



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 08:58 PM EST

PDB ID : 8G2A
Title : Crystal structure of the A2503-C2,C8-dimethylated *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A-site Phe-tRNA^{phe}, peptidyl P-site fMTHSMRC-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.45Å resolution
Authors : Aleksandrova, E.V.; Wu, K.J.Y.; Tresco, B.I.C.; Syroegin, E.A.; Killeavy, E.E.; Balasanyants, S.M.; Svetlov, M.S.; Gregory, S.T.; Atkinson, G.C.; Myers, A.G.; Polikanov, Y.S.
Deposited on : 2023-02-03
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

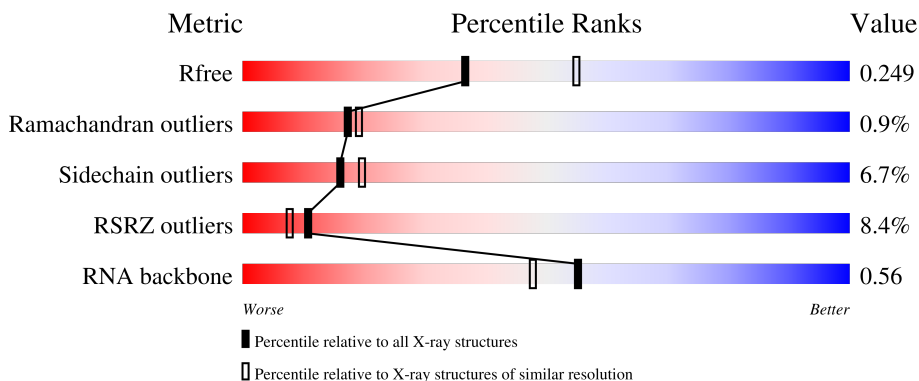
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)
RNA backbone	3102	1001 (2.80-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	2A	2915	
2	1B	121	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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Mol	Chain	Length	Quality of chain
2	2B	121	 2% 78% 21%
3	1D	276	 % 97%
3	2D	276	 % 96%
4	1E	206	 96%
4	2E	206	 6% 96%
5	1F	210	 89% 7%
5	2F	210	 93%
6	1G	182	 % 94% 5%
6	2G	182	 12% 88% 10%
7	1H	180	 % 94%
7	2H	180	 66% 94%
8	1I	148	 3% 89% 9%
8	2I	148	 4% 88% 10%
9	1N	140	 % 94% 6%
9	2N	140	 4% 92% 8%
10	1O	122	 98%
10	2O	122	 2% 94% 6%
11	1P	150	 % 93% 7%
11	2P	150	 8% 92% 7%
12	1Q	141	 % 99%
12	2Q	141	 20% 96%
13	1R	118	 97%
13	2R	118	 98%
14	1S	112	 92% 6%
14	2S	112	 9% 91% 6%

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Mol	Chain	Length	Quality of chain
15	1T	146	85% 5% 10%
15	2T	146	86% 10%
16	1U	118	96%
16	2U	118	94%
17	1V	101	97%
17	2V	101	97%
18	1W	113	96%
18	2W	113	97%
19	1X	96	95%
19	2X	96	97%
20	1Y	110	90% 7%
20	2Y	110	94%
21	1Z	206	68% 6% 25%
21	2Z	206	70% 7% 22%
22	10	85	98%
22	20	85	98%
23	11	98	97%
23	21	98	97%
24	12	72	93%
24	22	72	94%
25	13	60	93% 5%
25	23	60	90% 8%
26	14	71	85% 8%
26	24	71	79% 18%
27	15	60	93% 5%

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Mol	Chain	Length	Quality of chain
27	25	60	92% 7%
28	16	54	87% 11%
28	26	54	7% 89% 9%
29	17	49	6% 90% 8%
29	27	49	12% 90% 8%
30	18	65	91% 8%
30	28	65	5% 92% 6%
31	19	37	100%
31	29	37	76% 100%
32	1a	1521	5% 82% 16%
32	2a	1521	6% 81% 17%
33	1b	256	5% 78% 12% 10%
33	2b	256	13% 78% 12% 10%
34	1c	239	6% 80% 6% 14%
34	2c	239	21% 78% 8% 14%
35	1d	209	5% 89% 10%
35	2d	209	11% 92% 7%
36	1e	162	4% 84% 7% 9%
36	2e	162	7% 84% 7% 9%
37	1f	101	95%
37	2f	101	92% 7%
38	1g	156	10% 89% 10%
38	2g	156	17% 88% 12%
39	1h	138	4% 96%
39	2h	138	4% 93% 7%


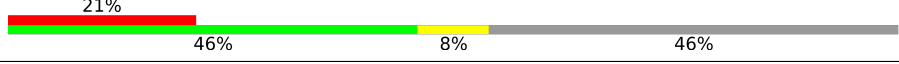
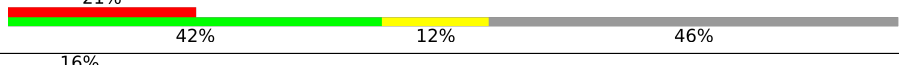


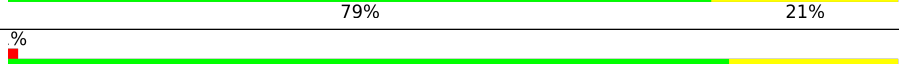
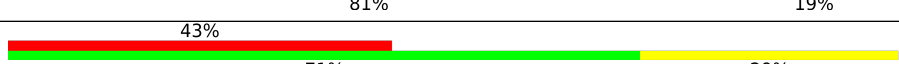
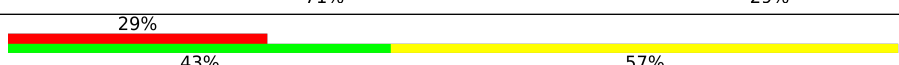
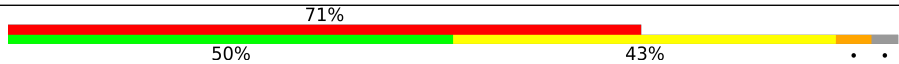


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Mol	Chain	Length	Quality of chain
40	1i	128	30% 91% 8%
40	2i	128	48% 90% 9%
41	1j	105	17% 81% 11% 8%
41	2j	105	46% 81% 10% 9%
42	1k	129	4% 84% 12%
42	2k	129	5% 83% 5% 12%
43	1l	132	5% 87% 5% 8%
43	2l	132	11% 86% 7% 8%
44	1m	126	7% 92% 5%
44	2m	126	20% 89% 7%
45	1n	61	31% 82% 15%
45	2n	61	84% 95%
46	1o	89	6% 97%
46	2o	89	4% 94%
47	1p	88	22% 91% 7%
47	2p	88	5% 88% 6% 7%
48	1q	105	11% 90% 6%
48	2q	105	5% 90% 6%
49	1r	88	74% 23%
49	2r	88	73% 5% 23%
50	1s	93	8% 87% 11%
50	2s	93	41% 82% 6% 11%
51	1t	106	34% 83% 7% 9%
51	2t	106	16% 87% 9%
52	1u	27	30% 81% 15%

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Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1z	7	
56	2z	7	
57	1y	76	
57	2y	76	

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	FME	1z	1	-	-	-	X
56	FME	2z	1	-	-	-	X
57	MIA	1y	37	-	-	-	X
57	5MU	1y	54	-	-	-	X
57	PSU	1y	55	-	-	-	X
57	PSU	2y	32	-	-	-	X
57	MIA	2y	37	-	-	-	X
57	5MU	2y	54	-	-	-	X
57	PSU	2y	55	-	-	-	X
58	MG	18	104	-	-	-	X
58	MG	1A	3178	-	-	-	X
58	MG	1A	3285	-	-	-	X
58	MG	1A	3339	-	-	-	X
58	MG	1A	3388	-	-	-	X
58	MG	1A	3416	-	-	-	X
58	MG	1A	3542	-	-	-	X
58	MG	1A	3547	-	-	-	X
58	MG	1A	3682	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1A	3890	-	-	-	X
58	MG	1A	3899	-	-	-	X
58	MG	1A	3975	-	-	-	X
58	MG	1A	4027	-	-	-	X
58	MG	1B	202	-	-	-	X
58	MG	1B	204	-	-	-	X
58	MG	27	103	-	-	-	X
58	MG	2A	3001	-	-	-	X
58	MG	2A	3004	-	-	-	X
58	MG	2A	3038	-	-	-	X
58	MG	2A	3044	-	-	-	X
58	MG	2A	3070	-	-	-	X
58	MG	2A	3073	-	-	-	X
58	MG	2A	3160	-	-	-	X
58	MG	2A	3189	-	-	-	X
58	MG	2A	3223	-	-	-	X
58	MG	2A	3268	-	-	-	X
58	MG	2A	3274	-	-	-	X
58	MG	2A	3304	-	-	-	X
58	MG	2A	3361	-	-	-	X
58	MG	2A	3374	-	-	-	X
58	MG	2A	3618	-	-	-	X
58	MG	2A	3691	-	-	-	X
58	MG	2D	301	-	-	-	X
58	MG	2a	1617	-	-	-	X
58	MG	2a	1721	-	-	-	X

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 300665 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
			61853	27532	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60323	26849	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
			Total	C	N	O	S			
5	1F	202	Total 1583	C 1009	N 297	O 275	S 2	0	0	0
5	2F	202	Total 1579	C 1007	N 296	O 274	S 2	0	0	0

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

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

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

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

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

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

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

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

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

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

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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
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MF-mRNA.

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

- Molecule 54 is a RNA chain called A-site Aminoacylated Phe-tRNA_{phe}.

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

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMTHSMRC-tRNA_{met} RNA-part.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
55	1x	77	Total 1646	C 734	N 298	O 536	P 77	S 1	0	0	0
55	2x	77	Total 1646	C 734	N 298	O 536	P 77	S 1	0	0	0

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMTHSMRC-tRNA_{met} Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
56	1z	7	Total 58	C 33	N 12	O 10	S 3	0	0	0
56	2z	7	Total 58	C 33	N 12	O 10	S 3	0	0	0

- Molecule 57 is a RNA chain called E-site Deacylated tRNA_{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
57	1y	74	Total 1585	C 707	N 285	O 518	P 74	S 1	0	0	0
57	2y	73	Total 1565	C 698	N 283	O 510	P 73	S 1	0	0	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1111	Total 1111	Mg 1111	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1B	37	Total Mg 37 37	0	0
58	1D	11	Total Mg 11 11	0	0
58	1E	13	Total Mg 13 13	0	0
58	1F	15	Total Mg 15 15	0	0
58	1G	4	Total Mg 4 4	0	0
58	1H	1	Total Mg 1 1	0	0
58	1I	1	Total Mg 1 1	0	0
58	1N	4	Total Mg 4 4	0	0
58	1O	6	Total Mg 6 6	0	0
58	1P	6	Total Mg 6 6	0	0
58	1Q	7	Total Mg 7 7	0	0
58	1R	6	Total Mg 6 6	0	0
58	1S	3	Total Mg 3 3	0	0
58	1T	4	Total Mg 4 4	0	0
58	1U	14	Total Mg 14 14	0	0
58	1V	8	Total Mg 8 8	0	0
58	1W	6	Total Mg 6 6	0	0
58	1X	6	Total Mg 6 6	0	0
58	1Y	2	Total Mg 2 2	0	0
58	1Z	3	Total Mg 3 3	0	0
58	10	12	Total Mg 12 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	11	5	Total Mg 5 5	0	0
58	12	2	Total Mg 2 2	0	0
58	13	3	Total Mg 3 3	0	0
58	14	1	Total Mg 1 1	0	0
58	15	8	Total Mg 8 8	0	0
58	16	2	Total Mg 2 2	0	0
58	17	4	Total Mg 4 4	0	0
58	18	4	Total Mg 4 4	0	0
58	19	1	Total Mg 1 1	0	0
58	1a	226	Total Mg 226 226	0	0
58	1b	1	Total Mg 1 1	0	0
58	1d	1	Total Mg 1 1	0	0
58	1e	2	Total Mg 2 2	0	0
58	1f	1	Total Mg 1 1	0	0
58	1k	1	Total Mg 1 1	0	0
58	1l	2	Total Mg 2 2	0	0
58	1m	1	Total Mg 1 1	0	0
58	1n	3	Total Mg 3 3	0	0
58	1r	1	Total Mg 1 1	0	0
58	1t	1	Total Mg 1 1	0	0
58	1v	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1w	8	Total Mg 8 8	0	0
58	1x	14	Total Mg 14 14	0	0
58	2A	826	Total Mg 826 826	0	0
58	2B	20	Total Mg 20 20	0	0
58	2D	6	Total Mg 6 6	0	0
58	2E	9	Total Mg 9 9	0	0
58	2F	8	Total Mg 8 8	0	0
58	2G	1	Total Mg 1 1	0	0
58	2O	1	Total Mg 1 1	0	0
58	2P	2	Total Mg 2 2	0	0
58	2Q	2	Total Mg 2 2	0	0
58	2R	2	Total Mg 2 2	0	0
58	2T	4	Total Mg 4 4	0	0
58	2U	2	Total Mg 2 2	0	0
58	2V	2	Total Mg 2 2	0	0
58	2W	2	Total Mg 2 2	0	0
58	2X	2	Total Mg 2 2	0	0
58	2Y	1	Total Mg 1 1	0	0
58	20	2	Total Mg 2 2	0	0
58	21	1	Total Mg 1 1	0	0
58	23	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	25	2	Total Mg 2 2	0	0
58	26	2	Total Mg 2 2	0	0
58	27	4	Total Mg 4 4	0	0
58	28	3	Total Mg 3 3	0	0
58	2a	241	Total Mg 241 241	0	0
58	2d	2	Total Mg 2 2	0	0
58	2e	2	Total Mg 2 2	0	0
58	2f	2	Total Mg 2 2	0	0
58	2j	1	Total Mg 1 1	0	0
58	2l	4	Total Mg 4 4	0	0
58	2n	2	Total Mg 2 2	0	0
58	2p	1	Total Mg 1 1	0	0
58	2q	1	Total Mg 1 1	0	0
58	2t	1	Total Mg 1 1	0	0
58	2v	3	Total Mg 3 3	0	0
58	2w	3	Total Mg 3 3	0	0
58	2x	8	Total Mg 8 8	0	0

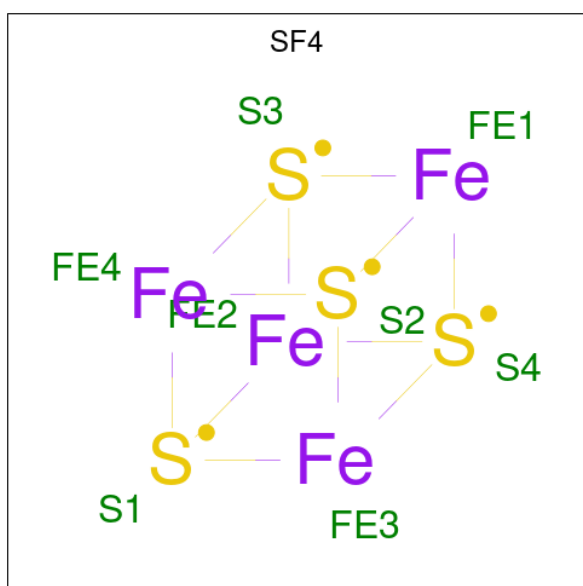
- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1	Total K 1 1	0	0
59	2A	1	Total K 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	2Y	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	2181	Total	O	0	0
			2181	2181		
62	1B	62	Total	O	0	0
			62	62		
62	1D	28	Total	O	0	0
			28	28		
62	1E	27	Total	O	0	0
			27	27		
62	1F	16	Total	O	0	0
			16	16		
62	1G	2	Total	O	0	0
			2	2		
62	1H	2	Total	O	0	0
			2	2		
62	1N	7	Total	O	0	0
			7	7		
62	1O	5	Total	O	0	0
			5	5		
62	1P	21	Total	O	0	0
			21	21		
62	1Q	12	Total	O	0	0
			12	12		
62	1R	12	Total	O	0	0
			12	12		
62	1S	4	Total	O	0	0
			4	4		
62	1T	11	Total	O	0	0
			11	11		
62	1U	13	Total	O	0	0
			13	13		
62	1V	9	Total	O	0	0
			9	9		
62	1W	9	Total	O	0	0
			9	9		
62	1X	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1Y	3	Total 3	O 3	0	0
62	1Z	2	Total 2	O 2	0	0
62	10	17	Total 17	O 17	0	0
62	11	8	Total 8	O 8	0	0
62	12	3	Total 3	O 3	0	0
62	13	4	Total 4	O 4	0	0
62	14	1	Total 1	O 1	0	0
62	15	6	Total 6	O 6	0	0
62	16	3	Total 3	O 3	0	0
62	17	9	Total 9	O 9	0	0
62	18	11	Total 11	O 11	0	0
62	1a	436	Total 436	O 436	0	0
62	1b	1	Total 1	O 1	0	0
62	1d	3	Total 3	O 3	0	0
62	1f	3	Total 3	O 3	0	0
62	1g	1	Total 1	O 1	0	0
62	1j	3	Total 3	O 3	0	0
62	1l	5	Total 5	O 5	0	0
62	1m	1	Total 1	O 1	0	0
62	1n	2	Total 2	O 2	0	0
62	1o	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1p	1	Total O 1 1	0	0
62	1q	2	Total O 2 2	0	0
62	1r	2	Total O 2 2	0	0
62	1t	1	Total O 1 1	0	0
62	1v	4	Total O 4 4	0	0
62	1w	12	Total O 12 12	0	0
62	1x	12	Total O 12 12	0	0
62	1z	5	Total O 5 5	0	0
62	1y	1	Total O 1 1	0	0
62	2A	1216	Total O 1216 1216	0	0
62	2B	20	Total O 20 20	0	0
62	2D	18	Total O 18 18	0	0
62	2E	18	Total O 18 18	0	0
62	2F	14	Total O 14 14	0	0
62	2N	1	Total O 1 1	0	0
62	2O	2	Total O 2 2	0	0
62	2P	12	Total O 12 12	0	0
62	2Q	2	Total O 2 2	0	0
62	2R	2	Total O 2 2	0	0
62	2T	6	Total O 6 6	0	0
62	2U	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2W	2	Total O 2 2	0	0
62	2X	1	Total O 1 1	0	0
62	2Y	2	Total O 2 2	0	0
62	20	1	Total O 1 1	0	0
62	21	4	Total O 4 4	0	0
62	23	1	Total O 1 1	0	0
62	27	3	Total O 3 3	0	0
62	28	3	Total O 3 3	0	0
62	29	1	Total O 1 1	0	0
62	2a	357	Total O 357 357	0	0
62	2c	1	Total O 1 1	0	0
62	2d	4	Total O 4 4	0	0
62	2e	3	Total O 3 3	0	0
62	2f	3	Total O 3 3	0	0
62	2j	2	Total O 2 2	0	0
62	2l	4	Total O 4 4	0	0
62	2n	2	Total O 2 2	0	0
62	2o	1	Total O 1 1	0	0
62	2p	2	Total O 2 2	0	0
62	2q	1	Total O 1 1	0	0
62	2r	2	Total O 2 2	0	0

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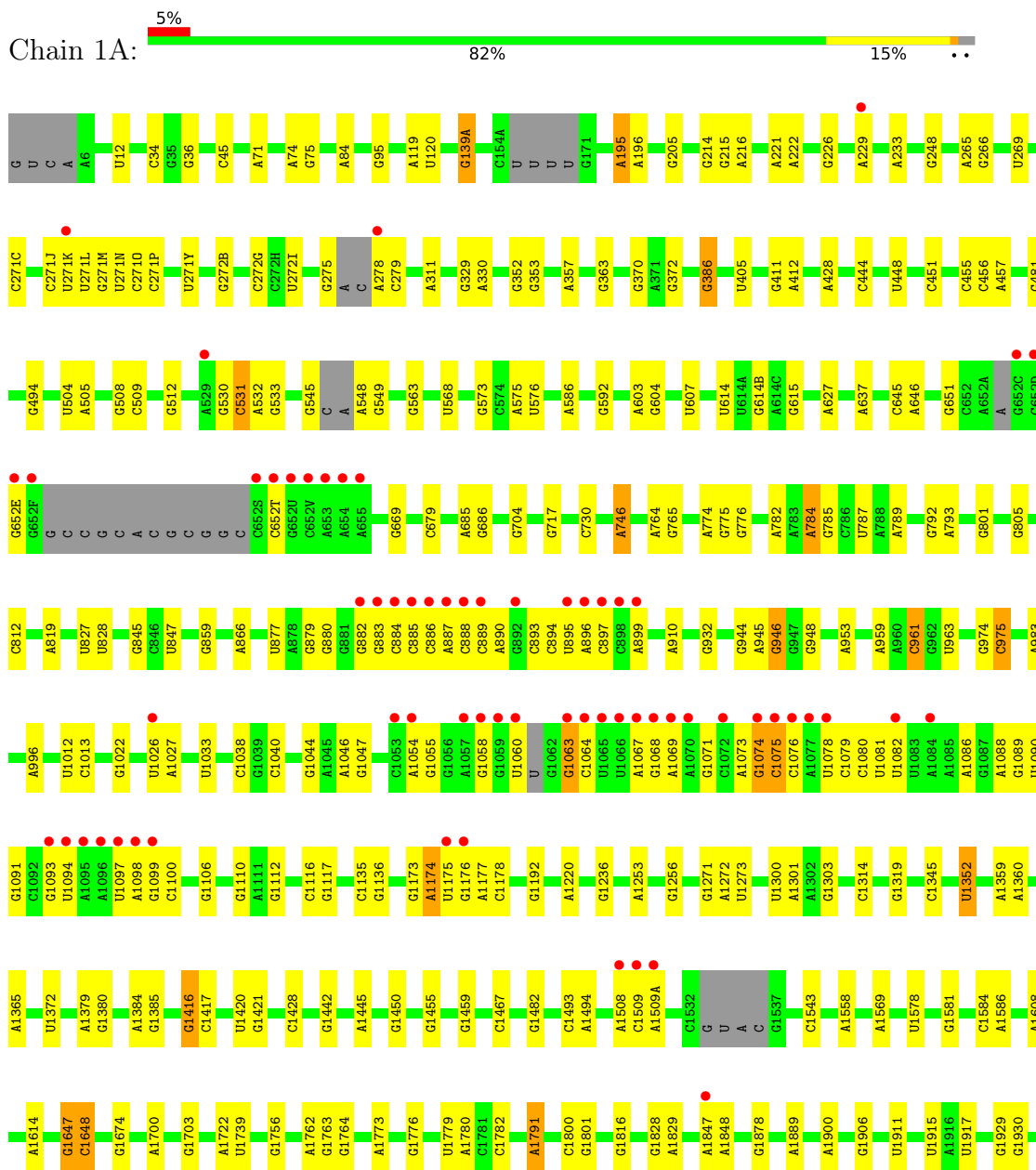
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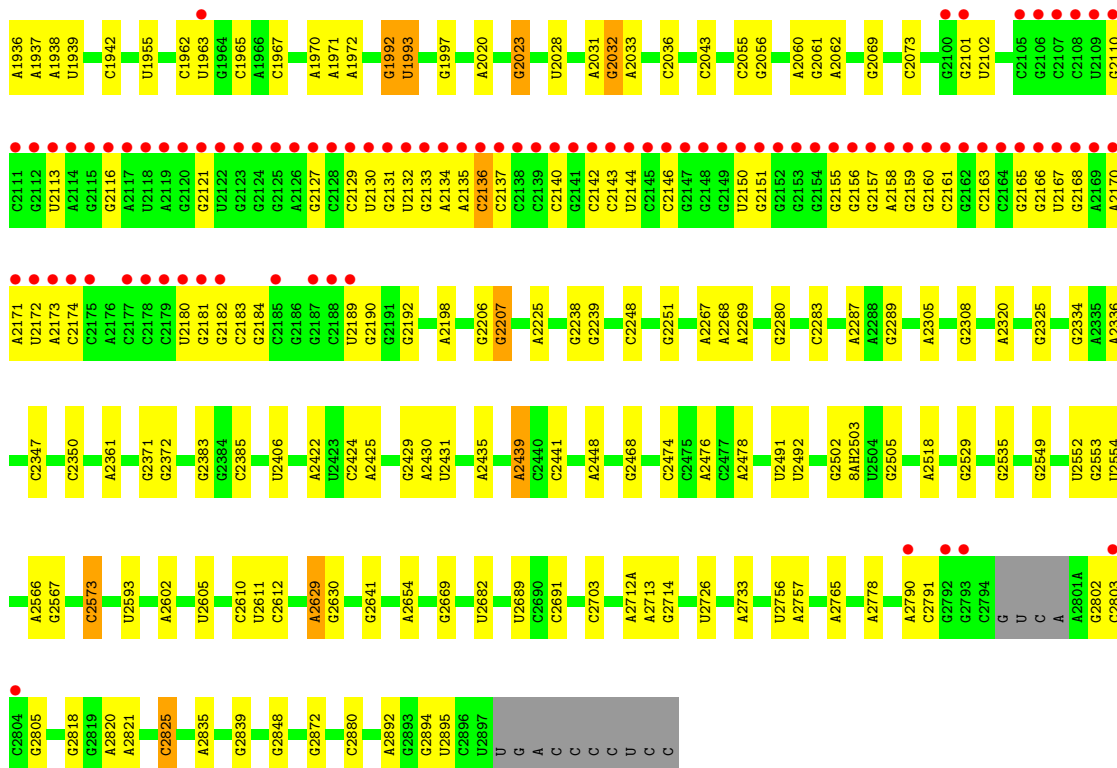
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2t	4	Total O 4 4	0	0
62	2v	3	Total O 3 3	0	0
62	2w	8	Total O 8 8	0	0
62	2x	3	Total O 3 3	0	0
62	2z	1	Total O 1 1	0	0

3 Residue-property plots [\(i\)](#)

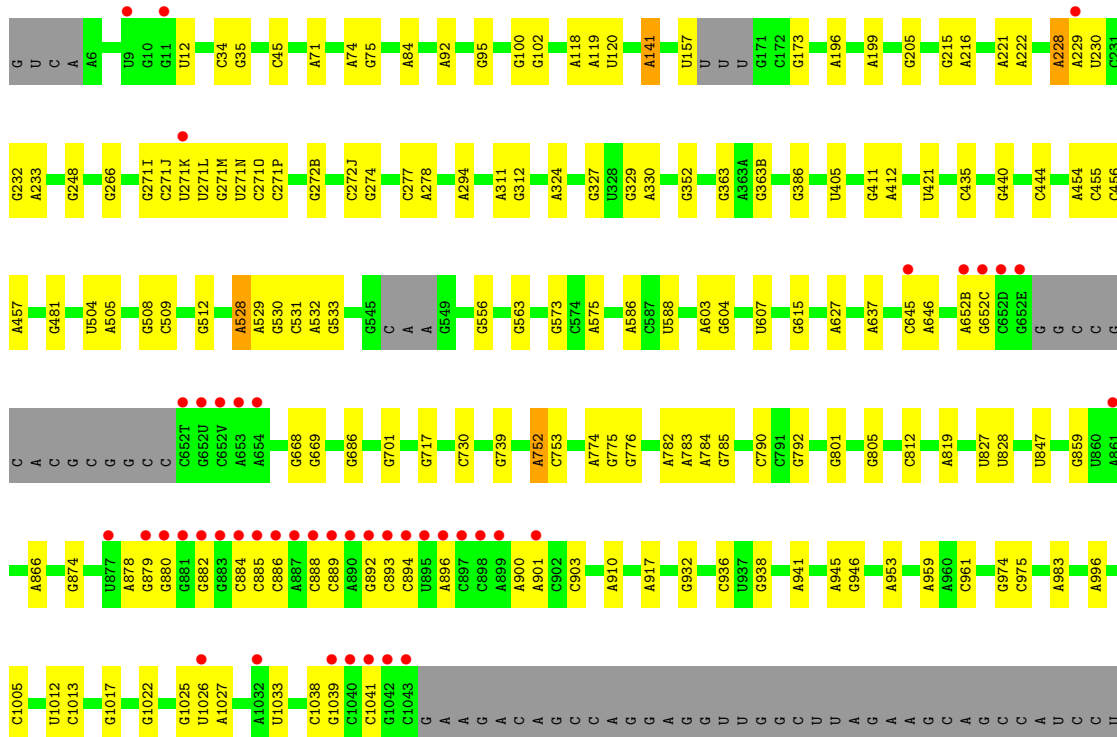
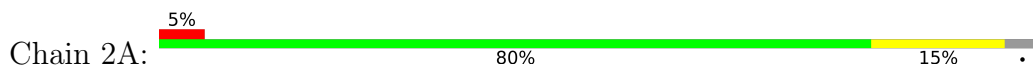
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

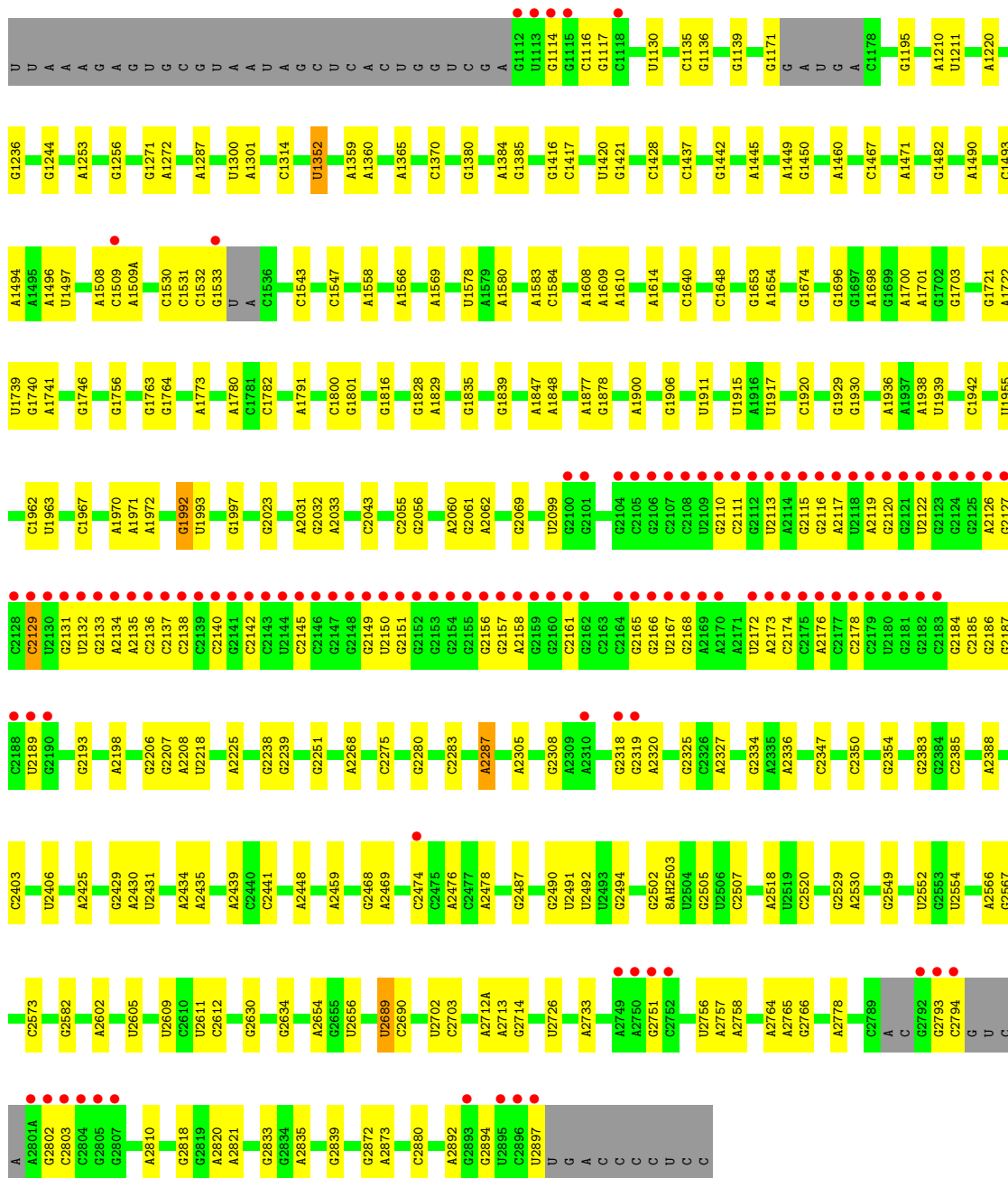
• Molecule 1: 23S Ribosomal RNA





● Molecule 1: 23S Ribosomal RNA

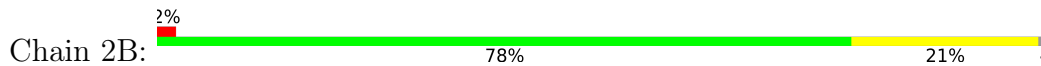


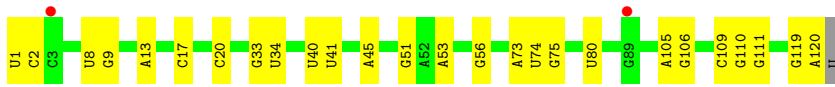


• Molecule 2: 5S Ribosomal RNA

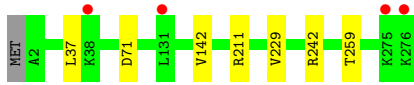


• Molecule 2: 5S Ribosomal RNA

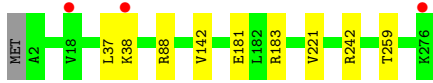




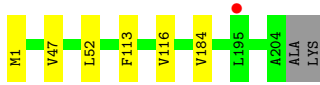
- Molecule 3: 50S ribosomal protein L2



- Molecule 3: 50S ribosomal protein L2



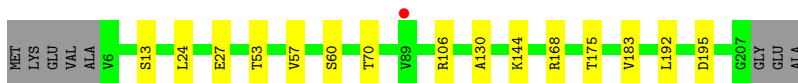
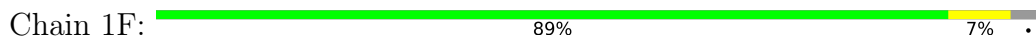
- Molecule 4: 50S ribosomal protein L3



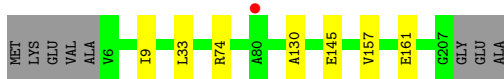
- Molecule 4: 50S ribosomal protein L3



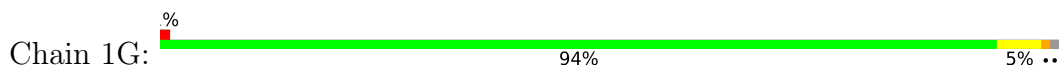
- Molecule 5: 50S ribosomal protein L4



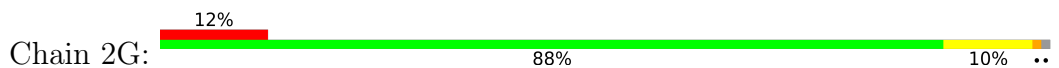
- Molecule 5: 50S ribosomal protein L4



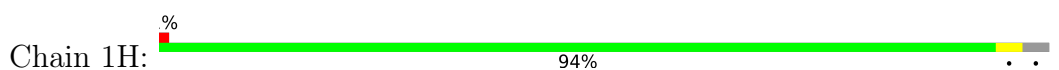
- Molecule 6: 50S ribosomal protein L5



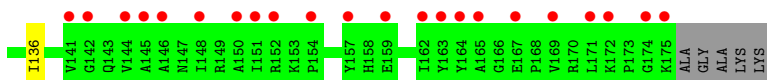
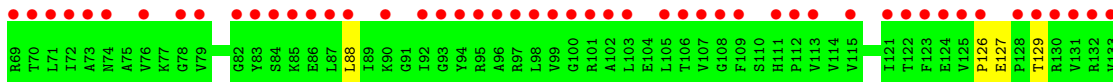
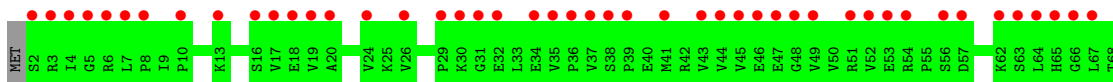
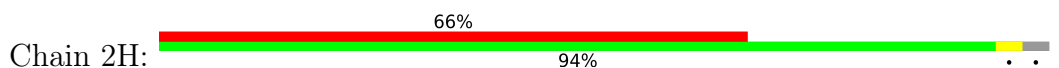
- Molecule 6: 50S ribosomal protein L5



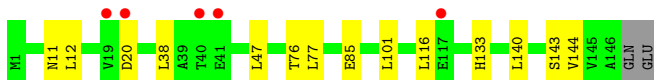
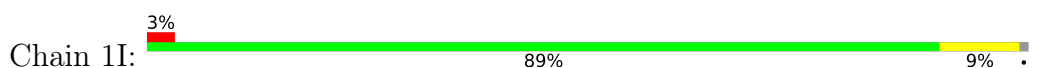
- Molecule 7: 50S ribosomal protein L6



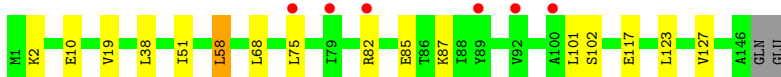
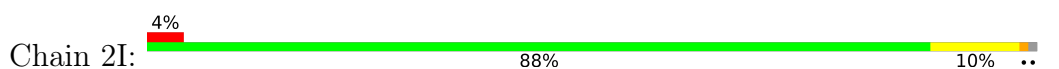
- Molecule 7: 50S ribosomal protein L6



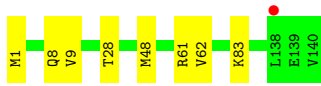
- Molecule 8: 50S ribosomal protein L9



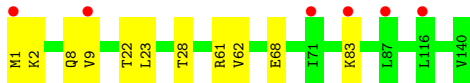
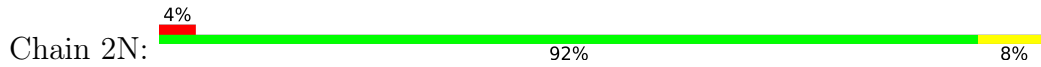
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



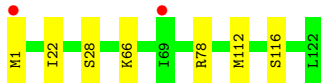
- Molecule 9: 50S ribosomal protein L13



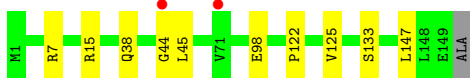
- Molecule 10: 50S ribosomal protein L14



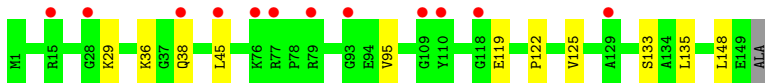
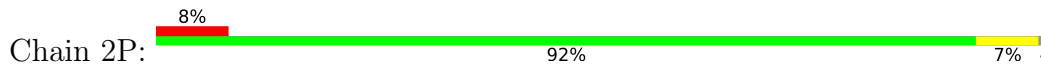
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15

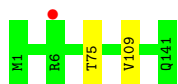


- Molecule 11: 50S ribosomal protein L15

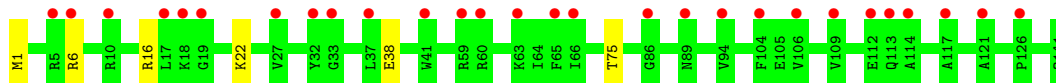


- Molecule 12: 50S ribosomal protein L16





- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



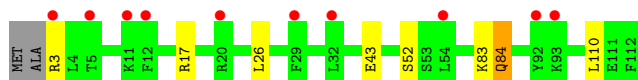
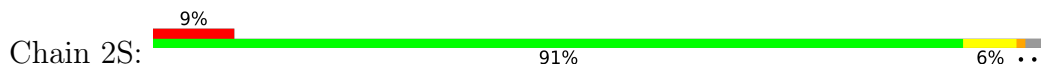
- Molecule 13: 50S ribosomal protein L17



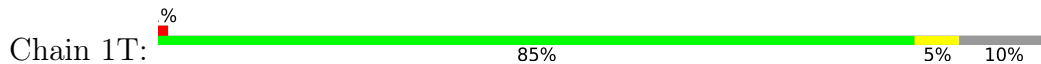
- Molecule 14: 50S ribosomal protein L18



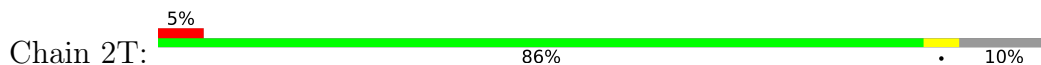
- Molecule 14: 50S ribosomal protein L18

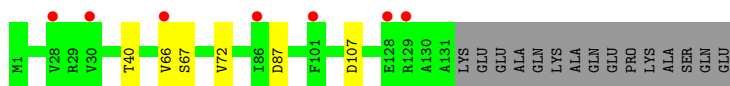


- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19

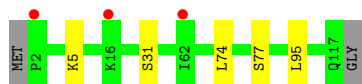




- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



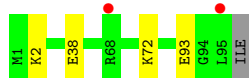
- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22



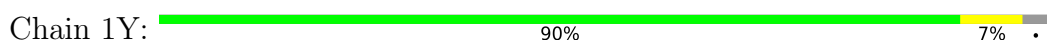
- Molecule 19: 50S ribosomal protein L23



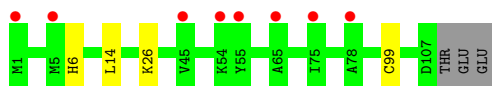
- Molecule 19: 50S ribosomal protein L23



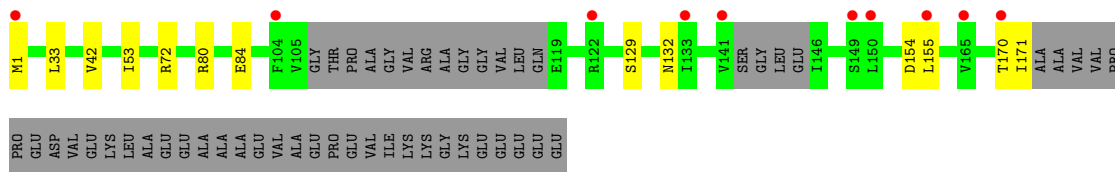
- Molecule 20: 50S ribosomal protein L24



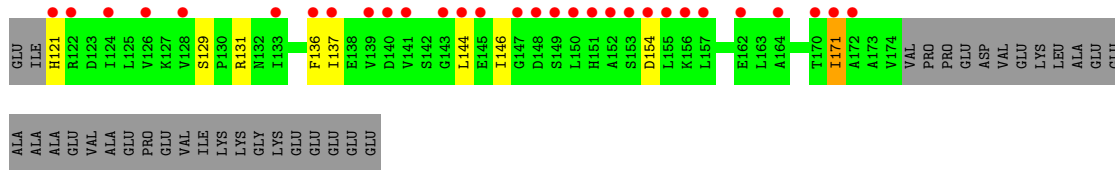
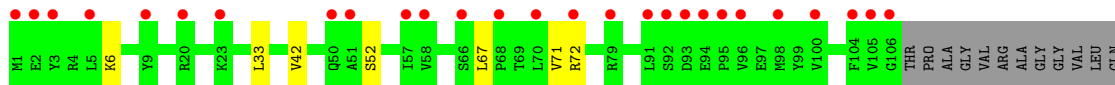
- Molecule 20: 50S ribosomal protein L24



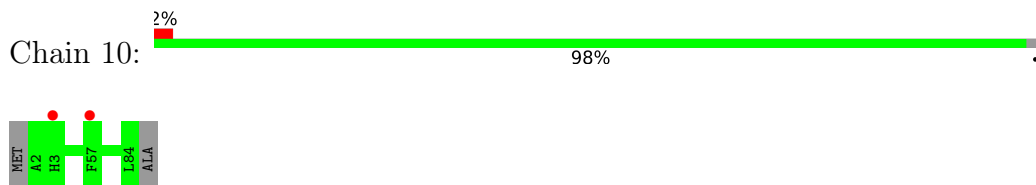
- Molecule 21: 50S ribosomal protein L25



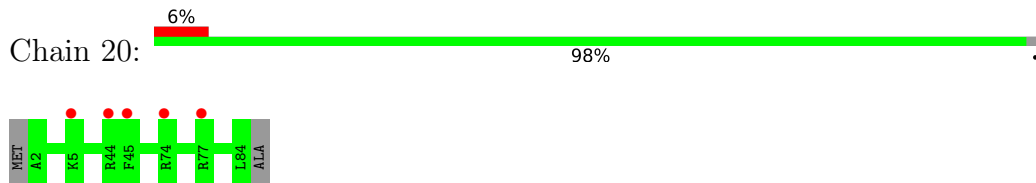
- Molecule 21: 50S ribosomal protein L25



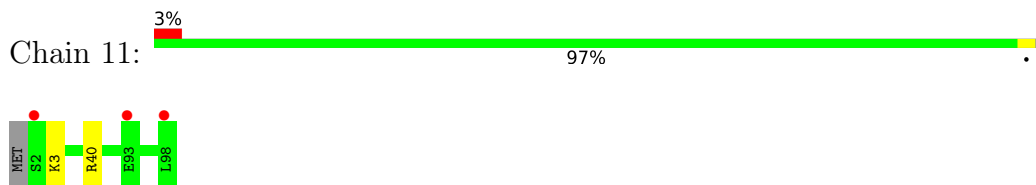
- Molecule 22: 50S ribosomal protein L27



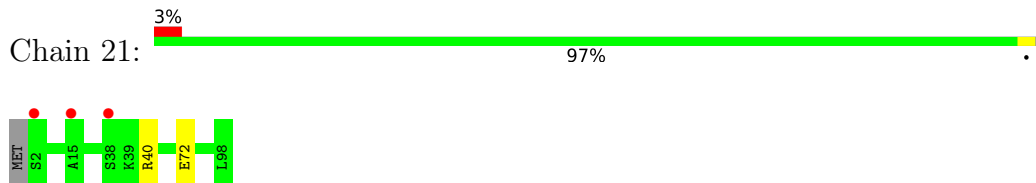
- Molecule 22: 50S ribosomal protein L27



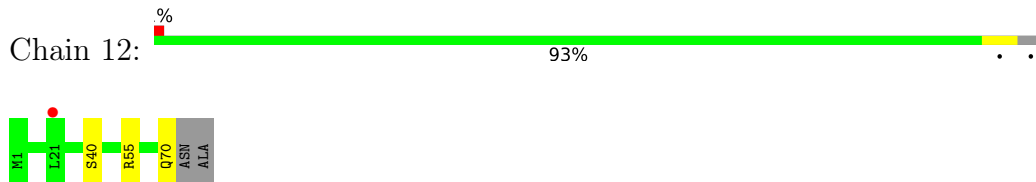
- Molecule 23: 50S ribosomal protein L28



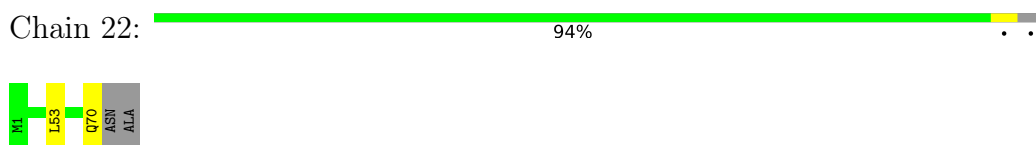
- Molecule 23: 50S ribosomal protein L28



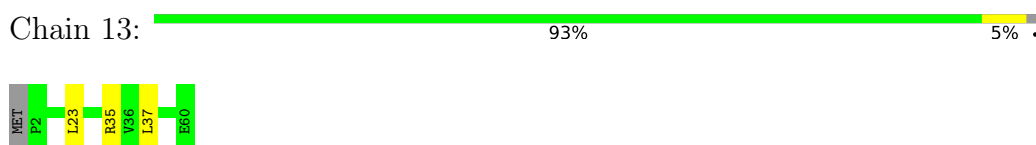
- Molecule 24: 50S ribosomal protein L29



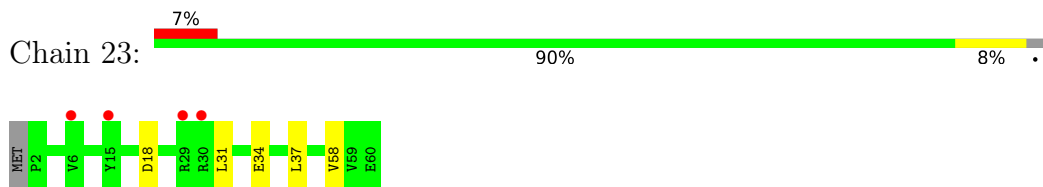
- Molecule 24: 50S ribosomal protein L29



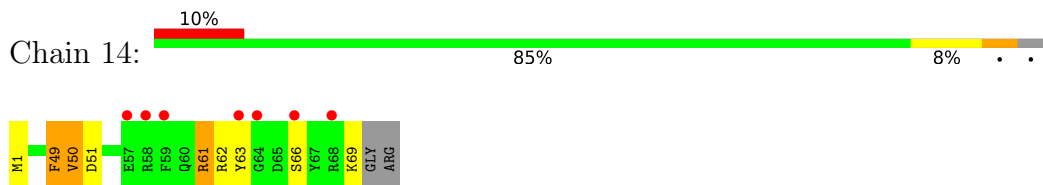
- Molecule 25: 50S ribosomal protein L30



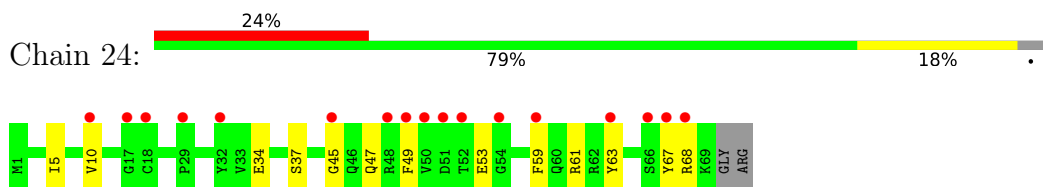
- Molecule 25: 50S ribosomal protein L30



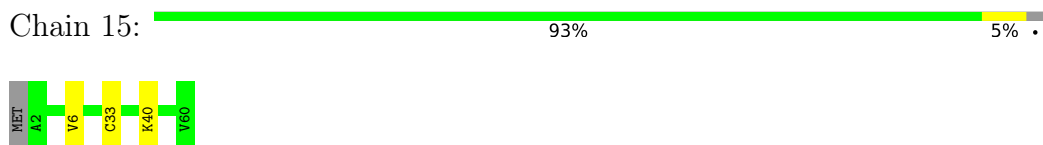
- Molecule 26: 50S ribosomal protein L31



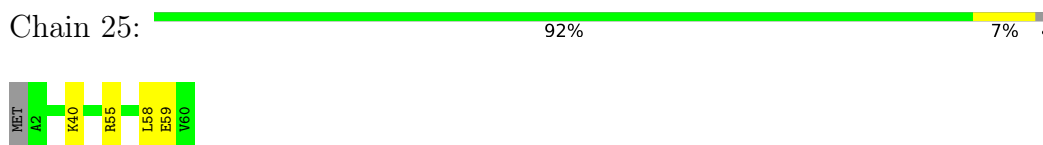
- Molecule 26: 50S ribosomal protein L31



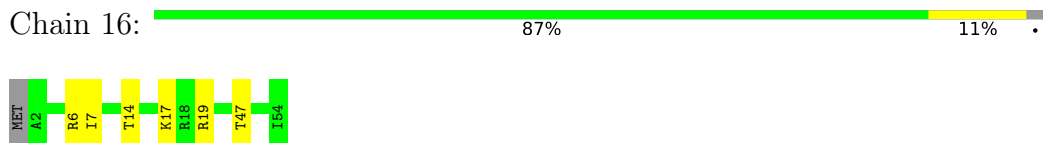
- Molecule 27: 50S ribosomal protein L32



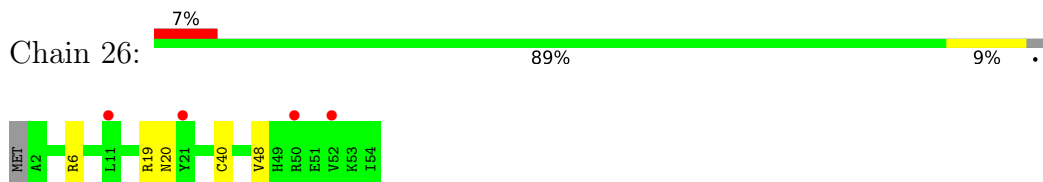
- Molecule 27: 50S ribosomal protein L32



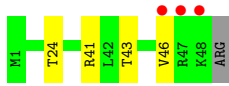
- Molecule 28: 50S ribosomal protein L33



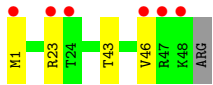
- Molecule 28: 50S ribosomal protein L33



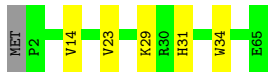
- Molecule 29: 50S ribosomal protein L34



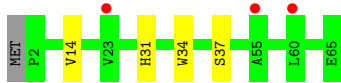
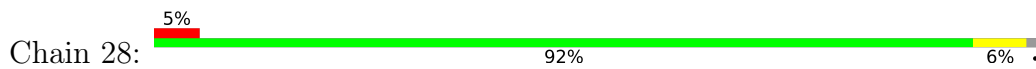
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

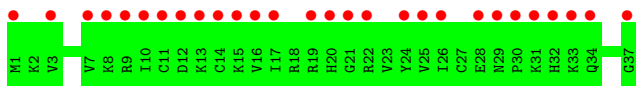
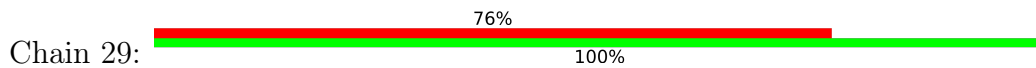


- Molecule 31: 50S ribosomal protein L36

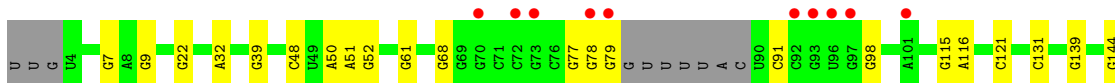
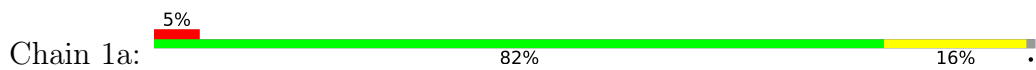


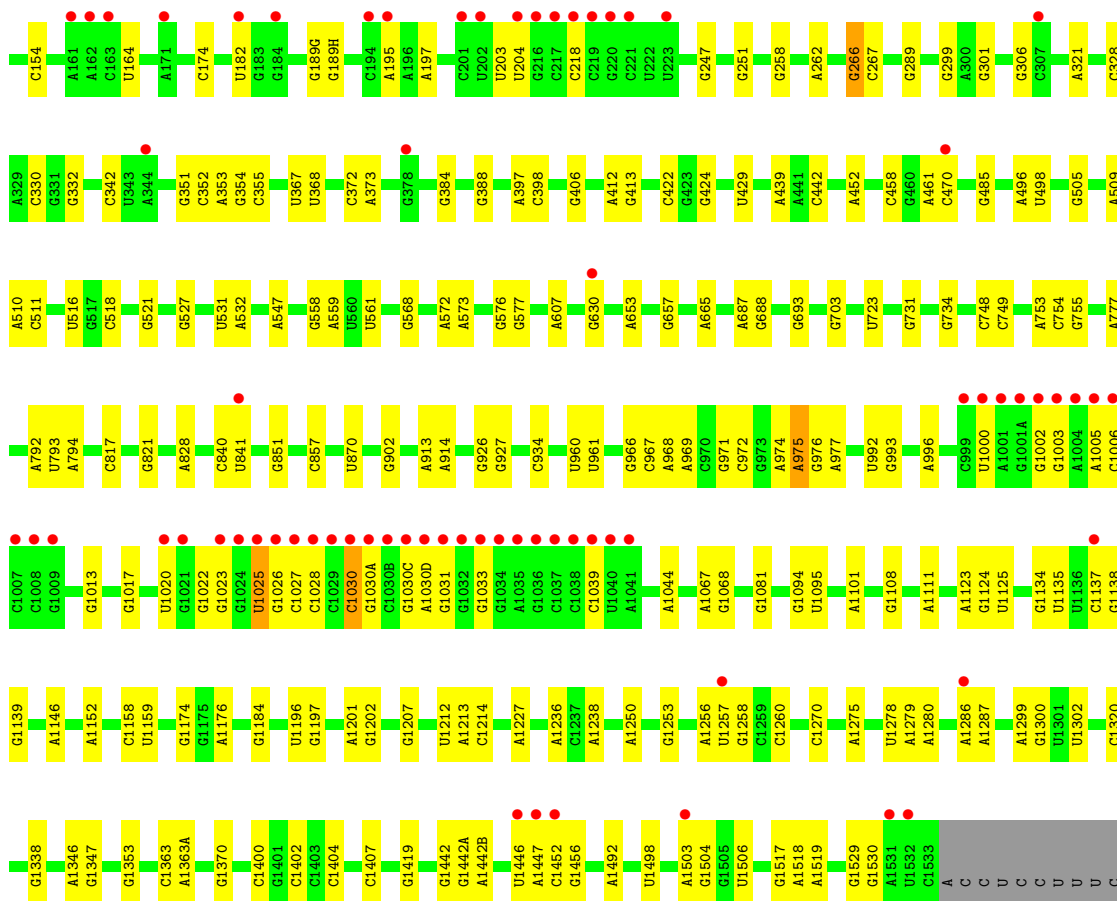
There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L36

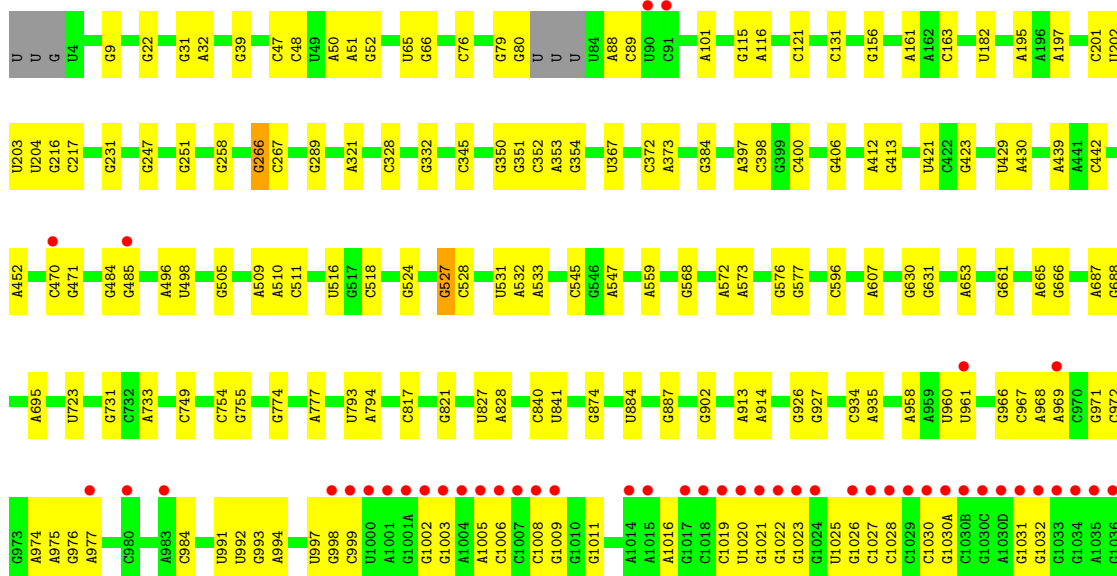
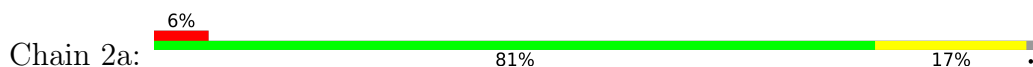


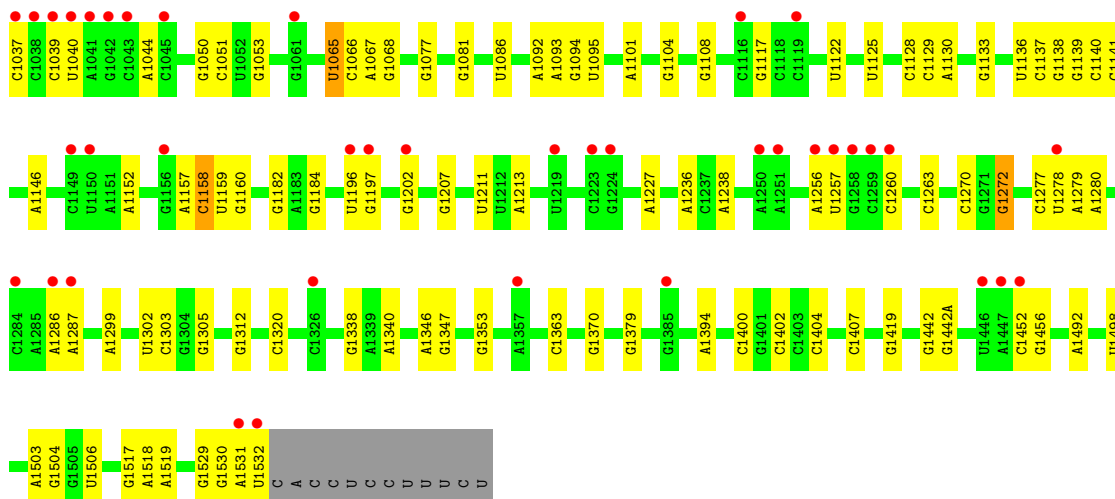
- Molecule 32: 16S Ribosomal RNA



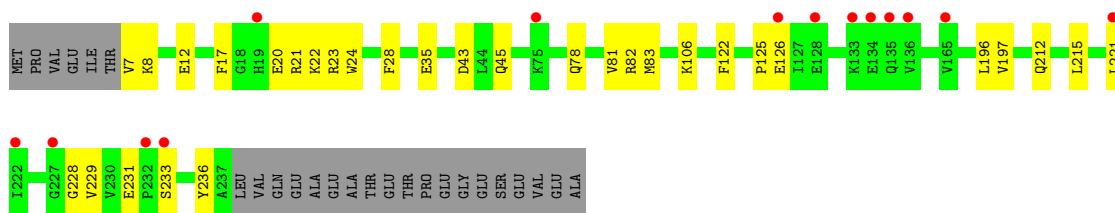
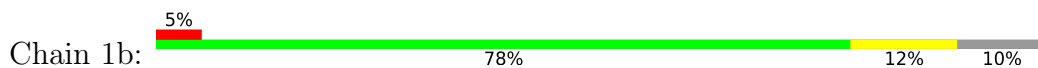


