,57,57,57	0
56	MG	2A	3338	1/1	0.92	1.03	64,64,64,64	0
56	MG	1a	1931	1/1	0.92	0.10	49,49,49,49	0
56	MG	2A	3881	1/1	0.92	0.14	71,71,71,71	0
56	MG	1A	3847	1/1	0.92	0.11	60,60,60,60	0
56	MG	1A	3983	1/1	0.92	0.20	73,73,73,73	0
56	MG	1a	1622	1/1	0.92	0.18	55,55,55,55	0
56	MG	1A	3341	1/1	0.92	0.21	46,46,46,46	0
56	MG	1A	3200	1/1	0.92	0.21	49,49,49,49	0
56	MG	1A	3851	1/1	0.92	0.19	45,45,45,45	0
56	MG	2A	3896	1/1	0.92	0.39	53,53,53,53	0
56	MG	2A	3347	1/1	0.92	0.15	51,51,51,51	0
56	MG	1A	3993	1/1	0.92	0.28	55,55,55,55	0
56	MG	2A	3586	1/1	0.92	0.17	60,60,60,60	0
56	MG	2A	3587	1/1	0.92	0.16	46,46,46,46	0
56	MG	1A	3019	1/1	0.92	0.20	45,45,45,45	0
56	MG	2A	3906	1/1	0.92	0.18	64,64,64,64	0
56	MG	1a	1785	1/1	0.92	0.07	71,71,71,71	0
56	MG	2a	3202	1/1	0.92	0.12	65,65,65,65	0
56	MG	1A	3731	1/1	0.92	0.19	57,57,57,57	0
56	MG	2A	3595	1/1	0.92	0.23	56,56,56,56	0
56	MG	2A	3912	1/1	0.92	0.09	41,41,41,41	0
56	MG	1w	106	1/1	0.92	0.10	63,63,63,63	0
56	MG	2A	3602	1/1	0.92	0.12	52,52,52,52	0
56	MG	2A	3182	1/1	0.92	0.14	62,62,62,62	0
56	MG	1a	1635	1/1	0.92	0.33	62,62,62,62	0
56	MG	1A	3732	1/1	0.92	0.16	35,35,35,35	0
56	MG	1w	110	1/1	0.92	0.16	78,78,78,78	0
56	MG	1B	222	1/1	0.92	0.14	59,59,59,59	0
56	MG	1x	101	1/1	0.92	0.25	45,45,45,45	0
56	MG	1A	4120	1/1	0.92	0.12	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3482	1/1	0.92	0.10	53,53,53,53	0
56	MG	2B	3016	1/1	0.92	0.15	63,63,63,63	0
56	MG	1A	3319	1/1	0.92	0.33	58,58,58,58	0
56	MG	2A	3626	1/1	0.92	0.29	48,48,48,48	0
56	MG	1A	4003	1/1	0.92	0.17	57,57,57,57	0
56	MG	2a	3236	1/1	0.92	0.10	65,65,65,65	0
56	MG	2D	302	1/1	0.92	0.13	27,27,27,27	0
56	MG	1A	3083	1/1	0.92	0.14	41,41,41,41	0
56	MG	2A	3640	1/1	0.92	0.25	45,45,45,45	0
56	MG	1A	4126	1/1	0.92	0.16	67,67,67,67	0
56	MG	1A	3134	1/1	0.92	0.16	45,45,45,45	0
56	MG	1A	3589	1/1	0.92	0.26	53,53,53,53	0
56	MG	2A	3651	1/1	0.92	0.07	61,61,61,61	0
56	MG	2G	3001	1/1	0.92	0.21	46,46,46,46	0
56	MG	1A	3746	1/1	0.92	0.10	51,51,51,51	0
56	MG	2Q	3001	1/1	0.92	0.08	59,59,59,59	0
56	MG	1a	1808	1/1	0.92	0.28	61,61,61,61	0
56	MG	1A	3135	1/1	0.92	0.29	39,39,39,39	0
56	MG	1A	3593	1/1	0.92	0.13	50,50,50,50	0
56	MG	1A	3376	1/1	0.92	0.15	48,48,48,48	0
56	MG	1A	3652	1/1	0.92	0.16	52,52,52,52	0
56	MG	1A	3596	1/1	0.92	0.22	44,44,44,44	0
56	MG	1A	3767	1/1	0.92	0.15	24,24,24,24	0
56	MG	2A	3674	1/1	0.92	0.16	49,49,49,49	0
56	MG	1A	3447	1/1	0.92	0.42	58,58,58,58	0
56	MG	1A	4018	1/1	0.92	0.13	45,45,45,45	0
56	MG	1A	3156	1/1	0.92	0.97	47,47,47,47	0
56	MG	23	3002	1/1	0.92	0.19	53,53,53,53	0
56	MG	23	3003	1/1	0.92	0.21	48,48,48,48	0
56	MG	2A	3681	1/1	0.92	0.20	66,66,66,66	0
56	MG	1A	3449	1/1	0.92	0.15	52,52,52,52	0
56	MG	2A	3008	1/1	0.92	0.15	41,41,41,41	0
56	MG	1a	1675	1/1	0.92	0.17	53,53,53,53	0
56	MG	2A	3392	1/1	0.92	0.18	72,72,72,72	0
56	MG	2a	3002	1/1	0.92	0.42	72,72,72,72	0
56	MG	1A	3158	1/1	0.92	0.14	47,47,47,47	0
56	MG	2A	3689	1/1	0.92	0.17	53,53,53,53	0
56	MG	1A	3673	1/1	0.92	0.11	50,50,50,50	0
56	MG	2A	3022	1/1	0.92	0.17	37,37,37,37	0
56	MG	2A	3023	1/1	0.92	0.14	57,57,57,57	0
56	MG	1A	4035	1/1	0.92	0.16	39,39,39,39	0
58	K	1A	4256	1/1	0.92	0.18	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3009	1/1	0.92	0.13	72,72,72,72	0
56	MG	2A	3224	1/1	0.92	0.21	55,55,55,55	0
56	MG	2A	3705	1/1	0.92	0.22	58,58,58,58	0
56	MG	1A	3887	1/1	0.93	0.21	29,29,29,29	0
56	MG	2a	3033	1/1	0.93	0.10	55,55,55,55	0
56	MG	2A	3070	1/1	0.93	0.16	34,34,34,34	0
56	MG	1a	1717	1/1	0.93	0.10	63,63,63,63	0
56	MG	2A	3269	1/1	0.93	0.20	50,50,50,50	0
56	MG	1X	101	1/1	0.93	0.15	38,38,38,38	0
56	MG	1A	3075	1/1	0.93	0.15	32,32,32,32	0
56	MG	1A	4101	1/1	0.93	0.07	61,61,61,61	0
56	MG	1A	4102	1/1	0.93	0.12	32,32,32,32	0
56	MG	2A	3275	1/1	0.93	0.14	67,67,67,67	0
56	MG	2a	3045	1/1	0.93	0.12	68,68,68,68	0
56	MG	1A	3163	1/1	0.93	0.26	49,49,49,49	0
56	MG	2A	3277	1/1	0.93	0.56	63,63,63,63	0
56	MG	1A	3790	1/1	0.93	0.18	46,46,46,46	0
56	MG	10	103	1/1	0.93	1.00	54,54,54,54	0
56	MG	2A	3480	1/1	0.93	0.37	50,50,50,50	0
56	MG	1A	3228	1/1	0.93	0.17	37,37,37,37	0
56	MG	1A	4005	1/1	0.93	0.13	58,58,58,58	0
56	MG	1A	3335	1/1	0.93	0.32	56,56,56,56	0
56	MG	1A	4109	1/1	0.93	0.12	40,40,40,40	0
56	MG	1a	1884	1/1	0.93	0.13	54,54,54,54	0
56	MG	2A	3488	1/1	0.93	0.31	53,53,53,53	0
56	MG	1A	3621	1/1	0.93	0.19	40,40,40,40	0
56	MG	2A	3491	1/1	0.93	0.34	37,37,37,37	0
56	MG	2A	3095	1/1	0.93	0.19	48,48,48,48	0
56	MG	2A	3496	1/1	0.93	0.21	51,51,51,51	0
56	MG	1a	1886	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3691	1/1	0.93	0.22	55,55,55,55	0
56	MG	1A	4229	1/1	0.93	0.44	45,45,45,45	0
56	MG	1A	4230	1/1	0.93	0.60	45,45,45,45	0
56	MG	1A	4231	1/1	0.93	0.40	55,55,55,55	0
56	MG	2a	3070	1/1	0.93	0.10	76,76,76,76	0
56	MG	1A	3507	1/1	0.93	0.29	72,72,72,72	0
56	MG	1A	3798	1/1	0.93	0.13	54,54,54,54	0
56	MG	2A	3107	1/1	0.93	0.40	50,50,50,50	0
56	MG	1A	3799	1/1	0.93	0.14	47,47,47,47	0
56	MG	2A	3808	1/1	0.93	0.09	60,60,60,60	0
56	MG	1A	3508	1/1	0.93	0.35	41,41,41,41	0
56	MG	1A	3511	1/1	0.93	0.44	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4246	1/1	0.93	0.43	40,40,40,40	0
56	MG	2A	3812	1/1	0.93	0.19	48,48,48,48	0
56	MG	1A	3571	1/1	0.93	0.29	58,58,58,58	0
56	MG	2A	3120	1/1	0.93	0.16	34,34,34,34	0
56	MG	1a	1904	1/1	0.93	0.08	56,56,56,56	0
56	MG	2A	3523	1/1	0.93	0.11	31,31,31,31	0
56	MG	2A	3524	1/1	0.93	0.10	49,49,49,49	0
56	MG	1a	1601	1/1	0.93	0.23	50,50,50,50	0
56	MG	1A	3138	1/1	0.93	0.87	49,49,49,49	0
56	MG	1A	3076	1/1	0.93	0.51	43,43,43,43	0
56	MG	2a	3095	1/1	0.93	0.26	50,50,50,50	0
56	MG	1A	3435	1/1	0.93	0.43	53,53,53,53	0
56	MG	1A	3141	1/1	0.93	0.28	43,43,43,43	0
56	MG	1A	3478	1/1	0.93	0.20	47,47,47,47	0
56	MG	2a	3102	1/1	0.93	0.25	63,63,63,63	0
56	MG	1a	1608	1/1	0.93	0.10	47,47,47,47	0
56	MG	2A	3320	1/1	0.93	0.21	55,55,55,55	0
56	MG	1a	1761	1/1	0.93	0.23	55,55,55,55	0
56	MG	1A	4027	1/1	0.93	0.13	41,41,41,41	0
56	MG	2A	3546	1/1	0.93	0.11	34,34,34,34	0
56	MG	1A	4028	1/1	0.93	0.08	46,46,46,46	0
56	MG	2A	3137	1/1	0.93	0.19	52,52,52,52	0
56	MG	1A	4032	1/1	0.93	0.12	57,57,57,57	0
56	MG	1A	3716	1/1	0.93	0.11	44,44,44,44	0
56	MG	2A	3142	1/1	0.93	0.12	51,51,51,51	0
56	MG	1a	1922	1/1	0.93	0.16	52,52,52,52	0
56	MG	1A	3578	1/1	0.93	0.23	61,61,61,61	0
56	MG	1a	1769	1/1	0.93	0.14	44,44,44,44	0
56	MG	1A	3045	1/1	0.93	0.15	38,38,38,38	0
56	MG	1a	1772	1/1	0.93	0.12	56,56,56,56	0
56	MG	2A	3336	1/1	0.93	0.13	62,62,62,62	0
56	MG	2A	3856	1/1	0.93	0.16	44,44,44,44	0
56	MG	1A	3932	1/1	0.93	0.08	40,40,40,40	0
56	MG	1A	3638	1/1	0.93	0.18	54,54,54,54	0
56	MG	1A	3062	1/1	0.93	0.32	56,56,56,56	0
56	MG	1A	3092	1/1	0.93	0.15	53,53,53,53	0
56	MG	2A	3163	1/1	0.93	0.34	55,55,55,55	0
56	MG	1A	3939	1/1	0.93	0.14	51,51,51,51	0
56	MG	2a	3136	1/1	0.93	0.24	83,83,83,83	0
56	MG	2A	3576	1/1	0.93	0.14	29,29,29,29	0
56	MG	2a	3138	1/1	0.93	0.12	83,83,83,83	0
56	MG	2A	3577	1/1	0.93	0.20	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3167	1/1	0.93	0.31	41,41,41,41	0
56	MG	1a	1779	1/1	0.93	0.16	56,56,56,56	0
56	MG	2A	3581	1/1	0.93	0.12	42,42,42,42	0
56	MG	1a	1626	1/1	0.93	0.21	48,48,48,48	0
56	MG	2A	3171	1/1	0.93	0.13	61,61,61,61	0
56	MG	2A	3349	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	4047	1/1	0.93	0.14	58,58,58,58	0
56	MG	1A	3940	1/1	0.93	0.33	47,47,47,47	0
56	MG	1A	4142	1/1	0.93	0.10	64,64,64,64	0
56	MG	1A	3241	1/1	0.93	0.22	37,37,37,37	0
56	MG	2A	3356	1/1	0.93	0.15	53,53,53,53	0
56	MG	2A	3594	1/1	0.93	0.07	45,45,45,45	0
56	MG	1B	231	1/1	0.93	0.18	56,56,56,56	0
56	MG	1A	3210	1/1	0.93	0.08	67,67,67,67	0
56	MG	1A	3833	1/1	0.93	0.14	37,37,37,37	0
56	MG	1a	1637	1/1	0.93	0.34	56,56,56,56	0
