



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 19, 2022 – 11:42 AM EST

PDB ID : 7RQC
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with protein Y, A-site aminoacyl-tRNA analog ACC-PMN, and P-site MFI-tripeptidyl-tRNA analog ACCA-IFM at 2.50Å resolution
Authors : Syroegin, E.A.; Flemmich, L.; Klepacki, D.; Vazquez-Laslop, N.; Micura, R.; Polikanov, Y.S.
Deposited on : 2021-08-06
Resolution : 2.50 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 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 : 2.25
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.25

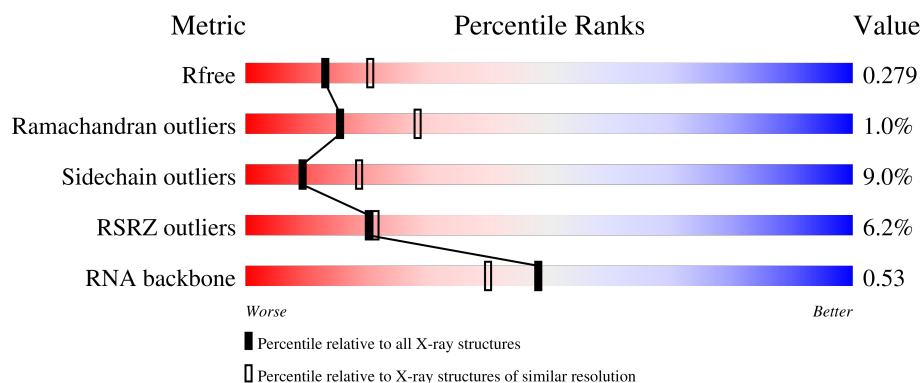
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>
1	2A	2915	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>..</div> </div> </div>
2	1B	121	<div> <div></div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>
2	2B	121	<div> <div></div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
3	1D	276	<div> <div>0%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>


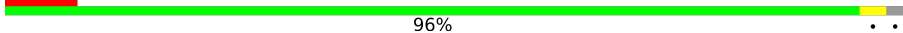

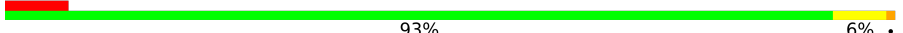











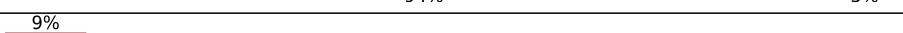
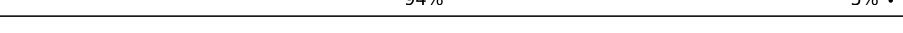
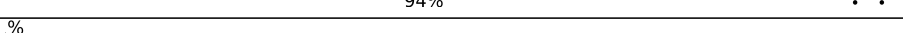







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Mol	Chain	Length	Quality of chain
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118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

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Mol	Chain	Length	Quality of chain
16	1U	118	 93% 5% .
16	2U	118	 96% . .
17	1V	101	 89% 10% .
17	2V	101	 93% 6% .
18	1W	113	 92% 7% .
18	2W	113	 93% 6% .
19	1X	96	 94% 5% .
19	2X	96	 96% . .
20	1Y	110	 85% 12% .
20	2Y	110	 89% 8% .
21	1Z	206	 88% 10% .
21	2Z	206	 88% 9% .
22	10	85	 94% . .
22	20	85	 93% 5% .
23	11	98	 94% 5% .
23	21	98	 94% 5% .
24	12	72	 94% . .
24	22	72	 86% 11% .
25	13	60	 92% 7% .
25	23	60	 88% 10% .
26	14	71	 82% 15% .
26	24	71	 79% 17% . .
27	15	60	 88% 10% .
27	25	60	 93% 5% .
28	16	54	 93% 6% .

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

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Mol	Chain	Length	Quality of chain
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	
53	1y	113	

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Mol	Chain	Length	Quality of chain
53	2y	113	
54	1w	4	
54	2w	4	
55	1x	4	
55	2x	4	
56	1v	3	
56	2v	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1a	3052	-	-	-	X
57	MG	2A	3246	-	-	-	X
57	MG	2A	3248	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 297682 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	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
			877	553	175	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
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			650	401	139	109	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

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

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

- Molecule 53 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1v	3	Total	C	N	O	S	0	0	0
			27	20	3	3	1			
56	2v	3	Total	C	N	O	S	0	0	0
			27	20	3	3	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1022	Total	Mg	0	0
			1022	1022		
57	1B	30	Total	Mg	0	0
			30	30		
57	1D	15	Total	Mg	0	0
			15	15		
57	1E	12	Total	Mg	0	0
			12	12		
57	1F	16	Total	Mg	0	0
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	4	Total 4	Mg 4	0	0
57	1H	2	Total 2	Mg 2	0	0
57	1N	4	Total 4	Mg 4	0	0
57	1O	1	Total 1	Mg 1	0	0
57	1P	5	Total 5	Mg 5	0	0
57	1Q	7	Total 7	Mg 7	0	0
57	1R	4	Total 4	Mg 4	0	0
57	1S	1	Total 1	Mg 1	0	0
57	1T	5	Total 5	Mg 5	0	0
57	1U	4	Total 4	Mg 4	0	0
57	1V	7	Total 7	Mg 7	0	0
57	1W	3	Total 3	Mg 3	0	0
57	1X	1	Total 1	Mg 1	0	0
57	1Y	1	Total 1	Mg 1	0	0
57	1Z	1	Total 1	Mg 1	0	0
57	10	9	Total 9	Mg 9	0	0
57	11	5	Total 5	Mg 5	0	0
57	13	3	Total 3	Mg 3	0	0
57	15	9	Total 9	Mg 9	0	0
57	17	6	Total 6	Mg 6	0	0
57	18	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	19	2	Total 2	Mg 2	0	0
57	1a	274	Total 274	Mg 274	0	0
57	1b	1	Total 1	Mg 1	0	0
57	1d	6	Total 6	Mg 6	0	0
57	1e	3	Total 3	Mg 3	0	0
57	1f	2	Total 2	Mg 2	0	0
57	1g	1	Total 1	Mg 1	0	0
57	1h	2	Total 2	Mg 2	0	0
57	1i	1	Total 1	Mg 1	0	0
57	1l	3	Total 3	Mg 3	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	3	Total 3	Mg 3	0	0
57	1o	2	Total 2	Mg 2	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1u	1	Total 1	Mg 1	0	0
57	1y	4	Total 4	Mg 4	0	0
57	1w	1	Total 1	Mg 1	0	0
57	1x	2	Total 2	Mg 2	0	0
57	2A	733	Total 733	Mg 733	0	0
57	2B	19	Total 19	Mg 19	0	0
57	2D	10	Total 10	Mg 10	0	0

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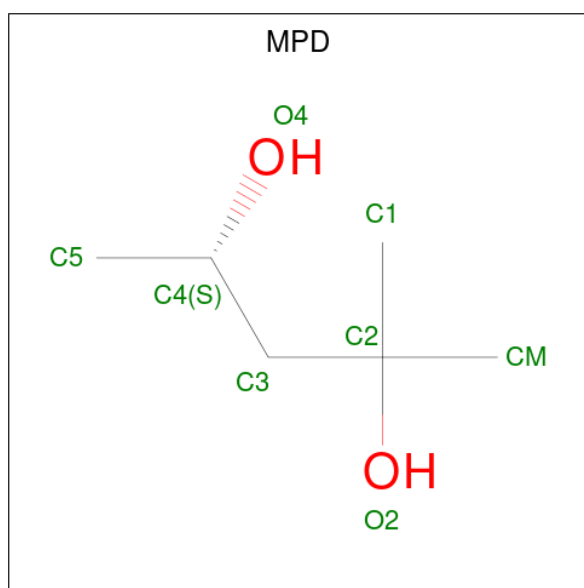
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2E	7	Total 7	Mg 7	0	0
57	2F	4	Total 4	Mg 4	0	0
57	2G	3	Total 3	Mg 3	0	0
57	2I	1	Total 1	Mg 1	0	0
57	2O	2	Total 2	Mg 2	0	0
57	2P	2	Total 2	Mg 2	0	0
57	2Q	4	Total 4	Mg 4	0	0
57	2R	3	Total 3	Mg 3	0	0
57	2T	3	Total 3	Mg 3	0	0
57	2U	1	Total 1	Mg 1	0	0
57	2V	3	Total 3	Mg 3	0	0
57	2W	3	Total 3	Mg 3	0	0
57	2X	1	Total 1	Mg 1	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	20	2	Total 2	Mg 2	0	0
57	21	1	Total 1	Mg 1	0	0
57	25	3	Total 3	Mg 3	0	0
57	27	2	Total 2	Mg 2	0	0
57	28	2	Total 2	Mg 2	0	0
57	2a	190	Total 190	Mg 190	0	0
57	2e	1	Total 1	Mg 1	0	0

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

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



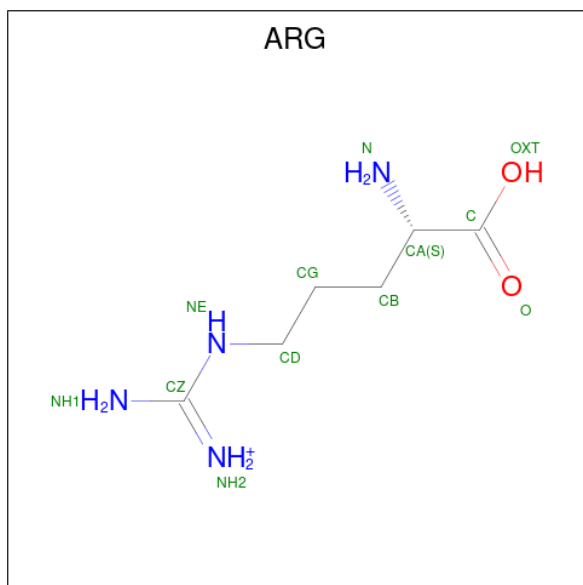
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total C O 8 6 2	0	0
58	18	1	Total C O 8 6 2	0	0
58	1a	1	Total C O 8 6 2	0	0
58	1a	1	Total C O 8 6 2	0	0

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

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



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

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

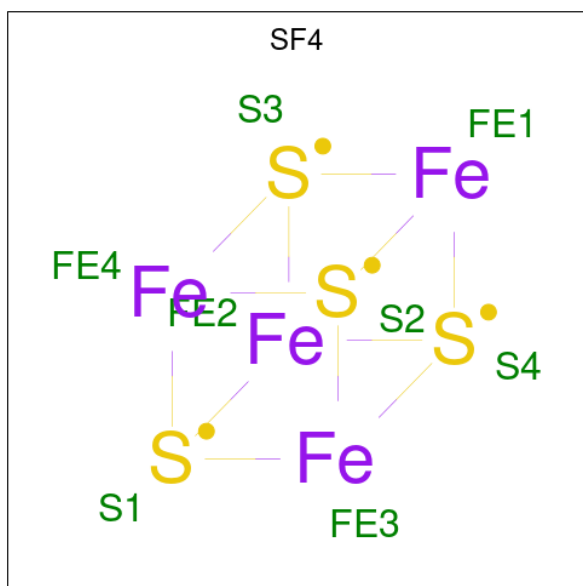
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		

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

- 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	3972	Total 3972	O 3972	0	0
62	1B	98	Total 98	O 98	0	0
62	1D	107	Total 107	O 107	0	0
62	1E	75	Total 75	O 75	0	0
62	1F	60	Total 60	O 60	0	0
62	1G	20	Total 20	O 20	0	0
62	1H	15	Total 15	O 15	0	0
62	1I	4	Total 4	O 4	0	0
62	1N	47	Total 47	O 47	0	0
62	1O	26	Total 26	O 26	0	0
62	1P	63	Total 63	O 63	0	0
62	1Q	37	Total 37	O 37	0	0
62	1R	34	Total 34	O 34	0	0
62	1S	15	Total 15	O 15	0	0
62	1T	32	Total 32	O 32	0	0
62	1U	45	Total 45	O 45	0	0
62	1V	36	Total 36	O 36	0	0
62	1W	25	Total 25	O 25	0	0
62	1X	26	Total 26	O 26	0	0
62	1Y	16	Total 16	O 16	0	0
62	1Z	8	Total 8	O 8	0	0
62	10	21	Total 21	O 21	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	11	26	Total 26	O 26	0	0
62	12	12	Total 12	O 12	0	0
62	13	21	Total 21	O 21	0	0
62	14	2	Total 2	O 2	0	0
62	15	25	Total 25	O 25	0	0
62	16	18	Total 18	O 18	0	0
62	17	13	Total 13	O 13	0	0
62	18	26	Total 26	O 26	0	0
62	19	5	Total 5	O 5	0	0
62	1a	509	Total 509	O 509	0	0
62	1b	1	Total 1	O 1	0	0
62	1d	10	Total 10	O 10	0	0
62	1e	3	Total 3	O 3	0	0
62	1f	3	Total 3	O 3	0	0
62	1h	1	Total 1	O 1	0	0
62	1j	2	Total 2	O 2	0	0
62	1l	4	Total 4	O 4	0	0
62	1m	1	Total 1	O 1	0	0
62	1o	4	Total 4	O 4	0	0
62	1p	3	Total 3	O 3	0	0
62	1t	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1u	1	Total 1	O 1	0	0
62	1y	8	Total 8	O 8	0	0
62	1w	3	Total 3	O 3	0	0
62	1x	3	Total 3	O 3	0	0
62	2A	2105	Total 2105	O 2105	0	0
62	2B	46	Total 46	O 46	0	0
62	2D	48	Total 48	O 48	0	0
62	2E	26	Total 26	O 26	0	0
62	2F	24	Total 24	O 24	0	0
62	2G	4	Total 4	O 4	0	0
62	2H	2	Total 2	O 2	0	0
62	2I	4	Total 4	O 4	0	0
62	2N	5	Total 5	O 5	0	0
62	2O	18	Total 18	O 18	0	0
62	2P	19	Total 19	O 19	0	0
62	2Q	18	Total 18	O 18	0	0
62	2R	22	Total 22	O 22	0	0
62	2S	3	Total 3	O 3	0	0
62	2T	7	Total 7	O 7	0	0
62	2U	10	Total 10	O 10	0	0
62	2V	7	Total 7	O 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2W	17	Total 17	O 17	0	0
62	2X	8	Total 8	O 8	0	0
62	2Y	5	Total 5	O 5	0	0
62	2Z	11	Total 11	O 11	0	0
62	20	12	Total 12	O 12	0	0
62	21	20	Total 20	O 20	0	0
62	22	1	Total 1	O 1	0	0
62	23	4	Total 4	O 4	0	0
62	25	10	Total 10	O 10	0	0
62	26	5	Total 5	O 5	0	0
62	27	8	Total 8	O 8	0	0
62	28	12	Total 12	O 12	0	0
62	29	2	Total 2	O 2	0	0
62	2a	291	Total 291	O 291	0	0
62	2d	3	Total 3	O 3	0	0
62	2f	3	Total 3	O 3	0	0
62	2j	2	Total 2	O 2	0	0
62	2l	2	Total 2	O 2	0	0
62	2m	2	Total 2	O 2	0	0
62	2o	4	Total 4	O 4	0	0
62	2p	2	Total 2	O 2	0	0

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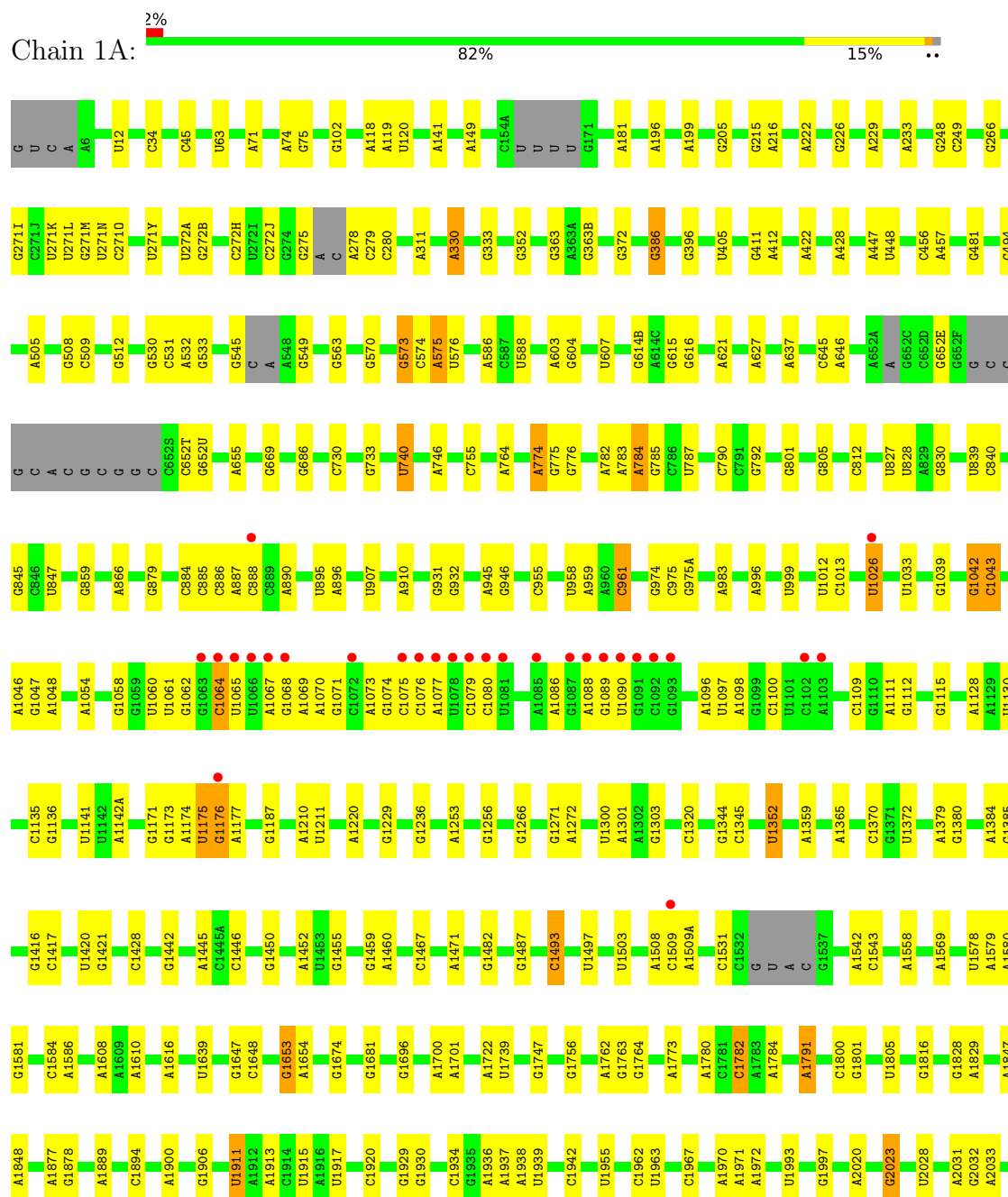
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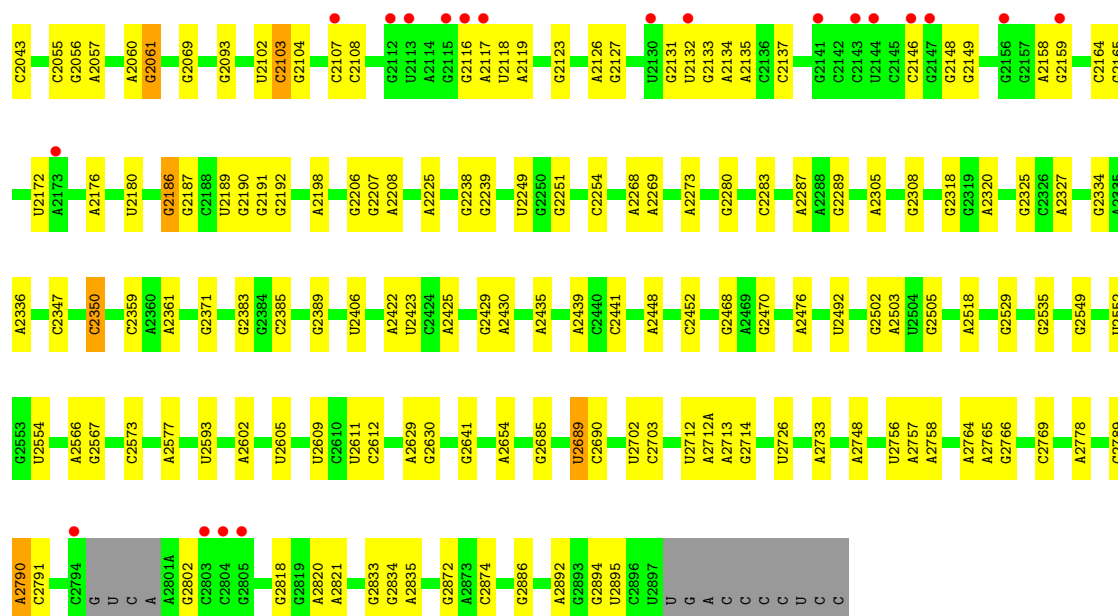
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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62	2r	3	Total 3	O 3	0	0
62	2t	2	Total 2	O 2	0	0
62	2y	3	Total 3	O 3	0	0
62	2w	3	Total 3	O 3	0	0
62	2x	1	Total 1	O 1	0	0

3 Residue-property plots

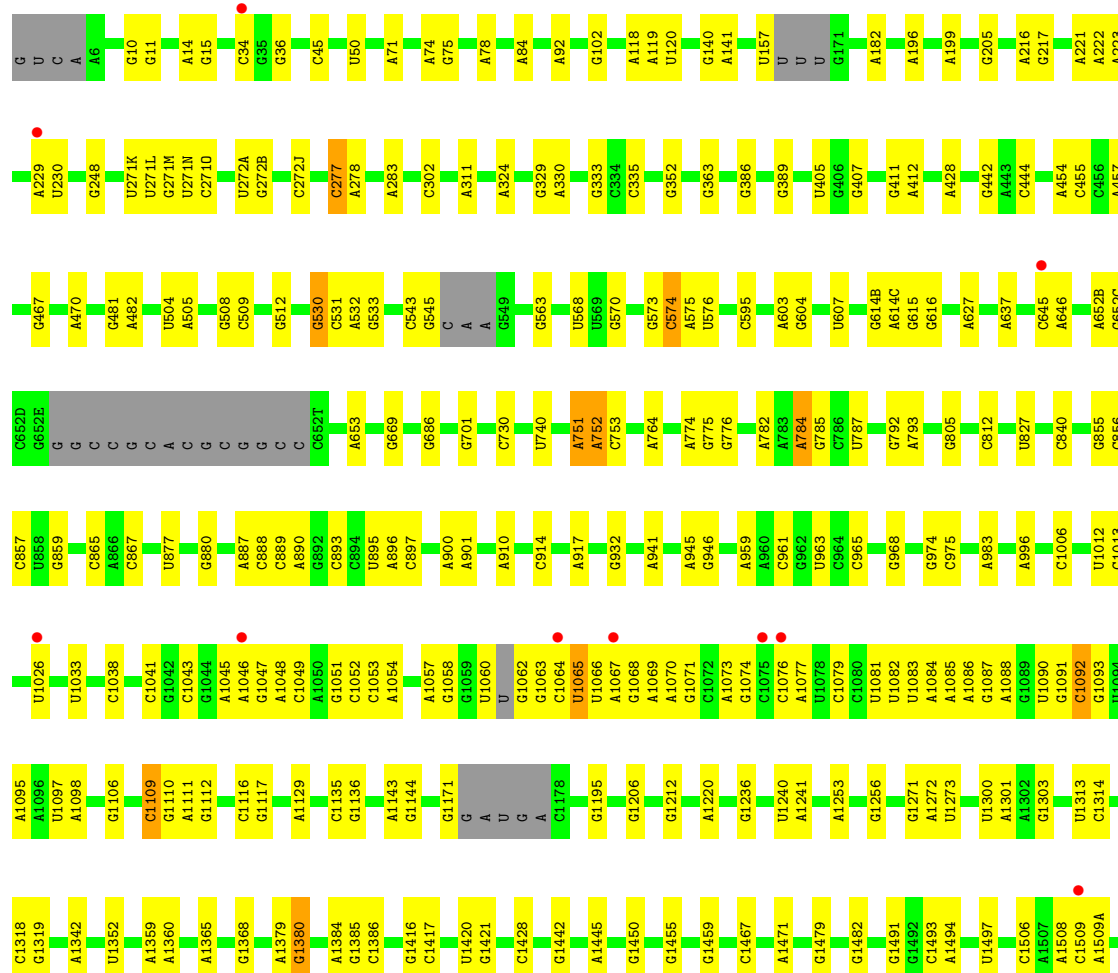
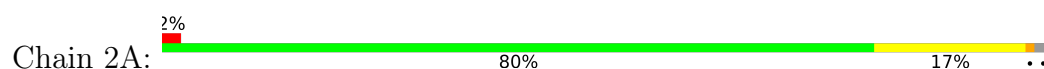
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S Ribosomal RNA

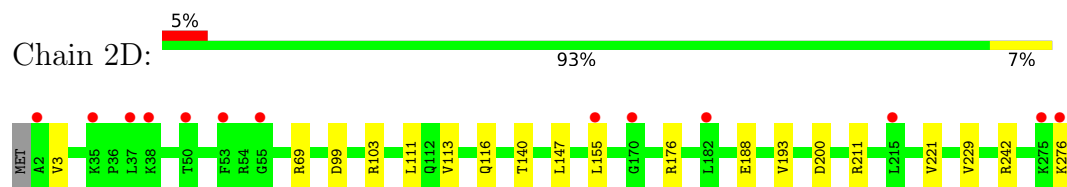




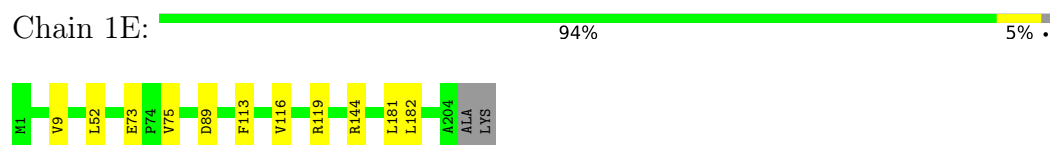
• Molecule 1: 23S Ribosomal RNA



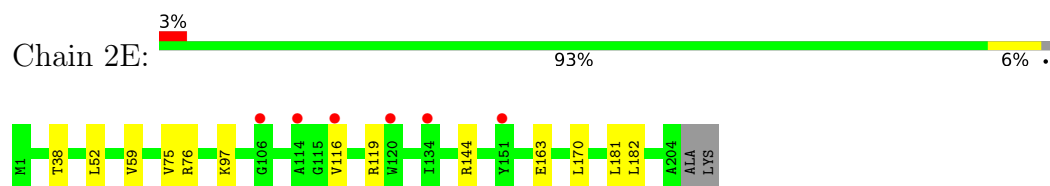
- Molecule 3: 50S ribosomal protein L2



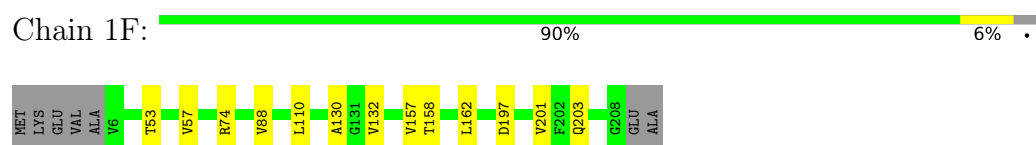
- Molecule 4: 50S ribosomal protein L3



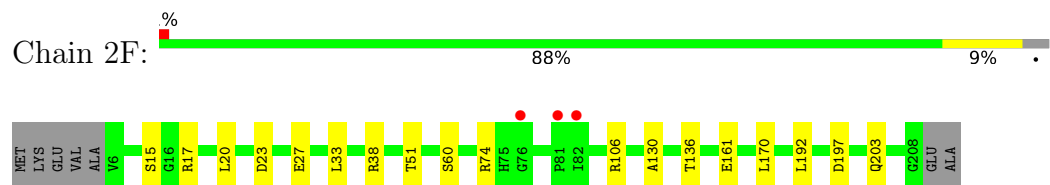
- Molecule 4: 50S ribosomal protein L3



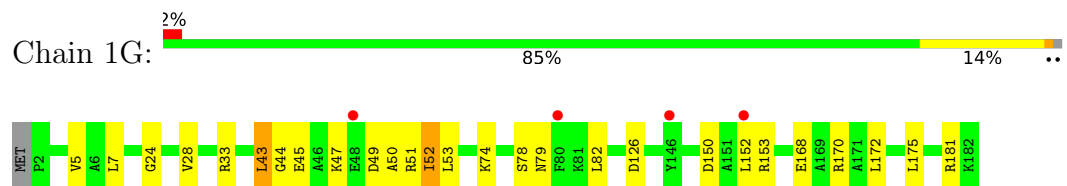
- Molecule 5: 50S ribosomal protein L4



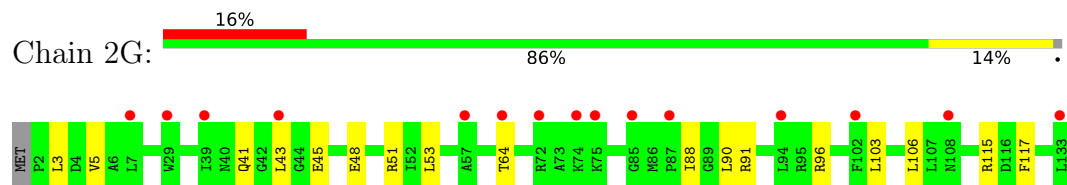
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5

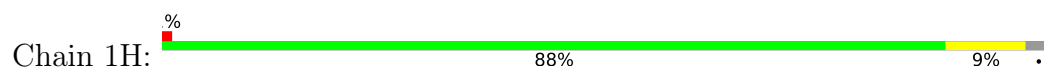


- Molecule 6: 50S ribosomal protein L5

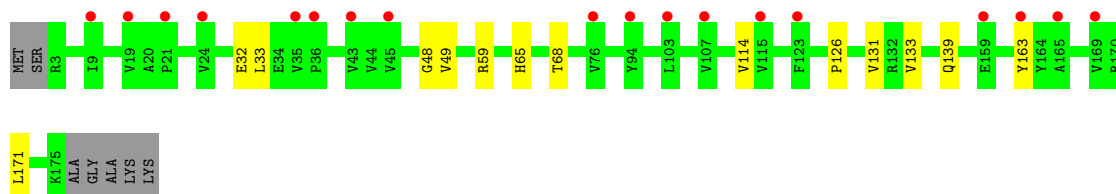
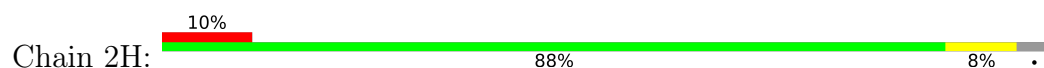




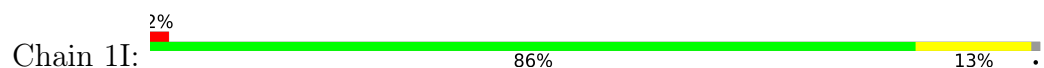
- Molecule 7: 50S ribosomal protein L6



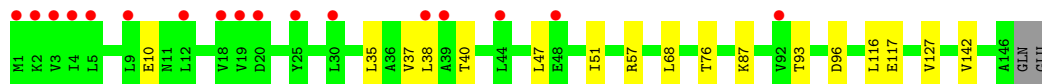
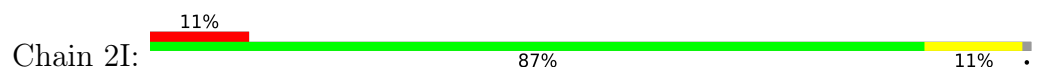
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



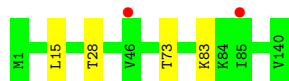
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



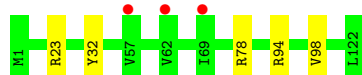
- Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14

Chain 1O:  97%

• Molecule 10: 50S ribosomal protein L14

Chain 2O:  96%

• Molecule 11: 50S ribosomal protein L15

Chain 1P:  95%

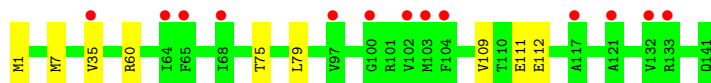
• Molecule 11: 50S ribosomal protein L15

Chain 2P:  91%

• Molecule 12: 50S ribosomal protein L16

Chain 1Q:  93%

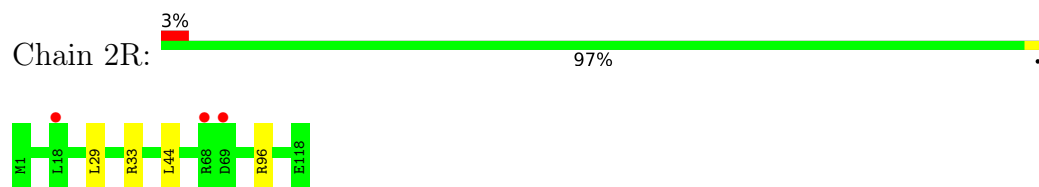
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:  94%

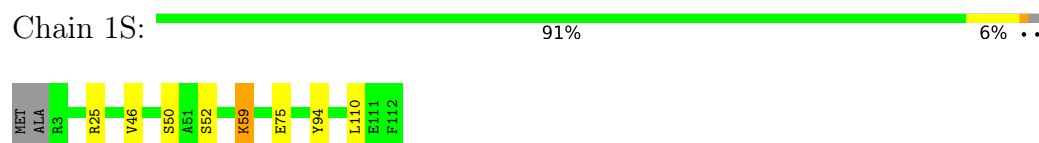
• Molecule 13: 50S ribosomal protein L17

Chain 1R:  92%

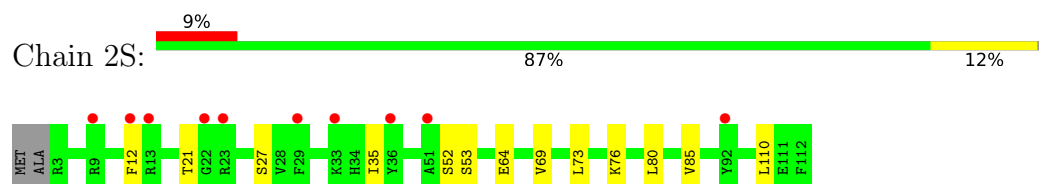
- Molecule 13: 50S ribosomal protein L17



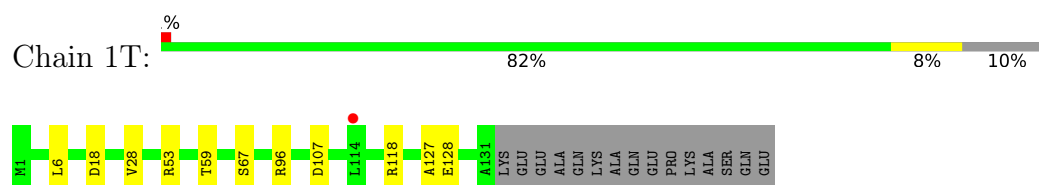
- Molecule 14: 50S ribosomal protein L18



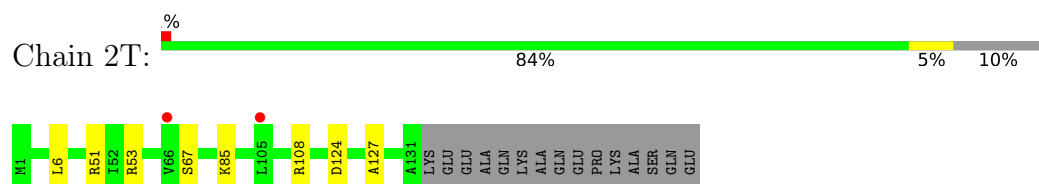
- Molecule 14: 50S ribosomal protein L18



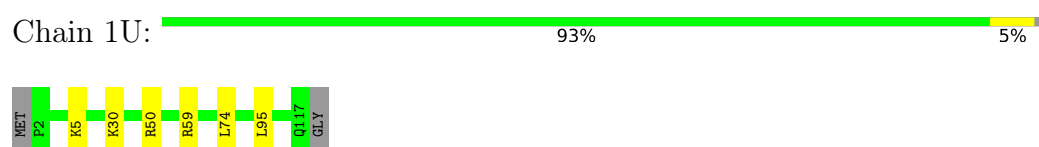
- Molecule 15: 50S ribosomal protein L19



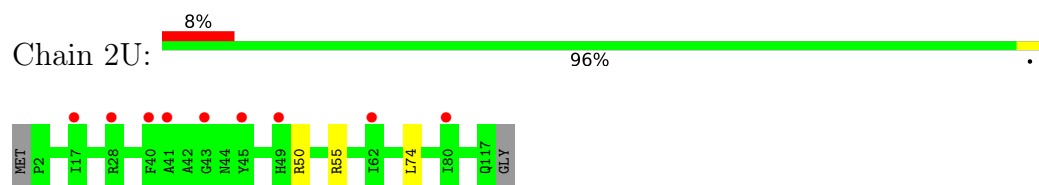
- Molecule 15: 50S ribosomal protein L19




- Molecule 16: 50S ribosomal protein L20

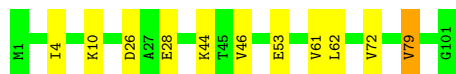


- Molecule 16: 50S ribosomal protein L20



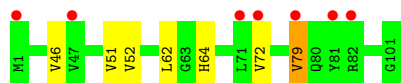
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  89% 10% .