• Molecule 32: 16S Ribosomal RNA

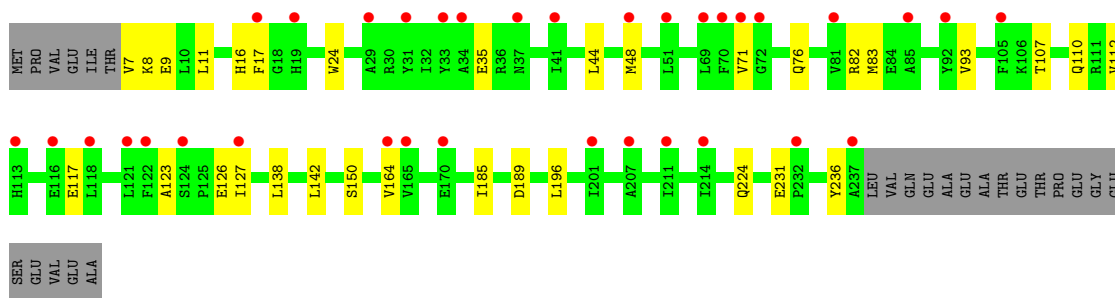
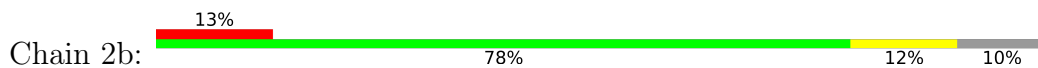




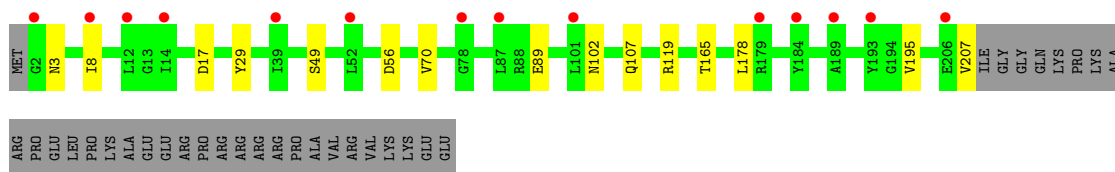
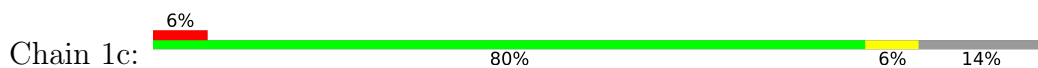
• Molecule 33: 30S ribosomal protein S2



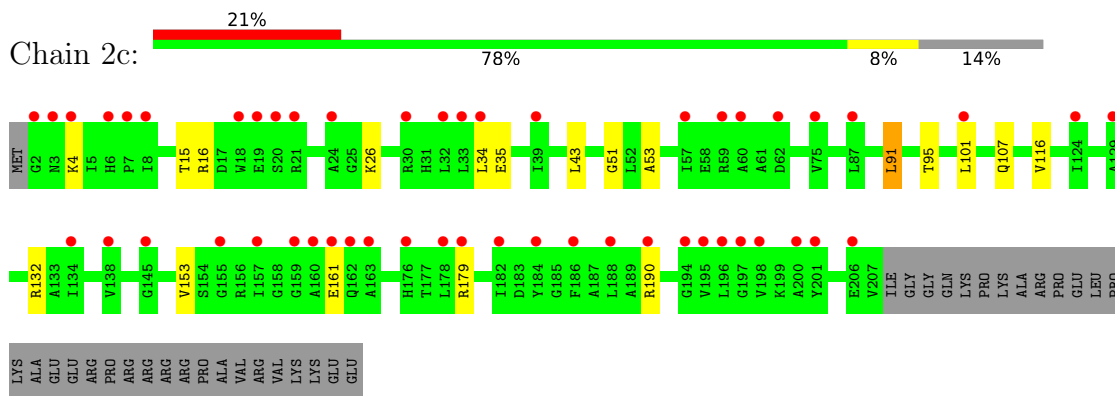
• Molecule 33: 30S ribosomal protein S2



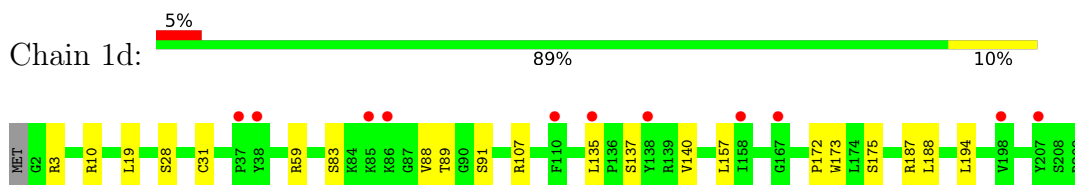
• Molecule 34: 30S ribosomal protein S3



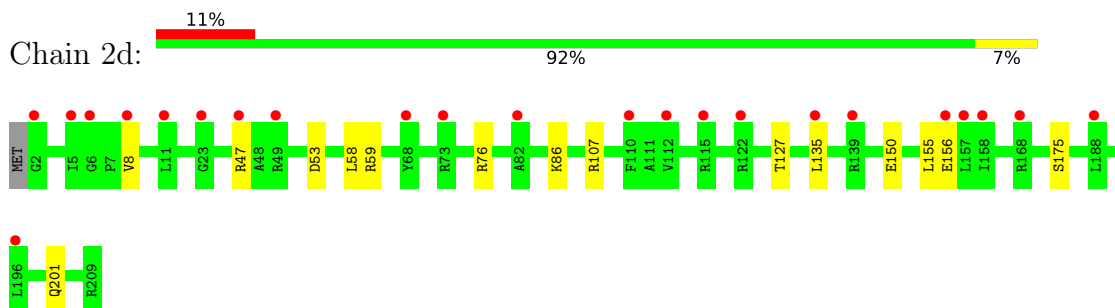
• Molecule 34: 30S ribosomal protein S3



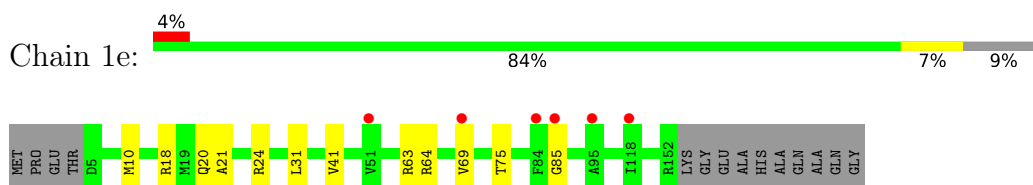
- Molecule 35: 30S ribosomal protein S4



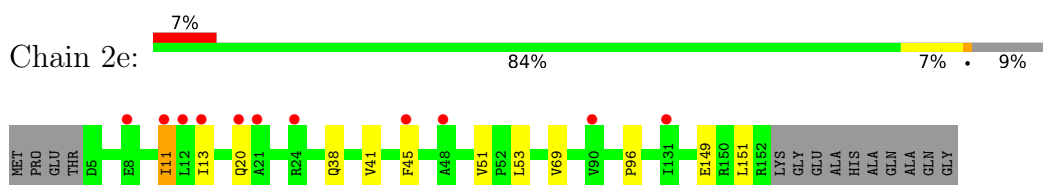
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6

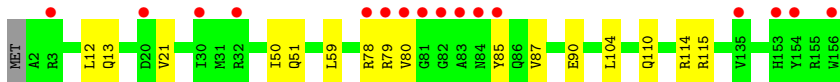
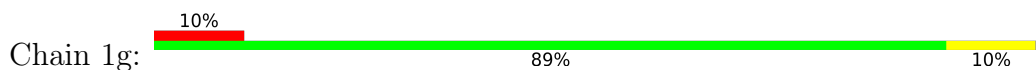




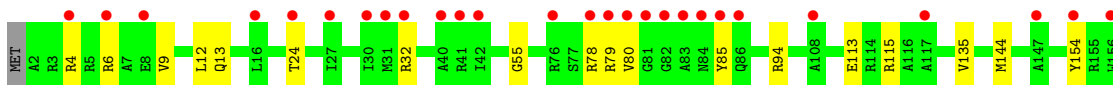
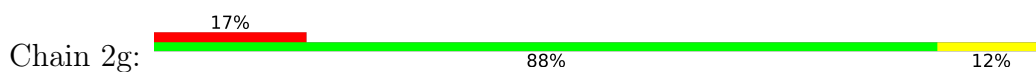
- Molecule 37: 30S ribosomal protein S6



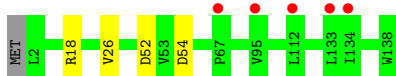
- Molecule 38: 30S ribosomal protein S7



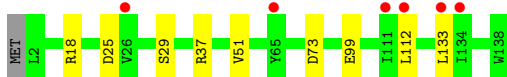
- Molecule 38: 30S ribosomal protein S7



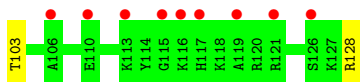
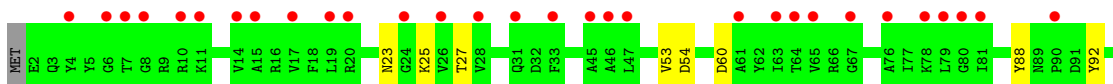
- Molecule 39: 30S ribosomal protein S8



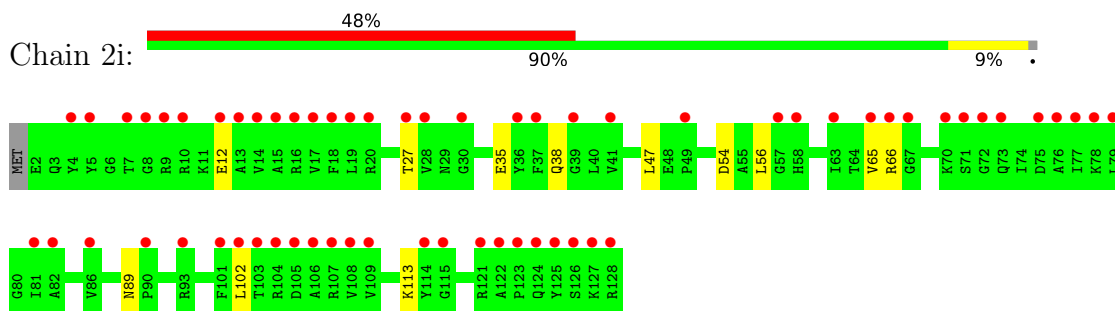
- Molecule 39: 30S ribosomal protein S8



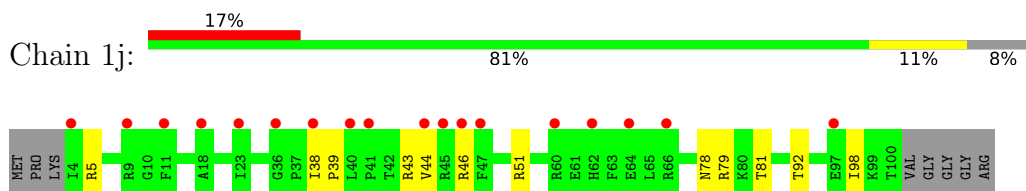
- Molecule 40: 30S ribosomal protein S9



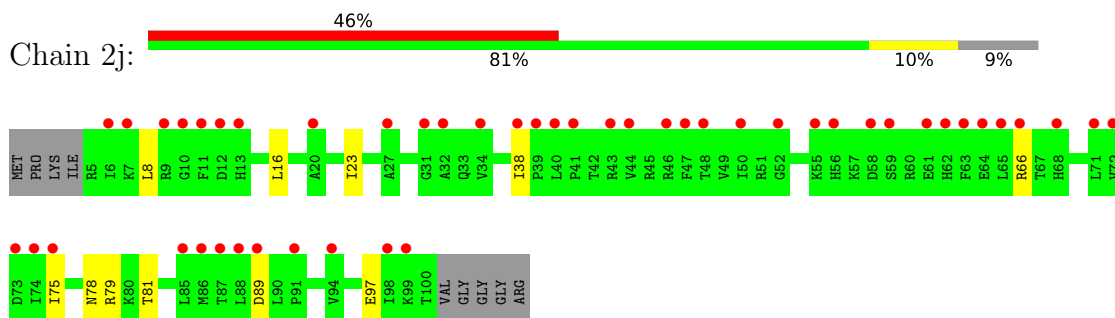
- Molecule 40: 30S ribosomal protein S9



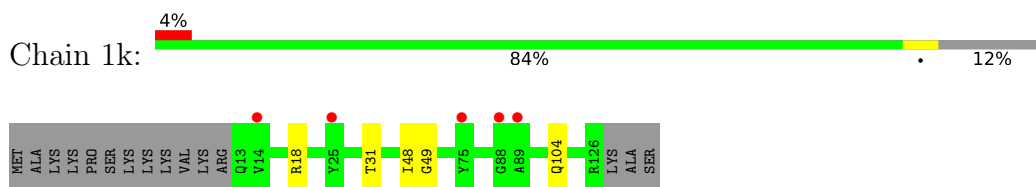
- Molecule 41: 30S ribosomal protein S10



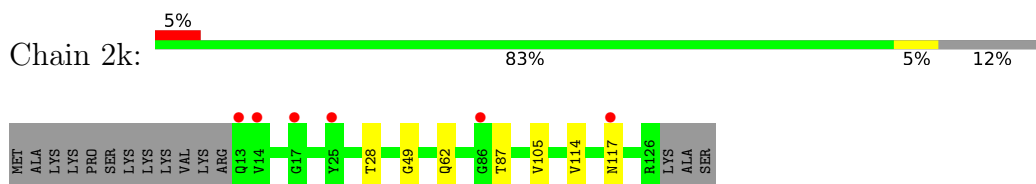
- Molecule 41: 30S ribosomal protein S10



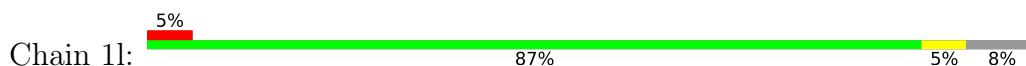
- Molecule 42: 30S ribosomal protein S11

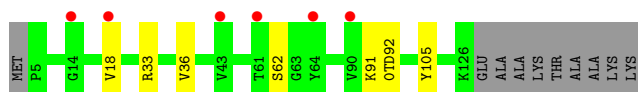


- Molecule 42: 30S ribosomal protein S11

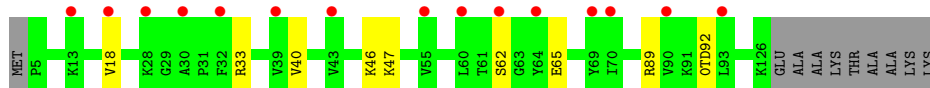
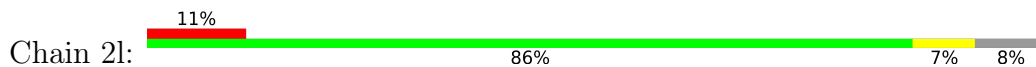


- Molecule 43: 30S ribosomal protein S12





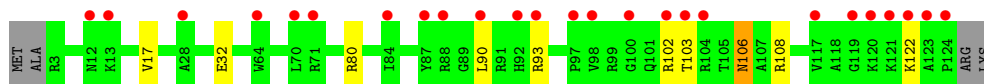
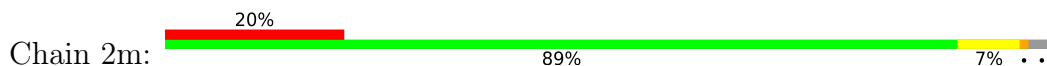
- Molecule 43: 30S ribosomal protein S12



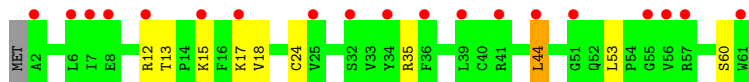
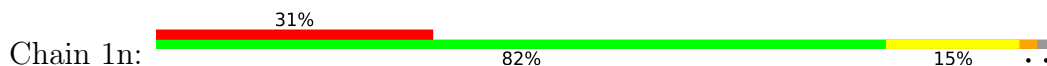
- Molecule 44: 30S ribosomal protein S13



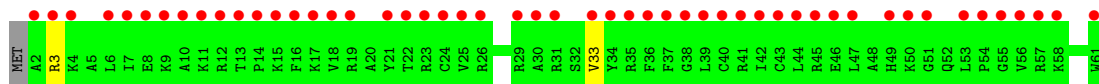
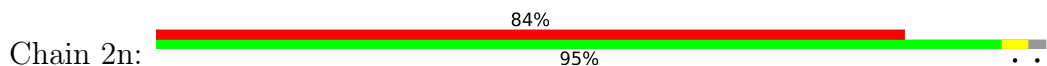
- Molecule 44: 30S ribosomal protein S13



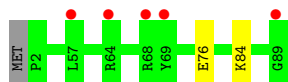
- Molecule 45: 30S ribosomal protein S14 type Z



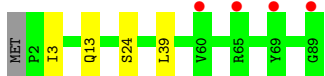
- Molecule 45: 30S ribosomal protein S14 type Z



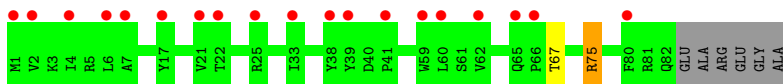
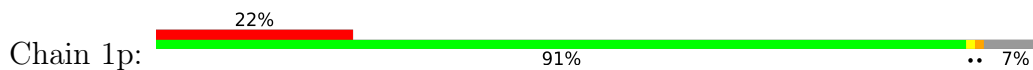
- Molecule 46: 30S ribosomal protein S15



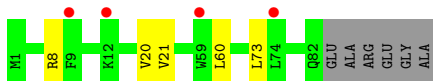
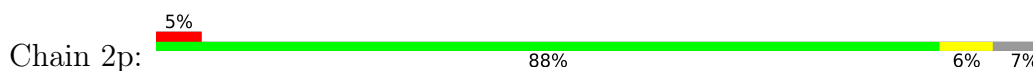
- Molecule 46: 30S ribosomal protein S15



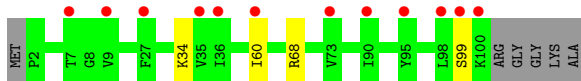
- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16



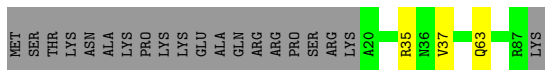
- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



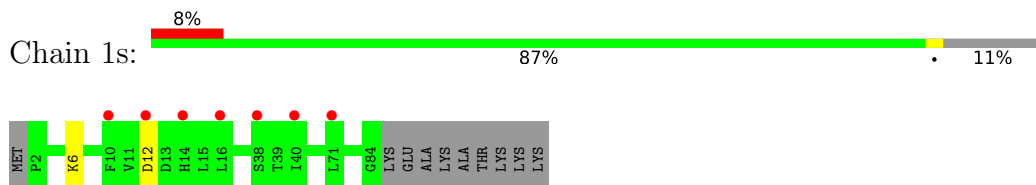
- Molecule 49: 30S ribosomal protein S18



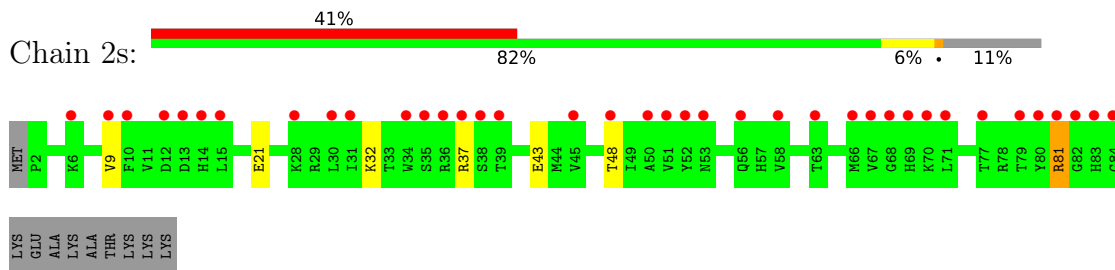
- Molecule 49: 30S ribosomal protein S18



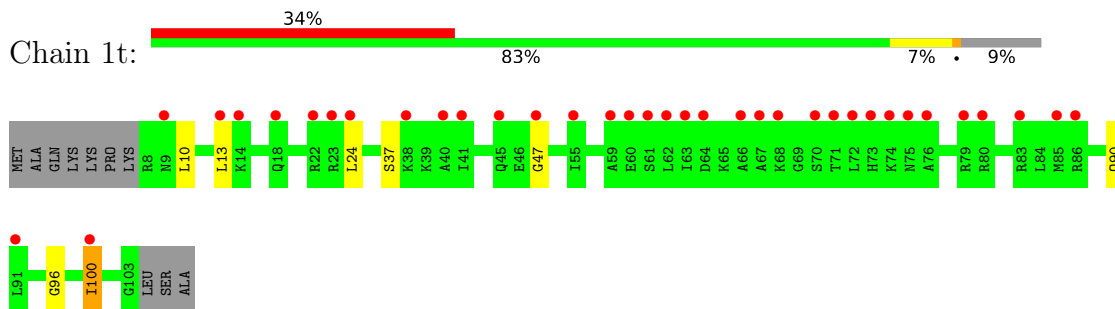
- Molecule 50: 30S ribosomal protein S19



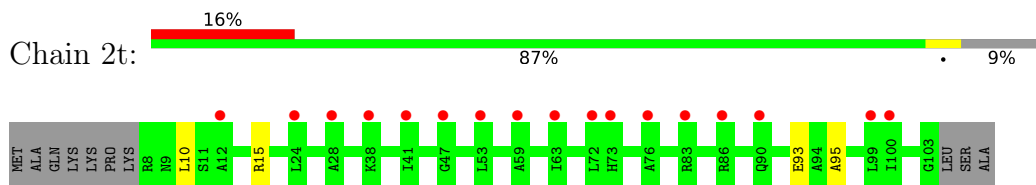
- Molecule 50: 30S ribosomal protein S19



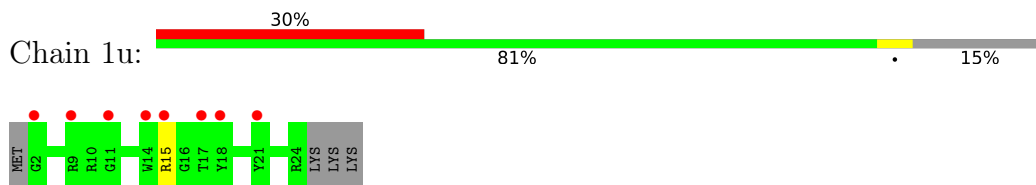
- Molecule 51: 30S ribosomal protein S20



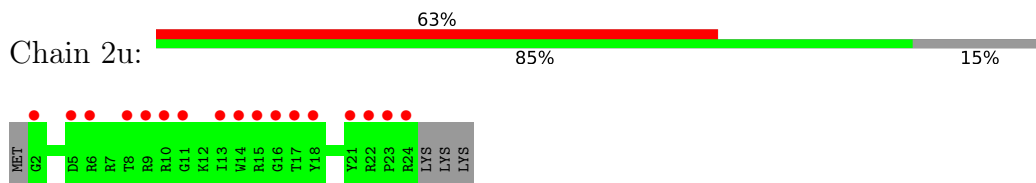
- Molecule 51: 30S ribosomal protein S20



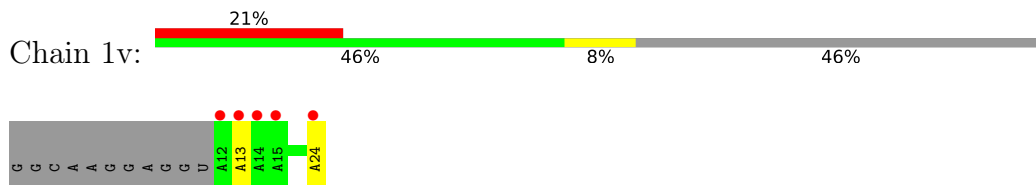
- Molecule 52: 30S ribosomal protein Thx



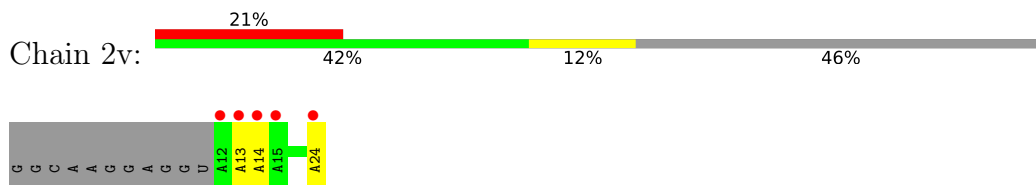
- Molecule 52: 30S ribosomal protein Thx



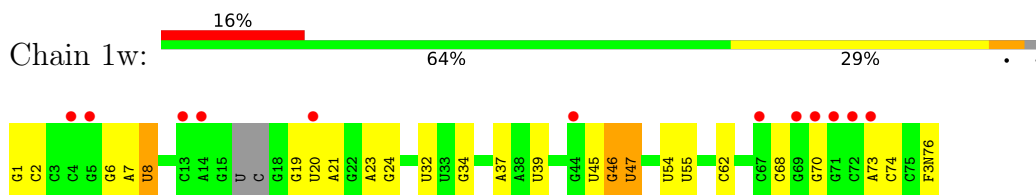
- Molecule 53: MF-mRNA



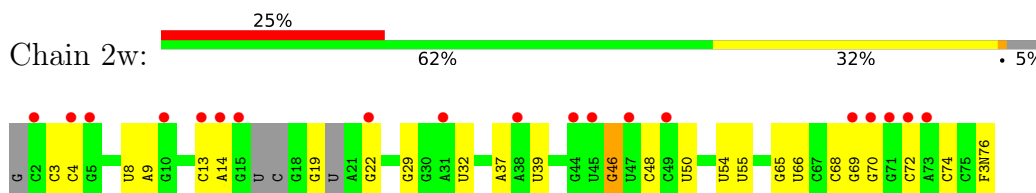
- Molecule 53: MF-mRNA



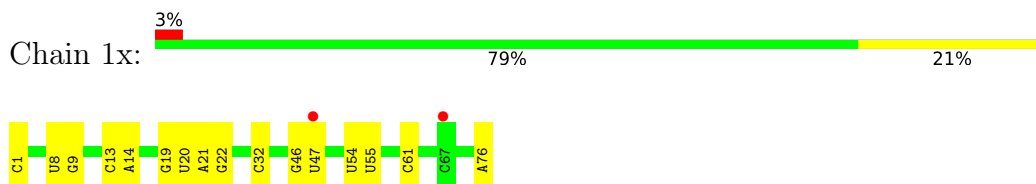
- Molecule 54: A-site Aminoacylated Phe-tRNA^{phe}



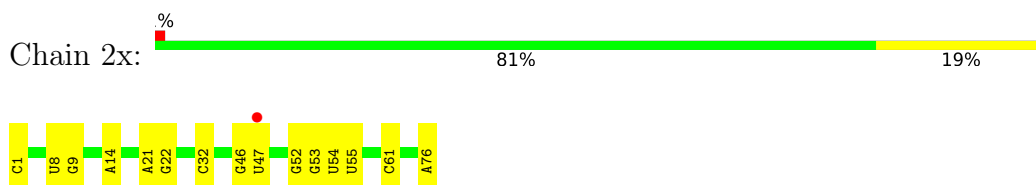
- Molecule 54: A-site Aminoacylated Phe-tRNA^{phe}



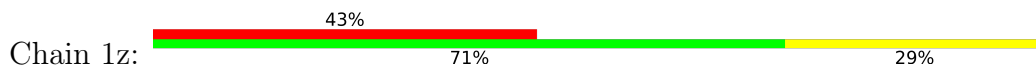
- Molecule 55: P-site Peptidyl-tRNA fMTHSMRC-tRNA^{met} RNA-part

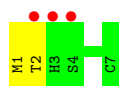


- Molecule 55: P-site Peptidyl-tRNA fMTHSMRC-tRNA^{met} RNA-part

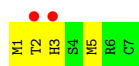
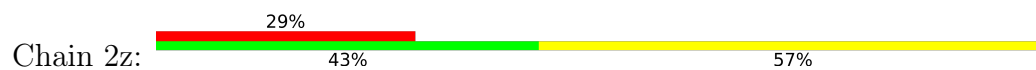


- Molecule 56: P-site Peptidyl-tRNA fMTHSMRC-tRNA^{met} Peptide-part

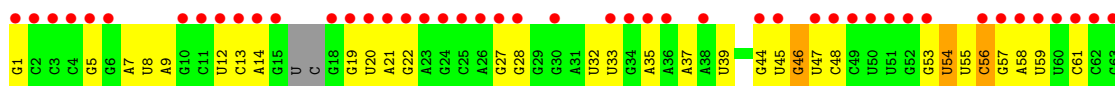
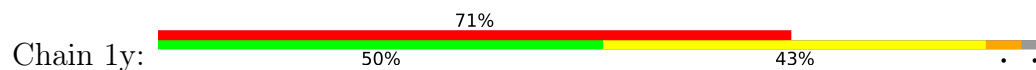




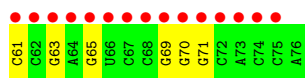
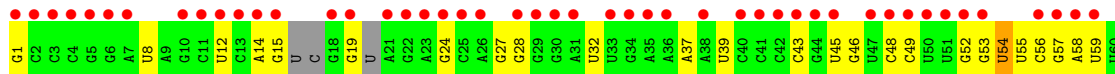
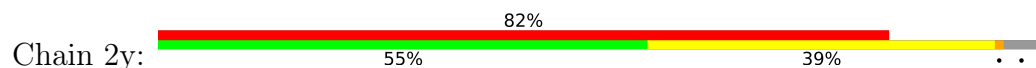
- Molecule 56: P-site Peptidyl-tRNA fMTHSMRC-tRNAmet Peptide-part



- Molecule 57: E-site Deacylated tRNAphe



- Molecule 57: E-site Deacylated tRNAphe



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.01Å 450.38Å 625.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	125.46 – 2.45 190.33 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.2 (125.46-2.45) 99.2 (190.33-2.45)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.212 , 0.249 0.212 , 0.249	Depositor DCC
R_{free} test set	106589 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtrriage
Anisotropy	0.182	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	300665	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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: OMC, 2MU, K, 4OC, 8AH, 2MG, UR3, MG, F3N, M2G, PSU, MA6, ZN, MIA, G7M, FME, 5MU, 0TD, SF4, OMG, 4SU, 8AN, 5MC

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	0.49	0/69010	0.95	97/107716 (0.1%)
1	2A	0.38	0/67294	0.85	25/105038 (0.0%)
2	1B	0.42	1/2882 (0.0%)	0.82	0/4494
2	2B	0.38	1/2879 (0.0%)	0.81	1/4487 (0.0%)
3	1D	0.36	0/2186	0.56	0/2944
3	2D	0.30	0/2186	0.52	0/2944
4	1E	0.33	0/1592	0.53	0/2149
4	2E	0.29	0/1592	0.49	0/2149
5	1F	0.33	0/1618	0.53	0/2191
5	2F	0.29	0/1614	0.49	0/2186
6	1G	0.30	0/1448	0.49	0/1957
6	2G	0.29	0/1453	0.46	0/1963
7	1H	0.31	0/1356	0.51	0/1834
7	2H	0.29	0/1356	0.45	0/1834
8	1I	0.31	0/1112	0.49	0/1514
8	2I	0.28	0/1079	0.51	1/1475 (0.1%)
9	1N	0.33	0/1144	0.51	0/1543
9	2N	0.28	0/1144	0.46	0/1543
10	1O	0.34	0/943	0.54	0/1269
10	2O	0.31	0/943	0.50	0/1269
11	1P	0.31	0/1152	0.59	0/1533
11	2P	0.29	0/1152	0.53	0/1533
12	1Q	0.35	0/1143	0.54	0/1527
12	2Q	0.29	0/1143	0.48	0/1527
13	1R	0.33	0/982	0.54	0/1312
13	2R	0.27	0/982	0.47	0/1312
14	1S	0.30	0/883	0.52	0/1176
14	2S	0.28	0/880	0.48	0/1172
15	1T	0.31	0/1105	0.51	0/1477
15	2T	0.29	0/1097	0.47	0/1468
16	1U	0.34	0/977	0.52	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.28	0/977	0.44	0/1301
17	1V	0.33	0/782	0.54	0/1049
17	2V	0.29	0/782	0.50	0/1049
18	1W	0.35	0/897	0.54	0/1205
18	2W	0.29	0/897	0.48	0/1205
19	1X	0.34	0/764	0.56	0/1025
19	2X	0.31	0/764	0.53	0/1025
20	1Y	0.33	0/819	0.52	0/1095
20	2Y	0.31	0/819	0.49	0/1095
21	1Z	0.32	0/1267	0.50	0/1717
21	2Z	0.30	0/1299	0.50	0/1763
22	10	0.33	0/662	0.52	0/881
22	20	0.29	0/662	0.46	0/881
23	11	0.33	0/762	0.50	0/1014
23	21	0.33	0/762	0.51	0/1014
24	12	0.32	0/590	0.47	0/781
24	22	0.27	0/590	0.42	0/781
25	13	0.33	0/474	0.54	0/635
25	23	0.27	0/469	0.43	0/630
26	14	0.34	0/565	0.56	0/761
26	24	0.32	0/545	0.52	0/737
27	15	0.30	0/469	0.58	0/635
27	25	0.29	0/469	0.50	0/635
28	16	0.32	0/460	0.52	0/613
28	26	0.28	0/456	0.50	0/608
29	17	0.35	0/426	0.55	0/561
29	27	0.32	0/426	0.49	0/561
30	18	0.31	0/525	0.52	0/691
30	28	0.29	0/525	0.49	0/691
31	19	0.33	0/310	0.51	0/407
31	29	0.27	0/310	0.49	0/407
32	1a	0.35	0/35795	0.85	14/55864 (0.0%)
32	2a	0.35	3/35886 (0.0%)	0.87	29/56005 (0.1%)
33	1b	0.31	0/1881	0.48	0/2542
33	2b	0.30	0/1860	0.47	0/2518
34	1c	0.29	0/1572	0.45	0/2126
34	2c	0.29	0/1566	0.46	0/2119
35	1d	0.29	0/1685	0.48	1/2262 (0.0%)
35	2d	0.28	0/1704	0.46	0/2284
36	1e	0.29	0/1145	0.52	0/1543
36	2e	0.30	0/1149	0.51	0/1548
37	1f	0.29	0/823	0.48	0/1115
37	2f	0.29	0/829	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.28	0/1250	0.43	0/1679
38	2g	0.28	0/1254	0.43	0/1683
39	1h	0.29	0/1108	0.48	0/1494
39	2h	0.26	0/1108	0.46	0/1494
40	1i	0.29	0/1002	0.49	0/1346
40	2i	0.30	0/997	0.48	0/1343
41	1j	0.27	0/722	0.45	0/982
41	2j	0.28	0/727	0.51	0/988
42	1k	0.29	0/844	0.49	0/1145
42	2k	0.27	0/848	0.47	0/1149
43	1l	0.30	0/937	0.51	0/1260
43	2l	0.28	0/937	0.47	0/1260
44	1m	0.27	0/969	0.49	0/1302
44	2m	0.29	0/961	0.47	0/1291
45	1n	0.30	0/501	0.53	1/664 (0.2%)
45	2n	0.30	0/501	0.51	0/664
46	1o	0.27	0/739	0.41	0/985
46	2o	0.26	0/739	0.41	0/985
47	1p	0.30	0/697	0.51	0/939
47	2p	0.28	0/693	0.48	0/935
48	1q	0.28	0/836	0.47	0/1117
48	2q	0.26	0/836	0.46	0/1117
49	1r	0.29	0/560	0.47	0/746
49	2r	0.26	0/560	0.50	0/746
50	1s	0.27	0/667	0.52	0/900
50	2s	0.30	0/661	0.56	0/893
51	1t	0.26	0/730	0.45	0/965
51	2t	0.28	0/729	0.42	0/965
52	1u	0.27	0/203	0.48	0/266
52	2u	0.29	0/203	0.48	0/266
53	1v	0.41	0/310	0.88	0/480
53	2v	0.40	0/310	0.87	0/480
54	1w	0.51	1/1581 (0.1%)	1.02	1/2458 (0.0%)
54	2w	0.43	0/1531	0.96	0/2379
55	1x	0.59	4/1723 (0.2%)	1.14	20/2684 (0.7%)
55	2x	0.54	1/1723 (0.1%)	1.06	15/2684 (0.6%)
56	1z	0.43	0/48	0.67	0/62
56	2z	0.33	0/48	0.60	0/62
57	1y	0.59	1/1606 (0.1%)	1.09	6/2497 (0.2%)
57	2y	0.54	1/1583 (0.1%)	0.98	0/2459
All	All	0.39	13/316728 (0.0%)	0.81	211/474153 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	1	C	OP3-P	-10.33	1.48	1.61
32	2a	1272	G	N1-C2	-10.28	1.29	1.37
55	2x	1	C	OP3-P	-10.19	1.49	1.61
54	1w	1	G	OP3-P	-10.19	1.49	1.61
32	2a	1272	G	C6-N1	-10.16	1.32	1.39
2	1B	1	U	OP3-P	-10.16	1.49	1.61
57	1y	1	G	OP3-P	-10.04	1.49	1.61
2	2B	1	U	OP3-P	-9.99	1.49	1.61
57	2y	1	G	OP3-P	-9.89	1.49	1.61
32	2a	1263	C	N3-C4	-6.93	1.29	1.33
55	1x	14	A	N7-C5	-5.68	1.35	1.39
55	1x	22	G	C8-N7	5.38	1.34	1.30
55	1x	14	A	C8-N7	-5.28	1.27	1.31

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	30.45	137.17	118.90
32	2a	1272	G	C5-C6-O6	23.87	142.92	128.60
32	2a	1272	G	N3-C2-N2	23.57	136.40	119.90
32	2a	1272	G	N1-C2-N2	-20.93	97.36	116.20
32	2a	1263	C	N3-C2-O2	-17.85	109.41	121.90
32	2a	1263	C	C2-N3-C4	17.43	128.62	119.90
32	2a	1272	G	N1-C6-O6	-14.63	111.12	119.90
32	2a	1272	G	C6-N1-C2	13.11	132.97	125.10
55	1x	46	G	C6-N1-C2	-12.58	117.55	125.10
32	2a	1263	C	C5-C6-N1	11.94	126.97	121.00
55	2x	46	G	C6-N1-C2	-11.20	118.38	125.10
32	2a	1272	G	C5-C6-N1	-11.17	105.92	111.50
1	1A	1075	C	N1-C2-O2	11.10	125.56	118.90
1	1A	1086	A	N1-C6-N6	-11.02	111.99	118.60
32	2a	1272	G	C2-N3-C4	-10.69	106.55	111.90
55	1x	14	A	C5-N7-C8	10.43	109.11	103.90
32	2a	1263	C	C5-C4-N4	10.36	127.45	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	14	A	C4-C5-C6	10.24	122.12	117.00
32	2a	1263	C	C4-C5-C6	-10.11	112.34	117.40
32	2a	1263	C	N3-C4-N4	-10.11	110.92	118.00
1	1A	1075	C	C2-N3-C4	10.05	124.93	119.90
32	2a	1263	C	C2-N1-C1'	9.88	129.67	118.80
55	1x	22	G	C5-N7-C8	-9.88	99.36	104.30
1	1A	2573	C	N1-C2-O2	-9.78	113.03	118.90
1	1A	512	G	O4'-C1'-N9	9.38	115.70	108.20
55	2x	14	A	C5-N7-C8	9.09	108.45	103.90
1	1A	946	G	O5'-P-OP1	-9.05	97.55	105.70
1	2A	2136	C	N1-C2-O2	9.00	124.30	118.90
1	1A	1352	U	O5'-P-OP1	-8.99	97.61	105.70
55	1x	46	G	N3-C2-N2	-8.98	113.61	119.90
1	1A	1063	G	C5-C6-O6	8.80	133.88	128.60
1	1A	2682	U	O5'-P-OP2	-8.77	97.81	105.70
2	2B	80	U	O4'-C1'-N1	8.71	115.17	108.20
55	2x	14	A	C4-C5-C6	8.65	121.33	117.00
1	1A	2492	U	O5'-P-OP1	-8.56	98.00	105.70
32	2a	1263	C	C6-N1-C2	-8.52	116.89	120.30
1	1A	531	C	O5'-P-OP2	-8.38	98.16	105.70
57	1y	33	U	C2-N1-C1'	8.34	127.71	117.70
32	2a	1263	C	N1-C2-N3	-8.28	113.40	119.20
1	1A	2036	C	O5'-P-OP1	-8.24	98.28	105.70
1	1A	2167	U	C2-N1-C1'	8.08	127.40	117.70
1	1A	576	U	O5'-P-OP1	-8.06	98.44	105.70
1	1A	1063	G	C6-N1-C2	8.02	129.91	125.10
55	2x	22	G	C5-N7-C8	-8.01	100.29	104.30
1	1A	793	A	O5'-P-OP2	-7.96	98.54	105.70
55	1x	46	G	C5-C6-N1	7.86	115.43	111.50
55	1x	14	A	C5-C6-N1	-7.75	113.83	117.70
32	2a	754	C	C2-N1-C1'	7.70	127.27	118.80
1	1A	975	C	N1-C2-O2	-7.67	114.30	118.90
1	1A	2269	A	O5'-P-OP1	-7.63	98.83	105.70
57	1y	56	C	N1-C2-O2	7.60	123.46	118.90
32	1a	558	G	O5'-P-OP1	-7.39	99.05	105.70
57	1y	33	U	N3-C2-O2	-7.34	117.06	122.20
1	2A	512	G	O4'-C1'-N9	7.30	114.04	108.20
1	1A	801	G	O5'-P-OP2	-7.28	99.15	105.70
57	1y	33	U	N1-C2-O2	7.16	127.81	122.80
1	1A	948	G	O5'-P-OP1	-7.16	99.26	105.70
1	1A	1993	U	O5'-P-OP1	-7.13	99.28	105.70
1	1A	2167	U	N1-C2-O2	7.10	127.77	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2136	C	N3-C2-O2	-6.98	117.01	121.90
55	1x	22	G	C5-C6-N1	6.97	114.99	111.50
1	1A	1063	G	N3-C2-N2	6.96	124.77	119.90
55	1x	22	G	C4-C5-C6	-6.84	114.69	118.80
32	2a	1272	G	C8-N9-C1'	-6.79	118.18	127.00
1	1A	1614	A	O5'-P-OP1	-6.78	99.60	105.70
55	1x	22	G	N7-C8-N9	6.75	116.48	113.10
32	1a	1025	U	N1-C2-O2	6.74	127.52	122.80
55	2x	46	G	N3-C2-N2	-6.73	115.19	119.90
32	2a	1272	G	C4-N9-C1'	6.68	135.19	126.50
1	1A	2610	C	N1-C2-O2	6.67	122.90	118.90
55	2x	46	G	C5-C6-N1	6.63	114.81	111.50
1	2A	847	U	C2-N1-C1'	6.62	125.65	117.70
32	1a	299	G	C5-C6-O6	-6.55	124.67	128.60
1	1A	787	U	O5'-P-OP1	-6.52	99.83	105.70
1	1A	1086	A	C5-C6-N6	6.49	128.90	123.70
1	1A	1776	G	O5'-P-OP2	-6.42	99.93	105.70
1	1A	975	C	C2-N1-C1'	-6.39	111.78	118.80
1	1A	2629	A	P-O3'-C3'	6.37	127.35	119.70
1	1A	2167	U	N3-C2-O2	-6.36	117.75	122.20
1	1A	1075	C	C5-C4-N4	6.34	124.64	120.20
55	2x	22	G	N1-C6-O6	-6.33	116.11	119.90
1	1A	2129	C	N1-C2-O2	6.32	122.69	118.90
55	1x	22	G	C4-C5-N7	6.31	113.32	110.80
8	2I	58	LEU	CA-CB-CG	6.27	129.73	115.30
55	2x	46	G	N1-C2-N3	6.26	127.65	123.90
1	2A	2129	C	N1-C2-O2	6.25	122.65	118.90
32	2a	1263	C	C6-N1-C1'	-6.19	113.37	120.80
1	1A	1080	C	N1-C2-O2	6.18	122.61	118.90
32	1a	1158	C	C2-N1-C1'	6.15	125.56	118.80
55	1x	46	G	N1-C2-N3	6.12	127.57	123.90
1	1A	1074	G	C5-C6-O6	-6.08	124.95	128.60
1	2A	1352	U	O5'-P-OP1	-6.08	100.23	105.70
55	2x	22	G	C4-C5-C6	-6.05	115.17	118.80
45	1n	44	LEU	CA-CB-CG	6.05	129.22	115.30
1	1A	1992	G	P-O3'-C3'	6.05	126.96	119.70
55	2x	22	G	N7-C8-N9	6.04	116.12	113.10
1	1A	1074	G	N3-C4-N9	6.02	129.61	126.00
1	2A	2689	U	N3-C2-O2	-6.02	117.98	122.20
32	2a	1067	A	P-O3'-C3'	6.01	126.91	119.70
1	1A	975	C	C6-N1-C1'	6.00	128.00	120.80
1	1A	2371	G	C5-C6-N1	5.97	114.49	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1075	C	N3-C2-O2	-5.96	117.72	121.90
1	2A	141	A	O4'-C1'-N9	5.96	112.97	108.20
1	1A	372	G	O4'-C1'-N9	5.95	112.96	108.20
1	2A	801	G	O5'-P-OP2	-5.94	100.35	105.70
1	1A	2028	U	N3-C4-O4	-5.94	115.25	119.40
54	1w	47	U	C2-N1-C1'	5.93	124.82	117.70
1	1A	614	U	N3-C2-O2	-5.92	118.05	122.20
55	1x	46	G	N9-C4-C5	5.89	107.76	105.40
55	2x	14	A	C5-C6-N1	-5.88	114.76	117.70
32	2a	754	C	C6-N1-C1'	-5.85	113.78	120.80
32	2a	1158	C	C2-N1-C1'	5.85	125.23	118.80
32	1a	1030	C	N1-C2-O2	5.78	122.37	118.90
1	2A	1698	A	O4'-C1'-N9	5.77	112.81	108.20
55	1x	14	A	C8-N9-C1'	-5.77	117.32	127.70
55	1x	46	G	C5-C6-O6	-5.74	125.15	128.60
1	1A	2848	G	O4'-C1'-N9	5.74	112.79	108.20
1	2A	2689	U	P-O3'-C3'	5.73	126.57	119.70
1	2A	885	C	C5-C6-N1	5.72	123.86	121.00
1	1A	2573	C	C2-N3-C4	-5.71	117.04	119.90
1	2A	1992	G	P-O3'-C3'	5.69	126.53	119.70
1	1A	386	G	O4'-C1'-N9	5.68	112.75	108.20
55	2x	22	G	C5-C6-N1	5.66	114.33	111.50
1	1A	2032	G	C5-N7-C8	5.64	107.12	104.30
1	1A	1648	C	O5'-P-OP1	-5.63	100.63	105.70
32	1a	1030	C	C2-N3-C4	5.62	122.71	119.90
32	2a	266	G	P-O3'-C3'	5.61	126.44	119.70
1	1A	2023	G	O5'-P-OP1	-5.61	100.65	105.70
1	1A	2825	C	C6-N1-C2	-5.60	118.06	120.30
1	1A	1779	U	O4'-C1'-N1	5.60	112.68	108.20
1	1A	1372	U	N3-C4-O4	5.60	123.32	119.40
1	2A	141	A	N7-C8-N9	5.59	116.59	113.80
1	1A	1174	A	OP1-P-O3'	5.58	117.47	105.20
57	1y	56	C	C2-N3-C4	5.58	122.69	119.90
1	1A	2129	C	C2-N1-C1'	5.57	124.93	118.80
1	2A	2492	U	O5'-P-OP1	-5.55	100.70	105.70
1	2A	2689	U	N1-C2-O2	5.54	126.68	122.80
1	2A	528	A	P-O3'-C3'	5.53	126.34	119.70
55	2x	14	A	C4-C5-N7	-5.51	107.94	110.70
1	1A	1074	G	N9-C4-C5	-5.50	103.20	105.40
1	1A	704	G	O4'-C1'-N9	5.49	112.59	108.20
1	1A	847	U	C2-N1-C1'	5.44	124.23	117.70
55	1x	14	A	C4-N9-C1'	5.43	136.08	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1614	A	O5'-P-OP1	-5.43	100.82	105.70
1	1A	1174	A	P-O3'-C3'	5.41	126.19	119.70
55	2x	14	A	C8-N9-C1'	-5.40	117.98	127.70
1	2A	228	A	P-O3'-C3'	5.37	126.14	119.70
1	1A	1936	A	O4'-C1'-N9	5.36	112.49	108.20
1	2A	2318	G	N3-C4-C5	-5.35	125.92	128.60
32	2a	115	G	P-O3'-C3'	5.33	126.10	119.70
1	1A	975	C	N1-C2-N3	5.32	122.93	119.20
55	2x	14	A	C4-N9-C1'	5.32	135.88	126.30
32	1a	754	C	C2-N1-C1'	5.32	124.65	118.80
35	1d	187	ARG	C-N-CA	-5.31	108.42	121.70
32	1a	913	A	P-O3'-C3'	5.31	126.07	119.70
55	1x	22	G	C8-N9-C1'	5.31	133.90	127.00
1	1A	2593	U	N3-C4-C5	5.30	117.78	114.60
1	1A	1064	C	C2-N1-C1'	5.29	124.62	118.80
1	1A	568	U	C5-C4-O4	-5.28	122.73	125.90
1	1A	1314	C	C2-N1-C1'	5.27	124.60	118.80
1	1A	271(Y)	U	O4'-C1'-N1	5.27	112.41	108.20
1	1A	226	G	O4'-C1'-N9	5.25	112.40	108.20
55	1x	14	A	C4-C5-N7	-5.25	108.07	110.70
1	1A	1416	G	O4'-C1'-N9	5.25	112.40	108.20
32	2a	754	C	N1-C2-O2	5.25	122.05	118.90
32	1a	1067	A	P-O3'-C3'	5.24	125.99	119.70
1	1A	975	C	C2-N3-C4	-5.23	117.28	119.90
1	1A	1082	U	N3-C4-O4	-5.23	115.74	119.40
32	1a	115	G	P-O3'-C3'	5.23	125.97	119.70
1	1A	1647	G	O4'-C1'-N9	-5.22	104.02	108.20
57	1y	33	U	C6-N1-C1'	-5.22	113.90	121.20
1	2A	752	A	P-O3'-C3'	5.22	125.96	119.70
32	2a	1065	U	P-O3'-C3'	5.22	125.96	119.70
1	2A	2287	A	O4'-C1'-N9	5.21	112.37	108.20
1	1A	2167	U	C6-N1-C1'	-5.21	113.91	121.20
1	1A	139(A)	G	C5-N7-C8	5.20	106.90	104.30
1	2A	528	A	OP1-P-O3'	5.20	116.63	105.20
32	2a	913	A	P-O3'-C3'	5.18	125.92	119.70
1	1A	1236	G	C8-N9-C4	5.18	108.47	106.40
1	1A	2129	C	N3-C2-O2	-5.17	118.28	121.90
1	1A	784	A	OP1-P-O3'	5.17	116.58	105.20
1	1A	1063	G	N1-C6-O6	-5.16	116.80	119.90
1	1A	847	U	N1-C2-O2	5.16	126.41	122.80
1	1A	1064	C	N1-C2-O2	5.16	122.00	118.90
1	1A	2439	A	OP1-P-O3'	5.16	116.55	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	368	U	O4'-C1'-N1	5.16	112.33	108.20
1	2A	141	A	C8-N9-C4	-5.16	103.74	105.80
1	1A	2553	G	N3-C4-N9	5.15	129.09	126.00
55	1x	46	G	C4-C5-N7	-5.14	108.74	110.80
1	1A	2136	C	N1-C2-O2	5.14	121.98	118.90
1	1A	961	C	O5'-P-OP2	-5.13	101.08	105.70
1	1A	1791	A	O5'-P-OP1	-5.13	101.08	105.70
1	1A	1100	C	C2-N1-C1'	5.13	124.44	118.80
1	1A	1074	G	C4-C5-N7	5.12	112.85	110.80
1	1A	944	G	C8-N9-C1'	-5.12	120.35	127.00
32	1a	266	G	P-O3'-C3'	5.11	125.84	119.70
1	1A	2248	C	O5'-P-OP2	-5.11	101.10	105.70
1	2A	228	A	OP1-P-O3'	5.10	116.42	105.20
1	1A	746	A	O4'-C1'-N9	5.08	112.27	108.20
32	1a	748	C	P-O3'-C3'	5.06	125.78	119.70
1	1A	845	G	O4'-C1'-N9	5.06	112.25	108.20
1	1A	1080	C	C2-N3-C4	5.05	122.43	119.90
1	1A	2073	C	OP2-P-O3'	5.05	116.32	105.20
1	1A	195	A	P-O3'-C3'	5.05	125.76	119.70
1	1A	679	C	N1-C2-O2	5.04	121.92	118.90
1	1A	975	C	C5-C6-N1	-5.03	118.48	121.00
32	1a	975	A	O4'-C1'-N9	-5.03	104.18	108.20
1	1A	2207	G	N1-C6-O6	5.03	122.92	119.90
1	1A	2610	C	N3-C2-O2	-5.03	118.38	121.90
1	1A	1192	G	C5-N7-C8	5.02	106.81	104.30
55	1x	22	G	N1-C6-O6	-5.01	116.89	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	122	PHE	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	29	34
4	2E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	29	34
5	1F	200/210 (95%)	196 (98%)	3 (2%)	1 (0%)	29	34
5	2F	200/210 (95%)	190 (95%)	9 (4%)	1 (0%)	29	34
6	1G	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	25	29
6	2G	179/182 (98%)	159 (89%)	15 (8%)	5 (3%)	5	2
7	1H	172/180 (96%)	162 (94%)	10 (6%)	0	100	100
7	2H	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	25	29
8	1I	144/148 (97%)	123 (85%)	20 (14%)	1 (1%)	22	25
8	2I	144/148 (97%)	125 (87%)	18 (12%)	1 (1%)	22	25
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	130 (94%)	6 (4%)	2 (1%)	11	9
10	1O	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	133 (90%)	11 (8%)	3 (2%)	7	5
11	2P	147/150 (98%)	133 (90%)	10 (7%)	4 (3%)	5	2
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
12	2Q	139/141 (99%)	127 (91%)	11 (8%)	1 (1%)	22	25
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	17	19
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	19	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	123 (95%)	6 (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	16
17	2V	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	3 (3%)	2 (2%)	6	4
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	14
20	1Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	148/206 (72%)	130 (88%)	17 (12%)	1 (1%)	22	25
21	2Z	156/206 (76%)	131 (84%)	21 (14%)	4 (3%)	5	3
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	14
23	21	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	0
26	24	67/71 (94%)	57 (85%)	7 (10%)	3 (4%)	2	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	194 (85%)	26 (11%)	9 (4%)	3	1
33	2b	229/256 (90%)	197 (86%)	28 (12%)	4 (2%)	9	7
34	1c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	29	34
34	2c	204/239 (85%)	176 (86%)	21 (10%)	7 (3%)	3	1
35	1d	206/209 (99%)	194 (94%)	9 (4%)	3 (2%)	10	9
35	2d	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
36	1e	146/162 (90%)	130 (89%)	13 (9%)	3 (2%)	7	5
36	2e	146/162 (90%)	133 (91%)	10 (7%)	3 (2%)	7	5
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	143 (94%)	9 (6%)	1 (1%)	22	25
38	2g	153/156 (98%)	139 (91%)	11 (7%)	3 (2%)	7	5
39	1h	135/138 (98%)	123 (91%)	12 (9%)	0	100	100
39	2h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	22	25
40	1i	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	19	22
40	2i	125/128 (98%)	115 (92%)	9 (7%)	1 (1%)	19	22
41	1j	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	4	1
41	2j	94/105 (90%)	78 (83%)	13 (14%)	3 (3%)	4	1
42	1k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	17	19
42	2k	112/129 (87%)	102 (91%)	7 (6%)	3 (3%)	5	2
43	1l	119/132 (90%)	113 (95%)	4 (3%)	2 (2%)	9	7
43	2l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
44	1m	121/126 (96%)	109 (90%)	10 (8%)	2 (2%)	9	7
44	2m	120/126 (95%)	110 (92%)	9 (8%)	1 (1%)	19	22
45	1n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	7
45	2n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
47	1p	80/88 (91%)	66 (82%)	13 (16%)	1 (1%)	12	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	15	16
48	2q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	15	16
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	69 (85%)	10 (12%)	2 (2%)	5	3
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	4	1
51	2t	94/106 (89%)	85 (90%)	7 (7%)	2 (2%)	7	5
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
56	1z	5/7 (71%)	5 (100%)	0	0	100	100
56	2z	5/7 (71%)	5 (100%)	0	0	100	100
All	All	11378/12142 (94%)	10554 (93%)	718 (6%)	106 (1%)	17	19

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	1Z	53	ILE
33	1b	17	PHE
33	1b	126	GLU
35	1d	173	TRP
40	1i	54	ASP
42	1k	49	GLY
44	1m	67	GLU
5	2F	130	ALA
12	2Q	16	ARG
26	24	45	GLY
33	2b	17	PHE
38	2g	4	ARG
38	2g	55	GLY
44	2m	106	ASN
5	1F	130	ALA
8	1I	11	ASN
11	1P	44	GLY
17	1V	43	GLU
19	1X	93	GLU

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Mol	Chain	Res	Type
23	11	3	LYS
26	14	61	ARG
36	1e	21	ALA
36	1e	85	GLY
45	1n	12	ARG
48	1q	68	ARG
6	2G	42	GLY
6	2G	43	LEU
6	2G	50	ALA
6	2G	51	ARG
11	2P	36	LYS
21	2Z	52	SER
33	2b	126	GLU
34	2c	107	GLN
40	2i	56	LEU
48	2q	68	ARG
50	2s	81	ARG
11	1P	38	GLN
26	14	49	PHE
26	14	62	ARG
33	1b	228	GLY
34	1c	107	GLN
38	1g	79	ARG
41	1j	79	ARG
47	1p	75	ARG
9	2N	2	LYS
9	2N	23	LEU
11	2P	38	GLN
19	2X	93	GLU
21	2Z	144	LEU
26	24	47	GLN
26	24	49	PHE
34	2c	43	LEU
36	2e	69	VAL
41	2j	78	ASN
41	2j	79	ARG
42	2k	49	GLY
4	1E	52	LEU
6	1G	43	LEU
33	1b	8	LYS
33	1b	22	LYS
33	1b	106	LYS

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Mol	Chain	Res	Type
35	1d	88	VAL
41	1j	78	ASN
43	1l	91	LYS
43	1l	105	TYR
44	1m	106	ASN
4	2E	52	LEU
14	2S	84	GLN
34	2c	91	LEU
34	2c	95	THR
38	2g	80	VAL
42	2k	117	ASN
51	2t	10	LEU
15	1T	55	ASN
19	1X	2	LYS
26	14	51	ASP
51	1t	47	GLY
6	2G	181	ARG
7	2H	126	PRO
11	2P	122	PRO
21	2Z	146	ILE
33	2b	123	ALA
34	2c	53	ALA
33	1b	20	GLU
51	1t	100	ILE
8	2I	10	GLU
11	2P	45	LEU
34	2c	179	ARG
51	2t	95	ALA
35	1d	172	PRO
33	2b	231	GLU
34	2c	51	GLY
41	2j	75	ILE
42	2k	105	VAL
41	1j	39	PRO
50	2s	9	VAL
11	1P	122	PRO
36	2e	11	ILE
39	2h	73	ASP
33	1b	231	GLU
36	1e	69	VAL
51	1t	96	GLY
21	2Z	171	ILE

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Mol	Chain	Res	Type
26	14	50	VAL
36	2e	96	PRO
33	1b	125	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	208 (97%)	7 (3%)	38	49
3	2D	215/218 (99%)	206 (96%)	9 (4%)	30	39
4	1E	164/166 (99%)	159 (97%)	5 (3%)	41	52
4	2E	164/166 (99%)	158 (96%)	6 (4%)	34	45
5	1F	160/166 (96%)	146 (91%)	14 (9%)	10	11
5	2F	159/166 (96%)	153 (96%)	6 (4%)	33	43
6	1G	143/156 (92%)	133 (93%)	10 (7%)	15	18
6	2G	143/156 (92%)	126 (88%)	17 (12%)	5	4
7	1H	144/148 (97%)	139 (96%)	5 (4%)	36	47
7	2H	144/148 (97%)	140 (97%)	4 (3%)	43	56
8	1I	113/124 (91%)	100 (88%)	13 (12%)	5	5
8	2I	105/124 (85%)	90 (86%)	15 (14%)	3	2
9	1N	118/119 (99%)	110 (93%)	8 (7%)	16	19
9	2N	118/119 (99%)	109 (92%)	9 (8%)	13	15
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	52
10	2O	100/100 (100%)	93 (93%)	7 (7%)	15	18
11	1P	115/116 (99%)	108 (94%)	7 (6%)	18	24
11	2P	115/116 (99%)	108 (94%)	7 (6%)	18	24
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	59	71
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	27	36
13	1R	101/101 (100%)	98 (97%)	3 (3%)	41	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	2R	101/101 (100%)	99 (98%)	2 (2%)	55	67
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11	13
14	2S	85/88 (97%)	77 (91%)	8 (9%)	8	9
15	1T	115/127 (91%)	109 (95%)	6 (5%)	23	30
15	2T	113/127 (89%)	107 (95%)	6 (5%)	22	29
16	1U	93/94 (99%)	90 (97%)	3 (3%)	39	50
16	2U	93/94 (99%)	88 (95%)	5 (5%)	22	28
17	1V	80/82 (98%)	78 (98%)	2 (2%)	47	60
17	2V	80/82 (98%)	77 (96%)	3 (4%)	33	43
18	1W	90/92 (98%)	87 (97%)	3 (3%)	38	49
18	2W	90/92 (98%)	88 (98%)	2 (2%)	52	64
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46	58
19	2X	77/78 (99%)	76 (99%)	1 (1%)	69	79
20	1Y	85/91 (93%)	77 (91%)	8 (9%)	8	9
20	2Y	85/91 (93%)	81 (95%)	4 (5%)	26	34
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	9	10
21	2Z	137/179 (76%)	124 (90%)	13 (10%)	8	9
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	65 (100%)	0	100	100
23	11	80/83 (96%)	79 (99%)	1 (1%)	69	79
23	21	80/83 (96%)	78 (98%)	2 (2%)	47	60
24	12	65/67 (97%)	62 (95%)	3 (5%)	27	35
24	22	65/67 (97%)	63 (97%)	2 (3%)	40	52
25	13	51/52 (98%)	48 (94%)	3 (6%)	19	25
25	23	50/52 (96%)	45 (90%)	5 (10%)	7	7
26	14	59/63 (94%)	52 (88%)	7 (12%)	5	4
26	24	53/63 (84%)	43 (81%)	10 (19%)	1	1
27	15	50/52 (96%)	47 (94%)	3 (6%)	19	24
27	25	50/52 (96%)	46 (92%)	4 (8%)	12	14
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	4
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	8
29	27	41/42 (98%)	37 (90%)	4 (10%)	8	8
30	18	54/55 (98%)	49 (91%)	5 (9%)	9	9
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	16
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	171 (89%)	21 (11%)	6	6
33	2b	187/220 (85%)	159 (85%)	28 (15%)	3	2
34	1c	142/188 (76%)	128 (90%)	14 (10%)	8	7
34	2c	140/188 (74%)	127 (91%)	13 (9%)	9	9
35	1d	169/181 (93%)	152 (90%)	17 (10%)	7	7
35	2d	173/181 (96%)	158 (91%)	15 (9%)	10	11
36	1e	113/123 (92%)	104 (92%)	9 (8%)	12	14
36	2e	114/123 (93%)	104 (91%)	10 (9%)	10	11
37	1f	84/90 (93%)	80 (95%)	4 (5%)	25	33
37	2f	85/90 (94%)	78 (92%)	7 (8%)	11	13
38	1g	119/127 (94%)	104 (87%)	15 (13%)	4	3
38	2g	120/127 (94%)	105 (88%)	15 (12%)	4	3
39	1h	114/119 (96%)	110 (96%)	4 (4%)	36	47
39	2h	114/119 (96%)	106 (93%)	8 (7%)	15	18
40	1i	90/99 (91%)	81 (90%)	9 (10%)	7	7
40	2i	89/99 (90%)	78 (88%)	11 (12%)	4	4
41	1j	66/92 (72%)	57 (86%)	9 (14%)	3	3
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5	5
42	1k	82/99 (83%)	78 (95%)	4 (5%)	25	32
42	2k	83/99 (84%)	79 (95%)	4 (5%)	25	33
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	39
43	2l	96/108 (89%)	88 (92%)	8 (8%)	11	12
44	1m	93/101 (92%)	87 (94%)	6 (6%)	17	21
44	2m	92/101 (91%)	82 (89%)	10 (11%)	6	6
45	1n	49/50 (98%)	40 (82%)	9 (18%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30	40
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46	58
46	2o	78/80 (98%)	74 (95%)	4 (5%)	24	31
47	1p	69/74 (93%)	67 (97%)	2 (3%)	42	53
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13	16
48	1q	94/97 (97%)	91 (97%)	3 (3%)	39	50
48	2q	94/97 (97%)	91 (97%)	3 (3%)	39	50
49	1r	59/77 (77%)	56 (95%)	3 (5%)	24	31
49	2r	59/77 (77%)	55 (93%)	4 (7%)	16	19
50	1s	69/80 (86%)	67 (97%)	2 (3%)	42	53
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	10
51	1t	70/82 (85%)	64 (91%)	6 (9%)	10	11
51	2t	70/82 (85%)	68 (97%)	2 (3%)	42	53
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	27
52	2u	18/22 (82%)	18 (100%)	0	100	100
56	1z	6/6 (100%)	5 (83%)	1 (17%)	2	1
56	2z	6/6 (100%)	3 (50%)	3 (50%)	0	0
All	All	9315/10076 (92%)	8687 (93%)	628 (7%)	16	20