56	MG	1a	1638	1/1	0.93	0.09	45,45,45,45	0
56	MG	1A	3527	1/1	0.93	0.17	55,55,55,55	0
56	MG	1D	308	1/1	0.93	0.51	56,56,56,56	0
56	MG	2A	3611	1/1	0.93	0.05	60,60,60,60	0
56	MG	1D	309	1/1	0.93	0.15	41,41,41,41	0
56	MG	1A	3836	1/1	0.93	0.20	42,42,42,42	0
56	MG	1a	1645	1/1	0.93	0.20	53,53,53,53	0
56	MG	1A	4056	1/1	0.93	0.20	51,51,51,51	0
56	MG	2A	3193	1/1	0.93	0.15	57,57,57,57	0
56	MG	1A	3054	1/1	0.93	0.17	53,53,53,53	0
56	MG	1E	304	1/1	0.93	0.19	51,51,51,51	0
56	MG	2A	3196	1/1	0.93	0.16	57,57,57,57	0
56	MG	2A	3629	1/1	0.93	0.17	56,56,56,56	0
56	MG	2A	3631	1/1	0.93	0.08	47,47,47,47	0
56	MG	2A	3635	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3948	1/1	0.93	0.14	53,53,53,53	0
56	MG	1a	1652	1/1	0.93	0.24	41,41,41,41	0
56	MG	1A	3949	1/1	0.93	0.50	41,41,41,41	0
56	MG	1A	3098	1/1	0.93	0.22	57,57,57,57	0
56	MG	2B	3008	1/1	0.93	0.11	50,50,50,50	0
56	MG	1A	3347	1/1	0.93	0.51	42,42,42,42	0
56	MG	1a	1661	1/1	0.93	0.18	73,73,73,73	0
56	MG	1A	3954	1/1	0.93	0.24	62,62,62,62	0
56	MG	1F	301	1/1	0.93	0.27	68,68,68,68	0
56	MG	2A	3660	1/1	0.93	0.16	57,57,57,57	0
56	MG	2A	3661	1/1	0.93	0.08	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3277	1/1	0.93	0.46	47,47,47,47	0
56	MG	1A	3379	1/1	0.93	0.13	64,64,64,64	0
56	MG	1A	3594	1/1	0.93	0.24	40,40,40,40	0
56	MG	2a	3203	1/1	0.93	0.25	50,50,50,50	0
56	MG	2A	3003	1/1	0.93	0.19	40,40,40,40	0
56	MG	1F	305	1/1	0.93	0.55	39,39,39,39	0
56	MG	2E	305	1/1	0.93	0.19	53,53,53,53	0
56	MG	2A	3391	1/1	0.93	0.11	58,58,58,58	0
56	MG	2a	3211	1/1	0.93	0.10	71,71,71,71	0
56	MG	2E	308	1/1	0.93	0.96	59,59,59,59	0
56	MG	1A	3349	1/1	0.93	0.21	41,41,41,41	0
56	MG	1A	3454	1/1	0.93	0.25	51,51,51,51	0
56	MG	1A	3655	1/1	0.93	0.21	50,50,50,50	0
56	MG	2A	3017	1/1	0.93	0.22	44,44,44,44	0
56	MG	2a	3220	1/1	0.93	0.12	62,62,62,62	0
56	MG	1A	3658	1/1	0.93	0.18	65,65,65,65	0
56	MG	2Q	3002	1/1	0.93	0.38	47,47,47,47	0
56	MG	1A	3753	1/1	0.93	0.16	32,32,32,32	0
56	MG	1a	1678	1/1	0.93	0.08	52,52,52,52	0
56	MG	2a	3226	1/1	0.93	0.16	79,79,79,79	0
56	MG	1A	3659	1/1	0.93	0.31	41,41,41,41	0
56	MG	1A	3414	1/1	0.93	0.37	62,62,62,62	0
56	MG	2a	3230	1/1	0.93	0.11	66,66,66,66	0
56	MG	2A	3406	1/1	0.93	0.08	52,52,52,52	0
56	MG	2a	3232	1/1	0.93	0.09	43,43,43,43	0
56	MG	2A	3221	1/1	0.93	0.12	49,49,49,49	0
56	MG	2A	3694	1/1	0.93	0.07	60,60,60,60	0
56	MG	1A	3187	1/1	0.93	0.61	51,51,51,51	0
56	MG	2Z	8001	1/1	0.93	0.06	65,65,65,65	0
56	MG	1A	3765	1/1	0.93	0.21	28,28,28,28	0
56	MG	2A	3699	1/1	0.93	0.12	64,64,64,64	0
56	MG	1A	3494	1/1	0.93	0.09	45,45,45,45	0
56	MG	1a	1843	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3119	1/1	0.93	0.16	41,41,41,41	0
56	MG	1N	3006	1/1	0.93	0.14	46,46,46,46	0
56	MG	2A	3710	1/1	0.93	0.19	28,28,28,28	0
56	MG	1A	3101	1/1	0.93	0.10	66,66,66,66	0
56	MG	25	105	1/1	0.93	0.10	55,55,55,55	0
56	MG	2t	3001	1/1	0.93	0.07	63,63,63,63	0
56	MG	1A	4189	1/1	0.93	0.14	33,33,33,33	0
56	MG	1A	3549	1/1	0.93	0.83	50,50,50,50	0
56	MG	2A	3233	1/1	0.93	0.20	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3982	1/1	0.93	0.13	32,32,32,32	0
56	MG	1a	1850	1/1	0.93	0.12	59,59,59,59	0
56	MG	2A	3238	1/1	0.93	0.29	43,43,43,43	0
56	MG	1A	3676	1/1	0.93	0.22	46,46,46,46	0
56	MG	2A	3048	1/1	0.93	0.18	53,53,53,53	0
56	MG	1a	1696	1/1	0.93	0.13	55,55,55,55	0
56	MG	2A	3052	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	4196	1/1	0.93	0.18	37,37,37,37	0
56	MG	2A	3054	1/1	0.93	0.11	44,44,44,44	0
56	MG	1a	1703	1/1	0.93	0.27	51,51,51,51	0
56	MG	1A	3005	1/1	0.93	0.22	53,53,53,53	0
56	MG	1A	4198	1/1	0.93	0.08	45,45,45,45	0
56	MG	1R	202	1/1	0.93	0.21	36,36,36,36	0
56	MG	2A	3250	1/1	0.93	0.69	62,62,62,62	0
56	MG	1R	203	1/1	0.93	0.12	36,36,36,36	0
56	MG	1a	1863	1/1	0.93	0.12	76,76,76,76	0
56	MG	1A	3133	1/1	0.93	0.35	36,36,36,36	0
56	MG	2A	3256	1/1	0.93	0.15	58,58,58,58	0
56	MG	1A	3193	1/1	0.93	0.44	44,44,44,44	0
56	MG	2y	3007	1/1	0.93	0.14	84,84,84,84	0
56	MG	1A	3328	1/1	0.93	0.34	53,53,53,53	0
56	MG	2A	3260	1/1	0.93	0.10	73,73,73,73	0
57	CPT	2A	3904	4/5	0.93	0.13	79,102,124,194	4
56	MG	1A	3103	1/1	0.93	0.84	47,47,47,47	0
58	K	2A	3922	1/1	0.93	0.13	72,72,72,72	0
56	MG	1U	203	1/1	0.93	0.62	46,46,46,46	0
56	MG	1U	204	1/1	0.93	0.90	66,66,66,66	0
56	MG	1A	3197	1/1	0.93	0.12	55,55,55,55	0
59	ZN	2n	102	1/1	0.93	0.04	85,85,85,85	0
56	MG	2A	3662	1/1	0.94	0.33	52,52,52,52	0
56	MG	1A	3528	1/1	0.94	0.20	35,35,35,35	0
56	MG	2A	3667	1/1	0.94	0.17	36,36,36,36	0
56	MG	1a	1640	1/1	0.94	0.16	52,52,52,52	0
56	MG	1A	3529	1/1	0.94	0.24	45,45,45,45	0
56	MG	1a	1799	1/1	0.94	0.09	62,62,62,62	0
56	MG	1A	3530	1/1	0.94	0.27	43,43,43,43	0
56	MG	1D	311	1/1	0.94	0.14	51,51,51,51	0
56	MG	2a	3001	1/1	0.94	0.20	62,62,62,62	0
56	MG	1a	1803	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	4042	1/1	0.94	0.06	51,51,51,51	0
56	MG	2A	3396	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3006	1/1	0.94	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3718	1/1	0.94	0.17	35,35,35,35	0
56	MG	2A	3402	1/1	0.94	0.26	47,47,47,47	0
56	MG	1A	3488	1/1	0.94	0.26	45,45,45,45	0
56	MG	1A	3010	1/1	0.94	0.15	41,41,41,41	0
56	MG	1A	3816	1/1	0.94	0.20	58,58,58,58	0
56	MG	2A	3012	1/1	0.94	0.12	35,35,35,35	0
56	MG	1A	3935	1/1	0.94	0.20	58,58,58,58	0
56	MG	2A	3693	1/1	0.94	0.10	49,49,49,49	0
56	MG	1E	310	1/1	0.94	0.69	49,49,49,49	0
56	MG	1A	3590	1/1	0.94	0.21	44,44,44,44	0
56	MG	1A	3938	1/1	0.94	0.11	60,60,60,60	0
56	MG	2A	3412	1/1	0.94	0.31	53,53,53,53	0
56	MG	2A	3020	1/1	0.94	0.28	50,50,50,50	0
56	MG	1A	4158	1/1	0.94	0.15	49,49,49,49	0
56	MG	1A	3825	1/1	0.94	0.14	49,49,49,49	0
56	MG	2A	3225	1/1	0.94	0.23	54,54,54,54	0
56	MG	1A	3415	1/1	0.94	0.14	57,57,57,57	0
56	MG	2A	3418	1/1	0.94	0.15	64,64,64,64	0
56	MG	1A	3452	1/1	0.94	0.12	55,55,55,55	0
56	MG	1a	1666	1/1	0.94	0.38	49,49,49,49	0
56	MG	1A	3942	1/1	0.94	0.21	49,49,49,49	0
56	MG	2A	3718	1/1	0.94	0.14	30,30,30,30	0
56	MG	1A	3264	1/1	0.94	0.43	57,57,57,57	0
56	MG	2A	3231	1/1	0.94	0.43	49,49,49,49	0
56	MG	1A	3157	1/1	0.94	0.48	51,51,51,51	0
56	MG	1A	3541	1/1	0.94	0.19	48,48,48,48	0
56	MG	1G	3001	1/1	0.94	0.07	41,41,41,41	0
56	MG	2A	3236	1/1	0.94	0.26	61,61,61,61	0
56	MG	1a	1674	1/1	0.94	0.16	66,66,66,66	0
56	MG	2A	3039	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	3027	1/1	0.94	0.13	59,59,59,59	0
56	MG	2A	3041	1/1	0.94	0.18	39,39,39,39	0
56	MG	1a	1836	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3736	1/1	0.94	0.10	36,36,36,36	0
56	MG	1a	1676	1/1	0.94	0.21	60,60,60,60	0
56	MG	2a	3049	1/1	0.94	0.22	50,50,50,50	0
56	MG	1A	3419	1/1	0.94	0.33	61,61,61,61	0
56	MG	2a	3051	1/1	0.94	0.09	54,54,54,54	0
56	MG	2A	3741	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3657	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3736	1/1	0.94	0.19	32,32,32,32	0
56	MG	2A	3051	1/1	0.94	0.30	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1681	1/1	0.94	0.28	60,60,60,60	0
56	MG	1A	3100	1/1	0.94	0.13	48,48,48,48	0
56	MG	2A	3752	1/1	0.94	0.30	45,45,45,45	0
56	MG	1N	3001	1/1	0.94	0.44	56,56,56,56	0
56	MG	1A	3839	1/1	0.94	0.08	50,50,50,50	0
56	MG	2A	3252	1/1	0.94	0.20	66,66,66,66	0
56	MG	1a	1685	1/1	0.94	0.31	53,53,53,53	0
56	MG	1A	4070	1/1	0.94	0.18	51,51,51,51	0
56	MG	1N	3004	1/1	0.94	1.17	60,60,60,60	0
56	MG	1A	4181	1/1	0.94	0.34	47,47,47,47	0
56	MG	1A	3114	1/1	0.94	0.23	48,48,48,48	0
56	MG	1A	4185	1/1	0.94	0.13	43,43,43,43	0
56	MG	1A	3842	1/1	0.94	0.13	58,58,58,58	0
56	MG	1A	4073	1/1	0.94	0.25	68,68,68,68	0
56	MG	1A	3272	1/1	0.94	0.33	55,55,55,55	0
56	MG	1P	202	1/1	0.94	0.31	39,39,39,39	0
56	MG	1A	4190	1/1	0.94	0.14	58,58,58,58	0