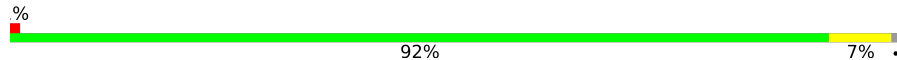


- Molecule 17: 50S ribosomal protein L21

Chain 2V:  7% 93% 6% .



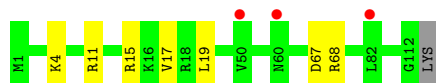
- Molecule 18: 50S ribosomal protein L22

Chain 1W:  % 92% 7% .



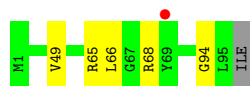
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  3% 93% 6% .



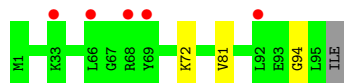
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  % 94% 5% .




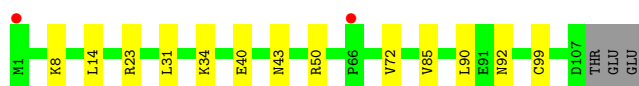
- Molecule 19: 50S ribosomal protein L23

Chain 2X:  5% 96% . .

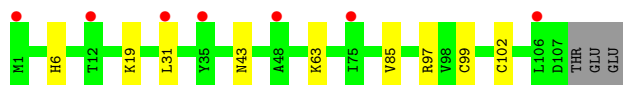
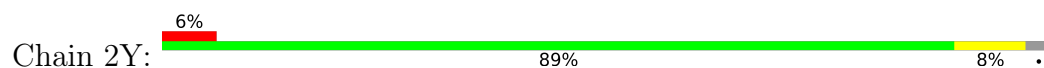


- Molecule 20: 50S ribosomal protein L24

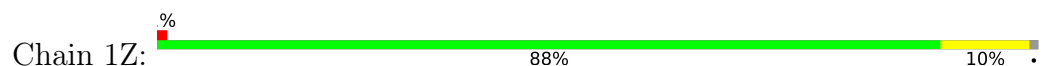
Chain 1Y:  2% 85% 12% .



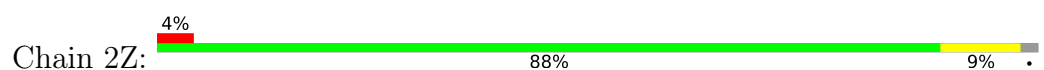
- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



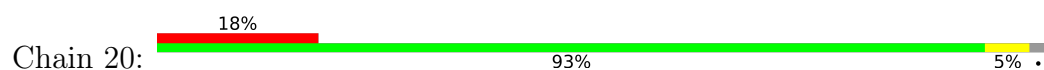
- Molecule 21: 50S ribosomal protein L25



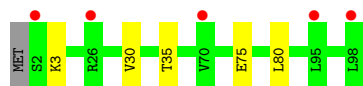
- Molecule 22: 50S ribosomal protein L27



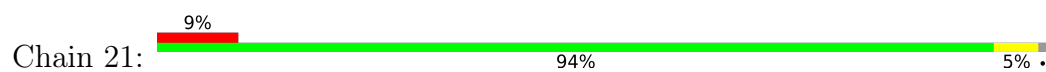
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



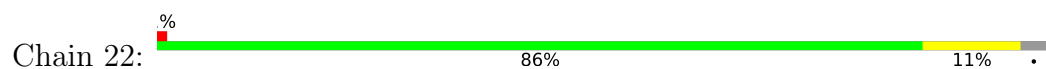
- Molecule 23: 50S ribosomal protein L28



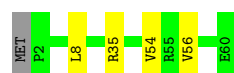
- Molecule 24: 50S ribosomal protein L29



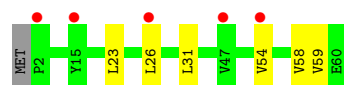
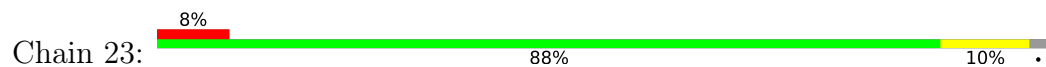
- Molecule 24: 50S ribosomal protein L29



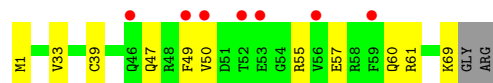
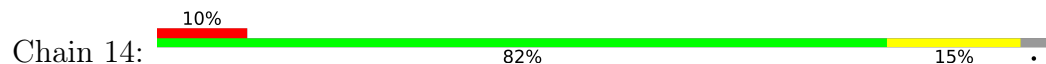
- Molecule 25: 50S ribosomal protein L30



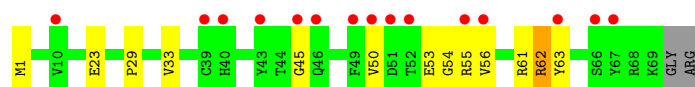
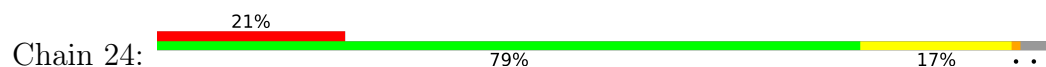
- Molecule 25: 50S ribosomal protein L30



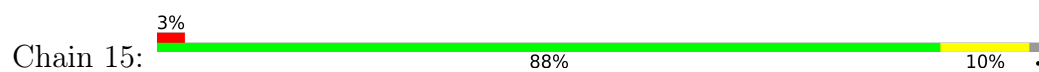
- Molecule 26: 50S ribosomal protein L31



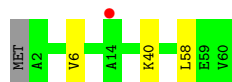
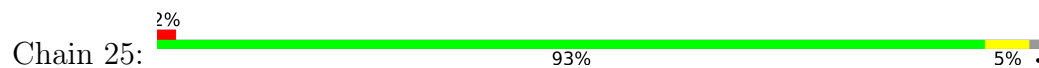
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



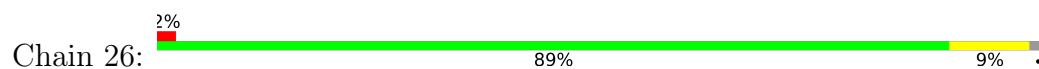
- Molecule 27: 50S ribosomal protein L32



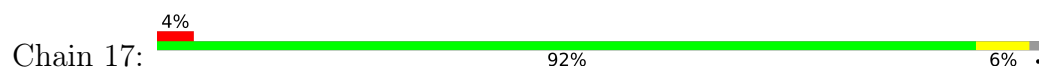
- Molecule 28: 50S ribosomal protein L33



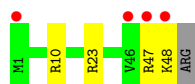
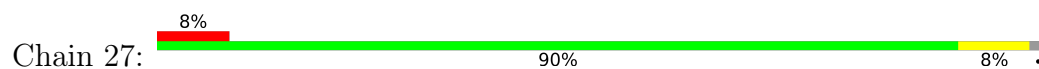
- Molecule 28: 50S ribosomal protein L33



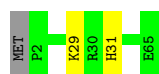
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



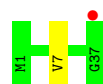
- Molecule 30: 50S ribosomal protein L35



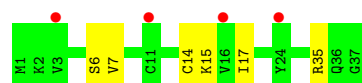
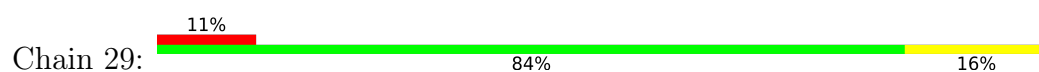
- Molecule 30: 50S ribosomal protein L35



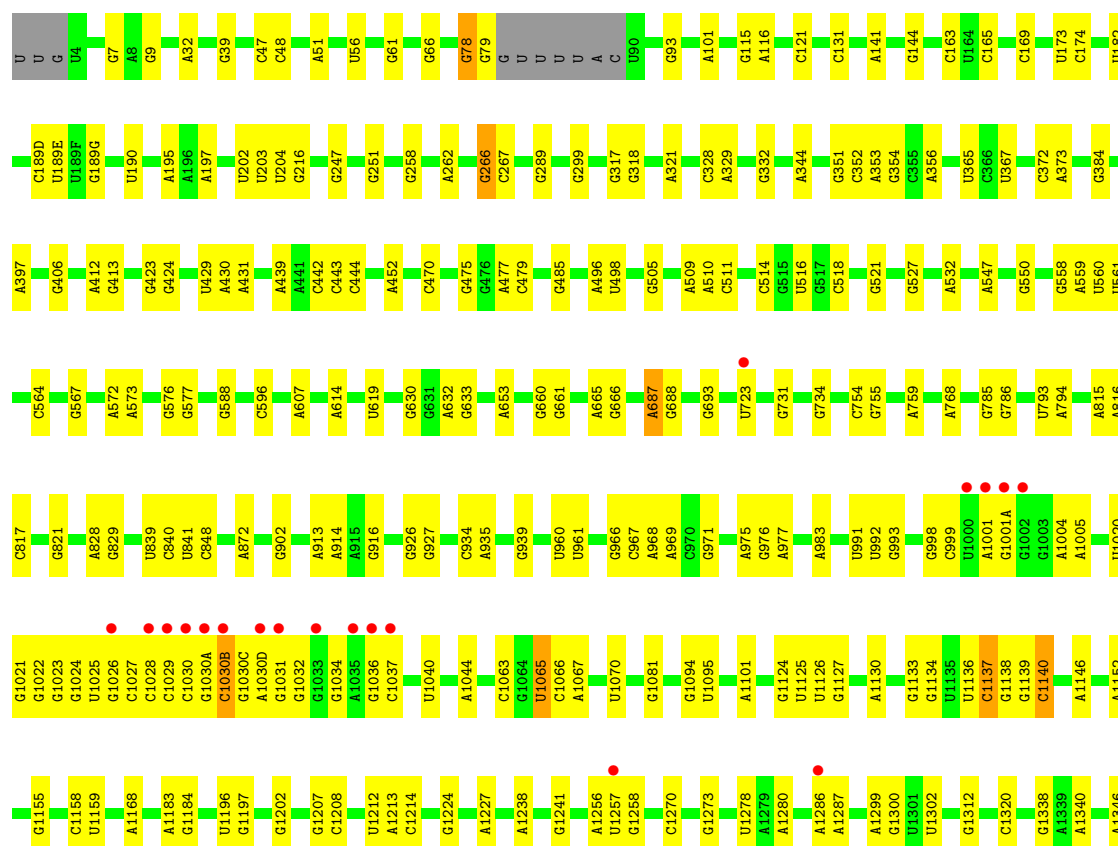
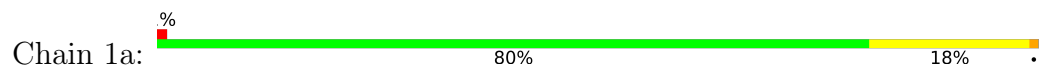
- Molecule 31: 50S ribosomal protein L36

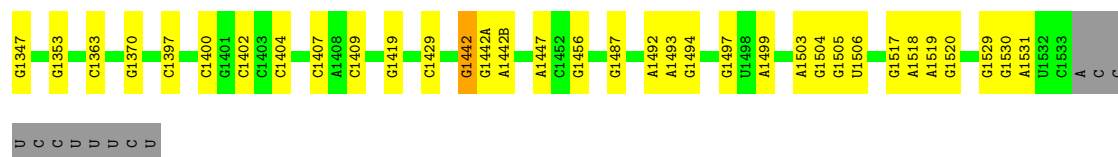


- Molecule 31: 50S ribosomal protein L36

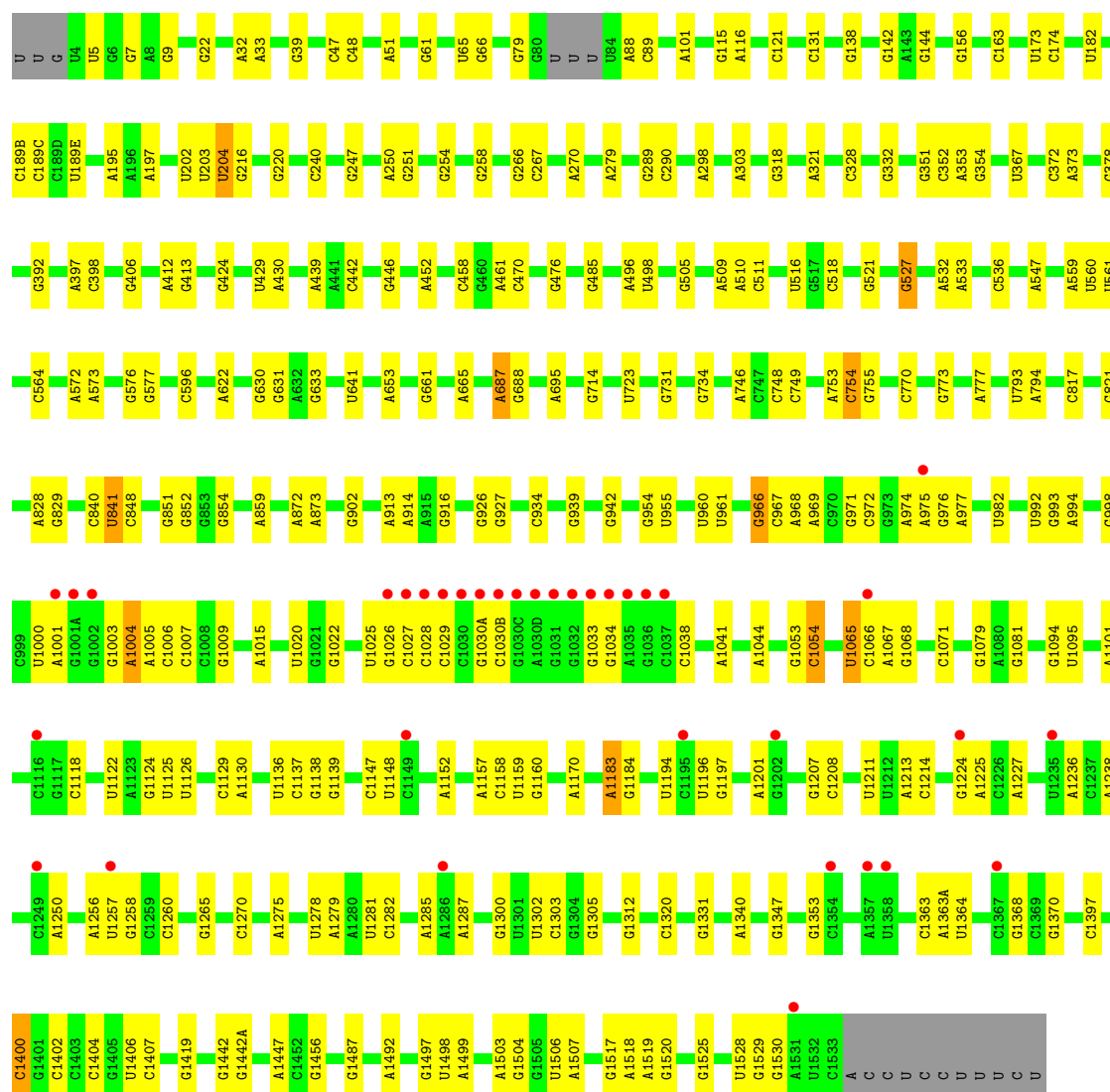
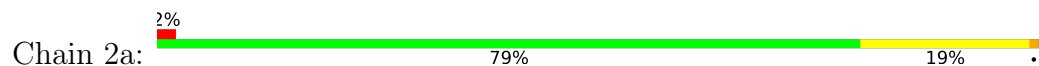


- Molecule 32: 16S Ribosomal RNA

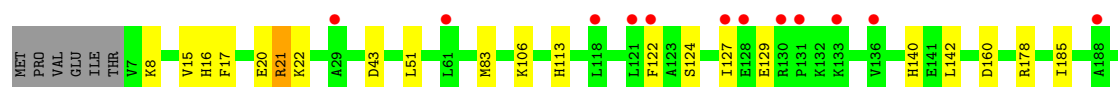
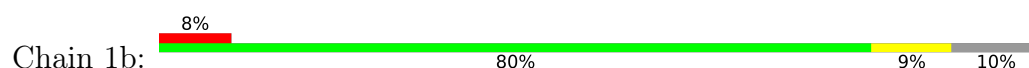


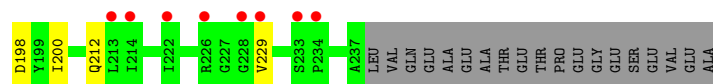


• Molecule 32: 16S Ribosomal RNA

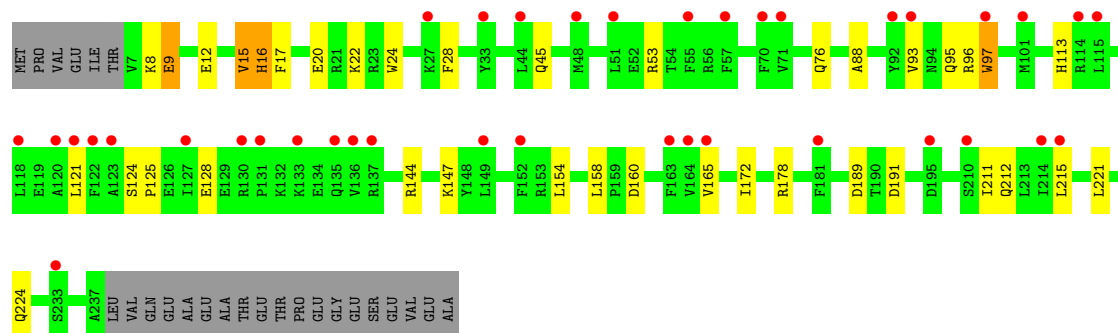
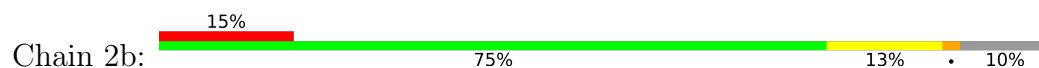


• Molecule 33: 30S ribosomal protein S2

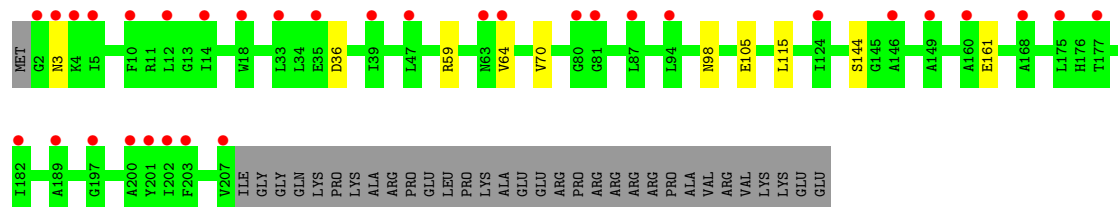
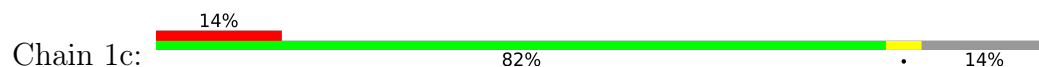




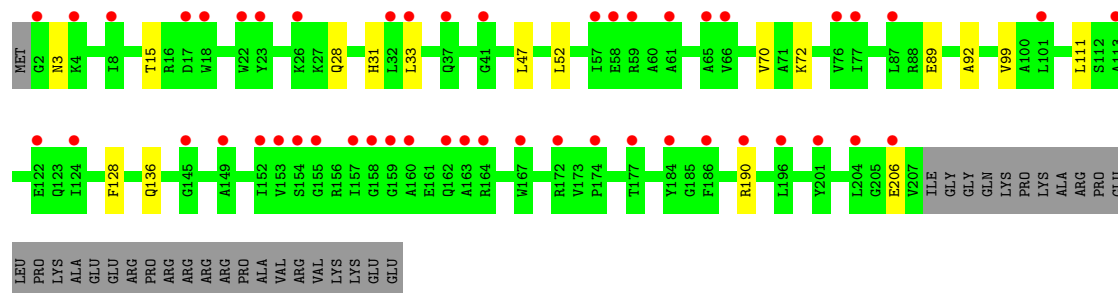
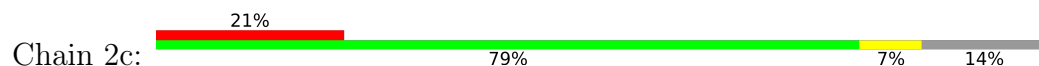
• Molecule 33: 30S ribosomal protein S2



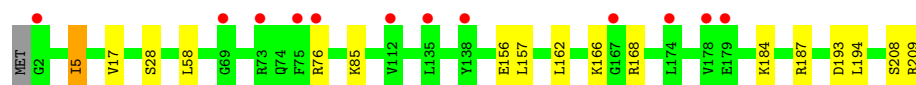
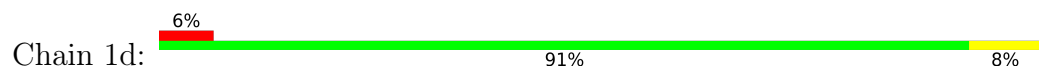
• Molecule 34: 30S ribosomal protein S3



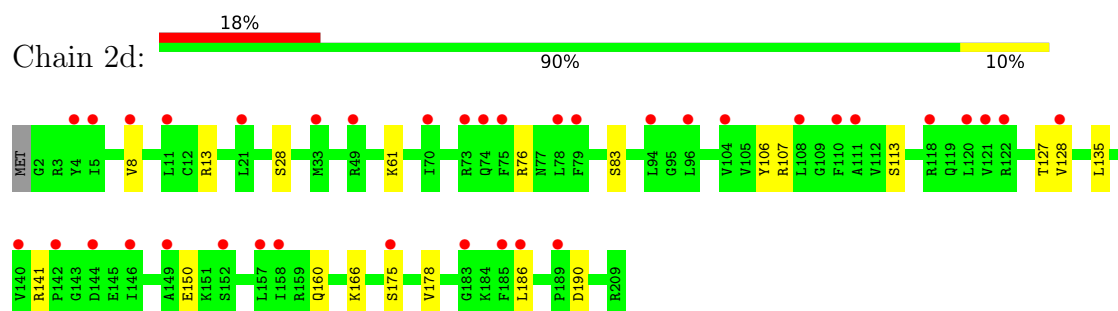
• Molecule 34: 30S ribosomal protein S3



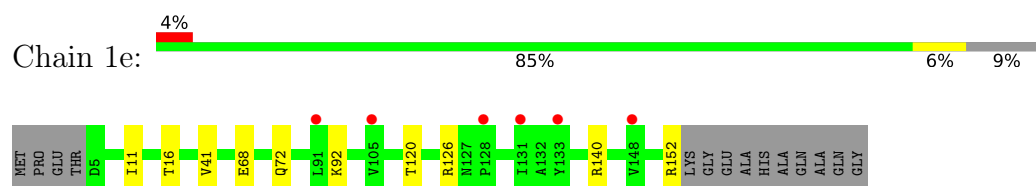
• Molecule 35: 30S ribosomal protein S4



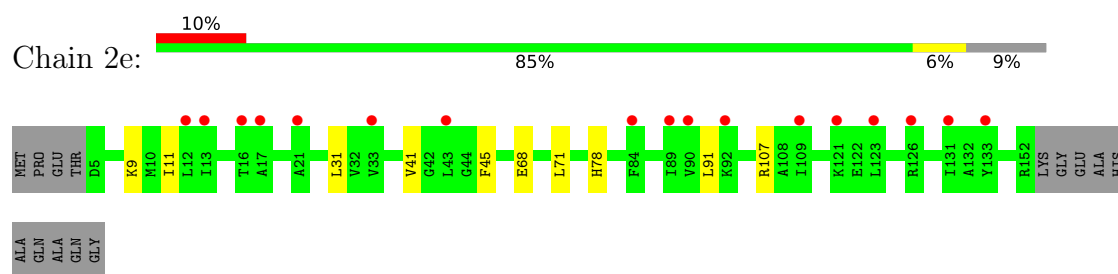
- Molecule 35: 30S ribosomal protein S4



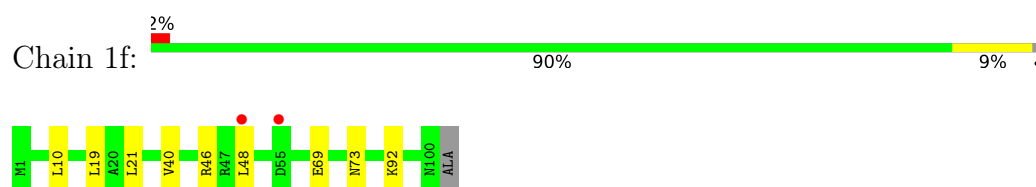
- Molecule 36: 30S ribosomal protein S5



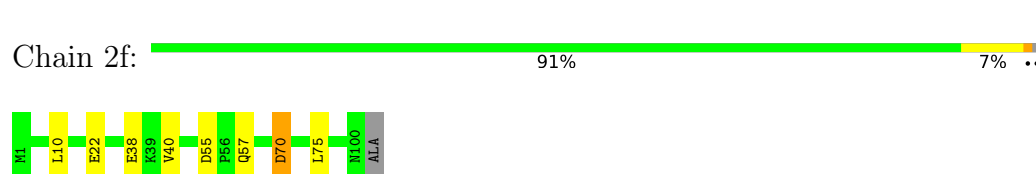
- Molecule 36: 30S ribosomal protein S5



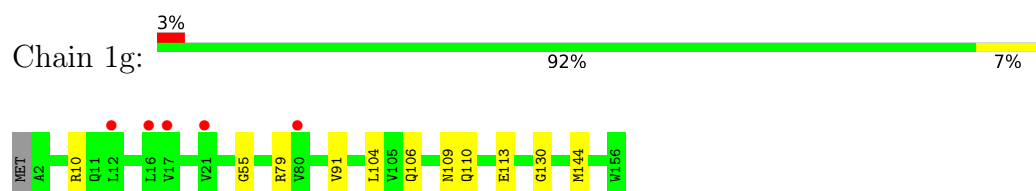
- Molecule 37: 30S ribosomal protein S6



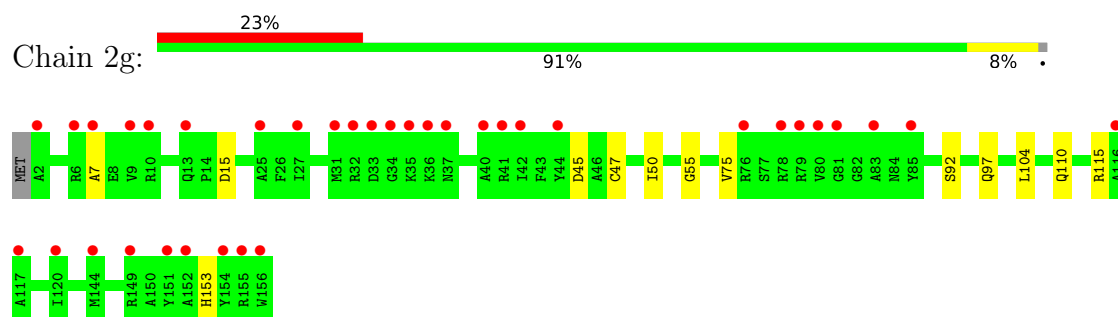
- Molecule 37: 30S ribosomal protein S6



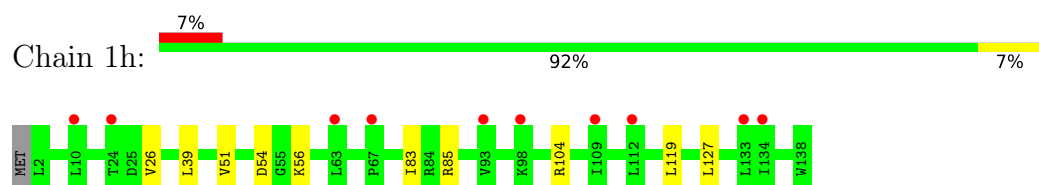
- Molecule 38: 30S ribosomal protein S7



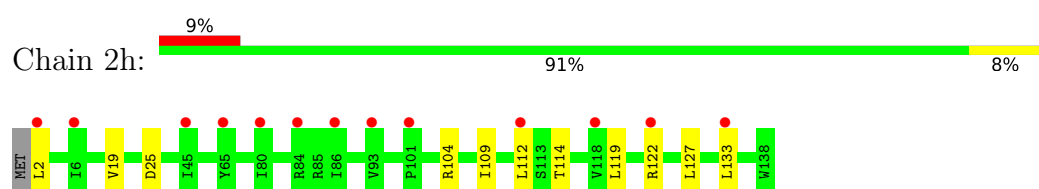
- Molecule 38: 30S ribosomal protein S7



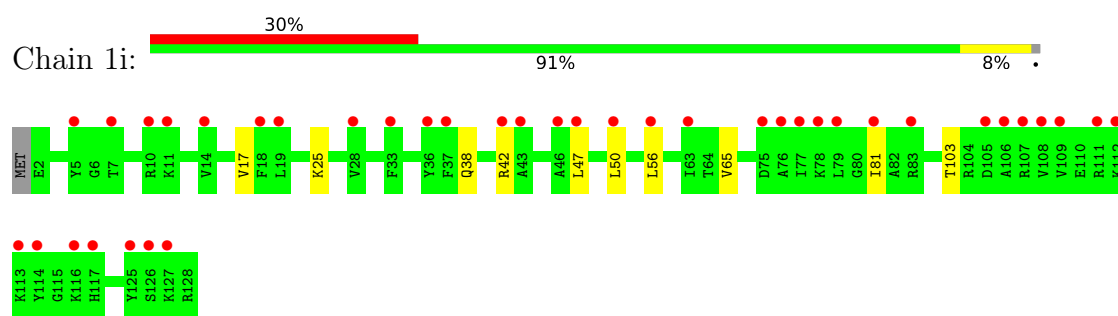
- Molecule 39: 30S ribosomal protein S8



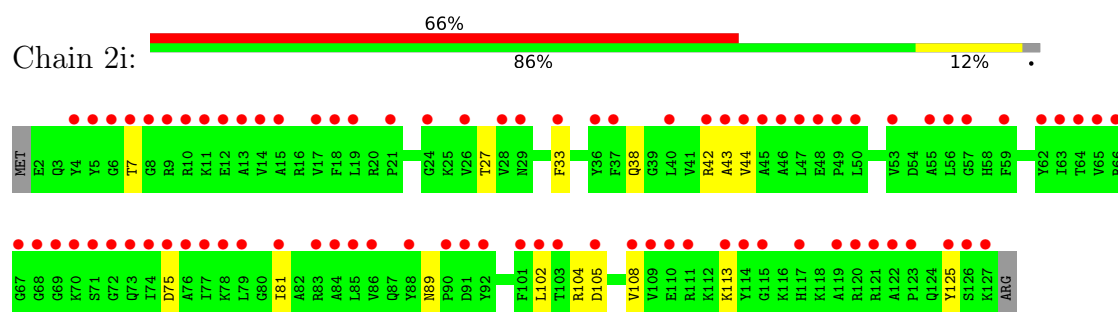
- Molecule 39: 30S ribosomal protein S8



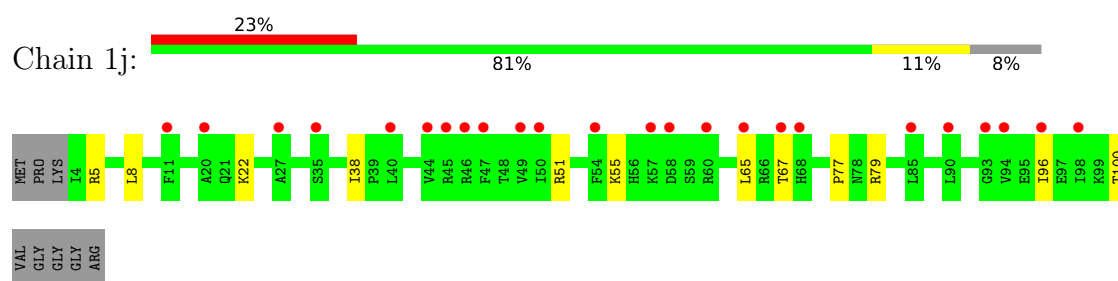
- Molecule 40: 30S ribosomal protein S9



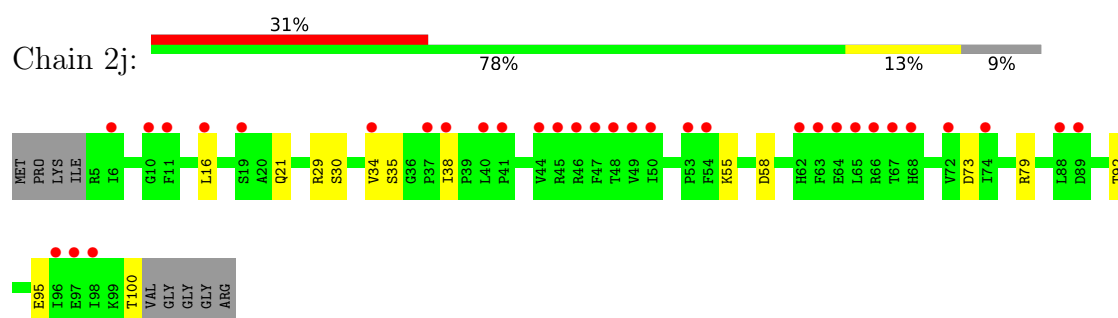
- Molecule 40: 30S ribosomal protein S9



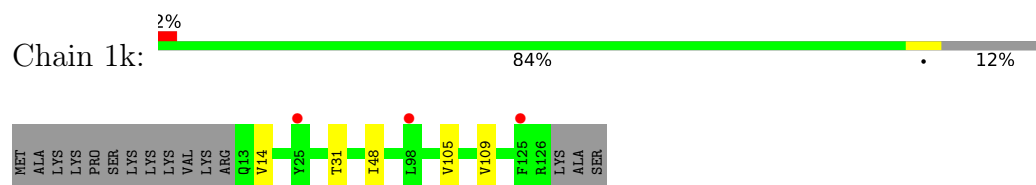
- Molecule 41: 30S ribosomal protein S10



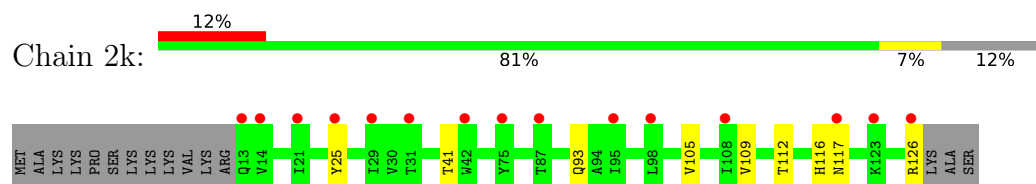
- Molecule 41: 30S ribosomal protein S10



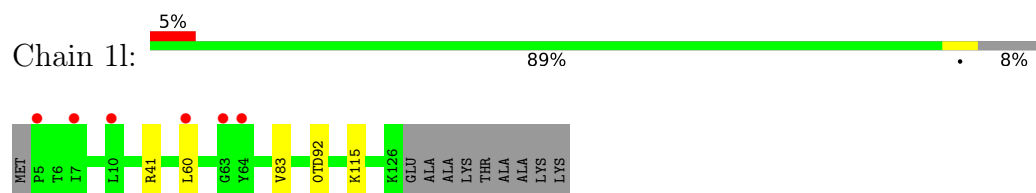
- Molecule 42: 30S ribosomal protein S11



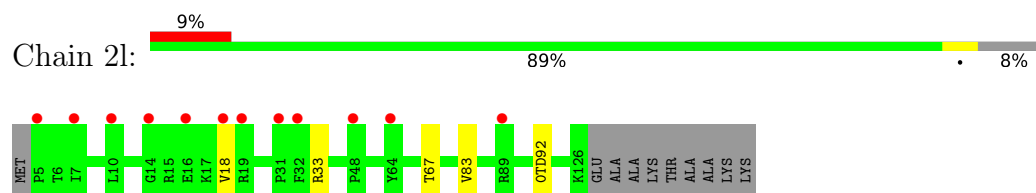
- Molecule 42: 30S ribosomal protein S11