All (628) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	37	LEU
3	1D	71	ASP
3	1D	142	VAL
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	1	MET
4	1E	47	VAL
4	1E	113	PHE
4	1E	116	VAL
4	1E	184	VAL
5	1F	13	SER
5	1F	24	LEU

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Mol	Chain	Res	Type
5	1F	27	GLU
5	1F	53	THR
5	1F	57	VAL
5	1F	60	SER
5	1F	70	THR
5	1F	106	ARG
5	1F	144	LYS
5	1F	168	ARG
5	1F	175	THR
5	1F	183	VAL
5	1F	192	LEU
5	1F	195	ASP
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	21	ARG
6	1G	22	ARG
6	1G	43	LEU
6	1G	91	ARG
6	1G	139	LEU
6	1G	159	VAL
6	1G	170	ARG
7	1H	95	ARG
7	1H	127	GLU
7	1H	134	SER
7	1H	149	ARG
7	1H	160	LYS
8	1I	12	LEU
8	1I	20	ASP
8	1I	38	LEU
8	1I	47	LEU
8	1I	76	THR
8	1I	77	LEU
8	1I	85	GLU
8	1I	101	LEU
8	1I	116	LEU
8	1I	133	HIS
8	1I	140	LEU
8	1I	143	SER
8	1I	144	VAL
9	1N	1	MET
9	1N	8	GLN

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Mol	Chain	Res	Type
9	1N	9	VAL
9	1N	28	THR
9	1N	48	MET
9	1N	61	ARG
9	1N	62	VAL
9	1N	83	LYS
10	1O	28	SER
10	1O	66	LYS
10	1O	113	LYS
11	1P	7	ARG
11	1P	15	ARG
11	1P	45	LEU
11	1P	98	GLU
11	1P	125	VAL
11	1P	133	SER
11	1P	147	LEU
12	1Q	75	THR
12	1Q	109	VAL
13	1R	24	GLN
13	1R	36	THR
13	1R	114	VAL
14	1S	3	ARG
14	1S	14	VAL
14	1S	17	ARG
14	1S	25	ARG
14	1S	46	VAL
14	1S	73	LEU
14	1S	110	LEU
15	1T	28	VAL
15	1T	36	GLU
15	1T	96	ARG
15	1T	107	ASP
15	1T	108	ARG
15	1T	115	ARG
16	1U	31	SER
16	1U	74	LEU
16	1U	95	LEU
17	1V	56	SER
17	1V	73	SER
18	1W	11	ARG
18	1W	17	VAL
18	1W	67	ASP

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Mol	Chain	Res	Type
19	1X	38	GLU
19	1X	72	LYS
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	31	LEU
20	1Y	64	GLU
20	1Y	67	LEU
20	1Y	91	GLU
20	1Y	92	ASN
20	1Y	99	CYS
21	1Z	1	MET
21	1Z	33	LEU
21	1Z	42	VAL
21	1Z	72	ARG
21	1Z	80	ARG
21	1Z	84	GLU
21	1Z	129	SER
21	1Z	132	ASN
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	171	ILE
23	11	40	ARG
24	12	40	SER
24	12	55	ARG
24	12	70	GLN
25	13	23	LEU
25	13	35	ARG
25	13	37	LEU
26	14	1	MET
26	14	49	PHE
26	14	50	VAL
26	14	61	ARG
26	14	63	TYR
26	14	66	SER
26	14	69	LYS
27	15	6	VAL
27	15	33	CYS
27	15	40	LYS
28	16	6	ARG
28	16	7	ILE
28	16	14	THR

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Mol	Chain	Res	Type
28	16	17	LYS
28	16	19	ARG
28	16	47	THR
29	17	24	THR
29	17	41	ARG
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	23	VAL
30	18	29	LYS
30	18	31	HIS
30	18	34	TRP
33	1b	7	VAL
33	1b	12	GLU
33	1b	21	ARG
33	1b	23	ARG
33	1b	24	TRP
33	1b	28	PHE
33	1b	35	GLU
33	1b	43	ASP
33	1b	45	GLN
33	1b	78	GLN
33	1b	81	VAL
33	1b	82	ARG
33	1b	83	MET
33	1b	196	LEU
33	1b	197	VAL
33	1b	212	GLN
33	1b	215	LEU
33	1b	221	LEU
33	1b	229	VAL
33	1b	233	SER
33	1b	236	TYR
34	1c	3	ASN
34	1c	8	ILE
34	1c	17	ASP
34	1c	29	TYR
34	1c	49	SER
34	1c	56	ASP
34	1c	70	VAL
34	1c	89	GLU
34	1c	102	ASN

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Mol	Chain	Res	Type
34	1c	119	ARG
34	1c	165	THR
34	1c	178	LEU
34	1c	195	VAL
34	1c	207	VAL
35	1d	3	ARG
35	1d	10	ARG
35	1d	19	LEU
35	1d	28	SER
35	1d	31	CYS
35	1d	59	ARG
35	1d	83	SER
35	1d	89	THR
35	1d	91	SER
35	1d	107	ARG
35	1d	135	LEU
35	1d	137	SER
35	1d	140	VAL
35	1d	157	LEU
35	1d	175	SER
35	1d	188	LEU
35	1d	194	LEU
36	1e	10	MET
36	1e	18	ARG
36	1e	20	GLN
36	1e	24	ARG
36	1e	31	LEU
36	1e	41	VAL
36	1e	63	ARG
36	1e	64	ARG
36	1e	75	THR
37	1f	72	VAL
37	1f	73	ASN
37	1f	75	LEU
37	1f	92	LYS
38	1g	12	LEU
38	1g	13	GLN
38	1g	21	VAL
38	1g	50	ILE
38	1g	51	GLN
38	1g	59	LEU
38	1g	78	ARG

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Mol	Chain	Res	Type
38	1g	80	VAL
38	1g	85	TYR
38	1g	87	VAL
38	1g	90	GLU
38	1g	104	LEU
38	1g	110	GLN
38	1g	114	ARG
38	1g	115	ARG
39	1h	18	ARG
39	1h	26	VAL
39	1h	52	ASP
39	1h	54	ASP
40	1i	23	ASN
40	1i	25	LYS
40	1i	27	THR
40	1i	53	VAL
40	1i	60	ASP
40	1i	88	TYR
40	1i	92	TYR
40	1i	103	THR
40	1i	128	ARG
41	1j	5	ARG
41	1j	38	ILE
41	1j	43	ARG
41	1j	44	VAL
41	1j	46	ARG
41	1j	51	ARG
41	1j	81	THR
41	1j	92	THR
41	1j	98	ILE
42	1k	18	ARG
42	1k	31	THR
42	1k	48	ILE
42	1k	104	GLN
43	1l	18	VAL
43	1l	33	ARG
43	1l	36	VAL
43	1l	62	SER
44	1m	4	ILE
44	1m	11	ARG
44	1m	43	THR
44	1m	70	LEU

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Mol	Chain	Res	Type
44	1m	106	ASN
44	1m	121	LYS
45	1n	13	THR
45	1n	15	LYS
45	1n	17	LYS
45	1n	18	VAL
45	1n	24	CYS
45	1n	35	ARG
45	1n	44	LEU
45	1n	53	LEU
45	1n	60	SER
46	1o	76	GLU
46	1o	84	LYS
47	1p	67	THR
47	1p	75	ARG
48	1q	34	LYS
48	1q	60	ILE
48	1q	99	SER
49	1r	35	ARG
49	1r	37	VAL
49	1r	63	GLN
50	1s	6	LYS
50	1s	12	ASP
51	1t	10	LEU
51	1t	13	LEU
51	1t	24	LEU
51	1t	37	SER
51	1t	90	GLN
51	1t	100	ILE
52	1u	15	ARG
56	1z	2	THR
3	2D	37	LEU
3	2D	38	LYS
3	2D	88	ARG
3	2D	142	VAL
3	2D	181	GLU
3	2D	183	ARG
3	2D	221	VAL
3	2D	242	ARG
3	2D	259	THR
4	2E	38	THR
4	2E	73	GLU

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Mol	Chain	Res	Type
4	2E	77	ILE
4	2E	87	GLU
4	2E	116	VAL
4	2E	145	LYS
5	2F	9	ILE
5	2F	33	LEU
5	2F	74	ARG
5	2F	145	GLU
5	2F	157	VAL
5	2F	161	GLU
6	2G	4	ASP
6	2G	5	VAL
6	2G	18	GLU
6	2G	28	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	51	ARG
6	2G	79	ASN
6	2G	91	ARG
6	2G	115	ARG
6	2G	124	SER
6	2G	130	ASN
6	2G	133	LEU
6	2G	140	ILE
6	2G	150	ASP
6	2G	152	LEU
6	2G	165	THR
7	2H	88	LEU
7	2H	127	GLU
7	2H	129	THR
7	2H	136	ILE
8	2I	2	LYS
8	2I	19	VAL
8	2I	38	LEU
8	2I	51	ILE
8	2I	58	LEU
8	2I	68	LEU
8	2I	75	LEU
8	2I	82	ARG
8	2I	85	GLU
8	2I	87	LYS
8	2I	101	LEU

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Mol	Chain	Res	Type
8	2I	102	SER
8	2I	117	GLU
8	2I	123	LEU
8	2I	127	VAL
9	2N	1	MET
9	2N	8	GLN
9	2N	9	VAL
9	2N	22	THR
9	2N	28	THR
9	2N	61	ARG
9	2N	62	VAL
9	2N	68	GLU
9	2N	83	LYS
10	2O	1	MET
10	2O	22	ILE
10	2O	28	SER
10	2O	66	LYS
10	2O	78	ARG
10	2O	112	MET
10	2O	116	SER
11	2P	29	LYS
11	2P	95	VAL
11	2P	119	GLU
11	2P	125	VAL
11	2P	133	SER
11	2P	135	LEU
11	2P	148	LEU
12	2Q	1	MET
12	2Q	6	ARG
12	2Q	22	LYS
12	2Q	38	GLU
12	2Q	75	THR
13	2R	36	THR
13	2R	114	VAL
14	2S	3	ARG
14	2S	17	ARG
14	2S	26	LEU
14	2S	43	GLU
14	2S	52	SER
14	2S	83	LYS
14	2S	84	GLN
14	2S	110	LEU

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Mol	Chain	Res	Type
15	2T	40	THR
15	2T	66	VAL
15	2T	67	SER
15	2T	72	VAL
15	2T	87	ASP
15	2T	107	ASP
16	2U	5	LYS
16	2U	31	SER
16	2U	74	LEU
16	2U	77	SER
16	2U	95	LEU
17	2V	53	GLU
17	2V	79	VAL
17	2V	98	GLU
18	2W	11	ARG
18	2W	17	VAL
19	2X	38	GLU
20	2Y	6	HIS
20	2Y	14	LEU
20	2Y	26	LYS
20	2Y	99	CYS
21	2Z	6	LYS
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	67	LEU
21	2Z	71	VAL
21	2Z	72	ARG
21	2Z	121	HIS
21	2Z	129	SER
21	2Z	131	ARG
21	2Z	136	PHE
21	2Z	137	ILE
21	2Z	154	ASP
21	2Z	171	ILE
23	21	40	ARG
23	21	72	GLU
24	22	53	LEU
24	22	70	GLN
25	23	18	ASP
25	23	31	LEU
25	23	34	GLU
25	23	37	LEU

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Mol	Chain	Res	Type
25	23	58	VAL
26	24	5	ILE
26	24	10	VAL
26	24	34	GLU
26	24	37	SER
26	24	53	GLU
26	24	59	PHE
26	24	61	ARG
26	24	63	TYR
26	24	67	TYR
26	24	68	ARG
27	25	40	LYS
27	25	55	ARG
27	25	58	LEU
27	25	59	GLU
28	26	6	ARG
28	26	19	ARG
28	26	20	ASN
28	26	40	CYS
28	26	48	VAL
29	27	1	MET
29	27	23	ARG
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	31	HIS
30	28	34	TRP
30	28	37	SER
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	11	LEU
33	2b	16	HIS
33	2b	24	TRP
33	2b	35	GLU
33	2b	44	LEU
33	2b	48	MET
33	2b	71	VAL
33	2b	76	GLN
33	2b	82	ARG
33	2b	83	MET
33	2b	93	VAL

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Mol	Chain	Res	Type
33	2b	107	THR
33	2b	110	GLN
33	2b	112	VAL
33	2b	117	GLU
33	2b	127	ILE
33	2b	138	LEU
33	2b	142	LEU
33	2b	150	SER
33	2b	164	VAL
33	2b	185	ILE
33	2b	189	ASP
33	2b	196	LEU
33	2b	224	GLN
33	2b	236	TYR
34	2c	4	LYS
34	2c	15	THR
34	2c	16	ARG
34	2c	26	LYS
34	2c	34	LEU
34	2c	35	GLU
34	2c	91	LEU
34	2c	101	LEU
34	2c	116	VAL
34	2c	132	ARG
34	2c	153	VAL
34	2c	161	GLU
34	2c	190	ARG
35	2d	8	VAL
35	2d	47	ARG
35	2d	53	ASP
35	2d	58	LEU
35	2d	59	ARG
35	2d	76	ARG
35	2d	86	LYS
35	2d	107	ARG
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	156	GLU
35	2d	175	SER
35	2d	201	GLN

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Mol	Chain	Res	Type
36	2e	11	ILE
36	2e	13	ILE
36	2e	20	GLN
36	2e	38	GLN
36	2e	41	VAL
36	2e	45	PHE
36	2e	51	VAL
36	2e	53	LEU
36	2e	149	GLU
36	2e	151	LEU
37	2f	10	LEU
37	2f	17	SER
37	2f	21	LEU
37	2f	45	LEU
37	2f	63	TYR
37	2f	69	GLU
37	2f	81	ILE
38	2g	6	ARG
38	2g	9	VAL
38	2g	12	LEU
38	2g	13	GLN
38	2g	24	THR
38	2g	32	ARG
38	2g	78	ARG
38	2g	79	ARG
38	2g	85	TYR
38	2g	94	ARG
38	2g	113	GLU
38	2g	115	ARG
38	2g	135	VAL
38	2g	144	MET
38	2g	154	TYR
39	2h	18	ARG
39	2h	25	ASP
39	2h	29	SER
39	2h	37	ARG
39	2h	51	VAL
39	2h	99	GLU
39	2h	112	LEU
39	2h	133	LEU
40	2i	12	GLU
40	2i	27	THR

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Mol	Chain	Res	Type
40	2i	35	GLU
40	2i	38	GLN
40	2i	47	LEU
40	2i	54	ASP
40	2i	65	VAL
40	2i	66	ARG
40	2i	89	ASN
40	2i	102	LEU
40	2i	113	LYS
41	2j	8	LEU
41	2j	16	LEU
41	2j	23	ILE
41	2j	38	ILE
41	2j	66	ARG
41	2j	81	THR
41	2j	89	ASP
41	2j	97	GLU
42	2k	28	THR
42	2k	62	GLN
42	2k	87	THR
42	2k	114	VAL
43	2l	18	VAL
43	2l	33	ARG
43	2l	40	VAL
43	2l	46	LYS
43	2l	47	LYS
43	2l	62	SER
43	2l	65	GLU
43	2l	89	ARG
44	2m	17	VAL
44	2m	32	GLU
44	2m	80	ARG
44	2m	90	LEU
44	2m	93	ARG
44	2m	102	ARG
44	2m	103	THR
44	2m	106	ASN
44	2m	108	ARG
44	2m	122	LYS
45	2n	3	ARG
45	2n	33	VAL
46	2o	3	ILE

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Mol	Chain	Res	Type
46	2o	13	GLN
46	2o	24	SER
46	2o	39	LEU
47	2p	8	ARG
47	2p	20	VAL
47	2p	21	VAL
47	2p	60	LEU
47	2p	73	LEU
48	2q	14	LYS
48	2q	60	ILE
48	2q	63	ARG
49	2r	31	LEU
49	2r	35	ARG
49	2r	41	LYS
49	2r	56	THR
50	2s	21	GLU
50	2s	32	LYS
50	2s	37	ARG
50	2s	43	GLU
50	2s	48	THR
50	2s	81	ARG
51	2t	15	ARG
51	2t	93	GLU
56	2z	2	THR
56	2z	3	HIS
56	2z	5	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	126	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
7	1H	74	ASN
8	1I	133	HIS
9	1N	8	GLN
12	1Q	12	GLN
12	1Q	57	HIS

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Mol	Chain	Res	Type
12	1Q	89	ASN
15	1T	58	ASN
16	1U	81	HIS
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
21	1Z	54	HIS
24	12	46	GLN
33	1b	16	HIS
33	1b	78	GLN
33	1b	94	ASN
33	1b	140	HIS
33	1b	212	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	102	ASN
34	1c	162	GLN
35	1d	45	GLN
35	1d	116	GLN
35	1d	125	HIS
35	1d	160	GLN
35	1d	161	ASN
36	1e	38	GLN
37	1f	57	GLN
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
39	1h	15	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	124	GLN
41	1j	56	HIS
41	1j	62	HIS
42	1k	104	GLN
43	1l	99	HIS
44	1m	92	HIS
49	1r	63	GLN
50	1s	83	HIS
51	1t	16	HIS

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Mol	Chain	Res	Type
51	1t	42	GLN
51	1t	90	GLN
56	1z	3	HIS
3	2D	87	ASN
4	2E	48	GLN
4	2E	143	ASN
5	2F	69	HIS
5	2F	75	HIS
5	2F	204	ASN
6	2G	41	GLN
6	2G	132	ASN
7	2H	139	GLN
9	2N	8	GLN
10	2O	3	GLN
10	2O	5	GLN
12	2Q	12	GLN
12	2Q	89	ASN
12	2Q	123	HIS
14	2S	38	GLN
14	2S	95	HIS
15	2T	58	ASN
15	2T	84	GLN
16	2U	94	ASN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
21	2Z	34	ASN
21	2Z	73	GLN
22	20	50	ASN
25	23	32	GLN
26	24	46	GLN
33	2b	76	GLN
33	2b	94	ASN
33	2b	135	GLN
34	2c	162	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
36	2e	38	GLN
36	2e	78	HIS

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Mol	Chain	Res	Type
37	2f	73	ASN
37	2f	100	ASN
38	2g	13	GLN
38	2g	28	ASN
38	2g	68	ASN
40	2i	3	GLN
40	2i	31	GLN
41	2j	33	GLN
41	2j	62	HIS
42	2k	104	GLN
42	2k	117	ASN
43	2l	99	HIS
44	2m	92	HIS
47	2p	16	HIS
47	2p	76	GLN
49	2r	63	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN
51	2t	90	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	404 (14%)	29 (1%)
1	2A	2789/2915 (95%)	431 (15%)	23 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	118/121 (97%)	24 (20%)	0
32	1a	1494/1521 (98%)	226 (15%)	0
32	2a	1498/1521 (98%)	255 (17%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	70/76 (92%)	18 (25%)	0
54	2w	67/76 (88%)	18 (26%)	0
55	1x	75/77 (97%)	7 (9%)	0
55	2x	75/77 (97%)	6 (8%)	0
57	1y	71/76 (93%)	29 (40%)	0
57	2y	69/76 (90%)	24 (34%)	0
All	All	9331/9620 (96%)	1456 (15%)	52 (0%)

All (1456) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	119	A
1	1A	120	U
1	1A	139(A)	G
1	1A	196	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	265	A
1	1A	269	U
1	1A	271(C)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(P)	C
1	1A	272(B)	G
1	1A	272(G)	C
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	353	G
1	1A	357	A
1	1A	363	G

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Mol	Chain	Res	Type
1	1A	370	G
1	1A	386	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	455	C
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	651	G
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	669	G

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Mol	Chain	Res	Type
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	764	A
1	1A	765	G
1	1A	774	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	877	U
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	893	C
1	1A	894	C
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	899	A
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G

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Mol	Chain	Res	Type
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1038	C
1	1A	1040	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1060	U
1	1A	1063	G
1	1A	1068	G
1	1A	1069	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1097	U
1	1A	1098	A

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Mol	Chain	Res	Type
1	1A	1099	G
1	1A	1106	G
1	1A	1110	G
1	1A	1112	G
1	1A	1116	C
1	1A	1117	G
1	1A	1135	C
1	1A	1136	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1220	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1319	G
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1459	G
1	1A	1467	C

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Mol	Chain	Res	Type
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1543	C
1	1A	1558	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1647	G
1	1A	1648	C
1	1A	1674	G
1	1A	1700	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
1	1A	1847	A
1	1A	1848	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A

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Mol	Chain	Res	Type
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2101	G
1	1A	2102	U
1	1A	2110	G
1	1A	2113	U
1	1A	2116	G
1	1A	2121	G
1	1A	2127	G
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2137	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C

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Mol	Chain	Res	Type
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2160	G
1	1A	2161	C
1	1A	2163	C
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2180	U
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2267	A
1	1A	2268	A
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A

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Mol	Chain	Res	Type
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2422	A
1	1A	2424	C
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2474	C
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2641	G
1	1A	2654	A
1	1A	2669	G
1	1A	2689	U
1	1A	2691	C

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Mol	Chain	Res	Type
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2765	A
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2803	C
1	1A	2805	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2825	C
1	1A	2835	A
1	1A	2839	G
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	13	A
2	1B	32	C
2	1B	35	U
2	1B	45	A
2	1B	50	G
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A

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Mol	Chain	Res	Type
32	1a	52	G
32	1a	61	G
32	1a	68	G
32	1a	77	G
32	1a	78	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	139	G
32	1a	144	G
32	1a	154	C
32	1a	164	U
32	1a	174	C
32	1a	182	U
32	1a	189(G)	G
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	218	C
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	262	A
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	306	G
32	1a	321	A
32	1a	328	C
32	1a	330	C
32	1a	332	G
32	1a	342	C
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G

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Mol	Chain	Res	Type
32	1a	355	C
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	388	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	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	521	G
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	607	A
32	1a	630	G
32	1a	653	A

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Mol	Chain	Res	Type
32	1a	657	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	703	G
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	749	C
32	1a	753	A
32	1a	755	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	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	857	C
32	1a	870	U
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	960	U
32	1a	961	U
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	992	U
32	1a	993	G
32	1a	996	A

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Mol	Chain	Res	Type
32	1a	1000	U
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1013	G
32	1a	1017	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1044	A
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	1111	A
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1134	G
32	1a	1135	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1174	G
32	1a	1176	A

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Mol	Chain	Res	Type
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1253	G
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	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1370	G
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C

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Mol	Chain	Res	Type
32	1a	1456	G
32	1a	1492	A
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	24	A
54	1w	2	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	23	A
54	1w	24	G
54	1w	34	G
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	62	C
54	1w	68	C
54	1w	70	G
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	13	C
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	47	U
55	1x	61	C
57	1y	5	G
57	1y	7	A
57	1y	9	A
57	1y	12	U
57	1y	13	C
57	1y	14	A
57	1y	19	G

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Mol	Chain	Res	Type
57	1y	20	U
57	1y	21	A
57	1y	22	G
57	1y	27	G
57	1y	28	G
57	1y	35	A
57	1y	44	G
57	1y	45	U
57	1y	46	G7M
57	1y	47	U
57	1y	48	C
57	1y	53	G
57	1y	54	5MU
57	1y	56	C
57	1y	57	G
57	1y	58	A
57	1y	59	U
57	1y	61	C
57	1y	66	U
57	1y	70	G
57	1y	71	G
57	1y	72	C
1	2A	12	U
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	92	A
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	141	A
1	2A	157	U
1	2A	173	G
1	2A	196	A
1	2A	199	A

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Mol	Chain	Res	Type
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	230	U
1	2A	232	G
1	2A	233	A
1	2A	248	G
1	2A	271(I)	G
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	271(P)	C
1	2A	272(B)	G
1	2A	272(J)	C
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	294	A
1	2A	311	A
1	2A	312	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	435	C
1	2A	440	G
1	2A	444	C

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Mol	Chain	Res	Type
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	528	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	556	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	615	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	701	G
1	2A	717	G
1	2A	730	C
1	2A	739	G
1	2A	752	A
1	2A	753	C
1	2A	775	G
1	2A	776	G

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Mol	Chain	Res	Type
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	859	G
1	2A	866	A
1	2A	874	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	882	G
1	2A	884	C
1	2A	886	C
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
1	2A	901	A
1	2A	903	C
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	936	C
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C

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Mol	Chain	Res	Type
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	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1114	G
1	2A	1116	C
1	2A	1117	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1171	G
1	2A	1195	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1236	G
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1370	C
1	2A	1380	G

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Mol	Chain	Res	Type
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
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	1674	G

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Mol	Chain	Res	Type
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1741	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	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1839	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	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U

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Mol	Chain	Res	Type
1	2A	1997	G
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2099	U
1	2A	2110	G
1	2A	2111	C
1	2A	2113	U
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2145	C
1	2A	2149	G
1	2A	2150	U
1	2A	2151	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C

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Mol	Chain	Res	Type
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2184	G
1	2A	2185	C
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2193	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2268	A
1	2A	2275	C
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A

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Mol	Chain	Res	Type
1	2A	2403	C
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2431	U
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2459	A
1	2A	2468	G
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2487	G
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2530	A
1	2A	2549	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2582	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2656	U

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Mol	Chain	Res	Type
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2757	A
1	2A	2758	A
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	2810	A
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2873	A
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	17	C
2	2B	20	C
2	2B	33	G
2	2B	34	U
2	2B	40	U

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Mol	Chain	Res	Type
2	2B	41	U
2	2B	45	A
2	2B	51	G
2	2B	53	A
2	2B	56	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	105	A
2	2B	106	G
2	2B	109	C
2	2B	110	G
2	2B	111	G
2	2B	119	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	31	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	65	U
32	2a	66	G
32	2a	76	C
32	2a	79	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	156	G
32	2a	161	A
32	2a	163	C
32	2a	182	U
32	2a	195	A
32	2a	197	A

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Mol	Chain	Res	Type
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	400	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	471	G
32	2a	484	G

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Mol	Chain	Res	Type
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	524	G
32	2a	527	G7M
32	2a	528	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	545	C
32	2a	547	A
32	2a	559	A
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	607	A
32	2a	630	G
32	2a	631	G
32	2a	653	A
32	2a	661	G
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A

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Mol	Chain	Res	Type
32	2a	817	C
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	874	G
32	2a	884	U
32	2a	887	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	984	C
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1008	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A

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Mol	Chain	Res	Type
32	2a	1019	C
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U
32	2a	1044	A
32	2a	1050	G
32	2a	1051	C
32	2a	1053	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1086	U
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1104	G
32	2a	1108	G
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1128	C
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C

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Mol	Chain	Res	Type
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1160	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	1213	A
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1270	C
32	2a	1272	G
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1312	G
32	2a	1320	C
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G

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Mol	Chain	Res	Type
32	2a	1363	C
32	2a	1370	G
32	2a	1379	G
32	2a	1394	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	24	A
54	2w	3	C
54	2w	4	C
54	2w	9	A
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	29	G
54	2w	46	G7M
54	2w	48	C
54	2w	50	U
54	2w	65	G
54	2w	66	U
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	72	C
54	2w	74	C
55	2x	9	G
55	2x	21	A
55	2x	47	U

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Mol	Chain	Res	Type
55	2x	52	G
55	2x	53	G
55	2x	61	C
57	2y	12	U
57	2y	14	A
57	2y	15	G
57	2y	19	G
57	2y	24	G
57	2y	27	G
57	2y	28	G
57	2y	43	C
57	2y	45	U
57	2y	48	C
57	2y	49	C
57	2y	52	G
57	2y	53	G
57	2y	54	5MU
57	2y	56	C
57	2y	57	G
57	2y	58	A
57	2y	59	U
57	2y	61	C
57	2y	63	G
57	2y	65	G
57	2y	69	G
57	2y	70	G
57	2y	71	G

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	271(J)	C
1	1A	278	A
1	1A	548	A
1	1A	573	G
1	1A	685	A
1	1A	746	A
1	1A	764	A
1	1A	774	A

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Mol	Chain	Res	Type
1	1A	974	G
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1379	A
1	1A	1420	U
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1762	A
1	1A	1992	G
1	1A	2170	A
1	1A	2183	C
1	1A	2406	U
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2430	A
1	2A	2439	A
1	2A	2689	U
1	2A	2756	U

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

90 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
54	PSU	1w	55	54	18,21,22	1.29	2 (11%)	22,30,33	1.97	4 (18%)
57	PSU	1y	32	57	18,21,22	1.32	2 (11%)	22,30,33	1.82	3 (13%)
43	0TD	2l	92	43	7,9,10	4.71	1 (14%)	6,11,13	5.15	3 (50%)
57	4SU	2y	8	57	18,21,22	1.71	4 (22%)	26,30,33	1.66	4 (15%)
57	MIA	2y	37	57	18,24,32	1.13	2 (11%)	18,35,47	1.20	2 (11%)
1	OMC	2A	1920	1	19,22,23	0.84	1 (5%)	26,31,34	0.89	1 (3%)
32	5MC	1a	1400	32	18,22,23	0.98	2 (11%)	26,32,35	1.12	2 (7%)
32	G7M	2a	527	32,58	20,26,27	1.24	2 (10%)	17,39,42	0.55	0
1	2MU	2A	2552	58,1	19,22,24	1.23	3 (15%)	26,31,36	1.74	6 (23%)
1	OMC	1A	1920	1	19,22,23	0.78	0	26,31,34	0.84	0
55	PSU	1x	55	55	18,21,22	1.33	2 (11%)	22,30,33	1.84	4 (18%)
1	5MC	2A	1942	1	18,22,23	0.98	2 (11%)	26,32,35	1.10	2 (7%)
57	5MU	2y	54	57	19,22,23	1.45	4 (21%)	28,32,35	1.91	6 (21%)
55	4SU	1x	8	55	18,21,22	2.24	6 (33%)	26,30,33	1.73	5 (19%)
54	4SU	2w	8	54	18,21,22	1.58	3 (16%)	26,30,33	2.29	5 (19%)
56	FME	2z	1	56	8,9,10	0.96	0	7,9,11	1.21	1 (14%)
55	8AN	2x	76	55,56,58	19,24,25	1.23	3 (15%)	13,35,38	1.99	3 (23%)
57	4SU	1y	8	57	18,21,22	1.65	5 (27%)	26,30,33	1.76	4 (15%)
1	5MC	2A	1962	58,1	18,22,23	0.99	2 (11%)	26,32,35	1.25	3 (11%)
32	M2G	1a	966	32	20,27,28	1.47	3 (15%)	22,40,43	1.01	3 (13%)
32	5MC	2a	1404	32	18,22,23	1.04	2 (11%)	26,32,35	1.18	2 (7%)
54	PSU	2w	32	54	18,21,22	1.34	2 (11%)	22,30,33	1.84	3 (13%)
32	G7M	1a	527	32,58	20,26,27	1.17	2 (10%)	17,39,42	0.63	0
54	4SU	1w	8	54	18,21,22	1.67	4 (22%)	26,30,33	2.08	4 (15%)
54	MIA	2w	37	54	20,27,32	1.85	3 (15%)	22,39,47	1.87	8 (36%)
1	5MC	1A	1962	58,1	18,22,23	0.96	2 (11%)	26,32,35	1.21	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	5MU	1y	54	57	19,22,23	1.49	4 (21%)	28,32,35	2.07	6 (21%)
32	5MC	1a	1404	32	18,22,23	0.99	2 (11%)	26,32,35	1.12	2 (7%)
1	5MU	2A	1939	58,1	19,22,23	1.48	6 (31%)	28,32,35	2.22	6 (21%)
54	5MU	1w	54	54	19,22,23	1.43	4 (21%)	28,32,35	1.96	6 (21%)
32	PSU	1a	516	32,58	18,21,22	1.36	2 (11%)	22,30,33	1.92	5 (22%)
1	PSU	2A	1917	1	18,21,22	1.32	2 (11%)	22,30,33	1.81	4 (18%)
55	4SU	2x	8	55	18,21,22	2.03	6 (33%)	26,30,33	1.33	5 (19%)
57	PSU	1y	39	57	18,21,22	1.38	2 (11%)	22,30,33	1.69	3 (13%)
1	OMG	2A	2251	55,58,1	18,26,27	0.93	1 (5%)	19,38,41	1.16	3 (15%)
1	2MU	1A	2552	58,1	19,22,24	1.18	2 (10%)	26,31,36	1.73	6 (23%)
54	PSU	2w	39	54	18,21,22	1.46	2 (11%)	22,30,33	1.43	3 (13%)
1	8AH	1A	2503	58,1	20,26,27	0.73	0	23,39,42	1.92	4 (17%)
54	PSU	1w	39	54	18,21,22	1.36	2 (11%)	22,30,33	1.66	3 (13%)
1	5MU	2A	1915	1	19,22,23	1.42	5 (26%)	28,32,35	2.27	6 (21%)
56	FME	1z	1	56	8,9,10	0.99	0	7,9,11	1.60	1 (14%)
32	PSU	2a	516	32,58	18,21,22	1.30	2 (11%)	22,30,33	1.94	4 (18%)
55	8AN	1x	76	55,56,58	19,24,25	1.27	2 (10%)	13,35,38	2.01	2 (15%)
32	5MC	1a	967	32	18,22,23	0.96	1 (5%)	26,32,35	1.11	2 (7%)
57	PSU	2y	32	57	18,21,22	1.34	2 (11%)	22,30,33	1.87	3 (13%)
32	M2G	2a	966	32	20,27,28	1.37	2 (10%)	22,40,43	1.00	2 (9%)
1	PSU	1A	1917	1	18,21,22	1.31	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	22,30,33	1.95	3 (13%)
32	5MC	2a	1407	32,58	18,22,23	0.96	2 (11%)	26,32,35	1.21	3 (11%)
32	UR3	2a	1498	32	19,22,23	1.07	2 (10%)	26,32,35	1.44	1 (3%)
57	PSU	2y	55	57	18,21,22	1.36	2 (11%)	22,30,33	1.80	5 (22%)
57	PSU	2y	39	42,57	18,21,22	1.33	2 (11%)	22,30,33	1.79	3 (13%)
57	G7M	1y	46	57	20,26,27	1.30	2 (10%)	17,39,42	0.59	0
55	5MC	2x	32	55	18,22,23	0.98	2 (11%)	26,32,35	1.25	3 (11%)
1	OMG	1A	2251	55,58,1	18,26,27	0.95	1 (5%)	19,38,41	1.03	2 (10%)
55	PSU	2x	55	55	18,21,22	1.35	3 (16%)	22,30,33	1.81	3 (13%)
32	2MG	2a	1207	32,58	18,26,27	0.95	1 (5%)	16,38,41	1.00	2 (12%)
55	5MC	1x	32	55	18,22,23	0.98	2 (11%)	26,32,35	1.22	2 (7%)
54	F3N	1w	76	1,54	30,36,37	1.43	5 (16%)	29,51,54	1.23	1 (3%)
57	MIA	1y	37	57	18,24,32	1.21	2 (11%)	18,35,47	1.22	2 (11%)
54	G7M	2w	46	54	20,26,27	1.23	2 (10%)	17,39,42	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	MIA	1w	37	54	24,31,32	2.10	3 (12%)	26,44,47	2.87	10 (38%)
55	5MU	2x	54	55	19,22,23	1.38	5 (26%)	28,32,35	2.14	6 (21%)
32	5MC	2a	1400	32	18,22,23	0.96	2 (11%)	26,32,35	1.26	3 (11%)
55	5MU	1x	54	55	19,22,23	1.47	4 (21%)	28,32,35	1.88	6 (21%)
54	PSU	1w	32	58,54	18,21,22	1.32	2 (11%)	22,30,33	1.89	4 (18%)
32	MA6	2a	1518	32	19,26,27	0.82	0	18,38,41	1.43	2 (11%)
32	4OC	2a	1402	32	20,23,24	0.80	0	26,32,35	0.96	1 (3%)
1	5MU	1A	1915	1	19,22,23	1.36	4 (21%)	28,32,35	2.10	7 (25%)
32	MA6	2a	1519	32	19,26,27	0.85	0	18,38,41	1.51	2 (11%)
54	G7M	1w	46	54	20,26,27	1.24	2 (10%)	17,39,42	0.60	0
1	5MC	1A	1942	1	18,22,23	0.97	2 (11%)	26,32,35	1.22	3 (11%)
32	5MC	2a	967	32	18,22,23	0.94	2 (11%)	26,32,35	1.12	4 (15%)
1	PSU	1A	1911	1	18,21,22	1.34	2 (11%)	22,30,33	1.94	5 (22%)
32	MA6	1a	1518	32	19,26,27	0.82	0	18,38,41	1.37	2 (11%)
32	5MC	1a	1407	32	18,22,23	1.00	2 (11%)	26,32,35	1.16	3 (11%)
32	2MG	1a	1207	32	18,26,27	0.94	1 (5%)	16,38,41	1.08	2 (12%)
32	4OC	1a	1402	32	20,23,24	0.75	0	26,32,35	0.94	1 (3%)
54	PSU	2w	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.82	3 (13%)
57	G7M	2y	46	57	20,26,27	1.38	2 (10%)	17,39,42	0.80	1 (5%)
32	UR3	1a	1498	32	19,22,23	0.98	2 (10%)	26,32,35	1.49	3 (11%)
1	PSU	1A	2605	58,1	18,21,22	1.47	2 (11%)	22,30,33	1.81	4 (18%)
32	MA6	1a	1519	32	19,26,27	0.81	0	18,38,41	1.47	2 (11%)
54	F3N	2w	76	1,54	30,36,37	1.44	6 (20%)	29,51,54	1.26	1 (3%)
43	0TD	1l	92	43	7,9,10	4.70	1 (14%)	6,11,13	2.11	3 (50%)
1	8AH	2A	2503	58,1	20,26,27	0.78	1 (5%)	23,39,42	1.91	4 (17%)
1	5MU	1A	1939	58,1	19,22,23	1.60	6 (31%)	28,32,35	2.11	7 (25%)
1	PSU	2A	2605	1	18,21,22	1.26	2 (11%)	22,30,33	2.11	4 (18%)
54	5MU	2w	54	54	19,22,23	1.30	4 (21%)	28,32,35	1.89	7 (25%)
57	PSU	1y	55	57	18,21,22	1.38	2 (11%)	22,30,33	1.90	3 (13%)

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
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
57	PSU	1y	32	57	-	2/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	4/7/12/14	-
57	4SU	2y	8	57	-	0/7/25/26	0/2/2/2
57	MIA	2y	37	57	-	1/3/25/34	0/3/3/3
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
32	G7M	2a	527	32,58	-	3/3/25/26	0/3/3/3
1	2MU	2A	2552	58,1	-	0/9/27/28	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
57	5MU	2y	54	57	-	2/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
56	FME	2z	1	56	-	4/7/9/11	-
55	8AN	2x	76	55,56,58	-	3/3/25/26	0/3/3/3
57	4SU	1y	8	57	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	58,1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,58	-	3/3/25/26	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/7/29/34	0/3/3/3
1	5MC	1A	1962	58,1	-	0/7/25/26	0/2/2/2
57	5MU	1y	54	57	-	2/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	58,1	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,58	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
57	PSU	1y	39	57	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,58,1	-	0/5/27/28	0/3/3/3
1	2MU	1A	2552	58,1	-	0/9/27/28	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	8AH	1A	2503	58,1	-	2/3/25/26	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
56	FME	1z	1	56	-	3/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	2a	516	32,58	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	55,56,58	-	3/3/25/26	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
57	PSU	2y	32	57	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32,58	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
57	PSU	2y	55	57	-	1/7/25/26	0/2/2/2
57	PSU	2y	39	42,57	-	0/7/25/26	0/2/2/2
57	G7M	1y	46	57	-	2/3/25/26	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	55,58,1	-	0/5/27/28	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32,58	-	0/5/27/28	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	1,54	-	0/15/37/38	0/4/4/4
57	MIA	1y	37	57	-	0/3/25/34	0/3/3/3
54	G7M	2w	46	54	-	1/3/25/26	0/3/3/3
54	MIA	1w	37	54	-	3/11/33/34	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	58,54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/5/27/28	0/3/3/3
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
57	G7M	2y	46	57	-	1/3/25/26	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	58,1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
54	F3N	2w	76	1,54	-	0/15/37/38	0/4/4/4
43	0TD	1l	92	43	-	3/7/12/14	-
1	8AH	2A	2503	58,1	-	1/3/25/26	0/3/3/3
1	5MU	1A	1939	58,1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
57	PSU	1y	55	57	-	2/7/25/26	0/2/2/2

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.16	1.69	1.82
43	1l	92	0TD	CB-SB	-12.05	1.70	1.82
54	1w	37	MIA	C13-C14	7.05	1.52	1.32
54	2w	37	MIA	C2-S10	-6.90	1.69	1.75
54	1w	37	MIA	C2-S10	-6.13	1.70	1.75
55	1x	8	4SU	C4-N3	-5.86	1.31	1.37
55	2x	8	4SU	C4-N3	-4.92	1.32	1.37
32	1a	966	M2G	C2-N3	4.71	1.36	1.30
54	2w	76	F3N	CB-CG	-4.53	1.40	1.51
54	1w	8	4SU	C4-S4	-4.41	1.60	1.68
32	2a	966	M2G	C2-N3	4.39	1.36	1.30
54	1w	76	F3N	CB-CG	-4.35	1.40	1.51
57	2y	8	4SU	C4-S4	-4.21	1.60	1.68
57	2y	46	G7M	C5-C4	4.21	1.47	1.39
54	2w	8	4SU	C4-S4	-4.15	1.60	1.68
55	1x	8	4SU	C2-N3	-4.07	1.30	1.38
57	1y	8	4SU	C4-S4	-4.05	1.60	1.68
57	1y	46	G7M	C5-C4	4.03	1.47	1.39
55	2x	8	4SU	C4-S4	-4.02	1.60	1.68
54	2w	39	PSU	C6-C5	3.96	1.39	1.35
55	1x	8	4SU	C4-S4	-3.93	1.60	1.68
57	1y	55	PSU	C6-C5	3.91	1.39	1.35
57	1y	39	PSU	C6-C5	3.84	1.39	1.35
54	2w	46	G7M	C5-C4	3.81	1.46	1.39
54	1w	46	G7M	C5-C4	3.77	1.46	1.39
57	1y	32	PSU	C6-C5	3.74	1.39	1.35
54	1w	76	F3N	O4'-C1'	3.73	1.46	1.41
32	2a	527	G7M	C5-C4	3.70	1.46	1.39
57	2y	39	PSU	C6-C5	3.70	1.39	1.35
57	2y	32	PSU	C6-C5	3.67	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2605	PSU	C6-C5	3.63	1.39	1.35
32	1a	516	PSU	C6-C5	3.61	1.39	1.35
54	2w	55	PSU	C6-C5	3.61	1.39	1.35
32	1a	527	G7M	C5-C4	3.57	1.46	1.39
1	1A	1911	PSU	C6-C5	3.56	1.39	1.35
32	2a	516	PSU	C6-C5	3.54	1.39	1.35
55	2x	55	PSU	C6-C5	3.48	1.39	1.35
54	1w	32	PSU	C6-C5	3.44	1.39	1.35
1	2A	1911	PSU	C6-C5	3.42	1.39	1.35
55	2x	8	4SU	C2-N3	-3.37	1.32	1.38
54	2w	32	PSU	C6-C5	3.35	1.39	1.35
55	1x	55	PSU	C6-C5	3.34	1.39	1.35
54	1w	55	PSU	C6-C5	3.26	1.39	1.35
32	2a	1404	5MC	C6-C5	3.25	1.39	1.34
57	1y	8	4SU	C4-N3	-3.21	1.34	1.37
1	1A	1939	5MU	C4-N3	-3.18	1.32	1.38
1	2A	1917	PSU	C6-C5	3.18	1.39	1.35
57	2y	8	4SU	C4-N3	-3.10	1.34	1.37
1	1A	1939	5MU	C2-N3	-3.06	1.32	1.38
57	2y	55	PSU	C6-C5	3.06	1.38	1.35
32	1a	967	5MC	C6-C5	3.05	1.39	1.34
54	1w	39	PSU	C6-C5	3.05	1.38	1.35
1	1A	1917	PSU	C6-C5	3.05	1.38	1.35
54	2w	76	F3N	O4'-C1'	3.04	1.45	1.41
57	1y	54	5MU	C6-C5	3.03	1.39	1.34
55	1x	54	5MU	C6-C5	3.01	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.99	1.33	1.38
57	1y	37	MIA	C5-C4	2.98	1.48	1.40
55	1x	76	8AN	C5-C4	-2.97	1.33	1.40
55	1x	8	4SU	C5-C4	-2.94	1.38	1.42
32	1a	1407	5MC	C6-C5	2.93	1.39	1.34
1	2A	1915	5MU	C6-C5	2.92	1.39	1.34
54	1w	8	4SU	C4-N3	-2.92	1.34	1.37
54	2w	76	F3N	C5-C4	-2.92	1.33	1.40
1	2A	1939	5MU	C6-C5	2.91	1.39	1.34
55	2x	8	4SU	C5-C4	-2.89	1.38	1.42
1	2A	1942	5MC	C6-C5	2.89	1.39	1.34
54	2w	39	PSU	C4-N3	-2.89	1.33	1.38
54	1w	39	PSU	C4-N3	-2.88	1.33	1.38
57	1y	37	MIA	C2-N3	2.87	1.36	1.32
32	1a	966	M2G	C2-N2	2.83	1.40	1.35
55	1x	54	5MU	C4-N3	-2.83	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	37	MIA	C5-C4	2.82	1.48	1.40
57	1y	54	5MU	C4-C5	2.79	1.49	1.44
32	2a	1407	5MC	C6-C5	2.79	1.39	1.34
54	2w	8	4SU	C4-N3	-2.78	1.34	1.37
57	2y	54	5MU	C6-C5	2.78	1.39	1.34
55	2x	54	5MU	C6-C5	2.78	1.39	1.34
55	2x	76	8AN	C5-C4	-2.78	1.33	1.40
1	2A	1939	5MU	C4-N3	-2.77	1.33	1.38
32	1a	1404	5MC	C6-C5	2.77	1.39	1.34
54	1w	54	5MU	C6-C5	2.77	1.39	1.34
1	1A	1915	5MU	C6-C5	2.76	1.39	1.34
57	2y	37	MIA	C5-C4	2.76	1.48	1.40
1	2A	2605	PSU	C6-C5	2.76	1.38	1.35
54	1w	76	F3N	C5-C4	-2.73	1.33	1.40
32	1a	1400	5MC	C6-C5	2.73	1.39	1.34
1	1A	1939	5MU	C6-C5	2.72	1.39	1.34
55	2x	32	5MC	C6-C5	2.71	1.39	1.34
1	2A	1917	PSU	C4-N3	-2.70	1.33	1.38
57	1y	54	5MU	C2-N1	2.70	1.42	1.38
55	1x	32	5MC	C6-C5	2.67	1.39	1.34
32	2a	1400	5MC	C6-C5	2.67	1.39	1.34
1	1A	1917	PSU	C4-N3	-2.66	1.33	1.38
57	2y	54	5MU	C4-C5	2.66	1.49	1.44
57	2y	37	MIA	C2-N3	2.66	1.36	1.32
57	2y	8	4SU	C5-C4	-2.65	1.39	1.42
1	1A	1939	5MU	C4-C5	2.64	1.49	1.44
54	1w	54	5MU	C4-C5	2.64	1.49	1.44
1	1A	2251	OMG	C6-N1	-2.63	1.34	1.37
54	1w	32	PSU	C4-N3	-2.63	1.34	1.38
54	1w	55	PSU	C4-N3	-2.63	1.34	1.38
54	1w	54	5MU	C4-N3	-2.62	1.34	1.38
1	1A	1942	5MC	C6-C5	2.61	1.38	1.34
32	2a	966	M2G	C2-N2	2.60	1.40	1.35
54	1w	37	MIA	C5-C4	2.60	1.47	1.40
1	1A	1962	5MC	C6-C5	2.60	1.38	1.34
55	2x	76	8AN	C6-C5	-2.59	1.33	1.43
32	1a	516	PSU	C4-N3	-2.59	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.58	1.34	1.38
1	1A	1911	PSU	C4-N3	-2.57	1.34	1.38
1	1A	1915	5MU	C2-N1	2.57	1.42	1.38
1	2A	2251	OMG	C6-N1	-2.57	1.34	1.37
1	2A	1962	5MC	C6-C5	2.57	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	54	5MU	C4-N3	-2.57	1.34	1.38
55	1x	54	5MU	C4-C5	2.57	1.49	1.44
1	1A	1962	5MC	C6-N1	-2.56	1.33	1.38
57	2y	55	PSU	C4-N3	-2.56	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.55	1.34	1.38
57	2y	54	5MU	C4-N3	-2.54	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.54	1.34	1.37
1	1A	1942	5MC	C6-N1	-2.53	1.33	1.38
55	1x	8	4SU	O2-C2	2.52	1.27	1.23
1	1A	2552	2MU	C4-N3	-2.52	1.34	1.38
57	1y	39	PSU	C4-N3	-2.51	1.34	1.38
1	1A	1939	5MU	C2-N1	2.51	1.42	1.38
54	2w	55	PSU	C4-N3	-2.49	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.49	1.33	1.38
54	2w	76	F3N	C6-C5	-2.48	1.34	1.43
55	2x	55	PSU	C4-N3	-2.48	1.34	1.38
55	2x	54	5MU	C4-C5	2.48	1.48	1.44
54	1w	46	G7M	C6-N1	-2.47	1.34	1.37
55	1x	55	PSU	C4-N3	-2.47	1.34	1.38
1	2A	1939	5MU	C2-N1	2.47	1.42	1.38
55	1x	76	8AN	C6-C5	-2.46	1.34	1.43
57	1y	54	5MU	C4-N3	-2.45	1.34	1.38
55	2x	54	5MU	C4-N3	-2.45	1.34	1.38
32	2a	967	5MC	C6-C5	2.45	1.38	1.34
57	2y	46	G7M	C6-N1	-2.45	1.34	1.37
55	1x	32	5MC	C6-N1	-2.44	1.33	1.38
32	2a	1207	2MG	C6-N1	-2.43	1.34	1.37
57	2y	54	5MU	C2-N1	2.43	1.42	1.38
55	2x	32	5MC	C6-N1	-2.43	1.33	1.38
1	2A	2552	2MU	C5-C4	2.42	1.49	1.43
32	1a	966	M2G	C6-N1	-2.42	1.34	1.37
1	2A	1962	5MC	C6-N1	-2.40	1.33	1.38
54	1w	76	F3N	C6-C5	-2.40	1.34	1.43
1	2A	1915	5MU	C4-C5	2.40	1.48	1.44
1	1A	1915	5MU	C4-N3	-2.39	1.34	1.38
57	1y	55	PSU	C4-N3	-2.38	1.34	1.38
1	1A	1939	5MU	C6-N1	-2.37	1.34	1.38
57	2y	39	PSU	C4-N3	-2.37	1.34	1.38
32	2a	967	5MC	C6-N1	-2.36	1.34	1.38
32	2a	527	G7M	C6-N1	-2.35	1.34	1.37
1	2A	1915	5MU	C2-N1	2.35	1.42	1.38
54	2w	32	PSU	C4-N3	-2.35	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2605	PSU	C4-N3	-2.35	1.34	1.38
57	1y	32	PSU	C4-N3	-2.34	1.34	1.38
54	2w	54	5MU	C6-C5	2.33	1.38	1.34
54	1w	8	4SU	C5-C4	-2.33	1.39	1.42
1	2A	1939	5MU	C4-C5	2.32	1.48	1.44
57	2y	32	PSU	C4-N3	-2.31	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.30	1.34	1.38
1	2A	2552	2MU	C4-N3	-2.29	1.34	1.38
32	2a	516	PSU	C4-N3	-2.29	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.28	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.27	1.34	1.38
54	1w	54	5MU	C2-N1	2.26	1.42	1.38
1	2A	2503	8AH	C5-C4	2.24	1.46	1.40
55	2x	54	5MU	C2-N1	2.23	1.42	1.38
1	1A	1915	5MU	C4-C5	2.22	1.48	1.44
1	2A	1942	5MC	C6-N1	-2.21	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.19	1.34	1.38
32	2a	1498	UR3	C2-N1	2.19	1.41	1.38
32	2a	1400	5MC	C6-N1	-2.19	1.34	1.38
55	1x	54	5MU	C2-N3	-2.18	1.34	1.38
54	2w	8	4SU	C5-C4	-2.18	1.39	1.42
57	1y	8	4SU	C5-C4	-2.17	1.39	1.42
32	2a	1404	5MC	C6-N1	-2.17	1.34	1.38
32	1a	1498	UR3	C2-N1	2.17	1.41	1.38
57	2y	8	4SU	C2-N3	-2.15	1.34	1.38
55	1x	8	4SU	C6-C5	2.14	1.40	1.35
1	2A	1915	5MU	C6-N1	-2.14	1.34	1.38
55	2x	8	4SU	C6-C5	2.13	1.40	1.35
32	1a	527	G7M	C6-N1	-2.13	1.34	1.37
54	2w	37	MIA	C2-N3	2.13	1.37	1.34
55	2x	8	4SU	O2-C2	2.12	1.26	1.23
32	1a	1407	5MC	C6-N1	-2.11	1.34	1.38
32	1a	1498	UR3	C6-C5	2.10	1.39	1.35
54	2w	54	5MU	C6-N1	-2.09	1.34	1.38
57	1y	8	4SU	C2-N3	-2.08	1.34	1.38
55	2x	54	5MU	C6-N1	-2.07	1.34	1.38
55	2x	55	PSU	C4-C5	2.05	1.50	1.44
55	2x	76	8AN	C5-N7	-2.04	1.32	1.39
54	1w	8	4SU	C2-N3	-2.04	1.34	1.38
54	1w	76	F3N	C5-N7	-2.04	1.32	1.39
57	1y	8	4SU	C6-C5	2.04	1.39	1.35
54	2w	46	G7M	C6-N1	-2.03	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	2MU	C2-N3	-2.02	1.34	1.38
1	1A	2552	2MU	C2-N3	-2.01	1.34	1.38
57	1y	46	G7M	C6-N1	-2.00	1.34	1.37
54	2w	76	F3N	C2'-C3'	-2.00	1.50	1.53
32	2a	1498	UR3	C6-C5	2.00	1.39	1.35
1	2A	1920	OMC	C6-C5	2.00	1.39	1.35
54	2w	76	F3N	C5-N7	-2.00	1.32	1.39
54	2w	54	5MU	C4-C5	2.00	1.48	1.44