56	MG	1a	1701	1/1	0.94	0.41	46,46,46,46	0
56	MG	2A	3472	1/1	0.94	0.34	55,55,55,55	0
56	MG	2A	3473	1/1	0.94	0.09	60,60,60,60	0
56	MG	1A	3313	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3020	1/1	0.94	0.24	38,38,38,38	0
56	MG	1A	3959	1/1	0.94	0.31	46,46,46,46	0
56	MG	2A	3777	1/1	0.94	0.14	55,55,55,55	0
56	MG	2A	3478	1/1	0.94	0.20	46,46,46,46	0
56	MG	2a	3084	1/1	0.94	0.25	62,62,62,62	0
56	MG	2A	3780	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	3747	1/1	0.94	0.16	32,32,32,32	0
56	MG	2A	3272	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	3749	1/1	0.94	0.12	44,44,44,44	0
56	MG	1A	4080	1/1	0.94	0.15	26,26,26,26	0
56	MG	1S	3003	1/1	0.94	0.17	72,72,72,72	0
56	MG	1A	3962	1/1	0.94	0.82	58,58,58,58	0
56	MG	1A	3664	1/1	0.94	0.19	51,51,51,51	0
56	MG	1a	1712	1/1	0.94	0.10	37,37,37,37	0
56	MG	1A	3665	1/1	0.94	0.12	40,40,40,40	0
56	MG	2A	3490	1/1	0.94	0.09	49,49,49,49	0
56	MG	1A	3666	1/1	0.94	0.22	43,43,43,43	0
56	MG	1A	3855	1/1	0.94	0.15	34,34,34,34	0
56	MG	1A	3668	1/1	0.94	0.17	48,48,48,48	0
56	MG	1V	201	1/1	0.94	0.22	41,41,41,41	0
56	MG	1W	3001	1/1	0.94	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3670	1/1	0.94	0.12	45,45,45,45	0
56	MG	1A	3761	1/1	0.94	0.15	26,26,26,26	0
56	MG	1A	4089	1/1	0.94	0.15	64,64,64,64	0
56	MG	1A	3763	1/1	0.94	0.09	37,37,37,37	0
56	MG	1A	3055	1/1	0.94	0.13	34,34,34,34	0
56	MG	2A	3508	1/1	0.94	0.05	35,35,35,35	0
56	MG	1A	4216	1/1	0.94	0.15	28,28,28,28	0
56	MG	2A	3510	1/1	0.94	0.22	26,26,26,26	0
56	MG	1A	3426	1/1	0.94	0.20	52,52,52,52	0
56	MG	1A	3118	1/1	0.94	0.20	49,49,49,49	0
56	MG	2A	3515	1/1	0.94	0.18	25,25,25,25	0
56	MG	2a	3125	1/1	0.94	0.22	48,48,48,48	0
56	MG	2a	3126	1/1	0.94	0.13	49,49,49,49	0
56	MG	2A	3295	1/1	0.94	0.40	43,43,43,43	0
56	MG	1a	1888	1/1	0.94	0.07	58,58,58,58	0
56	MG	1A	3674	1/1	0.94	0.08	33,33,33,33	0
56	MG	1a	1731	1/1	0.94	0.18	55,55,55,55	0
56	MG	2A	3110	1/1	0.94	0.16	46,46,46,46	0
56	MG	1A	3770	1/1	0.94	0.18	36,36,36,36	0
56	MG	2A	3302	1/1	0.94	0.37	57,57,57,57	0
56	MG	2A	3525	1/1	0.94	0.13	49,49,49,49	0
56	MG	1A	3986	1/1	0.94	0.21	39,39,39,39	0
56	MG	2A	3528	1/1	0.94	0.15	57,57,57,57	0
56	MG	2A	3826	1/1	0.94	0.10	81,81,81,81	0
56	MG	2A	3114	1/1	0.94	0.11	51,51,51,51	0
56	MG	2A	3305	1/1	0.94	0.25	55,55,55,55	0
56	MG	1a	1735	1/1	0.94	0.07	47,47,47,47	0
56	MG	2A	3534	1/1	0.94	0.11	40,40,40,40	0
56	MG	1a	1737	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3836	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3368	1/1	0.94	0.51	62,62,62,62	0
56	MG	2A	3839	1/1	0.94	0.19	33,33,33,33	0
56	MG	1A	3398	1/1	0.94	0.18	41,41,41,41	0
56	MG	2A	3542	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3990	1/1	0.94	0.14	44,44,44,44	0
56	MG	2A	3124	1/1	0.94	0.07	47,47,47,47	0
56	MG	2A	3845	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3877	1/1	0.94	0.09	40,40,40,40	0
56	MG	1A	3470	1/1	0.94	0.18	62,62,62,62	0
56	MG	1A	3223	1/1	0.94	0.65	43,43,43,43	0
56	MG	15	101	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	4239	1/1	0.94	0.64	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3163	1/1	0.94	0.13	46,46,46,46	0
56	MG	1A	3144	1/1	0.94	0.39	50,50,50,50	0
56	MG	2a	3165	1/1	0.94	0.10	68,68,68,68	0
56	MG	2A	3857	1/1	0.94	0.16	56,56,56,56	0
56	MG	1A	3780	1/1	0.94	0.16	55,55,55,55	0
56	MG	1A	4112	1/1	0.94	0.16	43,43,43,43	0
56	MG	2A	3554	1/1	0.94	0.22	33,33,33,33	0
56	MG	1A	3510	1/1	0.94	0.45	50,50,50,50	0
56	MG	1A	3682	1/1	0.94	0.14	40,40,40,40	0
56	MG	1A	4250	1/1	0.94	0.14	38,38,38,38	0
56	MG	1A	4251	1/1	0.94	0.52	49,49,49,49	0
56	MG	2A	3143	1/1	0.94	0.27	35,35,35,35	0
56	MG	2A	3331	1/1	0.94	0.20	64,64,64,64	0
56	MG	2a	3178	1/1	0.94	0.13	64,64,64,64	0
56	MG	2a	3179	1/1	0.94	0.09	80,80,80,80	0
56	MG	2A	3563	1/1	0.94	0.29	41,41,41,41	0
56	MG	2A	3564	1/1	0.94	0.16	70,70,70,70	0
56	MG	1A	4253	1/1	0.94	0.66	45,45,45,45	0
56	MG	2A	3568	1/1	0.94	0.14	31,31,31,31	0
56	MG	2a	3186	1/1	0.94	0.16	62,62,62,62	0
56	MG	2A	3333	1/1	0.94	0.16	53,53,53,53	0
56	MG	1A	3090	1/1	0.94	0.40	62,62,62,62	0
56	MG	2A	3151	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3201	1/1	0.94	0.17	28,28,28,28	0
56	MG	1a	1925	1/1	0.94	0.14	52,52,52,52	0
56	MG	1a	1760	1/1	0.94	0.20	48,48,48,48	0
56	MG	2A	3578	1/1	0.94	0.12	29,29,29,29	0
56	MG	2A	3155	1/1	0.94	0.26	56,56,56,56	0
56	MG	2A	3156	1/1	0.94	0.14	53,53,53,53	0
56	MG	2a	3199	1/1	0.94	0.31	62,62,62,62	0
56	MG	2A	3886	1/1	0.94	0.15	53,53,53,53	0
56	MG	2A	3157	1/1	0.94	0.24	45,45,45,45	0
56	MG	2A	3890	1/1	0.94	0.17	44,44,44,44	0
56	MG	1A	3787	1/1	0.94	0.07	35,35,35,35	0
56	MG	2A	3893	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3346	1/1	0.94	0.44	57,57,57,57	0
56	MG	2a	3207	1/1	0.94	0.12	71,71,71,71	0
56	MG	1A	3173	1/1	0.94	0.46	50,50,50,50	0
56	MG	1a	1764	1/1	0.94	0.19	36,36,36,36	0
56	MG	1A	3438	1/1	0.94	0.40	41,41,41,41	0
56	MG	1c	302	1/1	0.94	0.15	71,71,71,71	0
56	MG	2A	3591	1/1	0.94	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3166	1/1	0.94	0.11	47,47,47,47	0
56	MG	2A	3905	1/1	0.94	0.22	33,33,33,33	0
56	MG	1A	3902	1/1	0.94	0.07	59,59,59,59	0
56	MG	1A	3021	1/1	0.94	0.16	43,43,43,43	0
56	MG	2A	3909	1/1	0.94	0.21	51,51,51,51	0
56	MG	1A	4012	1/1	0.94	0.08	68,68,68,68	0
56	MG	2a	3223	1/1	0.94	0.12	57,57,57,57	0
56	MG	1a	1770	1/1	0.94	0.14	48,48,48,48	0
56	MG	2A	3600	1/1	0.94	0.16	62,62,62,62	0
56	MG	1l	204	1/1	0.94	0.21	49,49,49,49	0
56	MG	2A	3915	1/1	0.94	0.26	54,54,54,54	0
56	MG	1A	3630	1/1	0.94	0.30	39,39,39,39	0
56	MG	1B	213	1/1	0.94	0.13	80,80,80,80	0
56	MG	2A	3606	1/1	0.94	0.14	56,56,56,56	0
56	MG	1A	3122	1/1	0.94	0.23	53,53,53,53	0
56	MG	2a	3233	1/1	0.94	0.19	60,60,60,60	0
56	MG	1v	3001	1/1	0.94	0.20	64,64,64,64	0
56	MG	1B	219	1/1	0.94	0.15	63,63,63,63	0
56	MG	2B	3005	1/1	0.94	0.11	64,64,64,64	0
56	MG	2B	3007	1/1	0.94	0.14	53,53,53,53	0
56	MG	2A	3613	1/1	0.94	0.17	62,62,62,62	0
56	MG	1A	4127	1/1	0.94	0.07	38,38,38,38	0
56	MG	1A	3290	1/1	0.94	0.21	49,49,49,49	0
56	MG	2B	3012	1/1	0.94	0.12	58,58,58,58	0
56	MG	2B	3013	1/1	0.94	0.15	72,72,72,72	0
56	MG	2l	3004	1/1	0.94	0.14	61,61,61,61	0
56	MG	1a	1623	1/1	0.94	0.16	56,56,56,56	0
56	MG	2A	3620	1/1	0.94	0.21	40,40,40,40	0
56	MG	1A	3911	1/1	0.94	0.09	36,36,36,36	0
56	MG	2A	3368	1/1	0.94	0.36	65,65,65,65	0
56	MG	2A	3623	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	3124	1/1	0.94	0.43	39,39,39,39	0
56	MG	1A	3410	1/1	0.94	0.28	40,40,40,40	0
56	MG	2E	301	1/1	0.94	0.19	53,53,53,53	0
56	MG	2E	302	1/1	0.94	0.14	48,48,48,48	0
56	MG	2A	3372	1/1	0.94	0.14	54,54,54,54	0
56	MG	1A	3523	1/1	0.94	0.11	61,61,61,61	0
56	MG	2A	3190	1/1	0.94	0.24	64,64,64,64	0
56	MG	1A	3916	1/1	0.94	0.11	53,53,53,53	0
56	MG	2A	3636	1/1	0.94	0.16	60,60,60,60	0
56	MG	2A	3638	1/1	0.94	0.34	44,44,44,44	0
56	MG	1a	1631	1/1	0.94	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2F	304	1/1	0.94	0.62	52,52,52,52	0
56	MG	1A	3918	1/1	0.94	0.23	42,42,42,42	0
56	MG	1A	3131	1/1	0.94	0.25	45,45,45,45	0
56	MG	2P	201	1/1	0.94	0.19	57,57,57,57	0
56	MG	1x	108	1/1	0.94	0.23	73,73,73,73	0
56	MG	2A	3646	1/1	0.94	0.18	50,50,50,50	0
56	MG	2y	3001	1/1	0.94	0.10	58,58,58,58	0
56	MG	2A	3648	1/1	0.94	0.08	51,51,51,51	0
56	MG	2R	201	1/1	0.94	0.44	57,57,57,57	0
56	MG	2A	3649	1/1	0.94	0.15	58,58,58,58	0
56	MG	2A	3650	1/1	0.94	0.08	50,50,50,50	0
56	MG	2U	202	1/1	0.94	0.49	46,46,46,46	0
56	MG	1A	3293	1/1	0.94	0.17	57,57,57,57	0
56	MG	2U	206	1/1	0.94	0.39	49,49,49,49	0
56	MG	1A	3922	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3653	1/1	0.94	0.18	34,34,34,34	0
56	MG	2A	3655	1/1	0.94	0.18	58,58,58,58	0
56	MG	2A	3656	1/1	0.94	0.15	58,58,58,58	0