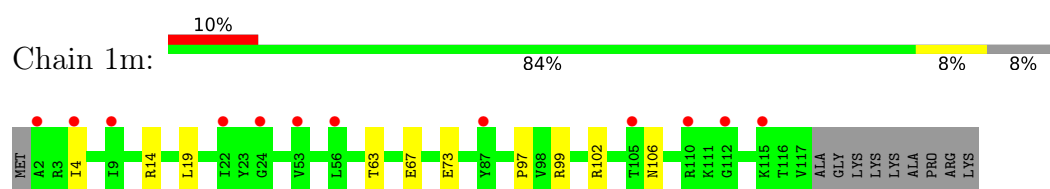
- Molecule 43: 30S ribosomal protein S12



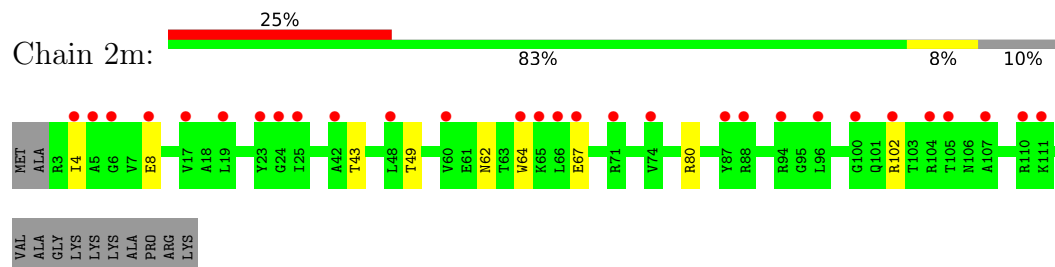
- Molecule 43: 30S ribosomal protein S12



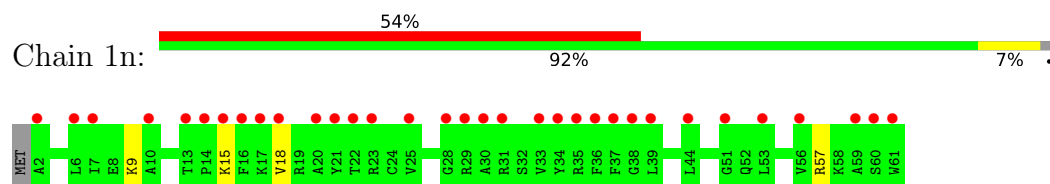
- Molecule 44: 30S ribosomal protein S13



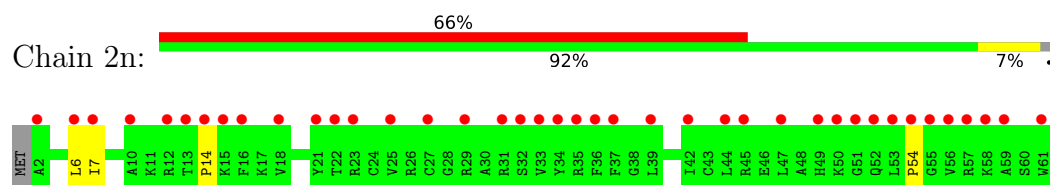
- Molecule 44: 30S ribosomal protein S13



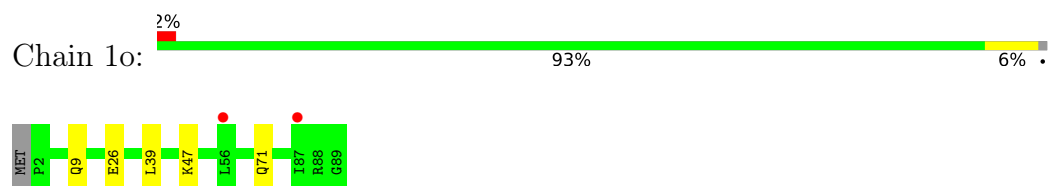
- Molecule 45: 30S ribosomal protein S14 type Z



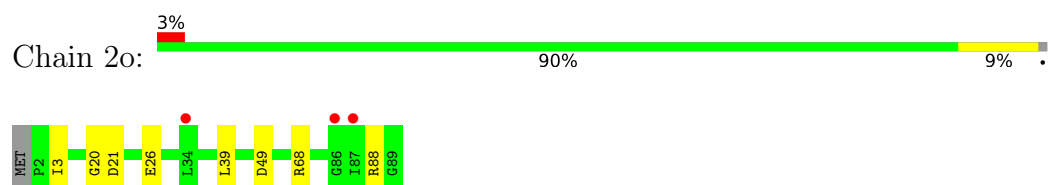
- Molecule 45: 30S ribosomal protein S14 type Z



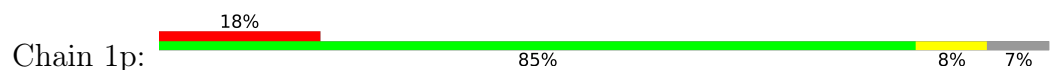
- Molecule 46: 30S ribosomal protein S15

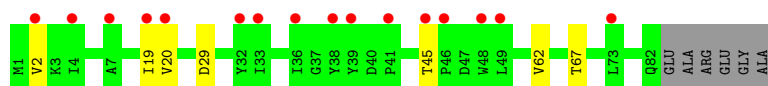


- Molecule 46: 30S ribosomal protein S15

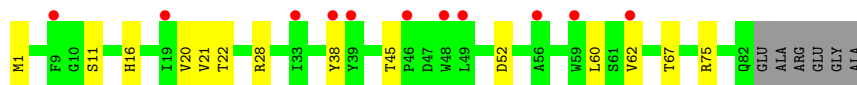
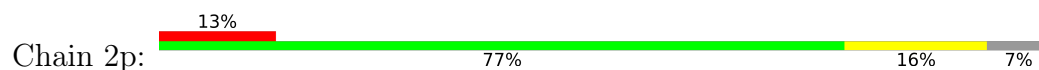


- Molecule 47: 30S ribosomal protein S16

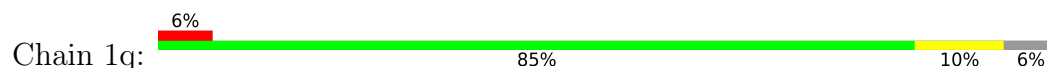




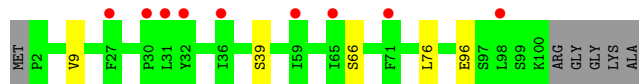
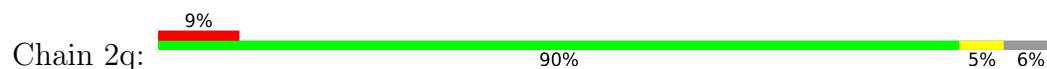
- Molecule 47: 30S ribosomal protein S16



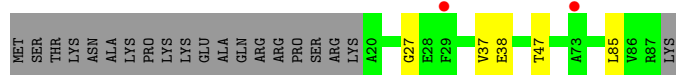
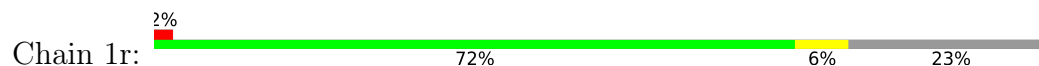
- Molecule 48: 30S ribosomal protein S17



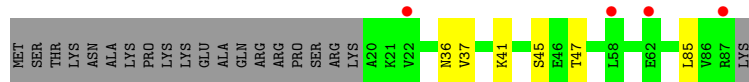
- Molecule 48: 30S ribosomal protein S17



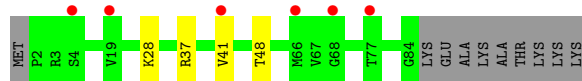
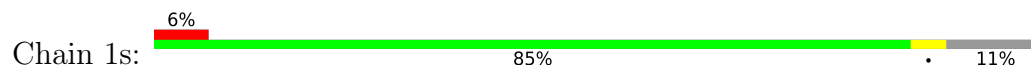
- Molecule 49: 30S ribosomal protein S18



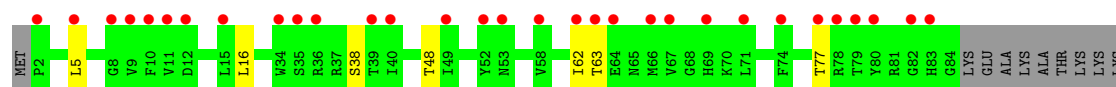
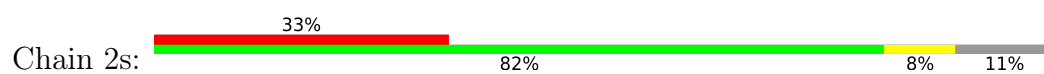
- Molecule 49: 30S ribosomal protein S18



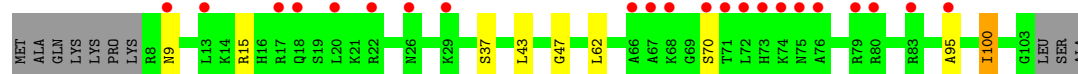
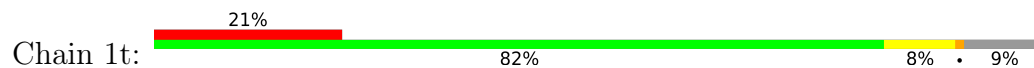
- Molecule 50: 30S ribosomal protein S19



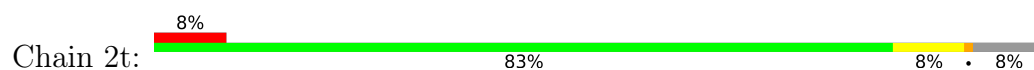
- Molecule 50: 30S ribosomal protein S19



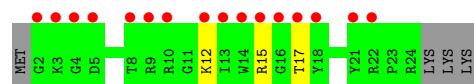
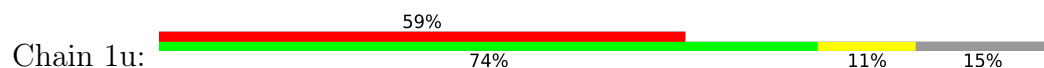
- Molecule 51: 30S ribosomal protein S20



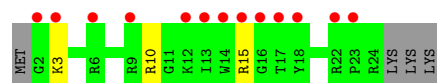
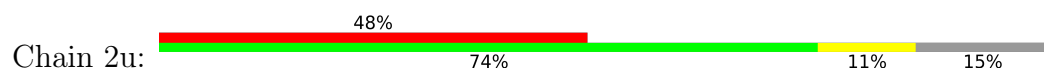
- Molecule 51: 30S ribosomal protein S20



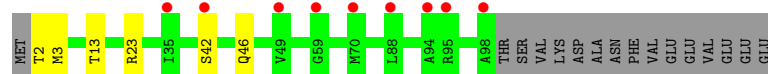
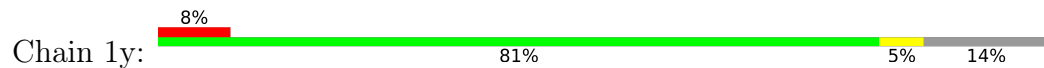
- Molecule 52: 30S ribosomal protein Thx



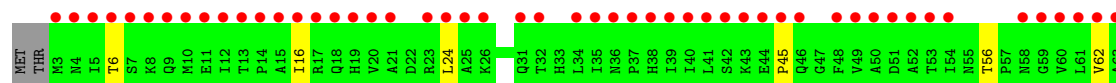
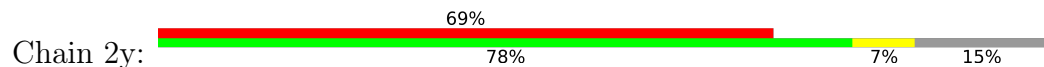
- Molecule 52: 30S ribosomal protein Thx

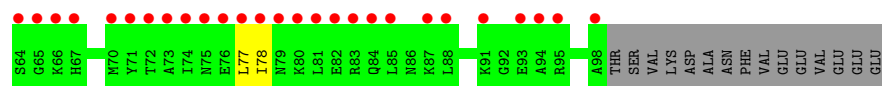


- Molecule 53: Ribosome-associated inhibitor A

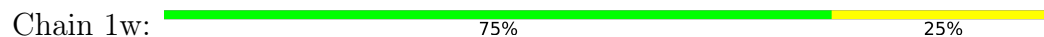


- Molecule 53: Ribosome-associated inhibitor A





- Molecule 54: A-site Aminoacyl-tRNA Analog



- Molecule 54: A-site Aminoacyl-tRNA Analog



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



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.32Å 449.63Å 620.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.05 – 2.50 310.11 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (155.05-2.50) 99.9 (310.11-2.50)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.230 , 0.278 0.231 , 0.279	Depositor DCC
R_{free} test set	99670 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	297682	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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 ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.51	4/69031 (0.0%)	1.00	88/107754 (0.1%)
1	2A	0.40	0/68903	0.90	44/107552 (0.0%)
2	1B	0.44	0/2876	0.94	0/4486
2	2B	0.35	0/2878	0.87	0/4490
3	1D	0.36	0/2181	0.58	0/2940
3	2D	0.33	0/2186	0.53	0/2944
4	1E	0.34	0/1592	0.54	0/2149
4	2E	0.31	0/1592	0.52	0/2149
5	1F	0.33	0/1619	0.52	0/2193
5	2F	0.29	0/1615	0.51	0/2188
6	1G	0.30	0/1451	0.49	0/1961
6	2G	0.29	0/1449	0.47	0/1957
7	1H	0.32	0/1356	0.51	0/1834
7	2H	0.30	0/1350	0.48	0/1826
8	1I	0.29	0/1109	0.49	0/1512
8	2I	0.30	0/1091	0.50	0/1490
9	1N	0.34	0/1148	0.53	0/1547
9	2N	0.30	0/1144	0.47	0/1543
10	1O	0.37	0/943	0.57	0/1269
10	2O	0.31	0/943	0.57	0/1269
11	1P	0.33	0/1152	0.54	0/1533
11	2P	0.31	0/1152	0.53	0/1533
12	1Q	0.36	0/1143	0.52	0/1527
12	2Q	0.30	0/1143	0.47	0/1527
13	1R	0.33	0/982	0.56	0/1312
13	2R	0.29	0/982	0.50	0/1312
14	1S	0.33	0/887	0.54	0/1180
14	2S	0.29	0/880	0.50	0/1172
15	1T	0.33	0/1105	0.56	1/1477 (0.1%)
15	2T	0.30	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	0.46	0/1301
17	1V	0.35	0/786	0.55	0/1053
17	2V	0.32	0/782	0.53	0/1049
18	1W	0.34	0/897	0.50	0/1205
18	2W	0.31	0/897	0.49	0/1205
19	1X	0.37	0/764	0.55	0/1025
19	2X	0.30	0/764	0.51	0/1025
20	1Y	0.34	0/823	0.55	0/1099
20	2Y	0.30	0/823	0.51	0/1100
21	1Z	0.31	0/1620	0.50	0/2200
21	2Z	0.29	0/1590	0.48	0/2162
22	10	0.37	0/662	0.55	0/881
22	20	0.30	0/659	0.53	0/877
23	11	0.31	0/761	0.51	0/1013
23	21	0.31	0/766	0.48	0/1018
24	12	0.30	0/590	0.48	0/781
24	22	0.30	0/594	0.45	0/785
25	13	0.34	0/474	0.54	0/635
25	23	0.27	0/469	0.47	0/630
26	14	0.30	0/559	0.54	0/754
26	24	0.35	0/549	0.56	0/741
27	15	0.35	0/473	0.57	0/639
27	25	0.30	0/469	0.53	0/635
28	16	0.33	0/460	0.55	0/613
28	26	0.31	0/456	0.49	0/608
29	17	0.36	0/426	0.56	0/561
29	27	0.29	0/426	0.52	0/561
30	18	0.34	0/525	0.53	0/691
30	28	0.29	0/525	0.49	0/691
31	19	0.36	0/310	0.53	0/407
31	29	0.30	0/310	0.55	0/407
32	1a	0.37	0/35795	0.89	21/55864 (0.0%)
32	2a	0.36	0/35890	0.88	29/56012 (0.1%)
33	1b	0.29	0/1876	0.49	0/2533
33	2b	0.30	0/1860	0.49	0/2518
34	1c	0.28	0/1582	0.46	0/2137
34	2c	0.28	0/1566	0.49	0/2119
35	1d	0.30	0/1695	0.49	0/2274
35	2d	0.29	0/1698	0.47	0/2277
36	1e	0.30	0/1149	0.52	0/1548
36	2e	0.29	0/1149	0.49	0/1548
37	1f	0.31	0/827	0.47	0/1120
37	2f	0.29	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.27	0/1254	0.42	0/1683
38	2g	0.28	0/1248	0.43	0/1676
39	1h	0.29	0/1118	0.49	0/1506
39	2h	0.28	0/1108	0.47	0/1494
40	1i	0.29	0/1005	0.47	0/1351
40	2i	0.30	0/985	0.49	0/1329
41	1j	0.26	0/732	0.50	0/993
41	2j	0.29	0/723	0.50	0/984
42	1k	0.29	0/849	0.49	0/1150
42	2k	0.29	0/848	0.50	0/1149
43	1l	0.32	0/937	0.52	0/1260
43	2l	0.27	0/937	0.50	0/1260
44	1m	0.28	0/924	0.48	0/1242
44	2m	0.27	0/905	0.49	0/1217
45	1n	0.30	0/501	0.49	0/664
45	2n	0.31	0/501	0.45	0/664
46	1o	0.28	0/739	0.43	0/985
46	2o	0.28	0/739	0.40	0/985
47	1p	0.27	0/697	0.52	0/939
47	2p	0.27	0/693	0.51	0/935
48	1q	0.29	0/836	0.48	0/1117
48	2q	0.30	0/836	0.46	0/1117
49	1r	0.29	0/560	0.49	0/746
49	2r	0.29	0/560	0.44	0/746
50	1s	0.27	0/663	0.50	0/895
50	2s	0.29	0/660	0.48	0/893
51	1t	0.27	0/734	0.45	0/969
51	2t	0.28	0/736	0.43	0/976
52	1u	0.25	0/203	0.46	0/266
52	2u	0.25	0/203	0.47	0/266
53	1y	0.28	0/776	0.48	0/1048
53	2y	0.27	0/761	0.45	0/1030
54	1w	0.50	0/44	0.95	0/67
54	2w	0.39	0/44	0.85	0/67
55	1x	0.40	0/44	0.99	0/67
55	2x	0.48	0/44	1.26	0/67
56	1v	0.35	0/27	0.47	0/34
56	2v	0.27	0/27	0.46	0/34
All	All	0.40	4/310260 (0.0%)	0.83	183/463691 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	0	1
17	2V	0	1
41	2j	0	1
47	1p	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	330	A	N9-C4	-7.05	1.33	1.37
1	1A	2790	A	N9-C4	5.63	1.41	1.37
1	1A	330	A	N3-C4	-5.36	1.31	1.34
1	1A	2249	U	C4-O4	-5.00	1.19	1.23

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1042	G	OP1-P-O3'	-12.02	78.76	105.20
1	1A	2577	A	O5'-P-OP1	-10.58	96.18	105.70
1	1A	588	U	O5'-P-OP2	-10.02	96.68	105.70
1	2A	576	U	O5'-P-OP1	-9.28	97.35	105.70
1	1A	330	A	C2-N3-C4	-9.14	106.03	110.60
1	1A	801	G	O5'-P-OP2	-9.09	97.52	105.70
1	2A	1092	C	C6-N1-C2	-8.77	116.79	120.30
1	1A	512	G	O4'-C1'-N9	8.68	115.14	108.20
1	1A	1372	U	C5-C4-O4	-8.48	120.81	125.90
1	2A	1092	C	C2-N1-C1'	8.38	128.01	118.80
1	1A	999	U	O5'-P-OP2	-8.36	98.18	105.70
32	2a	1158	C	N1-C2-O2	8.11	123.76	118.90
1	1A	1352	U	O5'-P-OP1	-8.09	98.42	105.70
1	1A	1043	C	OP1-P-OP2	8.01	131.61	119.60
1	2A	1092	C	N1-C2-O2	7.99	123.69	118.90
1	1A	740	U	O5'-P-OP2	-7.96	98.54	105.70
1	1A	1086	A	N1-C6-N6	-7.95	113.83	118.60
1	1A	1042	G	OP2-P-O3'	-7.78	88.09	105.20
32	2a	1158	C	C2-N1-C1'	7.70	127.27	118.80
1	1A	330	A	N1-C2-N3	7.64	133.12	129.30
1	2A	1639	U	O5'-P-OP2	-7.36	99.08	105.70
1	2A	1506	C	N1-C2-O2	7.36	123.31	118.90
1	1A	1372	U	N3-C4-O4	7.33	124.53	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2108	C	C2-N3-C4	7.26	123.53	119.90
1	2A	1648	C	O5'-P-OP1	-7.14	99.27	105.70
1	2A	1092	C	N3-C2-O2	-7.07	116.95	121.90
32	2a	254	G	O5'-P-OP1	-7.03	99.37	105.70
1	2A	574	C	N1-C2-O2	-7.00	114.70	118.90
1	2A	751	A	O5'-P-OP1	-6.99	99.41	105.70
1	1A	226	G	O4'-C1'-N9	6.99	113.79	108.20
1	2A	1092	C	C5-C6-N1	6.94	124.47	121.00
1	1A	576	U	O5'-P-OP1	-6.90	99.49	105.70
32	2a	1158	C	N3-C2-O2	-6.77	117.16	121.90
1	2A	2689	U	N3-C2-O2	-6.71	117.50	122.20
1	1A	2103	C	C2-N3-C4	6.69	123.24	119.90
32	2a	1158	C	C6-N1-C2	-6.64	117.64	120.30
1	2A	1506	C	C2-N1-C1'	6.62	126.09	118.80
1	1A	1176	G	OP1-P-O3'	6.61	119.74	105.20
1	2A	2108	C	N1-C2-O2	6.61	122.86	118.90
1	1A	2249	U	N3-C4-C5	6.47	118.48	114.60
1	2A	512	G	O4'-C1'-N9	6.41	113.33	108.20
1	1A	774	A	C8-N9-C4	-6.41	103.24	105.80
1	1A	2149	G	N3-C4-N9	-6.40	122.16	126.00
32	1a	299	G	C5-C6-O6	-6.40	124.76	128.60
1	2A	1313	U	C2-N1-C1'	6.39	125.37	117.70
1	1A	386	G	O4'-C1'-N9	6.30	113.24	108.20
1	2A	2501	C	C2-N1-C1'	-6.26	111.91	118.80
1	1A	2103	C	N1-C2-O2	6.19	122.61	118.90
1	2A	1313	U	N1-C2-O2	6.17	127.12	122.80
32	1a	558	G	O5'-P-OP1	-6.16	100.16	105.70
1	1A	330	A	N3-C4-N9	-6.15	122.48	127.40
1	1A	2371	G	N1-C6-O6	-6.13	116.22	119.90
1	1A	1653	G	C8-N9-C4	-6.09	103.97	106.40
1	1A	2028	U	N3-C4-O4	-6.03	115.18	119.40
32	2a	1003	G	C8-N9-C4	-5.97	104.01	106.40
1	1A	1064	C	N1-C2-O2	5.97	122.48	118.90
32	2a	841	U	C5-C6-N1	5.92	125.66	122.70
1	1A	784	A	P-O3'-C3'	5.90	126.78	119.70
1	2A	277	C	C2-N1-C1'	5.89	125.28	118.80
32	2a	1183	A	P-O3'-C3'	5.88	126.75	119.70
32	2a	1004	A	O4'-C1'-N9	5.87	112.90	108.20
32	1a	78	G	C8-N9-C1'	5.83	134.57	127.00
32	1a	78	G	O4'-C1'-N9	5.83	112.86	108.20
1	1A	1493	C	C2-N1-C1'	5.82	125.20	118.80
1	1A	2452	C	O5'-P-OP1	-5.82	100.47	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	271(Y)	U	O4'-C1'-N1	5.81	112.85	108.20
1	1A	2790	A	C2-N3-C4	5.80	113.50	110.60
1	1A	1782	C	O5'-P-OP1	-5.79	100.49	105.70
1	2A	277	C	N1-C2-O2	5.76	122.36	118.90
1	2A	1380	G	O5'-P-OP2	-5.76	100.52	105.70
1	1A	1026	U	N1-C2-O2	5.74	126.82	122.80
1	1A	961	C	O5'-P-OP2	-5.74	100.54	105.70
32	2a	754	C	C2-N1-C1'	5.73	125.11	118.80
1	1A	2254	C	N1-C2-O2	-5.72	115.47	118.90
1	1A	2350	C	C6-N1-C2	-5.69	118.02	120.30
1	1A	755	C	N1-C2-O2	-5.69	115.49	118.90
1	1A	12	U	N3-C2-O2	-5.67	118.23	122.20
1	2A	1506	C	N3-C2-O2	-5.67	117.93	121.90
1	1A	2712	U	O4'-C1'-N1	5.65	112.72	108.20
1	1A	1784	A	O5'-P-OP2	-5.62	100.64	105.70
32	2a	204	U	C2-N1-C1'	5.62	124.45	117.70
32	1a	1442	G	N3-C4-C5	-5.61	125.80	128.60
1	2A	1992	G	P-O3'-C3'	5.60	126.42	119.70
1	2A	1313	U	N3-C2-O2	-5.59	118.28	122.20
1	1A	494	G	C8-N9-C4	-5.59	104.16	106.40
1	1A	2492	U	O5'-P-OP1	-5.59	100.67	105.70
1	1A	2874	C	C2-N1-C1'	5.55	124.91	118.80
1	2A	2103	C	C2-N3-C4	5.54	122.67	119.90
1	1A	1805	U	O5'-P-OP2	-5.53	100.72	105.70
1	1A	1075	C	N1-C2-O2	5.50	122.20	118.90
1	1A	783	A	OP1-P-OP2	-5.50	111.35	119.60
1	1A	847	U	C2-N1-C1'	5.50	124.30	117.70
1	1A	955	C	O5'-P-OP2	-5.50	100.75	105.70
1	2A	1062	G	C4-N9-C1'	5.50	133.65	126.50
1	1A	570	G	C5-C6-N1	5.49	114.24	111.50
32	1a	1442	G	P-O3'-C3'	5.46	126.25	119.70
15	1T	18	ASP	C-N-CA	-5.44	108.10	121.70
1	1A	1266	G	OP1-P-O3'	5.43	117.15	105.20
1	1A	2249	U	N3-C4-O4	-5.43	115.60	119.40
1	1A	2186	G	C6-N1-C2	5.42	128.35	125.10
1	2A	2248	C	O5'-P-OP2	-5.42	100.82	105.70
32	2a	1009	G	C5-C6-O6	5.41	131.84	128.60
32	2a	79	G	C5-C6-O6	5.39	131.84	128.60
1	1A	2061	G	O5'-P-OP2	-5.39	100.85	105.70
32	1a	1036	G	C4-N9-C1'	5.36	133.47	126.50
1	2A	1065	U	P-O3'-C3'	5.36	126.13	119.70
32	1a	78	G	N3-C4-N9	-5.36	122.78	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	570	G	C5-C6-O6	-5.36	125.39	128.60
1	1A	1176	G	P-O3'-C3'	5.34	126.11	119.70
1	1A	2689	U	P-O3'-C3'	5.34	126.11	119.70
32	1a	913	A	P-O3'-C3'	5.33	126.10	119.70
32	2a	65	U	P-O3'-C3'	5.33	126.10	119.70
1	1A	1681	G	C8-N9-C4	5.32	108.53	106.40
1	1A	830	G	C8-N9-C4	-5.31	104.27	106.40
32	2a	1067	A	P-O3'-C3'	5.31	126.07	119.70
32	2a	1003	G	N3-C4-C5	-5.30	125.95	128.60
1	1A	1175	U	P-O3'-C3'	5.29	126.05	119.70
1	2A	2137	C	C5-C4-N4	5.29	123.91	120.20
1	1A	2023	G	O5'-P-OP1	-5.28	100.95	105.70
1	1A	2593	U	N3-C4-O4	-5.27	115.71	119.40
32	2a	1158	C	C5-C6-N1	5.26	123.63	121.00
1	1A	1681	G	N3-C4-C5	5.26	131.23	128.60
1	2A	752	A	P-O3'-C3'	5.26	126.02	119.70
1	1A	847	U	N1-C2-O2	5.26	126.48	122.80
32	1a	266	G	P-O3'-C3'	5.26	126.01	119.70
32	1a	1065	U	P-O3'-C3'	5.26	126.01	119.70
32	1a	365	U	C2-N1-C1'	5.25	124.00	117.70
1	2A	574	C	C2-N1-C1'	-5.25	113.02	118.80
1	1A	845	G	O4'-C1'-N9	5.24	112.39	108.20
32	1a	78	G	C4-N9-C1'	-5.23	119.70	126.50
1	2A	570	G	C4-C5-N7	5.23	112.89	110.80
32	1a	1040	U	C5-C4-O4	5.23	129.04	125.90
32	1a	1137	C	C6-N1-C2	-5.22	118.21	120.30
1	1A	2057	A	N1-C6-N6	-5.22	115.47	118.60
1	1A	330	A	N3-C4-C5	5.21	130.45	126.80
32	2a	913	A	P-O3'-C3'	5.21	125.95	119.70
32	2a	115	G	P-O3'-C3'	5.19	125.93	119.70
32	2a	754	C	N1-C2-O2	5.19	122.02	118.90
32	2a	1331	G	O4'-C1'-N9	5.19	112.35	108.20
32	2a	955	U	C2-N3-C4	5.18	130.11	127.00
1	1A	975(A)	G	O5'-P-OP2	-5.17	101.04	105.70
32	2a	1009	G	N1-C6-O6	-5.17	116.80	119.90
1	1A	575	A	O5'-P-OP1	-5.17	101.05	105.70
1	1A	1493	C	N1-C2-O2	5.17	122.00	118.90
32	1a	115	G	P-O3'-C3'	5.17	125.90	119.70
1	2A	2689	U	P-O3'-C3'	5.16	125.90	119.70
1	2A	2178	C	N1-C2-O2	5.16	122.00	118.90
32	2a	1065	U	P-O3'-C3'	5.15	125.89	119.70
32	1a	1030(B)	C	C6-N1-C2	-5.15	118.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	530	G	C4-N9-C1'	5.15	133.19	126.50
1	1A	1026	U	N3-C2-O2	-5.14	118.60	122.20
1	1A	2249	U	N1-C2-O2	5.14	126.40	122.80
1	1A	733	G	C5-N7-C8	5.12	106.86	104.30
1	1A	1344	G	C5-C6-O6	-5.12	125.53	128.60
1	1A	784	A	O4'-C1'-N9	5.12	112.29	108.20
1	1A	1791	A	O5'-P-OP1	-5.11	101.10	105.70
1	2A	787	U	O5'-P-OP1	-5.11	101.10	105.70
32	2a	1054	C	C2-N1-C1'	5.11	124.42	118.80
32	1a	687	A	P-O3'-C3'	5.10	125.83	119.70
1	2A	2104	G	C4-N9-C1'	5.10	133.13	126.50
1	1A	784	A	OP1-P-O3'	5.10	116.41	105.20
1	2A	784	A	OP1-P-O3'	5.10	116.41	105.20
1	1A	2685	G	N1-C6-O6	-5.09	116.84	119.90
1	1A	2149	G	N3-C2-N2	-5.09	116.34	119.90
1	1A	2359	C	C6-N1-C2	-5.09	118.27	120.30
1	1A	2874	C	C6-N1-C1'	-5.08	114.70	120.80
32	1a	299	G	C4-C5-N7	5.08	112.83	110.80
1	2A	2006	C	C6-N1-C2	-5.08	118.27	120.30
1	1A	787	U	O5'-P-OP1	-5.07	101.14	105.70
32	2a	1054	C	N1-C2-O2	5.06	121.94	118.90
32	2a	687	A	P-O3'-C3'	5.06	125.77	119.70
32	2a	1225	A	C5-C6-N6	5.06	127.75	123.70
1	1A	573	G	C5-C6-O6	-5.05	125.57	128.60
1	2A	1109	C	C2-N1-C1'	5.05	124.36	118.80
1	1A	2149	G	C4-N9-C1'	-5.05	119.93	126.50
32	1a	1137	C	C5-C6-N1	5.04	123.52	121.00
32	2a	1126	U	N1-C2-O2	5.04	126.33	122.80
1	2A	2130	U	C5-C6-N1	5.04	125.22	122.70
1	1A	2149	G	C8-N9-C1'	5.04	133.55	127.00
1	2A	1506	C	C6-N1-C2	-5.03	118.29	120.30
1	1A	1187	G	N1-C6-O6	-5.03	116.88	119.90
1	1A	783	A	O5'-P-OP2	5.01	116.71	110.70
32	1a	1140	C	C2-N1-C1'	5.01	124.31	118.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
47	1p	19	ILE	Peptide
11	2P	35	HIS	Peptide

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Mol	Chain	Res	Type	Group
17	2V	52	VAL	Peptide
41	2j	35	SER	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/276 (99%)	251 (92%)	22 (8%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	48
4	2E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	29	48
5	1F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	29	48
5	2F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	29	48
6	1G	179/182 (98%)	157 (88%)	14 (8%)	8 (4%)	2	3
6	2G	179/182 (98%)	145 (81%)	28 (16%)	6 (3%)	3	5
7	1H	172/180 (96%)	161 (94%)	8 (5%)	3 (2%)	9	16
7	2H	171/180 (95%)	148 (86%)	20 (12%)	3 (2%)	8	14
8	1I	145/148 (98%)	122 (84%)	21 (14%)	2 (1%)	11	20
8	2I	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	11	20
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
11	1P	147/150 (98%)	140 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	2P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	22	39
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
12	2Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	100 (93%)	6 (6%)	2 (2%)	8	13
14	2S	108/112 (96%)	100 (93%)	8 (7%)	0	100	100
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	19	35
15	2T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	19	35
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	92 (93%)	4 (4%)	3 (3%)	4	6
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	28
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14	26
19	2X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	14	26
20	1Y	105/110 (96%)	94 (90%)	11 (10%)	0	100	100
20	2Y	105/110 (96%)	95 (90%)	9 (9%)	1 (1%)	15	28
21	1Z	201/206 (98%)	183 (91%)	18 (9%)	0	100	100
21	2Z	199/206 (97%)	167 (84%)	31 (16%)	1 (0%)	29	48
22	10	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
22	20	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	13	24
23	11	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	14	26
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	1
26	24	67/71 (94%)	47 (70%)	14 (21%)	6 (9%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	192 (84%)	28 (12%)	9 (4%)	3	4
33	2b	229/256 (90%)	187 (82%)	30 (13%)	12 (5%)	2	2
34	1c	204/239 (85%)	187 (92%)	17 (8%)	0	100	100
34	2c	204/239 (85%)	174 (85%)	28 (14%)	2 (1%)	15	28
35	1d	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	29	48
35	2d	206/209 (99%)	188 (91%)	18 (9%)	0	100	100
36	1e	146/162 (90%)	138 (94%)	8 (6%)	0	100	100
36	2e	146/162 (90%)	136 (93%)	10 (7%)	0	100	100
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	3 (3%)	2 (2%)	7	12
38	1g	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	12	21
38	2g	153/156 (98%)	137 (90%)	14 (9%)	2 (1%)	12	21
39	1h	135/138 (98%)	128 (95%)	6 (4%)	1 (1%)	22	39
39	2h	135/138 (98%)	123 (91%)	12 (9%)	0	100	100
40	1i	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
40	2i	124/128 (97%)	108 (87%)	14 (11%)	2 (2%)	9	17
41	1j	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	4	5
41	2j	94/105 (90%)	79 (84%)	13 (14%)	2 (2%)	7	11
42	1k	112/129 (87%)	101 (90%)	11 (10%)	0	100	100
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	8	14
43	1l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	2l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
44	1m	114/126 (90%)	101 (89%)	11 (10%)	2 (2%)	8	14
44	2m	112/126 (89%)	96 (86%)	14 (12%)	2 (2%)	8	14
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	3 (5%)	2 (3%)	3	5
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	78 (91%)	6 (7%)	2 (2%)	6	10
47	1p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
47	2p	80/88 (91%)	67 (84%)	12 (15%)	1 (1%)	12	21
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
49	1r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	10	18
49	2r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	10	18
50	1s	81/93 (87%)	68 (84%)	13 (16%)	0	100	100
50	2s	81/93 (87%)	65 (80%)	16 (20%)	0	100	100
51	1t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	4	5
51	2t	96/106 (91%)	86 (90%)	7 (7%)	3 (3%)	4	5
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	17 (81%)	3 (14%)	1 (5%)	2	2
53	1y	95/113 (84%)	92 (97%)	3 (3%)	0	100	100
53	2y	94/113 (83%)	88 (94%)	5 (5%)	1 (1%)	14	26
56	1v	1/3 (33%)	1 (100%)	0	0	100	100
56	2v	1/3 (33%)	1 (100%)	0	0	100	100
All	All	11643/12360 (94%)	10680 (92%)	851 (7%)	112 (1%)	15	28

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
33	1b	17	PHE
33	1b	124	SER
33	1b	127	ILE
41	1j	55	LYS
44	1m	67	GLU