All (293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-11.82	81.05	102.44
54	1w	37	MIA	C12-C13-C14	-8.90	109.82	127.14
54	2w	8	4SU	C4-N3-C2	-7.30	120.24	127.34
1	2A	2503	8AH	C2-N3-C4	6.79	121.04	115.52
1	1A	2503	8AH	C2-N3-C4	6.63	120.91	115.52
1	2A	2605	PSU	N1-C2-N3	6.33	122.30	115.13
54	1w	8	4SU	C4-N3-C2	-6.31	121.21	127.34
1	1A	1911	PSU	N1-C2-N3	6.15	122.10	115.13
1	2A	1911	PSU	N1-C2-N3	6.14	122.08	115.13
32	1a	516	PSU	N1-C2-N3	6.06	122.00	115.13
57	1y	55	PSU	N1-C2-N3	6.04	121.97	115.13
54	1w	37	MIA	C12-N6-C6	-5.98	113.69	122.55
55	1x	76	8AN	N3-C2-N1	-5.97	119.34	128.68
54	2w	32	PSU	N1-C2-N3	5.93	121.84	115.13
1	1A	1917	PSU	N1-C2-N3	5.92	121.84	115.13
57	2y	32	PSU	N1-C2-N3	5.90	121.82	115.13
54	1w	32	PSU	N1-C2-N3	5.89	121.80	115.13
54	1w	76	F3N	N3-C2-N1	-5.89	119.48	128.68
32	2a	516	PSU	N1-C2-N3	5.87	121.79	115.13
54	1w	8	4SU	C5-C4-N3	5.86	120.13	114.69
32	1a	1498	UR3	C4-N3-C2	-5.83	119.08	124.56
55	1x	55	PSU	N1-C2-N3	5.82	121.72	115.13
54	1w	55	PSU	N1-C2-N3	5.81	121.71	115.13
54	2w	8	4SU	C5-C4-N3	5.80	120.07	114.69
32	2a	1498	UR3	C4-N3-C2	-5.79	119.11	124.56
54	2w	76	F3N	N3-C2-N1	-5.79	119.63	128.68
55	2x	55	PSU	N1-C2-N3	5.78	121.68	115.13
55	2x	76	8AN	N3-C2-N1	-5.77	119.66	128.68
1	2A	1915	5MU	C4-N3-C2	-5.71	119.96	127.35
54	2w	55	PSU	N1-C2-N3	5.65	121.54	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1939	5MU	C4-N3-C2	-5.65	120.04	127.35
57	2y	39	PSU	N1-C2-N3	5.56	121.42	115.13
1	2A	1917	PSU	N1-C2-N3	5.55	121.42	115.13
1	1A	2605	PSU	N1-C2-N3	5.50	121.36	115.13
57	1y	32	PSU	N1-C2-N3	5.46	121.32	115.13
57	2y	55	PSU	N1-C2-N3	5.42	121.27	115.13
55	2x	54	5MU	C4-N3-C2	-5.40	120.35	127.35
54	1w	39	PSU	N1-C2-N3	5.40	121.25	115.13
57	1y	39	PSU	N1-C2-N3	5.38	121.23	115.13
1	2A	1915	5MU	C5-C4-N3	5.31	119.84	115.31
57	1y	54	5MU	C4-N3-C2	-5.27	120.53	127.35
57	1y	54	5MU	N3-C2-N1	5.25	121.85	114.89
1	2A	1939	5MU	N3-C2-N1	5.18	121.77	114.89
1	1A	1939	5MU	C5-C4-N3	5.17	119.72	115.31
1	1A	1939	5MU	C4-N3-C2	-5.16	120.67	127.35
57	1y	8	4SU	C4-N3-C2	-5.14	122.35	127.34
1	2A	1939	5MU	C5-C4-N3	5.14	119.69	115.31
1	2A	1915	5MU	N3-C2-N1	5.11	121.68	114.89
1	1A	1915	5MU	C4-N3-C2	-5.11	120.73	127.35
55	2x	54	5MU	N3-C2-N1	5.10	121.66	114.89
57	2y	8	4SU	C5-C4-N3	5.08	119.40	114.69
54	1w	54	5MU	N3-C2-N1	5.05	121.60	114.89
1	1A	1915	5MU	N3-C2-N1	5.03	121.57	114.89
54	1w	54	5MU	C4-N3-C2	-4.90	121.01	127.35
32	2a	1519	MA6	N3-C2-N1	-4.85	121.10	128.68
1	1A	1939	5MU	C5-C6-N1	-4.82	118.38	123.34
1	2A	2552	2MU	N3-C2-N1	4.81	121.27	114.89
1	2A	2605	PSU	C4-N3-C2	-4.80	119.42	126.34
32	1a	1519	MA6	N3-C2-N1	-4.77	121.22	128.68
55	1x	54	5MU	N3-C2-N1	4.76	121.21	114.89
1	1A	2552	2MU	N3-C2-N1	4.75	121.19	114.89
32	2a	1518	MA6	N3-C2-N1	-4.74	121.27	128.68
57	1y	8	4SU	C5-C4-N3	4.71	119.06	114.69
1	1A	1939	5MU	N3-C2-N1	4.70	121.13	114.89
1	1A	1915	5MU	O4-C4-C5	-4.65	119.51	124.90
1	2A	1915	5MU	O4-C4-C5	-4.62	119.54	124.90
32	1a	1518	MA6	N3-C2-N1	-4.60	121.48	128.68
57	2y	54	5MU	C4-N3-C2	-4.60	121.40	127.35
54	2w	8	4SU	N3-C2-N1	4.57	120.95	114.89
55	1x	54	5MU	C4-N3-C2	-4.51	121.52	127.35
54	1w	37	MIA	C15-C14-C13	-4.49	109.68	122.65
54	2w	39	PSU	N1-C2-N3	4.47	120.20	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	54	5MU	C5-C4-N3	4.47	119.13	115.31
57	2y	54	5MU	N3-C2-N1	4.42	120.75	114.89
54	1w	55	PSU	C4-N3-C2	-4.41	119.98	126.34
54	2w	54	5MU	C4-N3-C2	-4.40	121.65	127.35
1	1A	1915	5MU	C5-C4-N3	4.35	119.02	115.31
57	1y	54	5MU	C5-C4-N3	4.28	118.97	115.31
1	2A	1939	5MU	O4-C4-C5	-4.27	119.95	124.90
54	1w	32	PSU	C4-N3-C2	-4.25	120.21	126.34
32	1a	516	PSU	C4-N3-C2	-4.24	120.22	126.34
55	1x	8	4SU	S4-C4-N3	-4.23	116.04	120.21
1	1A	1911	PSU	C4-N3-C2	-4.23	120.25	126.34
1	2A	2552	2MU	C4-N3-C2	-4.22	121.02	126.58
54	2w	37	MIA	C5-C6-N1	-4.21	117.32	120.81
1	2A	1939	5MU	C5-C6-N1	-4.20	119.02	123.34
1	1A	2552	2MU	C4-N3-C2	-4.19	121.06	126.58
57	2y	54	5MU	C5-C4-N3	4.16	118.86	115.31
54	2w	54	5MU	C5-C4-N3	4.15	118.86	115.31
54	2w	54	5MU	O4-C4-C5	-4.14	120.10	124.90
55	2x	54	5MU	O4-C4-C5	-4.12	120.12	124.90
32	2a	516	PSU	C4-N3-C2	-4.10	120.43	126.34
54	1w	37	MIA	C2-N3-C4	4.08	120.95	115.32
54	2w	54	5MU	N3-C2-N1	4.07	120.29	114.89
55	1x	54	5MU	C5-C6-N1	-4.05	119.17	123.34
55	1x	8	4SU	C6-C5-C4	-4.05	116.45	119.95
54	1w	54	5MU	C5-C4-N3	4.03	118.75	115.31
1	1A	1942	5MC	C5-C6-N1	-4.00	119.23	123.34
1	2A	1911	PSU	O2-C2-N1	-3.99	118.39	122.79
1	1A	1917	PSU	C4-N3-C2	-3.99	120.59	126.34
32	1a	967	5MC	C5-C6-N1	-3.99	119.24	123.34
55	1x	55	PSU	C4-N3-C2	-3.95	120.64	126.34
57	2y	8	4SU	C4-N3-C2	-3.95	123.51	127.34
1	2A	1915	5MU	C5-C6-N1	-3.93	119.30	123.34
55	2x	54	5MU	C5-C6-N1	-3.91	119.31	123.34
1	2A	1917	PSU	C4-N3-C2	-3.91	120.71	126.34
1	2A	1911	PSU	C4-N3-C2	-3.88	120.74	126.34
32	2a	1404	5MC	C5-C6-N1	-3.87	119.36	123.34
32	2a	1400	5MC	C5-C6-N1	-3.86	119.36	123.34
32	2a	516	PSU	O2-C2-N1	-3.86	118.54	122.79
57	2y	55	PSU	C4-N3-C2	-3.85	120.79	126.34
1	2A	2605	PSU	O2-C2-N1	-3.83	118.58	122.79
57	1y	54	5MU	C5-C6-N1	-3.82	119.41	123.34
55	1x	32	5MC	C5-C6-N1	-3.81	119.42	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	55	PSU	C4-N3-C2	-3.79	120.88	126.34
54	2w	32	PSU	C4-N3-C2	-3.77	120.91	126.34
57	1y	32	PSU	C4-N3-C2	-3.76	120.91	126.34
54	1w	37	MIA	C16-C14-C13	-3.76	111.77	122.65
1	1A	2605	PSU	C4-N3-C2	-3.75	120.93	126.34
56	1z	1	FME	CA-N-CN	3.75	128.59	122.82
1	2A	2503	8AH	C5-C6-N1	-3.73	118.56	121.01
55	2x	32	5MC	C5-C6-N1	-3.73	119.50	123.34
57	2y	32	PSU	O2-C2-N1	-3.72	118.69	122.79
54	2w	55	PSU	C4-N3-C2	-3.72	120.98	126.34
54	2w	37	MIA	C2-N3-C4	3.71	120.43	115.32
54	1w	8	4SU	N3-C2-N1	3.69	119.79	114.89
57	1y	55	PSU	C4-N3-C2	-3.68	121.04	126.34
55	1x	54	5MU	C5-C4-N3	3.68	118.45	115.31
57	2y	32	PSU	C4-N3-C2	-3.68	121.04	126.34
55	1x	8	4SU	O2-C2-N1	3.67	127.67	122.79
32	1a	1404	5MC	C5-C6-N1	-3.67	119.57	123.34
32	2a	1407	5MC	C5-C6-N1	-3.66	119.57	123.34
57	1y	55	PSU	O2-C2-N1	-3.65	118.78	122.79
57	1y	8	4SU	N3-C2-N1	3.65	119.73	114.89
1	1A	1917	PSU	O2-C2-N1	-3.64	118.78	122.79
57	2y	39	PSU	C4-N3-C2	-3.63	121.11	126.34
57	2y	54	5MU	C5-C6-N1	-3.57	119.67	123.34
1	1A	2503	8AH	C5-C6-N1	-3.57	118.67	121.01
54	1w	54	5MU	C5-C6-N1	-3.54	119.69	123.34
1	2A	1942	5MC	C5-C6-N1	-3.54	119.70	123.34
54	1w	8	4SU	C5-C4-S4	-3.54	119.91	124.47
54	1w	54	5MU	O4-C4-C5	-3.52	120.83	124.90
54	2w	8	4SU	C5-C4-S4	-3.47	120.00	124.47
57	1y	54	5MU	O4-C4-C5	-3.46	120.90	124.90
57	1y	39	PSU	C4-N3-C2	-3.41	121.43	126.34
32	1a	1400	5MC	C5-C6-N1	-3.40	119.84	123.34
43	2l	92	0TD	OD2-CG-CB	3.36	120.41	113.15
54	2w	37	MIA	C11-S10-C2	-3.36	99.76	102.27
54	2w	32	PSU	O2-C2-N1	-3.34	119.11	122.79
1	1A	1962	5MC	C5-C6-N1	-3.34	119.91	123.34
57	1y	37	MIA	N3-C2-N1	-3.34	123.46	128.68
32	1a	1407	5MC	C5-C6-N1	-3.34	119.91	123.34
57	2y	54	5MU	O4-C4-C5	-3.31	121.06	124.90
57	1y	32	PSU	O2-C2-N1	-3.26	119.20	122.79
57	2y	37	MIA	N3-C2-N1	-3.21	123.66	128.68
43	1l	92	0TD	CSB-SB-CB	-3.20	96.65	102.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	37	MIA	C5-C6-N1	-3.20	118.16	120.81
32	2a	1519	MA6	C4-C5-N7	-3.18	106.08	109.40
54	1w	37	MIA	C2-N1-C6	3.18	122.88	117.19
54	2w	55	PSU	O2-C2-N1	-3.15	119.33	122.79
54	1w	55	PSU	O2-C2-N1	-3.15	119.33	122.79
54	1w	39	PSU	C4-N3-C2	-3.14	121.81	126.34
1	2A	1917	PSU	O2-C2-N1	-3.14	119.33	122.79
55	2x	8	4SU	C5-C4-N3	3.12	117.58	114.69
55	1x	32	5MC	C5-C4-N3	-3.12	118.31	121.67
1	1A	2552	2MU	O4-C4-C5	-3.11	119.69	125.16
57	2y	55	PSU	O2-C2-N1	-3.10	119.38	122.79
55	2x	76	8AN	O4'-C1'-C2'	-3.09	102.41	106.93
32	2a	967	5MC	C5-C6-N1	-3.08	120.17	123.34
43	1l	92	0TD	OD2-CG-CB	3.06	119.76	113.15
54	2w	54	5MU	C5-C6-N1	-3.05	120.20	123.34
57	2y	39	PSU	O2-C2-N1	-3.03	119.46	122.79
55	2x	8	4SU	C6-C5-C4	-3.02	117.33	119.95
32	1a	1519	MA6	C4-C5-N7	-3.01	106.26	109.40
1	2A	1962	5MC	C5-C6-N1	-3.00	120.25	123.34
55	1x	54	5MU	O4-C4-C5	-2.98	121.44	124.90
1	1A	1915	5MU	C5-C6-N1	-2.97	120.28	123.34
1	2A	1962	5MC	C5-C4-N3	-2.94	118.50	121.67
32	1a	1404	5MC	C5-C4-N3	-2.91	118.53	121.67
57	2y	8	4SU	C5-C4-S4	-2.91	120.71	124.47
1	2A	2552	2MU	O2-C2-N1	-2.91	118.91	122.79
56	2z	1	FME	CA-N-CN	2.91	127.29	122.82
32	2a	1518	MA6	C4-C5-N7	-2.90	106.38	109.40
55	1x	8	4SU	C4-N3-C2	2.89	130.14	127.34
55	1x	55	PSU	O2-C2-N1	-2.87	119.63	122.79
54	2w	8	4SU	O2-C2-N1	-2.86	118.99	122.79
55	2x	54	5MU	O2-C2-N1	-2.84	119.01	122.79
1	2A	2552	2MU	C5-C4-N3	2.82	119.06	114.84
1	1A	1911	PSU	O2-C2-N1	-2.79	119.72	122.79
32	2a	1404	5MC	C5-C4-N3	-2.77	118.68	121.67
54	1w	39	PSU	O2-C2-N1	-2.76	119.75	122.79
55	2x	55	PSU	O2-C2-N1	-2.74	119.77	122.79
1	1A	1942	5MC	C5-C4-N3	-2.74	118.72	121.67
32	2a	1407	5MC	C5-C4-N3	-2.74	118.72	121.67
1	1A	2552	2MU	C5-C4-N3	2.71	118.89	114.84
55	2x	8	4SU	S4-C4-N3	-2.71	117.54	120.21
32	1a	516	PSU	O2-C2-N1	-2.71	119.81	122.79
54	2w	37	MIA	C12-N6-C6	-2.68	120.57	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	54	5MU	O2-C2-N1	-2.68	119.23	122.79
1	2A	1915	5MU	O2-C2-N1	-2.65	119.26	122.79
1	1A	2552	2MU	O2-C2-N1	-2.64	119.28	122.79
55	2x	32	5MC	C5-C4-N3	-2.62	118.85	121.67
32	1a	1407	5MC	C5-C4-N3	-2.61	118.86	121.67
32	1a	1207	2MG	C8-N7-C5	2.60	107.95	102.99
1	1A	1962	5MC	C5-C4-N3	-2.59	118.88	121.67
54	1w	54	5MU	O2-C2-N1	-2.59	119.34	122.79
32	1a	1402	4OC	C6-C5-C4	2.59	120.13	116.96
54	2w	37	MIA	C2-N1-C6	2.59	121.82	117.19
1	2A	2251	OMG	C5-C6-N1	2.58	118.51	113.95
54	1w	37	MIA	C11-S10-C2	-2.58	100.34	102.27
54	1w	37	MIA	C4-C5-N7	-2.58	106.71	109.40
54	1w	32	PSU	O2-C2-N1	-2.57	119.96	122.79
1	2A	2503	8AH	C4-C5-N7	-2.57	106.86	109.47
1	2A	2552	2MU	O4-C4-C5	-2.57	120.65	125.16
1	1A	2503	8AH	C4-C5-N7	-2.56	106.87	109.47
55	1x	8	4SU	C5-C4-N3	2.55	117.06	114.69
1	2A	1942	5MC	C5-C4-N3	-2.54	118.93	121.67
1	1A	2503	8AH	C2-N1-C6	2.52	122.02	118.08
54	1w	37	MIA	N3-C2-N1	-2.52	122.34	126.98
32	1a	1518	MA6	C4-C5-N7	-2.52	106.77	109.40
57	2y	37	MIA	C4-C5-N7	-2.52	106.77	109.40
32	2a	1400	5MC	O2-C2-N3	-2.51	118.25	122.33
1	1A	1939	5MU	O4-C4-C5	-2.51	122.00	124.90
57	1y	8	4SU	C5-C4-S4	-2.49	121.25	124.47
1	2A	2503	8AH	C2-N1-C6	2.47	121.93	118.08
32	1a	1400	5MC	C5-C4-N3	-2.46	119.02	121.67
1	2A	2251	OMG	C8-N7-C5	2.46	107.67	102.99
32	1a	1498	UR3	C3U-N3-C4	2.45	121.39	117.89
55	2x	8	4SU	O2-C2-N1	2.45	126.04	122.79
57	1y	37	MIA	C4-C5-N7	-2.44	106.85	109.40
57	2y	8	4SU	N3-C2-N1	2.41	118.08	114.89
1	2A	1939	5MU	O2-C2-N1	-2.40	119.59	122.79
32	1a	1407	5MC	O2-C2-N3	-2.38	118.46	122.33
54	2w	54	5MU	O2-C2-N1	-2.37	119.63	122.79
43	2l	92	0TD	OD1-CG-CB	-2.37	117.49	122.44
1	1A	1962	5MC	O2-C2-N3	-2.36	118.49	122.33
1	1A	1939	5MU	O2-C2-N3	-2.36	117.10	121.50
32	2a	966	M2G	C8-N7-C5	2.35	107.47	102.99
1	1A	2251	OMG	C8-N7-C5	2.34	107.44	102.99
54	2w	39	PSU	C4-N3-C2	-2.33	122.99	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	37	MIA	C4-C5-N7	-2.31	106.99	109.40
55	1x	76	8AN	O4'-C1'-C2'	-2.31	103.56	106.93
57	1y	54	5MU	O2-C2-N1	-2.30	119.72	122.79
32	2a	1207	2MG	C8-N7-C5	2.29	107.34	102.99
1	1A	1911	PSU	C5-C6-N1	-2.28	118.69	122.11
32	2a	1402	4OC	C6-C5-C4	2.27	119.74	116.96
32	1a	1207	2MG	C5-C6-N1	2.27	117.95	113.95
32	1a	516	PSU	C5-C6-N1	-2.26	118.71	122.11
32	2a	1407	5MC	O2-C2-N3	-2.25	118.67	122.33
32	1a	967	5MC	C5-C4-N3	-2.25	119.25	121.67
1	2A	1920	OMC	O2-C2-N3	-2.25	118.67	122.33
1	2A	2605	PSU	C5-C6-N1	-2.24	118.74	122.11
32	1a	966	M2G	C8-N7-C5	2.24	107.26	102.99
55	2x	32	5MC	O2-C2-N3	-2.24	118.69	122.33
57	2y	46	G7M	C3'-C2'-C1'	2.23	104.34	100.98
1	1A	1915	5MU	O2-C2-N1	-2.23	119.82	122.79
32	1a	966	M2G	C5-C6-N1	2.22	117.87	113.95
54	1w	55	PSU	C5-C6-N1	-2.22	118.78	122.11
57	2y	54	5MU	C5M-C5-C4	2.21	121.20	118.77
32	2a	967	5MC	C5-C4-N3	-2.20	119.30	121.67
32	1a	1498	UR3	C6-N1-C2	-2.19	119.83	121.79
1	2A	1962	5MC	N4-C4-N3	2.17	122.43	118.48
54	2w	39	PSU	C6-C5-C4	-2.15	116.69	118.20
1	2A	2552	2MU	C2'-C1'-N1	-2.15	110.06	114.22
32	2a	967	5MC	CM5-C5-C6	-2.14	119.99	122.85
32	2a	967	5MC	C1'-N1-C6	-2.14	117.57	121.12
32	2a	1207	2MG	C5-C6-N1	2.13	117.72	113.95
1	1A	2605	PSU	O2-C2-N1	-2.13	120.45	122.79
32	2a	966	M2G	C5-C6-N1	2.13	117.71	113.95
1	1A	1942	5MC	CM5-C5-C6	-2.12	120.01	122.85
1	2A	1917	PSU	C5-C6-N1	-2.12	118.93	122.11
32	1a	966	M2G	O6-C6-C5	-2.12	120.23	124.37
1	1A	2251	OMG	C5-C6-N1	2.11	117.68	113.95
43	1l	92	0TD	OD1-CG-CB	-2.11	118.03	122.44
57	1y	39	PSU	O2-C2-N1	-2.10	120.48	122.79
54	1w	32	PSU	C5-C6-N1	-2.09	118.97	122.11
57	2y	55	PSU	O4'-C1'-C2'	2.09	108.09	105.14
55	2x	76	8AN	O2'-C2'-C3'	2.09	116.91	111.47
32	2a	1400	5MC	C5-C4-N3	-2.08	119.43	121.67
1	1A	1911	PSU	O4'-C1'-C2'	2.08	108.08	105.14
54	2w	54	5MU	C5M-C5-C4	2.08	121.06	118.77
54	2w	37	MIA	C1'-N9-C4	2.07	130.28	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2y	55	PSU	C5-C6-N1	-2.06	119.02	122.11
1	2A	2251	OMG	O6-C6-C5	-2.05	120.37	124.37
32	1a	516	PSU	O4'-C1'-C2'	2.04	108.02	105.14
1	1A	2552	2MU	C2'-C1'-N1	-2.04	110.27	114.22
32	2a	516	PSU	O4'-C1'-C2'	2.03	108.01	105.14
1	1A	2605	PSU	C6-C5-C4	-2.03	116.78	118.20
55	1x	55	PSU	C5-C6-N1	-2.03	119.07	122.11
54	2w	37	MIA	N6-C6-N1	2.02	121.02	118.50
1	1A	1915	5MU	C1'-N1-C2	2.02	121.23	117.57
55	2x	8	4SU	C1'-N1-C2	2.02	121.23	117.57
1	1A	1939	5MU	C5M-C5-C4	2.00	120.97	118.77

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	SB-CB-CG-OD2
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
55	1x	76	8AN	O4'-C4'-C5'-O5'
55	1x	76	8AN	C3'-C4'-C5'-O5'
57	1y	46	G7M	C4'-C5'-O5'-P
57	1y	54	5MU	O4'-C4'-C5'-O5'
43	2l	92	0TD	O-C-CA-CB
43	2l	92	0TD	CG-CB-SB-CSB
54	2w	37	MIA	C5-C6-N6-C12
54	2w	37	MIA	N1-C6-N6-C12
55	2x	76	8AN	C3'-C4'-C5'-O5'
57	2y	54	5MU	O4'-C4'-C5'-O5'
56	1z	1	FME	N-CA-CB-CG
56	1z	1	FME	C-CA-CB-CG
56	2z	1	FME	O-C-CA-CB
54	1w	46	G7M	C4'-C5'-O5'-P
32	1a	1519	MA6	O4'-C4'-C5'-O5'
57	1y	54	5MU	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
55	2x	76	8AN	O4'-C4'-C5'-O5'
57	2y	54	5MU	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	C3'-C4'-C5'-O5'
56	2z	1	FME	CB-CG-SD-CE
32	1a	527	G7M	C3'-C4'-C5'-O5'
56	2z	1	FME	N-CA-CB-CG
32	2a	527	G7M	O4'-C4'-C5'-O5'
55	1x	76	8AN	C4'-C5'-O5'-P
43	1l	92	0TD	SB-CB-CG-OD1
54	2w	46	G7M	C4'-C5'-O5'-P
32	2a	527	G7M	C4'-C5'-O5'-P
57	2y	46	G7M	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
55	2x	76	8AN	C4'-C5'-O5'-P
56	1z	1	FME	CA-CB-CG-SD
56	2z	1	FME	CA-CB-CG-SD
57	1y	46	G7M	C3'-C4'-C5'-O5'
54	1w	37	MIA	N6-C12-C13-C14
57	1y	32	PSU	O4'-C1'-C5-C4
57	1y	55	PSU	O4'-C1'-C5-C4
43	2l	92	0TD	CA-CB-SB-CSB
32	1a	527	G7M	C4'-C5'-O5'-P
32	1a	1400	5MC	O4'-C4'-C5'-O5'
1	2A	2503	8AH	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
1	1A	2503	8AH	C4'-C5'-O5'-P
32	1a	527	G7M	O4'-C4'-C5'-O5'
57	2y	37	MIA	C3'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
57	1y	32	PSU	O4'-C1'-C5-C6
57	1y	55	PSU	O4'-C1'-C5-C6
57	2y	55	PSU	O4'-C1'-C5-C6
1	1A	2503	8AH	O4'-C4'-C5'-O5'
43	2l	92	0TD	SB-CB-CG-OD1
1	1A	1920	OMC	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 2765 ligands modelled in this entry, 2763 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	SF4	2d	303	35	0,12,12	-	-	-		
61	SF4	1d	302	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	2d	303	35	-	-	0/6/5/5
61	SF4	1d	302	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.

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%)	0.68	154 (5%) 25 23	24, 43, 98, 108	0
1	2A	2789/2915 (95%)	0.52	155 (5%) 24 21	39, 61, 97, 107	0
2	1B	120/121 (99%)	0.22	0 100 100	39, 58, 72, 91	0
2	2B	120/121 (99%)	-0.12	2 (1%) 70 67	68, 77, 86, 93	0
3	1D	275/276 (99%)	0.56	4 (1%) 73 71	26, 44, 57, 86	0
3	2D	275/276 (99%)	0.71	3 (1%) 80 80	36, 54, 65, 84	0
4	1E	204/206 (99%)	0.66	1 (0%) 91 92	26, 45, 64, 75	0
4	2E	204/206 (99%)	0.60	12 (5%) 22 19	42, 64, 76, 81	0
5	1F	202/210 (96%)	0.54	1 (0%) 91 92	24, 48, 70, 87	0
5	2F	202/210 (96%)	0.55	1 (0%) 91 92	41, 67, 80, 85	0
6	1G	181/182 (99%)	0.25	2 (1%) 80 80	48, 64, 75, 89	0
6	2G	181/182 (99%)	0.78	21 (11%) 4 3	66, 78, 85, 91	0
7	1H	174/180 (96%)	0.48	1 (0%) 89 89	44, 58, 71, 78	0
7	2H	174/180 (96%)	2.79	118 (67%) 0 0	72, 85, 93, 97	0
8	1I	146/148 (98%)	0.36	5 (3%) 45 41	51, 75, 82, 85	0
8	2I	146/148 (98%)	0.33	6 (4%) 37 34	55, 75, 83, 87	0
9	1N	140/140 (100%)	0.85	1 (0%) 87 88	32, 43, 63, 75	0
9	2N	140/140 (100%)	0.67	6 (4%) 35 32	52, 69, 81, 88	0
10	1O	122/122 (100%)	0.50	0 100 100	32, 46, 62, 66	0
10	2O	122/122 (100%)	0.69	2 (1%) 72 69	52, 64, 74, 80	0
11	1P	149/150 (99%)	0.50	2 (1%) 77 76	25, 54, 71, 77	0
11	2P	149/150 (99%)	0.77	12 (8%) 12 9	45, 69, 83, 89	0
12	1Q	141/141 (100%)	0.53	1 (0%) 87 88	31, 47, 62, 74	0
12	2Q	141/141 (100%)	1.28	28 (19%) 1 0	54, 70, 80, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.57	0 100 100	32, 41, 53, 62	0
13	2R	118/118 (100%)	0.42	0 100 100	47, 58, 68, 75	0
14	1S	110/112 (98%)	0.56	0 100 100	45, 58, 69, 73	0
14	2S	110/112 (98%)	0.76	10 (9%) 9 6	62, 74, 80, 83	0
15	1T	131/146 (89%)	0.42	1 (0%) 86 86	40, 50, 74, 83	0
15	2T	131/146 (89%)	0.53	7 (5%) 26 23	56, 66, 78, 83	0
16	1U	116/118 (98%)	0.77	1 (0%) 84 85	27, 35, 50, 69	0
16	2U	116/118 (98%)	0.55	3 (2%) 56 52	47, 67, 76, 81	0
17	1V	101/101 (100%)	0.54	0 100 100	28, 44, 59, 70	0
17	2V	101/101 (100%)	0.35	3 (2%) 50 46	46, 74, 80, 85	0
18	1W	112/113 (99%)	0.78	0 100 100	28, 36, 54, 82	0
18	2W	112/113 (99%)	0.86	5 (4%) 33 30	46, 54, 69, 95	0
19	1X	95/96 (98%)	0.89	2 (2%) 63 60	33, 44, 68, 80	0
19	2X	95/96 (98%)	0.65	2 (2%) 63 60	50, 63, 75, 84	0
20	1Y	107/110 (97%)	0.73	0 100 100	38, 56, 73, 82	0
20	2Y	107/110 (97%)	0.89	8 (7%) 14 11	62, 73, 83, 88	0
21	1Z	154/206 (74%)	0.53	10 (6%) 18 15	43, 69, 87, 91	0
21	2Z	160/206 (77%)	1.82	57 (35%) 0 0	71, 83, 90, 92	0
22	10	83/85 (97%)	0.68	2 (2%) 59 54	33, 44, 58, 67	0
22	20	83/85 (97%)	0.78	5 (6%) 21 18	47, 66, 75, 82	0
23	11	97/98 (98%)	0.62	3 (3%) 49 45	35, 52, 76, 82	0
23	21	97/98 (98%)	0.53	3 (3%) 49 45	43, 59, 76, 83	0
24	12	70/72 (97%)	0.92	1 (1%) 75 74	39, 54, 64, 76	0
24	22	70/72 (97%)	0.32	0 100 100	60, 71, 77, 85	0
25	13	59/60 (98%)	0.66	0 100 100	32, 41, 67, 82	0
25	23	59/60 (98%)	0.55	4 (6%) 17 13	60, 68, 77, 85	0
26	14	69/71 (97%)	0.41	7 (10%) 7 4	61, 80, 89, 91	0
26	24	69/71 (97%)	1.16	17 (24%) 0 0	76, 86, 91, 93	0
27	15	59/60 (98%)	0.76	0 100 100	26, 38, 57, 61	0
27	25	59/60 (98%)	0.56	0 100 100	42, 56, 72, 80	0
28	16	53/54 (98%)	0.41	0 100 100	41, 50, 65, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.62	4 (7%) 14 11	49, 62, 71, 75	0
29	17	48/49 (97%)	0.96	3 (6%) 20 16	27, 34, 60, 70	0
29	27	48/49 (97%)	1.12	6 (12%) 3 2	40, 46, 70, 75	0
30	18	64/65 (98%)	0.58	0 100 100	35, 41, 47, 62	0
30	28	64/65 (98%)	0.95	3 (4%) 31 29	50, 58, 65, 66	0
31	19	37/37 (100%)	0.60	0 100 100	36, 44, 59, 62	0
31	29	37/37 (100%)	2.80	28 (75%) 0 0	67, 74, 81, 83	0
32	1a	1488/1521 (97%)	0.36	80 (5%) 25 23	40, 71, 94, 108	0
32	2a	1491/1521 (98%)	0.33	86 (5%) 23 20	49, 76, 95, 108	0
33	1b	231/256 (90%)	0.40	14 (6%) 21 18	66, 80, 90, 94	0
33	2b	231/256 (90%)	0.77	34 (14%) 2 1	72, 86, 91, 94	0
34	1c	206/239 (86%)	0.61	14 (6%) 17 13	65, 76, 86, 89	0
34	2c	206/239 (86%)	1.24	51 (24%) 0 0	74, 83, 88, 94	0
35	1d	208/209 (99%)	0.57	11 (5%) 26 23	61, 72, 81, 88	0
35	2d	208/209 (99%)	0.71	23 (11%) 5 3	60, 70, 79, 87	0
36	1e	148/162 (91%)	0.56	6 (4%) 37 34	51, 67, 77, 82	0
36	2e	148/162 (91%)	0.71	11 (7%) 14 11	60, 74, 82, 91	0
37	1f	100/101 (99%)	0.14	0 100 100	60, 71, 78, 81	0
37	2f	100/101 (99%)	0.24	0 100 100	58, 69, 77, 87	0
38	1g	155/156 (99%)	0.88	16 (10%) 6 4	67, 75, 86, 90	0
38	2g	155/156 (99%)	1.00	27 (17%) 1 1	71, 80, 88, 94	0
39	1h	137/138 (99%)	0.43	5 (3%) 42 39	58, 69, 76, 82	0
39	2h	137/138 (99%)	0.54	6 (4%) 34 32	67, 76, 80, 84	0
40	1i	127/128 (99%)	1.49	39 (30%) 0 0	58, 80, 85, 89	0
40	2i	127/128 (99%)	2.14	62 (48%) 0 0	71, 85, 90, 93	0
41	1j	97/105 (92%)	1.07	18 (18%) 1 0	62, 80, 89, 91	0
41	2j	96/105 (91%)	2.30	48 (50%) 0 0	74, 88, 93, 96	0
42	1k	114/129 (88%)	0.68	5 (4%) 34 32	48, 69, 79, 81	0
42	2k	114/129 (88%)	0.46	6 (5%) 26 23	58, 74, 84, 88	0
43	1l	121/132 (91%)	0.57	6 (4%) 28 26	51, 57, 69, 76	0
43	2l	121/132 (91%)	0.87	15 (12%) 4 2	60, 68, 76, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.62	9 (7%) 15 11	59, 74, 82, 90	0
44	2m	122/126 (96%)	1.34	25 (20%) 1 0	73, 82, 87, 91	0
45	1n	60/61 (98%)	1.62	19 (31%) 0 0	67, 74, 82, 86	0
45	2n	60/61 (98%)	4.12	51 (85%) 0 0	77, 84, 89, 90	0
46	1o	88/89 (98%)	0.33	5 (5%) 23 20	50, 69, 76, 80	0
46	2o	88/89 (98%)	0.48	4 (4%) 33 30	59, 72, 82, 85	0
47	1p	82/88 (93%)	1.29	19 (23%) 0 0	64, 73, 80, 88	0
47	2p	82/88 (93%)	0.79	4 (4%) 29 27	63, 71, 78, 81	0
48	1q	99/105 (94%)	1.00	12 (12%) 4 2	57, 69, 77, 79	0
48	2q	99/105 (94%)	0.62	5 (5%) 28 25	62, 74, 82, 84	0
49	1r	68/88 (77%)	0.25	0 100 100	58, 68, 78, 82	0
49	2r	68/88 (77%)	0.31	0 100 100	63, 71, 80, 84	0
50	1s	83/93 (89%)	0.74	7 (8%) 11 8	67, 77, 85, 89	0
50	2s	83/93 (89%)	2.10	38 (45%) 0 0	78, 86, 91, 96	0
51	1t	96/106 (90%)	1.68	36 (37%) 0 0	63, 74, 82, 84	0
51	2t	96/106 (90%)	1.01	17 (17%) 1 1	63, 73, 84, 86	0
52	1u	23/27 (85%)	1.81	8 (34%) 0 0	67, 71, 76, 79	0
52	2u	23/27 (85%)	3.24	17 (73%) 0 0	70, 79, 83, 88	0
53	1v	13/24 (54%)	2.31	5 (38%) 0 0	52, 59, 93, 103	0
53	2v	13/24 (54%)	2.67	5 (38%) 0 0	65, 73, 97, 102	0
54	1w	66/76 (86%)	1.19	12 (18%) 1 0	34, 88, 99, 103	0
54	2w	64/76 (84%)	1.67	19 (29%) 0 0	50, 95, 100, 103	0
55	1x	72/77 (93%)	0.14	2 (2%) 53 49	31, 65, 83, 90	0
55	2x	72/77 (93%)	0.17	1 (1%) 75 74	48, 77, 88, 98	0
56	1z	6/7 (85%)	2.91	3 (50%) 0 0	33, 41, 67, 73	0
56	2z	6/7 (85%)	2.50	2 (33%) 0 0	52, 58, 77, 78	0
57	1y	67/76 (88%)	4.00	54 (80%) 0 0	62, 99, 103, 104	0
57	2y	66/76 (86%)	4.53	62 (93%) 0 0	70, 102, 104, 106	0
All	All	20883/21762 (95%)	0.70	1757 (8%) 11 8	24, 67, 90, 108	0

All (1757) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	18.1
1	2A	652(V)	C	17.8
44	1m	124	PRO	15.6
1	2A	652(U)	G	15.3
44	2m	124	PRO	15.0
1	1A	653	A	14.2
1	1A	652(C)	G	14.1
44	1m	123	ALA	13.9
57	2y	36	A	13.1
1	2A	653	A	12.8
45	2n	38	GLY	12.7
1	1A	652(V)	C	12.0
1	1A	652(S)	C	12.0
1	2A	652(C)	G	12.0
57	1y	36	A	11.3
32	2a	1030(B)	C	11.2
1	1A	652(U)	G	11.0
54	1w	70	G	10.9
1	1A	652(T)	C	10.4
57	1y	35	A	10.3
57	1y	34	G	10.2
32	2a	1030(A)	G	10.1
1	2A	2802	G	9.9
54	2w	71	G	9.9
1	2A	652(T)	C	9.6
45	2n	39	LEU	9.4
1	2A	654	A	9.3
1	1A	654	A	9.2
1	2A	888	C	9.2
57	2y	34	G	9.1
57	2y	35	A	8.9
32	2a	1001(A)	G	8.9
21	2Z	144	LEU	8.8
57	1y	24	G	8.7
1	2A	884	C	8.7
1	1A	2159	G	8.6
1	2A	2146	C	8.5
1	1A	2131	G	8.4
32	2a	1032	G	8.4
45	2n	11	LYS	8.4
32	2a	1033	G	8.3
45	1n	2	ALA	8.3
53	2v	12	A	8.2

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Mol	Chain	Res	Type	RSRZ
1	2A	2139	C	8.2
1	2A	883	G	8.2
1	2A	652(D)	C	8.2
45	2n	35	ARG	8.2
1	1A	1509	C	8.1
38	2g	154	TYR	8.1
1	2A	2145	C	8.0
38	2g	156	TRP	8.0
20	2Y	1	MET	8.0
57	1y	21	A	8.0
56	1z	2	THR	8.0
41	2j	47	PHE	7.8
44	1m	2	ALA	7.8
1	2A	2160	G	7.8
1	1A	2115	G	7.7
57	2y	1	G	7.7
38	2g	80	VAL	7.6
52	2u	16	GLY	7.6
57	1y	19	G	7.5
40	2i	8	GLY	7.5
54	1w	71	G	7.4
57	2y	19	G	7.4
1	1A	2166	G	7.3
7	2H	48	GLY	7.3
1	2A	885	C	7.3
1	1A	2116	G	7.3
26	24	63	TYR	7.3
45	2n	34	TYR	7.3
1	2A	2147	G	7.2
1	1A	2129	C	7.2
1	1A	2145	C	7.1
21	2Z	149	SER	7.1
41	2j	74	ILE	7.1
1	2A	2128	C	7.1
1	1A	2151	G	7.0
57	1y	38	A	7.0
53	1v	12	A	6.9
1	2A	887	A	6.9
50	2s	80	TYR	6.9
32	1a	1026	G	6.9
1	2A	2803	C	6.8
32	1a	1035	A	6.8

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Mol	Chain	Res	Type	RSRZ
45	2n	12	ARG	6.8
32	1a	1030(B)	C	6.8
45	2n	25	VAL	6.8
53	1v	13	A	6.8
7	2H	72	ILE	6.8
57	2y	62	C	6.7
40	1i	14	VAL	6.7
50	2s	50	ALA	6.7
7	2H	113	VAL	6.7
32	1a	1036	G	6.7
1	1A	2141	G	6.6
1	2A	2138	C	6.6
32	2a	1030	C	6.6
32	2a	1039	C	6.6
40	2i	15	ALA	6.6
3	1D	276	LYS	6.6
1	1A	2111	C	6.6
57	2y	21	A	6.6
57	2y	58	A	6.5
7	2H	128	PRO	6.5
32	2a	1257	U	6.5
54	2w	70	G	6.5
1	1A	884	C	6.5
32	1a	1001(A)	G	6.5
32	1a	1030(A)	G	6.5
1	1A	897	C	6.5
57	1y	1	G	6.5
1	1A	2128	C	6.4
32	1a	1001	A	6.4
38	1g	79	ARG	6.4
57	1y	5	G	6.4
57	1y	15	G	6.4
38	2g	82	GLY	6.4
32	1a	1003	G	6.4
38	1g	156	TRP	6.4
57	2y	5	G	6.4
1	2A	2127	G	6.3
40	1i	19	LEU	6.3
40	2i	14	VAL	6.3
57	2y	63	G	6.3
21	2Z	106	GLY	6.3
57	2y	57	G	6.3

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Mol	Chain	Res	Type	RSRZ
45	2n	13	THR	6.2
45	2n	2	ALA	6.2
12	2Q	33	GLY	6.2
1	2A	2110	G	6.2
32	2a	1035	A	6.1
1	1A	2168	G	6.1
41	2j	63	PHE	6.1
50	2s	84	GLY	6.1
1	2A	2116	G	6.1
57	1y	22	G	6.1
1	1A	1095	A	6.1
1	1A	2110	G	6.1
1	1A	2164	C	6.0
1	1A	2160	G	6.0
1	2A	2149	G	6.0
54	1w	20	U	6.0
1	1A	2135	A	6.0
21	2Z	96	VAL	6.0
32	1a	1034	G	6.0
1	1A	2132	U	6.0
23	2l	2	SER	6.0
32	1a	1028	C	6.0
50	2s	30	LEU	6.0
57	1y	13	C	5.9
1	1A	2181	G	5.9
1	2A	2112	G	5.9
1	2A	2117	A	5.9
44	2m	120	LYS	5.9
57	1y	75	C	5.9
38	2g	79	ARG	5.9
7	2H	123	PHE	5.9
1	2A	2801(A)	A	5.9
32	2a	1034	G	5.9
57	2y	53	G	5.9
1	2A	2125	G	5.8
1	1A	2130	U	5.8
54	2w	72	C	5.8
7	2H	6	ARG	5.8
57	1y	47	U	5.8
57	2y	33	U	5.8
57	2y	74	C	5.8
57	2y	18	G	5.8

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Mol	Chain	Res	Type	RSRZ
57	2y	56	C	5.8
45	2n	22	THR	5.8
1	1A	2140	C	5.8
1	2A	886	C	5.8
1	2A	2111	C	5.8
1	1A	2161	C	5.8
38	2g	81	GLY	5.8
1	2A	2123	G	5.7
54	1w	72	C	5.7
1	1A	1096	A	5.7
45	2n	36	PHE	5.7
1	1A	2117	A	5.7
45	2n	56	VAL	5.7
32	2a	1031	G	5.7
57	2y	52	G	5.7
1	2A	2133	G	5.7
1	1A	652(D)	C	5.6
1	2A	2792	G	5.6
32	2a	1002	G	5.6
57	2y	29	G	5.6
57	2y	6	G	5.6
32	1a	1027	C	5.6
41	2j	66	ARG	5.6
40	1i	15	ALA	5.6
1	1A	2162	G	5.6
1	2A	2793	G	5.6
45	2n	37	PHE	5.6
1	2A	894	C	5.6
1	2A	2159	G	5.5
44	2m	121	LYS	5.5
1	1A	2114	A	5.5
31	29	17	ILE	5.5
1	2A	2129	C	5.5
1	1A	2146	C	5.5
1	2A	2174	C	5.5
57	1y	71	G	5.5
40	2i	36	TYR	5.5
38	2g	32	ARG	5.5
26	24	49	PHE	5.5
7	2H	44	VAL	5.4
40	2i	128	ARG	5.4
34	2c	20	SER	5.4

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Mol	Chain	Res	Type	RSRZ
32	2a	1036	G	5.4
1	2A	2169	A	5.4
50	2s	13	ASP	5.4
1	1A	888	C	5.4
21	2Z	155	LEU	5.4
57	2y	15	G	5.4
7	2H	129	THR	5.4
32	1a	1447	A	5.4
21	2Z	51	ALA	5.4
1	1A	2108	C	5.4
52	2u	14	TRP	5.4
1	2A	896	A	5.4
57	1y	14	A	5.4
57	2y	65	G	5.3
32	1a	1029	C	5.3
56	2z	3	HIS	5.3
1	2A	1112	G	5.3
57	1y	20	U	5.3
21	2Z	147	GLY	5.3
31	29	16	VAL	5.3
45	2n	61	TRP	5.3
21	2Z	139	VAL	5.3
45	1n	25	VAL	5.3
40	2i	114	TYR	5.3
1	2A	2154	G	5.3
34	2c	4	LYS	5.2
1	1A	652(F)	G	5.2
1	1A	2147	G	5.2
7	2H	35	VAL	5.2
41	2j	85	LEU	5.2
1	1A	2165	G	5.2
57	1y	57	G	5.2
45	2n	50	LYS	5.2
52	2u	9	ARG	5.2
1	2A	1509	C	5.2
32	2a	1040	U	5.2
32	1a	1033	G	5.2
45	2n	42	ILE	5.2
52	2u	15	ARG	5.2
7	2H	142	GLY	5.2
38	1g	154	TYR	5.2
7	2H	2	SER	5.2

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Mol	Chain	Res	Type	RSRZ
57	2y	38	A	5.2
1	2A	2113	U	5.2
7	2H	125	VAL	5.2
21	1Z	1	MET	5.2
1	1A	896	A	5.1
57	2y	45	U	5.1
1	2A	1113	U	5.1
32	2a	1532	U	5.1
57	2y	2	C	5.1
7	2H	92	ILE	5.1
32	2a	1030(C)	G	5.1
38	1g	81	GLY	5.1
1	2A	2804	C	5.1
32	2a	1030(D)	A	5.1
52	2u	13	ILE	5.1
45	2n	43	CYS	5.1
1	1A	2109	U	5.1
57	1y	23	A	5.1
21	2Z	170	THR	5.1
51	1t	76	ALA	5.1
21	2Z	128	VAL	5.1
7	2H	105	LEU	5.1
21	2Z	153	SER	5.1
1	2A	2182	G	5.0
7	2H	52	VAL	5.0
1	1A	885	C	5.0
1	1A	2112	G	5.0
1	2A	2168	G	5.0
57	2y	66	U	5.0
7	2H	132	ARG	5.0
45	2n	57	ARG	5.0
1	2A	2896	C	5.0
1	1A	2158	A	5.0
50	2s	81	ARG	5.0
32	1a	1030(C)	G	5.0
7	2H	159	GLU	5.0
50	2s	71	LEU	5.0
57	2y	64	A	5.0
1	1A	652(E)	G	4.9
7	2H	141	VAL	4.9
41	2j	44	VAL	4.9
1	2A	2179	C	4.9

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Mol	Chain	Res	Type	RSRZ
32	2a	1286	A	4.9
51	2t	41	ILE	4.9
51	2t	59	ALA	4.9
1	1A	2133	G	4.9
40	2i	27	THR	4.9
32	1a	1024	G	4.9
34	2c	182	ILE	4.9
1	2A	882	G	4.9
56	2z	2	THR	4.9
41	2j	65	LEU	4.9
53	2v	24	A	4.9
7	2H	102	ALA	4.9
1	2A	892	G	4.9
32	1a	1025	U	4.9
29	17	48	LYS	4.9
50	1s	12	ASP	4.8
32	2a	1027	C	4.8
32	1a	1532	U	4.8
7	2H	131	VAL	4.8
38	2g	16	LEU	4.8
1	2A	1026	U	4.8
41	2j	59	SER	4.8
1	2A	229	A	4.8
1	2A	2165	G	4.8
21	2Z	93	ASP	4.8
7	2H	24	VAL	4.8
7	2H	82	GLY	4.8
35	1d	167	GLY	4.8
53	2v	14	A	4.8
52	2u	17	THR	4.8
40	2i	13	ALA	4.8
44	2m	122	LYS	4.8
57	1y	2	C	4.8
57	2y	3	C	4.8
34	1c	39	ILE	4.8
57	2y	14	A	4.7
1	2A	2148	G	4.7
21	2Z	141	VAL	4.7
41	2j	72	VAL	4.7
40	2i	105	ASP	4.7
1	1A	1094	U	4.7
21	2Z	140	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2161	C	4.7
33	1b	133	LYS	4.7
32	1a	1257	U	4.7
21	2Z	152	ALA	4.7
1	1A	2154	G	4.7
1	2A	652(E)	G	4.7
1	1A	2180	U	4.7
45	2n	18	VAL	4.7
7	2H	95	ARG	4.7
1	1A	2120	G	4.7
50	2s	12	ASP	4.7
7	2H	94	TYR	4.7
57	2y	61	C	4.7
34	2c	155	GLY	4.7
45	2n	7	ILE	4.7
1	2A	2109	U	4.7
1	2A	2141	G	4.7
32	2a	1021	G	4.7
57	1y	53	G	4.7
21	2Z	156	LYS	4.7
29	27	48	LYS	4.7
21	2Z	137	ILE	4.7
45	2n	44	LEU	4.7
45	2n	31	ARG	4.6
53	2v	15	A	4.6
40	2i	65	VAL	4.6
1	1A	889	C	4.6
32	2a	1003	G	4.6
45	2n	51	GLY	4.6
26	24	50	VAL	4.6
32	2a	1024	G	4.6
41	1j	46	ARG	4.6
51	1t	70	SER	4.6
1	1A	2174	C	4.6
7	2H	47	GLU	4.6
31	29	24	TYR	4.6
34	2c	198	VAL	4.6
48	2q	23	VAL	4.6
1	2A	889	C	4.6
40	2i	66	ARG	4.6
1	2A	2126	A	4.6
1	2A	2135	A	4.6

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Mol	Chain	Res	Type	RSRZ
53	2v	13	A	4.6
32	1a	204	U	4.6
1	2A	2100	G	4.6
40	2i	106	ALA	4.6
33	2b	33	TYR	4.6
21	2Z	148	ASP	4.6
57	2y	26	A	4.6
41	2j	40	LEU	4.6
21	2Z	145	GLU	4.6
57	1y	59	U	4.5
57	2y	44	G	4.5
1	1A	1098	A	4.5
40	2i	37	PHE	4.5
45	2n	24	CYS	4.5
54	2w	45	U	4.5
7	2H	45	VAL	4.5
45	1n	55	GLY	4.5
1	2A	2805	G	4.5
1	1A	1508	A	4.5
1	2A	897	C	4.5
45	2n	6	LEU	4.5
45	2n	4	LYS	4.5
1	2A	2164	C	4.5
7	2H	99	VAL	4.5
26	24	59	PHE	4.5
7	2H	145	ALA	4.5
26	24	68	ARG	4.5
32	1a	1531	A	4.5
40	2i	76	ALA	4.5
1	1A	2175	C	4.5
52	1u	9	ARG	4.5
32	1a	1286	A	4.5
40	2i	86	VAL	4.5
1	2A	895	U	4.4
1	2A	881	G	4.4
54	2w	73	A	4.4
7	2H	121	ILE	4.4
32	1a	1023	G	4.4
38	1g	83	ALA	4.4
40	1i	117	HIS	4.4
7	2H	96	ALA	4.4
7	2H	98	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
12	2Q	37	LEU	4.4
1	1A	1057	A	4.4
40	2i	82	ALA	4.4
57	2y	43	C	4.4
43	2l	39	VAL	4.4
40	2i	93	ARG	4.4
52	2u	8	THR	4.4
40	1i	8	GLY	4.4
1	1A	2144	U	4.4
57	2y	67	C	4.4
48	1q	98	LEU	4.4
41	2j	10	GLY	4.3
34	2c	6	HIS	4.3
57	1y	25	C	4.3
51	1t	9	ASN	4.3
1	2A	893	C	4.3
7	2H	37	VAL	4.3
57	1y	45	U	4.3
44	2m	70	LEU	4.3
51	1t	72	LEU	4.3
32	2a	1287	A	4.3
41	2j	55	LYS	4.3
57	1y	58	A	4.3
31	29	19	ARG	4.3
38	2g	78	ARG	4.3
44	2m	100	GLY	4.3
52	2u	11	GLY	4.3
57	2y	31	A	4.3
1	2A	1043	C	4.3
31	29	20	HIS	4.3
55	2x	47	U	4.3
7	2H	43	VAL	4.3
1	2A	2115	G	4.3
1	2A	2120	G	4.3
1	1A	2119	A	4.3
32	2a	1001	A	4.3
32	1a	1030	C	4.3
34	2c	39	ILE	4.3
1	2A	2167	U	4.3
32	1a	1031	G	4.3
38	2g	83	ALA	4.3
57	2y	24	G	4.3