59	ZN	14	501	1/1	0.94	0.08	104,104,104,104	0
56	MG	1A	3923	1/1	0.94	0.14	67,67,67,67	0
56	MG	1x	112	1/1	0.94	0.18	47,47,47,47	0
59	ZN	26	501	1/1	0.94	0.11	59,59,59,59	0
56	MG	1D	304	1/1	0.94	0.13	19,19,19,19	0
56	MG	1a	1794	1/1	0.94	0.34	52,52,52,52	0
56	MG	2A	3492	1/1	0.95	0.16	58,58,58,58	0
56	MG	2A	3493	1/1	0.95	0.39	45,45,45,45	0
56	MG	1A	3794	1/1	0.95	0.14	32,32,32,32	0
56	MG	2A	3111	1/1	0.95	0.13	34,34,34,34	0
56	MG	1A	3332	1/1	0.95	0.14	49,49,49,49	0
56	MG	1a	1905	1/1	0.95	0.08	56,56,56,56	0
56	MG	2a	3028	1/1	0.95	0.25	47,47,47,47	0
56	MG	2A	3500	1/1	0.95	0.37	33,33,33,33	0
56	MG	2A	3501	1/1	0.95	0.07	72,72,72,72	0
56	MG	1A	3694	1/1	0.95	0.21	36,36,36,36	0
56	MG	2A	3116	1/1	0.95	0.36	40,40,40,40	0
56	MG	1A	3910	1/1	0.95	0.10	35,35,35,35	0
56	MG	1a	1752	1/1	0.95	0.04	63,63,63,63	0
56	MG	2A	3767	1/1	0.95	0.25	52,52,52,52	0
56	MG	1a	1910	1/1	0.95	0.07	61,61,61,61	0
56	MG	1a	1911	1/1	0.95	0.06	57,57,57,57	0
56	MG	2A	3770	1/1	0.95	0.10	52,52,52,52	0
56	MG	1A	3022	1/1	0.95	0.12	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3566	1/1	0.95	0.07	46,46,46,46	0
56	MG	2A	3511	1/1	0.95	0.25	52,52,52,52	0
56	MG	2A	3307	1/1	0.95	0.09	48,48,48,48	0
56	MG	2a	3046	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3061	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3183	1/1	0.95	0.18	54,54,54,54	0
56	MG	1A	3705	1/1	0.95	0.21	42,42,42,42	0
56	MG	2A	3129	1/1	0.95	0.23	56,56,56,56	0
56	MG	1A	3917	1/1	0.95	0.18	36,36,36,36	0
56	MG	1A	3569	1/1	0.95	0.49	43,43,43,43	0
56	MG	2A	3314	1/1	0.95	0.12	48,48,48,48	0
56	MG	1A	3919	1/1	0.95	0.23	47,47,47,47	0
56	MG	1B	220	1/1	0.95	0.14	51,51,51,51	0
56	MG	2A	3788	1/1	0.95	0.06	47,47,47,47	0
56	MG	2A	3789	1/1	0.95	0.07	50,50,50,50	0
56	MG	1A	3250	1/1	0.95	0.08	58,58,58,58	0
56	MG	1a	1617	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3709	1/1	0.95	0.10	33,33,33,33	0
56	MG	1A	4022	1/1	0.95	0.07	60,60,60,60	0
56	MG	1A	4023	1/1	0.95	0.15	19,19,19,19	0
56	MG	2A	3532	1/1	0.95	0.15	49,49,49,49	0
56	MG	1A	3710	1/1	0.95	0.22	44,44,44,44	0
56	MG	1A	3216	1/1	0.95	0.16	52,52,52,52	0
56	MG	1A	3924	1/1	0.95	0.12	45,45,45,45	0
56	MG	2A	3147	1/1	0.95	0.09	44,44,44,44	0
56	MG	2A	3539	1/1	0.95	0.12	56,56,56,56	0
56	MG	2A	3150	1/1	0.95	0.21	38,38,38,38	0
56	MG	1A	4029	1/1	0.95	0.09	59,59,59,59	0
56	MG	1A	3925	1/1	0.95	0.13	32,32,32,32	0
56	MG	1A	3116	1/1	0.95	0.29	33,33,33,33	0
56	MG	1l	201	1/1	0.95	0.22	49,49,49,49	0
56	MG	1a	1628	1/1	0.95	0.25	51,51,51,51	0
56	MG	1A	3377	1/1	0.95	0.45	50,50,50,50	0
56	MG	1A	3014	1/1	0.95	0.20	32,32,32,32	0
56	MG	1D	303	1/1	0.95	0.50	45,45,45,45	0
56	MG	1A	3719	1/1	0.95	0.15	53,53,53,53	0
56	MG	1A	3820	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	3821	1/1	0.95	0.10	40,40,40,40	0
56	MG	1w	101	1/1	0.95	0.16	87,87,87,87	0
56	MG	1A	3186	1/1	0.95	0.24	50,50,50,50	0
56	MG	1D	310	1/1	0.95	0.34	27,27,27,27	0
56	MG	2a	3088	1/1	0.95	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3041	1/1	0.95	0.14	33,33,33,33	0
56	MG	1A	3030	1/1	0.95	0.25	40,40,40,40	0
56	MG	1A	3936	1/1	0.95	0.13	64,64,64,64	0
56	MG	2a	3092	1/1	0.95	0.18	77,77,77,77	0
56	MG	2A	3170	1/1	0.95	0.13	38,38,38,38	0
56	MG	2a	3094	1/1	0.95	0.20	61,61,61,61	0
56	MG	1w	109	1/1	0.95	0.05	61,61,61,61	0
56	MG	1a	1788	1/1	0.95	0.09	38,38,38,38	0
56	MG	2A	3566	1/1	0.95	0.12	51,51,51,51	0
56	MG	1A	3301	1/1	0.95	0.31	58,58,58,58	0
56	MG	2A	3829	1/1	0.95	0.09	34,34,34,34	0
56	MG	2A	3830	1/1	0.95	0.17	56,56,56,56	0
56	MG	1A	3120	1/1	0.95	0.61	41,41,41,41	0
56	MG	1a	1643	1/1	0.95	0.15	57,57,57,57	0
56	MG	1E	306	1/1	0.95	0.18	50,50,50,50	0
56	MG	2A	3572	1/1	0.95	0.12	40,40,40,40	0
56	MG	1A	4161	1/1	0.95	0.13	23,23,23,23	0
56	MG	1x	105	1/1	0.95	0.19	62,62,62,62	0
56	MG	2a	3111	1/1	0.95	0.23	67,67,67,67	0
56	MG	1x	106	1/1	0.95	0.35	50,50,50,50	0
56	MG	1A	3303	1/1	0.95	0.39	40,40,40,40	0
56	MG	2A	3184	1/1	0.95	0.14	58,58,58,58	0
56	MG	1a	1647	1/1	0.95	0.11	49,49,49,49	0
56	MG	2A	3364	1/1	0.95	0.16	56,56,56,56	0
56	MG	2A	3846	1/1	0.95	0.12	31,31,31,31	0
56	MG	1A	3521	1/1	0.95	0.30	71,71,71,71	0
56	MG	2A	3849	1/1	0.95	0.07	60,60,60,60	0
56	MG	1A	3729	1/1	0.95	0.10	48,48,48,48	0
56	MG	2A	3852	1/1	0.95	0.07	72,72,72,72	0
56	MG	1A	3477	1/1	0.95	0.14	44,44,44,44	0
56	MG	1A	3304	1/1	0.95	0.18	55,55,55,55	0
56	MG	2A	3369	1/1	0.95	0.11	52,52,52,52	0
56	MG	1A	3306	1/1	0.95	0.22	40,40,40,40	0
56	MG	1A	3066	1/1	0.95	0.17	46,46,46,46	0
56	MG	1A	3153	1/1	0.95	0.25	39,39,39,39	0
56	MG	2A	3859	1/1	0.95	0.26	41,41,41,41	0
56	MG	1A	4061	1/1	0.95	0.08	72,72,72,72	0
56	MG	1a	1807	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	4173	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	3653	1/1	0.95	0.13	50,50,50,50	0
56	MG	2A	3598	1/1	0.95	0.12	46,46,46,46	0
56	MG	1A	4175	1/1	0.95	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3843	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3350	1/1	0.95	0.74	39,39,39,39	0
56	MG	1A	3591	1/1	0.95	0.26	48,48,48,48	0
56	MG	1A	3434	1/1	0.95	0.18	51,51,51,51	0
56	MG	1G	3004	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	4183	1/1	0.95	0.36	33,33,33,33	0
56	MG	2a	3147	1/1	0.95	0.07	78,78,78,78	0
56	MG	2A	3007	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3848	1/1	0.95	0.21	57,57,57,57	0
56	MG	2A	3612	1/1	0.95	0.19	41,41,41,41	0
56	MG	2A	3009	1/1	0.95	0.16	33,33,33,33	0
56	MG	2A	3011	1/1	0.95	0.08	47,47,47,47	0
56	MG	2a	3154	1/1	0.95	0.14	48,48,48,48	0
56	MG	1A	3033	1/1	0.95	0.62	39,39,39,39	0
56	MG	2A	3390	1/1	0.95	0.23	43,43,43,43	0
56	MG	1A	3104	1/1	0.95	0.50	54,54,54,54	0
56	MG	1A	3661	1/1	0.95	0.47	61,61,61,61	0
56	MG	1A	3130	1/1	0.95	0.14	57,57,57,57	0
56	MG	2a	3160	1/1	0.95	0.07	77,77,77,77	0
56	MG	1A	3266	1/1	0.95	0.17	54,54,54,54	0
56	MG	2A	3889	1/1	0.95	0.13	25,25,25,25	0
56	MG	1A	4192	1/1	0.95	0.47	52,52,52,52	0
56	MG	1a	1680	1/1	0.95	0.51	48,48,48,48	0
56	MG	2A	3398	1/1	0.95	0.18	48,48,48,48	0
56	MG	2A	3399	1/1	0.95	0.13	49,49,49,49	0
56	MG	2A	3895	1/1	0.95	0.36	41,41,41,41	0
56	MG	1a	1830	1/1	0.95	0.19	36,36,36,36	0
56	MG	2A	3633	1/1	0.95	0.15	59,59,59,59	0
56	MG	2A	3634	1/1	0.95	0.16	39,39,39,39	0
56	MG	1A	3755	1/1	0.95	0.20	26,26,26,26	0
56	MG	1A	3597	1/1	0.95	0.50	49,49,49,49	0
56	MG	2A	3637	1/1	0.95	0.15	35,35,35,35	0
56	MG	1a	1835	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3230	1/1	0.95	0.26	39,39,39,39	0
56	MG	1a	1837	1/1	0.95	0.16	32,32,32,32	0
56	MG	2a	3180	1/1	0.95	0.11	70,70,70,70	0
56	MG	2A	3643	1/1	0.95	0.15	51,51,51,51	0
56	MG	1O	3002	1/1	0.95	0.46	59,59,59,59	0
56	MG	1A	3964	1/1	0.95	0.49	37,37,37,37	0
56	MG	2a	3184	1/1	0.95	0.10	58,58,58,58	0
56	MG	1A	3017	1/1	0.95	0.32	44,44,44,44	0
56	MG	1A	3071	1/1	0.95	0.31	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3038	1/1	0.95	0.22	36,36,36,36	0
56	MG	2A	3916	1/1	0.95	0.50	41,41,41,41	0
56	MG	2A	3917	1/1	0.95	0.19	52,52,52,52	0
56	MG	1a	1689	1/1	0.95	0.13	65,65,65,65	0
56	MG	2A	3919	1/1	0.95	0.12	39,39,39,39	0
56	MG	1P	203	1/1	0.95	0.38	44,44,44,44	0
56	MG	1A	3669	1/1	0.95	0.31	48,48,48,48	0
56	MG	1A	3969	1/1	0.95	0.12	44,44,44,44	0
56	MG	2A	3654	1/1	0.95	0.27	54,54,54,54	0
56	MG	2a	3198	1/1	0.95	0.18	68,68,68,68	0
56	MG	1A	3970	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	4203	1/1	0.95	0.71	50,50,50,50	0
56	MG	2B	3006	1/1	0.95	0.17	54,54,54,54	0
56	MG	1A	3443	1/1	0.95	0.12	42,42,42,42	0
56	MG	1A	3972	1/1	0.95	0.15	34,34,34,34	0
56	MG	1a	1697	1/1	0.95	0.18	45,45,45,45	0
56	MG	1S	3001	1/1	0.95	0.36	52,52,52,52	0
56	MG	1A	3602	1/1	0.95	0.27	56,56,56,56	0