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Mol	Chain	Res	Type
51	1t	47	GLY
26	24	56	VAL
26	24	62	ARG
33	2b	9	GLU
33	2b	17	PHE
33	2b	125	PRO
40	2i	43	ALA
40	2i	44	VAL
41	2j	79	ARG
42	2k	105	VAL
6	1G	50	ALA
7	1H	126	PRO
7	1H	159	GLU
14	1S	94	TYR
15	1T	127	ALA
19	1X	94	GLY
26	14	39	CYS
35	1d	5	ILE
51	1t	95	ALA
6	2G	117	PHE
17	2V	79	VAL
19	2X	94	GLY
21	2Z	120	ILE
33	2b	22	LYS
38	2g	55	GLY
41	2j	55	LYS
44	2m	67	GLU
49	2r	36	ASN
6	1G	44	GLY
7	1H	92	ILE
14	1S	59	LYS
17	1V	53	GLU
26	14	55	ARG
33	1b	21	ARG
6	2G	48	GLU
6	2G	115	ARG
33	2b	16	HIS
33	2b	88	ALA
33	2b	124	SER
34	2c	99	VAL
37	2f	38	GLU
38	2g	7	ALA

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Mol	Chain	Res	Type
42	2k	25	TYR
4	1E	52	LEU
5	1F	130	ALA
6	1G	43	LEU
6	1G	74	LYS
17	1V	26	ASP
26	14	47	GLN
33	1b	8	LYS
33	1b	16	HIS
33	1b	129	GLU
41	1j	79	ARG
44	1m	106	ASN
51	1t	100	ILE
6	2G	43	LEU
6	2G	96	ARG
7	2H	126	PRO
8	2I	10	GLU
8	2I	117	GLU
26	24	29	PRO
26	24	55	ARG
33	2b	15	VAL
33	2b	97	TRP
37	2f	70	ASP
45	2n	14	PRO
47	2p	52	ASP
51	2t	95	ALA
51	2t	100	ILE
52	2u	3	LYS
6	1G	51	ARG
17	1V	79	VAL
26	14	57	GLU
33	1b	20	GLU
33	1b	22	LYS
4	2E	52	LEU
5	2F	130	ALA
7	2H	48	GLY
22	20	4	LYS
26	24	45	GLY
33	2b	20	GLU
33	2b	95	GLN
34	2c	92	ALA
44	2m	8	GLU

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Mol	Chain	Res	Type
45	2n	54	PRO
53	2y	45	PRO
23	1l	3	LYS
38	1g	130	GLY
41	1j	77	PRO
6	2G	45	GLU
7	2H	65	HIS
15	2T	127	ALA
20	2Y	102	CYS
46	2o	49	ASP
51	2t	47	GLY
6	1G	52	ILE
49	1r	27	GLY
26	24	54	GLY
6	1G	24	GLY
38	1g	55	GLY
46	2o	20	GLY
33	2b	165	VAL
8	1I	111	PRO
8	1I	137	PRO
39	1h	83	ILE
11	2P	122	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/218 (98%)	193 (90%)	21 (10%)	8	15
3	2D	215/218 (99%)	196 (91%)	19 (9%)	10	19
4	1E	164/166 (99%)	154 (94%)	10 (6%)	18	36
4	2E	164/166 (99%)	152 (93%)	12 (7%)	14	27
5	1F	160/166 (96%)	148 (92%)	12 (8%)	13	26
5	2F	159/166 (96%)	142 (89%)	17 (11%)	6	13
6	1G	144/156 (92%)	123 (85%)	21 (15%)	3	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	2G	142/156 (91%)	123 (87%)	19 (13%)	4	7
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9	19
7	2H	143/148 (97%)	132 (92%)	11 (8%)	13	25
8	1I	111/124 (90%)	94 (85%)	17 (15%)	2	5
8	2I	108/124 (87%)	93 (86%)	15 (14%)	3	6
9	1N	119/119 (100%)	110 (92%)	9 (8%)	13	25
9	2N	118/119 (99%)	114 (97%)	4 (3%)	37	63
10	1O	100/100 (100%)	96 (96%)	4 (4%)	31	56
10	2O	100/100 (100%)	95 (95%)	5 (5%)	24	46
11	1P	115/116 (99%)	109 (95%)	6 (5%)	23	44
11	2P	115/116 (99%)	105 (91%)	10 (9%)	10	20
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	9	19
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11	23
13	1R	101/101 (100%)	91 (90%)	10 (10%)	8	15
13	2R	101/101 (100%)	97 (96%)	4 (4%)	31	56
14	1S	87/88 (99%)	80 (92%)	7 (8%)	12	23
14	2S	85/88 (97%)	72 (85%)	13 (15%)	2	5
15	1T	115/127 (91%)	106 (92%)	9 (8%)	12	24
15	2T	113/127 (89%)	106 (94%)	7 (6%)	18	35
16	1U	93/94 (99%)	87 (94%)	6 (6%)	17	33
16	2U	93/94 (99%)	90 (97%)	3 (3%)	39	65
17	1V	81/82 (99%)	72 (89%)	9 (11%)	6	11
17	2V	80/82 (98%)	74 (92%)	6 (8%)	13	26
18	1W	90/92 (98%)	82 (91%)	8 (9%)	9	19
18	2W	90/92 (98%)	83 (92%)	7 (8%)	12	24
19	1X	77/78 (99%)	73 (95%)	4 (5%)	23	44
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46	72
20	1Y	86/91 (94%)	73 (85%)	13 (15%)	3	5
20	2Y	86/91 (94%)	78 (91%)	8 (9%)	9	17
21	1Z	169/179 (94%)	148 (88%)	21 (12%)	4	9
21	2Z	165/179 (92%)	147 (89%)	18 (11%)	6	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	10	65/67 (97%)	62 (95%)	3 (5%)	27	50
22	20	64/67 (96%)	61 (95%)	3 (5%)	26	49
23	11	79/83 (95%)	75 (95%)	4 (5%)	24	45
23	21	81/83 (98%)	76 (94%)	5 (6%)	18	35
24	12	65/67 (97%)	63 (97%)	2 (3%)	40	67
24	22	66/67 (98%)	58 (88%)	8 (12%)	5	9
25	13	51/52 (98%)	47 (92%)	4 (8%)	12	24
25	23	50/52 (96%)	44 (88%)	6 (12%)	5	9
26	14	58/63 (92%)	51 (88%)	7 (12%)	5	9
26	24	54/63 (86%)	46 (85%)	8 (15%)	3	5
27	15	51/52 (98%)	45 (88%)	6 (12%)	5	10
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	37
28	16	51/52 (98%)	48 (94%)	3 (6%)	19	37
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	15
29	17	41/42 (98%)	38 (93%)	3 (7%)	14	27
29	27	41/42 (98%)	37 (90%)	4 (10%)	8	15
30	18	54/55 (98%)	52 (96%)	2 (4%)	34	60
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	27
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	69
31	29	34/34 (100%)	28 (82%)	6 (18%)	2	3
33	1b	191/220 (87%)	174 (91%)	17 (9%)	9	19
33	2b	187/220 (85%)	157 (84%)	30 (16%)	2	4
34	1c	144/188 (77%)	134 (93%)	10 (7%)	15	30
34	2c	140/188 (74%)	125 (89%)	15 (11%)	6	13
35	1d	171/181 (94%)	154 (90%)	17 (10%)	8	15
35	2d	172/181 (95%)	152 (88%)	20 (12%)	5	10
36	1e	114/123 (93%)	104 (91%)	10 (9%)	10	19
36	2e	114/123 (93%)	104 (91%)	10 (9%)	10	19
37	1f	85/90 (94%)	76 (89%)	9 (11%)	6	13
37	2f	85/90 (94%)	78 (92%)	7 (8%)	11	22
38	1g	120/127 (94%)	111 (92%)	9 (8%)	13	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	2g	119/127 (94%)	108 (91%)	11 (9%)	9	18
39	1h	116/119 (98%)	107 (92%)	9 (8%)	12	24
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	16
40	1i	91/99 (92%)	81 (89%)	10 (11%)	6	12
40	2i	88/99 (89%)	74 (84%)	14 (16%)	2	4
41	1j	68/92 (74%)	59 (87%)	9 (13%)	4	7
41	2j	68/92 (74%)	57 (84%)	11 (16%)	2	4
42	1k	83/99 (84%)	78 (94%)	5 (6%)	19	37
42	2k	83/99 (84%)	76 (92%)	7 (8%)	11	21
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	54
43	2l	96/108 (89%)	92 (96%)	4 (4%)	30	54
44	1m	90/101 (89%)	82 (91%)	8 (9%)	9	19
44	2m	87/101 (86%)	79 (91%)	8 (9%)	9	18
45	1n	49/50 (98%)	45 (92%)	4 (8%)	11	22
45	2n	49/50 (98%)	47 (96%)	2 (4%)	30	55
46	1o	78/80 (98%)	73 (94%)	5 (6%)	17	33
46	2o	78/80 (98%)	72 (92%)	6 (8%)	13	25
47	1p	69/74 (93%)	63 (91%)	6 (9%)	10	20
47	2p	68/74 (92%)	55 (81%)	13 (19%)	1	2
48	1q	94/97 (97%)	84 (89%)	10 (11%)	6	13
48	2q	94/97 (97%)	89 (95%)	5 (5%)	22	43
49	1r	59/77 (77%)	55 (93%)	4 (7%)	16	30
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10	21
50	1s	68/80 (85%)	64 (94%)	4 (6%)	19	37
50	2s	67/80 (84%)	60 (90%)	7 (10%)	7	13
51	1t	71/82 (87%)	64 (90%)	7 (10%)	8	15
51	2t	70/82 (85%)	62 (89%)	8 (11%)	5	11
52	1u	18/22 (82%)	15 (83%)	3 (17%)	2	4
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	11
53	1y	82/98 (84%)	76 (93%)	6 (7%)	14	27
53	2y	79/98 (81%)	72 (91%)	7 (9%)	9	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	1v	3/3 (100%)	3 (100%)	0	100	100
56	2v	3/3 (100%)	3 (100%)	0	100	100
All	All	9537/10266 (93%)	8682 (91%)	855 (9%)	9	19

All (855) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	7	LYS
3	1D	37	LEU
3	1D	54	ARG
3	1D	61	LEU
3	1D	69	ARG
3	1D	71	ASP
3	1D	88	ARG
3	1D	94	LEU
3	1D	111	LEU
3	1D	113	VAL
3	1D	115	GLN
3	1D	131	LEU
3	1D	155	LEU
3	1D	193	VAL
3	1D	211	ARG
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	237	GLU
3	1D	242	ARG
3	1D	259	THR
4	1E	9	VAL
4	1E	73	GLU
4	1E	75	VAL
4	1E	89	ASP
4	1E	113	PHE
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	181	LEU
4	1E	182	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG

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Mol	Chain	Res	Type
5	1F	88	VAL
5	1F	110	LEU
5	1F	132	VAL
5	1F	157	VAL
5	1F	158	THR
5	1F	162	LEU
5	1F	197	ASP
5	1F	201	VAL
5	1F	203	GLN
6	1G	5	VAL
6	1G	7	LEU
6	1G	28	VAL
6	1G	33	ARG
6	1G	43	LEU
6	1G	45	GLU
6	1G	49	ASP
6	1G	52	ILE
6	1G	53	LEU
6	1G	78	SER
6	1G	79	ASN
6	1G	82	LEU
6	1G	126	ASP
6	1G	150	ASP
6	1G	152	LEU
6	1G	153	ARG
6	1G	168	GLU
6	1G	170	ARG
6	1G	172	LEU
6	1G	175	LEU
6	1G	181	ARG
7	1H	3	ARG
7	1H	15	VAL
7	1H	23	ARG
7	1H	24	VAL
7	1H	45	VAL
7	1H	52	VAL
7	1H	95	ARG
7	1H	119	GLU
7	1H	124	GLU
7	1H	127	GLU
7	1H	129	THR
7	1H	132	ARG

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Mol	Chain	Res	Type
7	1H	139	GLN
8	1I	5	LEU
8	1I	12	LEU
8	1I	18	VAL
8	1I	38	LEU
8	1I	41	GLU
8	1I	43	ASN
8	1I	44	LEU
8	1I	47	LEU
8	1I	60	GLU
8	1I	61	ARG
8	1I	68	LEU
8	1I	78	THR
8	1I	92	VAL
8	1I	101	LEU
8	1I	109	ILE
8	1I	129	THR
8	1I	140	LEU
9	1N	1	MET
9	1N	14	VAL
9	1N	33	LEU
9	1N	59	LYS
9	1N	62	VAL
9	1N	68	GLU
9	1N	119	ARG
9	1N	121	LYS
9	1N	133	GLN
10	1O	10	VAL
10	1O	23	ARG
10	1O	42	SER
10	1O	97	ARG
11	1P	3	LEU
11	1P	57	THR
11	1P	83	VAL
11	1P	92	GLU
11	1P	101	VAL
11	1P	135	LEU
12	1Q	6	ARG
12	1Q	7	MET
12	1Q	18	LYS
12	1Q	21	THR
12	1Q	60	ARG

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Mol	Chain	Res	Type
12	1Q	63	LYS
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	112	GLU
12	1Q	115	MET
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	49	ASP
13	1R	67	LEU
13	1R	75	LEU
13	1R	96	ARG
13	1R	100	LEU
13	1R	114	VAL
14	1S	25	ARG
14	1S	46	VAL
14	1S	50	SER
14	1S	52	SER
14	1S	59	LYS
14	1S	75	GLU
14	1S	110	LEU
15	1T	6	LEU
15	1T	28	VAL
15	1T	53	ARG
15	1T	59	THR
15	1T	67	SER
15	1T	96	ARG
15	1T	107	ASP
15	1T	118	ARG
15	1T	128	GLU
16	1U	5	LYS
16	1U	30	LYS
16	1U	50	ARG
16	1U	59	ARG
16	1U	74	LEU
16	1U	95	LEU
17	1V	4	ILE
17	1V	10	LYS
17	1V	28	GLU
17	1V	44	LYS
17	1V	46	VAL

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Mol	Chain	Res	Type
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
18	1W	4	LYS
18	1W	11	ARG
18	1W	19	LEU
18	1W	65	LEU
18	1W	78	GLU
18	1W	85	VAL
18	1W	100	THR
18	1W	107	LEU
19	1X	49	VAL
19	1X	65	ARG
19	1X	66	LEU
19	1X	68	ARG
20	1Y	8	LYS
20	1Y	14	LEU
20	1Y	23	ARG
20	1Y	31	LEU
20	1Y	34	LYS
20	1Y	40	GLU
20	1Y	43	ASN
20	1Y	50	ARG
20	1Y	72	VAL
20	1Y	85	VAL
20	1Y	90	LEU
20	1Y	92	ASN
20	1Y	99	CYS
21	1Z	18	LEU
21	1Z	31	ARG
21	1Z	42	VAL
21	1Z	50	GLN
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	87	ASP
21	1Z	91	LEU
21	1Z	93	ASP
21	1Z	102	LEU
21	1Z	103	ARG
21	1Z	112	ARG
21	1Z	126	VAL

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Mol	Chain	Res	Type
21	1Z	129	SER
21	1Z	131	ARG
21	1Z	142	SER
21	1Z	155	LEU
21	1Z	161	VAL
21	1Z	170	THR
21	1Z	185	GLU
21	1Z	198	LYS
22	10	3	HIS
22	10	59	LEU
22	10	66	VAL
23	11	30	VAL
23	11	35	THR
23	11	75	GLU
23	11	80	LEU
24	12	32	LEU
24	12	53	LEU
25	13	8	LEU
25	13	35	ARG
25	13	54	VAL
25	13	56	VAL
26	14	1	MET
26	14	33	VAL
26	14	49	PHE
26	14	50	VAL
26	14	60	GLN
26	14	61	ARG
26	14	69	LYS
27	15	6	VAL
27	15	16	ARG
27	15	40	LYS
27	15	55	ARG
27	15	58	LEU
27	15	60	VAL
28	16	44	ARG
28	16	48	VAL
28	16	52	VAL
29	17	43	THR
29	17	47	ARG
29	17	48	LYS
30	18	29	LYS
30	18	31	HIS

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Mol	Chain	Res	Type
31	19	7	VAL
33	1b	15	VAL
33	1b	21	ARG
33	1b	43	ASP
33	1b	51	LEU
33	1b	83	MET
33	1b	106	LYS
33	1b	113	HIS
33	1b	122	PHE
33	1b	140	HIS
33	1b	142	LEU
33	1b	160	ASP
33	1b	178	ARG
33	1b	185	ILE
33	1b	198	ASP
33	1b	200	ILE
33	1b	212	GLN
33	1b	229	VAL
34	1c	3	ASN
34	1c	36	ASP
34	1c	59	ARG
34	1c	64	VAL
34	1c	70	VAL
34	1c	98	ASN
34	1c	105	GLU
34	1c	115	LEU
34	1c	144	SER
34	1c	161	GLU
35	1d	5	ILE
35	1d	17	VAL
35	1d	28	SER
35	1d	58	LEU
35	1d	76	ARG
35	1d	85	LYS
35	1d	156	GLU
35	1d	157	LEU
35	1d	162	LEU
35	1d	166	LYS
35	1d	168	ARG
35	1d	184	LYS
35	1d	187	ARG
35	1d	193	ASP

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Mol	Chain	Res	Type
35	1d	194	LEU
35	1d	208	SER
35	1d	209	ARG
36	1e	11	ILE
36	1e	16	THR
36	1e	41	VAL
36	1e	68	GLU
36	1e	72	GLN
36	1e	92	LYS
36	1e	120	THR
36	1e	126	ARG
36	1e	140	ARG
36	1e	152	ARG
37	1f	10	LEU
37	1f	19	LEU
37	1f	21	LEU
37	1f	40	VAL
37	1f	46	ARG
37	1f	48	LEU
37	1f	69	GLU
37	1f	73	ASN
37	1f	92	LYS
38	1g	10	ARG
38	1g	79	ARG
38	1g	91	VAL
38	1g	104	LEU
38	1g	106	GLN
38	1g	109	ASN
38	1g	110	GLN
38	1g	113	GLU
38	1g	144	MET
39	1h	26	VAL
39	1h	39	LEU
39	1h	51	VAL
39	1h	54	ASP
39	1h	56	LYS
39	1h	85	ARG
39	1h	104	ARG
39	1h	119	LEU
39	1h	127	LEU
40	1i	17	VAL
40	1i	25	LYS

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Mol	Chain	Res	Type
40	1i	38	GLN
40	1i	42	ARG
40	1i	47	LEU
40	1i	50	LEU
40	1i	56	LEU
40	1i	65	VAL
40	1i	81	ILE
40	1i	103	THR
41	1j	5	ARG
41	1j	8	LEU
41	1j	22	LYS
41	1j	38	ILE
41	1j	51	ARG
41	1j	65	LEU
41	1j	67	THR
41	1j	96	ILE
41	1j	100	THR
42	1k	14	VAL
42	1k	31	THR
42	1k	48	ILE
42	1k	105	VAL
42	1k	109	VAL
43	1l	41	ARG
43	1l	60	LEU
43	1l	83	VAL
43	1l	115	LYS
44	1m	4	ILE
44	1m	14	ARG
44	1m	19	LEU
44	1m	63	THR
44	1m	73	GLU
44	1m	97	PRO
44	1m	99	ARG
44	1m	102	ARG
45	1n	9	LYS
45	1n	15	LYS
45	1n	18	VAL
45	1n	57	ARG
46	1o	9	GLN
46	1o	26	GLU
46	1o	39	LEU
46	1o	47	LYS

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Mol	Chain	Res	Type
46	1o	71	GLN
47	1p	2	VAL
47	1p	20	VAL
47	1p	29	ASP
47	1p	45	THR
47	1p	62	VAL
47	1p	67	THR
48	1q	7	THR
48	1q	11	VAL
48	1q	36	ILE
48	1q	50	LYS
48	1q	61	GLU
48	1q	63	ARG
48	1q	66	SER
48	1q	76	LEU
48	1q	79	SER
48	1q	97	SER
49	1r	37	VAL
49	1r	38	GLU
49	1r	47	THR
49	1r	85	LEU
50	1s	28	LYS
50	1s	37	ARG
50	1s	41	VAL
50	1s	48	THR
51	1t	9	ASN
51	1t	15	ARG
51	1t	37	SER
51	1t	43	LEU
51	1t	62	LEU
51	1t	70	SER
51	1t	100	ILE
52	1u	12	LYS
52	1u	15	ARG
52	1u	17	THR
53	1y	2	THR
53	1y	3	MET
53	1y	13	THR
53	1y	23	ARG
53	1y	42	SER
53	1y	46	GLN
3	2D	3	VAL

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Mol	Chain	Res	Type
3	2D	69	ARG
3	2D	99	ASP
3	2D	103	ARG
3	2D	111	LEU
3	2D	113	VAL
3	2D	116	GLN
3	2D	140	THR
3	2D	147	LEU
3	2D	155	LEU
3	2D	176	ARG
3	2D	188	GLU
3	2D	193	VAL
3	2D	200	ASP
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	276	LYS
4	2E	38	THR
4	2E	59	VAL
4	2E	75	VAL
4	2E	76	ARG
4	2E	97	LYS
4	2E	116	VAL
4	2E	119	ARG
4	2E	144	ARG
4	2E	163	GLU
4	2E	170	LEU
4	2E	181	LEU
4	2E	182	LEU
5	2F	15	SER
5	2F	17	ARG
5	2F	20	LEU
5	2F	23	ASP
5	2F	27	GLU
5	2F	33	LEU
5	2F	38	ARG
5	2F	51	THR
5	2F	60	SER
5	2F	74	ARG
5	2F	106	ARG
5	2F	136	THR

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Mol	Chain	Res	Type
5	2F	161	GLU
5	2F	170	LEU
5	2F	192	LEU
5	2F	197	ASP
5	2F	203	GLN
6	2G	3	LEU
6	2G	5	VAL
6	2G	41	GLN
6	2G	51	ARG
6	2G	53	LEU
6	2G	64	THR
6	2G	88	ILE
6	2G	90	LEU
6	2G	91	ARG
6	2G	103	LEU
6	2G	106	LEU
6	2G	136	ARG
6	2G	139	LEU
6	2G	149	VAL
6	2G	159	VAL
6	2G	165	THR
6	2G	167	GLU
6	2G	172	LEU
6	2G	173	LEU
7	2H	32	GLU
7	2H	33	LEU
7	2H	49	VAL
7	2H	59	ARG
7	2H	68	THR
7	2H	114	VAL
7	2H	131	VAL
7	2H	133	VAL
7	2H	139	GLN
7	2H	163	TYR
7	2H	171	LEU
8	2I	35	LEU
8	2I	37	VAL
8	2I	38	LEU
8	2I	40	THR
8	2I	47	LEU
8	2I	51	ILE
8	2I	57	ARG

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Mol	Chain	Res	Type
8	2I	68	LEU
8	2I	76	THR
8	2I	87	LYS
8	2I	93	THR
8	2I	96	ASP
8	2I	116	LEU
8	2I	127	VAL
8	2I	142	VAL
9	2N	15	LEU
9	2N	28	THR
9	2N	73	THR
9	2N	83	LYS
10	2O	23	ARG
10	2O	32	TYR
10	2O	78	ARG
10	2O	94	ARG
10	2O	98	VAL
11	2P	29	LYS
11	2P	59	LEU
11	2P	65	ARG
11	2P	71	VAL
11	2P	83	VAL
11	2P	92	GLU
11	2P	95	VAL
11	2P	96	THR
11	2P	99	LEU
11	2P	149	GLU
12	2Q	1	MET
12	2Q	7	MET
12	2Q	35	VAL
12	2Q	60	ARG
12	2Q	75	THR
12	2Q	79	LEU
12	2Q	109	VAL
12	2Q	111	GLU
12	2Q	112	GLU
13	2R	29	LEU
13	2R	33	ARG
13	2R	44	LEU
13	2R	96	ARG
14	2S	12	PHE
14	2S	21	THR

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Mol	Chain	Res	Type
14	2S	27	SER
14	2S	35	ILE
14	2S	52	SER
14	2S	53	SER
14	2S	64	GLU
14	2S	69	VAL
14	2S	73	LEU
14	2S	76	LYS
14	2S	80	LEU
14	2S	85	VAL
14	2S	110	LEU
15	2T	6	LEU
15	2T	51	ARG
15	2T	53	ARG
15	2T	67	SER
15	2T	85	LYS
15	2T	108	ARG
15	2T	124	ASP
16	2U	50	ARG
16	2U	55	ARG
16	2U	74	LEU
17	2V	46	VAL
17	2V	51	VAL
17	2V	62	LEU
17	2V	64	HIS
17	2V	72	VAL
17	2V	79	VAL
18	2W	4	LYS
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	67	ASP
18	2W	68	ARG
19	2X	72	LYS
19	2X	81	VAL
20	2Y	6	HIS
20	2Y	19	LYS
20	2Y	31	LEU
20	2Y	43	ASN
20	2Y	63	LYS
20	2Y	85	VAL

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Mol	Chain	Res	Type
20	2Y	97	ARG
20	2Y	99	CYS
21	2Z	18	LEU
21	2Z	35	ARG
21	2Z	41	LEU
21	2Z	42	VAL
21	2Z	72	ARG
21	2Z	86	VAL
21	2Z	91	LEU
21	2Z	94	GLU
21	2Z	121	HIS
21	2Z	124	ILE
21	2Z	128	VAL
21	2Z	153	SER
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	162	GLU
21	2Z	175	VAL
21	2Z	185	GLU
21	2Z	190	GLU
22	20	14	ARG
22	20	53	MET
22	20	55	ARG
23	21	11	ARG
23	21	40	ARG
23	21	52	ARG
23	21	85	LEU
23	21	86	SER
24	22	4	SER
24	22	7	ARG
24	22	17	SER
24	22	19	VAL
24	22	27	GLU
24	22	32	LEU
24	22	53	LEU
24	22	64	LEU
25	23	23	LEU
25	23	26	LEU
25	23	31	LEU
25	23	54	VAL
25	23	58	VAL
25	23	59	VAL

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Mol	Chain	Res	Type
26	24	1	MET
26	24	23	GLU
26	24	33	VAL
26	24	50	VAL
26	24	53	GLU
26	24	61	ARG
26	24	62	ARG
26	24	63	TYR
27	25	6	VAL
27	25	40	LYS
27	25	58	LEU
28	26	14	THR
28	26	19	ARG
28	26	32	ASN
28	26	48	VAL
28	26	52	VAL
29	27	10	ARG
29	27	23	ARG
29	27	47	ARG
29	27	48	LYS
30	28	14	VAL
30	28	23	VAL
30	28	31	HIS
30	28	34	TRP
31	29	6	SER
31	29	7	VAL
31	29	14	CYS
31	29	15	LYS
31	29	17	ILE
31	29	35	ARG
33	2b	8	LYS
33	2b	9	GLU
33	2b	12	GLU
33	2b	15	VAL
33	2b	16	HIS
33	2b	24	TRP
33	2b	28	PHE
33	2b	45	GLN
33	2b	53	ARG
33	2b	76	GLN
33	2b	93	VAL
33	2b	96	ARG

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Mol	Chain	Res	Type
33	2b	97	TRP
33	2b	113	HIS
33	2b	121	LEU
33	2b	128	GLU
33	2b	144	ARG
33	2b	147	LYS
33	2b	154	LEU
33	2b	158	LEU
33	2b	160	ASP
33	2b	172	ILE
33	2b	178	ARG
33	2b	189	ASP
33	2b	191	ASP
33	2b	211	ILE
33	2b	212	GLN
33	2b	215	LEU
33	2b	221	LEU
33	2b	224	GLN
34	2c	3	ASN
34	2c	15	THR
34	2c	28	GLN
34	2c	31	HIS
34	2c	33	LEU
34	2c	47	LEU
34	2c	52	LEU
34	2c	70	VAL
34	2c	72	LYS
34	2c	89	GLU
34	2c	111	LEU
34	2c	128	PHE
34	2c	136	GLN
34	2c	190	ARG
34	2c	206	GLU
35	2d	8	VAL
35	2d	13	ARG
35	2d	28	SER
35	2d	61	LYS
35	2d	76	ARG
35	2d	83	SER
35	2d	106	TYR
35	2d	107	ARG
35	2d	113	SER

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Mol	Chain	Res	Type
35	2d	127	THR
35	2d	128	VAL
35	2d	135	LEU
35	2d	141	ARG
35	2d	150	GLU
35	2d	160	GLN
35	2d	166	LYS
35	2d	175	SER
35	2d	178	VAL
35	2d	186	LEU
35	2d	190	ASP
36	2e	9	LYS
36	2e	11	ILE
36	2e	31	LEU
36	2e	41	VAL
36	2e	45	PHE
36	2e	68	GLU
36	2e	71	LEU
36	2e	78	HIS
36	2e	91	LEU
36	2e	107	ARG
37	2f	10	LEU
37	2f	22	GLU
37	2f	40	VAL
37	2f	55	ASP
37	2f	57	GLN
37	2f	70	ASP
37	2f	75	LEU
38	2g	15	ASP
38	2g	45	ASP
38	2g	47	CYS
38	2g	50	ILE
38	2g	75	VAL
38	2g	92	SER
38	2g	97	GLN
38	2g	104	LEU
38	2g	110	GLN
38	2g	115	ARG
38	2g	153	HIS
39	2h	2	LEU
39	2h	19	VAL
39	2h	25	ASP

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Mol	Chain	Res	Type
39	2h	104	ARG
39	2h	109	ILE
39	2h	112	LEU
39	2h	114	THR
39	2h	119	LEU
39	2h	122	ARG
39	2h	127	LEU
39	2h	133	LEU
40	2i	7	THR
40	2i	27	THR
40	2i	33	PHE
40	2i	38	GLN
40	2i	42	ARG
40	2i	75	ASP
40	2i	81	ILE
40	2i	89	ASN
40	2i	102	LEU
40	2i	104	ARG
40	2i	105	ASP
40	2i	108	VAL
40	2i	113	LYS
40	2i	125	TYR
41	2j	16	LEU
41	2j	21	GLN
41	2j	29	ARG
41	2j	30	SER
41	2j	34	VAL
41	2j	38	ILE
41	2j	58	ASP
41	2j	73	ASP
41	2j	92	THR
41	2j	95	GLU
41	2j	100	THR
42	2k	41	THR
42	2k	93	GLN
42	2k	109	VAL
42	2k	112	THR
42	2k	116	HIS
42	2k	117	ASN
42	2k	126	ARG
43	2l	18	VAL
43	2l	33	ARG

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Mol	Chain	Res	Type
43	2l	67	THR
43	2l	83	VAL
44	2m	4	ILE
44	2m	43	THR
44	2m	49	THR
44	2m	62	ASN
44	2m	64	TRP
44	2m	80	ARG
44	2m	102	ARG
44	2m	116	THR
45	2n	6	LEU
45	2n	7	ILE
46	2o	3	ILE
46	2o	21	ASP
46	2o	26	GLU
46	2o	39	LEU
46	2o	68	ARG
46	2o	88	ARG
47	2p	1	MET
47	2p	11	SER
47	2p	16	HIS
47	2p	20	VAL
47	2p	21	VAL
47	2p	22	THR
47	2p	28	ARG
47	2p	38	TYR
47	2p	45	THR
47	2p	60	LEU
47	2p	62	VAL
47	2p	67	THR
47	2p	75	ARG
48	2q	9	VAL
48	2q	39	SER
48	2q	66	SER
48	2q	76	LEU
48	2q	96	GLU
49	2r	37	VAL
49	2r	41	LYS
49	2r	45	SER
49	2r	47	THR
49	2r	85	LEU
50	2s	5	LEU

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Mol	Chain	Res	Type
50	2s	16	LEU
50	2s	38	SER
50	2s	48	THR
50	2s	62	ILE
50	2s	63	THR
50	2s	77	THR
51	2t	15	ARG
51	2t	24	LEU
51	2t	62	LEU
51	2t	71	THR
51	2t	84	LEU
51	2t	86	ARG
51	2t	99	LEU
51	2t	100	ILE
52	2u	10	ARG
52	2u	15	ARG
53	2y	6	THR
53	2y	16	ILE
53	2y	24	LEU
53	2y	56	THR
53	2y	62	VAL
53	2y	77	LEU
53	2y	78	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	115	GLN
3	1D	253	GLN
4	1E	48	GLN
4	1E	121	ASN
5	1F	8	GLN
5	1F	69	HIS
5	1F	133	ASN
5	1F	203	GLN
6	1G	26	GLN
8	1I	105	HIS
10	1O	3	GLN
12	1Q	12	GLN
13	1R	50	HIS
14	1S	68	GLN

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Mol	Chain	Res	Type
14	1S	84	GLN
15	1T	43	GLN
15	1T	58	ASN
15	1T	123	GLN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	73	GLN
22	10	35	ASN
25	13	32	GLN
29	17	36	GLN
33	1b	78	GLN
33	1b	135	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	102	ASN
34	1c	123	GLN
35	1d	77	ASN
35	1d	123	HIS
35	1d	125	HIS
35	1d	129	ASN
37	1f	73	ASN
38	1g	28	ASN
38	1g	86	GLN
38	1g	110	GLN
38	1g	148	ASN
39	1h	70	GLN
40	1i	3	GLN
40	1i	38	GLN
40	1i	73	GLN
41	1j	13	HIS
41	1j	56	HIS
42	1k	93	GLN
43	1l	99	HIS
44	1m	40	ASN
44	1m	92	HIS
46	1o	9	GLN
46	1o	13	GLN
46	1o	28	GLN
46	1o	71	GLN
48	1q	93	GLN

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Mol	Chain	Res	Type
50	1s	47	HIS
50	1s	56	GLN
50	1s	69	HIS
50	1s	83	HIS
51	1t	18	GLN
53	1y	89	GLN
3	2D	87	ASN
3	2D	96	HIS
3	2D	253	GLN
4	2E	48	GLN
5	2F	69	HIS
5	2F	133	ASN
8	2I	54	GLN
8	2I	105	HIS
8	2I	133	HIS
8	2I	139	GLN
10	2O	3	GLN
12	2Q	141	GLN
13	2R	31	HIS
13	2R	71	GLN
15	2T	38	ASN
15	2T	58	ASN
15	2T	104	ASN
16	2U	94	ASN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	92	ASN
21	2Z	55	HIS
21	2Z	73	GLN
25	23	32	GLN
26	24	60	GLN
29	27	36	GLN
33	2b	19	HIS
33	2b	40	HIS
33	2b	204	ASN
34	2c	102	ASN
34	2c	139	GLN
35	2d	42	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	160	GLN
36	2e	78	HIS

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Mol	Chain	Res	Type
36	2e	127	ASN
37	2f	13	ASN
38	2g	86	GLN
38	2g	110	GLN
38	2g	148	ASN
40	2i	3	GLN
40	2i	38	GLN
40	2i	58	HIS
41	2j	62	HIS
41	2j	69	ASN
42	2k	26	ASN
43	2l	99	HIS
44	2m	62	ASN
44	2m	77	ASN
46	2o	9	GLN
46	2o	13	GLN
46	2o	28	GLN
46	2o	71	GLN
47	2p	76	GLN
48	2q	26	GLN
50	2s	23	ASN
50	2s	83	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	410 (14%)	27 (0%)
1	2A	2857/2915 (98%)	484 (16%)	30 (1%)
2	1B	119/121 (98%)	13 (10%)	0
2	2B	119/121 (98%)	17 (14%)	0
32	1a	1494/1521 (98%)	267 (17%)	0
32	2a	1498/1521 (98%)	278 (18%)	0
54	1w	2/4 (50%)	0	0
54	2w	2/4 (50%)	1 (50%)	0
55	1x	2/4 (50%)	1 (50%)	0
55	2x	2/4 (50%)	1 (50%)	0
All	All	8959/9130 (98%)	1472 (16%)	57 (0%)

All (1472) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	34	C
1	1A	45	C
1	1A	63	U
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	102	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	141	A
1	1A	149	A
1	1A	181	A
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	272(J)	C
1	1A	275	G
1	1A	279	C
1	1A	280	C
1	1A	311	A
1	1A	330	A
1	1A	333	G
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	372	G
1	1A	386	G

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Mol	Chain	Res	Type
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	422	A
1	1A	428	A
1	1A	447	A
1	1A	448	U
1	1A	456	C
1	1A	457	A
1	1A	481	G
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	574	C
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	616	G
1	1A	621	A
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	652(U)	G
1	1A	655	A
1	1A	669	G
1	1A	686	G

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Mol	Chain	Res	Type
1	1A	730	C
1	1A	740	U
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	890	A
1	1A	896	A
1	1A	907	U
1	1A	910	A
1	1A	931	G
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	958	U
1	1A	959	A
1	1A	961	C
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	1026	U
1	1A	1033	U
1	1A	1039	G
1	1A	1042	G

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Mol	Chain	Res	Type
1	1A	1043	C
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1058	G
1	1A	1060	U
1	1A	1061	U
1	1A	1062	G
1	1A	1064	C
1	1A	1065	U
1	1A	1067	A
1	1A	1068	G
1	1A	1069	A
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1076	C
1	1A	1077	A
1	1A	1079	C
1	1A	1080	C
1	1A	1088	A
1	1A	1090	U
1	1A	1096	A
1	1A	1097	U
1	1A	1098	A
1	1A	1100	C
1	1A	1109	C
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1141	U
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G

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Mol	Chain	Res	Type
1	1A	1177	A
1	1A	1210	A
1	1A	1211	U
1	1A	1220	A
1	1A	1229	G
1	1A	1236	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1320	C
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1365	A
1	1A	1370	C
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1446	C
1	1A	1450	G
1	1A	1452	A
1	1A	1455	G
1	1A	1459	G
1	1A	1460	A
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G
1	1A	1487	G
1	1A	1493	C
1	1A	1497	U
1	1A	1503	U
1	1A	1508	A

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Mol	Chain	Res	Type
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1531	C
1	1A	1542	A
1	1A	1543	C
1	1A	1558	A
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1616	A
1	1A	1639	U
1	1A	1647	G
1	1A	1648	C
1	1A	1654	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1722	A
1	1A	1739	U
1	1A	1747	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
1	1A	1847	A
1	1A	1848	A

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Mol	Chain	Res	Type
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1894	C
1	1A	1900	A
1	1A	1906	G
1	1A	1911	PSU
1	1A	1913	A
1	1A	1929	G
1	1A	1930	G
1	1A	1934	C
1	1A	1936	A
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2093	G
1	1A	2102	U
1	1A	2103	C
1	1A	2104	G
1	1A	2107	C
1	1A	2108	C
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U

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Mol	Chain	Res	Type
1	1A	2119	A
1	1A	2123	G
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2137	C
1	1A	2146	C
1	1A	2148	G
1	1A	2158	A
1	1A	2159	G
1	1A	2164	C
1	1A	2165	G
1	1A	2172	U
1	1A	2176	A
1	1A	2180	U
1	1A	2186	G
1	1A	2187	G
1	1A	2189	U
1	1A	2190	G
1	1A	2191	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2273	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	2318	G
1	1A	2320	A

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Mol	Chain	Res	Type
1	1A	2325	G
1	1A	2327	A
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2389	G
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2470	G
1	1A	2476	A
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	2609	U
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	2689	U

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Mol	Chain	Res	Type
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2748	A
1	1A	2757	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2769	C
1	1A	2778	A
1	1A	2789	C
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2834	G
1	1A	2835	A
1	1A	2872	G
1	1A	2886	G
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	7	G
2	1B	13	A
2	1B	35	U
2	1B	42	C
2	1B	53	A
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	106	G
2	1B	110	G

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Mol	Chain	Res	Type
2	1B	116	G
2	1B	120	A
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	56	U
32	1a	61	G
32	1a	66	G
32	1a	78	G
32	1a	79	G
32	1a	93	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	141	A
32	1a	144	G
32	1a	163	C
32	1a	165	C
32	1a	169	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	189(E)	U
32	1a	189(G)	G
32	1a	190	U
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	262	A
32	1a	266	G

Continued on next page...