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Mol	Chain	Res	Type	RSRZ
38	1g	80	VAL	4.2
50	2s	51	VAL	4.2
1	1A	2127	G	4.2
54	2w	44	G	4.2
31	29	25	VAL	4.2
51	1t	59	ALA	4.2
41	1j	47	PHE	4.2
1	1A	2149	G	4.2
1	1A	2169	A	4.2
1	1A	2170	A	4.2
53	1v	14	A	4.2
57	1y	70	G	4.2
57	1y	4	C	4.2
14	2S	3	ARG	4.2
40	2i	9	ARG	4.2
51	1t	80	ARG	4.2
43	1l	64	TYR	4.2
21	2Z	57	ILE	4.2
56	1z	3	HIS	4.2
12	2Q	6	ARG	4.2
45	2n	55	GLY	4.2
7	2H	169	VAL	4.2
33	1b	165	VAL	4.2
54	2w	4	C	4.2
1	1A	271(K)	U	4.1
57	2y	51	U	4.1
1	1A	2107	C	4.1
1	2A	2140	C	4.1
54	1w	73	A	4.1
1	1A	1068	G	4.1
31	29	22	ARG	4.1
1	2A	2170	A	4.1
57	2y	30	G	4.1
7	2H	106	THR	4.1
43	2l	18	VAL	4.1
1	1A	887	A	4.1
7	2H	171	LEU	4.1
40	1i	79	LEU	4.1
57	1y	12	U	4.1
12	2Q	59	ARG	4.1
21	2Z	1	MET	4.1
57	2y	72	C	4.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2189	U	4.1
32	1a	162	A	4.1
1	2A	2144	U	4.1
1	2A	2134	A	4.1
7	2H	19	VAL	4.1
12	2Q	109	VAL	4.1
1	2A	2153	G	4.0
32	2a	1150	U	4.0
57	2y	47	U	4.0
57	1y	56	C	4.0
57	2y	4	C	4.0
45	2n	16	PHE	4.0
34	2c	57	ILE	4.0
1	1A	2152	G	4.0
54	1w	69	G	4.0
57	1y	61	C	4.0
57	2y	28	G	4.0
7	2H	29	PRO	4.0
40	2i	90	PRO	4.0
51	1t	79	ARG	4.0
7	2H	7	LEU	4.0
7	2H	38	SER	4.0
34	2c	34	LEU	4.0
41	2j	98	ILE	4.0
1	1A	2167	U	4.0
11	2P	109	GLY	4.0
45	2n	40	CYS	4.0
1	1A	1069	A	4.0
21	2Z	151	HIS	4.0
11	2P	110	TYR	4.0
38	2g	85	TYR	4.0
44	2m	87	TYR	4.0
3	2D	38	LYS	4.0
43	2l	55	VAL	4.0
21	2Z	157	LEU	4.0
41	2j	88	LEU	4.0
33	2b	34	ALA	3.9
50	2s	14	HIS	3.9
7	2H	69	ARG	3.9
1	2A	2181	G	3.9
31	29	30	PRO	3.9
6	2G	3	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
7	2H	103	LEU	3.9
32	1a	1005	A	3.9
7	2H	71	LEU	3.9
1	1A	2142	C	3.9
21	2Z	164	ALA	3.9
23	11	2	SER	3.9
40	2i	115	GLY	3.9
40	1i	113	LYS	3.9
38	2g	76	ARG	3.9
45	2n	53	LEU	3.9
51	1t	22	ARG	3.9
34	2c	8	ILE	3.9
21	2Z	150	LEU	3.9
34	1c	87	LEU	3.9
1	1A	2106	G	3.8
45	2n	23	ARG	3.8
26	24	51	ASP	3.8
51	1t	38	LYS	3.8
32	2a	1531	A	3.8
51	2t	63	ILE	3.8
45	2n	30	ALA	3.8
52	2u	6	ARG	3.8
1	1A	2182	G	3.8
31	29	13	LYS	3.8
57	1y	44	G	3.8
45	2n	8	GLU	3.8
40	2i	103	THR	3.8
29	27	46	VAL	3.8
50	2s	79	THR	3.8
51	1t	74	LYS	3.8
40	1i	26	VAL	3.8
7	2H	157	TYR	3.8
22	20	45	PHE	3.8
50	2s	52	TYR	3.8
50	2s	70	LYS	3.8
40	1i	65	VAL	3.8
1	1A	1064	C	3.8
1	2A	2156	G	3.8
51	1t	67	ALA	3.7
1	2A	2142	C	3.7
1	1A	2157	G	3.7
7	2H	49	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
40	2i	108	VAL	3.7
41	2j	46	ARG	3.7
34	2c	160	ALA	3.7
1	1A	1060	U	3.7
1	1A	2113	U	3.7
1	1A	2189	U	3.7
1	2A	2118	U	3.7
32	1a	1037	C	3.7
7	2H	172	LYS	3.7
50	2s	36	ARG	3.7
1	1A	2148	G	3.7
32	1a	1032	G	3.7
33	2b	232	PRO	3.7
20	2Y	5	MET	3.7
57	2y	73	A	3.7
1	1A	2118	U	3.7
1	2A	2895	U	3.7
32	2a	1029	C	3.7
6	2G	2	PRO	3.7
1	2A	2190	G	3.7
32	1a	1002	G	3.7
41	2j	27	ALA	3.7
54	1w	44	G	3.7
7	2H	20	ALA	3.7
1	2A	2173	A	3.7
50	2s	28	LYS	3.7
7	2H	8	PRO	3.7
39	2h	133	LEU	3.7
43	2l	60	LEU	3.7
21	2Z	122	ARG	3.7
41	2j	73	ASP	3.7
33	2b	17	PHE	3.7
31	29	26	ILE	3.7
32	1a	1040	U	3.7
32	2a	1005	A	3.7
32	2a	1026	G	3.7
31	29	29	ASN	3.7
41	2j	39	PRO	3.7
40	1i	121	ARG	3.7
32	1a	1446	U	3.6
14	2S	92	TYR	3.6
33	2b	37	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
38	2g	40	ALA	3.6
41	2j	32	ALA	3.6
34	2c	157	ILE	3.6
43	2l	93	LEU	3.6
1	1A	278	A	3.6
52	2u	22	ARG	3.6
7	2H	5	GLY	3.6
57	2y	68	C	3.6
36	2e	21	ALA	3.6
12	2Q	63	LYS	3.6
1	1A	1059	G	3.6
1	1A	1063	G	3.6
1	2A	2107	C	3.6
50	2s	37	ARG	3.6
41	2j	48	THR	3.6
33	2b	81	VAL	3.6
40	2i	109	VAL	3.6
41	2j	62	HIS	3.6
54	2w	2	C	3.6
57	2y	25	C	3.6
42	1k	25	TYR	3.6
7	2H	133	VAL	3.6
50	2s	38	SER	3.6
32	1a	202	U	3.6
32	1a	79	G	3.6
12	2Q	117	ALA	3.6
51	1t	71	THR	3.6
45	2n	33	VAL	3.6
50	2s	35	SER	3.5
1	1A	2163	C	3.5
57	1y	74	C	3.5
12	2Q	114	ALA	3.5
57	1y	10	G	3.5
7	2H	16	SER	3.5
7	2H	112	PRO	3.5
1	1A	2172	U	3.5
3	2D	276	LYS	3.5
1	2A	2177	C	3.5
57	1y	3	C	3.5
38	1g	153	HIS	3.5
41	1j	41	PRO	3.5
34	2c	87	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
51	1t	24	LEU	3.5
51	1t	62	LEU	3.5
7	2H	53	GLU	3.5
1	1A	2188	C	3.5
40	1i	106	ALA	3.5
45	2n	10	ALA	3.5
50	2s	63	THR	3.5
12	2Q	32	TYR	3.5
38	2g	4	ARG	3.5
52	2u	5	ASP	3.5
1	1A	1082	U	3.5
23	11	98	LEU	3.5
7	2H	17	VAL	3.5
7	2H	79	VAL	3.5
57	2y	23	A	3.5
45	1n	57	ARG	3.5
57	2y	71	G	3.5
45	1n	56	VAL	3.5
50	2s	9	VAL	3.5
54	2w	31	A	3.4
21	2Z	20	ARG	3.4
29	17	47	ARG	3.4
8	2I	100	ALA	3.4
40	1i	45	ALA	3.4
9	2N	83	LYS	3.4
52	1u	14	TRP	3.4
21	2Z	143	GLY	3.4
43	1l	18	VAL	3.4
1	1A	1058	G	3.4
1	2A	2114	A	3.4
10	2O	69	ILE	3.4
32	1a	1007	C	3.4
33	2b	19	HIS	3.4
41	1j	40	LEU	3.4
38	2g	147	ALA	3.4
40	1i	46	ALA	3.4
40	1i	126	SER	3.4
35	1d	198	VAL	3.4
40	2i	10	ARG	3.4
12	2Q	113	GLN	3.4
1	2A	2131	G	3.4
40	2i	125	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
41	1j	38	ILE	3.4
1	2A	652(B)	A	3.4
32	2a	1004	A	3.4
48	1q	7	THR	3.4
21	2Z	104	PHE	3.4
38	1g	85	TYR	3.4
39	2h	134	ILE	3.4
1	1A	1066	U	3.4
1	1A	2171	A	3.4
1	1A	886	C	3.4
1	1A	2139	C	3.4
34	2c	75	VAL	3.4
34	2c	201	TYR	3.4
33	1b	135	GLN	3.4
1	1A	2792	G	3.4
1	2A	2157	G	3.4
11	2P	15	ARG	3.4
34	2c	186	PHE	3.4
51	1t	23	ARG	3.4
51	1t	63	ILE	3.4
1	1A	1065	U	3.4
1	1A	2153	G	3.4
1	2A	1114	G	3.4
21	2Z	126	VAL	3.4
32	1a	163	C	3.4
32	2a	1038	C	3.4
32	2a	1041	A	3.3
32	2a	1037	C	3.3
50	2s	82	GLY	3.3
1	1A	2123	G	3.3
57	1y	28	G	3.3
19	1X	95	LEU	3.3
41	2j	71	LEU	3.3
40	1i	119	ALA	3.3
12	2Q	5	ARG	3.3
31	29	37	GLY	3.3
1	1A	2134	A	3.3
1	1A	2136	C	3.3
1	2A	2143	C	3.3
32	2a	1149	C	3.3
11	2P	45	LEU	3.3
33	2b	121	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	2A	2152	G	3.3
32	1a	220	G	3.3
52	1u	2	GLY	3.3
47	1p	21	VAL	3.3
1	2A	2794	C	3.3
47	2p	74	LEU	3.3
53	1v	15	A	3.3
57	1y	11	C	3.3
35	2d	6	GLY	3.3
50	2s	67	VAL	3.3
52	2u	10	ARG	3.3
1	1A	1097	U	3.3
50	2s	31	ILE	3.3
1	2A	2175	C	3.3
57	1y	48	C	3.3
57	2y	7	A	3.3
45	2n	49	HIS	3.3
45	1n	51	GLY	3.3
6	2G	49	ASP	3.3
21	2Z	9	TYR	3.3
31	29	12	ASP	3.3
1	2A	2151	G	3.3
1	2A	2166	G	3.3
40	2i	126	SER	3.3
1	2A	2137	C	3.3
7	2H	124	GLU	3.3
7	2H	51	ARG	3.3
51	1t	64	ASP	3.3
47	2p	59	TRP	3.3
1	1A	2156	G	3.2
57	1y	30	G	3.2
14	2S	29	PHE	3.2
33	1b	227	GLY	3.2
47	1p	80	PHE	3.2
1	1A	1084	A	3.2
41	1j	44	VAL	3.2
1	1A	2150	U	3.2
21	2Z	171	ILE	3.2
33	2b	122	PHE	3.2
1	1A	2138	C	3.2
1	1A	229	A	3.2
7	2H	10	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
7	2H	101	ARG	3.2
7	2H	115	VAL	3.2
40	2i	17	VAL	3.2
44	2m	93	ARG	3.2
31	29	33	LYS	3.2
40	1i	80	GLY	3.2
40	1i	33	PHE	3.2
51	1t	55	ILE	3.2
32	2a	998	G	3.2
32	2a	1061	G	3.2
1	1A	1076	C	3.2
7	2H	3	ARG	3.2
32	2a	1018	C	3.2
33	2b	92	TYR	3.2
7	2H	76	VAL	3.2
19	2X	92	LEU	3.2
21	1Z	104	PHE	3.2
41	2j	13	HIS	3.2
33	2b	165	VAL	3.2
34	1c	193	TYR	3.2
31	29	11	CYS	3.2
44	1m	25	ILE	3.2
47	2p	9	PHE	3.2
45	2n	45	ARG	3.2
31	29	32	HIS	3.2
52	2u	2	GLY	3.2
40	2i	28	VAL	3.2
42	1k	89	ALA	3.2
51	1t	68	LYS	3.2
1	2A	2158	A	3.2
40	1i	81	ILE	3.2
57	1y	60	U	3.2
7	2H	63	SER	3.2
44	1m	122	LYS	3.2
7	2H	165	ALA	3.1
26	24	52	THR	3.1
40	2i	19	LEU	3.2
1	2A	2150	U	3.1
36	2e	11	ILE	3.1
21	2Z	121	HIS	3.1
41	2j	56	HIS	3.1
28	26	52	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
12	2Q	121	ALA	3.1
1	2A	2130	U	3.1
12	2Q	65	PHE	3.1
32	1a	999	C	3.1
57	1y	33	U	3.1
57	1y	62	C	3.1
15	2T	66	VAL	3.1
11	2P	38	GLN	3.1
26	24	32	TYR	3.1
12	2Q	19	GLY	3.1
40	2i	67	GLY	3.1
51	1t	75	ASN	3.1
1	1A	2178	C	3.1
32	2a	1006	C	3.1
45	2n	46	GLU	3.1
45	2n	17	LYS	3.1
41	2j	58	ASP	3.1
12	2Q	17	LEU	3.1
21	2Z	172	ALA	3.1
38	1g	32	ARG	3.1
50	2s	68	GLY	3.1
41	1j	62	HIS	3.1
1	2A	2136	C	3.1
32	2a	1007	C	3.1
57	2y	42	C	3.1
40	1i	31	GLN	3.1
32	1a	78	G	3.1
35	2d	168	ARG	3.1
40	1i	47	LEU	3.1
38	1g	84	ASN	3.1
41	1j	64	GLU	3.1
44	2m	102	ARG	3.1
26	24	66	SER	3.1
41	2j	11	PHE	3.1
43	2l	64	TYR	3.1
32	1a	92	C	3.1
35	2d	156	GLU	3.1
1	1A	1077	A	3.1
46	2o	60	VAL	3.1
1	1A	2155	G	3.1
7	2H	148	ILE	3.1
20	2Y	55	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
36	2e	13	ILE	3.1
8	2I	82	ARG	3.1
57	2y	13	C	3.1
4	1E	195	LEU	3.1
7	2H	146	ALA	3.1
25	23	29	ARG	3.0
32	1a	73	G	3.0
32	1a	630	G	3.0
57	1y	52	G	3.0
6	1G	146	TYR	3.0
33	2b	113	HIS	3.0
47	1p	22	THR	3.0
50	2s	39	THR	3.0
35	1d	86	LYS	3.0
32	1a	93	G	3.0
57	1y	18	G	3.0
33	2b	29	ALA	3.0
34	2c	101	LEU	3.0
47	1p	7	ALA	3.0
47	1p	60	LEU	3.0
19	2X	68	ARG	3.0
32	1a	1008	C	3.0
32	2a	1452	C	3.0
48	2q	9	VAL	3.0
1	1A	895	U	3.0
1	1A	1070	A	3.0
1	2A	2119	A	3.0
32	1a	344	A	3.0
32	1a	1000	U	3.0
51	1t	41	ILE	3.0
51	1t	100	ILE	3.0
32	2a	1023	G	3.0
34	2c	33	LEU	3.0
40	1i	90	PRO	3.0
1	1A	2143	C	3.0
1	1A	2179	C	3.0
47	1p	1	MET	3.0
44	2m	119	GLY	3.0
47	1p	38	TYR	3.0
7	2H	32	GLU	3.0
1	2A	2124	G	3.0
33	1b	136	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
42	1k	14	VAL	3.0
1	1A	2185	C	3.0
31	29	31	LYS	3.0
32	2a	1043	C	3.0
45	2n	58	LYS	3.0
57	2y	75	C	3.0
7	2H	4	ILE	3.0
50	2s	10	PHE	3.0
40	2i	58	HIS	3.0
1	2A	890	A	3.0
6	2G	78	SER	3.0
4	2E	196	VAL	3.0
12	2Q	89	ASN	3.0
30	28	23	VAL	3.0
1	1A	2125	G	3.0
1	2A	2108	C	3.0
54	2w	47	U	3.0
7	2H	64	LEU	3.0
36	2e	12	LEU	3.0
40	2i	122	ALA	3.0
7	2H	97	ARG	3.0
41	2j	9	ARG	3.0
35	2d	8	VAL	2.9
21	2Z	124	ILE	2.9
32	1a	1452	C	2.9
32	2a	1022	G	2.9
32	2a	1028	C	2.9
7	2H	150	ALA	2.9
14	2S	20	ARG	2.9
47	1p	6	LEU	2.9
52	1u	15	ARG	2.9
26	24	45	GLY	2.9
54	1w	14	A	2.9
44	2m	64	TRP	2.9
31	29	15	LYS	2.9
48	1q	100	LYS	2.9
1	2A	2132	U	2.9
32	1a	841	U	2.9
33	2b	105	PHE	2.9
33	2b	127	ILE	2.9
44	2m	84	ILE	2.9
48	1q	99	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	1A	2177	C	2.9
1	1A	2121	G	2.9
21	2Z	162	GLU	2.9
32	2a	1223	C	2.9
34	2c	178	LEU	2.9
41	2j	20	ALA	2.9
51	1t	13	LEU	2.9
15	2T	28	VAL	2.9
54	2w	14	A	2.9
38	2g	6	ARG	2.9
50	2s	56	GLN	2.9
1	1A	2137	C	2.9
31	29	8	LYS	2.9
57	1y	6	G	2.9
7	2H	144	VAL	2.9
21	2Z	105	VAL	2.9
33	2b	41	ILE	2.9
50	2s	48	THR	2.9
12	1Q	6	ARG	2.9
23	11	93	GLU	2.9
44	2m	104	ARG	2.9
57	2y	70	G	2.9
1	1A	899	A	2.9
7	2H	78	GLY	2.9
32	2a	1357	A	2.9
57	1y	51	U	2.9
40	2i	123	PRO	2.9
6	2G	181	ARG	2.9
7	2H	167	GLU	2.9
1	2A	645	C	2.9
1	2A	2188	C	2.9
52	1u	18	TYR	2.9
55	1x	67	C	2.9
1	1A	2100	G	2.9
34	1c	14	ILE	2.9
38	2g	27	ILE	2.9
48	1q	36	ILE	2.9
55	1x	47	U	2.9
45	2n	14	PRO	2.9
1	2A	898	C	2.8
7	2H	93	GLY	2.8
34	2c	138	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
40	2i	107	ARG	2.8
51	1t	83	ARG	2.8
51	2t	83	ARG	2.8
1	1A	1078	U	2.8
33	2b	201	ILE	2.8
45	1n	15	LYS	2.8
50	1s	40	ILE	2.8
1	2A	2106	G	2.8
1	2A	2121	G	2.8
1	2A	2162	G	2.8
32	1a	195	A	2.8
54	2w	5	G	2.8
57	2y	69	G	2.8
4	2E	148	GLY	2.8
21	2Z	100	VAL	2.8
26	24	10	VAL	2.8
40	1i	78	LYS	2.8
1	2A	2183	C	2.8
40	2i	124	GLN	2.8
7	2H	154	PRO	2.8
36	1e	84	PHE	2.8
45	1n	36	PHE	2.8
41	2j	64	GLU	2.8
32	2a	977	A	2.8
40	1i	11	LYS	2.8
57	1y	27	G	2.8
35	1d	38	TYR	2.8
42	2k	25	TYR	2.8
32	2a	1008	C	2.8
51	1t	60	GLU	2.8
4	2E	52	LEU	2.8
6	2G	133	LEU	2.8
14	2S	5	THR	2.8
40	1i	7	THR	2.8
51	2t	12	ALA	2.8
41	2j	7	LYS	2.8
50	2s	15	LEU	2.8
41	2j	31	GLY	2.8
1	2A	899	A	2.8
10	2O	1	MET	2.8
1	2A	2318	G	2.8
34	2c	195	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
34	2c	124	ILE	2.8
57	2y	59	U	2.8
34	2c	129	ALA	2.8
54	1w	4	C	2.8
54	2w	49	C	2.8
51	1t	45	GLN	2.8
33	2b	48	MET	2.8
1	1A	2173	A	2.8
7	2H	13	LYS	2.8
7	2H	54	ARG	2.8
45	2n	21	TYR	2.8
48	1q	95	TYR	2.8
32	1a	307	C	2.8
35	2d	135	LEU	2.8
29	27	1	MET	2.8
51	2t	73	HIS	2.8
53	1v	24	A	2.8
51	1t	18	GLN	2.8
34	2c	24	ALA	2.8
40	2i	72	GLY	2.8
41	1j	4	ILE	2.8
34	2c	196	LEU	2.8
54	2w	22	G	2.8
7	2H	56	SER	2.8
11	2P	76	LYS	2.8
22	20	44	ARG	2.8
34	1c	179	ARG	2.8
38	1g	78	ARG	2.8
8	1I	19	VAL	2.7
32	1a	223	U	2.7
40	2i	4	TYR	2.7
26	14	59	PHE	2.7
7	2H	88	LEU	2.7
28	26	11	LEU	2.7
46	1o	57	LEU	2.7
45	2n	3	ARG	2.7
32	1a	1039	C	2.7
32	2a	1045	C	2.7
57	2y	48	C	2.7
40	2i	39	GLY	2.7
1	2A	2897	U	2.7
7	2H	151	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
26	24	67	TYR	2.7
43	2l	30	ALA	2.7
39	1h	112	LEU	2.7
39	2h	112	LEU	2.7
21	2Z	94	GLU	2.7
11	2P	28	GLY	2.7
21	1Z	141	VAL	2.7
48	1q	9	VAL	2.7
31	29	9	ARG	2.7
30	28	55	ALA	2.7
36	2e	131	ILE	2.7
39	1h	134	ILE	2.7
44	1m	103	THR	2.7
21	2Z	66	SER	2.7
32	1a	1004	A	2.7
32	2a	999	C	2.7
40	2i	20	ARG	2.7
41	2j	94	VAL	2.7
47	1p	2	VAL	2.7
1	2A	2155	G	2.7
33	2b	207	ALA	2.7
44	2m	103	THR	2.7
17	2V	71	LEU	2.7
40	2i	102	LEU	2.7
44	2m	92	HIS	2.7
1	1A	1054	A	2.7
21	2Z	50	GLN	2.7
32	2a	1259	C	2.7
32	2a	90	U	2.7
32	2a	1020	U	2.7
2	2B	89	G	2.7
41	2j	50	ILE	2.7
45	1n	6	LEU	2.7
31	29	21	GLY	2.7
38	2g	31	MET	2.7
1	1A	1509(A)	A	2.7
1	2A	1032	A	2.7
26	24	18	CYS	2.7
40	2i	73	GLN	2.7
3	2D	18	VAL	2.7
1	2A	2180	U	2.7
12	2Q	112	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
7	2H	67	LEU	2.7
12	2Q	104	PHE	2.7
40	2i	121	ARG	2.7
48	2q	59	ILE	2.7
50	1s	14	HIS	2.7
3	1D	38	LYS	2.7
26	24	54	GLY	2.7
32	1a	216	G	2.7
40	1i	28	VAL	2.6
38	2g	41	ARG	2.6
7	2H	175	LYS	2.6
1	2A	2752	C	2.6
21	1Z	150	LEU	2.6
32	1a	1038	C	2.6
38	2g	84	ASN	2.6
54	1w	67	C	2.6
31	29	34	GLN	2.6
40	1i	4	TYR	2.6
32	2a	485	G	2.6
35	2d	73	ARG	2.6
47	1p	25	ARG	2.6
51	2t	86	ARG	2.6
21	2Z	92	SER	2.6
26	14	64	GLY	2.6
34	2c	3	ASN	2.6
44	1m	4	ILE	2.6
50	1s	10	PHE	2.6
31	29	28	GLU	2.6
32	1a	218	C	2.6
7	2H	83	TYR	2.6
52	2u	21	TYR	2.6
7	2H	30	LYS	2.6
29	27	47	ARG	2.6
1	1A	2124	G	2.6
7	2H	26	VAL	2.6
32	1a	1009	G	2.6
32	2a	1224	G	2.6
38	1g	135	VAL	2.6
57	2y	10	G	2.6
44	2m	12	ASN	2.6
6	2G	135	LEU	2.6
45	2n	47	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
7	1H	4	ILE	2.6
41	2j	6	ILE	2.6
45	2n	54	PRO	2.6
12	2Q	10	ARG	2.6
41	2j	43	ARG	2.6
51	2t	38	LYS	2.6
1	2A	1118	C	2.6
21	1Z	149	SER	2.6
5	1F	89	VAL	2.6
36	1e	69	VAL	2.6
51	1t	66	ALA	2.6
1	1A	1176	G	2.6
1	2A	2104	G	2.6
40	2i	70	LYS	2.6
54	2w	69	G	2.6
57	2y	12	U	2.6
47	1p	66	PRO	2.6
1	2A	1041	C	2.6
45	1n	8	GLU	2.6
12	2Q	27	VAL	2.6
45	2n	26	ARG	2.6
46	2o	65	ARG	2.6
32	1a	1020	U	2.6
7	2H	109	PHE	2.6
35	2d	158	ILE	2.6
1	1A	1075	C	2.6
51	1t	47	GLY	2.6
57	2y	11	C	2.6
34	2c	59	ARG	2.6
48	1q	35	VAL	2.6
7	2H	18	GLU	2.6
21	2Z	133	ILE	2.6
34	2c	134	ILE	2.6
32	2a	1250	A	2.6
41	2j	12	ASP	2.6
45	2n	29	ARG	2.6
8	1I	41	GLU	2.6
32	2a	1116	C	2.6
4	2E	195	LEU	2.5
14	2S	54	LEU	2.5
16	2U	2	PRO	2.5
43	1l	43	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
34	2c	32	LEU	2.5
51	1t	14	LYS	2.5
51	2t	72	LEU	2.5
41	2j	38	ILE	2.5
45	1n	7	ILE	2.5
11	2P	118	GLY	2.5
34	2c	145	GLY	2.5
43	1l	14	GLY	2.5
1	2A	2750	A	2.5
1	2A	1042	G	2.5
7	2H	164	TYR	2.5
22	20	5	LYS	2.5
25	23	15	TYR	2.5
32	2a	1256	A	2.5
6	2G	17	PRO	2.5
6	2G	160	VAL	2.5
45	1n	39	LEU	2.5
50	2s	45	VAL	2.5
1	1A	2122	U	2.5
1	2A	9	U	2.5
33	2b	214	ILE	2.5
35	2d	5	ILE	2.5
7	2H	34	GLU	2.5
34	2c	19	GLU	2.5
48	1q	27	PHE	2.5
33	1b	75	LYS	2.5
43	2l	13	LYS	2.5
47	1p	59	TRP	2.5
35	1d	138	TYR	2.5
41	2j	87	THR	2.5
43	1l	61	THR	2.5
43	2l	69	TYR	2.5
57	1y	64	A	2.5
7	2H	86	GLU	2.5
8	2I	75	LEU	2.5
22	20	74	ARG	2.5
33	2b	118	LEU	2.5
34	1c	52	LEU	2.5
41	1j	66	ARG	2.5
41	2j	61	GLU	2.5
4	2E	197	ILE	2.5
20	2Y	75	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
34	2c	2	GLY	2.5
40	2i	57	GLY	2.5
48	2q	80	GLY	2.5
38	2g	86	GLN	2.5
7	2H	39	PRO	2.5
42	1k	75	TYR	2.5
1	1A	1067	A	2.5
21	2Z	58	VAL	2.5
21	2Z	154	ASP	2.5
39	1h	133	LEU	2.5
39	2h	26	VAL	2.5
40	2i	75	ASP	2.5
32	1a	217	C	2.5
31	29	10	ILE	2.5
32	2a	1156	G	2.5
32	2a	1197	G	2.5
32	2a	1385	G	2.5
57	1y	63	G	2.5
8	1I	117	GLU	2.5
40	1i	10	ARG	2.5
40	2i	104	ARG	2.5
51	1t	86	ARG	2.5
20	2Y	65	ALA	2.5
21	2Z	70	LEU	2.5
34	1c	184	TYR	2.5
34	2c	159	GLY	2.5
40	2i	5	TYR	2.5
43	2l	43	VAL	2.5
50	2s	58	VAL	2.5
1	1A	898	C	2.5
34	1c	8	ILE	2.5
40	2i	63	ILE	2.5
34	2c	21	ARG	2.5
40	1i	20	ARG	2.5
45	1n	17	LYS	2.5
54	2w	10	G	2.5
5	2F	80	ALA	2.5
12	2Q	126	PRO	2.5
7	2H	70	THR	2.5
14	2S	32	LEU	2.5
31	29	3	VAL	2.5
33	1b	19	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
35	2d	11	LEU	2.5
7	2H	152	ARG	2.5
1	1A	655	A	2.5
1	1A	2126	A	2.5
7	2H	162	ILE	2.5
35	1d	158	ILE	2.5
50	2s	6	LYS	2.5
32	1a	221	C	2.5
57	2y	40	C	2.5
1	2A	880	G	2.5
1	2A	1533	G	2.5
1	2A	2319	G	2.5
6	2G	121	ASN	2.5
32	1a	70	G	2.5
33	1b	128	GLU	2.5
6	2G	152	LEU	2.4
50	1s	71	LEU	2.4
8	2I	92	VAL	2.4
33	2b	31	TYR	2.4
6	2G	140	ILE	2.4
32	1a	1030(D)	A	2.4
6	1G	48	GLU	2.4
7	2H	46	GLU	2.4
7	2H	74	ASN	2.4
32	2a	980	C	2.4
54	1w	13	C	2.4
54	2w	13	C	2.4
34	2c	163	ALA	2.4
35	2d	82	ALA	2.4
6	2G	182	LYS	2.4
44	2m	71	ARG	2.4
1	2A	2101	G	2.4
54	1w	5	G	2.4
54	2w	15	G	2.4
57	1y	69	G	2.4
11	1P	71	VAL	2.4
41	2j	34	VAL	2.4
1	1A	1026	U	2.4
1	2A	2122	U	2.4
1	2A	2172	U	2.4
32	2a	1196	U	2.4
36	2e	8	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
38	2g	30	ILE	2.4
41	2j	86	MET	2.4
1	1A	2790	A	2.4
35	2d	115	ARG	2.4
41	1j	18	ALA	2.4
9	2N	116	LEU	2.4
33	1b	233	SER	2.4
32	2a	1000	U	2.4
40	2i	127	LYS	2.4
7	2H	65	HIS	2.4
32	2a	969	A	2.4
7	2H	87	LEU	2.4
9	2N	87	LEU	2.4
51	1t	61	SER	2.4
43	2l	90	VAL	2.4
1	2A	271(K)	U	2.4
1	2A	877	U	2.4
11	2P	79	ARG	2.4
21	2Z	3	TYR	2.4
45	1n	34	TYR	2.4
1	1A	882	G	2.4
1	1A	1074	G	2.4
1	2A	1115	G	2.4
45	1n	61	TRP	2.4
7	2H	122	THR	2.4
26	14	66	SER	2.4
18	2W	92	ARG	2.4
32	2a	1014	A	2.4
32	2a	1119	C	2.4
34	2c	30	ARG	2.4
57	2y	49	C	2.4
36	2e	90	VAL	2.4
11	2P	93	GLY	2.4
34	1c	78	GLY	2.4
41	1j	36	GLY	2.4
6	2G	157	ILE	2.4
40	2i	81	ILE	2.4
47	1p	4	ILE	2.4
7	2H	36	PRO	2.4
40	2i	78	LYS	2.4
35	2d	49	ARG	2.4
46	1o	68	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
6	2G	62	LEU	2.4
1	2A	2178	C	2.4
12	2Q	94	VAL	2.4
32	1a	470	C	2.4
33	2b	71	VAL	2.4
34	1c	206	GLU	2.4
40	2i	30	GLY	2.4
43	2l	28	LYS	2.4
6	2G	142	PRO	2.4
21	2Z	136	PHE	2.4
26	14	63	TYR	2.4
33	2b	70	PHE	2.4
36	2e	24	ARG	2.4
8	1I	40	THR	2.4
40	1i	64	THR	2.4
18	2W	112	GLY	2.3
17	2V	72	VAL	2.3
32	1a	194	C	2.3
32	1a	219	C	2.3
41	2j	91	PRO	2.3
15	2T	129	ARG	2.3
43	2l	70	ILE	2.3
34	2c	184	TYR	2.3
35	1d	110	PHE	2.3
7	2H	85	LYS	2.3
9	1N	138	LEU	2.3
35	2d	23	GLY	2.3
1	1A	2101	G	2.3
32	1a	182	U	2.3
32	1a	184	G	2.3
32	2a	1009	G	2.3
39	1h	95	VAL	2.3
45	1n	12	ARG	2.3
50	2s	83	HIS	2.3
52	2u	24	ARG	2.3
57	1y	65	G	2.3
40	2i	49	PRO	2.3
9	2N	1	MET	2.3
32	1a	72	C	2.3
32	1a	1041	A	2.3
32	2a	91	C	2.3
51	1t	85	MET	2.3

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Mol	Chain	Res	Type	RSRZ
36	1e	95	ALA	2.3
40	2i	71	SER	2.3
7	2H	100	GLY	2.3
33	1b	221	LEU	2.3
12	2Q	41	TRP	2.3
34	2c	176	HIS	2.3
7	2H	126	PRO	2.3
47	1p	62	VAL	2.3
35	1d	85	LYS	2.3
57	2y	50	U	2.3
1	1A	2804	C	2.3
1	2A	2474	C	2.3
15	2T	101	PHE	2.3
32	2a	1019	C	2.3
57	1y	49	C	2.3
51	1t	40	ALA	2.3
38	1g	82	GLY	2.3
21	1Z	155	LEU	2.3
38	1g	3	ARG	2.3
32	2a	961	U	2.3
6	2G	39	ILE	2.3
17	2V	92	THR	2.3
21	1Z	122	ARG	2.3
34	2c	190	ARG	2.3
40	1i	67	GLY	2.3
45	2n	41	ARG	2.3
51	2t	76	ALA	2.3
32	1a	97	G	2.3
3	1D	275	LYS	2.3
45	2n	15	LYS	2.3
9	2N	9	VAL	2.3
20	2Y	45	VAL	2.3
25	23	6	VAL	2.3
32	1a	96	U	2.3
15	2T	128	GLU	2.3
46	1o	64	ARG	2.3
50	2s	53	ASN	2.3
41	1j	11	PHE	2.3
42	1k	88	GLY	2.3
50	1s	38	SER	2.3
51	2t	47	GLY	2.3
29	27	24	THR	2.3

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Mol	Chain	Res	Type	RSRZ
38	2g	24	THR	2.3
41	2j	89	ASP	2.3
52	1u	21	TYR	2.3
1	2A	2749	A	2.3
32	2a	1251	A	2.3
32	2a	1258	G	2.3
52	2u	23	PRO	2.3
34	2c	179	ARG	2.3
7	2H	41	MET	2.3
4	2E	176	ILE	2.3
16	2U	62	ILE	2.3
21	1Z	133	ILE	2.3
36	2e	48	ALA	2.3
50	2s	34	TRP	2.3
33	1b	126	GLU	2.3
34	1c	12	LEU	2.3
35	1d	135	LEU	2.3
39	2h	65	TYR	2.3
47	1p	17	TYR	2.3
52	2u	18	TYR	2.3
15	1T	111	ARG	2.2
29	27	23	ARG	2.2
32	2a	1447	A	2.2
1	1A	883	G	2.2
32	1a	1021	G	2.2
21	1Z	165	VAL	2.2
34	2c	194	GLY	2.2
42	2k	14	VAL	2.2
21	2Z	98	MET	2.2
57	1y	50	U	2.2
8	2I	79	ILE	2.2
38	2g	42	ILE	2.2
26	14	57	GLU	2.2
40	1i	110	GLU	2.2
40	2i	12	GLU	2.2
21	2Z	72	ARG	2.2
44	2m	13	LYS	2.2
44	2m	88	ARG	2.2
45	1n	44	LEU	2.2
47	1p	39	TYR	2.2
48	2q	75	ARG	2.2
21	2Z	95	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
42	2k	117	ASN	2.2
15	2T	30	VAL	2.2
32	1a	161	A	2.2
36	1e	85	GLY	2.2
1	2A	11	G	2.2
57	2y	22	G	2.2
39	2h	111	ILE	2.2
41	1j	23	ILE	2.2
20	2Y	54	LYS	2.2
35	2d	110	PHE	2.2
41	1j	45	ARG	2.2
34	2c	18	TRP	2.2
35	2d	196	LEU	2.2
44	2m	97	PRO	2.2
46	1o	69	TYR	2.2
7	2H	174	GLY	2.2
12	2Q	86	GLY	2.2
34	2c	62	ASP	2.2
40	1i	115	GLY	2.2
29	17	46	VAL	2.2
40	1i	17	VAL	2.2
1	2A	901	A	2.2
32	1a	101	A	2.2
32	2a	1015	A	2.2
6	2G	136	ARG	2.2
26	14	58	ARG	2.2
26	14	68	ARG	2.2
33	2b	211	ILE	2.2
34	2c	200	ALA	2.2
40	1i	76	ALA	2.2
36	2e	45	PHE	2.2
1	2A	879	G	2.2
34	2c	188	LEU	2.2
35	1d	37	PRO	2.2
8	1I	20	ASP	2.2
33	2b	72	GLY	2.2
35	2d	2	GLY	2.2
41	2j	52	GLY	2.2
14	2S	93	LYS	2.2
43	1l	90	VAL	2.2
4	2E	134	ILE	2.2
42	2k	13	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
14	2S	11	LYS	2.2
16	2U	16	LYS	2.2
40	1i	116	LYS	2.2
41	2j	99	LYS	2.2
1	1A	2187	G	2.2
12	2Q	60	ARG	2.2
26	24	48	ARG	2.2
44	1m	87	TYR	2.2
23	21	38	SER	2.2
7	2H	111	HIS	2.2
12	2Q	106	VAL	2.2
44	2m	98	VAL	2.2
33	2b	237	ALA	2.2
12	2Q	66	ILE	2.2
36	1e	118	ILE	2.2
41	2j	75	ILE	2.2
50	2s	77	THR	2.2
1	1A	1847	A	2.2
7	2H	31	GLY	2.2
21	2Z	5	LEU	2.2
45	2n	19	ARG	2.2
1	1A	892	G	2.2
1	2A	2751	G	2.2
32	2a	1042	G	2.2
33	2b	124	SER	2.2
45	1n	32	SER	2.2
31	29	1	MET	2.2
1	1A	1175	U	2.2
4	2E	104	VAL	2.2
44	2m	117	VAL	2.2
23	21	15	ALA	2.2
1	1A	1072	C	2.2
32	1a	1137	C	2.2
11	1P	44	GLY	2.2
43	2l	32	PHE	2.2
52	1u	11	GLY	2.2
33	1b	232	PRO	2.2
33	2b	69	LEU	2.2
7	2H	90	LYS	2.1
21	2Z	23	LYS	2.1
7	2H	163	TYR	2.1
44	2m	28	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
35	2d	47	ARG	2.1
35	2d	122	ARG	2.1
9	2N	71	ILE	2.1
1	1A	2803	C	2.1
33	1b	134	GLU	2.1
33	2b	116	GLU	2.1
34	2c	7	PRO	2.1
1	1A	529	A	2.1
38	1g	20	ASP	2.1
7	2H	130	ARG	2.1
22	20	77	ARG	2.1
35	2d	112	VAL	2.1
41	1j	60	ARG	2.1
32	2a	1219	U	2.1
51	2t	28	ALA	2.1
1	1A	1093	G	2.1
1	1A	1099	G	2.1
1	1A	2793	G	2.1
1	2A	2807	G	2.1
41	2j	41	PRO	2.1
24	12	21	LEU	2.1
30	28	60	LEU	2.1
40	2i	79	LEU	2.1
1	2A	2105	C	2.1
57	2y	41	C	2.1
25	23	30	ARG	2.1
32	1a	1503	A	2.1
32	2a	983	A	2.1
41	1j	9	ARG	2.1
50	2s	66	MET	2.1
7	2H	108	GLY	2.1
1	1A	1963	U	2.1
8	2I	89	TYR	2.1
40	1i	61	ALA	2.1
46	2o	69	TYR	2.1
52	1u	17	THR	2.1
4	2E	32	PRO	2.1
33	2b	170	GLU	2.1
40	2i	16	ARG	2.1
50	2s	69	HIS	2.1
51	1t	73	HIS	2.1
1	2A	1040	C	2.1