56	MG	2A	3663	1/1	0.95	0.14	43,43,43,43	0
56	MG	2B	3014	1/1	0.95	0.13	81,81,81,81	0
56	MG	2a	3210	1/1	0.95	0.08	58,58,58,58	0
56	MG	1a	1855	1/1	0.95	0.12	49,49,49,49	0
56	MG	2A	3242	1/1	0.95	0.16	46,46,46,46	0
56	MG	1A	3108	1/1	0.95	0.52	42,42,42,42	0
56	MG	2B	3018	1/1	0.95	0.17	42,42,42,42	0
56	MG	2B	3019	1/1	0.95	0.20	66,66,66,66	0
56	MG	2A	3669	1/1	0.95	0.09	37,37,37,37	0
56	MG	2B	3021	1/1	0.95	0.79	74,74,74,74	0
56	MG	1A	3976	1/1	0.95	0.16	42,42,42,42	0
56	MG	1A	3236	1/1	0.95	0.11	64,64,64,64	0
56	MG	1A	3871	1/1	0.95	0.27	37,37,37,37	0
56	MG	1A	3089	1/1	0.95	0.20	48,48,48,48	0
56	MG	1A	3607	1/1	0.95	0.10	62,62,62,62	0
56	MG	1A	4217	1/1	0.95	0.14	57,57,57,57	0
56	MG	1A	4092	1/1	0.95	0.15	57,57,57,57	0
56	MG	2A	3679	1/1	0.95	0.10	51,51,51,51	0
56	MG	2E	306	1/1	0.95	0.21	42,42,42,42	0
56	MG	2A	3680	1/1	0.95	0.10	51,51,51,51	0
56	MG	2A	3440	1/1	0.95	0.18	42,42,42,42	0
56	MG	2A	3441	1/1	0.95	0.28	36,36,36,36	0
56	MG	1A	3546	1/1	0.95	0.17	50,50,50,50	0
56	MG	1A	3547	1/1	0.95	0.32	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1W	3005	1/1	0.95	0.16	29,29,29,29	0
56	MG	2e	3001	1/1	0.95	0.07	66,66,66,66	0
56	MG	2A	3254	1/1	0.95	0.11	56,56,56,56	0
56	MG	1A	3111	1/1	0.95	0.30	38,38,38,38	0
56	MG	1A	3985	1/1	0.95	0.14	59,59,59,59	0
56	MG	1X	105	1/1	0.95	0.31	62,62,62,62	0
56	MG	2A	3451	1/1	0.95	0.19	54,54,54,54	0
56	MG	1A	4226	1/1	0.95	0.43	38,38,38,38	0
56	MG	1A	3612	1/1	0.95	0.22	41,41,41,41	0
56	MG	2n	101	1/1	0.95	0.18	70,70,70,70	0
56	MG	1a	1719	1/1	0.95	0.06	60,60,60,60	0
56	MG	1A	4228	1/1	0.95	0.08	42,42,42,42	0
56	MG	1A	3362	1/1	0.95	0.12	54,54,54,54	0
56	MG	2U	205	1/1	0.95	0.24	49,49,49,49	0
56	MG	2A	3078	1/1	0.95	0.28	41,41,41,41	0
56	MG	1A	3551	1/1	0.95	0.28	33,33,33,33	0
56	MG	1A	3167	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3711	1/1	0.95	0.23	73,73,73,73	0
56	MG	2A	3712	1/1	0.95	0.12	55,55,55,55	0
56	MG	2A	3084	1/1	0.95	0.18	54,54,54,54	0
56	MG	2w	101	1/1	0.95	0.22	65,65,65,65	0
56	MG	1A	3992	1/1	0.95	0.10	73,73,73,73	0
56	MG	1A	3136	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	4237	1/1	0.95	0.66	48,48,48,48	0
56	MG	2A	3467	1/1	0.95	0.26	56,56,56,56	0
56	MG	2A	3088	1/1	0.95	0.13	55,55,55,55	0
56	MG	2A	3720	1/1	0.95	0.21	57,57,57,57	0
56	MG	1A	3407	1/1	0.95	0.21	61,61,61,61	0
56	MG	1l	103	1/1	0.95	0.14	55,55,55,55	0
56	MG	2A	3723	1/1	0.95	0.17	50,50,50,50	0
56	MG	1A	3891	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3242	1/1	0.95	0.84	40,40,40,40	0
56	MG	1a	1733	1/1	0.95	0.23	41,41,41,41	0
56	MG	1A	3687	1/1	0.95	0.49	39,39,39,39	0
56	MG	1A	3999	1/1	0.95	0.42	32,32,32,32	0
56	MG	1a	1890	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	4000	1/1	0.95	0.18	29,29,29,29	0
56	MG	1A	3057	1/1	0.95	0.11	38,38,38,38	0
56	MG	15	105	1/1	0.95	0.17	62,62,62,62	0
56	MG	2A	3103	1/1	0.95	0.20	28,28,28,28	0
56	MG	2A	3483	1/1	0.95	0.20	52,52,52,52	0
56	MG	2a	3010	1/1	0.95	0.17	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3281	1/1	0.95	0.34	53,53,53,53	0
56	MG	2A	3742	1/1	0.95	0.13	43,43,43,43	0
56	MG	2A	3485	1/1	0.95	0.14	52,52,52,52	0
56	MG	2A	3105	1/1	0.95	0.08	44,44,44,44	0
56	MG	1A	3139	1/1	0.95	0.20	42,42,42,42	0
56	MG	2A	3289	1/1	0.95	0.39	52,52,52,52	0
56	MG	1A	4254	1/1	0.95	0.60	49,49,49,49	0
56	MG	17	104	1/1	0.95	0.17	41,41,41,41	0
56	MG	1A	3058	1/1	0.95	0.15	60,60,60,60	0
56	MG	2a	3041	1/1	0.96	0.34	43,43,43,43	0
56	MG	1A	3125	1/1	0.96	0.85	47,47,47,47	0
56	MG	1A	4148	1/1	0.96	0.11	43,43,43,43	0
56	MG	1D	301	1/1	0.96	0.18	46,46,46,46	0
56	MG	1A	3128	1/1	0.96	0.25	49,49,49,49	0
56	MG	2A	3161	1/1	0.96	0.08	54,54,54,54	0
56	MG	1A	3238	1/1	0.96	0.47	39,39,39,39	0
56	MG	1a	1634	1/1	0.96	0.21	14,14,14,14	0
56	MG	2A	3804	1/1	0.96	0.22	74,74,74,74	0
56	MG	1A	3129	1/1	0.96	0.11	41,41,41,41	0
56	MG	2A	3806	1/1	0.96	0.20	55,55,55,55	0
56	MG	1A	4152	1/1	0.96	0.15	24,24,24,24	0
56	MG	2A	3565	1/1	0.96	0.13	53,53,53,53	0
56	MG	1A	4033	1/1	0.96	0.17	49,49,49,49	0
56	MG	1A	3637	1/1	0.96	0.11	51,51,51,51	0
56	MG	1A	3712	1/1	0.96	0.31	39,39,39,39	0
56	MG	1a	1790	1/1	0.96	0.06	78,78,78,78	0
56	MG	1A	3286	1/1	0.96	0.36	62,62,62,62	0
56	MG	1A	3808	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3809	1/1	0.96	0.09	56,56,56,56	0
56	MG	1A	4160	1/1	0.96	0.16	72,72,72,72	0
56	MG	2A	3175	1/1	0.96	0.14	54,54,54,54	0
56	MG	1E	305	1/1	0.96	0.34	57,57,57,57	0
56	MG	1a	1796	1/1	0.96	0.16	51,51,51,51	0
56	MG	1A	3810	1/1	0.96	0.17	43,43,43,43	0
56	MG	2a	3067	1/1	0.96	0.05	62,62,62,62	0
56	MG	1A	3714	1/1	0.96	0.12	32,32,32,32	0
56	MG	1A	3715	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3287	1/1	0.96	0.13	51,51,51,51	0
56	MG	2A	3183	1/1	0.96	0.11	54,54,54,54	0
56	MG	2A	3584	1/1	0.96	0.27	25,25,25,25	0
56	MG	1a	1801	1/1	0.96	0.05	59,59,59,59	0
56	MG	1A	3025	1/1	0.96	0.35	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3522	1/1	0.96	0.44	51,51,51,51	0
56	MG	1A	3818	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3819	1/1	0.96	0.15	58,58,58,58	0
56	MG	1a	1655	1/1	0.96	0.17	42,42,42,42	0
56	MG	2A	3834	1/1	0.96	0.13	65,65,65,65	0
56	MG	2a	3081	1/1	0.96	0.16	52,52,52,52	0
56	MG	1a	1656	1/1	0.96	0.20	40,40,40,40	0
56	MG	1A	3581	1/1	0.96	0.08	39,39,39,39	0
56	MG	1A	3012	1/1	0.96	0.12	32,32,32,32	0
56	MG	1a	1660	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3822	1/1	0.96	0.20	34,34,34,34	0
56	MG	1A	3476	1/1	0.96	0.52	53,53,53,53	0
56	MG	1F	306	1/1	0.96	0.69	47,47,47,47	0
56	MG	2A	3386	1/1	0.96	0.55	68,68,68,68	0
56	MG	2A	3844	1/1	0.96	0.06	60,60,60,60	0
56	MG	1A	3381	1/1	0.96	0.26	38,38,38,38	0
56	MG	1A	3827	1/1	0.96	0.13	56,56,56,56	0
56	MG	2A	3607	1/1	0.96	0.24	51,51,51,51	0
56	MG	1A	4178	1/1	0.96	0.18	32,32,32,32	0
56	MG	2A	3006	1/1	0.96	0.19	51,51,51,51	0
56	MG	2a	3098	1/1	0.96	0.23	61,61,61,61	0
56	MG	1F	310	1/1	0.96	0.53	66,66,66,66	0
56	MG	1A	3013	1/1	0.96	0.55	34,34,34,34	0
56	MG	1a	1820	1/1	0.96	0.29	46,46,46,46	0
56	MG	2A	3615	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	3165	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3206	1/1	0.96	0.32	39,39,39,39	0
56	MG	2a	3106	1/1	0.96	0.19	66,66,66,66	0
56	MG	2A	3013	1/1	0.96	0.16	42,42,42,42	0
56	MG	1A	4182	1/1	0.96	0.27	57,57,57,57	0
56	MG	1A	3294	1/1	0.96	0.26	32,32,32,32	0
56	MG	1A	3832	1/1	0.96	0.05	48,48,48,48	0
56	MG	1A	3207	1/1	0.96	0.12	47,47,47,47	0
56	MG	1a	1829	1/1	0.96	0.18	27,27,27,27	0
56	MG	1A	3107	1/1	0.96	0.56	47,47,47,47	0
56	MG	1a	1831	1/1	0.96	0.18	29,29,29,29	0
56	MG	1A	3389	1/1	0.96	0.35	43,43,43,43	0
56	MG	1a	1833	1/1	0.96	0.38	70,70,70,70	0
56	MG	2a	3119	1/1	0.96	0.30	63,63,63,63	0
56	MG	1A	3537	1/1	0.96	0.18	33,33,33,33	0
56	MG	1A	4069	1/1	0.96	0.13	89,89,89,89	0
56	MG	2A	3871	1/1	0.96	0.28	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	4191	1/1	0.96	0.16	25,25,25,25	0
56	MG	1A	3733	1/1	0.96	0.18	21,21,21,21	0
56	MG	1A	3953	1/1	0.96	0.10	54,54,54,54	0
56	MG	1A	3656	1/1	0.96	0.28	53,53,53,53	0
56	MG	2A	3035	1/1	0.96	0.34	30,30,30,30	0
56	MG	2A	3641	1/1	0.96	0.11	36,36,36,36	0
56	MG	2a	3130	1/1	0.96	0.14	67,67,67,67	0
56	MG	1a	1841	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3840	1/1	0.96	0.14	44,44,44,44	0
56	MG	1A	3087	1/1	0.96	0.43	38,38,38,38	0
56	MG	1A	3043	1/1	0.96	0.28	34,34,34,34	0
56	MG	1A	3738	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3211	1/1	0.96	0.16	48,48,48,48	0
56	MG	2A	3043	1/1	0.96	0.11	50,50,50,50	0
56	MG	2A	3044	1/1	0.96	0.13	50,50,50,50	0
56	MG	1Q	201	1/1	0.96	0.16	37,37,37,37	0
56	MG	2A	3891	1/1	0.96	0.12	40,40,40,40	0
56	MG	1Q	202	1/1	0.96	0.34	35,35,35,35	0
56	MG	1A	3171	1/1	0.96	0.67	50,50,50,50	0