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Mol	Chain	Res	Type
32	1a	267	C
32	1a	289	G
32	1a	317	G
32	1a	318	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	344	A
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	431	A
32	1a	439	A
32	1a	442	C
32	1a	443	C
32	1a	444	C
32	1a	452	A
32	1a	470	C
32	1a	475	G
32	1a	477	A
32	1a	479	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

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Mol	Chain	Res	Type
32	1a	511	C
32	1a	514	C
32	1a	518	C
32	1a	521	G
32	1a	532	A
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	564	C
32	1a	567	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	588	G
32	1a	596	C
32	1a	607	A
32	1a	614	A
32	1a	619	U
32	1a	630	G
32	1a	632	A
32	1a	633	G
32	1a	653	A
32	1a	660	G
32	1a	661	G
32	1a	665	A
32	1a	666	G
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	754	C
32	1a	755	G
32	1a	759	A
32	1a	768	A
32	1a	785	G
32	1a	786	G
32	1a	793	U

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Mol	Chain	Res	Type
32	1a	794	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	872	A
32	1a	902	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	939	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	983	A
32	1a	991	U
32	1a	992	U
32	1a	993	G
32	1a	998	G
32	1a	999	C
32	1a	1001	A
32	1a	1001(A)	G
32	1a	1004	A
32	1a	1005	A
32	1a	1020	U
32	1a	1021	G
32	1a	1022	G
32	1a	1023	G

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Mol	Chain	Res	Type
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1031	G
32	1a	1032	G
32	1a	1034	G
32	1a	1037	C
32	1a	1044	A
32	1a	1063	C
32	1a	1065	U
32	1a	1066	C
32	1a	1067	A
32	1a	1070	U
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1124	G
32	1a	1125	U
32	1a	1126	U
32	1a	1127	G
32	1a	1130	A
32	1a	1133	G
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1155	G
32	1a	1158	C
32	1a	1159	U

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Mol	Chain	Res	Type
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1208	C
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1224	G
32	1a	1227	A
32	1a	1238	A
32	1a	1241	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1273	G
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1312	G
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1397	C
32	1a	1409	C
32	1a	1419	G
32	1a	1429	C
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A

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Mol	Chain	Res	Type
32	1a	1447	A
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1493	A
32	1a	1494	G
32	1a	1497	G
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
55	1x	74	C
1	2A	10	G
1	2A	11	G
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	36	G
1	2A	45	C
1	2A	50	U
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	78	A
1	2A	84	A
1	2A	92	A
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	140	G
1	2A	141	A
1	2A	157	U
1	2A	182	A
1	2A	196	A
1	2A	199	A

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Mol	Chain	Res	Type
1	2A	205	G
1	2A	216	A
1	2A	217	G
1	2A	221	A
1	2A	222	A
1	2A	223	A
1	2A	229	A
1	2A	230	U
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	302	C
1	2A	311	A
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	335	C
1	2A	352	G
1	2A	363	G
1	2A	386	G
1	2A	389	G
1	2A	405	U
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	442	G
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	467	G

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Mol	Chain	Res	Type
1	2A	470	A
1	2A	481	G
1	2A	482	A
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	543	C
1	2A	545	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	595	C
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	701	G
1	2A	730	C
1	2A	740	U
1	2A	751	A
1	2A	752	A
1	2A	753	C
1	2A	775	G

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Mol	Chain	Res	Type
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	793	A
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	855	G
1	2A	857	C
1	2A	859	G
1	2A	865	C
1	2A	867	C
1	2A	877	U
1	2A	880	G
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	895	U
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	932	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	959	A
1	2A	961	C
1	2A	963	U
1	2A	965	C
1	2A	968	G
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A

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Mol	Chain	Res	Type
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1041	C
1	2A	1043	C
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1049	C
1	2A	1051	G
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A
1	2A	1058	G
1	2A	1060	U
1	2A	1063	G
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1069	A
1	2A	1070	A
1	2A	1071	G
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
1	2A	1079	C
1	2A	1081	U
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1087	G
1	2A	1088	A
1	2A	1090	U

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Mol	Chain	Res	Type
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1095	A
1	2A	1097	U
1	2A	1098	A
1	2A	1106	G
1	2A	1109	C
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1117	G
1	2A	1129	A
1	2A	1135	C
1	2A	1136	G
1	2A	1144	G
1	2A	1171	G
1	2A	1195	G
1	2A	1206	G
1	2A	1212	G
1	2A	1220	A
1	2A	1236	G
1	2A	1241	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1318	C
1	2A	1319	G
1	2A	1342	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1380	G

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Mol	Chain	Res	Type
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1467	C
1	2A	1471	A
1	2A	1479	G
1	2A	1482	G
1	2A	1493	C
1	2A	1494	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1537	G
1	2A	1539	G
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
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	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1613	G
1	2A	1640	C
1	2A	1647	G

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Mol	Chain	Res	Type
1	2A	1648	C
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
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	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1902	C
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1918	A
1	2A	1929	G
1	2A	1930	G
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1985	G
1	2A	1993	U
1	2A	1997	G

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Mol	Chain	Res	Type
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2093	G
1	2A	2096	U
1	2A	2099	U
1	2A	2103	C
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2111	C
1	2A	2112	G
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2120	G
1	2A	2121	G
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2140	C
1	2A	2141	G
1	2A	2145	C

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Mol	Chain	Res	Type
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2152	G
1	2A	2153	G
1	2A	2155	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G
1	2A	2172	U
1	2A	2173	A
1	2A	2175	C
1	2A	2184	G
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2219	G
1	2A	2225	A
1	2A	2238	G
1	2A	2268	A
1	2A	2269	A
1	2A	2274	A
1	2A	2275	C
1	2A	2277	G
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2293	C
1	2A	2305	A
1	2A	2308	G

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Mol	Chain	Res	Type
1	2A	2311	A
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2343	C
1	2A	2347	C
1	2A	2372	G
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2406	U
1	2A	2410	G
1	2A	2414	G
1	2A	2422	A
1	2A	2424	C
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2465	C
1	2A	2470	G
1	2A	2476	A
1	2A	2487	G
1	2A	2491	U
1	2A	2492	U
1	2A	2498	C
1	2A	2502	G
1	2A	2505	G
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G

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Mol	Chain	Res	Type
1	2A	2549	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2630	G
1	2A	2654	A
1	2A	2660	A
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2732	G
1	2A	2733	A
1	2A	2744	G
1	2A	2752	C
1	2A	2757	A
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2794	C
1	2A	2802	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2872	G
1	2A	2880	C
1	2A	2891	G
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U

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Mol	Chain	Res	Type
2	2B	9	G
2	2B	12	C
2	2B	30	C
2	2B	33	G
2	2B	41	U
2	2B	42	C
2	2B	54	G
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	106	G
2	2B	109	C
2	2B	110	G
2	2B	115	G
2	2B	120	A
32	2a	5	U
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	33	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	61	G
32	2a	66	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	138	G
32	2a	142	G
32	2a	144	G
32	2a	156	G
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(B)	C

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Mol	Chain	Res	Type
32	2a	189(C)	C
32	2a	189(E)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	220	G
32	2a	240	C
32	2a	247	G
32	2a	250	A
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	270	A
32	2a	279	A
32	2a	289	G
32	2a	290	C
32	2a	298	A
32	2a	303	A
32	2a	318	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	378	G
32	2a	392	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	424	G
32	2a	429	U

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Mol	Chain	Res	Type
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	446	G
32	2a	452	A
32	2a	458	C
32	2a	461	A
32	2a	470	C
32	2a	476	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	527	G7M
32	2a	532	A
32	2a	533	A
32	2a	536	C
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	622	A
32	2a	630	G
32	2a	631	G
32	2a	633	G
32	2a	641	U
32	2a	653	A
32	2a	661	G
32	2a	665	A
32	2a	687	A
32	2a	688	G

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Mol	Chain	Res	Type
32	2a	695	A
32	2a	714	G
32	2a	723	U
32	2a	731	G
32	2a	734	G
32	2a	746	A
32	2a	748	C
32	2a	749	C
32	2a	753	A
32	2a	754	C
32	2a	755	G
32	2a	770	C
32	2a	773	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	852	G
32	2a	854	G
32	2a	859	A
32	2a	872	A
32	2a	873	A
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	939	G
32	2a	942	G
32	2a	954	G
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	968	A

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Mol	Chain	Res	Type
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	982	U
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	998	G
32	2a	1000	U
32	2a	1001	A
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1007	C
32	2a	1015	A
32	2a	1020	U
32	2a	1022	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1033	G
32	2a	1034	G
32	2a	1038	C
32	2a	1041	A
32	2a	1044	A
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1071	C
32	2a	1079	G
32	2a	1081	G
32	2a	1094	G

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Mol	Chain	Res	Type
32	2a	1095	U
32	2a	1101	A
32	2a	1118	C
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1147	C
32	2a	1148	U
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1170	A
32	2a	1183	A
32	2a	1184	G
32	2a	1194	U
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1208	C
32	2a	1211	U
32	2a	1213	A
32	2a	1214	C
32	2a	1224	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1265	G
32	2a	1270	C
32	2a	1275	A
32	2a	1278	U

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Mol	Chain	Res	Type
32	2a	1279	A
32	2a	1281	U
32	2a	1282	C
32	2a	1285	A
32	2a	1287	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1312	G
32	2a	1320	C
32	2a	1340	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1364	U
32	2a	1368	G
32	2a	1370	G
32	2a	1397	C
32	2a	1400	5MC
32	2a	1406	U
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1456	G
32	2a	1487	G
32	2a	1492	A
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1525	G
32	2a	1528	U
32	2a	1529	G
32	2a	1530	G
54	2w	74	C

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Mol	Chain	Res	Type
55	2x	74	C

All (57) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	249	C
1	1A	266	G
1	1A	278	A
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	839	U
1	1A	840	C
1	1A	887	A
1	1A	895	U
1	1A	974	G
1	1A	1047	G
1	1A	1065	U
1	1A	1089	G
1	1A	1142(A)	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1379	A
1	1A	1442	G
1	1A	1608	A
1	1A	1653	G
1	1A	2126	A
1	1A	2406	U
1	1A	2689	U
1	1A	2756	U
1	2A	196	A
1	2A	271(M)	G
1	2A	277	C
1	2A	752	A
1	2A	764	A
1	2A	774	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	900	A

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Mol	Chain	Res	Type
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1143	A
1	2A	1240	U
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1493	C
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2321	G
1	2A	2406	U
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PSU	1A	2605	1	17,21,22	1.56	4 (23%)	20,30,33	3.05	6 (30%)
1	PSU	2A	1911	1	17,21,22	1.57	2 (11%)	20,30,33	3.14	6 (30%)
32	2MG	1a	1207	32	19,26,27	1.30	2 (10%)	21,38,41	2.50	10 (47%)
1	PSU	2A	2605	1	17,21,22	1.63	3 (17%)	20,30,33	3.32	6 (30%)
32	MA6	2a	1518	32	19,26,27	0.80	0	18,38,41	1.40	2 (11%)
1	2MA	1A	2503	1,57	17,25,26	1.17	2 (11%)	19,37,40	1.83	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	2A	1939	1,57	15,22,23	1.22	1 (6%)	16,32,35	1.72	2 (12%)
1	OMC	2A	1920	1	15,22,23	0.67	0	17,31,34	1.35	2 (11%)
1	OMU	1A	2552	1,57	14,22,23	0.85	0	14,31,34	0.81	1 (7%)
32	5MC	1a	1400	32	15,22,23	1.38	1 (6%)	19,32,35	1.40	3 (15%)
32	MA6	1a	1518	32	19,26,27	0.82	0	18,38,41	1.34	2 (11%)
55	8AN	2x	76	57,55,56	19,24,25	1.19	3 (15%)	13,35,38	1.77	2 (15%)
32	PSU	1a	516	57,32	17,21,22	1.41	3 (17%)	20,30,33	3.19	6 (30%)
32	5MC	1a	967	32	15,22,23	1.28	1 (6%)	19,32,35	1.40	3 (15%)
1	5MU	1A	1939	1,57	15,22,23	1.21	2 (13%)	16,32,35	1.82	2 (12%)
32	G7M	1a	527	57,32	20,26,27	1.54	2 (10%)	20,39,42	2.01	5 (25%)
43	0TD	2l	92	43	4,9,10	3.07	1 (25%)	3,11,13	8.19	1 (33%)
1	OMG	1A	2251	1,57,55	18,26,27	1.21	2 (11%)	20,38,41	2.19	6 (30%)
1	OMC	1A	1920	1	15,22,23	0.66	0	17,31,34	1.49	2 (11%)
32	5MC	1a	1404	32	15,22,23	1.35	1 (6%)	19,32,35	1.24	3 (15%)
1	5MC	1A	1962	1,57	15,22,23	1.26	1 (6%)	19,32,35	1.29	2 (10%)
55	8AN	1x	76	57,55,56	19,24,25	1.30	4 (21%)	13,35,38	1.77	2 (15%)
32	MA6	1a	1519	32	19,26,27	0.80	0	18,38,41	1.42	2 (11%)
1	5MC	2A	1962	1,57	15,22,23	1.19	1 (6%)	19,32,35	1.58	4 (21%)
1	2MA	2A	2503	1,57	17,25,26	1.38	2 (11%)	19,37,40	2.16	3 (15%)
32	UR3	2a	1498	32	14,22,23	0.77	1 (7%)	15,32,35	0.73	1 (6%)
32	G7M	2a	527	57,32	20,26,27	1.51	2 (10%)	20,39,42	2.07	5 (25%)
32	4OC	2a	1402	32	16,23,24	0.69	0	17,32,35	1.32	2 (11%)
54	PPU	1w	76	54,1	32,40,41	0.87	1 (3%)	33,57,60	1.45	5 (15%)
54	PPU	2w	76	54,1	32,40,41	0.97	2 (6%)	33,57,60	1.37	6 (18%)
32	M2G	2a	966	57,32	20,27,28	1.49	3 (15%)	22,40,43	2.24	6 (27%)
32	5MC	2a	1407	32	15,22,23	1.38	1 (6%)	19,32,35	1.36	2 (10%)
1	5MU	1A	1915	1	15,22,23	1.04	1 (6%)	16,32,35	2.10	2 (12%)
32	5MC	2a	1400	32	15,22,23	1.33	1 (6%)	19,32,35	1.26	3 (15%)
32	4OC	1a	1402	32	16,23,24	0.61	0	17,32,35	1.17	1 (5%)
1	PSU	1A	1911	1	17,21,22	1.42	2 (11%)	20,30,33	3.05	7 (35%)
1	PSU	1A	1917	1	17,21,22	1.55	2 (11%)	20,30,33	3.19	6 (30%)
32	PSU	2a	516	57,32	17,21,22	1.63	3 (17%)	20,30,33	3.09	7 (35%)
32	5MC	1a	1407	32	15,22,23	1.37	1 (6%)	19,32,35	1.31	3 (15%)
1	5MC	2A	1942	1	15,22,23	1.40	1 (6%)	19,32,35	1.41	3 (15%)
32	UR3	1a	1498	32	14,22,23	0.69	0	15,32,35	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	1a	966	32	20,27,28	1.44	3 (15%)	22,40,43	2.19	6 (27%)
1	5MU	2A	1915	1	15,22,23	0.99	1 (6%)	16,32,35	2.03	1 (6%)
1	OMG	2A	2251	1,57,55	18,26,27	1.17	2 (11%)	20,38,41	2.08	6 (30%)
1	OMU	2A	2552	1,57	14,22,23	0.89	0	14,31,34	0.81	1 (7%)
1	PSU	2A	1917	1	17,21,22	1.55	3 (17%)	20,30,33	3.21	6 (30%)
1	5MC	1A	1942	1,57	15,22,23	1.26	1 (6%)	19,32,35	1.32	3 (15%)
32	2MG	2a	1207	32	19,26,27	1.25	2 (10%)	21,38,41	2.26	7 (33%)
32	5MC	2a	967	32	15,22,23	1.41	1 (6%)	19,32,35	1.28	2 (10%)
32	MA6	2a	1519	32	19,26,27	0.81	0	18,38,41	1.51	2 (11%)
43	0TD	1l	92	43	4,9,10	3.10	1 (25%)	3,11,13	3.43	1 (33%)
32	5MC	2a	1404	32	15,22,23	1.40	1 (6%)	19,32,35	1.33	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	1/5/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
1	2MA	1A	2503	1,57	-	2/3/25/26	0/3/3/3
1	5MU	2A	1939	1,57	-	0/5/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/7/27/28	0/2/2/2
1	OMU	1A	2552	1,57	-	0/7/27/28	0/2/2/2
32	5MC	1a	1400	32	-	0/5/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
55	8AN	2x	76	57,55,56	-	3/3/25/26	0/3/3/3
32	PSU	1a	516	57,32	-	1/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/5/25/26	0/2/2/2
1	5MU	1A	1939	1,57	-	1/5/25/26	0/2/2/2
32	G7M	1a	527	57,32	-	1/3/25/26	0/3/3/3
43	0TD	2l	92	43	-	1/3/12/14	-
1	OMG	1A	2251	1,57,55	-	0/5/27/28	0/3/3/3
1	OMC	1A	1920	1	-	1/7/27/28	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
1	5MC	1A	1962	1,57	-	2/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	8AN	1x	76	57,55,56	-	3/3/25/26	0/3/3/3
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
1	5MC	2A	1962	1,57	-	2/5/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	1/3/25/26	0/3/3/3
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
32	G7M	2a	527	57,32	-	2/3/25/26	0/3/3/3
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
54	PPU	1w	76	54,1	-	3/21/43/44	0/4/4/4
54	PPU	2w	76	54,1	-	2/21/43/44	0/4/4/4
32	M2G	2a	966	57,32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/5/25/26	0/2/2/2
32	5MC	2a	1400	32	-	4/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	3/9/29/30	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	57,32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
1	OMG	2A	2251	1,57,55	-	1/5/27/28	0/3/3/3
1	OMU	2A	2552	1,57	-	0/7/27/28	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
1	5MC	1A	1942	1,57	-	0/5/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
43	0TD	1l	92	43	-	1/3/12/14	-
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-5.87	1.69	1.84
43	1l	92	0TD	CB-SB	-5.84	1.70	1.84
32	2a	967	5MC	C5-C4	5.12	1.49	1.41
32	1a	527	G7M	C5-C4	5.08	1.46	1.39
1	2A	1942	5MC	C5-C4	5.05	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1404	5MC	C5-C4	5.04	1.49	1.41
32	1a	1400	5MC	C5-C4	4.92	1.49	1.41
32	1a	1404	5MC	C5-C4	4.86	1.48	1.41
32	2a	1407	5MC	C5-C4	4.82	1.48	1.41
32	1a	1407	5MC	C5-C4	4.80	1.48	1.41
1	2A	2503	2MA	C5-C6	4.78	1.48	1.41
32	2a	1400	5MC	C5-C4	4.74	1.48	1.41
32	2a	527	G7M	C5-C4	4.69	1.46	1.39
1	2A	2605	PSU	C5-C1'	-4.68	1.48	1.52
32	1a	967	5MC	C5-C4	4.55	1.48	1.41
1	1A	1962	5MC	C5-C4	4.52	1.48	1.41
32	2a	966	M2G	C5-C6	4.52	1.49	1.41
32	2a	1207	2MG	C5-C6	4.49	1.49	1.41
1	1A	1942	5MC	C5-C4	4.46	1.48	1.41
32	2a	516	PSU	C5-C1'	-4.43	1.48	1.52
1	1A	1917	PSU	C5-C1'	-4.26	1.48	1.52
32	1a	966	M2G	C5-C6	4.26	1.48	1.41
32	1a	1207	2MG	C5-C6	4.17	1.48	1.41
1	2A	1962	5MC	C5-C4	4.17	1.47	1.41
32	2a	527	G7M	C5-C6	4.11	1.48	1.41
1	2A	1939	5MU	C5-C4	4.08	1.50	1.41
1	1A	2251	OMG	C5-C6	4.04	1.48	1.41
1	2A	1911	PSU	C5-C1'	-4.03	1.48	1.52
32	1a	527	G7M	C5-C6	3.80	1.47	1.41
1	2A	1917	PSU	C5-C1'	-3.79	1.49	1.52
1	1A	2605	PSU	C5-C1'	-3.78	1.49	1.52
1	2A	2251	OMG	C5-C6	3.68	1.47	1.41
1	1A	1939	5MU	C5-C4	3.65	1.49	1.41
32	2a	516	PSU	C5-C4	3.62	1.49	1.41
1	2A	1917	PSU	C5-C4	3.60	1.49	1.41
1	1A	2503	2MA	C5-C6	3.58	1.46	1.41
1	2A	1911	PSU	C5-C4	3.58	1.49	1.41
32	1a	966	M2G	C2-N2	3.56	1.40	1.34
1	1A	2605	PSU	C5-C4	3.44	1.48	1.41
32	1a	516	PSU	C5-C4	3.43	1.48	1.41
32	2a	966	M2G	C2-N2	3.41	1.40	1.34
1	1A	1911	PSU	C5-C4	3.41	1.48	1.41
1	2A	2605	PSU	C5-C4	3.36	1.48	1.41
1	1A	1917	PSU	C5-C4	3.31	1.48	1.41
1	1A	1911	PSU	C5-C1'	-3.31	1.49	1.52
1	1A	1915	5MU	C5-C4	3.30	1.48	1.41
1	2A	1915	5MU	C5-C4	3.10	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	516	PSU	C5-C1'	-3.01	1.49	1.52
55	2x	76	8AN	C5-C4	-2.67	1.33	1.40
32	2a	966	M2G	C5-C4	2.67	1.48	1.40
54	2w	76	PPU	C5-C4	2.64	1.47	1.40
32	1a	966	M2G	C5-C4	2.58	1.47	1.40
55	2x	76	8AN	C6-C5	-2.50	1.34	1.43
55	1x	76	8AN	C6-C5	-2.50	1.34	1.43
1	2A	2251	OMG	C5-C4	2.48	1.47	1.40
32	2a	1207	2MG	C5-C4	2.47	1.47	1.40
55	1x	76	8AN	C5-C4	-2.45	1.34	1.40
54	1w	76	PPU	C5-C4	2.40	1.47	1.40
32	1a	1207	2MG	C5-C4	2.39	1.47	1.40
1	1A	2605	PSU	C2-N3	-2.36	1.33	1.38
55	1x	76	8AN	O4'-C1'	2.33	1.44	1.41
55	1x	76	8AN	C5-N7	-2.30	1.31	1.39
1	2A	2503	2MA	C5-C4	2.26	1.46	1.40
1	1A	1939	5MU	C2-N3	-2.23	1.33	1.38
55	2x	76	8AN	C5-N7	-2.22	1.31	1.39
1	2A	1917	PSU	C2-N1	-2.21	1.33	1.38
32	1a	516	PSU	O4'-C1'	-2.15	1.41	1.44
1	2A	2605	PSU	C2-N3	-2.15	1.33	1.38
1	1A	2605	PSU	C2-N1	-2.14	1.33	1.38
32	2a	516	PSU	O4'-C1'	-2.14	1.41	1.44
1	1A	2251	OMG	C5-C4	2.10	1.46	1.40
32	2a	1498	UR3	C4-N3	2.09	1.41	1.38
1	1A	2503	2MA	C5-C4	2.08	1.46	1.40
54	2w	76	PPU	C2-N3	2.02	1.35	1.32

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-14.12	74.08	101.85
32	1a	516	PSU	N3-C2-N1	-9.20	121.12	128.43
1	2A	2605	PSU	N3-C2-N1	-9.14	121.16	128.43
1	2A	1917	PSU	N3-C2-N1	-8.72	121.50	128.43
1	1A	1917	PSU	N3-C2-N1	-8.71	121.51	128.43
1	2A	1911	PSU	N3-C2-N1	-8.33	121.80	128.43
1	1A	1911	PSU	N3-C2-N1	-8.29	121.84	128.43
32	2a	516	PSU	N3-C2-N1	-8.16	121.94	128.43
1	1A	2605	PSU	N3-C2-N1	-8.09	122.00	128.43
1	1A	1915	5MU	C2-N3-C4	7.72	121.66	115.14
1	2A	1917	PSU	C2-N3-C4	7.56	121.52	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1915	5MU	C2-N3-C4	7.46	121.44	115.14
1	1A	1917	PSU	C2-N3-C4	6.80	120.89	115.14
1	1A	1911	PSU	C2-N3-C4	6.79	120.88	115.14
1	2A	1911	PSU	C2-N3-C4	6.75	120.84	115.14
1	2A	2503	2MA	C2-N3-C4	6.70	120.97	115.52
32	1a	516	PSU	C2-N3-C4	6.68	120.78	115.14
32	2a	516	PSU	C2-N3-C4	6.47	120.60	115.14
1	2A	2605	PSU	C2-N3-C4	6.34	120.50	115.14
1	2A	1939	5MU	C2-N3-C4	6.04	120.24	115.14
1	1A	1939	5MU	C2-N3-C4	5.79	120.03	115.14
1	1A	2605	PSU	C2-N3-C4	5.76	120.01	115.14
43	1l	92	0TD	CSB-SB-CB	-5.75	90.54	101.85
1	2A	1917	PSU	C5-C4-N3	-5.73	117.98	125.36
1	1A	2503	2MA	C2-N3-C4	5.72	120.17	115.52
55	2x	76	8AN	N3-C2-N1	-5.69	119.78	128.68
55	1x	76	8AN	N3-C2-N1	-5.64	119.86	128.68
32	2a	516	PSU	C5-C4-N3	-5.59	118.16	125.36
32	2a	527	G7M	C5-C6-N1	-5.57	115.81	123.43
32	1a	527	G7M	C5-C6-N1	-5.52	115.89	123.43
32	1a	966	M2G	C2-N1-C6	5.41	122.63	116.18
32	2a	966	M2G	C2-N1-C6	5.39	122.59	116.18
1	1A	1911	PSU	C5-C4-N3	-5.19	118.67	125.36
1	1A	1917	PSU	C5-C4-N3	-5.17	118.70	125.36
1	2A	1911	PSU	C5-C4-N3	-5.17	118.71	125.36
1	2A	2251	OMG	C2-N3-C4	5.14	121.23	115.36
32	1a	966	M2G	C2-N3-C4	5.03	120.98	115.28
1	1A	2251	OMG	C2-N3-C4	5.02	121.10	115.36
32	1a	516	PSU	C5-C4-N3	-4.97	118.96	125.36
32	2a	1519	MA6	N3-C2-N1	-4.82	121.14	128.68
1	2A	2605	PSU	C5-C1'-C2'	-4.77	106.80	115.32
1	1A	1920	OMC	C4-N3-C2	4.77	121.18	116.34
32	2a	966	M2G	C2-N3-C4	4.71	120.62	115.28
1	2A	2605	PSU	C6-N1-C2	4.67	123.06	115.36
1	2A	2605	PSU	C5-C6-N1	-4.66	118.71	124.44
1	2A	2503	2MA	C5-C6-N1	-4.64	118.19	123.06
32	2a	1518	MA6	N3-C2-N1	-4.64	121.43	128.68
32	2a	1207	2MG	C5-C6-N1	-4.63	117.09	123.43
32	1a	1518	MA6	N3-C2-N1	-4.63	121.44	128.68
32	1a	527	G7M	C2-N1-C6	4.61	123.26	115.93
32	1a	1207	2MG	C2-N3-C4	4.57	120.47	115.28
32	1a	516	PSU	C6-N1-C2	4.56	122.88	115.36
1	2A	2605	PSU	C5-C4-N3	-4.55	119.50	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	G7M	C2-N1-C6	4.52	123.12	115.93
1	1A	2605	PSU	C5-C4-N3	-4.51	119.55	125.36
32	2a	516	PSU	C5-C6-N1	-4.50	118.91	124.44
32	1a	1207	2MG	C2-N1-C6	4.50	123.24	115.18
32	2a	966	M2G	C5-C6-N1	-4.49	117.30	123.43
1	1A	2605	PSU	C6-N1-C2	4.48	122.74	115.36
32	1a	1207	2MG	C5-C6-N1	-4.45	117.34	123.43
1	1A	2605	PSU	C5-C6-N1	-4.45	118.97	124.44
1	1A	2503	2MA	C5-C6-N1	-4.45	118.40	123.06
32	1a	1519	MA6	N3-C2-N1	-4.44	121.73	128.68
1	1A	2605	PSU	C5-C1'-C2'	-4.38	107.51	115.32
32	2a	1207	2MG	C2-N3-C4	4.35	120.21	115.28
32	1a	1207	2MG	C4-C5-C6	-4.31	116.69	120.80
32	2a	516	PSU	C6-N1-C2	4.24	122.35	115.36
32	2a	1402	4OC	CM4-N4-C4	-4.23	119.33	122.97
32	1a	516	PSU	C5-C6-N1	-4.20	119.28	124.44
32	2a	1207	2MG	C2-N1-C6	4.11	122.55	115.18
1	1A	1917	PSU	C6-N1-C2	4.10	122.13	115.36
1	2A	1920	OMC	C4-N3-C2	4.05	120.45	116.34
1	2A	1911	PSU	C6-N1-C2	4.04	122.03	115.36
1	1A	2251	OMG	C2-N1-C6	4.00	122.28	115.93
1	1A	1917	PSU	C5-C6-N1	-3.99	119.53	124.44
1	2A	2251	OMG	C5-C6-N1	-3.96	118.02	123.43
32	1a	966	M2G	C5-C6-N1	-3.94	118.05	123.43
1	1A	1911	PSU	C6-N1-C2	3.91	121.81	115.36
1	2A	1911	PSU	C5-C6-N1	-3.90	119.64	124.44
32	2a	967	5MC	C4-N3-C2	3.89	120.71	116.02
32	2a	527	G7M	C2-N3-C4	3.88	119.79	115.36
32	2a	1407	5MC	C4-N3-C2	3.88	120.70	116.02
1	1A	2251	OMG	C5-C6-N1	-3.88	118.13	123.43
32	1a	966	M2G	C4-C5-C6	-3.87	117.11	120.80
1	2A	2251	OMG	C2-N1-C6	3.85	122.05	115.93
1	1A	1962	5MC	C4-N3-C2	3.85	120.66	116.02
32	1a	967	5MC	C4-N3-C2	3.80	120.60	116.02
1	2A	1962	5MC	N4-C4-N3	3.79	122.40	117.03
1	2A	1917	PSU	C6-N1-C2	3.76	121.57	115.36
32	2a	966	M2G	C4-C5-C6	-3.76	117.21	120.80
1	1A	1917	PSU	C5-C1'-C2'	-3.75	108.63	115.32
32	2a	1207	2MG	C4-C5-C6	-3.74	117.22	120.80
1	2A	1911	PSU	C5-C1'-C2'	-3.74	108.65	115.32
32	2a	1404	5MC	C4-N3-C2	3.72	120.50	116.02
1	1A	1911	PSU	C5-C6-N1	-3.71	119.88	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	76	PPU	N1-C6-N6	3.69	120.94	117.06
32	1a	527	G7M	C2-N3-C4	3.69	119.57	115.36
1	1A	2251	OMG	C4-C5-C6	-3.64	117.32	120.80
1	1A	1939	5MU	C5-C6-N1	-3.61	118.30	122.19
1	2A	1942	5MC	C5-C6-N1	-3.59	118.32	122.19
32	2a	1207	2MG	CM2-N2-C2	-3.55	119.31	123.59
1	2A	1962	5MC	C4-N3-C2	3.53	120.28	116.02
1	1A	2251	OMG	N3-C2-N1	-3.46	122.61	127.22
32	1a	1407	5MC	C4-N3-C2	3.45	120.19	116.02
32	1a	1402	4OC	CM4-N4-C4	-3.45	120.00	122.97
54	1w	76	PPU	N3-C2-N1	-3.44	123.30	128.68
32	1a	1400	5MC	C4-N3-C2	3.41	120.14	116.02
32	1a	1404	5MC	C4-N3-C2	3.40	120.12	116.02
54	2w	76	PPU	N1-C6-N6	3.38	120.61	117.06
1	2A	2251	OMG	N3-C2-N1	-3.37	122.72	127.22
54	1w	76	PPU	C3'-N3'-C	-3.34	118.17	123.21
1	2A	2503	2MA	C4-C5-N7	-3.30	105.96	109.40
32	2a	1519	MA6	C4-C5-N7	-3.28	105.98	109.40
32	1a	1519	MA6	C4-C5-N7	-3.22	106.04	109.40
54	2w	76	PPU	C4-C5-N7	-3.22	106.04	109.40
32	1a	1400	5MC	C5-C6-N1	-3.17	118.78	122.19
1	1A	2251	OMG	C4-C5-N7	-3.14	106.12	109.40
32	2a	1207	2MG	C4-C5-N7	-3.05	106.22	109.40
1	1A	1942	5MC	C4-N3-C2	3.05	119.70	116.02
32	2a	1400	5MC	C4-N3-C2	3.01	119.66	116.02
32	2a	966	M2G	C4-C5-N7	-2.99	106.28	109.40
1	2A	2251	OMG	C4-C5-C6	-2.98	117.96	120.80
32	1a	1207	2MG	C4-C5-N7	-2.94	106.33	109.40
32	1a	1207	2MG	CM2-N2-C2	-2.93	120.05	123.59
54	2w	76	PPU	N3-C2-N1	-2.91	124.13	128.68
32	2a	1518	MA6	C4-C5-N7	-2.90	106.38	109.40
54	1w	76	PPU	C4-C5-N7	-2.89	106.39	109.40
1	2A	1917	PSU	C5-C6-N1	-2.89	120.89	124.44
1	2A	1942	5MC	C4-N3-C2	2.88	119.50	116.02
32	1a	527	G7M	N3-C2-N1	-2.87	123.39	127.22
32	2a	527	G7M	N3-C2-N1	-2.83	123.45	127.22
1	1A	1942	5MC	N4-C4-N3	2.72	120.88	117.03
1	1A	1942	5MC	C5-C6-N1	-2.71	119.27	122.19
32	2a	1207	2MG	N2-C2-N1	2.70	119.55	116.96
32	1a	966	M2G	C4-C5-N7	-2.69	106.60	109.40
32	1a	967	5MC	N4-C4-N3	2.66	120.79	117.03
32	2a	1400	5MC	N4-C4-N3	2.65	120.77	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1404	5MC	N4-C4-N3	2.62	120.73	117.03
32	2a	1400	5MC	C5-C6-N1	-2.61	119.38	122.19
32	1a	1207	2MG	N2-C2-N1	2.56	119.42	116.96
32	1a	1207	2MG	C1'-N9-C4	-2.54	122.18	126.64
32	2a	966	M2G	N1-C2-N2	2.52	119.74	117.19
32	1a	1400	5MC	N4-C4-N3	2.48	120.53	117.03
1	1A	1962	5MC	N4-C4-N3	2.47	120.53	117.03
1	2A	1962	5MC	CM5-C5-C4	-2.47	119.22	121.72
32	2a	1407	5MC	N4-C4-N3	2.44	120.49	117.03
54	2w	76	PPU	CG-CB-CA	-2.42	109.09	114.13
1	1A	1911	PSU	C5-C1'-C2'	-2.41	111.02	115.32
1	2A	1942	5MC	N4-C4-N3	2.39	120.41	117.03
1	2A	1939	5MU	C5-C6-N1	-2.38	119.63	122.19
32	1a	1207	2MG	N3-C2-N1	-2.35	122.52	126.23
32	1a	1518	MA6	C4-C5-N7	-2.33	106.97	109.40
1	2A	1962	5MC	C5-C6-N1	-2.32	119.70	122.19
32	2a	516	PSU	C5-C1'-C2'	-2.31	111.21	115.32
54	2w	76	PPU	C3'-N3'-C	-2.30	119.75	123.21
1	1A	2552	OMU	C5-C4-N3	-2.28	118.29	123.31
1	2A	1917	PSU	C1'-C5-C4	2.26	125.38	121.12
1	2A	2552	OMU	C5-C4-N3	-2.25	118.35	123.31
32	1a	516	PSU	O4'-C1'-C2'	2.25	108.31	104.66
1	1A	1920	OMC	N4-C4-N3	2.25	120.04	116.49
55	1x	76	8AN	O4'-C1'-C2'	-2.24	103.65	106.93
54	1w	76	PPU	C10-N6-C6	-2.24	112.72	119.51
32	1a	1207	2MG	O3'-C3'-C2'	2.22	119.00	111.82
32	1a	1404	5MC	C5-C6-N1	-2.19	119.83	122.19
32	1a	1407	5MC	C5-C6-N1	-2.18	119.84	122.19
32	1a	967	5MC	C5-C6-N1	-2.15	119.88	122.19
1	1A	1915	5MU	C6-N1-C1'	-2.14	114.44	119.24
1	2A	2251	OMG	C4-C5-N7	-2.12	107.19	109.40
1	2A	1920	OMC	N4-C4-N3	2.11	119.82	116.49
32	1a	966	M2G	N3-C2-N2	2.10	119.31	117.18
32	2a	1404	5MC	C5-C6-N1	-2.08	119.95	122.19
1	1A	1911	PSU	O4'-C1'-C2'	2.06	108.00	104.66
55	2x	76	8AN	O4'-C1'-C2'	-2.06	103.92	106.93
32	1a	527	G7M	C4-C5-C6	-2.06	118.83	120.80
32	1a	1407	5MC	N4-C4-N3	2.05	119.94	117.03
32	2a	967	5MC	C5-C6-N1	-2.05	119.99	122.19
32	2a	516	PSU	O4'-C1'-C2'	2.04	107.97	104.66
32	2a	1498	UR3	C3U-N3-C4	2.04	120.82	118.12
54	2w	76	PPU	O4'-C4'-C3'	2.03	106.98	104.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1402	4OC	C5-C4-N3	-2.02	119.76	123.16
32	1a	1404	5MC	N4-C4-N3	2.01	119.88	117.03
32	2a	527	G7M	C4-C5-C6	-2.01	118.88	120.80