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Mol	Chain	Res	Type	RSRZ
57	1y	72	C	2.1
42	2k	86	GLY	2.1
7	2H	73	ALA	2.1
21	2Z	68	PRO	2.1
40	2i	7	THR	2.1
15	2T	86	ILE	2.1
40	1i	63	ILE	2.1
40	2i	77	ILE	2.1
3	1D	131	LEU	2.1
33	2b	51	LEU	2.1
35	2d	139	ARG	2.1
7	2H	66	GLY	2.1
32	2a	1017	G	2.1
32	2a	1284	C	2.1
40	1i	6	GLY	2.1
51	2t	90	GLN	2.1
1	2A	861	A	2.1
1	2A	2176	A	2.1
21	1Z	170	THR	2.1
33	2b	164	VAL	2.1
34	2c	161	GLU	2.1
35	1d	207	TYR	2.1
47	1p	41	PRO	2.1
18	2W	96	ILE	2.1
51	2t	100	ILE	2.1
6	2G	43	LEU	2.1
7	2H	84	SER	2.1
22	10	57	PHE	2.1
41	2j	68	HIS	2.1
43	2l	62	SER	2.1
50	1s	16	LEU	2.1
51	2t	99	LEU	2.1
18	2W	60	ASN	2.1
34	1c	2	GLY	2.1
46	1o	89	GLY	2.1
47	1p	65	GLN	2.1
21	2Z	2	GLU	2.1
32	2a	470	C	2.1
32	2a	1326	C	2.1
41	1j	97	GLU	2.1
6	2G	50	ALA	2.1
7	2H	62	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
7	2H	107	VAL	2.1
26	24	29	PRO	2.1
32	1a	378	G	2.1
34	2c	60	ALA	2.1
28	26	21	TYR	2.1
35	2d	68	TYR	2.1
4	2E	77	ILE	2.1
47	1p	33	ILE	2.1
48	1q	90	ILE	2.1
4	2E	5	LEU	2.1
14	2S	12	PHE	2.1
51	1t	91	LEU	2.1
51	2t	24	LEU	2.1
51	2t	53	LEU	2.1
34	2c	206	GLU	2.1
42	2k	17	GLY	2.1
21	2Z	79	ARG	2.1
45	2n	9	LYS	2.1
20	2Y	78	ALA	2.0
34	1c	189	ALA	2.0
38	2g	117	ALA	2.0
32	2a	1278	U	2.0
36	1e	51	VAL	2.0
48	1q	73	VAL	2.0
1	2A	1039	G	2.0
1	2A	2310	A	2.0
6	2G	60	LEU	2.0
32	1a	171	A	2.0
35	2d	157	LEU	2.0
35	2d	188	LEU	2.0
34	2c	197	GLY	2.0
40	1i	24	GLY	2.0
54	2w	38	A	2.0
19	1X	68	ARG	2.0
28	26	50	ARG	2.0
16	1U	69	CYS	2.0
7	2H	57	ASP	2.0
11	2P	129	ALA	2.0
39	1h	67	PRO	2.0
1	1A	1053	C	2.0
18	2W	47	VAL	2.0
22	10	3	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
31	29	7	VAL	2.0
32	1a	1006	C	2.0
32	2a	1260	C	2.0
32	2a	1446	U	2.0
36	2e	20	GLN	2.0
56	1z	4	SER	2.0
38	1g	30	ILE	2.0
11	2P	77	ARG	2.0
40	2i	101	PHE	2.0
45	1n	41	ARG	2.0
32	2a	1202	G	2.0
4	2E	1	MET	2.0
31	29	14	CYS	2.0
33	2b	85	ALA	2.0
38	2g	108	ALA	2.0
47	2p	12	LYS	2.0
40	2i	41	VAL	2.0
1	1A	2105	C	2.0
2	2B	3	C	2.0
26	24	17	GLY	2.0
32	1a	201	C	2.0
46	2o	89	GLY	2.0
21	2Z	91	LEU	2.0
33	1b	222	ILE	2.0
34	1c	101	LEU	2.0
44	1m	90	LEU	2.0
44	2m	90	LEU	2.0
48	1q	60	ILE	2.0
40	2i	18	PHE	2.0
38	2g	8	GLU	2.0
1	2A	2893	G	2.0
12	2Q	18	LYS	2.0
57	1y	26	A	2.0
34	2c	162	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
57	PSU	1y	55	20/21	0.60	0.50	98,101,103,116	0
57	MIA	2y	37	22/30	0.63	0.62	89,98,112,126	0
57	4SU	2y	8	20/21	0.64	0.29	97,104,109,125	0
57	PSU	2y	32	20/21	0.67	0.46	93,97,103,116	0
56	FME	1z	1	10/11	0.70	0.50	61,66,74,77	0
57	PSU	2y	55	20/21	0.71	0.41	94,99,102,107	0
57	5MU	1y	54	21/22	0.73	0.48	93,97,101,116	0
57	4SU	1y	8	20/21	0.74	0.31	98,100,110,115	0
57	G7M	1y	46	24/25	0.75	0.34	95,99,103,112	0
57	MIA	1y	37	22/30	0.76	0.57	89,96,105,116	0
56	FME	2z	1	10/11	0.76	0.63	70,75,82,82	0
57	G7M	2y	46	24/25	0.77	0.24	91,99,107,122	0
57	5MU	2y	54	21/22	0.79	0.49	96,100,108,126	0
54	G7M	2w	46	24/25	0.79	0.26	88,96,107,121	0
54	G7M	1w	46	24/25	0.80	0.18	79,86,100,116	0
54	4SU	2w	8	20/21	0.81	0.22	91,94,108,111	0
57	PSU	1y	39	20/21	0.81	0.40	88,94,106,106	0
57	PSU	2y	39	20/21	0.82	0.47	91,97,105,115	0
57	PSU	1y	32	20/21	0.82	0.36	90,93,105,108	0
54	PSU	2w	55	20/21	0.86	0.15	84,86,95,101	0
54	PSU	1w	55	20/21	0.87	0.19	60,73,84,85	0
54	4SU	1w	8	20/21	0.87	0.25	82,88,93,97	0
32	2MG	2a	1207	24/25	0.87	0.21	74,84,86,88	0
54	MIA	2w	37	25/30	0.89	0.29	63,75,83,105	0
55	PSU	1x	55	20/21	0.89	0.14	63,68,82,85	0
54	MIA	1w	37	29/30	0.90	0.33	56,63,77,92	0
32	PSU	2a	516	20/21	0.91	0.19	60,73,77,78	0
55	4SU	2x	8	20/21	0.91	0.16	79,82,85,87	0
55	PSU	2x	55	20/21	0.91	0.15	74,79,86,88	0
43	0TD	2l	92	10/11	0.92	0.20	64,67,70,75	0
54	5MU	2w	54	21/22	0.92	0.17	75,83,86,92	0
54	PSU	2w	32	20/21	0.93	0.24	75,82,86,89	0
55	5MU	2x	54	21/22	0.93	0.24	76,81,85,88	0
54	PSU	1w	32	20/21	0.93	0.17	59,65,74,75	0
54	PSU	2w	39	20/21	0.93	0.30	68,79,86,89	0
55	5MU	1x	54	21/22	0.94	0.16	66,70,75,81	0
43	0TD	1l	92	10/11	0.94	0.19	51,56,58,71	0
32	5MC	1a	967	21/22	0.94	0.20	49,56,62,63	0
54	5MU	1w	54	21/22	0.94	0.15	52,63,67,69	0
32	2MG	1a	1207	24/25	0.94	0.16	70,73,77,80	0
32	M2G	2a	966	25/26	0.94	0.26	61,67,76,80	0
32	5MC	2a	967	21/22	0.94	0.21	62,69,75,82	0
55	5MC	1x	32	21/22	0.95	0.19	56,60,66,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	PSU	1a	516	20/21	0.95	0.15	55,61,66,67	0
32	5MC	2a	1404	21/22	0.95	0.20	47,55,59,63	0
32	MA6	2a	1518	24/25	0.95	0.20	53,63,69,70	0
1	PSU	2A	1911	20/21	0.95	0.14	53,58,63,63	0
1	5MU	1A	1915	21/22	0.95	0.18	47,56,60,61	0
1	PSU	1A	1917	20/21	0.95	0.16	52,56,60,61	0
1	PSU	2A	1917	20/21	0.95	0.15	57,64,71,75	0
1	5MC	2A	1962	21/22	0.95	0.18	43,52,60,68	0
32	G7M	2a	527	24/25	0.95	0.20	61,68,71,74	0
55	4SU	1x	8	20/21	0.95	0.16	62,68,70,71	0
32	5MC	2a	1407	21/22	0.96	0.18	51,57,65,68	0
32	M2G	1a	966	25/26	0.96	0.22	51,55,63,66	0
32	MA6	2a	1519	24/25	0.96	0.23	55,62,65,66	0
1	5MU	2A	1915	21/22	0.96	0.17	62,66,70,73	0
32	5MC	2a	1400	21/22	0.96	0.28	64,69,76,80	0
32	4OC	2a	1402	22/23	0.96	0.18	56,61,64,68	0
1	OMC	2A	1920	21/22	0.96	0.19	49,60,64,67	0
1	5MC	2A	1942	21/22	0.96	0.18	53,59,65,71	0
54	F3N	2w	76	33/34	0.96	0.24	41,47,51,52	0
1	2MU	2A	2552	21/23	0.96	0.20	39,50,54,57	0
54	PSU	1w	39	20/21	0.96	0.25	61,66,76,78	0
55	5MC	2x	32	21/22	0.96	0.19	68,72,76,77	0
32	MA6	1a	1518	24/25	0.97	0.23	39,45,49,51	0
1	OMC	1A	1920	21/22	0.97	0.20	39,49,52,55	0
32	MA6	1a	1519	24/25	0.97	0.20	40,46,53,56	0
55	8AN	2x	76	22/23	0.97	0.20	41,48,54,61	0
55	8AN	1x	76	22/23	0.97	0.21	22,30,37,48	0
32	G7M	1a	527	24/25	0.97	0.18	49,56,61,63	0
1	PSU	2A	2605	20/21	0.97	0.20	36,43,50,52	0
32	UR3	2a	1498	21/22	0.97	0.23	53,58,62,63	0
32	5MC	1a	1400	21/22	0.97	0.20	49,56,59,63	0
1	5MU	1A	1939	21/22	0.98	0.21	25,33,37,39	0
1	5MU	2A	1939	21/22	0.98	0.20	35,43,49,51	0
1	5MC	1A	1942	21/22	0.98	0.20	35,45,49,56	0
32	UR3	1a	1498	21/22	0.98	0.22	39,45,50,52	0
1	5MC	1A	1962	21/22	0.98	0.20	31,40,43,49	0
32	4OC	1a	1402	22/23	0.98	0.19	44,50,52,53	0
1	OMG	2A	2251	24/25	0.98	0.19	39,46,49,58	0
1	8AH	1A	2503	24/25	0.98	0.23	21,29,33,37	0
1	8AH	2A	2503	24/25	0.98	0.22	39,44,48,52	0
32	5MC	1a	1404	21/22	0.98	0.20	38,45,49,50	0
1	PSU	1A	2605	20/21	0.98	0.20	27,32,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	F3N	1w	76	33/34	0.98	0.25	24,29,34,36	0
1	PSU	1A	1911	20/21	0.98	0.15	43,51,58,58	0
32	5MC	1a	1407	21/22	0.98	0.20	42,46,49,52	0
1	2MU	1A	2552	21/23	0.99	0.20	25,32,35,37	0
1	OMG	1A	2251	24/25	0.99	0.22	25,29,31,33	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(\AA^2)	Q<0.9
58	MG	2A	3395	1/1	0.12	0.36	88,88,88,88	0
58	MG	2A	3697	1/1	0.15	0.12	75,75,75,75	0
58	MG	1A	4009	1/1	0.18	0.10	60,60,60,60	0
58	MG	2A	3800	1/1	0.33	0.16	70,70,70,70	0
58	MG	2a	1714	1/1	0.34	0.20	69,69,69,69	0
58	MG	1A	3917	1/1	0.35	0.11	76,76,76,76	0
58	MG	1a	1811	1/1	0.35	0.17	76,76,76,76	0
58	MG	1A	3993	1/1	0.37	0.26	80,80,80,80	0
58	MG	2a	1747	1/1	0.37	0.18	83,83,83,83	0
58	MG	2v	102	1/1	0.38	0.20	87,87,87,87	0
58	MG	1A	3734	1/1	0.41	0.19	56,56,56,56	0
58	MG	1A	4029	1/1	0.42	0.23	68,68,68,68	0
58	MG	20	101	1/1	0.43	0.32	73,73,73,73	0
58	MG	2A	3185	1/1	0.44	0.23	85,85,85,85	0
58	MG	1a	1817	1/1	0.45	0.09	81,81,81,81	0
58	MG	2A	3228	1/1	0.47	0.23	67,67,67,67	0
58	MG	1A	4036	1/1	0.48	0.28	58,58,58,58	0
58	MG	1A	3761	1/1	0.48	0.25	79,79,79,79	0
58	MG	1A	3878	1/1	0.48	0.06	81,81,81,81	0
58	MG	2A	3605	1/1	0.49	0.30	87,87,87,87	0
58	MG	1A	3905	1/1	0.50	0.16	58,58,58,58	0
58	MG	1A	3469	1/1	0.50	0.26	73,73,73,73	0
58	MG	1T	203	1/1	0.51	0.37	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	2A	3604	1/1	0.51	0.12	83,83,83,83	0
58	MG	2A	3321	1/1	0.51	0.15	77,77,77,77	0
58	MG	2A	3817	1/1	0.52	0.08	78,78,78,78	0
58	MG	2A	3187	1/1	0.52	0.29	76,76,76,76	0
58	MG	2a	1704	1/1	0.52	0.22	78,78,78,78	0
58	MG	1A	3160	1/1	0.52	0.22	60,60,60,60	0
58	MG	1A	3291	1/1	0.52	0.18	58,58,58,58	0
58	MG	1A	3748	1/1	0.52	0.20	71,71,71,71	0
58	MG	2A	3327	1/1	0.53	0.23	74,74,74,74	0
58	MG	1A	4027	1/1	0.53	0.45	80,80,80,80	0
58	MG	2A	3284	1/1	0.53	0.20	68,68,68,68	0
58	MG	1A	3946	1/1	0.53	0.14	86,86,86,86	0
58	MG	1a	1680	1/1	0.54	0.09	75,75,75,75	0
58	MG	1a	1601	1/1	0.55	0.14	76,76,76,76	0
58	MG	2A	3487	1/1	0.55	0.20	86,86,86,86	0
58	MG	1S	203	1/1	0.55	0.14	77,77,77,77	0
58	MG	2A	3366	1/1	0.56	0.21	73,73,73,73	0
58	MG	1A	3979	1/1	0.56	0.13	68,68,68,68	0
58	MG	1w	103	1/1	0.56	0.18	87,87,87,87	0
58	MG	2a	1694	1/1	0.56	0.23	75,75,75,75	0
58	MG	2a	1679	1/1	0.57	0.18	64,64,64,64	0
58	MG	1a	1729	1/1	0.57	0.26	78,78,78,78	0
58	MG	2A	3551	1/1	0.57	0.21	66,66,66,66	0
58	MG	2A	3813	1/1	0.57	0.16	90,90,90,90	0
58	MG	1a	1672	1/1	0.57	0.17	74,74,74,74	0
58	MG	1A	3783	1/1	0.57	0.20	71,71,71,71	0
58	MG	1A	3616	1/1	0.58	0.24	44,44,44,44	0
58	MG	2A	3745	1/1	0.58	0.13	80,80,80,80	0
58	MG	1A	3542	1/1	0.58	0.59	69,69,69,69	0
58	MG	2A	3055	1/1	0.58	0.37	74,74,74,74	0
58	MG	2A	3356	1/1	0.58	0.25	71,71,71,71	0
58	MG	2A	3239	1/1	0.58	0.13	88,88,88,88	0
58	MG	2A	3180	1/1	0.59	0.19	78,78,78,78	0
58	MG	1A	3969	1/1	0.59	0.11	53,53,53,53	0
58	MG	2a	1605	1/1	0.59	0.23	75,75,75,75	0
58	MG	2A	3634	1/1	0.59	0.09	82,82,82,82	0
58	MG	1a	1759	1/1	0.59	0.09	81,81,81,81	0
58	MG	2A	3407	1/1	0.59	0.37	73,73,73,73	0
58	MG	2A	3751	1/1	0.59	0.12	55,55,55,55	0
58	MG	2a	1722	1/1	0.59	0.13	69,69,69,69	0
58	MG	2A	3324	1/1	0.59	0.14	82,82,82,82	0
58	MG	2A	3115	1/1	0.59	0.22	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3591	1/1	0.60	0.23	76,76,76,76	0
58	MG	1x	104	1/1	0.60	0.20	73,73,73,73	0
58	MG	1A	3889	1/1	0.60	0.10	69,69,69,69	0
58	MG	2B	208	1/1	0.60	0.15	76,76,76,76	0
58	MG	1A	4004	1/1	0.60	0.18	65,65,65,65	0
58	MG	1A	3493	1/1	0.60	0.26	71,71,71,71	0
58	MG	2a	1641	1/1	0.60	0.14	74,74,74,74	0
58	MG	1A	4096	1/1	0.61	0.13	53,53,53,53	0
58	MG	2A	3450	1/1	0.61	0.21	56,56,56,56	0
58	MG	1A	3325	1/1	0.61	0.37	70,70,70,70	0
58	MG	2a	1689	1/1	0.61	0.13	86,86,86,86	0
58	MG	2A	3497	1/1	0.61	0.38	77,77,77,77	0
58	MG	2A	3223	1/1	0.61	0.54	72,72,72,72	0
58	MG	2A	3094	1/1	0.61	0.13	82,82,82,82	0
58	MG	1A	3885	1/1	0.61	0.22	71,71,71,71	0
58	MG	2a	1723	1/1	0.61	0.10	72,72,72,72	0
58	MG	2B	216	1/1	0.61	0.23	85,85,85,85	0
58	MG	2v	101	1/1	0.61	0.21	65,65,65,65	0
58	MG	18	104	1/1	0.61	0.55	73,73,73,73	0
58	MG	1v	101	1/1	0.62	0.27	80,80,80,80	0
58	MG	1U	212	1/1	0.62	0.22	67,67,67,67	0
58	MG	2a	1619	1/1	0.62	0.31	63,63,63,63	0
58	MG	1a	1770	1/1	0.62	0.14	58,58,58,58	0
58	MG	1A	4059	1/1	0.62	0.15	58,58,58,58	0
58	MG	2a	1829	1/1	0.62	0.10	79,79,79,79	0
58	MG	2A	3089	1/1	0.62	0.15	85,85,85,85	0
58	MG	1A	3064	1/1	0.62	0.16	56,56,56,56	0
58	MG	2A	3328	1/1	0.63	0.20	72,72,72,72	0
58	MG	1A	3656	1/1	0.63	0.14	59,59,59,59	0
58	MG	2A	3313	1/1	0.63	0.18	78,78,78,78	0
58	MG	2A	3317	1/1	0.63	0.18	70,70,70,70	0
58	MG	1A	3682	1/1	0.63	0.43	70,70,70,70	0
58	MG	1A	3947	1/1	0.63	0.12	85,85,85,85	0
58	MG	1a	1623	1/1	0.63	0.25	75,75,75,75	0
58	MG	1A	3869	1/1	0.64	0.10	66,66,66,66	0
58	MG	1A	3553	1/1	0.64	0.17	65,65,65,65	0
58	MG	1A	3377	1/1	0.64	0.17	71,71,71,71	0
58	MG	1F	314	1/1	0.64	0.24	65,65,65,65	0
58	MG	1A	3006	1/1	0.64	0.27	67,67,67,67	0
58	MG	2a	1695	1/1	0.64	0.10	76,76,76,76	0
58	MG	2A	3781	1/1	0.64	0.12	83,83,83,83	0
58	MG	1x	102	1/1	0.64	0.23	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1687	1/1	0.64	0.15	69,69,69,69	0
58	MG	2A	3022	1/1	0.64	0.14	78,78,78,78	0
58	MG	1A	3965	1/1	0.64	0.16	77,77,77,77	0
58	MG	2A	3063	1/1	0.64	0.21	67,67,67,67	0
58	MG	2A	3080	1/1	0.64	0.19	90,90,90,90	0
58	MG	1A	3890	1/1	0.64	0.64	74,74,74,74	0
58	MG	2A	3691	1/1	0.65	0.45	84,84,84,84	0
58	MG	2A	3176	1/1	0.65	0.28	81,81,81,81	0
58	MG	1A	3155	1/1	0.65	0.29	74,74,74,74	0
58	MG	1a	1821	1/1	0.65	0.09	79,79,79,79	0
58	MG	1a	1731	1/1	0.65	0.13	64,64,64,64	0
58	MG	2a	1700	1/1	0.65	0.11	66,66,66,66	0
58	MG	1A	3980	1/1	0.65	0.14	53,53,53,53	0
58	MG	1A	3476	1/1	0.65	0.23	56,56,56,56	0
58	MG	2A	3335	1/1	0.65	0.30	63,63,63,63	0
58	MG	1A	3397	1/1	0.65	0.26	51,51,51,51	0
58	MG	2A	3628	1/1	0.65	0.23	84,84,84,84	0
58	MG	2A	3633	1/1	0.65	0.17	70,70,70,70	0
58	MG	1x	109	1/1	0.65	0.23	95,95,95,95	0
58	MG	2A	3651	1/1	0.65	0.27	90,90,90,90	0
58	MG	1W	206	1/1	0.66	0.34	56,56,56,56	0
58	MG	1a	1705	1/1	0.66	0.11	69,69,69,69	0
58	MG	2A	3006	1/1	0.66	0.21	66,66,66,66	0
58	MG	1A	3295	1/1	0.66	0.24	60,60,60,60	0
58	MG	2A	3762	1/1	0.66	0.22	76,76,76,76	0
58	MG	2l	202	1/1	0.66	0.15	74,74,74,74	0
58	MG	2A	3219	1/1	0.66	0.17	85,85,85,85	0
58	MG	1B	229	1/1	0.66	0.18	79,79,79,79	0
58	MG	2A	3589	1/1	0.67	0.11	65,65,65,65	0
58	MG	2a	1729	1/1	0.67	0.17	74,74,74,74	0
58	MG	2A	3157	1/1	0.67	0.12	78,78,78,78	0
58	MG	2a	1808	1/1	0.67	0.10	69,69,69,69	0
58	MG	1A	3610	1/1	0.67	0.22	52,52,52,52	0
58	MG	1a	1624	1/1	0.67	0.16	74,74,74,74	0
58	MG	1A	3782	1/1	0.67	0.26	78,78,78,78	0
58	MG	2A	3004	1/1	0.67	0.45	81,81,81,81	0
58	MG	2A	3217	1/1	0.68	0.14	82,82,82,82	0
58	MG	1A	3384	1/1	0.68	0.18	62,62,62,62	0
58	MG	2A	3797	1/1	0.68	0.11	74,74,74,74	0
58	MG	1a	1664	1/1	0.68	0.30	72,72,72,72	0
58	MG	1A	3087	1/1	0.68	0.14	77,77,77,77	0
58	MG	1A	3601	1/1	0.68	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4006	1/1	0.68	0.12	50,50,50,50	0
58	MG	1B	214	1/1	0.68	0.18	74,74,74,74	0
58	MG	1A	3977	1/1	0.68	0.10	46,46,46,46	0
58	MG	1A	3260	1/1	0.68	0.20	72,72,72,72	0
58	MG	2A	3198	1/1	0.68	0.25	76,76,76,76	0
58	MG	2A	3711	1/1	0.68	0.19	66,66,66,66	0
58	MG	2A	3512	1/1	0.68	0.20	71,71,71,71	0
58	MG	2A	3548	1/1	0.68	0.18	62,62,62,62	0
58	MG	1a	1666	1/1	0.69	0.26	77,77,77,77	0
58	MG	2A	3621	1/1	0.69	0.29	66,66,66,66	0
58	MG	11	105	1/1	0.69	0.25	59,59,59,59	0
58	MG	2a	1621	1/1	0.69	0.30	85,85,85,85	0
58	MG	2A	3121	1/1	0.69	0.14	52,52,52,52	0
58	MG	2A	3227	1/1	0.69	0.34	68,68,68,68	0
58	MG	1A	3530	1/1	0.69	0.32	46,46,46,46	0
58	MG	2A	3374	1/1	0.69	0.42	65,65,65,65	0
58	MG	2A	3392	1/1	0.69	0.24	74,74,74,74	0
58	MG	1A	3532	1/1	0.69	0.20	58,58,58,58	0
58	MG	2A	3405	1/1	0.69	0.24	54,54,54,54	0
58	MG	2A	3248	1/1	0.69	0.24	79,79,79,79	0
58	MG	2a	1718	1/1	0.69	0.22	70,70,70,70	0
58	MG	1A	3955	1/1	0.69	0.18	50,50,50,50	0
58	MG	2A	3305	1/1	0.69	0.17	76,76,76,76	0
58	MG	2A	3312	1/1	0.69	0.20	79,79,79,79	0
58	MG	1A	3940	1/1	0.69	0.22	43,43,43,43	0
58	MG	2A	3805	1/1	0.69	0.23	59,59,59,59	0
58	MG	1a	1659	1/1	0.69	0.15	66,66,66,66	0
58	MG	2A	3320	1/1	0.69	0.22	80,80,80,80	0
58	MG	10	112	1/1	0.69	0.22	78,78,78,78	0
58	MG	2A	3200	1/1	0.69	0.19	54,54,54,54	0
58	MG	2a	1686	1/1	0.70	0.12	75,75,75,75	0
58	MG	1A	3847	1/1	0.70	0.34	62,62,62,62	0
58	MG	1A	3488	1/1	0.70	0.18	68,68,68,68	0
58	MG	1A	3746	1/1	0.70	0.21	74,74,74,74	0
58	MG	1A	4089	1/1	0.70	0.18	72,72,72,72	0
58	MG	1A	3453	1/1	0.70	0.25	67,67,67,67	0
58	MG	2a	1708	1/1	0.70	0.10	80,80,80,80	0
58	MG	14	101	1/1	0.70	0.08	87,87,87,87	0
58	MG	2A	3111	1/1	0.70	0.19	63,63,63,63	0
58	MG	2A	3653	1/1	0.70	0.23	51,51,51,51	0
58	MG	2P	202	1/1	0.70	0.15	75,75,75,75	0
58	MG	1a	1693	1/1	0.70	0.18	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	2A	3504	1/1	0.70	0.31	77,77,77,77	0
58	MG	2a	1793	1/1	0.70	0.13	65,65,65,65	0
58	MG	2a	1801	1/1	0.70	0.07	88,88,88,88	0
58	MG	1A	3333	1/1	0.70	0.23	66,66,66,66	0
58	MG	1A	3956	1/1	0.70	0.16	59,59,59,59	0
58	MG	1A	3674	1/1	0.70	0.20	68,68,68,68	0
58	MG	2a	1675	1/1	0.70	0.18	71,71,71,71	0
58	MG	1A	3262	1/1	0.70	0.20	60,60,60,60	0
58	MG	2A	3071	1/1	0.71	0.16	64,64,64,64	0
58	MG	1A	3549	1/1	0.71	0.07	63,63,63,63	0
58	MG	1A	3135	1/1	0.71	0.23	52,52,52,52	0
58	MG	2A	3565	1/1	0.71	0.21	75,75,75,75	0
58	MG	2A	3587	1/1	0.71	0.28	80,80,80,80	0
58	MG	1B	202	1/1	0.71	0.41	59,59,59,59	0
58	MG	1a	1685	1/1	0.71	0.19	54,54,54,54	0
58	MG	1A	3521	1/1	0.71	0.30	67,67,67,67	0
58	MG	1a	1690	1/1	0.71	0.23	79,79,79,79	0
58	MG	2A	3271	1/1	0.71	0.30	66,66,66,66	0
58	MG	1B	228	1/1	0.71	0.23	47,47,47,47	0
58	MG	1A	3894	1/1	0.71	0.09	74,74,74,74	0
58	MG	1a	1716	1/1	0.71	0.13	62,62,62,62	0
58	MG	1A	3381	1/1	0.71	0.15	72,72,72,72	0
58	MG	1A	3864	1/1	0.71	0.22	64,64,64,64	0
58	MG	2a	1636	1/1	0.71	0.22	77,77,77,77	0
58	MG	2a	1637	1/1	0.71	0.11	75,75,75,75	0
58	MG	2d	301	1/1	0.71	0.11	71,71,71,71	0
58	MG	1A	3058	1/1	0.71	0.11	60,60,60,60	0
58	MG	2t	201	1/1	0.71	0.12	66,66,66,66	0
58	MG	2A	3501	1/1	0.71	0.22	80,80,80,80	0
58	MG	1A	3130	1/1	0.71	0.26	56,56,56,56	0
58	MG	1A	3319	1/1	0.72	0.19	68,68,68,68	0
58	MG	1A	3334	1/1	0.72	0.21	65,65,65,65	0
58	MG	1A	3197	1/1	0.72	0.12	58,58,58,58	0
58	MG	2a	1609	1/1	0.72	0.26	73,73,73,73	0
58	MG	2A	3301	1/1	0.72	0.20	66,66,66,66	0
58	MG	2A	3304	1/1	0.72	0.96	67,67,67,67	0
58	MG	2A	3583	1/1	0.72	0.29	83,83,83,83	0
58	MG	2A	3377	1/1	0.72	0.35	80,80,80,80	0
58	MG	2a	1789	1/1	0.72	0.20	71,71,71,71	0
58	MG	1B	209	1/1	0.72	0.18	49,49,49,49	0
58	MG	2a	1673	1/1	0.72	0.16	63,63,63,63	0
58	MG	1a	1721	1/1	0.72	0.19	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1825	1/1	0.72	0.21	83,83,83,83	0
58	MG	2a	1841	1/1	0.72	0.10	87,87,87,87	0
58	MG	2A	3045	1/1	0.72	0.23	47,47,47,47	0
58	MG	1a	1629	1/1	0.72	0.10	55,55,55,55	0
58	MG	1A	3794	1/1	0.72	0.19	62,62,62,62	0
58	MG	2A	3070	1/1	0.72	0.42	61,61,61,61	0
58	MG	2A	3242	1/1	0.72	0.32	78,78,78,78	0
58	MG	2x	105	1/1	0.72	0.13	86,86,86,86	0
58	MG	2W	201	1/1	0.73	0.37	74,74,74,74	0
58	MG	1A	3017	1/1	0.73	0.18	54,54,54,54	0
58	MG	2A	3298	1/1	0.73	0.36	71,71,71,71	0
58	MG	1A	3597	1/1	0.73	0.20	59,59,59,59	0
58	MG	2a	1610	1/1	0.73	0.13	84,84,84,84	0
58	MG	1A	3755	1/1	0.73	0.12	52,52,52,52	0
58	MG	1a	1702	1/1	0.73	0.24	83,83,83,83	0
58	MG	2a	1631	1/1	0.73	0.11	77,77,77,77	0
58	MG	2a	1633	1/1	0.73	0.08	63,63,63,63	0
58	MG	2A	3571	1/1	0.73	0.17	65,65,65,65	0
58	MG	2A	3308	1/1	0.73	0.16	79,79,79,79	0
58	MG	1A	3346	1/1	0.73	0.19	67,67,67,67	0
58	MG	2A	3183	1/1	0.73	0.25	64,64,64,64	0
58	MG	2A	3595	1/1	0.73	0.20	54,54,54,54	0
58	MG	2A	3314	1/1	0.73	0.36	78,78,78,78	0
58	MG	1A	3416	1/1	0.73	0.53	70,70,70,70	0
58	MG	1a	1613	1/1	0.73	0.15	68,68,68,68	0
58	MG	2A	3030	1/1	0.73	0.30	70,70,70,70	0
58	MG	1A	3427	1/1	0.73	0.32	71,71,71,71	0
58	MG	2a	1696	1/1	0.73	0.11	83,83,83,83	0
58	MG	2a	1698	1/1	0.73	0.27	55,55,55,55	0
58	MG	2A	3325	1/1	0.73	0.15	85,85,85,85	0
58	MG	2A	3210	1/1	0.73	0.19	64,64,64,64	0
58	MG	1A	4000	1/1	0.73	0.19	40,40,40,40	0
58	MG	2A	3665	1/1	0.73	0.14	76,76,76,76	0
58	MG	1A	3354	1/1	0.73	0.17	58,58,58,58	0
58	MG	1B	231	1/1	0.73	0.14	82,82,82,82	0
58	MG	2A	3224	1/1	0.73	0.19	56,56,56,56	0
58	MG	1A	3659	1/1	0.73	0.12	50,50,50,50	0
58	MG	2A	3079	1/1	0.73	0.08	72,72,72,72	0
58	MG	2A	3380	1/1	0.73	0.22	74,74,74,74	0
58	MG	1A	3218	1/1	0.73	0.23	67,67,67,67	0
58	MG	1A	3312	1/1	0.73	0.38	60,60,60,60	0
58	MG	2A	3246	1/1	0.73	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
58	MG	2a	1817	1/1	0.73	0.09	59,59,59,59	0
58	MG	1A	3487	1/1	0.73	0.23	70,70,70,70	0
58	MG	2A	3810	1/1	0.73	0.12	58,58,58,58	0
58	MG	2A	3253	1/1	0.73	0.28	79,79,79,79	0
58	MG	2e	202	1/1	0.73	0.12	84,84,84,84	0
58	MG	2A	3454	1/1	0.73	0.20	65,65,65,65	0
58	MG	2A	3268	1/1	0.73	0.46	68,68,68,68	0
58	MG	1A	3963	1/1	0.73	0.26	62,62,62,62	0
58	MG	2D	301	1/1	0.73	0.51	51,51,51,51	0
58	MG	2A	3273	1/1	0.73	0.21	71,71,71,71	0
58	MG	1A	3202	1/1	0.74	0.39	57,57,57,57	0
58	MG	2A	3315	1/1	0.74	0.36	81,81,81,81	0
58	MG	1a	1820	1/1	0.74	0.22	83,83,83,83	0
58	MG	1A	3714	1/1	0.74	0.21	48,48,48,48	0
58	MG	2A	3798	1/1	0.74	0.06	71,71,71,71	0
58	MG	1A	3293	1/1	0.74	0.29	65,65,65,65	0
58	MG	18	101	1/1	0.74	0.36	62,62,62,62	0
58	MG	1A	3545	1/1	0.74	0.13	61,61,61,61	0
58	MG	1A	3920	1/1	0.74	0.16	79,79,79,79	0
58	MG	1A	3506	1/1	0.74	0.25	63,63,63,63	0
58	MG	2A	3821	1/1	0.74	0.12	71,71,71,71	0
58	MG	2A	3160	1/1	0.74	0.84	67,67,67,67	0
58	MG	2A	3172	1/1	0.74	0.20	68,68,68,68	0
58	MG	1D	310	1/1	0.74	0.32	49,49,49,49	0
58	MG	2A	3272	1/1	0.74	0.23	78,78,78,78	0
58	MG	1A	3075	1/1	0.74	0.20	43,43,43,43	0
58	MG	2a	1733	1/1	0.74	0.08	92,92,92,92	0
58	MG	1A	4078	1/1	0.74	0.07	81,81,81,81	0
58	MG	2a	1771	1/1	0.74	0.30	77,77,77,77	0
58	MG	2A	3296	1/1	0.74	0.13	60,60,60,60	0
58	MG	1A	3574	1/1	0.74	0.20	56,56,56,56	0
58	MG	2A	3400	1/1	0.74	0.12	60,60,60,60	0
58	MG	1A	3285	1/1	0.74	0.44	63,63,63,63	0
58	MG	2a	1620	1/1	0.74	0.28	72,72,72,72	0
58	MG	1W	202	1/1	0.74	0.29	65,65,65,65	0
58	MG	2a	1622	1/1	0.74	0.12	66,66,66,66	0
58	MG	2a	1626	1/1	0.74	0.31	66,66,66,66	0
58	MG	1a	1805	1/1	0.74	0.07	76,76,76,76	0
58	MG	1a	1806	1/1	0.74	0.17	74,74,74,74	0
58	MG	2A	3709	1/1	0.74	0.10	92,92,92,92	0
58	MG	1A	4102	1/1	0.74	0.31	83,83,83,83	0
58	MG	2A	3742	1/1	0.74	0.12	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1813	1/1	0.74	0.07	74,74,74,74	0
58	MG	1A	3926	1/1	0.75	0.20	73,73,73,73	0
58	MG	1A	3681	1/1	0.75	0.13	70,70,70,70	0
58	MG	2B	209	1/1	0.75	0.10	77,77,77,77	0
58	MG	2B	210	1/1	0.75	0.25	83,83,83,83	0
58	MG	1a	1668	1/1	0.75	0.13	68,68,68,68	0
58	MG	2A	3171	1/1	0.75	0.15	78,78,78,78	0
58	MG	1A	3154	1/1	0.75	0.23	61,61,61,61	0
58	MG	2A	3175	1/1	0.75	0.24	66,66,66,66	0
58	MG	2A	3044	1/1	0.75	0.46	79,79,79,79	0
58	MG	1A	3298	1/1	0.75	0.19	66,66,66,66	0
58	MG	2A	3698	1/1	0.75	0.16	64,64,64,64	0
58	MG	2A	3708	1/1	0.75	0.20	80,80,80,80	0
58	MG	2a	1617	1/1	0.75	0.52	73,73,73,73	0
58	MG	1B	222	1/1	0.75	0.31	84,84,84,84	0
58	MG	1A	3345	1/1	0.75	0.36	58,58,58,58	0
58	MG	2A	3519	1/1	0.75	0.19	48,48,48,48	0
58	MG	1A	3422	1/1	0.75	0.30	69,69,69,69	0
58	MG	2A	3331	1/1	0.75	0.17	72,72,72,72	0
58	MG	2A	3276	1/1	0.75	0.32	76,76,76,76	0
58	MG	1A	3190	1/1	0.75	0.20	44,44,44,44	0
58	MG	1A	3351	1/1	0.75	0.23	41,41,41,41	0
58	MG	2a	1837	1/1	0.75	0.23	78,78,78,78	0
58	MG	1A	3248	1/1	0.75	0.20	45,45,45,45	0
58	MG	2A	3799	1/1	0.75	0.07	82,82,82,82	0
58	MG	2a	1649	1/1	0.75	0.16	67,67,67,67	0
58	MG	1A	3543	1/1	0.75	0.17	66,66,66,66	0
58	MG	1a	1625	1/1	0.75	0.19	69,69,69,69	0
58	MG	2A	3390	1/1	0.75	0.20	79,79,79,79	0
58	MG	1A	3074	1/1	0.75	0.24	61,61,61,61	0
58	MG	1A	3327	1/1	0.75	0.32	77,77,77,77	0
58	MG	2A	3598	1/1	0.76	0.16	71,71,71,71	0
58	MG	1A	3428	1/1	0.76	0.17	73,73,73,73	0
58	MG	1A	3933	1/1	0.76	0.16	38,38,38,38	0
58	MG	2A	3610	1/1	0.76	0.24	69,69,69,69	0
58	MG	2A	3618	1/1	0.76	0.44	63,63,63,63	0
58	MG	1A	3480	1/1	0.76	0.13	87,87,87,87	0
58	MG	2A	3625	1/1	0.76	0.13	79,79,79,79	0
58	MG	1B	237	1/1	0.76	0.21	49,49,49,49	0
58	MG	1A	4084	1/1	0.76	0.33	69,69,69,69	0
58	MG	1A	3430	1/1	0.76	0.23	74,74,74,74	0
58	MG	1A	3005	1/1	0.76	0.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4098	1/1	0.76	0.27	64,64,64,64	0
58	MG	1x	112	1/1	0.76	0.09	71,71,71,71	0
58	MG	1a	1653	1/1	0.76	0.12	71,71,71,71	0
58	MG	1a	1740	1/1	0.76	0.12	85,85,85,85	0
58	MG	2A	3509	1/1	0.76	0.33	69,69,69,69	0
58	MG	2A	3705	1/1	0.76	0.17	69,69,69,69	0
58	MG	1A	4100	1/1	0.76	0.19	52,52,52,52	0
58	MG	2A	3518	1/1	0.76	0.17	41,41,41,41	0
58	MG	1a	1760	1/1	0.76	0.18	83,83,83,83	0
58	MG	2A	3712	1/1	0.76	0.07	57,57,57,57	0
58	MG	2A	3716	1/1	0.76	0.06	82,82,82,82	0
58	MG	2A	3717	1/1	0.76	0.25	46,46,46,46	0
58	MG	2a	1830	1/1	0.76	0.13	79,79,79,79	0
58	MG	2A	3177	1/1	0.76	0.16	73,73,73,73	0
58	MG	2A	3743	1/1	0.76	0.12	67,67,67,67	0
58	MG	1A	3489	1/1	0.76	0.25	65,65,65,65	0
58	MG	1A	3899	1/1	0.76	0.54	81,81,81,81	0
58	MG	2j	201	1/1	0.76	0.12	83,83,83,83	0
58	MG	2A	3047	1/1	0.76	0.28	68,68,68,68	0
58	MG	1Z	301	1/1	0.76	0.12	64,64,64,64	0
58	MG	1A	3670	1/1	0.76	0.10	71,71,71,71	0
58	MG	1A	3254	1/1	0.76	0.21	65,65,65,65	0
58	MG	1A	3871	1/1	0.76	0.14	38,38,38,38	0
58	MG	1A	3975	1/1	0.77	0.51	73,73,73,73	0
58	MG	1a	1749	1/1	0.77	0.14	76,76,76,76	0
58	MG	1a	1626	1/1	0.77	0.10	67,67,67,67	0
58	MG	2A	3718	1/1	0.77	0.20	44,44,44,44	0
58	MG	1A	3037	1/1	0.77	0.24	70,70,70,70	0
58	MG	1E	306	1/1	0.77	0.23	57,57,57,57	0
58	MG	2A	3525	1/1	0.77	0.20	77,77,77,77	0
58	MG	2A	3049	1/1	0.77	0.21	68,68,68,68	0
58	MG	2A	3205	1/1	0.77	0.14	76,76,76,76	0
58	MG	1A	3482	1/1	0.77	0.12	61,61,61,61	0
58	MG	2A	3785	1/1	0.77	0.12	58,58,58,58	0
58	MG	1A	4095	1/1	0.77	0.27	51,51,51,51	0
58	MG	2A	3582	1/1	0.77	0.19	63,63,63,63	0
58	MG	1a	1809	1/1	0.77	0.16	82,82,82,82	0
58	MG	1A	3419	1/1	0.77	0.12	59,59,59,59	0
58	MG	2A	3804	1/1	0.77	0.14	63,63,63,63	0
58	MG	2A	3073	1/1	0.77	0.42	66,66,66,66	0
58	MG	2A	3593	1/1	0.77	0.18	66,66,66,66	0
58	MG	2A	3074	1/1	0.77	0.21	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3939	1/1	0.77	0.18	56,56,56,56	0
58	MG	1A	3618	1/1	0.77	0.23	45,45,45,45	0
58	MG	2A	3348	1/1	0.77	0.27	59,59,59,59	0
58	MG	2A	3241	1/1	0.77	0.37	62,62,62,62	0
58	MG	1A	3434	1/1	0.77	0.12	71,71,71,71	0
58	MG	1A	3451	1/1	0.77	0.16	68,68,68,68	0
58	MG	1B	207	1/1	0.77	0.16	75,75,75,75	0
58	MG	2A	3113	1/1	0.77	0.16	64,64,64,64	0
58	MG	2A	3254	1/1	0.77	0.18	63,63,63,63	0
58	MG	2a	1809	1/1	0.77	0.09	75,75,75,75	0
58	MG	1A	3420	1/1	0.77	0.19	60,60,60,60	0
58	MG	27	103	1/1	0.77	0.82	74,74,74,74	0
58	MG	2A	3636	1/1	0.77	0.16	80,80,80,80	0
58	MG	1A	4017	1/1	0.77	0.25	64,64,64,64	0
58	MG	2A	3156	1/1	0.77	0.09	76,76,76,76	0
58	MG	1A	3458	1/1	0.77	0.21	77,77,77,77	0
58	MG	1B	227	1/1	0.77	0.25	56,56,56,56	0
58	MG	1A	3388	1/1	0.77	0.72	63,63,63,63	0
58	MG	1A	3805	1/1	0.77	0.12	62,62,62,62	0
58	MG	2A	3479	1/1	0.77	0.11	47,47,47,47	0
58	MG	1A	3088	1/1	0.77	0.33	50,50,50,50	0
58	MG	1B	232	1/1	0.77	0.19	73,73,73,73	0
58	MG	2A	3017	1/1	0.77	0.17	60,60,60,60	0
58	MG	2a	1678	1/1	0.78	0.12	88,88,88,88	0
58	MG	1a	1768	1/1	0.78	0.06	75,75,75,75	0
58	MG	1a	1769	1/1	0.78	0.13	70,70,70,70	0
58	MG	1A	3780	1/1	0.78	0.14	47,47,47,47	0
58	MG	1a	1779	1/1	0.78	0.06	69,69,69,69	0
58	MG	2A	3189	1/1	0.78	0.40	71,71,71,71	0
58	MG	1A	3948	1/1	0.78	0.24	59,59,59,59	0
58	MG	1A	3178	1/1	0.78	0.40	46,46,46,46	0
58	MG	2B	202	1/1	0.78	0.23	81,81,81,81	0
58	MG	2A	3649	1/1	0.78	0.10	72,72,72,72	0
58	MG	1Y	201	1/1	0.78	0.38	76,76,76,76	0
58	MG	1A	3424	1/1	0.78	0.28	62,62,62,62	0
58	MG	2a	1716	1/1	0.78	0.14	66,66,66,66	0
58	MG	1A	3339	1/1	0.78	0.59	57,57,57,57	0
58	MG	2A	3675	1/1	0.78	0.08	76,76,76,76	0
58	MG	2F	304	1/1	0.78	0.17	60,60,60,60	0
58	MG	1A	3095	1/1	0.78	0.26	51,51,51,51	0
58	MG	2A	3511	1/1	0.78	0.31	77,77,77,77	0
58	MG	2A	3318	1/1	0.78	0.28	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1A	3907	1/1	0.78	0.09	61,61,61,61	0
58	MG	16	101	1/1	0.78	0.20	67,67,67,67	0
58	MG	1a	1824	1/1	0.78	0.13	87,87,87,87	0
58	MG	1A	3815	1/1	0.78	0.13	45,45,45,45	0
58	MG	2a	1807	1/1	0.78	0.10	78,78,78,78	0
58	MG	1A	3919	1/1	0.78	0.20	52,52,52,52	0
58	MG	2A	3561	1/1	0.78	0.17	79,79,79,79	0
58	MG	2a	1810	1/1	0.78	0.10	73,73,73,73	0
58	MG	1A	3241	1/1	0.78	0.27	60,60,60,60	0
58	MG	1A	3483	1/1	0.78	0.15	59,59,59,59	0
58	MG	1a	1618	1/1	0.78	0.12	60,60,60,60	0
58	MG	2A	3145	1/1	0.78	0.10	68,68,68,68	0
58	MG	1a	1725	1/1	0.78	0.22	58,58,58,58	0
58	MG	1A	3242	1/1	0.78	0.19	61,61,61,61	0
58	MG	1F	311	1/1	0.78	0.12	65,65,65,65	0
58	MG	1A	3046	1/1	0.78	0.23	55,55,55,55	0
58	MG	1A	3547	1/1	0.78	0.47	57,57,57,57	0
58	MG	1T	202	1/1	0.78	0.12	72,72,72,72	0
58	MG	2a	1668	1/1	0.78	0.15	67,67,67,67	0
58	MG	2A	3023	1/1	0.78	0.17	68,68,68,68	0
58	MG	1A	3200	1/1	0.78	0.20	71,71,71,71	0
58	MG	2A	3812	1/1	0.79	0.08	74,74,74,74	0
58	MG	1a	1754	1/1	0.79	0.07	66,66,66,66	0
58	MG	2A	3498	1/1	0.79	0.24	73,73,73,73	0
58	MG	1B	204	1/1	0.79	0.41	73,73,73,73	0
58	MG	1A	3663	1/1	0.79	0.21	67,67,67,67	0
58	MG	1O	201	1/1	0.79	0.19	72,72,72,72	0
58	MG	1A	3790	1/1	0.79	0.09	55,55,55,55	0
58	MG	2A	3260	1/1	0.79	0.20	64,64,64,64	0
58	MG	1A	3736	1/1	0.79	0.17	91,91,91,91	0
58	MG	1A	3539	1/1	0.79	0.20	80,80,80,80	0
58	MG	2a	1712	1/1	0.79	0.15	84,84,84,84	0
58	MG	2A	3001	1/1	0.79	0.42	69,69,69,69	0
58	MG	2G	201	1/1	0.79	0.09	73,73,73,73	0
58	MG	1A	3525	1/1	0.79	0.21	48,48,48,48	0
58	MG	2a	1721	1/1	0.79	0.45	80,80,80,80	0
58	MG	2T	202	1/1	0.79	0.13	73,73,73,73	0
58	MG	2A	3274	1/1	0.79	0.40	81,81,81,81	0
58	MG	2a	1725	1/1	0.79	0.12	82,82,82,82	0
58	MG	2a	1727	1/1	0.79	0.08	82,82,82,82	0
58	MG	2A	3556	1/1	0.79	0.21	65,65,65,65	0
58	MG	26	102	1/1	0.79	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3365	1/1	0.79	0.31	75,75,75,75	0
58	MG	1A	3898	1/1	0.79	0.11	54,54,54,54	0
58	MG	2a	1782	1/1	0.79	0.15	82,82,82,82	0
58	MG	2A	3102	1/1	0.79	0.17	74,74,74,74	0
58	MG	2A	3286	1/1	0.79	0.26	73,73,73,73	0
58	MG	1A	3653	1/1	0.79	0.20	34,34,34,34	0
58	MG	2A	3719	1/1	0.79	0.15	54,54,54,54	0
58	MG	1A	3900	1/1	0.79	0.10	58,58,58,58	0
58	MG	1A	3853	1/1	0.79	0.16	57,57,57,57	0
58	MG	1a	1815	1/1	0.79	0.12	78,78,78,78	0
58	MG	2a	1624	1/1	0.79	0.28	76,76,76,76	0
58	MG	2A	3220	1/1	0.79	0.11	84,84,84,84	0
58	MG	2a	1630	1/1	0.79	0.09	79,79,79,79	0
58	MG	2A	3038	1/1	0.79	0.41	75,75,75,75	0
58	MG	2A	3406	1/1	0.79	0.12	68,68,68,68	0
58	MG	1A	3328	1/1	0.79	0.12	72,72,72,72	0
58	MG	2A	3606	1/1	0.79	0.21	80,80,80,80	0
58	MG	2A	3434	1/1	0.79	0.16	42,42,42,42	0
58	MG	1A	3713	1/1	0.79	0.33	41,41,41,41	0
58	MG	1A	3363	1/1	0.79	0.14	69,69,69,69	0
58	MG	2A	3164	1/1	0.79	0.13	59,59,59,59	0
58	MG	1E	310	1/1	0.79	0.27	72,72,72,72	0
58	MG	2A	3489	1/1	0.79	0.24	65,65,65,65	0
58	MG	2A	3562	1/1	0.80	0.13	76,76,76,76	0
58	MG	2E	302	1/1	0.80	0.32	71,71,71,71	0
58	MG	1a	1816	1/1	0.80	0.10	69,69,69,69	0
58	MG	1A	3492	1/1	0.80	0.17	66,66,66,66	0
58	MG	2A	3580	1/1	0.80	0.11	74,74,74,74	0
58	MG	1A	3122	1/1	0.80	0.31	54,54,54,54	0
58	MG	2A	3230	1/1	0.80	0.15	76,76,76,76	0
58	MG	1A	3199	1/1	0.80	0.23	61,61,61,61	0
58	MG	1A	3176	1/1	0.80	0.21	45,45,45,45	0
58	MG	27	102	1/1	0.80	0.18	56,56,56,56	0
58	MG	2A	3050	1/1	0.80	0.21	57,57,57,57	0
58	MG	2A	3735	1/1	0.80	0.22	50,50,50,50	0
58	MG	1A	3055	1/1	0.80	0.30	54,54,54,54	0
58	MG	1a	1676	1/1	0.80	0.16	72,72,72,72	0
58	MG	1A	4018	1/1	0.80	0.19	44,44,44,44	0
58	MG	2A	3481	1/1	0.80	0.20	62,62,62,62	0
58	MG	1w	108	1/1	0.80	0.25	87,87,87,87	0
58	MG	1A	3417	1/1	0.80	0.20	66,66,66,66	0
58	MG	2A	3262	1/1	0.80	0.19	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3787	1/1	0.80	0.08	65,65,65,65	0
58	MG	2A	3794	1/1	0.80	0.10	66,66,66,66	0
58	MG	2a	1796	1/1	0.80	0.18	75,75,75,75	0
58	MG	1A	3531	1/1	0.80	0.24	60,60,60,60	0
58	MG	1A	3970	1/1	0.80	0.16	53,53,53,53	0
58	MG	1A	3486	1/1	0.80	0.44	49,49,49,49	0
58	MG	1a	1786	1/1	0.80	0.16	78,78,78,78	0
58	MG	1A	4067	1/1	0.80	0.19	61,61,61,61	0
58	MG	2a	1814	1/1	0.80	0.06	76,76,76,76	0
58	MG	1A	3372	1/1	0.80	0.13	53,53,53,53	0
58	MG	2a	1824	1/1	0.80	0.12	70,70,70,70	0
58	MG	2A	3639	1/1	0.80	0.20	69,69,69,69	0
58	MG	2a	1657	1/1	0.80	0.16	67,67,67,67	0
58	MG	2A	3361	1/1	0.80	0.44	63,63,63,63	0
58	MG	2A	3008	1/1	0.80	0.17	66,66,66,66	0
58	MG	1A	3344	1/1	0.80	0.23	45,45,45,45	0
58	MG	2A	3661	1/1	0.80	0.18	71,71,71,71	0
58	MG	2A	3537	1/1	0.80	0.22	62,62,62,62	0
58	MG	2A	3292	1/1	0.80	0.18	68,68,68,68	0
58	MG	1a	1718	1/1	0.80	0.19	46,46,46,46	0
58	MG	2a	1693	1/1	0.80	0.13	74,74,74,74	0
58	MG	1A	3799	1/1	0.80	0.10	75,75,75,75	0
58	MG	1A	3134	1/1	0.80	0.20	56,56,56,56	0
58	MG	2x	106	1/1	0.80	0.24	80,80,80,80	0
58	MG	2A	3259	1/1	0.81	0.38	82,82,82,82	0
58	MG	2a	1643	1/1	0.81	0.17	57,57,57,57	0
58	MG	2A	3749	1/1	0.81	0.15	67,67,67,67	0
58	MG	2A	3573	1/1	0.81	0.36	85,85,85,85	0
58	MG	2A	3576	1/1	0.81	0.17	63,63,63,63	0
58	MG	2a	1671	1/1	0.81	0.16	78,78,78,78	0
58	MG	2a	1672	1/1	0.81	0.11	64,64,64,64	0
58	MG	2A	3173	1/1	0.81	0.14	79,79,79,79	0
58	MG	1A	3139	1/1	0.81	0.26	49,49,49,49	0
58	MG	1a	1640	1/1	0.81	0.20	63,63,63,63	0
58	MG	2A	3270	1/1	0.81	0.36	63,63,63,63	0
58	MG	2A	3062	1/1	0.81	0.17	66,66,66,66	0
58	MG	1A	3385	1/1	0.81	0.37	47,47,47,47	0
58	MG	1a	1657	1/1	0.81	0.13	83,83,83,83	0
58	MG	1A	3866	1/1	0.81	0.14	78,78,78,78	0
58	MG	1A	3967	1/1	0.81	0.11	87,87,87,87	0
58	MG	1A	3916	1/1	0.81	0.18	79,79,79,79	0
58	MG	2A	3197	1/1	0.81	0.23	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	2A	3288	1/1	0.81	0.14	72,72,72,72	0
58	MG	1a	1761	1/1	0.81	0.10	70,70,70,70	0
58	MG	2A	3412	1/1	0.81	0.24	78,78,78,78	0
58	MG	2a	1709	1/1	0.81	0.14	54,54,54,54	0
58	MG	2A	3294	1/1	0.81	0.29	75,75,75,75	0
58	MG	1A	4060	1/1	0.81	0.12	64,64,64,64	0
58	MG	2B	207	1/1	0.81	0.17	72,72,72,72	0
58	MG	2A	3088	1/1	0.81	0.10	78,78,78,78	0
58	MG	1A	3387	1/1	0.81	0.16	64,64,64,64	0
58	MG	2A	3303	1/1	0.81	0.50	58,58,58,58	0
58	MG	1A	3171	1/1	0.81	0.28	42,42,42,42	0
58	MG	2B	219	1/1	0.81	0.11	78,78,78,78	0
58	MG	2A	3640	1/1	0.81	0.12	64,64,64,64	0
58	MG	2D	304	1/1	0.81	0.63	67,67,67,67	0
58	MG	2E	301	1/1	0.81	0.16	68,68,68,68	0
58	MG	2A	3218	1/1	0.81	0.31	86,86,86,86	0
58	MG	2A	3095	1/1	0.81	0.15	65,65,65,65	0
58	MG	1A	3237	1/1	0.81	0.24	69,69,69,69	0
58	MG	1a	1781	1/1	0.81	0.27	72,72,72,72	0
58	MG	1A	3497	1/1	0.81	0.26	62,62,62,62	0
58	MG	1A	3401	1/1	0.81	0.18	60,60,60,60	0
58	MG	2A	3685	1/1	0.81	0.21	69,69,69,69	0
58	MG	1A	3404	1/1	0.81	0.14	70,70,70,70	0
58	MG	2A	3692	1/1	0.81	0.14	51,51,51,51	0
58	MG	2A	3229	1/1	0.81	0.16	72,72,72,72	0
58	MG	1a	1609	1/1	0.81	0.17	62,62,62,62	0
58	MG	2a	1607	1/1	0.81	0.13	75,75,75,75	0
58	MG	2A	3700	1/1	0.81	0.41	60,60,60,60	0
58	MG	2a	1822	1/1	0.81	0.12	74,74,74,74	0
58	MG	2A	3236	1/1	0.81	0.21	81,81,81,81	0
58	MG	2a	1615	1/1	0.81	0.12	62,62,62,62	0
58	MG	2A	3521	1/1	0.81	0.16	61,61,61,61	0
58	MG	1A	3997	1/1	0.81	0.20	66,66,66,66	0
58	MG	1A	3893	1/1	0.81	0.12	56,56,56,56	0
58	MG	1A	3745	1/1	0.81	0.12	50,50,50,50	0
58	MG	2A	3714	1/1	0.81	0.27	63,63,63,63	0
58	MG	2A	3163	1/1	0.81	0.19	65,65,65,65	0
58	MG	1A	3895	1/1	0.81	0.11	70,70,70,70	0
58	MG	2A	3334	1/1	0.81	0.39	60,60,60,60	0
58	MG	1A	3409	1/1	0.81	0.30	57,57,57,57	0
58	MG	1A	3362	1/1	0.81	0.42	48,48,48,48	0
58	MG	2w	102	1/1	0.81	0.08	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	2w	103	1/1	0.81	0.25	98,98,98,98	0
58	MG	2A	3566	1/1	0.81	0.14	75,75,75,75	0
58	MG	2A	3568	1/1	0.81	0.15	71,71,71,71	0
59	K	2A	3368	1/1	0.81	0.11	73,73,73,73	0
58	MG	2A	3570	1/1	0.82	0.14	69,69,69,69	0
58	MG	2A	3332	1/1	0.82	0.21	51,51,51,51	0
58	MG	2A	3755	1/1	0.82	0.12	65,65,65,65	0
58	MG	2a	1669	1/1	0.82	0.18	66,66,66,66	0
58	MG	1x	106	1/1	0.82	0.18	72,72,72,72	0
58	MG	2A	3575	1/1	0.82	0.20	58,58,58,58	0
58	MG	2A	3240	1/1	0.82	0.20	60,60,60,60	0
58	MG	2A	3577	1/1	0.82	0.16	74,74,74,74	0
58	MG	2A	3337	1/1	0.82	0.25	60,60,60,60	0
58	MG	1A	4109	1/1	0.82	0.12	71,71,71,71	0
58	MG	1B	201	1/1	0.82	0.24	66,66,66,66	0
58	MG	2A	3585	1/1	0.82	0.22	49,49,49,49	0
58	MG	1A	3954	1/1	0.82	0.11	49,49,49,49	0
58	MG	2A	3125	1/1	0.82	0.17	71,71,71,71	0
58	MG	2A	3132	1/1	0.82	0.28	68,68,68,68	0
58	MG	1B	203	1/1	0.82	0.21	56,56,56,56	0
58	MG	2A	3257	1/1	0.82	0.30	71,71,71,71	0
58	MG	2A	3601	1/1	0.82	0.17	63,63,63,63	0
58	MG	2A	3378	1/1	0.82	0.33	78,78,78,78	0
58	MG	1A	3002	1/1	0.82	0.14	53,53,53,53	0
58	MG	1a	1665	1/1	0.82	0.09	80,80,80,80	0
58	MG	2A	3391	1/1	0.82	0.15	55,55,55,55	0
58	MG	2A	3261	1/1	0.82	0.22	76,76,76,76	0
58	MG	1A	3007	1/1	0.82	0.24	45,45,45,45	0
58	MG	1A	3680	1/1	0.82	0.15	69,69,69,69	0
58	MG	2B	213	1/1	0.82	0.20	76,76,76,76	0
58	MG	1A	3613	1/1	0.82	0.16	35,35,35,35	0
58	MG	1A	4034	1/1	0.82	0.18	79,79,79,79	0
58	MG	1a	1793	1/1	0.82	0.10	64,64,64,64	0
58	MG	1A	3177	1/1	0.82	0.21	51,51,51,51	0
58	MG	1A	3918	1/1	0.82	0.10	81,81,81,81	0
58	MG	1A	3617	1/1	0.82	0.14	42,42,42,42	0
58	MG	2a	1746	1/1	0.82	0.19	75,75,75,75	0
58	MG	2A	3645	1/1	0.82	0.10	81,81,81,81	0
58	MG	1A	3315	1/1	0.82	0.21	66,66,66,66	0
58	MG	2a	1778	1/1	0.82	0.15	62,62,62,62	0
58	MG	2A	3478	1/1	0.82	0.28	76,76,76,76	0
58	MG	2a	1787	1/1	0.82	0.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1A	3730	1/1	0.82	0.22	74,74,74,74	0
58	MG	2U	202	1/1	0.82	0.20	83,83,83,83	0
58	MG	1a	1608	1/1	0.82	0.30	74,74,74,74	0
58	MG	2A	3059	1/1	0.82	0.47	66,66,66,66	0
58	MG	2A	3666	1/1	0.82	0.21	67,67,67,67	0
58	MG	1A	4083	1/1	0.82	0.17	62,62,62,62	0
58	MG	1a	1708	1/1	0.82	0.14	55,55,55,55	0
58	MG	2A	3191	1/1	0.82	0.18	73,73,73,73	0
58	MG	1a	1818	1/1	0.82	0.14	74,74,74,74	0
58	MG	1A	3929	1/1	0.82	0.15	42,42,42,42	0
58	MG	1A	3342	1/1	0.82	0.53	61,61,61,61	0
58	MG	1A	3140	1/1	0.82	0.20	37,37,37,37	0
58	MG	2a	1616	1/1	0.82	0.15	75,75,75,75	0
58	MG	1a	1722	1/1	0.82	0.21	79,79,79,79	0
58	MG	2a	1618	1/1	0.82	0.12	75,75,75,75	0
58	MG	2a	1839	1/1	0.82	0.16	70,70,70,70	0
58	MG	1A	3180	1/1	0.82	0.48	49,49,49,49	0
58	MG	2A	3082	1/1	0.82	0.43	63,63,63,63	0
58	MG	2A	3084	1/1	0.82	0.25	54,54,54,54	0
58	MG	1A	3836	1/1	0.82	0.20	36,36,36,36	0
58	MG	2A	3222	1/1	0.82	0.21	85,85,85,85	0
58	MG	2l	204	1/1	0.82	0.15	69,69,69,69	0
58	MG	2q	201	1/1	0.82	0.24	79,79,79,79	0
58	MG	1A	3841	1/1	0.82	0.17	82,82,82,82	0
58	MG	1A	3251	1/1	0.82	0.10	70,70,70,70	0
58	MG	1x	103	1/1	0.82	0.16	60,60,60,60	0
58	MG	2A	3097	1/1	0.82	0.22	44,44,44,44	0
58	MG	2A	3101	1/1	0.82	0.29	61,61,61,61	0
58	MG	2x	103	1/1	0.82	0.18	77,77,77,77	0
58	MG	1a	1639	1/1	0.82	0.10	70,70,70,70	0
58	MG	2A	3235	1/1	0.82	0.42	83,83,83,83	0
58	MG	2A	3105	1/1	0.82	0.11	73,73,73,73	0
58	MG	1A	3084	1/1	0.83	0.14	69,69,69,69	0
58	MG	1a	1673	1/1	0.83	0.11	71,71,71,71	0
58	MG	1A	3698	1/1	0.83	0.17	44,44,44,44	0
58	MG	2a	1692	1/1	0.83	0.12	73,73,73,73	0
58	MG	2A	3825	1/1	0.83	0.18	63,63,63,63	0
58	MG	2A	3826	1/1	0.83	0.09	75,75,75,75	0
58	MG	2B	201	1/1	0.83	0.12	80,80,80,80	0
58	MG	1A	3398	1/1	0.83	0.35	55,55,55,55	0
58	MG	2A	3214	1/1	0.83	0.21	61,61,61,61	0
58	MG	1A	4055	1/1	0.83	0.19	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3011	1/1	0.83	0.09	61,61,61,61	0
58	MG	2a	1705	1/1	0.83	0.34	68,68,68,68	0
58	MG	2A	3015	1/1	0.83	0.28	52,52,52,52	0
58	MG	1a	1800	1/1	0.83	0.08	71,71,71,71	0
58	MG	2A	3657	1/1	0.83	0.23	60,60,60,60	0
58	MG	2A	3108	1/1	0.83	0.14	79,79,79,79	0
58	MG	1A	3259	1/1	0.83	0.30	61,61,61,61	0
58	MG	1A	3717	1/1	0.83	0.16	26,26,26,26	0
58	MG	2A	3668	1/1	0.83	0.17	72,72,72,72	0
58	MG	1A	4062	1/1	0.83	0.12	65,65,65,65	0
58	MG	2F	301	1/1	0.83	0.28	52,52,52,52	0
58	MG	1A	3172	1/1	0.83	0.21	62,62,62,62	0
58	MG	1A	3640	1/1	0.83	0.10	67,67,67,67	0
58	MG	2A	3126	1/1	0.83	0.26	54,54,54,54	0
58	MG	2A	3131	1/1	0.83	0.23	69,69,69,69	0
58	MG	1A	3335	1/1	0.83	0.29	67,67,67,67	0
58	MG	1A	3655	1/1	0.83	0.22	45,45,45,45	0
58	MG	2A	3048	1/1	0.83	0.10	72,72,72,72	0
58	MG	25	101	1/1	0.83	0.36	66,66,66,66	0
58	MG	1A	3300	1/1	0.83	0.18	58,58,58,58	0
58	MG	1A	3658	1/1	0.83	0.22	69,69,69,69	0
58	MG	2A	3243	1/1	0.83	0.21	74,74,74,74	0
58	MG	2a	1791	1/1	0.83	0.06	62,62,62,62	0
58	MG	2A	3162	1/1	0.83	0.35	71,71,71,71	0
58	MG	2A	3053	1/1	0.83	0.16	80,80,80,80	0
58	MG	2a	1798	1/1	0.83	0.09	92,92,92,92	0
58	MG	2A	3346	1/1	0.83	0.24	64,64,64,64	0
58	MG	1A	3994	1/1	0.83	0.30	70,70,70,70	0
58	MG	2A	3166	1/1	0.83	0.27	53,53,53,53	0
58	MG	2A	3360	1/1	0.83	0.13	84,84,84,84	0
58	MG	2A	3168	1/1	0.83	0.25	67,67,67,67	0
58	MG	2A	3737	1/1	0.83	0.19	43,43,43,43	0
58	MG	2A	3741	1/1	0.83	0.10	78,78,78,78	0
58	MG	1F	315	1/1	0.83	0.22	57,57,57,57	0
58	MG	1A	3378	1/1	0.83	0.14	55,55,55,55	0
58	MG	1A	3756	1/1	0.83	0.18	57,57,57,57	0
58	MG	1A	3661	1/1	0.83	0.40	60,60,60,60	0
58	MG	2A	3263	1/1	0.83	0.31	67,67,67,67	0
58	MG	1A	3261	1/1	0.83	0.15	44,44,44,44	0
58	MG	1A	3080	1/1	0.83	0.29	45,45,45,45	0
58	MG	1A	3277	1/1	0.83	0.10	62,62,62,62	0
58	MG	1A	3146	1/1	0.83	0.19	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3184	1/1	0.83	0.18	68,68,68,68	0
58	MG	2a	1639	1/1	0.83	0.14	76,76,76,76	0
58	MG	1A	4026	1/1	0.83	0.31	59,59,59,59	0
58	MG	2A	3795	1/1	0.83	0.21	81,81,81,81	0
58	MG	1A	3236	1/1	0.83	0.43	62,62,62,62	0
58	MG	2A	3281	1/1	0.83	0.71	66,66,66,66	0
58	MG	2A	3083	1/1	0.83	0.20	51,51,51,51	0
58	MG	2A	3190	1/1	0.83	0.28	64,64,64,64	0
58	MG	2A	3287	1/1	0.83	0.11	63,63,63,63	0
58	MG	10	109	1/1	0.83	0.51	72,72,72,72	0
58	MG	2A	3809	1/1	0.83	0.06	65,65,65,65	0
58	MG	2A	3086	1/1	0.83	0.16	82,82,82,82	0
58	MG	2A	3464	1/1	0.83	0.28	55,55,55,55	0
58	MG	1a	1611	1/1	0.84	0.09	79,79,79,79	0
58	MG	2a	1666	1/1	0.84	0.18	77,77,77,77	0
58	MG	2A	3136	1/1	0.84	0.27	69,69,69,69	0
58	MG	2A	3343	1/1	0.84	0.20	70,70,70,70	0
58	MG	2A	3789	1/1	0.84	0.17	69,69,69,69	0
58	MG	1A	4050	1/1	0.84	0.21	66,66,66,66	0
58	MG	2A	3148	1/1	0.84	0.19	53,53,53,53	0
58	MG	2A	3150	1/1	0.84	0.09	76,76,76,76	0
58	MG	2A	3153	1/1	0.84	0.11	55,55,55,55	0
58	MG	1A	3297	1/1	0.84	0.42	65,65,65,65	0
58	MG	1A	3686	1/1	0.84	0.14	55,55,55,55	0
58	MG	2a	1687	1/1	0.84	0.14	77,77,77,77	0
58	MG	1A	3897	1/1	0.84	0.14	79,79,79,79	0
58	MG	1A	3534	1/1	0.84	0.43	43,43,43,43	0
58	MG	2A	3806	1/1	0.84	0.17	52,52,52,52	0
58	MG	1A	3706	1/1	0.84	0.23	50,50,50,50	0
58	MG	1A	3537	1/1	0.84	0.15	49,49,49,49	0
58	MG	2A	3602	1/1	0.84	0.09	78,78,78,78	0
58	MG	1A	3972	1/1	0.84	0.10	63,63,63,63	0
58	MG	2A	3386	1/1	0.84	0.37	66,66,66,66	0
58	MG	1A	3198	1/1	0.84	0.27	45,45,45,45	0
58	MG	1G	202	1/1	0.84	0.21	68,68,68,68	0
58	MG	2A	3267	1/1	0.84	0.80	60,60,60,60	0
58	MG	2A	3393	1/1	0.84	0.18	71,71,71,71	0
58	MG	1N	202	1/1	0.84	0.21	52,52,52,52	0
58	MG	1A	3827	1/1	0.84	0.13	39,39,39,39	0
58	MG	1O	206	1/1	0.84	0.27	76,76,76,76	0
58	MG	2a	1717	1/1	0.84	0.33	70,70,70,70	0
58	MG	1A	3461	1/1	0.84	0.23	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1808	1/1	0.84	0.16	75,75,75,75	0
58	MG	2A	3409	1/1	0.84	0.15	69,69,69,69	0
58	MG	2A	3178	1/1	0.84	0.22	78,78,78,78	0
58	MG	2a	1724	1/1	0.84	0.38	76,76,76,76	0
58	MG	2A	3415	1/1	0.84	0.21	50,50,50,50	0
58	MG	1A	3383	1/1	0.84	0.33	70,70,70,70	0
58	MG	2A	3277	1/1	0.84	0.12	77,77,77,77	0
58	MG	1A	4097	1/1	0.84	0.11	44,44,44,44	0
58	MG	2a	1744	1/1	0.84	0.12	77,77,77,77	0
58	MG	1U	203	1/1	0.84	0.24	56,56,56,56	0
58	MG	2E	308	1/1	0.84	0.12	75,75,75,75	0
58	MG	1A	3347	1/1	0.84	1.26	59,59,59,59	0
58	MG	2A	3186	1/1	0.84	0.23	77,77,77,77	0
58	MG	1a	1675	1/1	0.84	0.27	64,64,64,64	0
58	MG	1V	203	1/1	0.84	0.42	48,48,48,48	0
58	MG	1a	1678	1/1	0.84	0.15	61,61,61,61	0
58	MG	1A	3848	1/1	0.84	0.15	65,65,65,65	0
58	MG	2V	201	1/1	0.84	0.72	54,54,54,54	0
58	MG	2A	3194	1/1	0.84	0.10	67,67,67,67	0
58	MG	1A	3348	1/1	0.84	0.15	59,59,59,59	0
58	MG	1A	3923	1/1	0.84	0.12	77,77,77,77	0
58	MG	2A	3508	1/1	0.84	0.27	72,72,72,72	0
58	MG	1A	3514	1/1	0.84	0.15	40,40,40,40	0
58	MG	2A	3701	1/1	0.84	0.12	59,59,59,59	0
58	MG	27	104	1/1	0.84	0.16	70,70,70,70	0
58	MG	1m	3001	1/1	0.84	0.10	66,66,66,66	0
58	MG	2A	3208	1/1	0.84	0.17	60,60,60,60	0
58	MG	10	105	1/1	0.84	0.30	62,62,62,62	0
58	MG	2A	3710	1/1	0.84	0.19	65,65,65,65	0
58	MG	1w	101	1/1	0.84	0.20	82,82,82,82	0
58	MG	1A	3374	1/1	0.84	0.19	65,65,65,65	0
58	MG	1A	3868	1/1	0.84	0.10	52,52,52,52	0
58	MG	2A	3534	1/1	0.84	0.32	46,46,46,46	0
58	MG	1A	3279	1/1	0.84	0.23	54,54,54,54	0
58	MG	2A	3538	1/1	0.84	0.31	57,57,57,57	0
58	MG	1a	1713	1/1	0.84	0.17	77,77,77,77	0
58	MG	2A	3721	1/1	0.84	0.26	41,41,41,41	0
58	MG	1A	3576	1/1	0.84	0.11	59,59,59,59	0
58	MG	1A	3526	1/1	0.84	0.50	54,54,54,54	0
58	MG	2a	1627	1/1	0.84	0.13	72,72,72,72	0
58	MG	1A	3529	1/1	0.84	0.20	66,66,66,66	0
58	MG	1A	4028	1/1	0.84	0.20	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3775	1/1	0.84	0.24	63,63,63,63	0
58	MG	1a	1728	1/1	0.84	0.13	78,78,78,78	0