56	MG	2A	3049	1/1	0.96	0.25	21,21,21,21	0
56	MG	1A	3742	1/1	0.96	0.14	43,43,43,43	0
56	MG	2A	3428	1/1	0.96	0.16	46,46,46,46	0
56	MG	1A	3743	1/1	0.96	0.25	43,43,43,43	0
56	MG	2A	3898	1/1	0.96	0.20	55,55,55,55	0
56	MG	2A	3658	1/1	0.96	0.31	36,36,36,36	0
56	MG	1A	3744	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3213	1/1	0.96	0.44	53,53,53,53	0
56	MG	2A	3435	1/1	0.96	0.23	44,44,44,44	0
56	MG	1A	3110	1/1	0.96	0.28	40,40,40,40	0
56	MG	1A	3254	1/1	0.96	0.24	56,56,56,56	0
56	MG	2A	3907	1/1	0.96	0.12	38,38,38,38	0
56	MG	2A	3664	1/1	0.96	0.13	62,62,62,62	0
56	MG	1A	3305	1/1	0.96	0.24	35,35,35,35	0
56	MG	2A	3666	1/1	0.96	0.10	47,47,47,47	0
56	MG	1a	1857	1/1	0.96	0.17	64,64,64,64	0
56	MG	2a	3161	1/1	0.96	0.08	70,70,70,70	0
56	MG	1A	3750	1/1	0.96	0.15	45,45,45,45	0
56	MG	1A	4212	1/1	0.96	0.16	32,32,32,32	0
56	MG	1a	1860	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3137	1/1	0.96	0.44	38,38,38,38	0
56	MG	1A	3175	1/1	0.96	0.46	43,43,43,43	0
56	MG	1A	3754	1/1	0.96	0.18	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3667	1/1	0.96	0.16	44,44,44,44	0
56	MG	1A	3009	1/1	0.96	0.20	33,33,33,33	0
56	MG	1A	3861	1/1	0.96	0.17	31,31,31,31	0
56	MG	2a	3172	1/1	0.96	0.07	62,62,62,62	0
56	MG	1A	3015	1/1	0.96	0.14	30,30,30,30	0
56	MG	1A	4095	1/1	0.96	0.29	51,51,51,51	0
56	MG	2B	3003	1/1	0.96	0.11	58,58,58,58	0
56	MG	1A	4096	1/1	0.96	0.19	17,17,17,17	0
56	MG	1A	4223	1/1	0.96	0.23	39,39,39,39	0
56	MG	1A	3864	1/1	0.96	0.18	24,24,24,24	0
56	MG	2A	3684	1/1	0.96	0.13	63,63,63,63	0
56	MG	2A	3074	1/1	0.96	0.08	38,38,38,38	0
56	MG	2A	3686	1/1	0.96	0.08	49,49,49,49	0
56	MG	1X	103	1/1	0.96	0.14	34,34,34,34	0
56	MG	1A	3606	1/1	0.96	0.15	54,54,54,54	0
56	MG	1A	3866	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3550	1/1	0.96	0.28	34,34,34,34	0
56	MG	1a	1721	1/1	0.96	0.10	41,41,41,41	0
56	MG	2A	3082	1/1	0.96	0.06	49,49,49,49	0
56	MG	2A	3695	1/1	0.96	0.09	43,43,43,43	0
56	MG	2A	3083	1/1	0.96	0.27	44,44,44,44	0
56	MG	1A	3869	1/1	0.96	0.18	26,26,26,26	0
56	MG	2A	3698	1/1	0.96	0.18	32,32,32,32	0
56	MG	1A	3762	1/1	0.96	0.11	29,29,29,29	0
56	MG	1A	3608	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3702	1/1	0.96	0.15	45,45,45,45	0
56	MG	1A	3873	1/1	0.96	0.18	57,57,57,57	0
56	MG	2a	3197	1/1	0.96	0.14	63,63,63,63	0
56	MG	2A	3704	1/1	0.96	0.13	50,50,50,50	0
56	MG	1A	4235	1/1	0.96	0.55	37,37,37,37	0
56	MG	1A	4236	1/1	0.96	0.20	37,37,37,37	0
56	MG	1A	3046	1/1	0.96	0.17	33,33,33,33	0
56	MG	1A	3989	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3032	1/1	0.96	0.86	47,47,47,47	0
56	MG	1A	4242	1/1	0.96	0.22	53,53,53,53	0
56	MG	2a	3205	1/1	0.96	0.18	59,59,59,59	0
56	MG	2A	3094	1/1	0.96	0.12	45,45,45,45	0
56	MG	1A	3221	1/1	0.96	0.17	46,46,46,46	0
56	MG	2A	3096	1/1	0.96	0.09	42,42,42,42	0
56	MG	1A	3093	1/1	0.96	0.23	26,26,26,26	0
56	MG	1A	3077	1/1	0.96	0.50	39,39,39,39	0
56	MG	1A	4247	1/1	0.96	0.15	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1738	1/1	0.96	0.09	51,51,51,51	0
56	MG	1A	3772	1/1	0.96	0.06	47,47,47,47	0
56	MG	1a	1895	1/1	0.96	0.06	58,58,58,58	0
56	MG	1A	3883	1/1	0.96	0.20	47,47,47,47	0
56	MG	1a	1741	1/1	0.96	0.07	51,51,51,51	0
56	MG	2R	202	1/1	0.96	0.34	50,50,50,50	0
56	MG	1a	1898	1/1	0.96	0.20	43,43,43,43	0
56	MG	1A	3614	1/1	0.96	0.09	40,40,40,40	0
56	MG	1A	3885	1/1	0.96	0.20	36,36,36,36	0
56	MG	2A	3731	1/1	0.96	0.24	62,62,62,62	0
56	MG	2U	204	1/1	0.96	0.37	42,42,42,42	0
56	MG	2A	3732	1/1	0.96	0.11	53,53,53,53	0
56	MG	1a	1744	1/1	0.96	0.14	45,45,45,45	0
56	MG	1A	3775	1/1	0.96	0.28	30,30,30,30	0
56	MG	1A	3095	1/1	0.96	0.27	47,47,47,47	0
56	MG	1A	3097	1/1	0.96	0.20	31,31,31,31	0
56	MG	18	102	1/1	0.96	0.27	45,45,45,45	0
56	MG	2X	102	1/1	0.96	0.23	66,66,66,66	0
56	MG	1A	3078	1/1	0.96	0.08	46,46,46,46	0
56	MG	1B	203	1/1	0.96	0.20	45,45,45,45	0
56	MG	2A	3504	1/1	0.96	0.12	47,47,47,47	0
56	MG	20	103	1/1	0.96	0.16	55,55,55,55	0
56	MG	2A	3117	1/1	0.96	0.10	54,54,54,54	0
56	MG	1A	3050	1/1	0.96	0.25	24,24,24,24	0
56	MG	2A	3306	1/1	0.96	0.14	44,44,44,44	0
56	MG	2A	3747	1/1	0.96	0.34	47,47,47,47	0
56	MG	2A	3119	1/1	0.96	0.11	48,48,48,48	0
56	MG	2A	3750	1/1	0.96	0.30	44,44,44,44	0
56	MG	1A	3619	1/1	0.96	0.31	41,41,41,41	0
56	MG	27	101	1/1	0.96	0.18	45,45,45,45	0
56	MG	1A	3896	1/1	0.96	0.18	38,38,38,38	0
56	MG	2q	201	1/1	0.96	0.07	55,55,55,55	0
56	MG	1A	3080	1/1	0.96	0.36	44,44,44,44	0
56	MG	1A	3563	1/1	0.96	0.57	44,44,44,44	0
56	MG	2A	3513	1/1	0.96	0.16	28,28,28,28	0
56	MG	1a	1606	1/1	0.96	0.09	68,68,68,68	0
56	MG	2A	3125	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3622	1/1	0.96	0.12	54,54,54,54	0
56	MG	2A	3518	1/1	0.96	0.14	32,32,32,32	0
56	MG	2A	3316	1/1	0.96	0.38	52,52,52,52	0
56	MG	1A	3623	1/1	0.96	0.07	36,36,36,36	0
56	MG	1a	1918	1/1	0.96	0.12	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1B	212	1/1	0.96	0.09	42,42,42,42	0
56	MG	2A	3130	1/1	0.96	0.20	47,47,47,47	0
56	MG	1A	3001	1/1	0.96	0.08	47,47,47,47	0
56	MG	1A	4131	1/1	0.96	0.12	24,24,24,24	0
56	MG	2a	3015	1/1	0.96	0.13	63,63,63,63	0
56	MG	1A	3461	1/1	0.96	0.38	45,45,45,45	0
56	MG	1a	1924	1/1	0.96	0.18	43,43,43,43	0
56	MG	1A	3194	1/1	0.96	0.22	49,49,49,49	0
56	MG	2A	3136	1/1	0.96	0.13	41,41,41,41	0
56	MG	2A	3327	1/1	0.96	0.20	54,54,54,54	0
56	MG	1A	3123	1/1	0.96	0.55	41,41,41,41	0
56	MG	1A	4016	1/1	0.96	0.16	58,58,58,58	0
56	MG	1A	3628	1/1	0.96	0.16	49,49,49,49	0
56	MG	2A	3140	1/1	0.96	0.06	45,45,45,45	0
56	MG	2A	3778	1/1	0.96	0.16	53,53,53,53	0
56	MG	1A	3003	1/1	0.96	0.20	30,30,30,30	0
56	MG	1a	1768	1/1	0.96	0.18	47,47,47,47	0
56	MG	1A	3696	1/1	0.96	0.13	49,49,49,49	0
56	MG	1A	4020	1/1	0.96	0.10	65,65,65,65	0
56	MG	1A	3698	1/1	0.96	0.21	48,48,48,48	0
56	MG	1A	3234	1/1	0.96	0.17	62,62,62,62	0
56	MG	1a	1625	1/1	0.96	0.16	50,50,50,50	0
56	MG	2A	3547	1/1	0.96	0.12	28,28,28,28	0
56	MG	1A	3235	1/1	0.96	0.23	52,52,52,52	0
59	ZN	1Y	501	1/1	0.96	0.11	79,79,79,79	0
56	MG	2A	3341	1/1	0.96	0.13	56,56,56,56	0
56	MG	1a	1775	1/1	0.96	0.29	60,60,60,60	0
56	MG	1A	3572	1/1	0.96	0.21	39,39,39,39	0
56	MG	1B	233	1/1	0.96	0.16	82,82,82,82	0
56	MG	1n	502	1/1	0.96	0.10	41,41,41,41	0
56	MG	2a	3040	1/1	0.96	0.25	44,44,44,44	0
56	MG	16	103	1/1	0.97	0.10	53,53,53,53	0
56	MG	2A	3099	1/1	0.97	0.29	44,44,44,44	0
56	MG	2A	3708	1/1	0.97	0.09	55,55,55,55	0
56	MG	2A	3709	1/1	0.97	0.06	59,59,59,59	0
56	MG	1A	3462	1/1	0.97	0.12	43,43,43,43	0
56	MG	2A	3535	1/1	0.97	0.20	37,37,37,37	0
56	MG	1a	1823	1/1	0.97	0.21	51,51,51,51	0
56	MG	1A	3261	1/1	0.97	0.08	56,56,56,56	0
56	MG	2A	3538	1/1	0.97	0.15	48,48,48,48	0
56	MG	2a	3101	1/1	0.97	0.23	40,40,40,40	0
56	MG	1D	306	1/1	0.97	0.23	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3716	1/1	0.97	0.14	29,29,29,29	0
56	MG	1w	102	1/1	0.97	0.22	77,77,77,77	0
56	MG	1A	3758	1/1	0.97	0.10	36,36,36,36	0
56	MG	1A	3166	1/1	0.97	0.64	42,42,42,42	0
56	MG	1a	1828	1/1	0.97	0.14	67,67,67,67	0
56	MG	1A	3760	1/1	0.97	0.16	29,29,29,29	0
56	MG	1A	4039	1/1	0.97	0.14	51,51,51,51	0
56	MG	1A	3145	1/1	0.97	0.42	45,45,45,45	0
56	MG	1A	3963	1/1	0.97	0.41	38,38,38,38	0
56	MG	1A	3556	1/1	0.97	0.53	45,45,45,45	0
56	MG	1A	4044	1/1	0.97	0.11	50,50,50,50	0
56	MG	1A	4122	1/1	0.97	0.12	48,48,48,48	0
56	MG	2A	3728	1/1	0.97	0.11	32,32,32,32	0
56	MG	2A	3729	1/1	0.97	0.10	48,48,48,48	0
56	MG	2a	3118	1/1	0.97	0.15	70,70,70,70	0
56	MG	1A	3168	1/1	0.97	0.27	36,36,36,36	0
56	MG	1A	3824	1/1	0.97	0.09	65,65,65,65	0
56	MG	1A	3764	1/1	0.97	0.10	40,40,40,40	0
56	MG	2a	3122	1/1	0.97	0.14	53,53,53,53	0
56	MG	1A	3525	1/1	0.97	0.48	47,47,47,47	0
56	MG	2A	3556	1/1	0.97	0.12	59,59,59,59	0