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1920	OMC	C2'-C1'-N1-C6
1	1A	1939	5MU	O4'-C1'-N1-C6
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
1	2A	1920	OMC	C2'-C1'-N1-C6
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6
32	2a	1402	4OC	C5-C4-N4-CM4
55	1x	76	8AN	C3'-C4'-C5'-O5'
55	2x	76	8AN	C3'-C4'-C5'-O5'
54	2w	76	PPU	C3'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'
54	2w	76	PPU	O4'-C4'-C5'-O5'
55	2x	76	8AN	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
55	1x	76	8AN	O4'-C4'-C5'-O5'
55	1x	76	8AN	C4'-C5'-O5'-P
55	2x	76	8AN	C4'-C5'-O5'-P
32	2a	1402	4OC	N3-C4-N4-CM4
54	1w	76	PPU	N-CA-CB-CG
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
32	1a	1402	4OC	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
1	2A	1917	PSU	C2'-C1'-C5-C6
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	1a	516	PSU	O4'-C4'-C5'-O5'
32	1a	1207	2MG	C3'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
1	1A	2503	2MA	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	1w	76	PPU	O-C-N3'-C3'
54	1w	76	PPU	C2'-C3'-N3'-C

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 2521 ligands modelled in this entry, 2510 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	MPD	18	104	-	7,7,7	0.33	0	9,10,10	0.53	0
59	ARG	1B	231	57	7,11,11	0.25	0	6,13,13	0.52	0
58	MPD	1a	3276	-	7,7,7	0.36	0	9,10,10	0.41	0
58	MPD	1A	4023	-	7,7,7	0.26	0	9,10,10	0.40	0
58	MPD	2A	3735	-	7,7,7	0.27	0	9,10,10	0.27	0
58	MPD	2B	220	-	7,7,7	0.33	0	9,10,10	0.32	0
61	SF4	1d	307	35	0,12,12	-	-	-	-	-
61	SF4	2d	501	35	0,12,12	-	-	-	-	-
59	ARG	1F	317	57	7,11,11	0.25	0	6,13,13	0.28	0
58	MPD	1a	3275	-	7,7,7	0.27	0	9,10,10	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	MPD	2A	3734	-	7,7,7	0.30	0	9,10,10	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	MPD	18	104	-	-	0/5/5/5	-
59	ARG	1B	231	57	-	1/7/11/11	-
58	MPD	1a	3276	-	-	3/5/5/5	-
58	MPD	1A	4023	-	-	0/5/5/5	-
58	MPD	2A	3735	-	-	4/5/5/5	-
58	MPD	2B	220	-	-	0/5/5/5	-
61	SF4	1d	307	35	-	-	0/6/5/5
61	SF4	2d	501	35	-	-	0/6/5/5
59	ARG	1F	317	57	-	0/7/11/11	-
58	MPD	1a	3275	-	-	1/5/5/5	-
58	MPD	2A	3734	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1a	3276	MPD	C2-C3-C4-O4
58	2A	3735	MPD	O2-C2-C3-C4
59	1B	231	ARG	CA-CB-CG-CD
58	1a	3276	MPD	CM-C2-C3-C4
58	2A	3735	MPD	C1-C2-C3-C4
58	2A	3735	MPD	CM-C2-C3-C4
58	1a	3276	MPD	O2-C2-C3-C4
58	2A	3734	MPD	O2-C2-C3-C4
58	1a	3275	MPD	C2-C3-C4-C5
58	2A	3735	MPD	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	2861/2915 (98%)	0.28	48 (1%) 70 72	19, 36, 84, 98	0
1	2A	2856/2915 (97%)	0.12	64 (2%) 62 65	33, 55, 87, 99	0
2	1B	120/121 (99%)	-0.03	0 100 100	29, 47, 61, 78	0
2	2B	120/121 (99%)	-0.22	0 100 100	57, 71, 79, 84	0
3	1D	275/276 (99%)	0.59	4 (1%) 73 75	22, 36, 51, 61	0
3	2D	275/276 (99%)	0.70	13 (4%) 31 33	29, 50, 61, 74	0
4	1E	204/206 (99%)	0.51	0 100 100	20, 40, 58, 70	0
4	2E	204/206 (99%)	0.47	6 (2%) 51 55	31, 53, 68, 76	0
5	1F	203/210 (96%)	0.43	0 100 100	19, 41, 64, 77	0
5	2F	203/210 (96%)	0.46	3 (1%) 73 75	33, 62, 74, 79	0
6	1G	181/182 (99%)	0.32	4 (2%) 62 65	43, 59, 71, 78	0
6	2G	181/182 (99%)	0.93	29 (16%) 1 1	64, 74, 79, 83	0
7	1H	174/180 (96%)	0.38	2 (1%) 80 82	38, 51, 62, 66	0
7	2H	173/180 (96%)	0.83	18 (10%) 6 6	65, 72, 77, 84	0
8	1I	147/148 (99%)	0.25	3 (2%) 65 68	43, 67, 74, 77	0
8	2I	146/148 (98%)	0.49	17 (11%) 4 4	57, 70, 78, 80	0
9	1N	140/140 (100%)	0.53	0 100 100	23, 38, 56, 67	0
9	2N	140/140 (100%)	0.54	2 (1%) 75 77	43, 60, 71, 75	0
10	1O	122/122 (100%)	0.46	0 100 100	29, 40, 58, 68	0
10	2O	122/122 (100%)	0.42	3 (2%) 57 61	41, 53, 65, 68	0
11	1P	149/150 (99%)	0.44	0 100 100	19, 45, 64, 71	0
11	2P	149/150 (99%)	0.59	8 (5%) 25 27	37, 61, 74, 82	0
12	1Q	141/141 (100%)	0.55	0 100 100	25, 39, 52, 60	0
12	2Q	141/141 (100%)	0.82	13 (9%) 9 9	45, 60, 68, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.53	0 100 100	25, 35, 47, 60	0
13	2R	118/118 (100%)	0.62	3 (2%) 57 61	38, 50, 60, 67	0
14	1S	110/112 (98%)	0.32	0 100 100	35, 48, 58, 63	0
14	2S	110/112 (98%)	0.70	10 (9%) 9 9	60, 67, 73, 74	0
15	1T	131/146 (89%)	0.34	1 (0%) 86 87	31, 45, 62, 73	0
15	2T	131/146 (89%)	0.35	2 (1%) 73 75	45, 55, 69, 75	0
16	1U	116/118 (98%)	0.57	0 100 100	21, 29, 46, 59	0
16	2U	116/118 (98%)	0.73	9 (7%) 13 13	38, 56, 68, 71	0
17	1V	101/101 (100%)	0.45	0 100 100	20, 42, 56, 64	0
17	2V	101/101 (100%)	0.49	7 (6%) 16 17	40, 63, 70, 74	0
18	1W	112/113 (99%)	0.55	1 (0%) 84 86	23, 33, 50, 74	0
18	2W	112/113 (99%)	0.66	3 (2%) 54 58	37, 48, 62, 80	0
19	1X	95/96 (98%)	0.55	1 (1%) 80 82	25, 36, 57, 71	0
19	2X	95/96 (98%)	0.78	5 (5%) 26 28	48, 57, 68, 75	0
20	1Y	107/110 (97%)	0.45	2 (1%) 66 69	36, 47, 61, 71	0
20	2Y	107/110 (97%)	0.67	7 (6%) 18 19	56, 65, 72, 73	0
21	1Z	203/206 (98%)	0.30	3 (1%) 73 75	37, 55, 67, 76	0
21	2Z	201/206 (97%)	0.43	8 (3%) 38 41	60, 70, 76, 81	0
22	10	83/85 (97%)	0.57	1 (1%) 79 80	26, 35, 50, 56	0
22	20	83/85 (97%)	1.14	15 (18%) 1 1	41, 57, 66, 70	0
23	11	97/98 (98%)	0.83	5 (5%) 27 29	28, 43, 61, 68	0
23	21	97/98 (98%)	0.84	9 (9%) 8 8	38, 54, 69, 73	0
24	12	70/72 (97%)	0.31	0 100 100	36, 47, 57, 73	0
24	22	70/72 (97%)	0.24	1 (1%) 75 77	56, 63, 68, 70	0
25	13	59/60 (98%)	0.41	0 100 100	26, 36, 59, 65	0
25	23	59/60 (98%)	0.87	5 (8%) 10 10	48, 58, 69, 75	0
26	14	69/71 (97%)	0.51	7 (10%) 7 6	50, 70, 81, 84	0
26	24	69/71 (97%)	1.17	15 (21%) 0 0	73, 79, 86, 89	0
27	15	59/60 (98%)	0.54	2 (3%) 45 48	20, 34, 49, 59	0
27	25	59/60 (98%)	0.47	1 (1%) 70 72	34, 49, 63, 69	0
28	16	53/54 (98%)	0.35	0 100 100	31, 41, 52, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.33	1 (1%) 66 69	48, 56, 65, 66	0
29	17	48/49 (97%)	0.70	2 (4%) 36 39	20, 28, 47, 52	0
29	27	48/49 (97%)	0.69	4 (8%) 11 11	32, 41, 57, 65	0
30	18	64/65 (98%)	0.61	0 100 100	25, 34, 40, 51	0
30	28	64/65 (98%)	1.01	8 (12%) 3 3	45, 51, 58, 64	0
31	19	37/37 (100%)	0.66	1 (2%) 54 58	28, 39, 54, 59	0
31	29	37/37 (100%)	1.30	4 (10%) 5 5	51, 61, 68, 71	0
32	1a	1488/1521 (97%)	0.03	19 (1%) 77 79	35, 64, 84, 98	0
32	2a	1492/1521 (98%)	0.12	35 (2%) 60 63	48, 71, 86, 97	0
33	1b	231/256 (90%)	0.63	20 (8%) 10 10	60, 71, 79, 84	0
33	2b	231/256 (90%)	0.88	38 (16%) 1 1	64, 76, 81, 84	0
34	1c	206/239 (86%)	0.93	33 (16%) 1 1	56, 67, 74, 82	0
34	2c	206/239 (86%)	1.31	49 (23%) 0 0	66, 76, 81, 84	0
35	1d	208/209 (99%)	0.64	12 (5%) 23 24	52, 65, 74, 82	0
35	2d	208/209 (99%)	1.04	37 (17%) 1 1	56, 67, 73, 78	0
36	1e	148/162 (91%)	0.58	6 (4%) 37 40	48, 62, 69, 76	0
36	2e	148/162 (91%)	0.84	17 (11%) 4 4	55, 68, 74, 82	0
37	1f	100/101 (99%)	0.26	2 (2%) 65 68	50, 60, 70, 72	0
37	2f	100/101 (99%)	0.20	0 100 100	56, 66, 72, 78	0
38	1g	155/156 (99%)	0.37	5 (3%) 47 51	55, 66, 71, 76	0
38	2g	155/156 (99%)	1.01	36 (23%) 0 0	66, 74, 79, 81	0
39	1h	137/138 (99%)	0.61	10 (7%) 15 15	50, 63, 69, 71	0
39	2h	137/138 (99%)	0.87	13 (9%) 8 8	62, 68, 74, 77	0
40	1i	127/128 (99%)	1.44	39 (30%) 0 0	55, 70, 76, 79	0
40	2i	126/128 (98%)	2.94	85 (67%) 0 0	69, 77, 82, 87	0
41	1j	97/105 (92%)	1.20	24 (24%) 0 0	56, 69, 79, 81	0
41	2j	96/105 (91%)	2.09	33 (34%) 0 0	68, 77, 81, 85	0
42	1k	114/129 (88%)	0.39	3 (2%) 56 59	44, 60, 68, 73	0
42	2k	114/129 (88%)	1.02	15 (13%) 3 3	57, 68, 75, 77	0
43	1l	121/132 (91%)	0.56	6 (4%) 28 30	48, 57, 68, 72	0
43	2l	121/132 (91%)	0.68	12 (9%) 7 7	54, 62, 68, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.73	12 (10%) 6 6	56, 67, 74, 79	0
44	2m	114/126 (90%)	1.33	31 (27%) 0 0	69, 76, 80, 81	0
45	1n	60/61 (98%)	2.22	33 (55%) 0 0	56, 65, 71, 72	0
45	2n	60/61 (98%)	2.91	40 (66%) 0 0	69, 75, 80, 85	0
46	1o	88/89 (98%)	0.53	2 (2%) 60 63	45, 60, 70, 75	0
46	2o	88/89 (98%)	0.59	3 (3%) 45 48	56, 66, 74, 77	0
47	1p	82/88 (93%)	1.24	16 (19%) 1 1	60, 66, 75, 83	0
47	2p	82/88 (93%)	1.01	11 (13%) 3 2	57, 66, 72, 79	0
48	1q	99/105 (94%)	0.82	6 (6%) 21 22	51, 62, 69, 74	0
48	2q	99/105 (94%)	0.69	9 (9%) 9 9	57, 65, 73, 75	0
49	1r	68/88 (77%)	0.45	2 (2%) 51 55	52, 59, 72, 76	0
49	2r	68/88 (77%)	0.78	4 (5%) 22 23	62, 70, 76, 80	0
50	1s	83/93 (89%)	0.71	6 (7%) 15 16	57, 68, 75, 79	0
50	2s	83/93 (89%)	1.63	31 (37%) 0 0	70, 77, 82, 84	0
51	1t	96/106 (90%)	1.12	22 (22%) 0 0	57, 65, 73, 74	0
51	2t	98/106 (92%)	0.85	8 (8%) 11 11	54, 65, 74, 78	0
52	1u	23/27 (85%)	2.40	16 (69%) 0 0	61, 67, 71, 73	0
52	2u	23/27 (85%)	2.59	13 (56%) 0 0	72, 75, 79, 80	0
53	1y	97/113 (85%)	0.72	9 (9%) 8 8	46, 59, 68, 79	0
53	2y	96/113 (84%)	3.64	78 (81%) 0 0	69, 78, 83, 91	0
54	1w	3/4 (75%)	-0.06	0 100 100	36, 36, 42, 43	0
54	2w	3/4 (75%)	-0.23	0 100 100	49, 49, 52, 64	0
55	1x	3/4 (75%)	-0.17	0 100 100	36, 36, 37, 48	0
55	2x	3/4 (75%)	0.65	0 100 100	49, 49, 54, 65	0
56	1v	3/3 (100%)	1.56	1 (33%) 0 0	32, 32, 32, 38	0
56	2v	3/3 (100%)	2.98	3 (100%) 0 0	48, 48, 54, 60	0
All	All	20796/21490 (96%)	0.49	1285 (6%) 20 21	19, 60, 80, 99	0

All (1285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
53	2y	88	LEU	8.6
53	2y	12	ILE	8.1

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Mol	Chain	Res	Type	RSRZ
45	2n	61	TRP	8.1
40	2i	115	GLY	8.0
1	1A	1076	C	7.7
53	2y	50	ALA	7.5
41	2j	65	LEU	7.3
40	2i	109	VAL	7.3
53	2y	40	ILE	7.3
40	2i	75	ASP	7.2
42	2k	98	LEU	7.2
40	1i	46	ALA	7.2
1	1A	1087	G	7.1
41	2j	96	ILE	7.1
50	2s	9	VAL	7.1
45	2n	13	THR	6.9
53	2y	10	MET	6.9
53	2y	78	ILE	6.9
41	2j	67	THR	6.8
32	2a	1030(A)	G	6.7
40	2i	76	ALA	6.7
53	2y	3	MET	6.6
40	2i	7	THR	6.5
39	2h	2	LEU	6.5
40	2i	63	ILE	6.5
45	2n	34	TYR	6.5
53	2y	39	ILE	6.4
53	2y	41	LEU	6.3
33	2b	123	ALA	6.2
40	2i	71	SER	6.2
53	2y	5	ILE	6.2
53	2y	51	ASP	6.1
41	2j	47	PHE	6.1
53	2y	74	ILE	6.1
53	2y	77	LEU	6.1
1	2A	2138	C	6.0
53	2y	63	ALA	6.0
40	2i	40	LEU	6.0
1	2A	2140	C	5.9
32	2a	1030(B)	C	5.9
53	2y	49	VAL	5.8
40	2i	56	LEU	5.7
53	2y	80	LYS	5.7
8	2I	3	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2142	C	5.6
45	2n	25	VAL	5.6
41	2j	44	VAL	5.6
1	2A	2146	C	5.6
41	2j	46	ARG	5.4
23	2l	2	SER	5.4
45	1n	25	VAL	5.4
34	2c	33	LEU	5.4
53	2y	52	ALA	5.3
1	2A	1067	A	5.3
52	2u	2	GLY	5.3
6	2G	57	ALA	5.3
19	2X	92	LEU	5.3
53	2y	58	ASN	5.3
40	2i	92	TYR	5.3
53	1y	98	ALA	5.3
53	2y	8	LYS	5.3
40	2i	66	ARG	5.2
1	2A	2169	A	5.2
53	2y	73	ALA	5.2
40	2i	72	GLY	5.2
52	2u	14	TRP	5.2
53	2y	7	SER	5.1
26	24	56	VAL	5.1
32	1a	1036	G	5.1
40	2i	47	LEU	5.1
40	2i	33	PHE	5.1
32	2a	1030	C	5.1
6	2G	39	ILE	5.1
38	1g	16	LEU	5.0
41	2j	34	VAL	5.0
23	1l	2	SER	5.0
40	2i	18	PHE	5.0
1	1A	1068	G	5.0
53	2y	48	PHE	5.0
53	2y	4	ASN	5.0
40	2i	91	ASP	5.0
40	2i	74	ILE	5.0
40	2i	69	GLY	5.0
1	1A	2116	G	4.9
32	2a	1036	G	4.9
41	1j	49	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
41	2j	54	PHE	4.9
52	2u	13	ILE	4.9
6	1G	48	GLU	4.9
26	24	49	PHE	4.9
36	2e	13	ILE	4.9
53	2y	9	GLN	4.9
41	2j	38	ILE	4.9
32	2a	1257	U	4.8
41	2j	45	ARG	4.8
19	2X	68	ARG	4.8
53	2y	42	SER	4.8
40	1i	126	SER	4.8
34	2c	160	ALA	4.8
1	1A	1064	C	4.8
26	14	59	PHE	4.8
32	1a	1030(B)	C	4.8
33	2b	122	PHE	4.8
38	2g	154	TYR	4.8
6	2G	133	LEU	4.8
50	2s	49	ILE	4.8
53	2y	87	LYS	4.7
34	2c	163	ALA	4.7
33	2b	118	LEU	4.7
40	2i	10	ARG	4.7
53	2y	79	ASN	4.7
45	2n	2	ALA	4.7
51	1t	76	ALA	4.7
41	2j	16	LEU	4.7
34	2c	159	GLY	4.7
48	2q	98	LEU	4.7
53	2y	81	LEU	4.7
45	1n	18	VAL	4.7
52	2u	15	ARG	4.6
22	20	52	GLY	4.6
38	2g	80	VAL	4.6
52	1u	13	ILE	4.6
51	1t	73	HIS	4.6
45	1n	14	PRO	4.6
45	2n	44	LEU	4.6
40	2i	126	SER	4.6
40	2i	85	LEU	4.6
44	2m	87	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
41	2j	62	HIS	4.6
32	1a	1257	U	4.5
45	1n	2	ALA	4.5
53	2y	64	SER	4.5
44	2m	6	GLY	4.5
45	1n	21	TYR	4.5
34	1c	2	GLY	4.5
38	2g	2	ALA	4.5
7	2H	19	VAL	4.5
41	1j	45	ARG	4.5
40	2i	42	ARG	4.5
40	2i	49	PRO	4.5
40	2i	8	GLY	4.5
34	2c	23	TYR	4.4
45	2n	42	ILE	4.4
45	2n	29	ARG	4.4
47	1p	19	ILE	4.4
32	1a	1030	C	4.4
40	2i	4	TYR	4.4
40	2i	68	GLY	4.4
45	2n	18	VAL	4.4
33	1b	214	ILE	4.4
40	2i	36	TYR	4.4
41	1j	20	ALA	4.4
41	2j	66	ARG	4.4
51	1t	72	LEU	4.4
45	2n	37	PHE	4.4
53	2y	35	ILE	4.4
26	14	49	PHE	4.4
32	2a	1031	G	4.4
45	2n	6	LEU	4.3
51	1t	18	GLN	4.3
53	2y	38	HIS	4.3
31	29	16	VAL	4.3
33	1b	128	GLU	4.3
33	2b	163	PHE	4.3
50	2s	10	PHE	4.3
45	2n	7	ILE	4.3
40	1i	109	VAL	4.3
1	2A	2174	C	4.2
40	2i	114	TYR	4.2
45	2n	10	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
41	2j	19	SER	4.2
45	2n	53	LEU	4.2
41	2j	64	GLU	4.2
1	2A	2159	G	4.2
34	2c	32	LEU	4.2
26	24	50	VAL	4.2
35	2d	140	VAL	4.2
1	2A	2141	G	4.2
32	2a	1026	G	4.1
50	2s	15	LEU	4.1
40	2i	110	GLU	4.1
12	2Q	104	PHE	4.1
40	2i	59	PHE	4.1
45	1n	34	TYR	4.1
1	2A	2124	G	4.1
44	1m	2	ALA	4.1
19	2X	69	TYR	4.1
34	2c	65	ALA	4.1
44	2m	5	ALA	4.1
45	1n	10	ALA	4.1
40	2i	127	LYS	4.1
36	2e	84	PHE	4.1
38	2g	155	ARG	4.1
1	2A	2132	U	4.1
41	2j	63	PHE	4.1
1	2A	2147	G	4.0
29	27	48	LYS	4.0
1	2A	2136	C	4.0
42	2k	123	LYS	4.0
53	2y	20	VAL	4.0
40	2i	73	GLN	4.0
53	2y	70	MET	4.0
40	1i	108	VAL	4.0
33	1b	121	LEU	4.0
41	2j	48	THR	4.0
1	2A	2139	C	4.0
52	1u	2	GLY	4.0
44	2m	116	THR	4.0
56	2v	1	MET	4.0
53	2y	71	TYR	4.0
32	2a	1030(C)	G	4.0
41	2j	40	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
38	2g	6	ARG	3.9
34	2c	157	ILE	3.9
41	1j	27	ALA	3.9
53	2y	21	ALA	3.9
1	2A	2126	A	3.9
50	2s	82	GLY	3.9
29	27	47	ARG	3.9
34	1c	168	ALA	3.9
40	2i	108	VAL	3.9
50	2s	11	VAL	3.9
52	2u	17	THR	3.9
33	1b	122	PHE	3.9
53	2y	60	VAL	3.9
44	2m	64	TRP	3.9
52	2u	9	ARG	3.9
1	1A	1090	U	3.9
50	2s	80	TYR	3.9
34	1c	63	ASN	3.8
34	2c	152	ILE	3.8
40	2i	113	LYS	3.8
53	2y	72	THR	3.8
34	2c	8	ILE	3.8
53	1y	95	ARG	3.8
32	2a	1033	G	3.8
35	2d	158	ILE	3.8
40	2i	77	ILE	3.8
34	2c	2	GLY	3.8
53	2y	65	GLY	3.8
26	14	52	THR	3.8
34	2c	201	TYR	3.8
35	1d	179	GLU	3.8
40	2i	105	ASP	3.8
6	2G	152	LEU	3.8
45	2n	27	CYS	3.8
52	2u	22	ARG	3.7
1	2A	1076	C	3.7
32	2a	1034	G	3.7
1	2A	2173	A	3.7
44	2m	102	ARG	3.7
45	2n	35	ARG	3.7
44	2m	66	LEU	3.7
1	2A	2154	G	3.7

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Mol	Chain	Res	Type	RSRZ
32	2a	1032	G	3.7
50	2s	77	THR	3.7
12	2Q	121	ALA	3.7
34	1c	203	PHE	3.7
53	2y	11	GLU	3.7
21	2Z	155	LEU	3.7
33	2b	121	LEU	3.7
35	1d	178	VAL	3.7
45	1n	17	LYS	3.7
29	27	1	MET	3.7
1	2A	2125	G	3.7
34	2c	101	LEU	3.7
53	2y	6	THR	3.7
34	1c	146	ALA	3.7
29	17	1	MET	3.7
41	2j	74	ILE	3.7
53	2y	59	GLY	3.7
7	2H	43	VAL	3.7
34	2c	186	PHE	3.6
45	2n	23	ARG	3.6
52	1u	18	TYR	3.6
53	2y	61	LEU	3.6
52	1u	14	TRP	3.6
36	2e	16	THR	3.6
26	14	46	GLN	3.6
53	2y	82	GLU	3.6
1	1A	2107	C	3.6
1	2A	2803	C	3.6
47	2p	9	PHE	3.6
40	2i	70	LYS	3.6
53	2y	19	HIS	3.6
22	20	51	VAL	3.6
40	2i	53	VAL	3.6
40	2i	78	LYS	3.6
6	2G	43	LEU	3.6
44	1m	87	TYR	3.6
53	2y	32	THR	3.6
40	1i	28	VAL	3.6
53	2y	16	ILE	3.6
34	2c	58	GLU	3.6
38	2g	81	GLY	3.6
50	2s	69	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	1A	1075	C	3.6
32	1a	1001(A)	G	3.6
35	1d	2	GLY	3.6
45	1n	33	VAL	3.6
33	1b	222	ILE	3.5
34	1c	10	PHE	3.5
40	2i	101	PHE	3.5
45	1n	15	LYS	3.5
47	1p	7	ALA	3.5
32	2a	1028	C	3.5
41	2j	72	VAL	3.5
50	2s	67	VAL	3.5
20	2Y	1	MET	3.5
40	2i	28	VAL	3.5
36	2e	109	ILE	3.5
45	2n	55	GLY	3.5
44	1m	56	LEU	3.5
32	2a	1030(D)	A	3.5
23	1l	98	LEU	3.5
49	2r	58	LEU	3.5
1	1A	2147	G	3.5
32	2a	1001(A)	G	3.5
35	2d	149	ALA	3.5
45	1n	20	ALA	3.5
33	2b	233	SER	3.5
50	2s	66	MET	3.5
41	1j	50	ILE	3.5
45	1n	59	ALA	3.5
53	2y	94	ALA	3.5
35	2d	175	SER	3.5
8	2l	18	VAL	3.5
40	1i	63	ILE	3.4
36	2e	12	LEU	3.4
40	2i	102	LEU	3.4
53	2y	34	LEU	3.4
26	24	51	ASP	3.4
44	2m	65	LYS	3.4
43	2l	18	VAL	3.4
32	1a	1001	A	3.4
33	2b	152	PHE	3.4
41	2j	6	ILE	3.4
45	2n	31	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
34	1c	189	ALA	3.4
53	2y	53	THR	3.4
34	2c	145	GLY	3.4
39	1h	93	VAL	3.4
41	2j	49	VAL	3.4
34	2c	57	ILE	3.4
1	2A	229	A	3.4
38	2g	9	VAL	3.4
45	2n	36	PHE	3.4
40	2i	19	LEU	3.4
43	1l	64	TYR	3.4
1	1A	1077	A	3.4
1	2A	2145	C	3.4
40	2i	90	PRO	3.4
40	2i	65	VAL	3.4
40	1i	47	LEU	3.4
44	2m	23	TYR	3.4
45	2n	51	GLY	3.4
47	1p	73	LEU	3.4
50	2s	71	LEU	3.4
34	2c	4	LYS	3.4
45	2n	57	ARG	3.4
33	2b	181	PHE	3.4
38	2g	34	GLY	3.4
33	1b	233	SER	3.4
38	2g	25	ALA	3.4
1	1A	1063	G	3.4
23	2l	70	VAL	3.4
38	2g	36	LYS	3.4
3	2D	182	LEU	3.3
34	2c	184	TYR	3.3
47	1p	32	TYR	3.3
52	2u	18	TYR	3.3
43	2l	19	ARG	3.3
7	2H	35	VAL	3.3
53	2y	62	VAL	3.3
1	2A	2793	G	3.3
43	2l	5	PRO	3.3
35	2d	4	TYR	3.3
14	2S	33	LYS	3.3
40	2i	50	LEU	3.3
1	2A	2109	U	3.3

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Mol	Chain	Res	Type	RSRZ
38	2g	33	ASP	3.3
45	2n	54	PRO	3.3
52	1u	10	ARG	3.3
40	2i	64	THR	3.3
41	2j	68	HIS	3.3
42	2k	75	TYR	3.3
26	24	52	THR	3.3
40	1i	43	ALA	3.3
42	2k	29	ILE	3.3
1	2A	2107	C	3.3
51	1t	74	LYS	3.3
40	2i	24	GLY	3.3
1	2A	2127	G	3.3
40	1i	107	ARG	3.3
40	2i	83	ARG	3.3
40	2i	111	ARG	3.3
8	1I	3	VAL	3.3
35	2d	70	ILE	3.3
40	2i	9	ARG	3.3
40	2i	5	TYR	3.3
45	2n	33	VAL	3.3
53	2y	24	LEU	3.2
47	2p	19	ILE	3.2
12	2Q	103	MET	3.2
1	1A	2117	A	3.2
53	2y	45	PRO	3.2
43	2l	10	LEU	3.2
39	2h	112	LEU	3.2
33	1b	188	ALA	3.2
38	2g	7	ALA	3.2
53	2y	25	ALA	3.2
6	2G	157	ILE	3.2
1	2A	2153	G	3.2
35	1d	167	GLY	3.2
7	2H	9	ILE	3.2
36	2e	121	LYS	3.2
45	1n	60	SER	3.2
1	1A	1089	G	3.2
22	20	76	GLY	3.2
40	2i	21	PRO	3.2
1	2A	2143	C	3.2
26	24	46	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
36	2e	123	LEU	3.2
1	1A	1065	U	3.2
47	2p	33	ILE	3.2
34	2c	37	GLN	3.2
40	1i	14	VAL	3.2
1	2A	1509	C	3.2
46	2o	34	LEU	3.2
53	2y	23	ARG	3.2
34	2c	124	ILE	3.2
42	2k	42	TRP	3.2
47	1p	48	TRP	3.2
38	1g	12	LEU	3.2
40	2i	46	ALA	3.1
50	2s	79	THR	3.1
38	2g	27	ILE	3.1
40	1i	37	PHE	3.1
40	2i	81	ILE	3.1
53	2y	18	GLN	3.1
9	2N	46	VAL	3.1
21	2Z	191	VAL	3.1
33	2b	115	LEU	3.1
34	2c	76	VAL	3.1
40	2i	62	TYR	3.1
33	2b	57	PHE	3.1
35	2d	146	ILE	3.1
48	1q	27	PHE	3.1
8	2I	1	MET	3.1
14	2S	51	ALA	3.1
40	1i	79	LEU	3.1
42	1k	25	TYR	3.1
40	2i	67	GLY	3.1
51	1t	9	ASN	3.1
1	1A	2805	G	3.1
52	1u	3	LYS	3.1
53	2y	43	LYS	3.1
34	1c	160	ALA	3.1
34	2c	66	VAL	3.1
40	2i	14	VAL	3.1
7	2H	159	GLU	3.1
17	2V	81	TYR	3.1
34	1c	201	TYR	3.1
34	1c	5	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
50	2s	62	ILE	3.1
53	2y	54	ILE	3.1
45	1n	39	LEU	3.1
44	1m	112	GLY	3.1
35	2d	75	PHE	3.1
39	1h	134	ILE	3.1
1	1A	2146	C	3.1
8	2I	19	VAL	3.1
26	24	66	SER	3.1
33	2b	97	TRP	3.1
41	1j	46	ARG	3.1
1	2A	1075	C	3.1
32	2a	1027	C	3.1
3	2D	37	LEU	3.1
15	2T	105	LEU	3.1
50	2s	12	ASP	3.0
53	2y	76	GLU	3.0
34	2c	59	ARG	3.0
40	1i	77	ILE	3.0
47	2p	48	TRP	3.0
48	1q	25	ARG	3.0
26	24	63	TYR	3.0
38	2g	44	TYR	3.0
34	1c	12	LEU	3.0
49	2r	62	GLU	3.0
53	1y	94	ALA	3.0
45	2n	12	ARG	3.0
20	2Y	75	ILE	3.0
30	28	16	ILE	3.0
41	2j	11	PHE	3.0
47	2p	39	TYR	3.0
34	1c	80	GLY	3.0
45	2n	49	HIS	3.0
39	2h	118	VAL	3.0
53	2y	37	PRO	3.0
6	2G	178	PHE	3.0
41	2j	50	ILE	3.0
26	24	43	TYR	3.0
42	2k	25	TYR	3.0
1	2A	2110	G	3.0
33	1b	133	LYS	3.0
35	2d	152	SER	3.0