58	MG	2A	3329	1/1	0.84	0.11	69,69,69,69	0
58	MG	1a	1603	1/1	0.84	0.14	63,63,63,63	0
58	MG	1A	3449	1/1	0.84	0.20	47,47,47,47	0
58	MG	1A	3390	1/1	0.84	0.24	63,63,63,63	0
58	MG	2A	3767	1/1	0.84	0.13	82,82,82,82	0
58	MG	2A	3814	1/1	0.85	0.09	69,69,69,69	0
58	MG	2A	3637	1/1	0.85	0.35	77,77,77,77	0
58	MG	2A	3820	1/1	0.85	0.23	79,79,79,79	0
58	MG	1a	1650	1/1	0.85	0.19	71,71,71,71	0
58	MG	2a	1680	1/1	0.85	0.10	57,57,57,57	0
58	MG	1A	3444	1/1	0.85	0.14	58,58,58,58	0
58	MG	2A	3644	1/1	0.85	0.28	68,68,68,68	0
58	MG	1a	1765	1/1	0.85	0.08	73,73,73,73	0
58	MG	2A	3128	1/1	0.85	0.28	52,52,52,52	0
58	MG	1A	3763	1/1	0.85	0.12	53,53,53,53	0
58	MG	1B	210	1/1	0.85	0.53	64,64,64,64	0
58	MG	1a	1662	1/1	0.85	0.26	66,66,66,66	0
58	MG	2A	3142	1/1	0.85	0.22	63,63,63,63	0
58	MG	1A	3343	1/1	0.85	0.30	46,46,46,46	0
58	MG	1A	3643	1/1	0.85	0.08	50,50,50,50	0
58	MG	2B	218	1/1	0.85	0.26	87,87,87,87	0
58	MG	2A	3322	1/1	0.85	0.11	77,77,77,77	0
58	MG	1A	3550	1/1	0.85	0.24	55,55,55,55	0
58	MG	2A	3676	1/1	0.85	0.22	63,63,63,63	0
58	MG	2D	306	1/1	0.85	0.34	64,64,64,64	0
58	MG	1A	3350	1/1	0.85	0.20	50,50,50,50	0
58	MG	1A	3784	1/1	0.85	0.12	56,56,56,56	0
58	MG	1a	1801	1/1	0.85	0.11	64,64,64,64	0
58	MG	2A	3531	1/1	0.85	0.34	67,67,67,67	0
58	MG	1A	3452	1/1	0.85	0.47	55,55,55,55	0
58	MG	2F	305	1/1	0.85	0.34	60,60,60,60	0
58	MG	1A	3386	1/1	0.85	0.18	59,59,59,59	0
58	MG	2A	3051	1/1	0.85	0.12	59,59,59,59	0
58	MG	2A	3540	1/1	0.85	0.25	51,51,51,51	0
58	MG	2A	3546	1/1	0.85	0.22	50,50,50,50	0
58	MG	1B	235	1/1	0.85	0.18	76,76,76,76	0
58	MG	2A	3252	1/1	0.85	0.14	74,74,74,74	0
58	MG	2a	1735	1/1	0.85	0.24	86,86,86,86	0
58	MG	1B	236	1/1	0.85	0.15	57,57,57,57	0
58	MG	2A	3560	1/1	0.85	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	2A	3340	1/1	0.85	0.20	71,71,71,71	0
58	MG	2a	1764	1/1	0.85	0.14	78,78,78,78	0
58	MG	1A	3426	1/1	0.85	0.25	56,56,56,56	0
58	MG	2A	3256	1/1	0.85	0.13	67,67,67,67	0
58	MG	1a	1812	1/1	0.85	0.19	90,90,90,90	0
58	MG	28	103	1/1	0.85	0.30	56,56,56,56	0
58	MG	1a	1684	1/1	0.85	0.16	58,58,58,58	0
58	MG	1A	3996	1/1	0.85	0.18	73,73,73,73	0
58	MG	1A	3660	1/1	0.85	0.12	67,67,67,67	0
58	MG	1A	4094	1/1	0.85	0.09	57,57,57,57	0
58	MG	2a	1612	1/1	0.85	0.14	74,74,74,74	0
58	MG	1a	1605	1/1	0.85	0.17	68,68,68,68	0
58	MG	2a	1802	1/1	0.85	0.08	70,70,70,70	0
58	MG	1E	311	1/1	0.85	0.24	49,49,49,49	0
58	MG	1A	3813	1/1	0.85	0.13	47,47,47,47	0
58	MG	1A	3149	1/1	0.85	0.24	61,61,61,61	0
58	MG	1A	3116	1/1	0.85	0.28	37,37,37,37	0
58	MG	1A	3949	1/1	0.85	0.18	39,39,39,39	0
58	MG	1A	4015	1/1	0.85	0.17	53,53,53,53	0
58	MG	2A	3087	1/1	0.85	0.16	64,64,64,64	0
58	MG	2a	1823	1/1	0.85	0.14	79,79,79,79	0
58	MG	1A	3187	1/1	0.85	0.39	72,72,72,72	0
58	MG	1A	3839	1/1	0.85	0.22	34,34,34,34	0
58	MG	1a	1723	1/1	0.85	0.17	71,71,71,71	0
58	MG	1A	3512	1/1	0.85	0.44	46,46,46,46	0
58	MG	1A	3960	1/1	0.85	0.12	66,66,66,66	0
58	MG	2a	1632	1/1	0.85	0.12	79,79,79,79	0
58	MG	1a	1630	1/1	0.85	0.27	70,70,70,70	0
58	MG	1a	1636	1/1	0.85	0.11	76,76,76,76	0
58	MG	2A	3103	1/1	0.85	0.23	54,54,54,54	0
58	MG	2A	3410	1/1	0.85	0.20	75,75,75,75	0
58	MG	1a	1638	1/1	0.85	0.19	65,65,65,65	0
58	MG	2n	101	1/1	0.85	0.17	74,74,74,74	0
58	MG	2p	101	1/1	0.85	0.19	76,76,76,76	0
58	MG	1a	1741	1/1	0.85	0.10	59,59,59,59	0
58	MG	2A	3297	1/1	0.85	0.29	61,61,61,61	0
58	MG	2a	1654	1/1	0.85	0.10	65,65,65,65	0
58	MG	1A	3205	1/1	0.85	0.13	48,48,48,48	0
58	MG	2a	1665	1/1	0.85	0.19	86,86,86,86	0
58	MG	2A	3300	1/1	0.85	0.54	69,69,69,69	0
58	MG	2x	102	1/1	0.85	0.21	49,49,49,49	0
58	MG	2A	3216	1/1	0.85	0.29	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3438	1/1	0.85	0.27	58,58,58,58	0
58	MG	2A	3635	1/1	0.85	0.19	67,67,67,67	0
58	MG	1a	1644	1/1	0.85	0.11	62,62,62,62	0
60	ZN	24	501	1/1	0.85	0.07	126,126,126,126	0
58	MG	2A	3299	1/1	0.86	0.17	72,72,72,72	0
58	MG	2A	3736	1/1	0.86	0.16	65,65,65,65	0
58	MG	1A	3120	1/1	0.86	0.24	52,52,52,52	0
58	MG	2A	3738	1/1	0.86	0.11	61,61,61,61	0
58	MG	2A	3527	1/1	0.86	0.13	79,79,79,79	0
58	MG	2A	3037	1/1	0.86	0.14	56,56,56,56	0
58	MG	1A	3903	1/1	0.86	0.18	51,51,51,51	0
58	MG	2A	3040	1/1	0.86	0.10	77,77,77,77	0
58	MG	1a	1733	1/1	0.86	0.12	62,62,62,62	0
58	MG	1A	3209	1/1	0.86	0.28	57,57,57,57	0
58	MG	2A	3542	1/1	0.86	0.13	51,51,51,51	0
58	MG	1A	3792	1/1	0.86	0.16	64,64,64,64	0
58	MG	1a	1745	1/1	0.86	0.10	60,60,60,60	0
58	MG	2A	3775	1/1	0.86	0.15	73,73,73,73	0
58	MG	2A	3779	1/1	0.86	0.22	61,61,61,61	0
58	MG	1a	1746	1/1	0.86	0.12	61,61,61,61	0
58	MG	2A	3552	1/1	0.86	0.14	67,67,67,67	0
58	MG	1A	3456	1/1	0.86	0.17	36,36,36,36	0
58	MG	1A	3689	1/1	0.86	0.25	30,30,30,30	0
58	MG	1A	4016	1/1	0.86	0.14	70,70,70,70	0
58	MG	1A	3382	1/1	0.86	0.21	49,49,49,49	0
58	MG	2A	3058	1/1	0.86	0.19	38,38,38,38	0
58	MG	1A	3808	1/1	0.86	0.20	61,61,61,61	0
58	MG	2A	3323	1/1	0.86	0.16	79,79,79,79	0
58	MG	1A	3316	1/1	0.86	0.21	49,49,49,49	0
58	MG	1A	3708	1/1	0.86	0.23	28,28,28,28	0
58	MG	1A	3817	1/1	0.86	0.09	45,45,45,45	0
58	MG	2a	1697	1/1	0.86	0.17	65,65,65,65	0
58	MG	1a	1627	1/1	0.86	0.13	66,66,66,66	0
58	MG	1E	302	1/1	0.86	0.28	47,47,47,47	0
58	MG	1A	3049	1/1	0.86	0.47	57,57,57,57	0
58	MG	2A	3078	1/1	0.86	0.19	59,59,59,59	0
58	MG	2A	3333	1/1	0.86	0.32	63,63,63,63	0
58	MG	1A	3473	1/1	0.86	0.45	47,47,47,47	0
58	MG	1A	3715	1/1	0.86	0.24	35,35,35,35	0
58	MG	1F	304	1/1	0.86	0.22	63,63,63,63	0
58	MG	1A	3716	1/1	0.86	0.20	37,37,37,37	0
58	MG	2A	3592	1/1	0.86	0.21	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1803	1/1	0.86	0.11	75,75,75,75	0
58	MG	1F	312	1/1	0.86	0.29	42,42,42,42	0
58	MG	1F	313	1/1	0.86	0.12	54,54,54,54	0
58	MG	2A	3353	1/1	0.86	0.29	70,70,70,70	0
58	MG	1A	3846	1/1	0.86	0.16	57,57,57,57	0
58	MG	1a	1655	1/1	0.86	0.23	76,76,76,76	0
58	MG	1a	1810	1/1	0.86	0.16	73,73,73,73	0
58	MG	1A	3085	1/1	0.86	0.13	68,68,68,68	0
58	MG	1A	3728	1/1	0.86	0.19	67,67,67,67	0
58	MG	2A	3372	1/1	0.86	0.25	60,60,60,60	0
58	MG	2a	1738	1/1	0.86	0.27	60,60,60,60	0
58	MG	1I	201	1/1	0.86	0.08	67,67,67,67	0
58	MG	2B	220	1/1	0.86	0.13	74,74,74,74	0
58	MG	1A	3631	1/1	0.86	0.19	49,49,49,49	0
58	MG	2a	1756	1/1	0.86	0.19	64,64,64,64	0
58	MG	1A	3014	1/1	0.86	0.38	50,50,50,50	0
58	MG	1A	3194	1/1	0.86	0.12	65,65,65,65	0
58	MG	2A	3382	1/1	0.86	0.20	75,75,75,75	0
58	MG	1Q	204	1/1	0.86	0.28	72,72,72,72	0
58	MG	2a	1786	1/1	0.86	0.15	71,71,71,71	0
58	MG	2A	3109	1/1	0.86	0.24	70,70,70,70	0
58	MG	1a	1669	1/1	0.86	0.19	47,47,47,47	0
58	MG	1a	1670	1/1	0.86	0.17	73,73,73,73	0
58	MG	1R	203	1/1	0.86	0.32	44,44,44,44	0
58	MG	2A	3118	1/1	0.86	0.07	64,64,64,64	0
58	MG	2A	3120	1/1	0.86	0.51	51,51,51,51	0
58	MG	2a	1800	1/1	0.86	0.20	67,67,67,67	0
58	MG	2A	3647	1/1	0.86	0.19	66,66,66,66	0
58	MG	1R	206	1/1	0.86	0.07	75,75,75,75	0
58	MG	1A	3743	1/1	0.86	0.20	27,27,27,27	0
58	MG	1n	101	1/1	0.86	0.17	59,59,59,59	0
58	MG	1A	3164	1/1	0.86	0.20	40,40,40,40	0
58	MG	1A	3961	1/1	0.86	0.17	78,78,78,78	0
58	MG	26	101	1/1	0.86	0.11	68,68,68,68	0
58	MG	1A	3870	1/1	0.86	0.09	66,66,66,66	0
58	MG	1w	107	1/1	0.86	0.13	59,59,59,59	0
58	MG	1U	205	1/1	0.86	0.32	54,54,54,54	0
58	MG	2A	3269	1/1	0.86	0.15	60,60,60,60	0
58	MG	1A	3246	1/1	0.86	0.18	77,77,77,77	0
58	MG	2A	3147	1/1	0.86	0.22	67,67,67,67	0
58	MG	2A	3689	1/1	0.86	0.27	63,63,63,63	0
58	MG	2A	3467	1/1	0.86	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
58	MG	1A	3025	1/1	0.86	0.19	77,77,77,77	0
58	MG	2a	1611	1/1	0.86	0.20	77,77,77,77	0
58	MG	1A	3437	1/1	0.86	0.16	52,52,52,52	0
58	MG	1A	3888	1/1	0.86	0.18	34,34,34,34	0
58	MG	1x	108	1/1	0.86	0.21	32,32,32,32	0
58	MG	1X	101	1/1	0.86	0.48	50,50,50,50	0
58	MG	2A	3490	1/1	0.86	0.28	60,60,60,60	0
58	MG	2A	3493	1/1	0.86	0.17	62,62,62,62	0
58	MG	1A	3370	1/1	0.86	0.15	49,49,49,49	0
58	MG	1A	3439	1/1	0.86	0.11	52,52,52,52	0
58	MG	1A	3092	1/1	0.86	0.23	71,71,71,71	0
58	MG	1A	3978	1/1	0.86	0.08	52,52,52,52	0
58	MG	2a	1625	1/1	0.86	0.18	70,70,70,70	0
58	MG	1A	3446	1/1	0.86	0.20	64,64,64,64	0
58	MG	1A	3059	1/1	0.86	0.23	67,67,67,67	0
58	MG	2a	1629	1/1	0.86	0.16	73,73,73,73	0
58	MG	2x	104	1/1	0.86	0.26	68,68,68,68	0
58	MG	1A	3781	1/1	0.86	0.12	63,63,63,63	0
58	MG	1A	3083	1/1	0.86	0.35	49,49,49,49	0
58	MG	1B	208	1/1	0.86	0.11	68,68,68,68	0
58	MG	1A	3587	1/1	0.86	0.28	56,56,56,56	0
58	MG	1A	3747	1/1	0.87	0.19	52,52,52,52	0
58	MG	1A	3027	1/1	0.87	0.18	42,42,42,42	0
58	MG	1A	3754	1/1	0.87	0.20	69,69,69,69	0
58	MG	1A	3951	1/1	0.87	0.13	32,32,32,32	0
58	MG	2A	3264	1/1	0.87	0.19	61,61,61,61	0
58	MG	2A	3265	1/1	0.87	0.13	85,85,85,85	0
58	MG	1A	3952	1/1	0.87	0.24	48,48,48,48	0
58	MG	1A	3307	1/1	0.87	0.19	51,51,51,51	0
58	MG	2A	3815	1/1	0.87	0.12	77,77,77,77	0
58	MG	2A	3031	1/1	0.87	0.27	49,49,49,49	0
58	MG	2A	3402	1/1	0.87	0.14	77,77,77,77	0
58	MG	2A	3032	1/1	0.87	0.32	53,53,53,53	0
58	MG	1A	3440	1/1	0.87	0.20	46,46,46,46	0
58	MG	1a	1634	1/1	0.87	0.37	81,81,81,81	0
58	MG	1A	3552	1/1	0.87	0.24	43,43,43,43	0
58	MG	1A	3402	1/1	0.87	0.14	59,59,59,59	0
58	MG	1A	3882	1/1	0.87	0.20	59,59,59,59	0
58	MG	1A	3555	1/1	0.87	0.13	41,41,41,41	0
58	MG	2a	1702	1/1	0.87	0.21	59,59,59,59	0
58	MG	1A	4091	1/1	0.87	0.06	46,46,46,46	0
58	MG	2A	3449	1/1	0.87	0.24	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3494	1/1	0.87	0.17	80,80,80,80	0
58	MG	1Q	203	1/1	0.87	0.14	45,45,45,45	0
58	MG	2A	3462	1/1	0.87	0.15	52,52,52,52	0
58	MG	1A	3309	1/1	0.87	0.25	48,48,48,48	0
58	MG	1a	1790	1/1	0.87	0.06	57,57,57,57	0
58	MG	2A	3181	1/1	0.87	0.21	70,70,70,70	0
58	MG	1A	3684	1/1	0.87	0.05	60,60,60,60	0
58	MG	2D	305	1/1	0.87	0.15	68,68,68,68	0
58	MG	1A	3891	1/1	0.87	0.12	71,71,71,71	0
58	MG	1A	3240	1/1	0.87	0.09	62,62,62,62	0
58	MG	1a	1663	1/1	0.87	0.27	70,70,70,70	0
58	MG	2E	306	1/1	0.87	0.20	73,73,73,73	0
58	MG	1A	3974	1/1	0.87	0.18	59,59,59,59	0
58	MG	1A	3414	1/1	0.87	0.19	61,61,61,61	0
58	MG	2a	1730	1/1	0.87	0.20	80,80,80,80	0
58	MG	1T	204	1/1	0.87	0.13	65,65,65,65	0
58	MG	2A	3302	1/1	0.87	0.47	83,83,83,83	0
58	MG	2A	3678	1/1	0.87	0.15	67,67,67,67	0
58	MG	1A	4107	1/1	0.87	0.18	53,53,53,53	0
58	MG	2R	201	1/1	0.87	0.12	70,70,70,70	0
58	MG	1A	3038	1/1	0.87	0.17	38,38,38,38	0
58	MG	2A	3505	1/1	0.87	0.25	69,69,69,69	0
58	MG	1U	207	1/1	0.87	0.32	41,41,41,41	0
58	MG	2a	1765	1/1	0.87	0.21	68,68,68,68	0
58	MG	1A	3704	1/1	0.87	0.31	60,60,60,60	0
58	MG	1A	3077	1/1	0.87	0.30	53,53,53,53	0
58	MG	2A	3204	1/1	0.87	0.46	68,68,68,68	0
58	MG	2a	1784	1/1	0.87	0.09	80,80,80,80	0
58	MG	2A	3515	1/1	0.87	0.23	59,59,59,59	0
58	MG	1A	3522	1/1	0.87	0.61	68,68,68,68	0
58	MG	2A	3706	1/1	0.87	0.10	79,79,79,79	0
58	MG	1A	3050	1/1	0.87	0.14	58,58,58,58	0
58	MG	2A	3520	1/1	0.87	0.20	76,76,76,76	0
58	MG	1A	3082	1/1	0.87	0.23	46,46,46,46	0
58	MG	2a	1602	1/1	0.87	0.23	77,77,77,77	0
58	MG	2A	3212	1/1	0.87	0.19	61,61,61,61	0
58	MG	1A	3051	1/1	0.87	0.18	53,53,53,53	0
58	MG	1A	3294	1/1	0.87	0.28	59,59,59,59	0
58	MG	1A	3425	1/1	0.87	0.34	53,53,53,53	0
58	MG	1B	212	1/1	0.87	0.38	69,69,69,69	0
58	MG	1A	3727	1/1	0.87	0.21	61,61,61,61	0
58	MG	1d	301	1/1	0.87	0.11	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1813	1/1	0.87	0.16	75,75,75,75	0
58	MG	1e	201	1/1	0.87	0.20	81,81,81,81	0
58	MG	1l	202	1/1	0.87	0.19	62,62,62,62	0
58	MG	2a	1818	1/1	0.87	0.10	67,67,67,67	0
58	MG	1a	1691	1/1	0.87	0.12	69,69,69,69	0
58	MG	1A	3829	1/1	0.87	0.20	40,40,40,40	0
58	MG	1r	101	1/1	0.87	0.07	81,81,81,81	0
58	MG	12	102	1/1	0.87	0.28	54,54,54,54	0
58	MG	1A	3103	1/1	0.87	0.16	38,38,38,38	0
58	MG	2A	3233	1/1	0.87	0.16	57,57,57,57	0
58	MG	1a	1706	1/1	0.87	0.13	79,79,79,79	0
58	MG	15	108	1/1	0.87	0.13	64,64,64,64	0
58	MG	1A	3479	1/1	0.87	0.17	79,79,79,79	0
58	MG	1A	3356	1/1	0.87	0.38	77,77,77,77	0
58	MG	1A	3845	1/1	0.87	0.27	34,34,34,34	0
58	MG	1A	3233	1/1	0.87	0.44	50,50,50,50	0
58	MG	2A	3771	1/1	0.87	0.34	72,72,72,72	0
58	MG	1A	4019	1/1	0.87	0.11	30,30,30,30	0
58	MG	2n	102	1/1	0.87	0.09	79,79,79,79	0
58	MG	1A	3109	1/1	0.87	0.74	60,60,60,60	0
58	MG	1A	3934	1/1	0.87	0.16	64,64,64,64	0
58	MG	2A	3364	1/1	0.87	0.40	51,51,51,51	0
58	MG	1D	306	1/1	0.87	0.33	42,42,42,42	0
58	MG	1A	3391	1/1	0.87	0.19	72,72,72,72	0
58	MG	2a	1645	1/1	0.87	0.14	50,50,50,50	0
58	MG	2A	3371	1/1	0.87	0.16	57,57,57,57	0
58	MG	1A	3369	1/1	0.87	0.31	52,52,52,52	0
58	MG	2A	3005	1/1	0.87	0.20	70,70,70,70	0
58	MG	2a	1662	1/1	0.87	0.31	57,57,57,57	0
58	MG	2A	3588	1/1	0.87	0.22	60,60,60,60	0
58	MG	1A	3861	1/1	0.87	0.19	33,33,33,33	0
58	MG	1a	1739	1/1	0.87	0.15	77,77,77,77	0
58	MG	2A	3801	1/1	0.87	0.05	67,67,67,67	0
58	MG	2A	3611	1/1	0.88	0.38	70,70,70,70	0
58	MG	1A	3360	1/1	0.88	0.13	36,36,36,36	0
58	MG	2A	3424	1/1	0.88	0.18	54,54,54,54	0
58	MG	1A	3789	1/1	0.88	0.10	70,70,70,70	0
58	MG	1A	3607	1/1	0.88	0.24	34,34,34,34	0
58	MG	2a	1681	1/1	0.88	0.26	69,69,69,69	0
58	MG	1A	3226	1/1	0.88	0.34	56,56,56,56	0
58	MG	1A	4092	1/1	0.88	0.28	81,81,81,81	0
58	MG	2A	3457	1/1	0.88	0.22	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4093	1/1	0.88	0.10	66,66,66,66	0
58	MG	1A	3465	1/1	0.88	0.24	48,48,48,48	0
58	MG	1A	3308	1/1	0.88	0.21	56,56,56,56	0
58	MG	2A	3206	1/1	0.88	0.08	69,69,69,69	0
58	MG	1x	101	1/1	0.88	0.24	70,70,70,70	0
58	MG	1a	1738	1/1	0.88	0.09	59,59,59,59	0
58	MG	2A	3486	1/1	0.88	0.09	68,68,68,68	0
58	MG	1A	3803	1/1	0.88	0.25	62,62,62,62	0
58	MG	1A	3364	1/1	0.88	0.19	56,56,56,56	0
58	MG	1R	201	1/1	0.88	0.24	45,45,45,45	0
58	MG	1A	3282	1/1	0.88	0.39	62,62,62,62	0
58	MG	1A	3173	1/1	0.88	0.14	58,58,58,58	0
58	MG	1a	1748	1/1	0.88	0.10	73,73,73,73	0
58	MG	1x	113	1/1	0.88	0.13	71,71,71,71	0
58	MG	1a	1642	1/1	0.88	0.20	64,64,64,64	0
58	MG	1A	3432	1/1	0.88	0.19	52,52,52,52	0
58	MG	1A	3289	1/1	0.88	0.08	45,45,45,45	0
58	MG	2A	3226	1/1	0.88	0.19	63,63,63,63	0
58	MG	2E	305	1/1	0.88	0.23	76,76,76,76	0
58	MG	1A	3252	1/1	0.88	0.15	73,73,73,73	0
58	MG	1A	3984	1/1	0.88	0.11	59,59,59,59	0
58	MG	1A	3986	1/1	0.88	0.34	45,45,45,45	0
58	MG	2A	3517	1/1	0.88	0.21	71,71,71,71	0
58	MG	1A	3909	1/1	0.88	0.14	47,47,47,47	0
58	MG	2F	308	1/1	0.88	0.30	69,69,69,69	0
58	MG	2A	3232	1/1	0.88	0.22	66,66,66,66	0
58	MG	2A	3129	1/1	0.88	0.23	45,45,45,45	0
58	MG	1A	3912	1/1	0.88	0.34	64,64,64,64	0
58	MG	2a	1737	1/1	0.88	0.16	53,53,53,53	0
58	MG	2T	201	1/1	0.88	0.15	69,69,69,69	0
58	MG	2A	3702	1/1	0.88	0.21	65,65,65,65	0
58	MG	2T	203	1/1	0.88	0.24	60,60,60,60	0
58	MG	2A	3018	1/1	0.88	0.27	43,43,43,43	0
58	MG	1A	3174	1/1	0.88	0.22	71,71,71,71	0
58	MG	2a	1763	1/1	0.88	0.15	75,75,75,75	0
58	MG	2V	202	1/1	0.88	0.32	67,67,67,67	0
58	MG	2A	3137	1/1	0.88	0.29	56,56,56,56	0
58	MG	2X	102	1/1	0.88	0.18	53,53,53,53	0
58	MG	2A	3533	1/1	0.88	0.08	65,65,65,65	0
58	MG	1a	1771	1/1	0.88	0.12	52,52,52,52	0
58	MG	1A	3406	1/1	0.88	0.23	50,50,50,50	0
58	MG	2A	3338	1/1	0.88	0.44	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3175	1/1	0.88	0.10	77,77,77,77	0
58	MG	1A	3546	1/1	0.88	0.22	43,43,43,43	0
58	MG	1A	3144	1/1	0.88	0.17	42,42,42,42	0
58	MG	2A	3151	1/1	0.88	0.23	72,72,72,72	0
58	MG	2A	3352	1/1	0.88	0.07	78,78,78,78	0
58	MG	2A	3152	1/1	0.88	0.15	53,53,53,53	0
58	MG	2A	3724	1/1	0.88	0.14	49,49,49,49	0
58	MG	2A	3727	1/1	0.88	0.19	47,47,47,47	0
58	MG	1A	3491	1/1	0.88	0.34	57,57,57,57	0
58	MG	2a	1804	1/1	0.88	0.30	79,79,79,79	0
58	MG	2a	1806	1/1	0.88	0.06	66,66,66,66	0
58	MG	1A	3141	1/1	0.88	0.33	46,46,46,46	0
58	MG	1A	3928	1/1	0.88	0.23	34,34,34,34	0
58	MG	1A	3665	1/1	0.88	0.16	61,61,61,61	0
58	MG	1A	3331	1/1	0.88	0.13	63,63,63,63	0
58	MG	2a	1812	1/1	0.88	0.12	53,53,53,53	0
58	MG	1A	3855	1/1	0.88	0.15	61,61,61,61	0
58	MG	2A	3567	1/1	0.88	0.19	69,69,69,69	0
58	MG	1A	3857	1/1	0.88	0.13	45,45,45,45	0
58	MG	2A	3748	1/1	0.88	0.10	67,67,67,67	0
58	MG	1A	3450	1/1	0.88	0.61	56,56,56,56	0
58	MG	2A	3750	1/1	0.88	0.24	74,74,74,74	0
58	MG	1a	1682	1/1	0.88	0.19	69,69,69,69	0
58	MG	15	102	1/1	0.88	0.24	47,47,47,47	0
58	MG	2A	3756	1/1	0.88	0.23	50,50,50,50	0
58	MG	2a	1834	1/1	0.88	0.23	85,85,85,85	0
58	MG	2a	1835	1/1	0.88	0.12	69,69,69,69	0
58	MG	1A	3677	1/1	0.88	0.09	49,49,49,49	0
58	MG	1A	3213	1/1	0.88	0.17	47,47,47,47	0
58	MG	1A	3505	1/1	0.88	0.16	58,58,58,58	0
58	MG	1A	3771	1/1	0.88	0.17	54,54,54,54	0
58	MG	2A	3387	1/1	0.88	0.31	67,67,67,67	0
58	MG	2A	3388	1/1	0.88	0.22	38,38,38,38	0
58	MG	2A	3782	1/1	0.88	0.15	62,62,62,62	0
58	MG	2A	3389	1/1	0.88	0.17	62,62,62,62	0
58	MG	1A	3142	1/1	0.88	0.47	44,44,44,44	0
58	MG	2a	1640	1/1	0.88	0.14	69,69,69,69	0
58	MG	2A	3068	1/1	0.88	0.15	62,62,62,62	0
58	MG	1A	3778	1/1	0.88	0.24	63,63,63,63	0
58	MG	1a	1703	1/1	0.88	0.18	69,69,69,69	0
58	MG	2A	3182	1/1	0.88	0.21	64,64,64,64	0
58	MG	1a	1604	1/1	0.88	0.22	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3278	1/1	0.88	0.21	81,81,81,81	0
58	MG	2A	3600	1/1	0.88	0.29	62,62,62,62	0
58	MG	2a	1663	1/1	0.88	0.15	76,76,76,76	0
58	MG	1A	3421	1/1	0.88	0.17	50,50,50,50	0
58	MG	1A	3357	1/1	0.88	0.47	50,50,50,50	0
58	MG	1A	3687	1/1	0.88	0.12	64,64,64,64	0
58	MG	1A	3957	1/1	0.88	0.20	45,45,45,45	0
58	MG	1A	3457	1/1	0.88	0.37	45,45,45,45	0
60	ZN	2Y	202	1/1	0.88	0.14	96,96,96,96	0
58	MG	2A	3289	1/1	0.88	0.11	85,85,85,85	0
58	MG	2A	3077	1/1	0.89	0.15	73,73,73,73	0
58	MG	1A	3467	1/1	0.89	0.12	57,57,57,57	0
58	MG	1a	1602	1/1	0.89	0.21	56,56,56,56	0
58	MG	1a	1695	1/1	0.89	0.19	56,56,56,56	0
58	MG	1a	1699	1/1	0.89	0.16	82,82,82,82	0
58	MG	1A	3902	1/1	0.89	0.20	72,72,72,72	0
58	MG	1F	306	1/1	0.89	0.24	43,43,43,43	0
58	MG	2a	1656	1/1	0.89	0.20	68,68,68,68	0
58	MG	1A	3744	1/1	0.89	0.20	48,48,48,48	0
58	MG	2a	1659	1/1	0.89	0.28	73,73,73,73	0
58	MG	1a	1606	1/1	0.89	0.25	70,70,70,70	0
58	MG	1l	201	1/1	0.89	0.11	81,81,81,81	0
58	MG	1A	3832	1/1	0.89	0.20	33,33,33,33	0
58	MG	1A	3569	1/1	0.89	0.27	39,39,39,39	0
58	MG	2A	3326	1/1	0.89	0.19	76,76,76,76	0
58	MG	1a	1715	1/1	0.89	0.10	67,67,67,67	0
58	MG	1A	3376	1/1	0.89	0.23	51,51,51,51	0
58	MG	2A	3770	1/1	0.89	0.18	96,96,96,96	0
58	MG	2A	3098	1/1	0.89	0.11	76,76,76,76	0
58	MG	1A	3667	1/1	0.89	0.16	56,56,56,56	0
58	MG	1G	201	1/1	0.89	0.21	42,42,42,42	0
58	MG	1A	3212	1/1	0.89	0.18	53,53,53,53	0
58	MG	1A	3751	1/1	0.89	0.10	51,51,51,51	0
58	MG	1A	3106	1/1	0.89	0.33	56,56,56,56	0
58	MG	1A	3320	1/1	0.89	0.48	51,51,51,51	0
58	MG	2A	3110	1/1	0.89	0.30	71,71,71,71	0
58	MG	2A	3564	1/1	0.89	0.22	63,63,63,63	0
58	MG	1A	3992	1/1	0.89	0.23	31,31,31,31	0
58	MG	1A	3527	1/1	0.89	0.15	44,44,44,44	0
58	MG	2A	3344	1/1	0.89	0.30	65,65,65,65	0
58	MG	2A	3345	1/1	0.89	0.32	79,79,79,79	0
58	MG	2A	3234	1/1	0.89	0.29	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3347	1/1	0.89	0.17	77,77,77,77	0
58	MG	1A	3599	1/1	0.89	0.25	41,41,41,41	0
58	MG	2a	1699	1/1	0.89	0.24	72,72,72,72	0
58	MG	2A	3574	1/1	0.89	0.15	49,49,49,49	0
58	MG	2A	3349	1/1	0.89	0.28	63,63,63,63	0
58	MG	2a	1703	1/1	0.89	0.19	74,74,74,74	0
58	MG	2A	3808	1/1	0.89	0.24	87,87,87,87	0
58	MG	1Q	206	1/1	0.89	0.17	57,57,57,57	0
58	MG	2A	3238	1/1	0.89	0.19	76,76,76,76	0
58	MG	1x	107	1/1	0.89	0.19	60,60,60,60	0
58	MG	2A	3581	1/1	0.89	0.14	71,71,71,71	0
58	MG	2A	3358	1/1	0.89	0.28	67,67,67,67	0
58	MG	2A	3359	1/1	0.89	0.26	59,59,59,59	0
58	MG	1A	3924	1/1	0.89	0.12	73,73,73,73	0
58	MG	2A	3123	1/1	0.89	0.30	50,50,50,50	0
58	MG	2a	1720	1/1	0.89	0.35	71,71,71,71	0
58	MG	1A	3215	1/1	0.89	0.32	63,63,63,63	0
58	MG	1x	111	1/1	0.89	0.12	49,49,49,49	0
58	MG	2A	3244	1/1	0.89	0.49	63,63,63,63	0
58	MG	1R	204	1/1	0.89	0.17	53,53,53,53	0
58	MG	1A	3858	1/1	0.89	0.14	39,39,39,39	0
58	MG	2A	3250	1/1	0.89	0.36	74,74,74,74	0
58	MG	2A	3251	1/1	0.89	0.18	76,76,76,76	0
58	MG	1A	3606	1/1	0.89	0.20	31,31,31,31	0
58	MG	2A	3003	1/1	0.89	0.38	56,56,56,56	0
58	MG	1A	3326	1/1	0.89	0.22	58,58,58,58	0
58	MG	2B	215	1/1	0.89	0.10	77,77,77,77	0
58	MG	2A	3383	1/1	0.89	0.23	49,49,49,49	0
58	MG	2A	3384	1/1	0.89	0.19	73,73,73,73	0
58	MG	1A	3217	1/1	0.89	0.31	40,40,40,40	0
58	MG	1a	1651	1/1	0.89	0.10	50,50,50,50	0
58	MG	2A	3007	1/1	0.89	0.21	56,56,56,56	0
58	MG	2A	3620	1/1	0.89	0.16	59,59,59,59	0
58	MG	1a	1757	1/1	0.89	0.12	86,86,86,86	0
58	MG	1A	3447	1/1	0.89	0.26	60,60,60,60	0
58	MG	2A	3149	1/1	0.89	0.24	60,60,60,60	0
58	MG	2a	1774	1/1	0.89	0.10	83,83,83,83	0
58	MG	1a	1654	1/1	0.89	0.18	68,68,68,68	0
58	MG	2E	303	1/1	0.89	0.20	48,48,48,48	0
58	MG	1A	3192	1/1	0.89	0.21	44,44,44,44	0
58	MG	1A	3224	1/1	0.89	0.40	67,67,67,67	0
58	MG	2A	3396	1/1	0.89	0.18	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3266	1/1	0.89	0.19	72,72,72,72	0
58	MG	2F	302	1/1	0.89	0.38	78,78,78,78	0
58	MG	2A	3401	1/1	0.89	0.20	72,72,72,72	0
58	MG	2A	3021	1/1	0.89	0.61	58,58,58,58	0
58	MG	1A	3119	1/1	0.89	0.22	64,64,64,64	0
58	MG	1A	3626	1/1	0.89	0.19	62,62,62,62	0
58	MG	1A	3711	1/1	0.89	0.21	46,46,46,46	0
58	MG	1B	218	1/1	0.89	0.16	57,57,57,57	0
58	MG	1a	1776	1/1	0.89	0.14	60,60,60,60	0
58	MG	1A	3283	1/1	0.89	0.21	68,68,68,68	0
58	MG	1A	3638	1/1	0.89	0.19	29,29,29,29	0
58	MG	2A	3421	1/1	0.89	0.44	65,65,65,65	0
58	MG	2A	3663	1/1	0.89	0.08	65,65,65,65	0
58	MG	2A	3664	1/1	0.89	0.19	77,77,77,77	0
58	MG	1a	1785	1/1	0.89	0.20	71,71,71,71	0
58	MG	2A	3427	1/1	0.89	0.17	83,83,83,83	0
58	MG	1A	3096	1/1	0.89	0.45	58,58,58,58	0
58	MG	2A	3669	1/1	0.89	0.17	46,46,46,46	0
58	MG	1a	1787	1/1	0.89	0.22	83,83,83,83	0
58	MG	1a	1788	1/1	0.89	0.14	61,61,61,61	0
58	MG	1A	3310	1/1	0.89	0.19	60,60,60,60	0
58	MG	2A	3682	1/1	0.89	0.09	67,67,67,67	0
58	MG	1A	3311	1/1	0.89	0.30	59,59,59,59	0
58	MG	10	107	1/1	0.89	0.09	63,63,63,63	0
58	MG	2a	1831	1/1	0.89	0.12	74,74,74,74	0
58	MG	1A	4043	1/1	0.89	0.13	58,58,58,58	0
58	MG	2A	3179	1/1	0.89	0.13	66,66,66,66	0
58	MG	2A	3695	1/1	0.89	0.09	59,59,59,59	0
58	MG	2A	3474	1/1	0.89	0.24	44,44,44,44	0
58	MG	2A	3290	1/1	0.89	0.10	86,86,86,86	0
58	MG	2A	3052	1/1	0.89	0.10	51,51,51,51	0
58	MG	2A	3480	1/1	0.89	0.28	73,73,73,73	0
58	MG	1A	4047	1/1	0.89	0.08	57,57,57,57	0
58	MG	2A	3054	1/1	0.89	0.11	74,74,74,74	0
58	MG	1A	3495	1/1	0.89	0.29	54,54,54,54	0
58	MG	1A	3110	1/1	0.89	0.16	45,45,45,45	0
58	MG	1a	1679	1/1	0.89	0.24	81,81,81,81	0
58	MG	1A	3314	1/1	0.89	0.28	65,65,65,65	0
58	MG	2A	3496	1/1	0.89	0.17	71,71,71,71	0
58	MG	1D	308	1/1	0.89	0.17	52,52,52,52	0
58	MG	1A	3814	1/1	0.89	0.21	51,51,51,51	0
58	MG	2A	3715	1/1	0.89	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3500	1/1	0.89	0.21	54,54,54,54	0
58	MG	1A	3462	1/1	0.89	0.20	63,63,63,63	0
58	MG	2x	101	1/1	0.89	0.67	76,76,76,76	0
58	MG	1a	1686	1/1	0.89	0.24	63,63,63,63	0
58	MG	1A	4064	1/1	0.89	0.15	60,60,60,60	0
58	MG	2A	3306	1/1	0.89	0.62	62,62,62,62	0
58	MG	2A	3723	1/1	0.89	0.39	67,67,67,67	0
58	MG	1A	3258	1/1	0.89	0.41	67,67,67,67	0
58	MG	2A	3310	1/1	0.89	0.16	54,54,54,54	0
58	MG	2A	3311	1/1	0.89	0.46	70,70,70,70	0
58	MG	2a	1638	1/1	0.89	0.21	56,56,56,56	0
58	MG	1a	1621	1/1	0.90	0.16	54,54,54,54	0
58	MG	2A	3772	1/1	0.90	0.19	65,65,65,65	0
58	MG	2A	3114	1/1	0.90	0.30	65,65,65,65	0
58	MG	1A	3475	1/1	0.90	0.50	38,38,38,38	0
58	MG	2A	3363	1/1	0.90	0.11	70,70,70,70	0
58	MG	1A	3229	1/1	0.90	0.10	47,47,47,47	0
58	MG	2A	3784	1/1	0.90	0.21	77,77,77,77	0
58	MG	1A	3536	1/1	0.90	0.52	46,46,46,46	0
58	MG	2A	3786	1/1	0.90	0.08	62,62,62,62	0
58	MG	1A	3896	1/1	0.90	0.21	58,58,58,58	0
58	MG	1A	3435	1/1	0.90	0.41	56,56,56,56	0
58	MG	2A	3792	1/1	0.90	0.17	66,66,66,66	0
58	MG	2a	1674	1/1	0.90	0.38	74,74,74,74	0
58	MG	2A	3793	1/1	0.90	0.19	80,80,80,80	0
58	MG	1x	110	1/1	0.90	0.21	72,72,72,72	0
58	MG	2A	3578	1/1	0.90	0.21	45,45,45,45	0
58	MG	1A	3722	1/1	0.90	0.23	67,67,67,67	0
58	MG	1A	3287	1/1	0.90	0.47	59,59,59,59	0
58	MG	1Q	201	1/1	0.90	0.28	40,40,40,40	0
58	MG	1a	1744	1/1	0.90	0.24	74,74,74,74	0
58	MG	2A	3002	1/1	0.90	0.59	71,71,71,71	0
58	MG	1a	1635	1/1	0.90	0.09	55,55,55,55	0
58	MG	1A	3211	1/1	0.90	0.23	49,49,49,49	0
58	MG	2A	3141	1/1	0.90	0.25	57,57,57,57	0
58	MG	1A	3290	1/1	0.90	0.20	60,60,60,60	0
58	MG	1A	3826	1/1	0.90	0.17	39,39,39,39	0
58	MG	1A	3061	1/1	0.90	0.23	48,48,48,48	0
58	MG	1A	3983	1/1	0.90	0.13	53,53,53,53	0
58	MG	1a	1643	1/1	0.90	0.16	67,67,67,67	0
58	MG	2A	3012	1/1	0.90	0.19	51,51,51,51	0
58	MG	2a	1701	1/1	0.90	0.27	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3105	1/1	0.90	0.15	40,40,40,40	0
58	MG	2A	3816	1/1	0.90	0.19	77,77,77,77	0
58	MG	1A	4105	1/1	0.90	0.13	40,40,40,40	0
58	MG	2A	3818	1/1	0.90	0.14	70,70,70,70	0
58	MG	1A	3445	1/1	0.90	0.21	54,54,54,54	0
58	MG	1A	3411	1/1	0.90	0.16	43,43,43,43	0
58	MG	1A	3163	1/1	0.90	0.21	52,52,52,52	0
58	MG	2A	3159	1/1	0.90	0.18	70,70,70,70	0
58	MG	2A	3613	1/1	0.90	0.14	67,67,67,67	0
58	MG	2A	3403	1/1	0.90	0.48	56,56,56,56	0
58	MG	2A	3619	1/1	0.90	0.20	74,74,74,74	0
58	MG	1A	3052	1/1	0.90	0.23	44,44,44,44	0
58	MG	2A	3029	1/1	0.90	0.24	52,52,52,52	0
58	MG	1A	3047	1/1	0.90	0.26	35,35,35,35	0
58	MG	2B	212	1/1	0.90	0.16	78,78,78,78	0
58	MG	1a	1775	1/1	0.90	0.09	66,66,66,66	0
58	MG	2A	3629	1/1	0.90	0.14	37,37,37,37	0
58	MG	2A	3630	1/1	0.90	0.22	59,59,59,59	0
58	MG	1A	3418	1/1	0.90	0.18	52,52,52,52	0
58	MG	2A	3034	1/1	0.90	0.24	44,44,44,44	0
58	MG	2a	1731	1/1	0.90	0.28	70,70,70,70	0
58	MG	2a	1732	1/1	0.90	0.12	68,68,68,68	0
58	MG	1A	3222	1/1	0.90	0.12	58,58,58,58	0
58	MG	2A	3419	1/1	0.90	0.31	58,58,58,58	0
58	MG	1a	1780	1/1	0.90	0.08	57,57,57,57	0
58	MG	1A	3299	1/1	0.90	0.18	36,36,36,36	0
58	MG	2A	3174	1/1	0.90	0.17	76,76,76,76	0
58	MG	2A	3041	1/1	0.90	0.22	59,59,59,59	0
58	MG	1A	3851	1/1	0.90	0.22	30,30,30,30	0
58	MG	2a	1755	1/1	0.90	0.20	66,66,66,66	0
58	MG	1V	208	1/1	0.90	0.23	55,55,55,55	0
58	MG	2a	1757	1/1	0.90	0.17	57,57,57,57	0
58	MG	1W	201	1/1	0.90	0.40	63,63,63,63	0
58	MG	1A	3502	1/1	0.90	0.21	45,45,45,45	0
58	MG	2A	3461	1/1	0.90	0.25	72,72,72,72	0
58	MG	2a	1770	1/1	0.90	0.14	77,77,77,77	0
58	MG	1A	4011	1/1	0.90	0.09	73,73,73,73	0
58	MG	1a	1791	1/1	0.90	0.13	66,66,66,66	0
58	MG	2a	1776	1/1	0.90	0.29	79,79,79,79	0
58	MG	1A	3247	1/1	0.90	0.31	37,37,37,37	0
58	MG	2A	3473	1/1	0.90	0.18	50,50,50,50	0
58	MG	1A	3856	1/1	0.90	0.20	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1B	221	1/1	0.90	0.22	69,69,69,69	0
58	MG	2A	3667	1/1	0.90	0.33	63,63,63,63	0
58	MG	1A	3932	1/1	0.90	0.21	37,37,37,37	0
58	MG	1a	1804	1/1	0.90	0.11	63,63,63,63	0
58	MG	1A	3757	1/1	0.90	0.14	68,68,68,68	0
58	MG	2A	3307	1/1	0.90	0.28	80,80,80,80	0
58	MG	2a	1797	1/1	0.90	0.06	78,78,78,78	0
58	MG	2A	3188	1/1	0.90	0.31	49,49,49,49	0
58	MG	2A	3681	1/1	0.90	0.05	72,72,72,72	0
58	MG	2A	3309	1/1	0.90	0.16	62,62,62,62	0
58	MG	10	108	1/1	0.90	0.15	49,49,49,49	0
58	MG	2A	3491	1/1	0.90	0.13	70,70,70,70	0
58	MG	2a	1805	1/1	0.90	0.10	77,77,77,77	0
58	MG	2A	3061	1/1	0.90	0.13	60,60,60,60	0
58	MG	1A	3330	1/1	0.90	0.11	59,59,59,59	0
58	MG	1A	4024	1/1	0.90	0.30	65,65,65,65	0
58	MG	1a	1681	1/1	0.90	0.18	70,70,70,70	0
58	MG	2A	3069	1/1	0.90	0.17	63,63,63,63	0
58	MG	2A	3316	1/1	0.90	0.12	78,78,78,78	0
58	MG	11	104	1/1	0.90	0.12	68,68,68,68	0
58	MG	2A	3201	1/1	0.90	0.15	46,46,46,46	0
58	MG	2A	3507	1/1	0.90	0.26	79,79,79,79	0
58	MG	1B	230	1/1	0.90	0.45	83,83,83,83	0
58	MG	1A	3938	1/1	0.90	0.13	43,43,43,43	0
58	MG	1A	3304	1/1	0.90	0.16	61,61,61,61	0
58	MG	2A	3076	1/1	0.90	0.14	47,47,47,47	0
58	MG	1A	3767	1/1	0.90	0.18	31,31,31,31	0
58	MG	1A	3459	1/1	0.90	0.25	63,63,63,63	0
58	MG	1A	3361	1/1	0.90	0.13	65,65,65,65	0
58	MG	17	104	1/1	0.90	0.22	67,67,67,67	0
58	MG	1A	3280	1/1	0.90	0.16	52,52,52,52	0
58	MG	1a	1823	1/1	0.90	0.07	69,69,69,69	0
58	MG	1A	3099	1/1	0.90	0.31	46,46,46,46	0
58	MG	2A	3085	1/1	0.90	0.40	69,69,69,69	0
58	MG	1a	1701	1/1	0.90	0.12	82,82,82,82	0
58	MG	1A	4044	1/1	0.90	0.26	57,57,57,57	0
58	MG	1A	3608	1/1	0.90	0.18	30,30,30,30	0
58	MG	2A	3336	1/1	0.90	0.30	47,47,47,47	0
58	MG	1a	1704	1/1	0.90	0.26	71,71,71,71	0
58	MG	1A	3875	1/1	0.90	0.16	49,49,49,49	0
58	MG	1A	4051	1/1	0.90	0.22	68,68,68,68	0
58	MG	1A	3699	1/1	0.90	0.23	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1n	103	1/1	0.90	0.14	85,85,85,85	0
58	MG	2A	3549	1/1	0.90	0.18	49,49,49,49	0
58	MG	2A	3550	1/1	0.90	0.18	75,75,75,75	0
58	MG	2a	1634	1/1	0.90	0.21	74,74,74,74	0
58	MG	2a	1635	1/1	0.90	0.17	82,82,82,82	0
58	MG	1A	3393	1/1	0.90	0.18	46,46,46,46	0
58	MG	1A	3396	1/1	0.90	0.18	55,55,55,55	0
58	MG	2A	3555	1/1	0.90	0.22	52,52,52,52	0
58	MG	1A	3472	1/1	0.90	0.42	39,39,39,39	0
58	MG	2A	3104	1/1	0.90	0.33	63,63,63,63	0
58	MG	1A	3709	1/1	0.90	0.15	44,44,44,44	0
58	MG	1A	3210	1/1	0.90	0.29	42,42,42,42	0
58	MG	2x	108	1/1	0.90	0.17	61,61,61,61	0
58	MG	1A	3474	1/1	0.90	0.36	53,53,53,53	0
60	ZN	14	102	1/1	0.90	0.04	110,110,110,110	0
58	MG	1a	1620	1/1	0.90	0.15	56,56,56,56	0
58	MG	1a	1724	1/1	0.90	0.20	81,81,81,81	0
58	MG	1A	3935	1/1	0.91	0.40	53,53,53,53	0
58	MG	1a	1819	1/1	0.91	0.08	81,81,81,81	0
58	MG	1A	3936	1/1	0.91	0.38	74,74,74,74	0
58	MG	2A	3090	1/1	0.91	0.09	72,72,72,72	0
58	MG	1A	3091	1/1	0.91	0.15	47,47,47,47	0
58	MG	1A	3673	1/1	0.91	0.19	76,76,76,76	0
58	MG	2A	3355	1/1	0.91	0.19	57,57,57,57	0
58	MG	1A	4071	1/1	0.91	0.18	65,65,65,65	0
58	MG	2A	3758	1/1	0.91	0.22	54,54,54,54	0
58	MG	1A	4076	1/1	0.91	0.20	41,41,41,41	0
58	MG	2A	3766	1/1	0.91	0.14	61,61,61,61	0
58	MG	1U	204	1/1	0.91	0.20	42,42,42,42	0
58	MG	1A	3024	1/1	0.91	0.17	64,64,64,64	0
58	MG	1e	202	1/1	0.91	0.33	63,63,63,63	0
58	MG	1A	3675	1/1	0.91	0.24	65,65,65,65	0
58	MG	1A	3850	1/1	0.91	0.14	40,40,40,40	0
58	MG	1A	3481	1/1	0.91	0.19	62,62,62,62	0
58	MG	1A	3678	1/1	0.91	0.23	34,34,34,34	0
58	MG	2a	1677	1/1	0.91	0.17	80,80,80,80	0
58	MG	1A	3156	1/1	0.91	0.44	47,47,47,47	0
58	MG	1A	3602	1/1	0.91	0.22	51,51,51,51	0
58	MG	1A	3337	1/1	0.91	0.20	57,57,57,57	0
58	MG	2A	3249	1/1	0.91	0.25	73,73,73,73	0
58	MG	2a	1683	1/1	0.91	0.19	65,65,65,65	0
58	MG	1A	3250	1/1	0.91	0.27	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3764	1/1	0.91	0.18	44,44,44,44	0
58	MG	1A	3863	1/1	0.91	0.18	39,39,39,39	0
58	MG	1A	3685	1/1	0.91	0.12	66,66,66,66	0
58	MG	1A	3159	1/1	0.91	0.31	37,37,37,37	0
58	MG	2A	3385	1/1	0.91	0.31	50,50,50,50	0
58	MG	2A	3796	1/1	0.91	0.10	56,56,56,56	0
58	MG	1A	3772	1/1	0.91	0.18	55,55,55,55	0
58	MG	1A	3964	1/1	0.91	0.12	72,72,72,72	0
58	MG	1a	1707	1/1	0.91	0.58	70,70,70,70	0
58	MG	2A	3590	1/1	0.91	0.11	78,78,78,78	0
58	MG	2A	3591	1/1	0.91	0.20	64,64,64,64	0
58	MG	1x	105	1/1	0.91	0.17	62,62,62,62	0
58	MG	1A	4106	1/1	0.91	0.17	66,66,66,66	0
58	MG	1A	3072	1/1	0.91	0.20	50,50,50,50	0
58	MG	1A	3776	1/1	0.91	0.21	66,66,66,66	0
58	MG	2A	3133	1/1	0.91	0.17	67,67,67,67	0
58	MG	2a	1707	1/1	0.91	0.32	68,68,68,68	0
58	MG	1A	3230	1/1	0.91	0.19	34,34,34,34	0
58	MG	1A	3779	1/1	0.91	0.24	53,53,53,53	0
58	MG	1A	3696	1/1	0.91	0.16	43,43,43,43	0
58	MG	1A	3697	1/1	0.91	0.23	51,51,51,51	0
58	MG	1A	3884	1/1	0.91	0.16	66,66,66,66	0
58	MG	17	101	1/1	0.91	0.18	42,42,42,42	0
58	MG	1A	3001	1/1	0.91	0.16	48,48,48,48	0
58	MG	1A	3886	1/1	0.91	0.09	51,51,51,51	0
58	MG	2A	3617	1/1	0.91	0.19	43,43,43,43	0
58	MG	1A	3540	1/1	0.91	0.53	67,67,67,67	0
58	MG	2A	3823	1/1	0.91	0.24	66,66,66,66	0
58	MG	1A	3234	1/1	0.91	0.12	48,48,48,48	0
58	MG	1A	3982	1/1	0.91	0.13	53,53,53,53	0
58	MG	1A	3785	1/1	0.91	0.11	48,48,48,48	0
58	MG	2A	3622	1/1	0.91	0.11	58,58,58,58	0
58	MG	2A	3623	1/1	0.91	0.10	59,59,59,59	0
58	MG	2A	3624	1/1	0.91	0.23	60,60,60,60	0
58	MG	1B	219	1/1	0.91	0.34	52,52,52,52	0
58	MG	1A	3788	1/1	0.91	0.17	77,77,77,77	0
58	MG	2A	3158	1/1	0.91	0.33	65,65,65,65	0
58	MG	1A	3705	1/1	0.91	0.24	24,24,24,24	0
58	MG	1A	3433	1/1	0.91	0.17	57,57,57,57	0
58	MG	2a	1740	1/1	0.91	0.07	66,66,66,66	0
58	MG	1A	3015	1/1	0.91	0.26	55,55,55,55	0
58	MG	2A	3443	1/1	0.91	0.17	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3296	1/1	0.91	0.38	67,67,67,67	0
58	MG	2a	1749	1/1	0.91	0.14	66,66,66,66	0
58	MG	1A	3795	1/1	0.91	0.34	55,55,55,55	0
58	MG	2A	3453	1/1	0.91	0.27	55,55,55,55	0
58	MG	2A	3291	1/1	0.91	0.18	72,72,72,72	0
58	MG	2a	1760	1/1	0.91	0.10	73,73,73,73	0
58	MG	1A	3436	1/1	0.91	0.36	66,66,66,66	0
58	MG	1a	1753	1/1	0.91	0.16	63,63,63,63	0
58	MG	2A	3646	1/1	0.91	0.19	64,64,64,64	0
58	MG	2a	1769	1/1	0.91	0.10	64,64,64,64	0
58	MG	2A	3169	1/1	0.91	0.27	64,64,64,64	0
58	MG	1a	1619	1/1	0.91	0.09	51,51,51,51	0
58	MG	1a	1756	1/1	0.91	0.13	78,78,78,78	0
58	MG	1A	3102	1/1	0.91	0.20	35,35,35,35	0
58	MG	2E	307	1/1	0.91	0.18	53,53,53,53	0
58	MG	2a	1781	1/1	0.91	0.23	70,70,70,70	0
58	MG	2A	3656	1/1	0.91	0.22	43,43,43,43	0
58	MG	1A	4003	1/1	0.91	0.11	39,39,39,39	0
58	MG	2A	3659	1/1	0.91	0.31	53,53,53,53	0
58	MG	2A	3660	1/1	0.91	0.16	71,71,71,71	0
58	MG	2A	3475	1/1	0.91	0.17	47,47,47,47	0
58	MG	2A	3662	1/1	0.91	0.12	55,55,55,55	0
58	MG	1A	3804	1/1	0.91	0.37	41,41,41,41	0
58	MG	1A	3648	1/1	0.91	0.17	37,37,37,37	0
58	MG	1A	3238	1/1	0.91	0.28	67,67,67,67	0
58	MG	1A	3904	1/1	0.91	0.11	38,38,38,38	0
58	MG	2A	3485	1/1	0.91	0.15	59,59,59,59	0
58	MG	1A	3009	1/1	0.91	0.22	27,27,27,27	0
58	MG	1A	3906	1/1	0.91	0.13	39,39,39,39	0
58	MG	2A	3674	1/1	0.91	0.10	71,71,71,71	0
58	MG	1A	3509	1/1	0.91	0.12	65,65,65,65	0
58	MG	1a	1773	1/1	0.91	0.07	66,66,66,66	0
58	MG	1A	3657	1/1	0.91	0.16	62,62,62,62	0
58	MG	1A	3816	1/1	0.91	0.29	39,39,39,39	0
58	MG	2A	3495	1/1	0.91	0.19	70,70,70,70	0
58	MG	1E	313	1/1	0.91	0.14	38,38,38,38	0
58	MG	2A	3687	1/1	0.91	0.12	75,75,75,75	0
58	MG	27	101	1/1	0.91	0.35	52,52,52,52	0
58	MG	1A	3023	1/1	0.91	0.31	38,38,38,38	0
58	MG	1A	3818	1/1	0.91	0.15	41,41,41,41	0
58	MG	1F	310	1/1	0.91	0.13	62,62,62,62	0
58	MG	2a	1820	1/1	0.91	0.11	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3822	1/1	0.91	0.32	46,46,46,46	0
58	MG	2A	3696	1/1	0.91	0.10	82,82,82,82	0
58	MG	2a	1603	1/1	0.91	0.14	68,68,68,68	0
58	MG	2a	1826	1/1	0.91	0.31	58,58,58,58	0
58	MG	2a	1827	1/1	0.91	0.12	74,74,74,74	0
58	MG	2a	1604	1/1	0.91	0.09	75,75,75,75	0
58	MG	1A	3560	1/1	0.91	0.14	43,43,43,43	0
58	MG	1A	3441	1/1	0.91	0.29	46,46,46,46	0
58	MG	2a	1608	1/1	0.91	0.23	66,66,66,66	0
58	MG	2A	3506	1/1	0.91	0.20	45,45,45,45	0
58	MG	2a	1836	1/1	0.91	0.19	81,81,81,81	0
58	MG	1a	1789	1/1	0.91	0.14	73,73,73,73	0
58	MG	2A	3195	1/1	0.91	0.60	51,51,51,51	0
58	MG	2A	3704	1/1	0.91	0.19	68,68,68,68	0
58	MG	2A	3196	1/1	0.91	0.55	75,75,75,75	0
58	MG	1A	4031	1/1	0.91	0.21	73,73,73,73	0
58	MG	2f	201	1/1	0.91	0.19	45,45,45,45	0
58	MG	1A	3921	1/1	0.91	0.07	66,66,66,66	0
58	MG	1a	1792	1/1	0.91	0.10	56,56,56,56	0
58	MG	2l	203	1/1	0.91	0.41	74,74,74,74	0
58	MG	2A	3066	1/1	0.91	0.11	55,55,55,55	0
58	MG	1A	4035	1/1	0.91	0.26	66,66,66,66	0
58	MG	1A	3828	1/1	0.91	0.07	43,43,43,43	0
58	MG	1G	203	1/1	0.91	0.17	72,72,72,72	0
58	MG	1a	1656	1/1	0.91	0.17	63,63,63,63	0
58	MG	2A	3523	1/1	0.91	0.15	47,47,47,47	0
58	MG	1A	4038	1/1	0.91	0.16	35,35,35,35	0
58	MG	1A	3302	1/1	0.91	0.27	35,35,35,35	0
58	MG	2A	3528	1/1	0.91	0.14	50,50,50,50	0
58	MG	2A	3720	1/1	0.91	0.23	50,50,50,50	0
58	MG	1A	3831	1/1	0.91	0.28	40,40,40,40	0
58	MG	1O	203	1/1	0.91	0.12	55,55,55,55	0
58	MG	1A	3133	1/1	0.91	0.18	52,52,52,52	0
58	MG	1A	4048	1/1	0.91	0.15	52,52,52,52	0
58	MG	2A	3729	1/1	0.91	0.09	71,71,71,71	0
58	MG	1A	3664	1/1	0.91	0.13	47,47,47,47	0
58	MG	1A	3585	1/1	0.91	0.07	58,58,58,58	0
58	MG	1A	4052	1/1	0.91	0.13	58,58,58,58	0
58	MG	1A	4053	1/1	0.91	0.11	71,71,71,71	0
58	MG	1A	3477	1/1	0.91	0.19	64,64,64,64	0
58	MG	1A	3844	1/1	0.91	0.30	54,54,54,54	0
58	MG	2A	3791	1/1	0.92	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3413	1/1	0.92	0.14	57,57,57,57	0
58	MG	2A	3414	1/1	0.92	0.10	58,58,58,58	0
58	MG	1a	1667	1/1	0.92	0.09	71,71,71,71	0
58	MG	2A	3416	1/1	0.92	0.23	66,66,66,66	0
58	MG	2A	3417	1/1	0.92	0.12	70,70,70,70	0
58	MG	1A	3557	1/1	0.92	0.18	63,63,63,63	0
58	MG	10	101	1/1	0.92	0.21	54,54,54,54	0
58	MG	10	103	1/1	0.92	0.19	50,50,50,50	0
58	MG	2A	3425	1/1	0.92	0.14	59,59,59,59	0
58	MG	1a	1795	1/1	0.92	0.07	88,88,88,88	0
58	MG	2A	3431	1/1	0.92	0.11	74,74,74,74	0
58	MG	2a	1688	1/1	0.92	0.23	64,64,64,64	0
58	MG	1A	3062	1/1	0.92	0.43	61,61,61,61	0
58	MG	2a	1690	1/1	0.92	0.14	73,73,73,73	0
58	MG	1A	3966	1/1	0.92	0.13	61,61,61,61	0
58	MG	1A	3562	1/1	0.92	0.12	59,59,59,59	0
58	MG	1B	233	1/1	0.92	0.21	67,67,67,67	0
58	MG	10	111	1/1	0.92	0.14	60,60,60,60	0
58	MG	1A	3563	1/1	0.92	0.19	30,30,30,30	0
58	MG	2A	3456	1/1	0.92	0.20	50,50,50,50	0
58	MG	1A	3013	1/1	0.92	0.17	33,33,33,33	0
58	MG	2A	3631	1/1	0.92	0.15	65,65,65,65	0
58	MG	1A	3971	1/1	0.92	0.21	63,63,63,63	0
58	MG	12	101	1/1	0.92	0.25	51,51,51,51	0
58	MG	1D	305	1/1	0.92	0.34	43,43,43,43	0
58	MG	2A	3819	1/1	0.92	0.16	73,73,73,73	0
58	MG	13	103	1/1	0.92	0.23	57,57,57,57	0
58	MG	2A	3469	1/1	0.92	0.17	59,59,59,59	0
58	MG	2a	1706	1/1	0.92	0.40	81,81,81,81	0
58	MG	2A	3638	1/1	0.92	0.14	75,75,75,75	0
58	MG	1A	3572	1/1	0.92	0.15	49,49,49,49	0
58	MG	1A	3973	1/1	0.92	0.13	29,29,29,29	0
58	MG	2a	1710	1/1	0.92	0.31	73,73,73,73	0
58	MG	15	103	1/1	0.92	0.21	37,37,37,37	0
58	MG	1A	3179	1/1	0.92	0.20	58,58,58,58	0
58	MG	2B	205	1/1	0.92	0.26	72,72,72,72	0
58	MG	2B	206	1/1	0.92	0.14	78,78,78,78	0
58	MG	1A	3910	1/1	0.92	0.13	41,41,41,41	0
58	MG	1A	3976	1/1	0.92	0.09	52,52,52,52	0
58	MG	1A	4066	1/1	0.92	0.12	69,69,69,69	0
58	MG	2A	3482	1/1	0.92	0.28	52,52,52,52	0
58	MG	2A	3199	1/1	0.92	0.22	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3389	1/1	0.92	0.18	60,60,60,60	0
58	MG	1A	3915	1/1	0.92	0.21	66,66,66,66	0
58	MG	19	101	1/1	0.92	0.28	60,60,60,60	0
58	MG	1A	3117	1/1	0.92	0.46	42,42,42,42	0
58	MG	1A	3270	1/1	0.92	0.60	45,45,45,45	0
58	MG	1A	3225	1/1	0.92	0.62	56,56,56,56	0
58	MG	2A	3494	1/1	0.92	0.16	42,42,42,42	0
58	MG	1A	3147	1/1	0.92	0.30	38,38,38,38	0
58	MG	1A	3371	1/1	0.92	0.16	46,46,46,46	0
58	MG	1a	1711	1/1	0.92	0.31	60,60,60,60	0
58	MG	1A	3079	1/1	0.92	0.32	33,33,33,33	0
58	MG	2A	3093	1/1	0.92	0.14	64,64,64,64	0
58	MG	2a	1741	1/1	0.92	0.21	81,81,81,81	0
58	MG	1A	3991	1/1	0.92	0.13	54,54,54,54	0
58	MG	2A	3671	1/1	0.92	0.39	52,52,52,52	0
58	MG	2A	3672	1/1	0.92	0.28	67,67,67,67	0
58	MG	1A	3672	1/1	0.92	0.10	57,57,57,57	0
58	MG	2A	3096	1/1	0.92	0.29	63,63,63,63	0
58	MG	2E	309	1/1	0.92	0.07	77,77,77,77	0
58	MG	2A	3221	1/1	0.92	0.10	75,75,75,75	0
58	MG	2a	1759	1/1	0.92	0.26	73,73,73,73	0
58	MG	1A	3373	1/1	0.92	0.13	63,63,63,63	0
58	MG	2a	1762	1/1	0.92	0.14	66,66,66,66	0
58	MG	1A	3797	1/1	0.92	0.20	59,59,59,59	0
58	MG	1a	1616	1/1	0.92	0.13	70,70,70,70	0
58	MG	2F	306	1/1	0.92	0.25	54,54,54,54	0
58	MG	2A	3683	1/1	0.92	0.09	64,64,64,64	0
58	MG	1a	1617	1/1	0.92	0.12	52,52,52,52	0
58	MG	1A	3927	1/1	0.92	0.28	64,64,64,64	0
58	MG	2Q	201	1/1	0.92	0.10	63,63,63,63	0
58	MG	2A	3513	1/1	0.92	0.17	67,67,67,67	0
58	MG	1A	3798	1/1	0.92	0.13	63,63,63,63	0
58	MG	2a	1779	1/1	0.92	0.20	71,71,71,71	0
58	MG	1A	3538	1/1	0.92	0.40	44,44,44,44	0
58	MG	1N	204	1/1	0.92	0.28	52,52,52,52	0
58	MG	1A	3138	1/1	0.92	0.24	41,41,41,41	0
58	MG	1A	3676	1/1	0.92	0.16	47,47,47,47	0
58	MG	1a	1734	1/1	0.92	0.22	76,76,76,76	0
58	MG	1O	205	1/1	0.92	0.12	68,68,68,68	0
58	MG	1A	4104	1/1	0.92	0.14	33,33,33,33	0
58	MG	2a	1792	1/1	0.92	0.23	72,72,72,72	0
58	MG	1A	3022	1/1	0.92	0.40	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	20	102	1/1	0.92	0.14	74,74,74,74	0
58	MG	2A	3703	1/1	0.92	0.20	71,71,71,71	0
58	MG	1A	3877	1/1	0.92	0.18	75,75,75,75	0
58	MG	2A	3350	1/1	0.92	0.45	65,65,65,65	0
58	MG	1a	1743	1/1	0.92	0.12	66,66,66,66	0
58	MG	1A	3405	1/1	0.92	0.10	73,73,73,73	0
58	MG	2a	1803	1/1	0.92	0.14	77,77,77,77	0
58	MG	2A	3354	1/1	0.92	0.30	49,49,49,49	0
58	MG	1a	1633	1/1	0.92	0.15	70,70,70,70	0
58	MG	1A	3679	1/1	0.92	0.15	29,29,29,29	0
58	MG	2a	1601	1/1	0.92	0.18	62,62,62,62	0
58	MG	2A	3357	1/1	0.92	0.45	77,77,77,77	0
58	MG	1A	3611	1/1	0.92	0.18	53,53,53,53	0
58	MG	2A	3547	1/1	0.92	0.16	58,58,58,58	0
58	MG	2A	3127	1/1	0.92	0.32	66,66,66,66	0
58	MG	2A	3247	1/1	0.92	0.13	70,70,70,70	0
58	MG	1A	3121	1/1	0.92	0.19	71,71,71,71	0
58	MG	1A	3286	1/1	0.92	0.26	42,42,42,42	0
58	MG	1R	205	1/1	0.92	0.24	61,61,61,61	0
58	MG	1A	3352	1/1	0.92	0.26	58,58,58,58	0
58	MG	1a	1641	1/1	0.92	0.12	69,69,69,69	0
58	MG	1A	3470	1/1	0.92	0.28	70,70,70,70	0
58	MG	1A	3821	1/1	0.92	0.28	43,43,43,43	0
58	MG	1A	3016	1/1	0.92	0.10	57,57,57,57	0
58	MG	1a	1648	1/1	0.92	0.15	50,50,50,50	0
58	MG	2A	3143	1/1	0.92	0.21	43,43,43,43	0
58	MG	2A	3014	1/1	0.92	0.27	48,48,48,48	0
58	MG	2A	3381	1/1	0.92	0.19	33,33,33,33	0
58	MG	2a	1832	1/1	0.92	0.06	90,90,90,90	0
58	MG	2a	1833	1/1	0.92	0.07	63,63,63,63	0
58	MG	2A	3740	1/1	0.92	0.21	37,37,37,37	0
58	MG	2A	3146	1/1	0.92	0.24	69,69,69,69	0
58	MG	1A	3355	1/1	0.92	0.30	60,60,60,60	0
58	MG	1B	211	1/1	0.92	0.12	60,60,60,60	0
58	MG	1A	3636	1/1	0.92	0.26	34,34,34,34	0
58	MG	2a	1840	1/1	0.92	0.21	60,60,60,60	0
58	MG	1B	213	1/1	0.92	0.41	69,69,69,69	0
58	MG	1a	1772	1/1	0.92	0.22	70,70,70,70	0
58	MG	1A	3255	1/1	0.92	0.16	54,54,54,54	0
58	MG	1B	215	1/1	0.92	0.20	64,64,64,64	0
58	MG	2A	3754	1/1	0.92	0.37	46,46,46,46	0
58	MG	1A	3443	1/1	0.92	0.32	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1778	1/1	0.92	0.20	87,87,87,87	0
58	MG	2A	3757	1/1	0.92	0.14	54,54,54,54	0
58	MG	1a	1658	1/1	0.92	0.22	68,68,68,68	0
58	MG	1A	3769	1/1	0.92	0.10	42,42,42,42	0
58	MG	2A	3763	1/1	0.92	0.17	65,65,65,65	0
58	MG	2A	3035	1/1	0.92	0.15	55,55,55,55	0
58	MG	1a	1660	1/1	0.92	0.12	70,70,70,70	0
58	MG	1a	1782	1/1	0.92	0.07	72,72,72,72	0
58	MG	1a	1784	1/1	0.92	0.15	77,77,77,77	0
58	MG	2v	103	1/1	0.92	0.21	72,72,72,72	0
58	MG	2w	101	1/1	0.92	0.08	86,86,86,86	0
58	MG	2a	1646	1/1	0.92	0.09	52,52,52,52	0
58	MG	1A	3216	1/1	0.92	0.21	51,51,51,51	0
58	MG	2A	3279	1/1	0.92	0.53	59,59,59,59	0
58	MG	2A	3778	1/1	0.92	0.10	74,74,74,74	0
58	MG	2A	3404	1/1	0.92	0.27	63,63,63,63	0
58	MG	2A	3280	1/1	0.92	0.33	69,69,69,69	0
58	MG	2A	3042	1/1	0.92	0.18	51,51,51,51	0
58	MG	1A	4037	1/1	0.92	0.06	54,54,54,54	0
58	MG	2A	3596	1/1	0.92	0.10	83,83,83,83	0
58	MG	1B	223	1/1	0.92	0.31	60,60,60,60	0
58	MG	1A	3647	1/1	0.92	0.25	57,57,57,57	0
58	MG	2A	3788	1/1	0.92	0.24	65,65,65,65	0
58	MG	1A	3773	1/1	0.92	0.19	59,59,59,59	0
58	MG	1A	3078	1/1	0.93	0.21	31,31,31,31	0
58	MG	2A	3780	1/1	0.93	0.18	56,56,56,56	0
58	MG	1A	3329	1/1	0.93	0.16	41,41,41,41	0
58	MG	2a	1670	1/1	0.93	0.29	75,75,75,75	0
58	MG	1a	1732	1/1	0.93	0.08	56,56,56,56	0
58	MG	1A	3768	1/1	0.93	0.11	39,39,39,39	0
58	MG	1A	3516	1/1	0.93	0.31	39,39,39,39	0
58	MG	1A	3860	1/1	0.93	0.18	39,39,39,39	0
58	MG	1A	3519	1/1	0.93	0.22	61,61,61,61	0
58	MG	2A	3275	1/1	0.93	0.09	56,56,56,56	0
58	MG	1A	3596	1/1	0.93	0.17	35,35,35,35	0
58	MG	1A	3093	1/1	0.93	0.33	71,71,71,71	0
58	MG	2A	3411	1/1	0.93	0.19	49,49,49,49	0
58	MG	1A	3056	1/1	0.93	0.32	54,54,54,54	0
58	MG	2a	1682	1/1	0.93	0.30	72,72,72,72	0
58	MG	1A	3468	1/1	0.93	0.38	57,57,57,57	0
58	MG	1A	3777	1/1	0.93	0.12	60,60,60,60	0
58	MG	1A	3958	1/1	0.93	0.20	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3131	1/1	0.93	0.44	44,44,44,44	0
58	MG	1G	204	1/1	0.93	0.17	68,68,68,68	0
58	MG	1a	1752	1/1	0.93	0.20	60,60,60,60	0
58	MG	1A	4070	1/1	0.93	0.07	74,74,74,74	0
58	MG	2A	3614	1/1	0.93	0.15	61,61,61,61	0
58	MG	1A	3605	1/1	0.93	0.22	40,40,40,40	0
58	MG	1A	3305	1/1	0.93	0.24	45,45,45,45	0