56	MG	1a	1610	1/1	0.97	0.45	64,64,64,64	0
56	MG	1A	4049	1/1	0.97	0.13	63,63,63,63	0
56	MG	2A	3259	1/1	0.97	0.20	59,59,59,59	0
56	MG	1a	1727	1/1	0.97	0.11	38,38,38,38	0
56	MG	2B	3010	1/1	0.97	0.12	59,59,59,59	0
56	MG	1E	311	1/1	0.97	0.08	34,34,34,34	0
56	MG	2A	3562	1/1	0.97	0.16	23,23,23,23	0
56	MG	1A	4214	1/1	0.97	0.21	47,47,47,47	0
56	MG	1A	3439	1/1	0.97	0.14	43,43,43,43	0
56	MG	2A	3745	1/1	0.97	0.15	51,51,51,51	0
56	MG	1A	3047	1/1	0.97	0.13	30,30,30,30	0
56	MG	1A	3561	1/1	0.97	0.72	42,42,42,42	0
56	MG	2A	3407	1/1	0.97	0.14	62,62,62,62	0
56	MG	1A	3769	1/1	0.97	0.23	27,27,27,27	0
56	MG	2A	3267	1/1	0.97	0.12	56,56,56,56	0
56	MG	2A	3570	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3048	1/1	0.97	0.15	34,34,34,34	0
56	MG	1A	4055	1/1	0.97	0.12	47,47,47,47	0
56	MG	1A	4134	1/1	0.97	0.05	36,36,36,36	0
56	MG	1y	3001	1/1	0.97	0.60	42,42,42,42	0
56	MG	2A	3575	1/1	0.97	0.06	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1y	3002	1/1	0.97	0.09	55,55,55,55	0
56	MG	1A	3771	1/1	0.97	0.17	25,25,25,25	0
56	MG	1A	3907	1/1	0.97	0.27	35,35,35,35	0
56	MG	1A	4224	1/1	0.97	0.41	49,49,49,49	0
56	MG	1A	4225	1/1	0.97	0.35	35,35,35,35	0
56	MG	2A	3763	1/1	0.97	0.14	49,49,49,49	0
56	MG	2F	301	1/1	0.97	0.21	44,44,44,44	0
56	MG	1A	3268	1/1	0.97	0.23	43,43,43,43	0
56	MG	1A	3773	1/1	0.97	0.13	54,54,54,54	0
56	MG	1A	4060	1/1	0.97	0.09	52,52,52,52	0
56	MG	1A	3835	1/1	0.97	0.20	37,37,37,37	0
56	MG	1A	3564	1/1	0.97	0.35	40,40,40,40	0
56	MG	2O	8001	1/1	0.97	0.12	50,50,50,50	0
56	MG	2A	3144	1/1	0.97	0.25	39,39,39,39	0
56	MG	1A	3675	1/1	0.97	0.15	53,53,53,53	0
56	MG	2A	3588	1/1	0.97	0.26	36,36,36,36	0
56	MG	1A	3914	1/1	0.97	0.15	41,41,41,41	0
56	MG	1A	3008	1/1	0.97	0.20	26,26,26,26	0
56	MG	2A	3149	1/1	0.97	0.26	35,35,35,35	0
56	MG	2A	3010	1/1	0.97	0.12	47,47,47,47	0
56	MG	2A	3776	1/1	0.97	0.20	33,33,33,33	0
56	MG	2A	3430	1/1	0.97	0.34	57,57,57,57	0
56	MG	1A	3531	1/1	0.97	0.28	34,34,34,34	0
56	MG	2a	3171	1/1	0.97	0.10	71,71,71,71	0
56	MG	1A	3150	1/1	0.97	0.19	43,43,43,43	0
56	MG	1A	3068	1/1	0.97	0.08	55,55,55,55	0
56	MG	1A	4238	1/1	0.97	0.45	39,39,39,39	0
56	MG	2V	201	1/1	0.97	0.13	50,50,50,50	0
56	MG	2A	3601	1/1	0.97	0.14	38,38,38,38	0
56	MG	2A	3015	1/1	0.97	0.13	34,34,34,34	0
56	MG	1A	3727	1/1	0.97	0.12	26,26,26,26	0
56	MG	1A	3641	1/1	0.97	0.12	40,40,40,40	0
56	MG	2X	101	1/1	0.97	0.10	45,45,45,45	0
56	MG	2A	3786	1/1	0.97	0.05	42,42,42,42	0
56	MG	2A	3787	1/1	0.97	0.04	51,51,51,51	0
56	MG	2A	3605	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3991	1/1	0.97	0.45	53,53,53,53	0
56	MG	1A	3534	1/1	0.97	0.25	19,19,19,19	0
56	MG	2A	3608	1/1	0.97	0.09	57,57,57,57	0
56	MG	1A	3323	1/1	0.97	0.23	43,43,43,43	0
56	MG	1A	4155	1/1	0.97	0.15	19,19,19,19	0
56	MG	1P	201	1/1	0.97	0.56	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3190	1/1	0.97	0.18	46,46,46,46	0
56	MG	1A	3784	1/1	0.97	0.12	65,65,65,65	0
56	MG	2A	3164	1/1	0.97	0.50	43,43,43,43	0
56	MG	2A	3614	1/1	0.97	0.17	54,54,54,54	0
56	MG	1A	3174	1/1	0.97	0.40	47,47,47,47	0
56	MG	1A	4249	1/1	0.97	0.29	46,46,46,46	0
56	MG	28	102	1/1	0.97	0.16	55,55,55,55	0
56	MG	1A	3786	1/1	0.97	0.21	48,48,48,48	0
56	MG	1A	3298	1/1	0.97	0.24	49,49,49,49	0
56	MG	1A	4252	1/1	0.97	0.29	24,24,24,24	0
56	MG	1a	1653	1/1	0.97	0.09	48,48,48,48	0
56	MG	2A	3034	1/1	0.97	0.16	41,41,41,41	0
56	MG	1A	3927	1/1	0.97	0.07	65,65,65,65	0
56	MG	2A	3624	1/1	0.97	0.12	45,45,45,45	0
56	MG	2A	3625	1/1	0.97	0.12	53,53,53,53	0
56	MG	1A	3195	1/1	0.97	0.61	39,39,39,39	0
56	MG	1A	3789	1/1	0.97	0.29	39,39,39,39	0
56	MG	2A	3462	1/1	0.97	0.25	42,42,42,42	0
56	MG	1A	3734	1/1	0.97	0.12	55,55,55,55	0
56	MG	2a	3012	1/1	0.97	0.14	57,57,57,57	0
56	MG	2A	3630	1/1	0.97	0.19	35,35,35,35	0
56	MG	2A	3464	1/1	0.97	0.04	53,53,53,53	0
56	MG	1B	201	1/1	0.97	0.11	24,24,24,24	0
56	MG	1A	3450	1/1	0.97	0.15	51,51,51,51	0
56	MG	1A	3161	1/1	0.97	0.21	46,46,46,46	0
56	MG	2a	3215	1/1	0.97	0.18	69,69,69,69	0
56	MG	2A	3468	1/1	0.97	0.35	62,62,62,62	0
56	MG	2a	3217	1/1	0.97	0.27	45,45,45,45	0
56	MG	2a	3218	1/1	0.97	0.09	49,49,49,49	0
56	MG	1A	3177	1/1	0.97	0.12	42,42,42,42	0
56	MG	1A	4167	1/1	0.97	0.13	47,47,47,47	0
56	MG	1B	206	1/1	0.97	0.37	51,51,51,51	0
56	MG	1U	202	1/1	0.97	0.43	35,35,35,35	0
56	MG	1A	3689	1/1	0.97	0.34	30,30,30,30	0
56	MG	1A	3509	1/1	0.97	0.25	38,38,38,38	0
56	MG	1U	205	1/1	0.97	0.34	42,42,42,42	0
56	MG	2A	3187	1/1	0.97	0.14	38,38,38,38	0
56	MG	2A	3477	1/1	0.97	0.36	44,44,44,44	0
56	MG	2a	3228	1/1	0.97	0.29	66,66,66,66	0
56	MG	2A	3647	1/1	0.97	0.25	39,39,39,39	0
56	MG	1A	3796	1/1	0.97	0.09	32,32,32,32	0
56	MG	1A	3740	1/1	0.97	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3833	1/1	0.97	0.06	34,34,34,34	0
56	MG	1V	202	1/1	0.97	0.18	65,65,65,65	0
56	MG	1A	3453	1/1	0.97	0.25	42,42,42,42	0
56	MG	1a	1903	1/1	0.97	0.16	49,49,49,49	0
56	MG	1A	3178	1/1	0.97	0.16	18,18,18,18	0
56	MG	1W	3003	1/1	0.97	0.53	45,45,45,45	0
56	MG	1A	3179	1/1	0.97	0.11	39,39,39,39	0
56	MG	1A	4176	1/1	0.97	0.17	55,55,55,55	0
56	MG	1a	1908	1/1	0.97	0.13	56,56,56,56	0
56	MG	2A	3337	1/1	0.97	0.15	53,53,53,53	0
56	MG	2A	3199	1/1	0.97	0.44	55,55,55,55	0
56	MG	1B	217	1/1	0.97	0.08	28,28,28,28	0
56	MG	2l	3003	1/1	0.97	0.12	68,68,68,68	0
56	MG	1B	218	1/1	0.97	0.28	22,22,22,22	0
56	MG	1A	3654	1/1	0.97	0.28	52,52,52,52	0
56	MG	1A	3162	1/1	0.97	0.79	40,40,40,40	0
56	MG	2A	3494	1/1	0.97	0.17	59,59,59,59	0
56	MG	1Y	502	1/1	0.97	0.08	50,50,50,50	0
56	MG	1A	3868	1/1	0.97	0.18	38,38,38,38	0
56	MG	2A	3497	1/1	0.97	0.45	58,58,58,58	0
56	MG	1A	3039	1/1	0.97	0.52	33,33,33,33	0
56	MG	1a	1686	1/1	0.97	0.17	42,42,42,42	0
56	MG	1Z	303	1/1	0.97	0.14	62,62,62,62	0
56	MG	1A	3697	1/1	0.97	0.24	34,34,34,34	0
56	MG	1B	224	1/1	0.97	0.16	76,76,76,76	0
56	MG	2A	3673	1/1	0.97	0.17	33,33,33,33	0
56	MG	1A	3748	1/1	0.97	0.13	56,56,56,56	0
56	MG	2A	3351	1/1	0.97	0.29	48,48,48,48	0
56	MG	2A	3075	1/1	0.97	0.33	46,46,46,46	0
56	MG	2A	3353	1/1	0.97	0.42	73,73,73,73	0
56	MG	2A	3678	1/1	0.97	0.11	29,29,29,29	0
56	MG	1A	3806	1/1	0.97	0.14	33,33,33,33	0
56	MG	1A	3064	1/1	0.97	0.11	37,37,37,37	0
56	MG	1a	1923	1/1	0.97	0.15	69,69,69,69	0
56	MG	2A	3079	1/1	0.97	0.15	47,47,47,47	0
56	MG	10	107	1/1	0.97	0.15	55,55,55,55	0
56	MG	1A	3584	1/1	0.97	0.26	57,57,57,57	0
56	MG	1A	3702	1/1	0.97	0.15	56,56,56,56	0
56	MG	1A	3284	1/1	0.97	0.34	40,40,40,40	0
56	MG	1A	4026	1/1	0.97	0.12	30,30,30,30	0
56	MG	1a	1698	1/1	0.97	0.17	36,36,36,36	0
56	MG	2A	3517	1/1	0.97	0.10	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1699	1/1	0.97	0.33	38,38,38,38	0
56	MG	2A	3880	1/1	0.97	0.05	55,55,55,55	0
56	MG	1A	3311	1/1	0.97	0.20	53,53,53,53	0
56	MG	1A	4107	1/1	0.97	0.09	36,36,36,36	0
57	CPT	1A	4209	4/5	0.97	0.21	75,78,104,121	4
56	MG	1d	502	1/1	0.97	0.34	55,55,55,55	0
56	MG	2A	3884	1/1	0.97	0.29	32,32,32,32	0
56	MG	1e	3001	1/1	0.97	0.14	61,61,61,61	0
57	CPT	2I	201	4/5	0.97	0.13	67,68,96,140	4
56	MG	1a	1702	1/1	0.97	0.23	42,42,42,42	0
56	MG	2A	3887	1/1	0.97	0.11	54,54,54,54	0
56	MG	1B	235	1/1	0.97	0.12	52,52,52,52	0
56	MG	1A	3880	1/1	0.97	0.21	32,32,32,32	0
56	MG	2A	3700	1/1	0.97	0.09	56,56,56,56	0
56	MG	1A	3154	1/1	0.97	0.23	49,49,49,49	0
56	MG	1D	302	1/1	0.97	0.42	44,44,44,44	0
56	MG	1a	1819	1/1	0.97	0.12	46,46,46,46	0
56	MG	1A	3882	1/1	0.97	0.20	59,59,59,59	0
56	MG	1Y	503	1/1	0.98	0.68	54,54,54,54	0
56	MG	1A	4025	1/1	0.98	0.05	53,53,53,53	0
56	MG	2A	3531	1/1	0.98	0.20	21,21,21,21	0
56	MG	2A	3438	1/1	0.98	0.35	44,44,44,44	0
56	MG	1B	214	1/1	0.98	0.14	46,46,46,46	0
56	MG	2A	3838	1/1	0.98	0.17	31,31,31,31	0
56	MG	1A	3031	1/1	0.98	0.17	27,27,27,27	0