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Mol	Chain	Res	Type	RSRZ
44	2m	104	ARG	3.0
33	1b	213	LEU	3.0
8	2I	92	VAL	3.0
1	1A	1067	A	3.0
45	2n	52	GLN	3.0
40	2i	17	VAL	3.0
53	1y	49	VAL	3.0
1	1A	2143	C	3.0
53	2y	84	GLN	3.0
35	2d	79	PHE	3.0
38	2g	42	ILE	3.0
50	2s	35	SER	3.0
7	2H	165	ALA	3.0
23	2l	82	LEU	3.0
40	1i	106	ALA	3.0
40	2i	55	ALA	3.0
45	1n	22	THR	3.0
52	1u	12	LYS	3.0
6	2G	159	VAL	3.0
34	1c	81	GLY	3.0
43	2l	89	ARG	3.0
1	2A	2802	G	3.0
32	2a	1202	G	3.0
8	2I	4	ILE	3.0
6	1G	146	TYR	3.0
33	2b	120	ALA	3.0
38	2g	40	ALA	3.0
44	1m	115	LYS	3.0
53	2y	26	LYS	3.0
33	1b	130	ARG	3.0
34	2c	22	TRP	3.0
44	1m	110	ARG	3.0
36	2e	33	VAL	2.9
8	2I	20	ASP	2.9
1	1A	1066	U	2.9
22	20	3	HIS	2.9
40	2i	117	HIS	2.9
1	2A	2106	G	2.9
53	2y	75	ASN	2.9
53	2y	93	GLU	2.9
6	1G	80	PHE	2.9
1	2A	2148	G	2.9

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Mol	Chain	Res	Type	RSRZ
1	2A	2168	G	2.9
7	2H	21	PRO	2.9
22	20	75	LEU	2.9
26	24	67	TYR	2.9
52	2u	23	PRO	2.9
7	1H	2	SER	2.9
46	2o	87	ILE	2.9
21	2Z	188	ALA	2.9
1	1A	1102	C	2.9
35	2d	96	LEU	2.9
43	1l	10	LEU	2.9
1	1A	1091	G	2.9
32	1a	1031	G	2.9
40	2i	26	VAL	2.9
1	2A	2130	U	2.9
34	2c	61	ALA	2.9
41	2j	41	PRO	2.9
48	1q	89	LEU	2.9
53	2y	67	HIS	2.9
1	1A	1176	G	2.9
1	2A	2162	G	2.9
5	2F	76	GLY	2.9
12	2Q	100	GLY	2.9
34	1c	182	ILE	2.9
8	1I	38	LEU	2.9
34	2c	87	LEU	2.9
44	2m	67	GLU	2.9
45	1n	53	LEU	2.9
40	2i	125	TYR	2.9
7	2H	24	VAL	2.9
26	24	10	VAL	2.9
33	2b	70	PHE	2.9
40	1i	81	ILE	2.9
41	2j	98	ILE	2.9
35	2d	120	LEU	2.9
1	1A	1080	C	2.8
9	2N	85	ILE	2.8
40	2i	119	ALA	2.8
44	2m	96	LEU	2.8
45	2n	39	LEU	2.8
47	2p	49	LEU	2.8
3	2D	55	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
33	1b	136	VAL	2.8
33	2b	114	ARG	2.8
41	1j	44	VAL	2.8
40	2i	11	LYS	2.8
48	1q	36	ILE	2.8
31	29	11	CYS	2.8
19	2X	66	LEU	2.8
45	2n	22	THR	2.8
26	24	45	GLY	2.8
36	1e	133	TYR	2.8
41	1j	94	VAL	2.8
56	2v	3	ILE	2.8
3	1D	276	LYS	2.8
7	2H	103	LEU	2.8
40	1i	112	LYS	2.8
48	1q	84	LEU	2.8
53	1y	88	LEU	2.8
11	2P	15	ARG	2.8
32	1a	1028	C	2.8
38	2g	41	ARG	2.8
41	1j	90	LEU	2.8
45	1n	44	LEU	2.8
22	20	73	GLY	2.8
17	2V	47	VAL	2.8
40	1i	117	HIS	2.8
40	2i	123	PRO	2.8
45	1n	56	VAL	2.8
13	2R	69	ASP	2.8
30	28	58	ILE	2.8
22	10	7	LEU	2.8
51	1t	13	LEU	2.8
51	1t	20	LEU	2.8
7	2H	169	VAL	2.8
34	1c	64	VAL	2.8
35	2d	8	VAL	2.8
47	1p	46	PRO	2.8
36	2e	17	ALA	2.8
40	2i	84	ALA	2.8
40	2i	122	ALA	2.8
43	2l	14	GLY	2.8
45	2n	16	PHE	2.8
1	1A	1093	G	2.8

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Mol	Chain	Res	Type	RSRZ
32	1a	1002	G	2.8
35	1d	174	LEU	2.8
35	2d	186	LEU	2.8
51	1t	70	SER	2.8
7	2H	36	PRO	2.8
38	2g	85	TYR	2.7
40	2i	88	TYR	2.7
35	2d	185	PHE	2.7
36	2e	21	ALA	2.7
40	2i	37	PHE	2.7
47	1p	4	ILE	2.7
48	2q	71	PHE	2.7
53	2y	13	THR	2.7
17	2V	71	LEU	2.7
1	2A	2108	C	2.7
3	1D	275	LYS	2.7
17	2V	72	VAL	2.7
23	11	70	VAL	2.7
44	2m	17	VAL	2.7
20	2Y	48	ALA	2.7
41	1j	47	PHE	2.7
52	1u	17	THR	2.7
32	2a	1286	A	2.7
32	2a	1029	C	2.7
35	2d	189	PRO	2.7
25	23	54	VAL	2.7
1	1A	2144	U	2.7
21	2Z	192	ALA	2.7
19	1X	69	TYR	2.7
44	1m	4	ILE	2.7
33	1b	61	LEU	2.7
6	2G	29	TRP	2.7
1	2A	2170	A	2.7
52	2u	12	LYS	2.7
6	2G	136	ARG	2.7
26	14	56	VAL	2.7
29	27	46	VAL	2.7
40	2i	15	ALA	2.7
6	2G	135	LEU	2.7
6	2G	140	ILE	2.7
8	2I	38	LEU	2.7
34	1c	94	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
42	1k	125	PHE	2.7
45	1n	36	PHE	2.7
26	24	40	HIS	2.7
32	2a	1001	A	2.7
44	2m	8	GLU	2.7
45	2n	45	ARG	2.7
32	1a	1029	C	2.7
1	2A	2144	U	2.7
1	2A	2116	G	2.7
40	1i	125	TYR	2.7
40	2i	12	GLU	2.7
53	2y	91	LYS	2.7
34	2c	17	ASP	2.7
35	1d	112	VAL	2.7
1	2A	2129	C	2.7
38	2g	116	ALA	2.7
53	1y	42	SER	2.7
30	28	7	HIS	2.7
34	2c	196	LEU	2.7
40	1i	111	ARG	2.7
44	2m	24	GLY	2.7
50	2s	34	TRP	2.7
1	2A	1046	A	2.6
22	20	77	ARG	2.6
8	2I	2	LYS	2.6
44	2m	105	THR	2.6
50	2s	63	THR	2.6
1	1A	1072	C	2.6
34	1c	175	LEU	2.6
40	1i	75	ASP	2.6
1	1A	2156	G	2.6
1	2A	2805	G	2.6
11	2P	79	ARG	2.6
45	1n	29	ARG	2.6
44	2m	60	VAL	2.6
38	2g	152	ALA	2.6
1	2A	1026	U	2.6
6	2G	139	LEU	2.6
13	2R	18	LEU	2.6
35	2d	183	GLY	2.6
41	2j	53	PRO	2.6
6	2G	146	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
21	2Z	199	LYS	2.6
50	1s	4	SER	2.6
27	15	60	VAL	2.6
38	2g	117	ALA	2.6
41	1j	68	HIS	2.6
41	1j	67	THR	2.6
44	2m	42	ALA	2.6
53	2y	98	ALA	2.6
34	2c	158	GLY	2.6
1	1A	2132	U	2.6
1	2A	2118	U	2.6
1	2A	2176	A	2.6
30	28	2	PRO	2.6
43	2l	7	ILE	2.6
40	1i	83	ARG	2.6
49	2r	22	VAL	2.6
41	1j	57	LYS	2.6
41	1j	85	LEU	2.6
33	2b	130	ARG	2.6
47	1p	38	TYR	2.6
34	2c	162	GLN	2.6
11	2P	118	GLY	2.6
52	1u	15	ARG	2.6
34	1c	33	LEU	2.6
35	2d	11	LEU	2.6
40	1i	56	LEU	2.6
34	2c	167	TRP	2.6
41	1j	54	PHE	2.6
51	2t	55	ILE	2.6
1	2A	2135	A	2.6
40	1i	127	LYS	2.6
1	1A	1509	C	2.6
1	1A	2803	C	2.6
1	2A	2137	C	2.6
38	2g	32	ARG	2.6
44	1m	53	VAL	2.6
45	2n	47	LEU	2.6
36	1e	131	ILE	2.6
44	1m	22	ILE	2.6
45	1n	61	TRP	2.6
45	2n	50	LYS	2.6
40	2i	120	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
25	23	15	TYR	2.6
40	1i	5	TYR	2.6
32	2a	1116	C	2.6
30	28	22	VAL	2.5
36	2e	90	VAL	2.5
30	28	21	LYS	2.5
33	2b	51	LEU	2.5
40	1i	11	LYS	2.5
40	1i	19	LEU	2.5
51	2t	72	LEU	2.5
45	1n	37	PHE	2.5
14	2S	23	ARG	2.5
53	2y	83	ARG	2.5
17	2V	1	MET	2.5
38	2g	156	TRP	2.5
6	2G	74	LYS	2.5
44	2m	107	ALA	2.5
45	2n	15	LYS	2.5
7	2H	45	VAL	2.5
34	2c	174	PRO	2.5
32	1a	1000	U	2.5
34	2c	172	ARG	2.5
12	2Q	68	ILE	2.5
34	1c	35	GLU	2.5
43	2l	32	PHE	2.5
53	1y	59	GLY	2.5
6	2G	75	LYS	2.5
33	1b	131	PRO	2.5
22	20	72	ARG	2.5
1	1A	1092	C	2.5
35	2d	21	LEU	2.5
51	1t	79	ARG	2.5
51	2t	84	LEU	2.5
38	2g	144	MET	2.5
35	2d	73	ARG	2.5
39	1h	67	PRO	2.5
40	1i	7	THR	2.5
51	1t	95	ALA	2.5
16	2U	45	TYR	2.5
40	1i	114	TYR	2.5
4	2E	116	VAL	2.5
21	2Z	125	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
39	1h	63	LEU	2.5
41	1j	40	LEU	2.5
47	1p	20	VAL	2.5
1	1A	2794	C	2.5
32	2a	1002	G	2.5
38	2g	13	GLN	2.5
42	2k	13	GLN	2.5
40	1i	76	ALA	2.5
45	1n	30	ALA	2.5
15	1T	114	LEU	2.5
40	2i	57	GLY	2.5
1	1A	1026	U	2.5
1	2A	34	C	2.5
16	2U	80	ILE	2.5
35	2d	110	PHE	2.5
38	2g	10	ARG	2.5
1	1A	2159	G	2.5
51	1t	68	LYS	2.5
3	1D	254	THR	2.5
3	2D	50	THR	2.5
51	2t	32	ALA	2.5
11	2P	116	GLY	2.5
52	1u	16	GLY	2.5
12	2Q	97	VAL	2.5
35	2d	104	VAL	2.5
42	1k	98	LEU	2.5
11	2P	68	GLN	2.5
12	2Q	133	ARG	2.5
40	1i	10	ARG	2.5
41	1j	60	ARG	2.5
42	2k	126	ARG	2.5
44	1m	9	ILE	2.5
48	2q	59	ILE	2.5
20	1Y	1	MET	2.5
32	2a	1367	C	2.5
33	2b	195	ASP	2.5
35	2d	144	ASP	2.5
1	1A	2112	G	2.5
1	2A	2133	G	2.5
40	2i	6	GLY	2.5
42	2k	14	VAL	2.4
45	2n	21	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
6	2G	144	ILE	2.4
38	2g	120	ILE	2.4
42	2k	95	ILE	2.4
32	1a	1030(D)	A	2.4
40	2i	13	ALA	2.4
44	2m	71	ARG	2.4
52	1u	22	ARG	2.4
1	2A	2152	G	2.4
39	2h	93	VAL	2.4
40	2i	44	VAL	2.4
43	2l	64	TYR	2.4
5	2F	82	ILE	2.4
47	1p	33	ILE	2.4
50	2s	64	GLU	2.4
3	2D	35	LYS	2.4
5	2F	81	PRO	2.4
16	2U	43	GLY	2.4
22	20	46	LYS	2.4
3	2D	2	ALA	2.4
27	25	14	ALA	2.4
42	2k	87	THR	2.4
47	1p	45	THR	2.4
52	1u	8	THR	2.4
36	1e	91	LEU	2.4
44	2m	19	LEU	2.4
23	2l	8	SER	2.4
33	2b	164	VAL	2.4
34	2c	206	GLU	2.4
35	2d	121	VAL	2.4
47	2p	38	TYR	2.4
41	1j	98	ILE	2.4
30	28	46	ARG	2.4
51	2t	9	ASN	2.4
22	20	2	ALA	2.4
1	1A	888	C	2.4
3	2D	155	LEU	2.4
33	2b	149	LEU	2.4
17	2V	79	VAL	2.4
33	1b	229	VAL	2.4
45	1n	23	ARG	2.4
36	2e	89	ILE	2.4
36	2e	133	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
42	2k	117	ASN	2.4
33	2b	101	MET	2.4
1	1A	2115	G	2.4
26	24	39	CYS	2.4
40	1i	113	LYS	2.4
1	1A	1088	A	2.4
1	1A	2804	C	2.4
34	2c	164	ARG	2.4
40	1i	42	ARG	2.4
23	2l	49	VAL	2.4
45	1n	51	GLY	2.4
4	2E	151	TYR	2.4
21	1Z	197	ILE	2.4
6	2G	87	PRO	2.4
18	1W	111	HIS	2.4
43	2l	48	PRO	2.4
33	2b	133	LYS	2.4
1	2A	2160	G	2.4
35	1d	76	ARG	2.4
39	2h	133	LEU	2.4
25	23	47	VAL	2.4
26	14	50	VAL	2.4
34	2c	41	GLY	2.4
51	1t	75	ASN	2.4
34	1c	4	LYS	2.4
34	1c	14	ILE	2.4
34	1c	124	ILE	2.4
11	2P	110	TYR	2.4
39	2h	101	PRO	2.4
21	2Z	79	ARG	2.4
34	1c	200	ALA	2.4
53	2y	17	ARG	2.4
50	2s	39	THR	2.4
34	2c	154	SER	2.4
47	2p	59	TRP	2.4
23	1l	95	LEU	2.4
47	1p	49	LEU	2.4
40	1i	78	LYS	2.3
44	2m	100	GLY	2.3
50	2s	53	ASN	2.3
14	2S	13	ARG	2.3
33	2b	127	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
33	2b	137	ARG	2.3
33	2b	214	ILE	2.3
39	2h	86	ILE	2.3
44	2m	4	ILE	2.3
44	2m	114	ARG	2.3
47	1p	36	ILE	2.3
50	2s	40	ILE	2.3
20	2Y	35	TYR	2.3
23	2l	64	ALA	2.3
34	1c	87	LEU	2.3
22	20	79	VAL	2.3
1	2A	2167	U	2.3
35	2d	118	ARG	2.3
49	2r	87	ARG	2.3
52	1u	9	ARG	2.3
43	1l	7	ILE	2.3
48	2q	36	ILE	2.3
53	1y	35	ILE	2.3
14	2S	12	PHE	2.3
40	1i	18	PHE	2.3
34	1c	149	ALA	2.3
47	1p	39	TYR	2.3
34	2c	177	THR	2.3
14	2S	22	GLY	2.3
50	2s	78	ARG	2.3
51	1t	17	ARG	2.3
53	2y	44	GLU	2.3
33	2b	71	VAL	2.3
40	2i	86	VAL	2.3
35	2d	33	MET	2.3
40	1i	116	LYS	2.3
32	1a	1026	G	2.3
33	2b	210	SER	2.3
40	2i	45	ALA	2.3
53	2y	15	ALA	2.3
52	2u	16	GLY	2.3
3	2D	215	LEU	2.3
6	1G	152	LEU	2.3
39	1h	112	LEU	2.3
44	2m	88	ARG	2.3
50	2s	36	ARG	2.3
51	2t	25	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
52	2u	6	ARG	2.3
12	2Q	35	VAL	2.3
41	2j	37	PRO	2.3
47	1p	41	PRO	2.3
6	2G	155	MET	2.3
33	1b	29	ALA	2.3
40	2i	29	ASN	2.3
49	1r	73	ALA	2.3
50	2s	8	GLY	2.3
1	2A	2894	G	2.3
32	1a	1286	A	2.3
8	2I	30	LEU	2.3
33	2b	27	LYS	2.3
33	2b	215	LEU	2.3
34	2c	204	LEU	2.3
41	1j	65	LEU	2.3
43	1l	60	LEU	2.3
7	2H	107	VAL	2.3
1	1A	2113	U	2.3
4	2E	134	ILE	2.3
3	2D	53	PHE	2.3
51	1t	29	LYS	2.3
53	2y	46	GLN	2.3
7	2H	163	TYR	2.3
14	2S	36	TYR	2.3
48	2q	32	TYR	2.3
44	2m	48	LEU	2.3
51	2t	62	LEU	2.3
33	2b	93	VAL	2.3
3	2D	275	LYS	2.3
14	2S	29	PHE	2.3
53	2y	31	GLN	2.3
34	1c	177	THR	2.3
40	1i	36	TYR	2.3
32	2a	1354	C	2.3
44	2m	110	ARG	2.2
52	2u	3	LYS	2.2
32	2a	1224	G	2.2
18	2W	50	VAL	2.2
23	2l	4	VAL	2.2
41	1j	93	GLY	2.2
35	2d	111	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
36	2e	131	ILE	2.2
39	1h	109	ILE	2.2
48	2q	27	PHE	2.2
34	2c	18	TRP	2.2
19	2X	33	LYS	2.2
20	2Y	31	LEU	2.2
34	2c	26	LYS	2.2
35	2d	94	LEU	2.2
36	2e	43	LEU	2.2
38	2g	76	ARG	2.2
53	2y	95	ARG	2.2
46	2o	86	GLY	2.2
12	2Q	102	VAL	2.2
29	17	46	VAL	2.2
33	2b	165	VAL	2.2
45	2n	56	VAL	2.2
1	1A	1078	U	2.2
32	1a	723	U	2.2
1	1A	2141	G	2.2
10	2O	69	ILE	2.2
16	2U	41	ALA	2.2
34	1c	202	ILE	2.2
42	2k	21	ILE	2.2
45	1n	7	ILE	2.2
40	1i	33	PHE	2.2
44	1m	105	THR	2.2
13	2R	68	ARG	2.2
4	2E	120	TRP	2.2
20	2Y	106	LEU	2.2
25	23	26	LEU	2.2
35	1d	135	LEU	2.2
33	1b	228	GLY	2.2
48	1q	33	GLY	2.2
31	29	3	VAL	2.2
50	2s	58	VAL	2.2
1	1A	2130	U	2.2
32	2a	1357	A	2.2
34	1c	39	ILE	2.2
34	2c	190	ARG	2.2
35	2d	122	ARG	2.2
12	2Q	65	PHE	2.2
20	2Y	12	THR	2.2

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Mol	Chain	Res	Type	RSRZ
39	1h	24	THR	2.2
25	23	2	PRO	2.2
45	2n	14	PRO	2.2
37	1f	55	ASP	2.2
1	1A	1079	C	2.2
7	2H	76	VAL	2.2
23	11	26	ARG	2.2
35	2d	49	ARG	2.2
36	1e	148	VAL	2.2
38	1g	17	VAL	2.2
48	2q	65	ILE	2.2
6	2G	94	LEU	2.2
20	1Y	66	PRO	2.2
33	2b	131	PRO	2.2
38	2g	37	ASN	2.2
39	1h	133	LEU	2.2
50	2s	2	PRO	2.2
53	2y	66	LYS	2.2
22	20	78	TYR	2.2
10	2O	57	VAL	2.2
35	2d	128	VAL	2.2
38	1g	21	VAL	2.2
32	1a	1037	C	2.2
41	2j	97	GLU	2.2
33	1b	127	ILE	2.2
39	2h	6	ILE	2.2
16	2U	40	PHE	2.2
44	2m	111	LYS	2.2
8	2I	12	LEU	2.2
34	2c	155	GLY	2.2
35	1d	69	GLY	2.2
1	2A	2120	G	2.2
32	1a	1030(A)	G	2.2
34	1c	18	TRP	2.2
50	2s	52	TYR	2.2
10	2O	62	VAL	2.2
33	2b	136	VAL	2.2
45	1n	13	THR	2.2
53	2y	36	ASN	2.2
21	1Z	80	ARG	2.2
23	21	61	ARG	2.2
33	1b	234	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	2A	2134	A	2.2
8	2I	5	LEU	2.2
18	2W	82	LEU	2.2
33	1b	118	LEU	2.2
41	2j	88	LEU	2.2
38	2g	35	LYS	2.1
16	2U	49	HIS	2.1
33	2b	92	TYR	2.1
35	1d	138	TYR	2.1
3	1D	221	VAL	2.1
34	1c	3	ASN	2.1
38	2g	83	ALA	2.1
44	2m	94	ARG	2.1
16	2U	62	ILE	2.1
1	2A	645	C	2.1
1	2A	1064	C	2.1
47	2p	46	PRO	2.1
56	2v	2	PHE	2.1
37	1f	48	LEU	2.1
48	2q	31	LEU	2.1
3	2D	276	LYS	2.1
17	2V	82	ARG	2.1
33	2b	48	MET	2.1
41	2j	89	ASP	2.1
8	2I	39	ALA	2.1
21	2Z	196	VAL	2.1
40	2i	121	ARG	2.1
44	2m	74	VAL	2.1
47	1p	2	VAL	2.1
47	2p	56	ALA	2.1
50	1s	19	VAL	2.1
31	19	37	GLY	2.1
50	1s	68	GLY	2.1
51	1t	66	ALA	2.1
3	2D	38	LYS	2.1
22	20	45	PHE	2.1
45	1n	16	PHE	2.1
49	1r	29	PHE	2.1
50	2s	74	PHE	2.1
8	2I	44	LEU	2.1
35	2d	78	LEU	2.1
45	1n	6	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
32	2a	1066	C	2.1
32	1a	1035	A	2.1
45	1n	35	ARG	2.1
53	1y	70	MET	2.1
39	2h	65	TYR	2.1
41	2j	10	GLY	2.1
1	1A	1081	U	2.1
32	2a	1235	U	2.1
40	2i	103	THR	2.1
51	1t	71	THR	2.1
35	2d	142	PRO	2.1
35	1d	75	PHE	2.1
6	2G	7	LEU	2.1
34	1c	47	LEU	2.1
39	1h	10	LEU	2.1
41	1j	58	ASP	2.1
51	1t	83	ARG	2.1
45	2n	58	LYS	2.1
44	1m	24	GLY	2.1
45	1n	28	GLY	2.1
12	2Q	132	VAL	2.1
50	1s	77	THR	2.1
52	1u	21	TYR	2.1
16	2U	17	ILE	2.1
44	2m	25	ILE	2.1
6	2G	102	PHE	2.1
7	1H	105	LEU	2.1
8	2I	48	GLU	2.1
11	2P	59	LEU	2.1
16	2U	28	ARG	2.1
23	2I	26	ARG	2.1
26	14	53	GLU	2.1
33	2b	55	PHE	2.1
38	2g	149	ARG	2.1
45	1n	38	GLY	2.1
6	2G	64	THR	2.1
30	28	23	VAL	2.1
34	2c	113	ALA	2.1
40	2i	43	ALA	2.1
32	2a	1358	U	2.1
14	2S	92	TYR	2.1
48	2q	30	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
45	1n	31	ARG	2.1
8	1I	109	ILE	2.1
24	22	41	ILE	2.1
36	2e	92	LYS	2.1
39	1h	98	LYS	2.1
39	2h	45	ILE	2.1
3	2D	170	GLY	2.1
34	1c	197	GLY	2.1
6	2G	138	GLN	2.1
38	2g	31	MET	2.1
12	2Q	117	ALA	2.1
22	20	49	LYS	2.1
26	24	55	ARG	2.1
35	1d	73	ARG	2.1
36	2e	126	ARG	2.1
43	2l	31	PRO	2.1
51	1t	67	ALA	2.1
7	2H	115	VAL	2.1
52	1u	5	ASP	2.1
1	2A	2119	A	2.1
32	2a	1035	A	2.1
8	2I	9	LEU	2.1
35	2d	108	LEU	2.1
46	1o	56	LEU	2.1
35	2d	74	GLN	2.1
6	2G	72	ARG	2.1
1	2A	2804	C	2.0
6	2G	158	ALA	2.0
21	1Z	192	ALA	2.0
27	15	18	ALA	2.0
34	2c	149	ALA	2.0
53	2y	14	PRO	2.0
34	1c	207	VAL	2.0
36	1e	105	VAL	2.0
47	2p	62	VAL	2.0
50	1s	41	VAL	2.0
1	2A	2123	G	2.0
31	29	24	TYR	2.0
32	1a	1033	G	2.0
28	26	54	ILE	2.0
33	2b	33	TYR	2.0
39	2h	80	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
40	2i	48	GLU	2.0
41	1j	35	SER	2.0
42	2k	108	ILE	2.0
46	1o	87	ILE	2.0
1	1A	1085	A	2.0
1	1A	1103	A	2.0
32	2a	975	A	2.0
52	1u	4	GLY	2.0
14	2S	9	ARG	2.0
39	2h	84	ARG	2.0
51	1t	80	ARG	2.0
50	1s	66	MET	2.0
43	1l	5	PRO	2.0
11	2P	125	VAL	2.0
15	2T	66	VAL	2.0
32	2a	1037	C	2.0
32	2a	1149	C	2.0
32	2a	1195	C	2.0
32	2a	1249	C	2.0
43	2l	16	GLU	2.0
50	2s	83	HIS	2.0
6	2G	108	ASN	2.0
33	2b	135	GLN	2.0
7	2H	94	TYR	2.0
8	2I	25	TYR	2.0
12	2Q	64	ILE	2.0
22	20	36	ILE	2.0
33	1b	226	ARG	2.0
33	2b	44	LEU	2.0
34	2c	77	ILE	2.0
41	1j	96	ILE	2.0
50	2s	5	LEU	2.0
51	2t	10	LEU	2.0
53	2y	85	LEU	2.0
1	2A	2151	G	2.0
7	2H	123	PHE	2.0
41	1j	11	PHE	2.0
32	2a	1531	A	2.0
6	2G	137	GLU	2.0
4	2E	114	ALA	2.0
45	2n	59	ALA	2.0
42	2k	31	THR	2.0