58	MG	2A	3426	1/1	0.93	0.22	49,49,49,49	0
58	MG	2A	3807	1/1	0.93	0.12	70,70,70,70	0
58	MG	1A	3395	1/1	0.93	0.40	52,52,52,52	0
58	MG	2A	3429	1/1	0.93	0.11	58,58,58,58	0
58	MG	2A	3430	1/1	0.93	0.13	51,51,51,51	0
58	MG	1a	1758	1/1	0.93	0.14	70,70,70,70	0
58	MG	2A	3432	1/1	0.93	0.11	54,54,54,54	0
58	MG	2A	3433	1/1	0.93	0.20	70,70,70,70	0
58	MG	1A	4081	1/1	0.93	0.14	47,47,47,47	0
58	MG	1A	3086	1/1	0.93	0.18	60,60,60,60	0
58	MG	2A	3446	1/1	0.93	0.26	48,48,48,48	0
58	MG	1A	3368	1/1	0.93	0.55	58,58,58,58	0
58	MG	1P	202	1/1	0.93	0.26	38,38,38,38	0
58	MG	1A	3883	1/1	0.93	0.16	44,44,44,44	0
58	MG	1A	3284	1/1	0.93	0.07	61,61,61,61	0
58	MG	2a	1711	1/1	0.93	0.21	72,72,72,72	0
58	MG	2A	3039	1/1	0.93	0.39	60,60,60,60	0
58	MG	2A	3824	1/1	0.93	0.22	68,68,68,68	0
58	MG	1A	3691	1/1	0.93	0.20	33,33,33,33	0
58	MG	1Q	205	1/1	0.93	0.19	63,63,63,63	0
58	MG	1A	3786	1/1	0.93	0.24	66,66,66,66	0
58	MG	2a	1719	1/1	0.93	0.23	82,82,82,82	0
58	MG	1A	3695	1/1	0.93	0.26	47,47,47,47	0
58	MG	2A	3465	1/1	0.93	0.12	58,58,58,58	0
58	MG	1a	1646	1/1	0.93	0.11	63,63,63,63	0
58	MG	1A	3533	1/1	0.93	0.17	68,68,68,68	0
58	MG	1a	1649	1/1	0.93	0.07	56,56,56,56	0
58	MG	1A	3204	1/1	0.93	0.17	43,43,43,43	0
58	MG	1A	3112	1/1	0.93	0.30	45,45,45,45	0
58	MG	2a	1728	1/1	0.93	0.14	78,78,78,78	0
58	MG	2B	211	1/1	0.93	0.06	76,76,76,76	0
58	MG	2A	3476	1/1	0.93	0.12	41,41,41,41	0
58	MG	2A	3654	1/1	0.93	0.10	66,66,66,66	0
58	MG	2B	214	1/1	0.93	0.17	71,71,71,71	0
58	MG	2A	3655	1/1	0.93	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3478	1/1	0.93	0.20	62,62,62,62	0
58	MG	1S	201	1/1	0.93	0.67	59,59,59,59	0
58	MG	2A	3658	1/1	0.93	0.55	58,58,58,58	0
58	MG	1A	3702	1/1	0.93	0.22	72,72,72,72	0
58	MG	1T	201	1/1	0.93	0.18	66,66,66,66	0
58	MG	1A	3619	1/1	0.93	0.16	32,32,32,32	0
58	MG	2A	3483	1/1	0.93	0.18	45,45,45,45	0
58	MG	2A	3484	1/1	0.93	0.19	46,46,46,46	0
58	MG	2A	3056	1/1	0.93	0.33	71,71,71,71	0
58	MG	2a	1750	1/1	0.93	0.14	77,77,77,77	0
58	MG	1A	3622	1/1	0.93	0.24	31,31,31,31	0
58	MG	1A	3206	1/1	0.93	0.15	53,53,53,53	0
58	MG	2A	3488	1/1	0.93	0.21	40,40,40,40	0
58	MG	1A	3113	1/1	0.93	0.24	51,51,51,51	0
58	MG	1A	3114	1/1	0.93	0.20	40,40,40,40	0
58	MG	1A	3710	1/1	0.93	0.17	34,34,34,34	0
58	MG	2A	3064	1/1	0.93	0.26	47,47,47,47	0
58	MG	1A	4110	1/1	0.93	0.12	57,57,57,57	0
58	MG	1A	4111	1/1	0.93	0.13	49,49,49,49	0
58	MG	1A	3442	1/1	0.93	0.43	46,46,46,46	0
58	MG	2A	3677	1/1	0.93	0.17	59,59,59,59	0
58	MG	1a	1798	1/1	0.93	0.18	73,73,73,73	0
58	MG	1A	3989	1/1	0.93	0.16	47,47,47,47	0
58	MG	1A	3812	1/1	0.93	0.07	58,58,58,58	0
58	MG	2P	201	1/1	0.93	0.17	61,61,61,61	0
58	MG	1A	3639	1/1	0.93	0.22	36,36,36,36	0
58	MG	2a	1780	1/1	0.93	0.29	60,60,60,60	0
58	MG	2A	3211	1/1	0.93	0.33	51,51,51,51	0
58	MG	1A	3408	1/1	0.93	0.22	54,54,54,54	0
58	MG	2a	1783	1/1	0.93	0.20	71,71,71,71	0
58	MG	2A	3213	1/1	0.93	0.31	64,64,64,64	0
58	MG	2a	1785	1/1	0.93	0.04	81,81,81,81	0
58	MG	1a	1671	1/1	0.93	0.08	73,73,73,73	0
58	MG	2A	3215	1/1	0.93	0.09	67,67,67,67	0
58	MG	2a	1788	1/1	0.93	0.12	72,72,72,72	0
58	MG	1A	3641	1/1	0.93	0.27	31,31,31,31	0
58	MG	2a	1790	1/1	0.93	0.09	88,88,88,88	0
58	MG	1a	1807	1/1	0.93	0.08	70,70,70,70	0
58	MG	1A	3375	1/1	0.93	0.60	53,53,53,53	0
58	MG	1A	3644	1/1	0.93	0.19	40,40,40,40	0
58	MG	2a	1794	1/1	0.93	0.17	72,72,72,72	0
58	MG	2A	3514	1/1	0.93	0.20	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3998	1/1	0.93	0.27	56,56,56,56	0
58	MG	2A	3516	1/1	0.93	0.18	72,72,72,72	0
58	MG	23	101	1/1	0.93	0.34	67,67,67,67	0
58	MG	1a	1677	1/1	0.93	0.21	56,56,56,56	0
58	MG	10	102	1/1	0.93	0.15	59,59,59,59	0
58	MG	1A	3645	1/1	0.93	0.23	33,33,33,33	0
58	MG	10	104	1/1	0.93	0.40	49,49,49,49	0
58	MG	1A	3098	1/1	0.93	0.16	33,33,33,33	0
58	MG	2A	3522	1/1	0.93	0.27	52,52,52,52	0
58	MG	1A	3042	1/1	0.93	0.20	36,36,36,36	0
58	MG	28	101	1/1	0.93	0.28	58,58,58,58	0
58	MG	2A	3351	1/1	0.93	0.46	63,63,63,63	0
58	MG	1A	3649	1/1	0.93	0.18	29,29,29,29	0
58	MG	1A	3548	1/1	0.93	0.40	69,69,69,69	0
58	MG	1A	3415	1/1	0.93	0.37	50,50,50,50	0
58	MG	1A	4013	1/1	0.93	0.21	41,41,41,41	0
58	MG	2a	1815	1/1	0.93	0.11	63,63,63,63	0
58	MG	1a	1688	1/1	0.93	0.16	62,62,62,62	0
58	MG	2a	1606	1/1	0.93	0.23	73,73,73,73	0
58	MG	1A	3448	1/1	0.93	0.13	59,59,59,59	0
58	MG	2a	1821	1/1	0.93	0.05	88,88,88,88	0
58	MG	1A	3004	1/1	0.93	0.20	37,37,37,37	0
58	MG	1B	226	1/1	0.93	0.20	63,63,63,63	0
58	MG	1a	1694	1/1	0.93	0.09	67,67,67,67	0
58	MG	2a	1825	1/1	0.93	0.10	77,77,77,77	0
58	MG	1A	3379	1/1	0.93	0.28	54,54,54,54	0
58	MG	1f	201	1/1	0.93	0.18	51,51,51,51	0
58	MG	2a	1828	1/1	0.93	0.12	69,69,69,69	0
58	MG	2a	1614	1/1	0.93	0.18	70,70,70,70	0
58	MG	1A	3349	1/1	0.93	0.41	40,40,40,40	0
58	MG	2A	3106	1/1	0.93	0.23	39,39,39,39	0
58	MG	2A	3734	1/1	0.93	0.17	71,71,71,71	0
58	MG	1A	3838	1/1	0.93	0.19	29,29,29,29	0
58	MG	1A	3925	1/1	0.93	0.21	73,73,73,73	0
58	MG	1A	3170	1/1	0.93	0.11	51,51,51,51	0
58	MG	2A	3373	1/1	0.93	0.08	70,70,70,70	0
58	MG	2A	3739	1/1	0.93	0.20	55,55,55,55	0
58	MG	15	107	1/1	0.93	0.19	41,41,41,41	0
58	MG	2A	3375	1/1	0.93	0.52	57,57,57,57	0
58	MG	1A	3323	1/1	0.93	0.27	39,39,39,39	0
58	MG	1t	201	1/1	0.93	0.11	63,63,63,63	0
58	MG	2A	3744	1/1	0.93	0.25	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3843	1/1	0.93	0.22	40,40,40,40	0
58	MG	2A	3747	1/1	0.93	0.30	81,81,81,81	0
58	MG	1A	3501	1/1	0.93	0.38	56,56,56,56	0
58	MG	1A	3930	1/1	0.93	0.20	46,46,46,46	0
58	MG	1A	4032	1/1	0.93	0.16	59,59,59,59	0
58	MG	1a	1712	1/1	0.93	0.26	68,68,68,68	0
58	MG	18	103	1/1	0.93	0.24	60,60,60,60	0
58	MG	1A	3264	1/1	0.93	0.22	63,63,63,63	0
58	MG	1A	3567	1/1	0.93	0.26	34,34,34,34	0
58	MG	1A	3266	1/1	0.93	0.28	58,58,58,58	0
58	MG	1a	1719	1/1	0.93	0.10	43,43,43,43	0
58	MG	2A	3759	1/1	0.93	0.10	72,72,72,72	0
58	MG	1D	309	1/1	0.93	0.34	37,37,37,37	0
58	MG	1A	3669	1/1	0.93	0.21	29,29,29,29	0
58	MG	2A	3765	1/1	0.93	0.19	76,76,76,76	0
58	MG	2a	1647	1/1	0.93	0.14	74,74,74,74	0
58	MG	2a	1648	1/1	0.93	0.11	65,65,65,65	0
58	MG	1A	3760	1/1	0.93	0.12	32,32,32,32	0
58	MG	2a	1650	1/1	0.93	0.12	70,70,70,70	0
58	MG	2a	1652	1/1	0.93	0.24	54,54,54,54	0
58	MG	1A	3423	1/1	0.93	0.15	67,67,67,67	0
58	MG	2A	3768	1/1	0.93	0.15	62,62,62,62	0
58	MG	1A	3069	1/1	0.93	0.16	33,33,33,33	0
58	MG	1a	1607	1/1	0.93	0.21	59,59,59,59	0
58	MG	2A	3398	1/1	0.93	0.34	60,60,60,60	0
58	MG	2A	3584	1/1	0.93	0.26	65,65,65,65	0
58	MG	2A	3399	1/1	0.93	0.25	54,54,54,54	0
60	ZN	29	501	1/1	0.93	0.09	81,81,81,81	0
60	ZN	2n	103	1/1	0.93	0.07	97,97,97,97	0
58	MG	2A	3773	1/1	0.94	0.19	71,71,71,71	0
58	MG	2a	1664	1/1	0.94	0.25	47,47,47,47	0
58	MG	1a	1674	1/1	0.94	0.32	66,66,66,66	0
58	MG	2A	3776	1/1	0.94	0.24	70,70,70,70	0
58	MG	2A	3777	1/1	0.94	0.13	70,70,70,70	0
58	MG	1A	3513	1/1	0.94	0.13	52,52,52,52	0
58	MG	1X	102	1/1	0.94	0.21	48,48,48,48	0
58	MG	1X	104	1/1	0.94	0.16	49,49,49,49	0
58	MG	1a	1814	1/1	0.94	0.23	66,66,66,66	0
58	MG	1X	106	1/1	0.94	0.23	61,61,61,61	0
58	MG	1A	4014	1/1	0.94	0.28	58,58,58,58	0
58	MG	1A	3632	1/1	0.94	0.19	30,30,30,30	0
58	MG	1A	3143	1/1	0.94	0.22	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3586	1/1	0.94	0.36	55,55,55,55	0
58	MG	1A	3637	1/1	0.94	0.23	30,30,30,30	0
58	MG	1a	1683	1/1	0.94	0.13	67,67,67,67	0
58	MG	1A	3410	1/1	0.94	0.48	47,47,47,47	0
58	MG	1a	1822	1/1	0.94	0.28	77,77,77,77	0
58	MG	1A	3558	1/1	0.94	0.17	39,39,39,39	0
58	MG	1A	4022	1/1	0.94	0.17	62,62,62,62	0
58	MG	2A	3258	1/1	0.94	0.48	69,69,69,69	0
58	MG	10	106	1/1	0.94	0.19	57,57,57,57	0
58	MG	1A	4023	1/1	0.94	0.35	60,60,60,60	0
58	MG	2A	3112	1/1	0.94	0.17	54,54,54,54	0
58	MG	2a	1691	1/1	0.94	0.17	82,82,82,82	0
58	MG	1B	220	1/1	0.94	0.17	44,44,44,44	0
58	MG	1A	3249	1/1	0.94	0.12	36,36,36,36	0
58	MG	10	110	1/1	0.94	0.18	70,70,70,70	0
58	MG	2A	3802	1/1	0.94	0.10	79,79,79,79	0
58	MG	2A	3803	1/1	0.94	0.20	42,42,42,42	0
58	MG	2A	3117	1/1	0.94	0.18	52,52,52,52	0
58	MG	1A	3862	1/1	0.94	0.21	42,42,42,42	0
58	MG	2A	3119	1/1	0.94	0.28	57,57,57,57	0
58	MG	2A	3609	1/1	0.94	0.16	43,43,43,43	0
58	MG	1A	3937	1/1	0.94	0.13	68,68,68,68	0
58	MG	1a	1698	1/1	0.94	0.18	42,42,42,42	0
58	MG	2A	3418	1/1	0.94	0.20	46,46,46,46	0
58	MG	2A	3122	1/1	0.94	0.20	60,60,60,60	0
58	MG	11	103	1/1	0.94	0.09	40,40,40,40	0
58	MG	2A	3422	1/1	0.94	0.33	49,49,49,49	0
58	MG	1A	3201	1/1	0.94	0.26	45,45,45,45	0
58	MG	1A	3053	1/1	0.94	0.30	51,51,51,51	0
58	MG	1A	3523	1/1	0.94	0.17	56,56,56,56	0
58	MG	1A	3568	1/1	0.94	0.05	64,64,64,64	0
58	MG	1A	3019	1/1	0.94	0.12	26,26,26,26	0
58	MG	1w	102	1/1	0.94	0.15	69,69,69,69	0
58	MG	1A	3571	1/1	0.94	0.21	32,32,32,32	0
58	MG	2A	3822	1/1	0.94	0.23	56,56,56,56	0
58	MG	1A	3791	1/1	0.94	0.08	66,66,66,66	0
58	MG	1A	3950	1/1	0.94	0.20	27,27,27,27	0
58	MG	1a	1709	1/1	0.94	0.29	75,75,75,75	0
58	MG	2A	3440	1/1	0.94	0.22	71,71,71,71	0
58	MG	2A	3827	1/1	0.94	0.19	70,70,70,70	0
58	MG	2A	3441	1/1	0.94	0.21	69,69,69,69	0
58	MG	2A	3140	1/1	0.94	0.40	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3285	1/1	0.94	0.28	62,62,62,62	0
58	MG	2A	3447	1/1	0.94	0.21	69,69,69,69	0
58	MG	1A	3874	1/1	0.94	0.07	44,44,44,44	0
58	MG	1A	3253	1/1	0.94	0.07	66,66,66,66	0
58	MG	2A	3451	1/1	0.94	0.23	51,51,51,51	0
58	MG	2A	3452	1/1	0.94	0.20	53,53,53,53	0
58	MG	2A	3642	1/1	0.94	0.37	75,75,75,75	0
58	MG	1A	3793	1/1	0.94	0.09	55,55,55,55	0
58	MG	1A	4046	1/1	0.94	0.13	53,53,53,53	0
58	MG	2A	3455	1/1	0.94	0.18	45,45,45,45	0
58	MG	17	103	1/1	0.94	0.18	40,40,40,40	0
58	MG	1A	3573	1/1	0.94	0.13	55,55,55,55	0
58	MG	1D	307	1/1	0.94	0.26	55,55,55,55	0
58	MG	1A	3169	1/1	0.94	0.30	27,27,27,27	0
58	MG	1A	4049	1/1	0.94	0.13	56,56,56,56	0
58	MG	1A	3183	1/1	0.94	0.15	53,53,53,53	0
58	MG	2D	303	1/1	0.94	0.56	44,44,44,44	0
58	MG	2A	3466	1/1	0.94	0.23	39,39,39,39	0
58	MG	1E	301	1/1	0.94	0.22	34,34,34,34	0
58	MG	1A	3577	1/1	0.94	0.14	31,31,31,31	0
58	MG	2A	3472	1/1	0.94	0.20	46,46,46,46	0
58	MG	2A	3155	1/1	0.94	0.17	78,78,78,78	0
58	MG	1a	1727	1/1	0.94	0.16	44,44,44,44	0
58	MG	1A	3718	1/1	0.94	0.15	60,60,60,60	0
58	MG	2a	1761	1/1	0.94	0.29	65,65,65,65	0
58	MG	1A	3232	1/1	0.94	0.58	43,43,43,43	0
58	MG	2A	3477	1/1	0.94	0.20	66,66,66,66	0
58	MG	1a	1730	1/1	0.94	0.16	78,78,78,78	0
58	MG	1A	3887	1/1	0.94	0.14	30,30,30,30	0
58	MG	2a	1766	1/1	0.94	0.28	71,71,71,71	0
58	MG	2a	1768	1/1	0.94	0.24	75,75,75,75	0
58	MG	1E	312	1/1	0.94	0.20	57,57,57,57	0
58	MG	1A	4057	1/1	0.94	0.12	49,49,49,49	0
58	MG	2F	303	1/1	0.94	0.23	71,71,71,71	0
58	MG	1A	3207	1/1	0.94	0.29	46,46,46,46	0
58	MG	2A	3009	1/1	0.94	0.17	43,43,43,43	0
58	MG	2a	1777	1/1	0.94	0.26	67,67,67,67	0
58	MG	1A	3588	1/1	0.94	0.20	27,27,27,27	0
58	MG	1F	309	1/1	0.94	0.19	35,35,35,35	0
58	MG	2A	3170	1/1	0.94	0.11	56,56,56,56	0
58	MG	1A	3590	1/1	0.94	0.22	63,63,63,63	0
58	MG	1a	1614	1/1	0.94	0.10	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3016	1/1	0.94	0.39	54,54,54,54	0
58	MG	1a	1742	1/1	0.94	0.12	51,51,51,51	0
58	MG	2R	202	1/1	0.94	0.28	54,54,54,54	0
58	MG	1A	3810	1/1	0.94	0.17	47,47,47,47	0
58	MG	1A	3043	1/1	0.94	0.19	42,42,42,42	0
58	MG	1A	3594	1/1	0.94	0.18	36,36,36,36	0
58	MG	1A	4068	1/1	0.94	0.25	71,71,71,71	0
58	MG	2A	3688	1/1	0.94	0.11	38,38,38,38	0
58	MG	2A	3025	1/1	0.94	0.30	58,58,58,58	0
58	MG	1A	4069	1/1	0.94	0.08	54,54,54,54	0
58	MG	2W	202	1/1	0.94	0.45	63,63,63,63	0
58	MG	2X	101	1/1	0.94	0.20	71,71,71,71	0
58	MG	1A	3235	1/1	0.94	0.27	58,58,58,58	0
58	MG	1a	1750	1/1	0.94	0.07	70,70,70,70	0
58	MG	1A	3666	1/1	0.94	0.23	55,55,55,55	0
58	MG	2A	3033	1/1	0.94	0.14	50,50,50,50	0
58	MG	1A	4072	1/1	0.94	0.07	74,74,74,74	0
58	MG	25	102	1/1	0.94	0.17	60,60,60,60	0
58	MG	1A	3188	1/1	0.94	0.22	41,41,41,41	0
58	MG	1A	3535	1/1	0.94	0.67	53,53,53,53	0
58	MG	1A	4079	1/1	0.94	0.23	36,36,36,36	0
58	MG	1a	1628	1/1	0.94	0.19	50,50,50,50	0
58	MG	2A	3510	1/1	0.94	0.18	72,72,72,72	0
58	MG	1N	203	1/1	0.94	0.28	43,43,43,43	0
58	MG	1A	3189	1/1	0.94	0.39	41,41,41,41	0
58	MG	2A	3192	1/1	0.94	0.38	56,56,56,56	0
58	MG	1A	3332	1/1	0.94	0.25	52,52,52,52	0
58	MG	1A	3603	1/1	0.94	0.20	60,60,60,60	0
58	MG	1a	1767	1/1	0.94	0.17	58,58,58,58	0
58	MG	2A	3341	1/1	0.94	0.43	68,68,68,68	0
58	MG	2a	1816	1/1	0.94	0.20	83,83,83,83	0
58	MG	1A	4086	1/1	0.94	0.12	79,79,79,79	0
58	MG	1A	3065	1/1	0.94	0.30	31,31,31,31	0
58	MG	1A	4090	1/1	0.94	0.20	49,49,49,49	0
58	MG	1P	206	1/1	0.94	0.27	57,57,57,57	0
58	MG	1A	3018	1/1	0.94	0.20	54,54,54,54	0
58	MG	2A	3203	1/1	0.94	0.14	49,49,49,49	0
58	MG	1A	3274	1/1	0.94	0.33	50,50,50,50	0
58	MG	2A	3526	1/1	0.94	0.14	66,66,66,66	0
58	MG	2a	1613	1/1	0.94	0.10	81,81,81,81	0
58	MG	1A	3981	1/1	0.94	0.16	39,39,39,39	0
58	MG	1A	3431	1/1	0.94	0.18	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3758	1/1	0.94	0.25	57,57,57,57	0
58	MG	1Q	207	1/1	0.94	0.17	50,50,50,50	0
58	MG	2A	3732	1/1	0.94	0.23	56,56,56,56	0
58	MG	1A	3908	1/1	0.94	0.28	64,64,64,64	0
58	MG	1A	3609	1/1	0.94	0.20	30,30,30,30	0
58	MG	1A	3987	1/1	0.94	0.19	32,32,32,32	0
58	MG	1A	3833	1/1	0.94	0.10	39,39,39,39	0
58	MG	1A	3834	1/1	0.94	0.13	54,54,54,54	0
58	MG	2A	3545	1/1	0.94	0.31	65,65,65,65	0
58	MG	1A	3070	1/1	0.94	0.11	28,28,28,28	0
58	MG	1S	202	1/1	0.94	0.16	62,62,62,62	0
58	MG	1A	3544	1/1	0.94	0.48	68,68,68,68	0
58	MG	1A	3278	1/1	0.94	0.16	45,45,45,45	0
58	MG	2e	201	1/1	0.94	0.08	81,81,81,81	0
58	MG	1A	3995	1/1	0.94	0.17	20,20,20,20	0
58	MG	1A	4108	1/1	0.94	0.10	70,70,70,70	0
58	MG	2f	202	1/1	0.94	0.10	82,82,82,82	0
58	MG	2A	3746	1/1	0.94	0.22	39,39,39,39	0
58	MG	1A	3340	1/1	0.94	0.45	54,54,54,54	0
58	MG	1A	3100	1/1	0.94	0.40	33,33,33,33	0
58	MG	2A	3075	1/1	0.94	0.08	62,62,62,62	0
58	MG	2A	3557	1/1	0.94	0.24	78,78,78,78	0
58	MG	2A	3559	1/1	0.94	0.17	83,83,83,83	0
58	MG	2A	3752	1/1	0.94	0.11	49,49,49,49	0
58	MG	1A	3245	1/1	0.94	0.22	58,58,58,58	0
58	MG	1a	1796	1/1	0.94	0.11	68,68,68,68	0
58	MG	2a	1642	1/1	0.94	0.22	75,75,75,75	0
58	MG	1A	4112	1/1	0.94	0.09	55,55,55,55	0
58	MG	2a	1644	1/1	0.94	0.20	59,59,59,59	0
58	MG	2A	3563	1/1	0.94	0.18	70,70,70,70	0
58	MG	1A	3508	1/1	0.94	0.21	23,23,23,23	0
58	MG	1A	3158	1/1	0.94	0.15	36,36,36,36	0
58	MG	1a	1802	1/1	0.94	0.18	70,70,70,70	0
58	MG	1U	214	1/1	0.94	0.98	81,81,81,81	0
58	MG	1A	3624	1/1	0.94	0.15	31,31,31,31	0
58	MG	2a	1651	1/1	0.94	0.10	62,62,62,62	0
58	MG	1V	206	1/1	0.94	0.40	60,60,60,60	0
58	MG	1A	3774	1/1	0.94	0.33	54,54,54,54	0
58	MG	2a	1655	1/1	0.94	0.24	58,58,58,58	0
58	MG	2A	3572	1/1	0.94	0.17	67,67,67,67	0
58	MG	1B	205	1/1	0.94	0.18	62,62,62,62	0
58	MG	1A	3041	1/1	0.94	0.16	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	2a	1660	1/1	0.94	0.15	60,60,60,60	0
58	MG	2a	1661	1/1	0.94	0.21	58,58,58,58	0
58	MG	1A	3694	1/1	0.94	0.22	69,69,69,69	0
58	MG	2a	1685	1/1	0.95	0.19	58,58,58,58	0
58	MG	2A	3065	1/1	0.95	0.32	49,49,49,49	0
58	MG	1A	3471	1/1	0.95	0.12	33,33,33,33	0
58	MG	2A	3067	1/1	0.95	0.21	37,37,37,37	0
58	MG	13	102	1/1	0.95	0.29	44,44,44,44	0
58	MG	1A	3030	1/1	0.95	0.20	34,34,34,34	0
58	MG	2A	3648	1/1	0.95	0.49	57,57,57,57	0
58	MG	1A	4073	1/1	0.95	0.24	44,44,44,44	0
58	MG	2A	3650	1/1	0.95	0.17	58,58,58,58	0
58	MG	1A	3633	1/1	0.95	0.21	65,65,65,65	0
58	MG	2A	3652	1/1	0.95	0.40	76,76,76,76	0
58	MG	2A	3072	1/1	0.95	0.30	54,54,54,54	0
58	MG	1a	1689	1/1	0.95	0.11	60,60,60,60	0
58	MG	1A	4077	1/1	0.95	0.18	35,35,35,35	0
58	MG	1A	3690	1/1	0.95	0.15	41,41,41,41	0
58	MG	1A	3634	1/1	0.95	0.13	41,41,41,41	0
58	MG	1A	3564	1/1	0.95	0.19	41,41,41,41	0
58	MG	16	102	1/1	0.95	0.16	53,53,53,53	0
58	MG	2A	3342	1/1	0.95	0.32	67,67,67,67	0
58	MG	1A	3517	1/1	0.95	0.31	43,43,43,43	0
58	MG	1A	3990	1/1	0.95	0.14	50,50,50,50	0
58	MG	1A	3208	1/1	0.95	0.34	41,41,41,41	0
58	MG	1A	4088	1/1	0.95	0.16	43,43,43,43	0
58	MG	1A	3191	1/1	0.95	0.26	27,27,27,27	0
58	MG	1A	3054	1/1	0.95	0.27	27,27,27,27	0
58	MG	1A	3412	1/1	0.95	0.35	39,39,39,39	0
58	MG	1A	3922	1/1	0.95	0.10	43,43,43,43	0
58	MG	1H	201	1/1	0.95	0.36	70,70,70,70	0
58	MG	2B	217	1/1	0.95	0.14	74,74,74,74	0
58	MG	2a	1715	1/1	0.95	0.32	64,64,64,64	0
58	MG	1A	3852	1/1	0.95	0.17	68,68,68,68	0
58	MG	1a	1826	1/1	0.95	0.18	64,64,64,64	0
58	MG	1b	301	1/1	0.95	0.20	78,78,78,78	0
58	MG	2A	3225	1/1	0.95	0.17	68,68,68,68	0
58	MG	1A	3701	1/1	0.95	0.17	32,32,32,32	0
58	MG	1A	3642	1/1	0.95	0.16	49,49,49,49	0
58	MG	1A	3999	1/1	0.95	0.14	64,64,64,64	0
58	MG	2A	3679	1/1	0.95	0.23	77,77,77,77	0
58	MG	2A	3680	1/1	0.95	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
58	MG	1A	3413	1/1	0.95	0.23	47,47,47,47	0
58	MG	1A	3317	1/1	0.95	0.32	57,57,57,57	0
58	MG	2E	304	1/1	0.95	0.14	45,45,45,45	0
58	MG	2A	3231	1/1	0.95	0.28	72,72,72,72	0
58	MG	2A	3362	1/1	0.95	0.21	50,50,50,50	0
58	MG	2A	3099	1/1	0.95	0.26	69,69,69,69	0
58	MG	1A	3318	1/1	0.95	0.32	54,54,54,54	0
58	MG	1a	1610	1/1	0.95	0.17	55,55,55,55	0
58	MG	2a	1734	1/1	0.95	0.08	71,71,71,71	0
58	MG	2A	3690	1/1	0.95	0.10	69,69,69,69	0
58	MG	1A	3859	1/1	0.95	0.24	33,33,33,33	0
58	MG	2A	3367	1/1	0.95	0.35	58,58,58,58	0
58	MG	2a	1739	1/1	0.95	0.05	65,65,65,65	0
58	MG	2A	3694	1/1	0.95	0.09	72,72,72,72	0
58	MG	2A	3369	1/1	0.95	0.31	58,58,58,58	0
58	MG	2a	1742	1/1	0.95	0.15	49,49,49,49	0
58	MG	1a	1720	1/1	0.95	0.11	72,72,72,72	0
58	MG	2F	307	1/1	0.95	0.38	55,55,55,55	0
58	MG	1A	4008	1/1	0.95	0.25	35,35,35,35	0
58	MG	1P	205	1/1	0.95	0.27	53,53,53,53	0
58	MG	2A	3699	1/1	0.95	0.21	51,51,51,51	0
58	MG	2a	1751	1/1	0.95	0.16	60,60,60,60	0
58	MG	2a	1752	1/1	0.95	0.19	57,57,57,57	0
58	MG	1A	3256	1/1	0.95	0.18	39,39,39,39	0
58	MG	2A	3530	1/1	0.95	0.11	73,73,73,73	0
58	MG	2Q	202	1/1	0.95	0.16	56,56,56,56	0
58	MG	1A	3931	1/1	0.95	0.22	26,26,26,26	0
58	MG	2A	3532	1/1	0.95	0.20	50,50,50,50	0
58	MG	1A	4012	1/1	0.95	0.18	46,46,46,46	0
58	MG	1a	1726	1/1	0.95	0.11	43,43,43,43	0
58	MG	2A	3535	1/1	0.95	0.16	59,59,59,59	0
58	MG	2T	204	1/1	0.95	0.08	70,70,70,70	0
58	MG	1A	3193	1/1	0.95	0.27	43,43,43,43	0
58	MG	1A	3127	1/1	0.95	0.27	34,34,34,34	0
58	MG	1A	3195	1/1	0.95	0.21	27,27,27,27	0
58	MG	1A	3214	1/1	0.95	0.17	43,43,43,43	0
58	MG	2A	3544	1/1	0.95	0.16	52,52,52,52	0
58	MG	2A	3713	1/1	0.95	0.08	62,62,62,62	0
58	MG	2A	3116	1/1	0.95	0.13	55,55,55,55	0
58	MG	2a	1775	1/1	0.95	0.09	67,67,67,67	0
58	MG	2Y	201	1/1	0.95	0.36	69,69,69,69	0
58	MG	1A	3865	1/1	0.95	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3239	1/1	0.95	0.33	47,47,47,47	0
58	MG	1A	3129	1/1	0.95	0.44	57,57,57,57	0
58	MG	1A	3595	1/1	0.95	0.14	33,33,33,33	0
58	MG	1a	1737	1/1	0.95	0.16	67,67,67,67	0
58	MG	1A	3359	1/1	0.95	0.26	34,34,34,34	0
58	MG	1A	3942	1/1	0.95	0.45	33,33,33,33	0
58	MG	2A	3722	1/1	0.95	0.12	57,57,57,57	0
58	MG	1A	3490	1/1	0.95	0.21	58,58,58,58	0
58	MG	1a	1631	1/1	0.95	0.30	79,79,79,79	0
58	MG	1a	1632	1/1	0.95	0.19	36,36,36,36	0
58	MG	2A	3728	1/1	0.95	0.17	46,46,46,46	0
58	MG	28	102	1/1	0.95	0.24	56,56,56,56	0
58	MG	1A	3066	1/1	0.95	0.25	17,17,17,17	0
58	MG	1x	114	1/1	0.95	0.16	70,70,70,70	0
58	MG	1A	3726	1/1	0.95	0.18	36,36,36,36	0
58	MG	1A	3455	1/1	0.95	0.29	35,35,35,35	0
58	MG	1A	4030	1/1	0.95	0.12	61,61,61,61	0
58	MG	1a	1637	1/1	0.95	0.21	59,59,59,59	0
58	MG	1A	3076	1/1	0.95	0.21	37,37,37,37	0
58	MG	2A	3138	1/1	0.95	0.29	63,63,63,63	0
58	MG	2A	3139	1/1	0.95	0.15	78,78,78,78	0
58	MG	1A	3880	1/1	0.95	0.12	43,43,43,43	0
58	MG	2A	3569	1/1	0.95	0.11	38,38,38,38	0
58	MG	1A	3801	1/1	0.95	0.27	35,35,35,35	0
58	MG	2A	3408	1/1	0.95	0.11	66,66,66,66	0
58	MG	1A	3244	1/1	0.95	0.21	31,31,31,31	0
58	MG	1A	3276	1/1	0.95	0.16	30,30,30,30	0
58	MG	1a	1755	1/1	0.95	0.06	73,73,73,73	0
58	MG	1U	208	1/1	0.95	0.26	43,43,43,43	0
58	MG	1U	210	1/1	0.95	0.15	33,33,33,33	0
58	MG	1A	3496	1/1	0.95	0.30	38,38,38,38	0
58	MG	2a	1811	1/1	0.95	0.14	64,64,64,64	0
58	MG	1a	1647	1/1	0.95	0.13	53,53,53,53	0
58	MG	1A	3740	1/1	0.95	0.19	22,22,22,22	0
58	MG	1A	3303	1/1	0.95	0.19	34,34,34,34	0
58	MG	1A	3959	1/1	0.95	0.23	53,53,53,53	0
58	MG	2A	3282	1/1	0.95	0.35	72,72,72,72	0
58	MG	2A	3420	1/1	0.95	0.20	27,27,27,27	0
58	MG	2A	3283	1/1	0.95	0.25	58,58,58,58	0
58	MG	2a	1819	1/1	0.95	0.20	76,76,76,76	0
58	MG	1A	3460	1/1	0.95	0.31	84,84,84,84	0
58	MG	2A	3760	1/1	0.95	0.12	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1652	1/1	0.95	0.18	62,62,62,62	0
58	MG	1B	224	1/1	0.95	0.30	60,60,60,60	0
58	MG	2A	3764	1/1	0.95	0.30	63,63,63,63	0
58	MG	2A	3026	1/1	0.95	0.19	45,45,45,45	0
58	MG	2A	3028	1/1	0.95	0.27	72,72,72,72	0
58	MG	1B	225	1/1	0.95	0.24	59,59,59,59	0
58	MG	1W	205	1/1	0.95	0.25	32,32,32,32	0
58	MG	1A	3671	1/1	0.95	0.12	52,52,52,52	0
58	MG	1A	3067	1/1	0.95	0.48	35,35,35,35	0
58	MG	1A	3503	1/1	0.95	0.54	56,56,56,56	0
58	MG	1X	103	1/1	0.95	0.39	47,47,47,47	0
58	MG	2A	3774	1/1	0.95	0.11	64,64,64,64	0
58	MG	2A	3438	1/1	0.95	0.14	65,65,65,65	0
58	MG	2A	3167	1/1	0.95	0.13	42,42,42,42	0
58	MG	1a	1777	1/1	0.95	0.11	49,49,49,49	0
58	MG	2A	3603	1/1	0.95	0.17	64,64,64,64	0
58	MG	1A	3892	1/1	0.95	0.21	50,50,50,50	0
58	MG	2A	3444	1/1	0.95	0.22	55,55,55,55	0
58	MG	1X	105	1/1	0.95	0.23	38,38,38,38	0
58	MG	2A	3608	1/1	0.95	0.16	61,61,61,61	0
58	MG	1A	3168	1/1	0.95	0.22	43,43,43,43	0
58	MG	2A	3448	1/1	0.95	0.18	61,61,61,61	0
58	MG	1A	3749	1/1	0.95	0.18	25,25,25,25	0
58	MG	2a	1653	1/1	0.95	0.23	57,57,57,57	0
58	MG	1A	3750	1/1	0.95	0.17	21,21,21,21	0
58	MG	1Z	303	1/1	0.95	0.20	67,67,67,67	0
58	MG	2A	3616	1/1	0.95	0.22	41,41,41,41	0
58	MG	2A	3790	1/1	0.95	0.20	53,53,53,53	0
58	MG	1A	3223	1/1	0.95	0.23	59,59,59,59	0
58	MG	1A	4056	1/1	0.95	0.09	77,77,77,77	0
58	MG	2A	3046	1/1	0.95	0.24	77,77,77,77	0
58	MG	1A	3614	1/1	0.95	0.14	33,33,33,33	0
58	MG	1A	4058	1/1	0.95	0.28	58,58,58,58	0
58	MG	1D	301	1/1	0.95	0.28	53,53,53,53	0
58	MG	1A	3507	1/1	0.95	0.31	34,34,34,34	0
58	MG	1A	3008	1/1	0.95	0.23	29,29,29,29	0
58	MG	2a	1667	1/1	0.95	0.30	64,64,64,64	0
58	MG	1A	4061	1/1	0.95	0.13	43,43,43,43	0
58	MG	2A	3626	1/1	0.95	0.17	47,47,47,47	0
58	MG	2A	3627	1/1	0.95	0.28	52,52,52,52	0
58	MG	1A	3554	1/1	0.95	0.17	36,36,36,36	0
58	MG	1A	3108	1/1	0.95	0.23	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3759	1/1	0.95	0.26	70,70,70,70	0
58	MG	1A	3510	1/1	0.95	0.19	47,47,47,47	0
58	MG	2A	3470	1/1	0.95	0.14	41,41,41,41	0
58	MG	2x	107	1/1	0.95	0.15	57,57,57,57	0
58	MG	2A	3057	1/1	0.95	0.26	58,58,58,58	0
58	MG	1a	1799	1/1	0.95	0.08	66,66,66,66	0
58	MG	1l	102	1/1	0.95	0.11	48,48,48,48	0
58	MG	1A	3151	1/1	0.95	0.21	35,35,35,35	0
58	MG	1A	3625	1/1	0.95	0.14	31,31,31,31	0
58	MG	1E	308	1/1	0.95	0.19	26,26,26,26	0
58	MG	1A	3028	1/1	0.95	0.18	35,35,35,35	0
58	MG	2A	3670	1/1	0.96	0.23	51,51,51,51	0
58	MG	1A	3627	1/1	0.96	0.15	57,57,57,57	0
58	MG	1A	3692	1/1	0.96	0.16	24,24,24,24	0
58	MG	2A	3673	1/1	0.96	0.22	63,63,63,63	0
58	MG	1A	4045	1/1	0.96	0.14	68,68,68,68	0
58	MG	1A	3628	1/1	0.96	0.14	30,30,30,30	0
58	MG	1A	3629	1/1	0.96	0.37	69,69,69,69	0
58	MG	1A	3036	1/1	0.96	0.50	35,35,35,35	0
58	MG	1A	3338	1/1	0.96	0.36	43,43,43,43	0
58	MG	1A	3565	1/1	0.96	0.19	12,12,12,12	0
58	MG	1D	302	1/1	0.96	0.28	45,45,45,45	0
58	MG	1A	3306	1/1	0.96	0.23	45,45,45,45	0
58	MG	1A	3635	1/1	0.96	0.16	36,36,36,36	0
58	MG	2a	1713	1/1	0.96	0.15	63,63,63,63	0
58	MG	1l	101	1/1	0.96	0.52	44,44,44,44	0
58	MG	1A	3125	1/1	0.96	0.12	50,50,50,50	0
58	MG	2A	3686	1/1	0.96	0.13	83,83,83,83	0
58	MG	1A	3872	1/1	0.96	0.14	57,57,57,57	0
58	MG	1A	3703	1/1	0.96	0.23	51,51,51,51	0
58	MG	1A	3126	1/1	0.96	0.20	51,51,51,51	0
58	MG	1A	3162	1/1	0.96	0.24	44,44,44,44	0
58	MG	1A	3181	1/1	0.96	0.19	39,39,39,39	0
58	MG	1E	305	1/1	0.96	0.27	41,41,41,41	0
58	MG	2A	3693	1/1	0.96	0.09	64,64,64,64	0
58	MG	1a	1696	1/1	0.96	0.09	87,87,87,87	0
58	MG	2A	3529	1/1	0.96	0.14	43,43,43,43	0
58	MG	1a	1697	1/1	0.96	0.16	50,50,50,50	0
58	MG	2A	3091	1/1	0.96	0.22	35,35,35,35	0
58	MG	1A	3227	1/1	0.96	0.20	38,38,38,38	0
58	MG	1A	3528	1/1	0.96	0.30	39,39,39,39	0
58	MG	15	101	1/1	0.96	0.41	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1E	309	1/1	0.96	0.19	33,33,33,33	0
58	MG	1A	3071	1/1	0.96	0.22	51,51,51,51	0
58	MG	2A	3237	1/1	0.96	0.10	71,71,71,71	0
58	MG	15	105	1/1	0.96	0.20	45,45,45,45	0
58	MG	2a	1736	1/1	0.96	0.07	73,73,73,73	0
58	MG	2A	3541	1/1	0.96	0.18	51,51,51,51	0
58	MG	1A	3968	1/1	0.96	0.16	57,57,57,57	0
58	MG	2A	3707	1/1	0.96	0.08	69,69,69,69	0
58	MG	2A	3100	1/1	0.96	0.26	48,48,48,48	0
58	MG	1A	4065	1/1	0.96	0.16	28,28,28,28	0
58	MG	1k	3100	1/1	0.96	0.16	55,55,55,55	0
58	MG	2a	1743	1/1	0.96	0.09	77,77,77,77	0
58	MG	1A	3484	1/1	0.96	0.44	44,44,44,44	0
58	MG	1F	303	1/1	0.96	0.21	40,40,40,40	0
58	MG	2A	3245	1/1	0.96	0.28	59,59,59,59	0
58	MG	1A	3578	1/1	0.96	0.12	45,45,45,45	0
58	MG	17	102	1/1	0.96	0.33	37,37,37,37	0
58	MG	2A	3107	1/1	0.96	0.19	45,45,45,45	0
58	MG	1n	102	1/1	0.96	0.15	70,70,70,70	0
58	MG	2a	1754	1/1	0.96	0.12	79,79,79,79	0
58	MG	1F	305	1/1	0.96	0.17	36,36,36,36	0
58	MG	2A	3394	1/1	0.96	0.34	69,69,69,69	0
58	MG	2A	3558	1/1	0.96	0.22	71,71,71,71	0
58	MG	1A	3581	1/1	0.96	0.21	30,30,30,30	0
58	MG	1A	3584	1/1	0.96	0.11	23,23,23,23	0
58	MG	2A	3397	1/1	0.96	0.12	49,49,49,49	0
58	MG	2l	101	1/1	0.96	0.66	56,56,56,56	0
58	MG	1A	3485	1/1	0.96	0.36	39,39,39,39	0
58	MG	1A	3586	1/1	0.96	0.25	41,41,41,41	0
58	MG	1A	3802	1/1	0.96	0.24	41,41,41,41	0
58	MG	1A	3651	1/1	0.96	0.12	58,58,58,58	0
58	MG	2a	1767	1/1	0.96	0.21	62,62,62,62	0
58	MG	1w	105	1/1	0.96	0.12	80,80,80,80	0
58	MG	1w	106	1/1	0.96	0.19	82,82,82,82	0
58	MG	1A	4074	1/1	0.96	0.17	53,53,53,53	0
58	MG	1A	3719	1/1	0.96	0.18	20,20,20,20	0
58	MG	2a	1772	1/1	0.96	0.16	81,81,81,81	0
58	MG	2a	1773	1/1	0.96	0.18	81,81,81,81	0
58	MG	1A	3380	1/1	0.96	0.37	49,49,49,49	0
58	MG	1A	3807	1/1	0.96	0.16	53,53,53,53	0
58	MG	1A	3184	1/1	0.96	0.66	41,41,41,41	0
58	MG	1A	4080	1/1	0.96	0.08	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3128	1/1	0.96	0.29	38,38,38,38	0
58	MG	1A	3166	1/1	0.96	0.28	36,36,36,36	0
58	MG	1N	201	1/1	0.96	0.23	41,41,41,41	0
58	MG	1A	3592	1/1	0.96	0.28	28,28,28,28	0
58	MG	1A	4085	1/1	0.96	0.29	43,43,43,43	0
58	MG	2A	3130	1/1	0.96	0.21	58,58,58,58	0
58	MG	1A	3733	1/1	0.96	0.09	38,38,38,38	0
58	MG	1A	3593	1/1	0.96	0.18	35,35,35,35	0
58	MG	1O	202	1/1	0.96	0.23	52,52,52,52	0
58	MG	1A	3901	1/1	0.96	0.15	52,52,52,52	0
58	MG	1O	204	1/1	0.96	0.15	57,57,57,57	0
58	MG	1A	3094	1/1	0.96	0.21	36,36,36,36	0
58	MG	1A	3737	1/1	0.96	0.13	53,53,53,53	0
58	MG	1P	201	1/1	0.96	0.29	36,36,36,36	0
58	MG	1A	3738	1/1	0.96	0.14	53,53,53,53	0
58	MG	1P	203	1/1	0.96	0.15	27,27,27,27	0
58	MG	1A	3819	1/1	0.96	0.16	41,41,41,41	0
58	MG	2A	3144	1/1	0.96	0.40	57,57,57,57	0
58	MG	1A	3104	1/1	0.96	0.22	40,40,40,40	0
58	MG	2A	3761	1/1	0.96	0.21	58,58,58,58	0
58	MG	2A	3594	1/1	0.96	0.12	56,56,56,56	0
58	MG	1A	3742	1/1	0.96	0.20	35,35,35,35	0
58	MG	1A	3825	1/1	0.96	0.10	72,72,72,72	0
58	MG	2A	3597	1/1	0.96	0.20	35,35,35,35	0
58	MG	2A	3010	1/1	0.96	0.27	60,60,60,60	0
58	MG	1A	3257	1/1	0.96	0.30	44,44,44,44	0
58	MG	2A	3436	1/1	0.96	0.19	46,46,46,46	0
58	MG	2A	3769	1/1	0.96	0.22	58,58,58,58	0
58	MG	2A	3437	1/1	0.96	0.16	64,64,64,64	0
58	MG	1A	3010	1/1	0.96	0.20	39,39,39,39	0
58	MG	2A	3439	1/1	0.96	0.14	38,38,38,38	0
58	MG	1a	1751	1/1	0.96	0.12	68,68,68,68	0
58	MG	1A	3032	1/1	0.96	0.16	50,50,50,50	0
58	MG	1A	3913	1/1	0.96	0.19	53,53,53,53	0
58	MG	1A	4103	1/1	0.96	0.11	58,58,58,58	0
58	MG	1R	202	1/1	0.96	0.17	31,31,31,31	0
58	MG	2A	3019	1/1	0.96	0.10	56,56,56,56	0
58	MG	1A	3914	1/1	0.96	0.18	62,62,62,62	0
58	MG	1A	4002	1/1	0.96	0.18	21,21,21,21	0
58	MG	1A	3107	1/1	0.96	0.26	32,32,32,32	0
58	MG	1A	3152	1/1	0.96	0.26	33,33,33,33	0
58	MG	2A	3783	1/1	0.96	0.18	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3034	1/1	0.96	0.17	26,26,26,26	0
58	MG	2A	3027	1/1	0.96	0.97	62,62,62,62	0
58	MG	2A	3165	1/1	0.96	0.15	68,68,68,68	0
58	MG	1A	3500	1/1	0.96	0.31	38,38,38,38	0
58	MG	1a	1764	1/1	0.96	0.08	73,73,73,73	0
58	MG	1A	3263	1/1	0.96	0.23	33,33,33,33	0
58	MG	2A	3458	1/1	0.96	0.18	40,40,40,40	0
58	MG	1a	1766	1/1	0.96	0.23	60,60,60,60	0
58	MG	1A	4010	1/1	0.96	0.19	22,22,22,22	0
58	MG	1A	3429	1/1	0.96	0.22	38,38,38,38	0
58	MG	1A	3752	1/1	0.96	0.14	30,30,30,30	0
58	MG	1A	3463	1/1	0.96	0.14	45,45,45,45	0
58	MG	2A	3036	1/1	0.96	0.21	35,35,35,35	0
58	MG	1A	3840	1/1	0.96	0.15	26,26,26,26	0
58	MG	2A	3632	1/1	0.96	0.19	45,45,45,45	0
58	MG	1A	3464	1/1	0.96	0.21	63,63,63,63	0
58	MG	2a	1838	1/1	0.96	0.13	72,72,72,72	0
58	MG	1A	3842	1/1	0.96	0.09	42,42,42,42	0
58	MG	1A	3196	1/1	0.96	0.20	47,47,47,47	0
58	MG	1A	3551	1/1	0.96	0.16	33,33,33,33	0
58	MG	2A	3319	1/1	0.96	0.32	67,67,67,67	0
58	MG	1A	3612	1/1	0.96	0.21	41,41,41,41	0
58	MG	1U	211	1/1	0.96	0.46	39,39,39,39	0
58	MG	1A	4021	1/1	0.96	0.29	56,56,56,56	0
58	MG	1A	3265	1/1	0.96	0.26	44,44,44,44	0
58	MG	2A	3643	1/1	0.96	0.12	69,69,69,69	0
58	MG	1A	3136	1/1	0.96	0.29	39,39,39,39	0
58	MG	1A	3301	1/1	0.96	0.36	73,73,73,73	0
58	MG	1A	3849	1/1	0.96	0.18	42,42,42,42	0
58	MG	1A	3366	1/1	0.96	0.12	34,34,34,34	0
58	MG	1a	1661	1/1	0.96	0.14	62,62,62,62	0
58	MG	2a	1676	1/1	0.96	0.08	63,63,63,63	0
58	MG	1B	217	1/1	0.96	0.21	59,59,59,59	0
58	MG	2A	3330	1/1	0.96	0.46	55,55,55,55	0
58	MG	1W	204	1/1	0.96	0.19	44,44,44,44	0
58	MG	1A	3269	1/1	0.96	0.23	41,41,41,41	0
58	MG	1A	3683	1/1	0.96	0.18	54,54,54,54	0
58	MG	1A	3403	1/1	0.96	0.11	57,57,57,57	0
58	MG	1A	3854	1/1	0.96	0.16	54,54,54,54	0
58	MG	1A	3621	1/1	0.96	0.10	30,30,30,30	0
58	MG	1a	1794	1/1	0.96	0.12	69,69,69,69	0
58	MG	2A	3060	1/1	0.96	0.28	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4033	1/1	0.96	0.27	49,49,49,49	0
58	MG	1A	3559	1/1	0.96	0.19	64,64,64,64	0
58	MG	1a	1797	1/1	0.96	0.08	65,65,65,65	0
58	MG	2A	3499	1/1	0.96	0.22	40,40,40,40	0
58	MG	1A	3243	1/1	0.96	0.21	56,56,56,56	0
58	MG	2B	204	1/1	0.96	0.17	68,68,68,68	0
59	K	1A	3504	1/1	0.96	0.21	69,69,69,69	0
58	MG	1A	3688	1/1	0.96	0.07	60,60,60,60	0
58	MG	2A	3503	1/1	0.96	0.20	62,62,62,62	0
60	ZN	1n	104	1/1	0.96	0.17	78,78,78,78	0
58	MG	1A	3561	1/1	0.96	0.11	47,47,47,47	0
58	MG	1A	3063	1/1	0.96	0.17	35,35,35,35	0
58	MG	2A	3207	1/1	0.96	0.11	82,82,82,82	0
58	MG	1A	4039	1/1	0.96	0.10	32,32,32,32	0
58	MG	1A	3365	1/1	0.97	0.19	32,32,32,32	0
58	MG	1A	4041	1/1	0.97	0.17	41,41,41,41	0
58	MG	2U	201	1/1	0.97	0.32	57,57,57,57	0
58	MG	2a	1726	1/1	0.97	0.12	64,64,64,64	0
58	MG	1A	3646	1/1	0.97	0.26	26,26,26,26	0
58	MG	2A	3202	1/1	0.97	0.63	55,55,55,55	0
58	MG	1a	1615	1/1	0.97	0.21	67,67,67,67	0
58	MG	1A	3598	1/1	0.97	0.20	57,57,57,57	0
58	MG	1A	3115	1/1	0.97	0.19	35,35,35,35	0
58	MG	1B	216	1/1	0.97	0.08	68,68,68,68	0
58	MG	1A	3275	1/1	0.97	0.13	54,54,54,54	0
58	MG	1A	3700	1/1	0.97	0.17	26,26,26,26	0
58	MG	2A	3209	1/1	0.97	0.13	54,54,54,54	0
58	MG	1A	3090	1/1	0.97	0.23	23,23,23,23	0
58	MG	1a	1622	1/1	0.97	0.15	49,49,49,49	0
58	MG	1A	3765	1/1	0.97	0.14	30,30,30,30	0
58	MG	2A	3463	1/1	0.97	0.25	40,40,40,40	0
58	MG	1A	3556	1/1	0.97	0.13	37,37,37,37	0
58	MG	1A	3835	1/1	0.97	0.19	54,54,54,54	0
58	MG	1A	3654	1/1	0.97	0.19	47,47,47,47	0
58	MG	2A	3753	1/1	0.97	0.18	50,50,50,50	0
58	MG	2A	3607	1/1	0.97	0.09	68,68,68,68	0
58	MG	2a	1745	1/1	0.97	0.11	76,76,76,76	0
58	MG	1A	3837	1/1	0.97	0.17	37,37,37,37	0
58	MG	1a	1736	1/1	0.97	0.13	56,56,56,56	0
58	MG	2a	1748	1/1	0.97	0.08	83,83,83,83	0
58	MG	1U	201	1/1	0.97	0.30	36,36,36,36	0
58	MG	2A	3471	1/1	0.97	0.24	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1U	202	1/1	0.97	0.45	44,44,44,44	0
58	MG	2A	3339	1/1	0.97	0.25	72,72,72,72	0
58	MG	2a	1753	1/1	0.97	0.15	69,69,69,69	0
58	MG	1A	3012	1/1	0.97	0.16	26,26,26,26	0
58	MG	1A	3518	1/1	0.97	0.28	73,73,73,73	0
58	MG	1A	3081	1/1	0.97	0.11	35,35,35,35	0
58	MG	1U	206	1/1	0.97	0.25	45,45,45,45	0
58	MG	2a	1758	1/1	0.97	0.15	76,76,76,76	0
58	MG	1A	3407	1/1	0.97	0.26	47,47,47,47	0
58	MG	1A	3073	1/1	0.97	0.23	27,27,27,27	0
58	MG	1U	209	1/1	0.97	0.19	41,41,41,41	0
58	MG	1A	3157	1/1	0.97	0.27	42,42,42,42	0
58	MG	1A	3281	1/1	0.97	0.26	49,49,49,49	0
58	MG	1A	3911	1/1	0.97	0.14	55,55,55,55	0
58	MG	1U	213	1/1	0.97	0.33	39,39,39,39	0
58	MG	1A	4063	1/1	0.97	0.10	82,82,82,82	0
58	MG	1B	234	1/1	0.97	0.16	64,64,64,64	0
58	MG	1V	204	1/1	0.97	0.38	37,37,37,37	0
58	MG	1V	205	1/1	0.97	0.18	34,34,34,34	0
58	MG	1a	1645	1/1	0.97	0.08	58,58,58,58	0
58	MG	1A	3712	1/1	0.97	0.17	32,32,32,32	0
58	MG	1V	207	1/1	0.97	0.19	39,39,39,39	0
58	MG	2A	3492	1/1	0.97	0.21	59,59,59,59	0
58	MG	1A	3341	1/1	0.97	0.42	43,43,43,43	0
58	MG	1A	3985	1/1	0.97	0.24	33,33,33,33	0
58	MG	2a	1623	1/1	0.97	0.26	67,67,67,67	0
58	MG	1A	3011	1/1	0.97	0.15	33,33,33,33	0
58	MG	2A	3124	1/1	0.97	0.20	47,47,47,47	0
58	MG	1A	3566	1/1	0.97	0.22	44,44,44,44	0
58	MG	1a	1762	1/1	0.97	0.14	62,62,62,62	0
58	MG	2a	1628	1/1	0.97	0.11	73,73,73,73	0
58	MG	2A	3641	1/1	0.97	0.23	45,45,45,45	0
58	MG	1D	304	1/1	0.97	0.20	44,44,44,44	0
58	MG	1A	3045	1/1	0.97	0.11	20,20,20,20	0
58	MG	1A	3123	1/1	0.97	0.20	44,44,44,44	0
58	MG	1A	3668	1/1	0.97	0.28	45,45,45,45	0
58	MG	1A	3313	1/1	0.97	0.38	44,44,44,44	0
58	MG	2A	3370	1/1	0.97	0.18	27,27,27,27	0
58	MG	1A	3570	1/1	0.97	0.19	37,37,37,37	0
58	MG	1A	3723	1/1	0.97	0.14	45,45,45,45	0
58	MG	2A	3134	1/1	0.97	0.38	47,47,47,47	0
58	MG	2A	3135	1/1	0.97	0.24	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1D	311	1/1	0.97	0.10	60,60,60,60	0
58	MG	2A	3376	1/1	0.97	0.13	50,50,50,50	0
58	MG	1A	4075	1/1	0.97	0.29	35,35,35,35	0
58	MG	2A	3255	1/1	0.97	0.15	72,72,72,72	0
58	MG	2A	3379	1/1	0.97	0.55	57,57,57,57	0
58	MG	1Y	202	1/1	0.97	0.39	52,52,52,52	0
58	MG	1a	1774	1/1	0.97	0.06	54,54,54,54	0
58	MG	1A	3725	1/1	0.97	0.15	26,26,26,26	0
58	MG	1E	304	1/1	0.97	0.19	33,33,33,33	0
58	MG	1A	3620	1/1	0.97	0.22	29,29,29,29	0
58	MG	1A	3161	1/1	0.97	0.23	18,18,18,18	0
58	MG	1E	307	1/1	0.97	0.21	35,35,35,35	0
58	MG	1A	3124	1/1	0.97	0.31	47,47,47,47	0
58	MG	1A	3060	1/1	0.97	0.31	56,56,56,56	0
58	MG	2A	3524	1/1	0.97	0.24	57,57,57,57	0
58	MG	1A	3732	1/1	0.97	0.19	46,46,46,46	0
58	MG	1a	1783	1/1	0.97	0.10	89,89,89,89	0
58	MG	1A	4082	1/1	0.97	0.15	63,63,63,63	0
58	MG	2a	1658	1/1	0.97	0.22	58,58,58,58	0
58	MG	1A	4001	1/1	0.97	0.08	45,45,45,45	0
58	MG	1A	3020	1/1	0.97	0.16	54,54,54,54	0
58	MG	1A	3111	1/1	0.97	0.65	51,51,51,51	0
58	MG	1A	3167	1/1	0.97	0.12	36,36,36,36	0
58	MG	2A	3154	1/1	0.97	0.16	69,69,69,69	0
58	MG	1A	4087	1/1	0.97	0.34	65,65,65,65	0
58	MG	1A	3145	1/1	0.97	0.44	44,44,44,44	0
58	MG	1F	308	1/1	0.97	0.18	34,34,34,34	0
58	MG	2A	3536	1/1	0.97	0.22	47,47,47,47	0
58	MG	1A	3580	1/1	0.97	0.19	31,31,31,31	0
58	MG	1A	3800	1/1	0.97	0.19	30,30,30,30	0
58	MG	1A	3739	1/1	0.97	0.17	51,51,51,51	0
58	MG	1A	3322	1/1	0.97	0.30	42,42,42,42	0
58	MG	1A	3741	1/1	0.97	0.22	26,26,26,26	0
58	MG	2A	3543	1/1	0.97	0.16	54,54,54,54	0
58	MG	1A	3583	1/1	0.97	0.14	39,39,39,39	0
58	MG	1A	3039	1/1	0.97	0.37	34,34,34,34	0
58	MG	1A	3873	1/1	0.97	0.20	44,44,44,44	0
58	MG	1A	3324	1/1	0.97	0.19	46,46,46,46	0
58	MG	1A	3035	1/1	0.97	0.16	34,34,34,34	0
58	MG	1A	3943	1/1	0.97	0.20	27,27,27,27	0
58	MG	1A	4101	1/1	0.97	0.19	51,51,51,51	0
58	MG	15	106	1/1	0.97	0.29	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3945	1/1	0.97	0.06	58,58,58,58	0
58	MG	2A	3553	1/1	0.97	0.29	73,73,73,73	0
58	MG	2a	1684	1/1	0.97	0.14	51,51,51,51	0
58	MG	2A	3554	1/1	0.97	0.28	55,55,55,55	0
58	MG	1A	4020	1/1	0.97	0.27	42,42,42,42	0
58	MG	1A	3809	1/1	0.97	0.21	51,51,51,51	0
58	MG	1A	3148	1/1	0.97	0.14	45,45,45,45	0
58	MG	2A	3293	1/1	0.97	0.23	60,60,60,60	0
58	MG	1A	3879	1/1	0.97	0.18	40,40,40,40	0
58	MG	2A	3295	1/1	0.97	0.18	59,59,59,59	0
58	MG	1A	3089	1/1	0.97	0.13	40,40,40,40	0
58	MG	1A	4025	1/1	0.97	0.14	46,46,46,46	0
58	MG	1A	3881	1/1	0.97	0.26	35,35,35,35	0
58	MG	2A	3423	1/1	0.97	0.20	45,45,45,45	0
58	MG	1A	3394	1/1	0.97	0.16	59,59,59,59	0
58	MG	18	102	1/1	0.97	0.20	43,43,43,43	0
58	MG	1A	3268	1/1	0.97	0.28	36,36,36,36	0
58	MG	1A	3953	1/1	0.97	0.17	32,32,32,32	0
58	MG	2A	3428	1/1	0.97	0.21	48,48,48,48	0
58	MG	1A	3219	1/1	0.97	0.20	39,39,39,39	0
58	MG	1A	3150	1/1	0.97	0.18	36,36,36,36	0
58	MG	1A	3273	1/1	0.97	0.26	36,36,36,36	0
58	MG	1P	204	1/1	0.97	0.29	39,39,39,39	0
58	MG	1A	3753	1/1	0.97	0.31	33,33,33,33	0
58	MG	1a	1710	1/1	0.97	0.18	61,61,61,61	0
58	MG	1A	3399	1/1	0.97	0.18	61,61,61,61	0
58	MG	1B	206	1/1	0.97	0.13	52,52,52,52	0
58	MG	1A	3693	1/1	0.97	0.28	56,56,56,56	0
58	MG	2A	3579	1/1	0.97	0.28	56,56,56,56	0
58	MG	2A	3193	1/1	0.97	0.24	72,72,72,72	0
58	MG	1a	1714	1/1	0.97	0.18	59,59,59,59	0
58	MG	1A	3400	1/1	0.97	0.31	39,39,39,39	0
58	MG	2O	201	1/1	0.97	0.16	65,65,65,65	0
58	MG	2A	3442	1/1	0.97	0.21	60,60,60,60	0
58	MG	1A	3823	1/1	0.97	0.31	38,38,38,38	0
58	MG	1a	1717	1/1	0.97	0.12	41,41,41,41	0
58	MG	2A	3730	1/1	0.97	0.13	50,50,50,50	0
58	MG	2A	3731	1/1	0.97	0.13	64,64,64,64	0
58	MG	2A	3445	1/1	0.97	0.15	61,61,61,61	0
58	MG	2A	3733	1/1	0.97	0.14	68,68,68,68	0
58	MG	1A	3962	1/1	0.97	0.10	67,67,67,67	0
58	MG	1A	3367	1/1	0.98	0.32	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3498	1/1	0.98	0.14	35,35,35,35	0
58	MG	1A	3735	1/1	0.98	0.21	24,24,24,24	0
58	MG	1A	3787	1/1	0.98	0.29	37,37,37,37	0
58	MG	1A	3604	1/1	0.98	0.11	45,45,45,45	0
58	MG	1E	303	1/1	0.98	0.24	37,37,37,37	0
58	MG	2A	3684	1/1	0.98	0.09	56,56,56,56	0
58	MG	1A	3044	1/1	0.98	0.17	41,41,41,41	0
58	MG	1A	3203	1/1	0.98	0.28	39,39,39,39	0
58	MG	1A	3221	1/1	0.98	0.26	32,32,32,32	0
58	MG	1A	4099	1/1	0.98	0.15	56,56,56,56	0
58	MG	1A	3031	1/1	0.98	0.21	36,36,36,36	0
58	MG	1A	3132	1/1	0.98	0.21	15,15,15,15	0
58	MG	1A	3040	1/1	0.98	0.28	35,35,35,35	0
58	MG	2A	3502	1/1	0.98	0.14	56,56,56,56	0
58	MG	1A	3652	1/1	0.98	0.23	31,31,31,31	0
58	MG	1A	3796	1/1	0.98	0.22	23,23,23,23	0
58	MG	1a	1763	1/1	0.98	0.13	61,61,61,61	0
58	MG	2A	3599	1/1	0.98	0.20	64,64,64,64	0
58	MG	1A	3101	1/1	0.98	0.09	43,43,43,43	0
58	MG	1w	104	1/1	0.98	0.10	67,67,67,67	0
58	MG	1V	201	1/1	0.98	0.31	35,35,35,35	0
58	MG	1F	301	1/1	0.98	0.27	43,43,43,43	0
58	MG	2a	1799	1/1	0.98	0.14	57,57,57,57	0
58	MG	1a	1612	1/1	0.98	0.13	31,31,31,31	0
58	MG	1A	4040	1/1	0.98	0.10	71,71,71,71	0
58	MG	1A	3068	1/1	0.98	0.18	18,18,18,18	0
58	MG	1A	4042	1/1	0.98	0.11	58,58,58,58	0
58	MG	1A	3541	1/1	0.98	0.43	32,32,32,32	0
58	MG	2A	3161	1/1	0.98	0.26	36,36,36,36	0
58	MG	1a	1692	1/1	0.98	0.14	44,44,44,44	0
58	MG	1F	307	1/1	0.98	0.21	45,45,45,45	0
58	MG	2A	3612	1/1	0.98	0.43	65,65,65,65	0
58	MG	1A	3575	1/1	0.98	0.26	30,30,30,30	0
58	MG	1A	3615	1/1	0.98	0.19	28,28,28,28	0
58	MG	2A	3615	1/1	0.98	0.19	39,39,39,39	0
58	MG	1W	203	1/1	0.98	0.19	39,39,39,39	0
58	MG	1A	3026	1/1	0.98	0.37	35,35,35,35	0
58	MG	2A	3081	1/1	0.98	0.39	49,49,49,49	0
58	MG	1A	3137	1/1	0.98	0.24	39,39,39,39	0
58	MG	1A	3511	1/1	0.98	0.24	48,48,48,48	0
58	MG	1a	1700	1/1	0.98	0.20	63,63,63,63	0
58	MG	1A	3579	1/1	0.98	0.16	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3435	1/1	0.98	0.16	43,43,43,43	0
58	MG	1A	3806	1/1	0.98	0.10	50,50,50,50	0
58	MG	1A	3662	1/1	0.98	0.21	19,19,19,19	0
58	MG	1A	3454	1/1	0.98	0.40	60,60,60,60	0
58	MG	1A	3988	1/1	0.98	0.18	45,45,45,45	0
58	MG	2A	3725	1/1	0.98	0.23	56,56,56,56	0
58	MG	2A	3726	1/1	0.98	0.12	63,63,63,63	0
58	MG	1A	4054	1/1	0.98	0.12	60,60,60,60	0
58	MG	1A	3867	1/1	0.98	0.17	45,45,45,45	0
58	MG	2A	3092	1/1	0.98	0.26	67,67,67,67	0
58	MG	2B	203	1/1	0.98	0.30	69,69,69,69	0
58	MG	1A	3353	1/1	0.98	0.24	34,34,34,34	0
58	MG	1A	3582	1/1	0.98	0.16	60,60,60,60	0
58	MG	1Z	302	1/1	0.98	0.21	58,58,58,58	0
58	MG	1A	3811	1/1	0.98	0.19	30,30,30,30	0
58	MG	2A	3539	1/1	0.98	0.20	43,43,43,43	0
58	MG	1A	3623	1/1	0.98	0.14	27,27,27,27	0
58	MG	1A	3033	1/1	0.98	0.16	47,47,47,47	0
58	MG	1A	3515	1/1	0.98	0.23	42,42,42,42	0
58	MG	2A	3013	1/1	0.98	0.13	50,50,50,50	0
58	MG	1A	3288	1/1	0.98	0.21	35,35,35,35	0
58	MG	1A	3267	1/1	0.98	0.26	38,38,38,38	0
58	MG	1A	3762	1/1	0.98	0.36	36,36,36,36	0
58	MG	1A	3231	1/1	0.98	0.12	41,41,41,41	0
58	MG	2d	302	1/1	0.98	0.19	68,68,68,68	0
58	MG	1A	3358	1/1	0.98	0.39	32,32,32,32	0
58	MG	1A	3820	1/1	0.98	0.18	43,43,43,43	0
58	MG	1A	3630	1/1	0.98	0.20	26,26,26,26	0
58	MG	1A	3766	1/1	0.98	0.17	33,33,33,33	0
58	MG	2A	3459	1/1	0.98	0.27	38,38,38,38	0
58	MG	2l	201	1/1	0.98	0.09	71,71,71,71	0
58	MG	2D	302	1/1	0.98	0.19	39,39,39,39	0
58	MG	2A	3460	1/1	0.98	0.30	52,52,52,52	0
58	MG	1A	3520	1/1	0.98	0.18	41,41,41,41	0
58	MG	2A	3024	1/1	0.98	0.16	56,56,56,56	0
58	MG	1A	4005	1/1	0.98	0.15	49,49,49,49	0
58	MG	1A	3944	1/1	0.98	0.16	45,45,45,45	0
58	MG	1A	3824	1/1	0.98	0.15	40,40,40,40	0
58	MG	1A	3021	1/1	0.98	0.17	17,17,17,17	0
58	MG	1Q	202	1/1	0.98	0.28	33,33,33,33	0
58	MG	2A	3468	1/1	0.98	0.30	58,58,58,58	0
58	MG	1A	3336	1/1	0.98	0.23	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3770	1/1	0.98	0.13	41,41,41,41	0
58	MG	13	101	1/1	0.98	0.17	37,37,37,37	0
58	MG	1A	3720	1/1	0.98	0.21	33,33,33,33	0
58	MG	1A	3721	1/1	0.98	0.08	47,47,47,47	0
58	MG	1A	3830	1/1	0.98	0.23	29,29,29,29	0
58	MG	1a	1735	1/1	0.98	0.18	47,47,47,47	0
58	MG	1A	3057	1/1	0.98	0.33	40,40,40,40	0
58	MG	1A	3524	1/1	0.98	0.11	51,51,51,51	0
58	MG	1A	3724	1/1	0.98	0.13	36,36,36,36	0
58	MG	1A	3271	1/1	0.98	0.32	37,37,37,37	0
58	MG	1A	3182	1/1	0.98	0.28	44,44,44,44	0
58	MG	1A	3466	1/1	0.98	0.13	30,30,30,30	0
58	MG	2A	3043	1/1	0.98	0.21	34,34,34,34	0
60	ZN	1Y	203	1/1	0.98	0.16	78,78,78,78	0
58	MG	1A	3097	1/1	0.98	0.24	39,39,39,39	0
60	ZN	15	109	1/1	0.98	0.17	50,50,50,50	0
58	MG	1A	3729	1/1	0.98	0.16	33,33,33,33	0
58	MG	1A	3118	1/1	0.98	0.36	44,44,44,44	0
58	MG	1A	3731	1/1	0.98	0.16	45,45,45,45	0
58	MG	1A	3186	1/1	0.98	0.15	40,40,40,40	0
58	MG	1a	1747	1/1	0.98	0.07	69,69,69,69	0
58	MG	1A	4007	1/1	0.99	0.21	19,19,19,19	0
58	MG	1A	3029	1/1	0.99	0.32	37,37,37,37	0
58	MG	2A	3020	1/1	0.99	0.21	28,28,28,28	0
58	MG	1A	3707	1/1	0.99	0.25	48,48,48,48	0
58	MG	1A	3185	1/1	0.99	0.36	33,33,33,33	0
58	MG	1A	3165	1/1	0.99	0.30	44,44,44,44	0
58	MG	1D	303	1/1	0.99	0.17	21,21,21,21	0
58	MG	1A	3600	1/1	0.99	0.11	51,51,51,51	0
58	MG	1F	302	1/1	0.99	0.20	35,35,35,35	0
58	MG	1A	3272	1/1	0.99	0.49	39,39,39,39	0
58	MG	1A	3321	1/1	0.99	0.54	41,41,41,41	0
58	MG	1A	3153	1/1	0.99	0.46	39,39,39,39	0
58	MG	1A	3589	1/1	0.99	0.19	15,15,15,15	0
58	MG	1V	202	1/1	0.99	0.25	35,35,35,35	0
58	MG	1A	3650	1/1	0.99	0.18	15,15,15,15	0
58	MG	1A	3941	1/1	0.99	0.17	19,19,19,19	0
58	MG	1A	3292	1/1	0.99	0.31	37,37,37,37	0
58	MG	2A	3811	1/1	0.99	0.16	50,50,50,50	0
58	MG	15	104	1/1	0.99	0.24	34,34,34,34	0
58	MG	1A	3048	1/1	0.99	0.29	30,30,30,30	0
58	MG	1A	3499	1/1	0.99	0.23	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1795	1/1	0.99	0.16	57,57,57,57	0
60	ZN	19	102	1/1	0.99	0.25	58,58,58,58	0
58	MG	1A	3003	1/1	0.99	0.17	27,27,27,27	0
58	MG	1A	3392	1/1	0.99	0.25	41,41,41,41	0
58	MG	1A	3220	1/1	0.99	0.30	33,33,33,33	0
60	ZN	25	103	1/1	0.99	0.21	71,71,71,71	0
60	ZN	26	103	1/1	0.99	0.17	65,65,65,65	0
58	MG	1A	3228	1/1	0.99	0.20	32,32,32,32	0
58	MG	1A	3876	1/1	0.99	0.17	13,13,13,13	0
61	SF4	1d	302	8/8	0.99	0.17	65,72,75,76	0
61	SF4	2d	303	8/8	0.99	0.13	62,70,76,82	0
60	ZN	16	103	1/1	1.00	0.21	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.