56	MG	2A	3632	1/1	0.98	0.20	34,34,34,34	0
56	MG	2A	3180	1/1	0.98	0.18	22,22,22,22	0
56	MG	10	101	1/1	0.98	0.04	51,51,51,51	0
56	MG	1B	216	1/1	0.98	0.14	37,37,37,37	0
56	MG	2A	3737	1/1	0.98	0.11	58,58,58,58	0
56	MG	1A	3388	1/1	0.98	0.41	45,45,45,45	0
56	MG	1A	3271	1/1	0.98	0.31	47,47,47,47	0
56	MG	1A	3176	1/1	0.98	0.18	42,42,42,42	0
56	MG	2A	3639	1/1	0.98	0.30	49,49,49,49	0
56	MG	2P	202	1/1	0.98	0.06	41,41,41,41	0
56	MG	2A	3850	1/1	0.98	0.13	68,68,68,68	0
56	MG	2a	3079	1/1	0.98	0.13	40,40,40,40	0
56	MG	2A	3541	1/1	0.98	0.08	29,29,29,29	0
56	MG	1A	4030	1/1	0.98	0.07	29,29,29,29	0
56	MG	1A	4170	1/1	0.98	0.21	13,13,13,13	0
56	MG	2A	3021	1/1	0.98	0.21	34,34,34,34	0
56	MG	1A	4031	1/1	0.98	0.05	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3453	1/1	0.98	0.24	53,53,53,53	0
56	MG	2A	3749	1/1	0.98	0.11	49,49,49,49	0
56	MG	2a	3087	1/1	0.98	0.11	64,64,64,64	0
56	MG	1A	3146	1/1	0.98	0.25	32,32,32,32	0
56	MG	1A	3872	1/1	0.98	0.12	55,55,55,55	0
56	MG	1A	3072	1/1	0.98	0.18	15,15,15,15	0
56	MG	1A	3035	1/1	0.98	0.08	54,54,54,54	0
56	MG	2A	3278	1/1	0.98	0.14	57,57,57,57	0
56	MG	1a	1786	1/1	0.98	0.04	53,53,53,53	0
56	MG	1b	3001	1/1	0.98	0.07	62,62,62,62	0
56	MG	1b	3002	1/1	0.98	0.06	65,65,65,65	0
56	MG	2A	3197	1/1	0.98	0.13	44,44,44,44	0
56	MG	2A	3867	1/1	0.98	0.11	33,33,33,33	0
56	MG	1A	3042	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	3096	1/1	0.98	0.15	46,46,46,46	0
56	MG	1a	1651	1/1	0.98	0.23	39,39,39,39	0
56	MG	1A	3994	1/1	0.98	0.13	44,44,44,44	0
56	MG	1e	3002	1/1	0.98	0.53	65,65,65,65	0
56	MG	2A	3037	1/1	0.98	0.18	33,33,33,33	0
56	MG	1a	1862	1/1	0.98	0.10	49,49,49,49	0
56	MG	1A	3182	1/1	0.98	0.19	58,58,58,58	0
56	MG	1A	4041	1/1	0.98	0.07	71,71,71,71	0
56	MG	1B	232	1/1	0.98	0.13	44,44,44,44	0
56	MG	1O	3004	1/1	0.98	0.21	54,54,54,54	0
56	MG	1a	1657	1/1	0.98	0.19	48,48,48,48	0
56	MG	17	101	1/1	0.98	0.16	38,38,38,38	0
56	MG	1A	4233	1/1	0.98	0.32	47,47,47,47	0
56	MG	2A	3046	1/1	0.98	0.04	37,37,37,37	0
56	MG	1A	3023	1/1	0.98	0.29	46,46,46,46	0
56	MG	2A	3299	1/1	0.98	0.13	58,58,58,58	0
56	MG	1A	3752	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3086	1/1	0.98	0.39	56,56,56,56	0
56	MG	1A	3724	1/1	0.98	0.20	31,31,31,31	0
56	MG	1A	3037	1/1	0.98	0.19	21,21,21,21	0
56	MG	1A	3283	1/1	0.98	0.27	42,42,42,42	0
56	MG	2d	502	1/1	0.98	0.09	58,58,58,58	0
56	MG	19	103	1/1	0.98	0.16	41,41,41,41	0
56	MG	2f	3001	1/1	0.98	0.20	41,41,41,41	0
56	MG	1A	4187	1/1	0.98	0.17	28,28,28,28	0
56	MG	1a	1736	1/1	0.98	0.23	44,44,44,44	0
56	MG	1a	1668	1/1	0.98	0.10	48,48,48,48	0
56	MG	1a	1669	1/1	0.98	0.05	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3038	1/1	0.98	0.42	46,46,46,46	0
56	MG	1A	3852	1/1	0.98	0.18	48,48,48,48	0
56	MG	1D	307	1/1	0.98	0.21	25,25,25,25	0
56	MG	1A	3307	1/1	0.98	0.16	53,53,53,53	0
56	MG	1A	3965	1/1	0.98	0.16	45,45,45,45	0
56	MG	2A	3791	1/1	0.98	0.10	46,46,46,46	0
56	MG	2A	3315	1/1	0.98	0.33	62,62,62,62	0
56	MG	1A	4143	1/1	0.98	0.20	36,36,36,36	0
56	MG	2q	203	1/1	0.98	0.24	72,72,72,72	0
56	MG	2a	3135	1/1	0.98	0.22	95,95,95,95	0
56	MG	2A	3794	1/1	0.98	0.08	74,74,74,74	0
56	MG	2A	3590	1/1	0.98	0.17	30,30,30,30	0
56	MG	2v	101	1/1	0.98	0.27	55,55,55,55	0
56	MG	2A	3690	1/1	0.98	0.06	43,43,43,43	0
56	MG	1A	4144	1/1	0.98	0.18	34,34,34,34	0
56	MG	2A	3148	1/1	0.98	0.15	45,45,45,45	0
56	MG	1A	3524	1/1	0.98	0.39	43,43,43,43	0
56	MG	1A	3700	1/1	0.98	0.07	55,55,55,55	0
56	MG	1A	3701	1/1	0.98	0.13	31,31,31,31	0
56	MG	2A	3914	1/1	0.98	0.49	38,38,38,38	0
56	MG	2A	3596	1/1	0.98	0.14	29,29,29,29	0
56	MG	2A	3597	1/1	0.98	0.09	28,28,28,28	0
56	MG	1A	3127	1/1	0.98	0.38	46,46,46,46	0
56	MG	1a	1613	1/1	0.98	0.17	18,18,18,18	0
56	MG	2A	3071	1/1	0.98	0.28	31,31,31,31	0
56	MG	1a	1893	1/1	0.98	0.12	36,36,36,36	0
56	MG	1A	3895	1/1	0.98	0.07	48,48,48,48	0
56	MG	1A	3060	1/1	0.98	0.16	50,50,50,50	0
56	MG	1a	1616	1/1	0.98	0.14	36,36,36,36	0
56	MG	1A	4200	1/1	0.98	0.06	55,55,55,55	0
56	MG	2A	3707	1/1	0.98	0.10	50,50,50,50	0
56	MG	1A	3897	1/1	0.98	0.41	44,44,44,44	0
56	MG	1A	3973	1/1	0.98	0.16	41,41,41,41	0
56	MG	2a	3042	1/1	0.98	0.10	81,81,81,81	0
56	MG	1A	3142	1/1	0.98	0.21	22,22,22,22	0
56	MG	1A	3028	1/1	0.98	0.37	28,28,28,28	0
56	MG	1A	3289	1/1	0.98	0.41	59,59,59,59	0
56	MG	2A	3818	1/1	0.98	0.08	55,55,55,55	0
56	MG	1A	3977	1/1	0.98	0.10	45,45,45,45	0
56	MG	1W	3004	1/1	0.98	0.28	39,39,39,39	0
57	CPT	1I	3002	4/5	0.98	0.11	70,77,97,175	0
56	MG	1A	4110	1/1	0.98	0.12	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	CPT	2A	3903	4/5	0.98	0.13	70,73,87,100	4
56	MG	1A	3901	1/1	0.98	0.13	60,60,60,60	0
56	MG	1A	3191	1/1	0.98	0.54	48,48,48,48	0
57	CPT	2a	3235	4/5	0.98	0.12	85,87,90,125	0
56	MG	1A	3070	1/1	0.98	0.20	25,25,25,25	0
56	MG	1X	104	1/1	0.98	0.50	48,48,48,48	0
56	MG	1A	3249	1/1	0.98	0.20	44,44,44,44	0
56	MG	1a	1838	1/1	0.98	0.14	39,39,39,39	0
59	ZN	15	103	1/1	0.98	0.17	46,46,46,46	0
56	MG	1A	3905	1/1	0.98	0.12	27,27,27,27	0
56	MG	2A	3432	1/1	0.98	0.17	38,38,38,38	0
56	MG	2A	3526	1/1	0.98	0.10	48,48,48,48	0
56	MG	1A	3711	1/1	0.98	0.19	51,51,51,51	0
56	MG	2A	3434	1/1	0.98	0.32	46,46,46,46	0
60	SF4	2d	501	8/8	0.98	0.12	58,66,75,87	0
56	MG	1A	3432	1/1	0.99	0.36	40,40,40,40	0
56	MG	1A	3813	1/1	0.99	0.18	34,34,34,34	0
56	MG	2a	3153	1/1	0.99	0.13	43,43,43,43	0
56	MG	1A	3280	1/1	0.99	0.21	29,29,29,29	0
56	MG	1A	3886	1/1	0.99	0.21	26,26,26,26	0
56	MG	1A	3815	1/1	0.99	0.13	44,44,44,44	0
56	MG	1A	3099	1/1	0.99	0.27	57,57,57,57	0
56	MG	1A	3908	1/1	0.99	0.08	47,47,47,47	0
56	MG	1A	3229	1/1	0.99	0.17	47,47,47,47	0
56	MG	2A	3060	1/1	0.99	0.26	50,50,50,50	0
56	MG	1A	4036	1/1	0.99	0.06	71,71,71,71	0
56	MG	2A	3397	1/1	0.99	0.06	36,36,36,36	0
56	MG	2A	3691	1/1	0.99	0.16	66,66,66,66	0
56	MG	2a	3114	1/1	0.99	0.10	69,69,69,69	0
56	MG	2A	3437	1/1	0.99	0.24	45,45,45,45	0
56	MG	2A	3027	1/1	0.99	0.10	27,27,27,27	0
56	MG	2A	3738	1/1	0.99	0.08	63,63,63,63	0
56	MG	2A	3028	1/1	0.99	0.45	47,47,47,47	0
56	MG	2A	3876	1/1	0.99	0.10	62,62,62,62	0
56	MG	1A	3262	1/1	0.99	0.10	58,58,58,58	0
56	MG	1A	3951	1/1	0.99	0.08	43,43,43,43	0
56	MG	15	104	1/1	0.99	0.30	42,42,42,42	0
56	MG	2A	3443	1/1	0.99	0.19	43,43,43,43	0
56	MG	2A	3444	1/1	0.99	0.31	32,32,32,32	0
56	MG	1A	3845	1/1	0.99	0.20	25,25,25,25	0
56	MG	1W	3006	1/1	0.99	0.13	35,35,35,35	0
56	MG	1A	3892	1/1	0.99	0.06	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3141	1/1	0.99	0.24	35,35,35,35	0
56	MG	1A	3126	1/1	0.99	0.19	40,40,40,40	0
56	MG	1w	105	1/1	0.99	0.11	58,58,58,58	0
56	MG	2A	3619	1/1	0.99	0.13	44,44,44,44	0
56	MG	1A	3894	1/1	0.99	0.20	34,34,34,34	0
56	MG	1A	4241	1/1	0.99	0.15	23,23,23,23	0
56	MG	1A	3876	1/1	0.99	0.22	48,48,48,48	0
56	MG	1A	3708	1/1	0.99	0.27	16,16,16,16	0
56	MG	1A	3309	1/1	0.99	0.43	47,47,47,47	0
56	MG	2A	3847	1/1	0.99	0.15	30,30,30,30	0
56	MG	1A	4245	1/1	0.99	0.19	46,46,46,46	0
56	MG	1A	4001	1/1	0.99	0.16	32,32,32,32	0
56	MG	1A	3863	1/1	0.99	0.12	59,59,59,59	0
56	MG	2A	3115	1/1	0.99	0.21	46,46,46,46	0
56	MG	1A	4094	1/1	0.99	0.09	22,22,22,22	0
56	MG	1A	3310	1/1	0.99	0.18	42,42,42,42	0
56	MG	1A	3823	1/1	0.99	0.18	28,28,28,28	0
59	ZN	19	102	1/1	0.99	0.10	27,27,27,27	0
59	ZN	1n	501	1/1	0.99	0.15	59,59,59,59	0
56	MG	1E	301	1/1	0.99	0.18	14,14,14,14	0
56	MG	2a	3097	1/1	0.99	0.24	48,48,48,48	0
59	ZN	25	102	1/1	0.99	0.13	61,61,61,61	0
56	MG	1A	4097	1/1	0.99	0.08	23,23,23,23	0
56	MG	2A	3016	1/1	0.99	0.12	52,52,52,52	0
56	MG	1A	3203	1/1	0.99	0.15	38,38,38,38	0
60	SF4	1d	501	8/8	0.99	0.18	55,59,67,69	0
56	MG	2A	3234	1/1	0.99	0.14	62,62,62,62	0
59	ZN	16	101	1/1	1.00	0.16	47,47,47,47	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.