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Mol	Chain	Res	Type	RSRZ
18	2W	60	ASN	2.0
34	2c	153	VAL	2.0
38	1g	80	VAL	2.0
45	2n	32	SER	2.0
51	1t	26	ASN	2.0
4	2E	106	GLY	2.0
6	2G	85	GLY	2.0
38	2g	78	ARG	2.0
38	2g	79	ARG	2.0
39	2h	122	ARG	2.0
43	1l	63	GLY	2.0
51	1t	22	ARG	2.0
35	2d	5	ILE	2.0
35	2d	157	LEU	2.0
40	1i	50	LEU	2.0
40	2i	79	LEU	2.0
38	2g	151	TYR	2.0
34	2c	122	GLU	2.0
40	1i	105	ASP	2.0
1	1A	2173	A	2.0
1	2A	2801(A)	A	2.0
36	1e	128	PRO	2.0
56	1v	1	MET	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	M2G	2a	966	25/26	0.89	0.20	58,71,83,94	0
32	2MG	2a	1207	24/25	0.89	0.14	72,77,87,90	0
1	5MU	2A	1915	21/22	0.90	0.12	73,80,85,96	0
1	PSU	2A	1917	20/21	0.90	0.12	64,74,85,92	0
32	5MC	2a	967	21/22	0.91	0.22	65,69,74,76	0
1	PSU	2A	1911	20/21	0.92	0.11	63,68,81,82	0
1	5MU	1A	1915	21/22	0.92	0.14	62,71,74,87	0
32	2MG	1a	1207	24/25	0.92	0.16	59,68,73,75	0
43	0TD	2l	92	10/11	0.92	0.15	63,65,69,72	0
1	PSU	1A	1917	20/21	0.93	0.14	62,67,70,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	5MC	2a	1404	21/22	0.93	0.19	51,61,66,72	0
32	PSU	2a	516	20/21	0.93	0.11	68,70,79,81	0
43	0TD	1l	92	10/11	0.94	0.17	54,59,62,71	0
1	OMC	2A	1920	21/22	0.94	0.13	57,65,69,72	0
32	5MC	2a	1400	21/22	0.94	0.27	61,70,75,78	0
32	4OC	2a	1402	22/23	0.94	0.18	60,66,69,73	0
32	5MC	1a	967	21/22	0.94	0.19	56,64,70,75	0
1	PSU	1A	1911	20/21	0.94	0.14	59,61,66,67	0
32	G7M	2a	527	24/25	0.95	0.14	60,63,67,71	0
32	PSU	1a	516	20/21	0.95	0.18	53,62,66,70	0
1	5MC	2A	1942	21/22	0.95	0.18	43,52,58,58	0
32	5MC	2a	1407	21/22	0.95	0.14	54,65,68,69	0
32	M2G	1a	966	25/26	0.95	0.19	53,57,62,65	0
32	5MC	1a	1404	21/22	0.96	0.16	44,50,54,56	0
32	UR3	1a	1498	21/22	0.96	0.18	43,49,52,55	0
32	UR3	2a	1498	21/22	0.96	0.18	57,61,66,69	0
1	OMC	1A	1920	21/22	0.96	0.18	38,54,60,63	0
55	8AN	1x	76	22/23	0.96	0.21	28,35,41,48	0
55	8AN	2x	76	22/23	0.96	0.22	41,45,53,58	0
32	MA6	1a	1519	24/25	0.97	0.21	41,49,53,55	0
1	5MU	2A	1939	21/22	0.97	0.17	33,39,43,43	0
32	G7M	1a	527	24/25	0.97	0.17	43,55,60,61	0
1	OMG	2A	2251	24/25	0.97	0.20	30,38,42,45	0
1	2MA	2A	2503	23/24	0.97	0.20	30,35,39,41	0
1	OMU	2A	2552	21/22	0.97	0.18	33,40,44,45	0
1	PSU	2A	2605	20/21	0.97	0.23	29,38,42,44	0
32	MA6	2a	1518	24/25	0.97	0.17	58,63,66,69	0
32	MA6	2a	1519	24/25	0.97	0.24	57,65,69,74	0
32	5MC	1a	1407	21/22	0.97	0.17	38,51,57,60	0
54	PPU	2w	76	37/38	0.97	0.23	30,41,45,51	0
32	4OC	1a	1402	22/23	0.97	0.18	43,50,52,68	0
32	MA6	1a	1518	24/25	0.97	0.20	42,47,50,50	0
32	5MC	1a	1400	21/22	0.98	0.18	48,52,57,60	0
1	OMU	1A	2552	21/22	0.98	0.18	21,27,33,33	0
1	PSU	1A	2605	20/21	0.98	0.18	24,28,32,35	0
1	5MU	1A	1939	21/22	0.98	0.18	23,28,31,34	0
1	5MC	1A	1942	21/22	0.98	0.19	30,36,42,46	0
1	5MC	1A	1962	21/22	0.98	0.19	33,38,43,44	0
54	PPU	1w	76	37/38	0.98	0.21	23,28,32,33	0
1	5MC	2A	1962	21/22	0.98	0.17	41,47,54,57	0
1	OMG	1A	2251	24/25	0.98	0.22	20,25,29,30	0
1	2MA	1A	2503	23/24	0.98	0.21	17,21,24,28	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	MG	2A	3677	1/1	0.25	0.26	63,63,63,63	0
57	MG	2A	3584	1/1	0.26	0.08	55,55,55,55	0
57	MG	2A	3646	1/1	0.35	0.11	55,55,55,55	0
57	MG	1A	3681	1/1	0.41	0.10	58,58,58,58	0
57	MG	2A	3668	1/1	0.49	0.08	51,51,51,51	0
57	MG	2T	201	1/1	0.49	0.20	66,66,66,66	0
57	MG	1A	3883	1/1	0.51	0.09	46,46,46,46	0
57	MG	1a	3199	1/1	0.53	0.22	59,59,59,59	0
57	MG	1A	3796	1/1	0.53	0.10	70,70,70,70	0
57	MG	1a	3100	1/1	0.54	0.18	78,78,78,78	0
57	MG	2a	3010	1/1	0.55	0.28	81,81,81,81	0
57	MG	1A	3389	1/1	0.57	0.14	31,31,31,31	0
57	MG	1b	301	1/1	0.57	0.11	75,75,75,75	0
57	MG	2A	3377	1/1	0.58	0.13	39,39,39,39	0
57	MG	2A	3528	1/1	0.58	0.21	65,65,65,65	0
57	MG	1A	4019	1/1	0.59	0.20	80,80,80,80	0
57	MG	2a	3164	1/1	0.60	0.18	71,71,71,71	0
57	MG	1A	3597	1/1	0.61	0.13	41,41,41,41	0
57	MG	1A	3421	1/1	0.61	0.12	33,33,33,33	0
57	MG	1A	3572	1/1	0.61	0.15	42,42,42,42	0
57	MG	1A	3866	1/1	0.61	0.16	70,70,70,70	0
57	MG	1a	3273	1/1	0.61	0.16	63,63,63,63	0
57	MG	2A	3542	1/1	0.63	0.18	64,64,64,64	0
57	MG	2A	3570	1/1	0.63	0.21	63,63,63,63	0
57	MG	1a	3145	1/1	0.63	0.12	67,67,67,67	0
57	MG	2A	3731	1/1	0.64	0.16	64,64,64,64	0
57	MG	1A	3011	1/1	0.65	0.17	50,50,50,50	0
57	MG	1A	3275	1/1	0.65	0.20	62,62,62,62	0
57	MG	2a	3157	1/1	0.65	0.09	68,68,68,68	0
57	MG	1A	3994	1/1	0.65	0.11	72,72,72,72	0
57	MG	15	3108	1/1	0.66	0.12	48,48,48,48	0
57	MG	2a	3154	1/1	0.66	0.10	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2B	206	1/1	0.66	0.14	74,74,74,74	0
57	MG	2A	3530	1/1	0.66	0.30	75,75,75,75	0
57	MG	1a	3220	1/1	0.67	0.23	76,76,76,76	0
57	MG	1a	3052	1/1	0.67	0.45	76,76,76,76	0
57	MG	2a	3132	1/1	0.67	0.20	81,81,81,81	0
57	MG	2a	3170	1/1	0.67	0.16	82,82,82,82	0
57	MG	2a	3064	1/1	0.68	0.11	75,75,75,75	0
57	MG	1a	3077	1/1	0.68	0.17	60,60,60,60	0
57	MG	2A	3666	1/1	0.68	0.17	75,75,75,75	0
57	MG	2A	3575	1/1	0.69	0.18	62,62,62,62	0
57	MG	1a	3020	1/1	0.69	0.14	57,57,57,57	0
57	MG	2A	3137	1/1	0.69	0.14	67,67,67,67	0
57	MG	2B	218	1/1	0.69	0.12	70,70,70,70	0
57	MG	1A	3779	1/1	0.69	0.13	34,34,34,34	0
57	MG	2A	3457	1/1	0.69	0.19	71,71,71,71	0
57	MG	2a	3186	1/1	0.69	0.08	67,67,67,67	0
57	MG	1A	3644	1/1	0.70	0.32	60,60,60,60	0
57	MG	1A	3871	1/1	0.70	0.14	50,50,50,50	0
57	MG	1A	3222	1/1	0.70	0.17	59,59,59,59	0
57	MG	1A	3425	1/1	0.70	0.17	35,35,35,35	0
57	MG	1A	3624	1/1	0.70	0.20	29,29,29,29	0
58	MPD	2B	220	8/8	0.70	0.25	53,65,71,77	0
57	MG	1A	3393	1/1	0.71	0.23	29,29,29,29	0
57	MG	1a	3011	1/1	0.71	0.09	69,69,69,69	0
57	MG	2A	3114	1/1	0.71	0.17	70,70,70,70	0
57	MG	2A	3543	1/1	0.71	0.10	67,67,67,67	0
57	MG	1A	3381	1/1	0.71	0.17	44,44,44,44	0
57	MG	2A	3191	1/1	0.71	0.12	72,72,72,72	0
57	MG	1A	3377	1/1	0.71	0.09	66,66,66,66	0
57	MG	1a	3059	1/1	0.71	0.26	60,60,60,60	0
57	MG	1a	3226	1/1	0.72	0.11	60,60,60,60	0
57	MG	2A	3614	1/1	0.72	0.12	62,62,62,62	0
57	MG	2A	3645	1/1	0.72	0.11	70,70,70,70	0
57	MG	2A	3494	1/1	0.72	0.15	42,42,42,42	0
57	MG	1A	3462	1/1	0.72	0.16	35,35,35,35	0
57	MG	1a	3094	1/1	0.72	0.14	69,69,69,69	0
57	MG	1a	3032	1/1	0.72	0.10	60,60,60,60	0
57	MG	1A	3851	1/1	0.72	0.22	61,61,61,61	0
57	MG	1A	3658	1/1	0.72	0.21	44,44,44,44	0
57	MG	1a	3067	1/1	0.72	0.14	54,54,54,54	0
57	MG	2a	3162	1/1	0.73	0.10	57,57,57,57	0
57	MG	2A	3619	1/1	0.73	0.35	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3168	1/1	0.73	0.15	66,66,66,66	0
57	MG	2A	3635	1/1	0.73	0.08	68,68,68,68	0
57	MG	1A	3979	1/1	0.73	0.10	29,29,29,29	0
57	MG	2A	3169	1/1	0.73	0.15	62,62,62,62	0
57	MG	2a	3009	1/1	0.74	0.13	70,70,70,70	0
57	MG	1x	102	1/1	0.74	0.11	41,41,41,41	0
57	MG	2a	3062	1/1	0.74	0.22	69,69,69,69	0
57	MG	2A	3084	1/1	0.74	0.17	63,63,63,63	0
57	MG	2A	3104	1/1	0.74	0.15	63,63,63,63	0
57	MG	1a	3150	1/1	0.74	0.14	56,56,56,56	0
57	MG	1F	312	1/1	0.74	0.21	52,52,52,52	0
57	MG	2A	3157	1/1	0.74	0.30	63,63,63,63	0
57	MG	2A	3688	1/1	0.74	0.16	59,59,59,59	0
57	MG	1a	3081	1/1	0.74	0.18	72,72,72,72	0
57	MG	1A	4011	1/1	0.74	0.08	53,53,53,53	0
57	MG	1A	3843	1/1	0.74	0.20	56,56,56,56	0
57	MG	1B	219	1/1	0.74	0.16	43,43,43,43	0
57	MG	2A	3096	1/1	0.75	0.18	54,54,54,54	0
57	MG	2A	3463	1/1	0.75	0.13	61,61,61,61	0
57	MG	1A	3278	1/1	0.75	0.17	47,47,47,47	0
57	MG	1B	230	1/1	0.75	0.14	61,61,61,61	0
57	MG	2A	3327	1/1	0.75	0.18	65,65,65,65	0
57	MG	1a	3133	1/1	0.75	0.17	63,63,63,63	0
57	MG	28	102	1/1	0.76	0.20	52,52,52,52	0
57	MG	1A	3507	1/1	0.76	0.15	76,76,76,76	0
57	MG	1A	3483	1/1	0.76	0.20	31,31,31,31	0
57	MG	1B	227	1/1	0.76	0.12	74,74,74,74	0
57	MG	1A	4004	1/1	0.76	0.37	51,51,51,51	0
57	MG	2a	3101	1/1	0.76	0.32	64,64,64,64	0
57	MG	2a	3124	1/1	0.76	0.10	56,56,56,56	0
57	MG	2A	3663	1/1	0.76	0.10	70,70,70,70	0
57	MG	2A	3326	1/1	0.76	0.10	63,63,63,63	0
57	MG	2A	3551	1/1	0.76	0.08	60,60,60,60	0
57	MG	2A	3564	1/1	0.76	0.20	66,66,66,66	0
57	MG	1a	3168	1/1	0.76	0.13	60,60,60,60	0
57	MG	1a	3176	1/1	0.76	0.10	74,74,74,74	0
57	MG	1A	3920	1/1	0.76	0.12	49,49,49,49	0
57	MG	2A	3606	1/1	0.76	0.11	56,56,56,56	0
57	MG	1a	3096	1/1	0.76	0.20	69,69,69,69	0
57	MG	1G	203	1/1	0.77	0.21	67,67,67,67	0
57	MG	1a	3121	1/1	0.77	0.14	52,52,52,52	0
57	MG	2A	3112	1/1	0.77	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3391	1/1	0.77	0.19	53,53,53,53	0
57	MG	1A	3942	1/1	0.77	0.28	67,67,67,67	0
57	MG	2A	3577	1/1	0.77	0.07	61,61,61,61	0
57	MG	1A	3129	1/1	0.77	0.13	47,47,47,47	0
57	MG	2A	3699	1/1	0.77	0.15	71,71,71,71	0
57	MG	2A	3603	1/1	0.77	0.15	51,51,51,51	0
57	MG	1A	3865	1/1	0.77	0.34	46,46,46,46	0
57	MG	1A	3490	1/1	0.77	0.10	40,40,40,40	0
57	MG	2Q	202	1/1	0.77	0.26	53,53,53,53	0
57	MG	1A	3931	1/1	0.77	0.11	60,60,60,60	0
57	MG	2A	3209	1/1	0.77	0.27	53,53,53,53	0
57	MG	2a	3008	1/1	0.77	0.14	64,64,64,64	0
57	MG	1A	3196	1/1	0.78	0.27	66,66,66,66	0
57	MG	2A	3561	1/1	0.78	0.15	58,58,58,58	0
57	MG	2A	3190	1/1	0.78	0.16	58,58,58,58	0
57	MG	1P	203	1/1	0.78	0.26	51,51,51,51	0
57	MG	1A	3885	1/1	0.78	0.33	53,53,53,53	0
57	MG	2A	3442	1/1	0.78	0.13	56,56,56,56	0
57	MG	2A	3246	1/1	0.78	0.44	62,62,62,62	0
57	MG	2a	3013	1/1	0.79	0.19	66,66,66,66	0
57	MG	2a	3015	1/1	0.79	0.14	61,61,61,61	0
57	MG	2a	3016	1/1	0.79	0.14	62,62,62,62	0
57	MG	1a	3060	1/1	0.79	0.33	65,65,65,65	0
57	MG	2A	3003	1/1	0.79	0.25	62,62,62,62	0
57	MG	2A	3698	1/1	0.79	0.09	72,72,72,72	0
57	MG	2A	3345	1/1	0.79	0.09	63,63,63,63	0
57	MG	2A	3167	1/1	0.79	0.37	56,56,56,56	0
57	MG	2A	3628	1/1	0.79	0.09	49,49,49,49	0
57	MG	1A	3523	1/1	0.79	0.14	54,54,54,54	0
57	MG	2a	3158	1/1	0.79	0.09	67,67,67,67	0
57	MG	2A	3644	1/1	0.79	0.09	48,48,48,48	0
57	MG	1A	3197	1/1	0.79	0.25	64,64,64,64	0
57	MG	1A	3933	1/1	0.79	0.11	51,51,51,51	0
57	MG	1S	201	1/1	0.79	0.14	48,48,48,48	0
57	MG	1A	3625	1/1	0.79	0.16	52,52,52,52	0
57	MG	2A	3248	1/1	0.79	0.42	67,67,67,67	0
57	MG	1A	3599	1/1	0.80	0.15	48,48,48,48	0
57	MG	2A	3525	1/1	0.80	0.15	50,50,50,50	0
57	MG	1a	3175	1/1	0.80	0.12	63,63,63,63	0
57	MG	2a	3033	1/1	0.80	0.15	57,57,57,57	0
57	MG	2a	3037	1/1	0.80	0.17	66,66,66,66	0
57	MG	2a	3049	1/1	0.80	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3918	1/1	0.80	0.13	34,34,34,34	0
57	MG	2A	3615	1/1	0.80	0.07	71,71,71,71	0
57	MG	1a	3178	1/1	0.80	0.14	70,70,70,70	0
57	MG	2B	203	1/1	0.80	0.15	71,71,71,71	0
57	MG	2A	3622	1/1	0.80	0.12	53,53,53,53	0
57	MG	2B	216	1/1	0.80	0.12	63,63,63,63	0
57	MG	1a	3040	1/1	0.80	0.14	66,66,66,66	0
57	MG	1A	3768	1/1	0.80	0.16	55,55,55,55	0
57	MG	2Q	203	1/1	0.80	0.15	62,62,62,62	0
57	MG	1a	3104	1/1	0.80	0.33	61,61,61,61	0
57	MG	1A	3638	1/1	0.80	0.70	38,38,38,38	0
57	MG	1A	3605	1/1	0.80	0.13	52,52,52,52	0
57	MG	1A	3010	1/1	0.80	0.16	50,50,50,50	0
57	MG	1A	3978	1/1	0.80	0.06	46,46,46,46	0
57	MG	2A	3730	1/1	0.81	0.21	52,52,52,52	0
57	MG	1A	3983	1/1	0.81	0.12	55,55,55,55	0
57	MG	1A	3880	1/1	0.81	0.19	54,54,54,54	0
57	MG	1a	3022	1/1	0.81	0.26	73,73,73,73	0
57	MG	2B	212	1/1	0.81	0.14	67,67,67,67	0
57	MG	1A	3210	1/1	0.81	0.11	52,52,52,52	0
57	MG	1a	3153	1/1	0.81	0.08	71,71,71,71	0
57	MG	2A	3160	1/1	0.81	0.14	63,63,63,63	0
57	MG	1A	3812	1/1	0.81	0.32	55,55,55,55	0
57	MG	2Q	204	1/1	0.81	0.09	67,67,67,67	0
57	MG	1a	3042	1/1	0.81	0.18	71,71,71,71	0
57	MG	2A	3181	1/1	0.81	0.28	74,74,74,74	0
57	MG	2A	3583	1/1	0.81	0.09	52,52,52,52	0
57	MG	1A	3899	1/1	0.81	0.06	49,49,49,49	0
57	MG	1A	3835	1/1	0.81	0.13	44,44,44,44	0
57	MG	1A	3459	1/1	0.81	0.12	53,53,53,53	0
57	MG	2A	3611	1/1	0.81	0.18	43,43,43,43	0
57	MG	2A	3223	1/1	0.81	0.15	57,57,57,57	0
57	MG	1a	3209	1/1	0.81	0.14	68,68,68,68	0
57	MG	1a	3214	1/1	0.81	0.12	71,71,71,71	0
57	MG	2A	3277	1/1	0.81	0.10	73,73,73,73	0
57	MG	1B	228	1/1	0.81	0.11	52,52,52,52	0
57	MG	2A	3629	1/1	0.81	0.07	69,69,69,69	0
57	MG	2a	3068	1/1	0.81	0.13	75,75,75,75	0
57	MG	1A	3921	1/1	0.81	0.12	50,50,50,50	0
57	MG	1A	3271	1/1	0.81	0.35	49,49,49,49	0
57	MG	1A	3614	1/1	0.81	0.18	43,43,43,43	0
57	MG	1d	304	1/1	0.81	0.17	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3221	1/1	0.81	0.18	65,65,65,65	0
57	MG	2A	3454	1/1	0.81	0.12	45,45,45,45	0
57	MG	1A	3595	1/1	0.81	0.14	69,69,69,69	0
57	MG	2A	3043	1/1	0.81	0.18	71,71,71,71	0
57	MG	1A	3875	1/1	0.81	0.15	39,39,39,39	0
57	MG	2A	3090	1/1	0.81	0.14	70,70,70,70	0
57	MG	1a	3117	1/1	0.81	0.07	55,55,55,55	0
57	MG	2A	3729	1/1	0.81	0.25	53,53,53,53	0
57	MG	1a	3158	1/1	0.82	0.12	55,55,55,55	0
57	MG	2a	3002	1/1	0.82	0.10	57,57,57,57	0
57	MG	17	105	1/1	0.82	0.42	62,62,62,62	0
57	MG	1B	224	1/1	0.82	0.12	38,38,38,38	0
57	MG	1a	3019	1/1	0.82	0.16	58,58,58,58	0
57	MG	2a	3011	1/1	0.82	0.13	58,58,58,58	0
57	MG	1A	3203	1/1	0.82	0.26	44,44,44,44	0
57	MG	1A	3991	1/1	0.82	0.13	50,50,50,50	0
57	MG	1A	3563	1/1	0.82	0.10	51,51,51,51	0
57	MG	2a	3021	1/1	0.82	0.10	62,62,62,62	0
57	MG	2a	3028	1/1	0.82	0.20	56,56,56,56	0
57	MG	1D	313	1/1	0.82	0.20	50,50,50,50	0
57	MG	1a	3218	1/1	0.82	0.13	71,71,71,71	0
57	MG	2a	3039	1/1	0.82	0.14	82,82,82,82	0
57	MG	2A	3334	1/1	0.82	0.15	52,52,52,52	0
57	MG	2A	3126	1/1	0.82	0.24	65,65,65,65	0
57	MG	2A	3132	1/1	0.82	0.09	60,60,60,60	0
57	MG	1A	3682	1/1	0.82	0.08	68,68,68,68	0
57	MG	2A	3588	1/1	0.82	0.09	54,54,54,54	0
57	MG	2A	3408	1/1	0.82	0.30	52,52,52,52	0
57	MG	1A	4007	1/1	0.82	0.05	54,54,54,54	0
57	MG	2a	3153	1/1	0.82	0.11	63,63,63,63	0
57	MG	2A	3447	1/1	0.82	0.15	64,64,64,64	0
57	MG	1A	3973	1/1	0.82	0.17	55,55,55,55	0
57	MG	1A	3857	1/1	0.82	0.12	51,51,51,51	0
57	MG	2G	202	1/1	0.82	0.08	66,66,66,66	0
57	MG	1d	303	1/1	0.82	0.14	64,64,64,64	0
57	MG	2A	3468	1/1	0.82	0.16	40,40,40,40	0
57	MG	1A	3717	1/1	0.82	0.13	58,58,58,58	0
57	MG	2a	3174	1/1	0.82	0.07	54,54,54,54	0
57	MG	2R	203	1/1	0.82	0.12	54,54,54,54	0
58	MPD	1a	3275	8/8	0.82	0.23	57,66,67,71	0
57	MG	2A	3523	1/1	0.82	0.12	48,48,48,48	0
57	MG	2G	201	1/1	0.83	0.19	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1B	222	1/1	0.83	0.13	74,74,74,74	0
57	MG	1A	3687	1/1	0.83	0.13	56,56,56,56	0
57	MG	2A	3581	1/1	0.83	0.30	62,62,62,62	0
57	MG	1a	3004	1/1	0.83	0.11	55,55,55,55	0
57	MG	1A	3990	1/1	0.83	0.14	47,47,47,47	0
57	MG	2A	3091	1/1	0.83	0.49	84,84,84,84	0
57	MG	2A	3597	1/1	0.83	0.05	64,64,64,64	0
57	MG	2A	3357	1/1	0.83	0.11	47,47,47,47	0
57	MG	2a	3005	1/1	0.83	0.17	66,66,66,66	0
57	MG	2A	3369	1/1	0.83	0.10	36,36,36,36	0
57	MG	1A	3457	1/1	0.83	0.13	44,44,44,44	0
57	MG	2A	3381	1/1	0.83	0.14	48,48,48,48	0
57	MG	1A	3932	1/1	0.83	0.18	51,51,51,51	0
57	MG	1a	3099	1/1	0.83	0.14	59,59,59,59	0
57	MG	1a	3187	1/1	0.83	0.09	60,60,60,60	0
57	MG	1a	3192	1/1	0.83	0.11	63,63,63,63	0
57	MG	2a	3020	1/1	0.83	0.12	59,59,59,59	0
57	MG	1a	3193	1/1	0.83	0.11	59,59,59,59	0
57	MG	2a	3027	1/1	0.83	0.17	68,68,68,68	0
57	MG	2A	3630	1/1	0.83	0.09	55,55,55,55	0
57	MG	1A	3391	1/1	0.83	0.15	43,43,43,43	0
57	MG	1A	3771	1/1	0.83	0.11	36,36,36,36	0
57	MG	1A	3494	1/1	0.83	0.10	32,32,32,32	0
57	MG	2A	3475	1/1	0.83	0.13	58,58,58,58	0
57	MG	2A	3648	1/1	0.83	0.15	53,53,53,53	0
57	MG	2A	3478	1/1	0.83	0.18	64,64,64,64	0
57	MG	1a	3119	1/1	0.83	0.19	69,69,69,69	0
57	MG	2A	3495	1/1	0.83	0.20	57,57,57,57	0
57	MG	2A	3519	1/1	0.83	0.11	50,50,50,50	0
57	MG	1A	3415	1/1	0.83	0.12	35,35,35,35	0
57	MG	2A	3174	1/1	0.83	0.12	63,63,63,63	0
57	MG	2A	3175	1/1	0.83	0.10	70,70,70,70	0
57	MG	1a	3123	1/1	0.83	0.16	78,78,78,78	0
57	MG	1a	3256	1/1	0.83	0.10	61,61,61,61	0
57	MG	1a	3129	1/1	0.83	0.12	64,64,64,64	0
57	MG	1A	3517	1/1	0.83	0.08	36,36,36,36	0
57	MG	2A	3558	1/1	0.83	0.09	40,40,40,40	0
57	MG	1a	3135	1/1	0.83	0.10	79,79,79,79	0
57	MG	1a	3141	1/1	0.83	0.20	60,60,60,60	0
57	MG	2a	3184	1/1	0.83	0.17	67,67,67,67	0
57	MG	1W	201	1/1	0.83	0.20	59,59,59,59	0
57	MG	2D	306	1/1	0.83	0.28	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2F	302	1/1	0.83	0.20	51,51,51,51	0
57	MG	1A	3398	1/1	0.84	0.10	44,44,44,44	0
57	MG	2A	3062	1/1	0.84	0.08	70,70,70,70	0
57	MG	1A	3868	1/1	0.84	0.13	40,40,40,40	0
57	MG	1a	3087	1/1	0.84	0.19	57,57,57,57	0
57	MG	2A	3596	1/1	0.84	0.11	39,39,39,39	0
57	MG	1A	3941	1/1	0.84	0.18	47,47,47,47	0
57	MG	2A	3375	1/1	0.84	0.13	40,40,40,40	0
57	MG	1a	3095	1/1	0.84	0.30	63,63,63,63	0
57	MG	1a	3184	1/1	0.84	0.13	69,69,69,69	0
57	MG	1a	3006	1/1	0.84	0.09	63,63,63,63	0
57	MG	2a	3007	1/1	0.84	0.14	60,60,60,60	0
57	MG	2A	3397	1/1	0.84	0.14	37,37,37,37	0
57	MG	1A	3050	1/1	0.84	0.26	39,39,39,39	0
57	MG	1A	3330	1/1	0.84	0.15	61,61,61,61	0
57	MG	1A	3671	1/1	0.84	0.13	52,52,52,52	0
57	MG	1a	3106	1/1	0.84	0.10	59,59,59,59	0
57	MG	2A	3143	1/1	0.84	0.15	53,53,53,53	0
57	MG	1A	3816	1/1	0.84	0.13	56,56,56,56	0
57	MG	2A	3640	1/1	0.84	0.13	59,59,59,59	0
57	MG	2A	3465	1/1	0.84	0.12	63,63,63,63	0
57	MG	2a	3023	1/1	0.84	0.14	69,69,69,69	0
57	MG	1A	3527	1/1	0.84	0.23	59,59,59,59	0
57	MG	1a	3035	1/1	0.84	0.22	52,52,52,52	0
57	MG	1A	3353	1/1	0.84	0.11	31,31,31,31	0
57	MG	2A	3662	1/1	0.84	0.10	61,61,61,61	0
57	MG	2a	3038	1/1	0.84	0.11	61,61,61,61	0
57	MG	1a	3231	1/1	0.84	0.12	53,53,53,53	0
57	MG	2a	3045	1/1	0.84	0.15	54,54,54,54	0
57	MG	1A	3623	1/1	0.84	0.16	30,30,30,30	0
57	MG	2a	3056	1/1	0.84	0.22	74,74,74,74	0
57	MG	1a	3051	1/1	0.84	0.16	56,56,56,56	0
57	MG	2A	3675	1/1	0.84	0.17	45,45,45,45	0
57	MG	1a	3274	1/1	0.84	0.15	68,68,68,68	0
57	MG	2a	3073	1/1	0.84	0.11	69,69,69,69	0
57	MG	2a	3084	1/1	0.84	0.10	79,79,79,79	0
57	MG	1A	3014	1/1	0.84	0.17	39,39,39,39	0
57	MG	2A	3527	1/1	0.84	0.17	59,59,59,59	0
57	MG	1A	4001	1/1	0.84	0.13	47,47,47,47	0
57	MG	2A	3718	1/1	0.84	0.13	71,71,71,71	0
57	MG	2A	3726	1/1	0.84	0.07	69,69,69,69	0
57	MG	2A	3216	1/1	0.84	0.14	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3860	1/1	0.84	0.11	50,50,50,50	0
57	MG	2a	3161	1/1	0.84	0.07	65,65,65,65	0
57	MG	2A	3233	1/1	0.84	0.14	63,63,63,63	0
57	MG	2A	3733	1/1	0.84	0.17	59,59,59,59	0
57	MG	2A	3238	1/1	0.84	0.09	58,58,58,58	0
57	MG	1A	3577	1/1	0.84	0.12	27,27,27,27	0
57	MG	2A	3247	1/1	0.84	0.11	54,54,54,54	0
57	MG	2a	3180	1/1	0.84	0.06	61,61,61,61	0
57	MG	2A	3001	1/1	0.84	0.17	55,55,55,55	0
57	MG	1a	3068	1/1	0.84	0.13	67,67,67,67	0
57	MG	2A	3313	1/1	0.84	0.17	68,68,68,68	0
57	MG	2A	3032	1/1	0.84	0.15	50,50,50,50	0
57	MG	1T	203	1/1	0.85	0.14	65,65,65,65	0
57	MG	1A	3620	1/1	0.85	0.12	37,37,37,37	0
57	MG	2A	3103	1/1	0.85	0.11	56,56,56,56	0
57	MG	1a	3083	1/1	0.85	0.30	76,76,76,76	0
57	MG	10	107	1/1	0.85	0.09	55,55,55,55	0
57	MG	1a	3189	1/1	0.85	0.15	77,77,77,77	0
57	MG	2A	3406	1/1	0.85	0.13	63,63,63,63	0
57	MG	1A	3621	1/1	0.85	0.28	37,37,37,37	0
57	MG	1A	3692	1/1	0.85	0.11	47,47,47,47	0
57	MG	1A	3707	1/1	0.85	0.19	65,65,65,65	0
57	MG	1A	3571	1/1	0.85	0.14	65,65,65,65	0
57	MG	1A	3736	1/1	0.85	0.13	47,47,47,47	0
57	MG	1A	3959	1/1	0.85	0.21	65,65,65,65	0
57	MG	1A	3513	1/1	0.85	0.21	31,31,31,31	0
57	MG	1a	3109	1/1	0.85	0.18	72,72,72,72	0
57	MG	1A	3193	1/1	0.85	0.16	61,61,61,61	0
57	MG	1a	3232	1/1	0.85	0.19	47,47,47,47	0
57	MG	2A	3479	1/1	0.85	0.12	45,45,45,45	0
57	MG	1A	3123	1/1	0.85	0.22	49,49,49,49	0
57	MG	2A	3189	1/1	0.85	0.18	59,59,59,59	0
57	MG	2A	3515	1/1	0.85	0.09	59,59,59,59	0
57	MG	1D	311	1/1	0.85	0.18	52,52,52,52	0
57	MG	1A	3090	1/1	0.85	0.20	43,43,43,43	0
57	MG	2A	3196	1/1	0.85	0.14	55,55,55,55	0
57	MG	1E	309	1/1	0.85	0.14	25,25,25,25	0
57	MG	2A	3215	1/1	0.85	0.18	53,53,53,53	0
57	MG	1a	3132	1/1	0.85	0.07	57,57,57,57	0
57	MG	1A	3537	1/1	0.85	0.18	61,61,61,61	0
57	MG	1l	201	1/1	0.85	0.65	68,68,68,68	0
57	MG	2a	3120	1/1	0.85	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3557	1/1	0.85	0.11	46,46,46,46	0
57	MG	2A	3556	1/1	0.85	0.10	53,53,53,53	0
57	MG	2a	3147	1/1	0.85	0.12	53,53,53,53	0
57	MG	1a	3056	1/1	0.85	0.15	52,52,52,52	0
57	MG	2B	209	1/1	0.85	0.13	61,61,61,61	0
57	MG	1G	204	1/1	0.85	0.11	50,50,50,50	0
57	MG	1A	3676	1/1	0.85	0.09	48,48,48,48	0
57	MG	1R	202	1/1	0.85	0.15	35,35,35,35	0
57	MG	2A	3287	1/1	0.85	0.10	67,67,67,67	0
57	MG	2E	301	1/1	0.85	0.30	47,47,47,47	0
57	MG	1A	3358	1/1	0.85	0.13	22,22,22,22	0
57	MG	2A	3317	1/1	0.85	0.12	50,50,50,50	0
57	MG	2A	3063	1/1	0.85	0.15	46,46,46,46	0
57	MG	2A	3064	1/1	0.85	0.34	49,49,49,49	0
57	MG	2A	3077	1/1	0.85	0.37	57,57,57,57	0
57	MG	1a	3069	1/1	0.85	0.16	61,61,61,61	0
57	MG	1a	3074	1/1	0.85	0.11	60,60,60,60	0
57	MG	2A	3368	1/1	0.85	0.10	60,60,60,60	0
60	ZN	24	501	1/1	0.85	0.11	119,119,119,119	0
57	MG	1A	3491	1/1	0.86	0.12	59,59,59,59	0
57	MG	2A	3050	1/1	0.86	0.10	66,66,66,66	0
57	MG	2A	3053	1/1	0.86	0.07	48,48,48,48	0
57	MG	2A	3057	1/1	0.86	0.16	51,51,51,51	0
57	MG	1A	3439	1/1	0.86	0.18	57,57,57,57	0
57	MG	2A	3343	1/1	0.86	0.12	56,56,56,56	0
57	MG	1a	3156	1/1	0.86	0.28	64,64,64,64	0
57	MG	1A	3951	1/1	0.86	0.08	60,60,60,60	0
57	MG	2A	3609	1/1	0.86	0.15	48,48,48,48	0
57	MG	1a	3160	1/1	0.86	0.11	60,60,60,60	0
57	MG	1A	3444	1/1	0.86	0.11	55,55,55,55	0
57	MG	1A	3171	1/1	0.86	0.17	45,45,45,45	0
57	MG	1G	201	1/1	0.86	0.07	62,62,62,62	0
57	MG	1A	3974	1/1	0.86	0.12	44,44,44,44	0
57	MG	1A	3975	1/1	0.86	0.19	52,52,52,52	0
57	MG	1A	3188	1/1	0.86	0.23	42,42,42,42	0
57	MG	1a	3082	1/1	0.86	0.14	80,80,80,80	0
57	MG	1a	3191	1/1	0.86	0.11	69,69,69,69	0
57	MG	2A	3426	1/1	0.86	0.08	65,65,65,65	0
57	MG	1A	3583	1/1	0.86	0.18	48,48,48,48	0
57	MG	1a	3084	1/1	0.86	0.13	50,50,50,50	0
57	MG	2a	3035	1/1	0.86	0.23	59,59,59,59	0
57	MG	2a	3036	1/1	0.86	0.14	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1R	204	1/1	0.86	0.17	50,50,50,50	0
57	MG	1a	3201	1/1	0.86	0.11	72,72,72,72	0
57	MG	1A	3626	1/1	0.86	0.20	49,49,49,49	0
57	MG	1A	3988	1/1	0.86	0.33	48,48,48,48	0
57	MG	2A	3665	1/1	0.86	0.11	37,37,37,37	0
57	MG	1A	3989	1/1	0.86	0.16	32,32,32,32	0
57	MG	1A	3627	1/1	0.86	0.19	22,22,22,22	0
57	MG	1A	3587	1/1	0.86	0.10	48,48,48,48	0
57	MG	1a	3228	1/1	0.86	0.22	72,72,72,72	0
57	MG	1A	3772	1/1	0.86	0.13	37,37,37,37	0
57	MG	1A	3419	1/1	0.86	0.17	25,25,25,25	0
57	MG	2A	3496	1/1	0.86	0.13	47,47,47,47	0
57	MG	1a	3243	1/1	0.86	0.07	47,47,47,47	0
57	MG	2A	3723	1/1	0.86	0.13	65,65,65,65	0
57	MG	2a	3131	1/1	0.86	0.30	72,72,72,72	0
57	MG	1A	3884	1/1	0.86	0.12	42,42,42,42	0
57	MG	1A	3793	1/1	0.86	0.09	45,45,45,45	0
57	MG	1A	3151	1/1	0.86	0.12	43,43,43,43	0
57	MG	2A	3214	1/1	0.86	0.23	60,60,60,60	0
57	MG	1A	3803	1/1	0.86	0.11	52,52,52,52	0
57	MG	1B	201	1/1	0.86	0.14	43,43,43,43	0
57	MG	2A	3541	1/1	0.86	0.14	60,60,60,60	0
57	MG	2A	3218	1/1	0.86	0.27	53,53,53,53	0
57	MG	1A	3811	1/1	0.86	0.21	42,42,42,42	0
57	MG	2B	215	1/1	0.86	0.08	72,72,72,72	0
57	MG	1d	306	1/1	0.86	0.07	78,78,78,78	0
57	MG	1g	201	1/1	0.86	0.17	62,62,62,62	0
57	MG	1A	3317	1/1	0.86	0.21	37,37,37,37	0
57	MG	1B	223	1/1	0.86	0.07	44,44,44,44	0
57	MG	1A	3675	1/1	0.86	0.11	71,71,71,71	0
57	MG	2A	3254	1/1	0.86	0.19	57,57,57,57	0
57	MG	1A	3555	1/1	0.86	0.14	45,45,45,45	0
57	MG	1A	3842	1/1	0.86	0.16	45,45,45,45	0
57	MG	2A	3098	1/1	0.87	0.15	54,54,54,54	0
57	MG	2A	3568	1/1	0.87	0.14	43,43,43,43	0
57	MG	1a	3134	1/1	0.87	0.10	43,43,43,43	0
57	MG	1A	3324	1/1	0.87	0.11	35,35,35,35	0
57	MG	1A	3739	1/1	0.87	0.10	42,42,42,42	0
57	MG	2A	3579	1/1	0.87	0.15	55,55,55,55	0
57	MG	1a	3234	1/1	0.87	0.25	63,63,63,63	0
57	MG	2A	3350	1/1	0.87	0.10	46,46,46,46	0
57	MG	1a	3237	1/1	0.87	0.26	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3129	1/1	0.87	0.17	46,46,46,46	0
57	MG	2A	3591	1/1	0.87	0.13	50,50,50,50	0
57	MG	1A	3433	1/1	0.87	0.17	32,32,32,32	0
57	MG	2A	3136	1/1	0.87	0.14	59,59,59,59	0
57	MG	1A	3518	1/1	0.87	0.08	50,50,50,50	0
57	MG	1A	3636	1/1	0.87	0.18	43,43,43,43	0
57	MG	2A	3384	1/1	0.87	0.10	57,57,57,57	0
57	MG	2A	3385	1/1	0.87	0.11	37,37,37,37	0
57	MG	1a	3010	1/1	0.87	0.15	58,58,58,58	0
57	MG	1A	3776	1/1	0.87	0.20	22,22,22,22	0
57	MG	1a	3086	1/1	0.87	0.10	61,61,61,61	0
57	MG	2A	3620	1/1	0.87	0.14	54,54,54,54	0
57	MG	1a	3014	1/1	0.87	0.14	47,47,47,47	0
57	MG	1A	3926	1/1	0.87	0.10	51,51,51,51	0
57	MG	1A	3498	1/1	0.87	0.13	52,52,52,52	0
57	MG	1h	202	1/1	0.87	0.15	66,66,66,66	0
57	MG	1A	3787	1/1	0.87	0.09	28,28,28,28	0
57	MG	2A	3636	1/1	0.87	0.10	53,53,53,53	0
57	MG	1t	201	1/1	0.87	0.12	65,65,65,65	0
57	MG	2A	3643	1/1	0.87	0.12	55,55,55,55	0
57	MG	2A	3458	1/1	0.87	0.10	49,49,49,49	0
57	MG	1a	3181	1/1	0.87	0.20	63,63,63,63	0
57	MG	1A	3357	1/1	0.87	0.15	25,25,25,25	0
57	MG	2A	3201	1/1	0.87	0.13	61,61,61,61	0
57	MG	1A	3691	1/1	0.87	0.20	53,53,53,53	0
57	MG	1a	3101	1/1	0.87	0.16	57,57,57,57	0
57	MG	2a	3050	1/1	0.87	0.14	54,54,54,54	0
57	MG	1A	3799	1/1	0.87	0.08	45,45,45,45	0
57	MG	2a	3057	1/1	0.87	0.21	68,68,68,68	0
57	MG	2a	3058	1/1	0.87	0.10	64,64,64,64	0
57	MG	1N	203	1/1	0.87	0.10	58,58,58,58	0
57	MG	2A	3667	1/1	0.87	0.07	50,50,50,50	0
57	MG	1A	3949	1/1	0.87	0.10	38,38,38,38	0
57	MG	1A	3650	1/1	0.87	0.10	49,49,49,49	0
57	MG	2a	3082	1/1	0.87	0.17	58,58,58,58	0
57	MG	2A	3499	1/1	0.87	0.13	44,44,44,44	0
57	MG	2A	3678	1/1	0.87	0.13	54,54,54,54	0
57	MG	2a	3109	1/1	0.87	0.08	62,62,62,62	0
57	MG	2a	3114	1/1	0.87	0.21	62,62,62,62	0
57	MG	2A	3508	1/1	0.87	0.08	72,72,72,72	0
57	MG	2a	3123	1/1	0.87	0.07	55,55,55,55	0
57	MG	2A	3695	1/1	0.87	0.35	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3696	1/1	0.87	0.22	62,62,62,62	0
57	MG	2A	3224	1/1	0.87	0.27	42,42,42,42	0
57	MG	2a	3134	1/1	0.87	0.11	63,63,63,63	0
57	MG	2a	3139	1/1	0.87	0.19	76,76,76,76	0
57	MG	2A	3516	1/1	0.87	0.09	74,74,74,74	0
57	MG	2A	3700	1/1	0.87	0.28	80,80,80,80	0
57	MG	1a	3053	1/1	0.87	0.16	71,71,71,71	0
57	MG	2a	3155	1/1	0.87	0.14	61,61,61,61	0
57	MG	1a	3203	1/1	0.87	0.12	75,75,75,75	0
57	MG	1a	3204	1/1	0.87	0.13	63,63,63,63	0
57	MG	2A	3728	1/1	0.87	0.26	76,76,76,76	0
57	MG	2A	3067	1/1	0.87	0.13	47,47,47,47	0
57	MG	1A	3876	1/1	0.87	0.16	27,27,27,27	0
57	MG	2A	3252	1/1	0.87	0.10	66,66,66,66	0
57	MG	2A	3732	1/1	0.87	0.20	66,66,66,66	0
57	MG	2a	3173	1/1	0.87	0.16	71,71,71,71	0
57	MG	2A	3083	1/1	0.87	0.15	55,55,55,55	0
57	MG	2A	3268	1/1	0.87	0.12	55,55,55,55	0
57	MG	2A	3270	1/1	0.87	0.22	56,56,56,56	0
57	MG	1B	212	1/1	0.87	0.11	48,48,48,48	0
57	MG	1A	3531	1/1	0.87	0.07	52,52,52,52	0
57	MG	1A	3664	1/1	0.87	0.06	46,46,46,46	0
57	MG	1X	101	1/1	0.87	0.38	48,48,48,48	0
57	MG	1A	3996	1/1	0.88	0.17	56,56,56,56	0
57	MG	2B	207	1/1	0.88	0.18	70,70,70,70	0
57	MG	1A	3758	1/1	0.88	0.24	70,70,70,70	0
57	MG	2B	211	1/1	0.88	0.09	59,59,59,59	0
57	MG	1A	4002	1/1	0.88	0.15	54,54,54,54	0
57	MG	1A	3761	1/1	0.88	0.10	49,49,49,49	0
57	MG	1A	3145	1/1	0.88	0.19	50,50,50,50	0
57	MG	1A	3146	1/1	0.88	0.13	31,31,31,31	0
57	MG	2B	219	1/1	0.88	0.12	66,66,66,66	0
57	MG	2A	3234	1/1	0.88	0.20	46,46,46,46	0
57	MG	2A	3552	1/1	0.88	0.09	50,50,50,50	0
57	MG	2E	307	1/1	0.88	0.18	63,63,63,63	0
57	MG	1a	3023	1/1	0.88	0.14	61,61,61,61	0
57	MG	1A	3588	1/1	0.88	0.12	40,40,40,40	0
57	MG	1A	4022	1/1	0.88	0.08	36,36,36,36	0
57	MG	2O	202	1/1	0.88	0.18	69,69,69,69	0
57	MG	2A	3005	1/1	0.88	0.10	62,62,62,62	0
57	MG	2A	3017	1/1	0.88	0.12	47,47,47,47	0
57	MG	2A	3028	1/1	0.88	0.22	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3886	1/1	0.88	0.12	48,48,48,48	0
57	MG	1A	3775	1/1	0.88	0.10	32,32,32,32	0
57	MG	1A	3912	1/1	0.88	0.06	42,42,42,42	0
57	MG	1A	3589	1/1	0.88	0.17	43,43,43,43	0
57	MG	1A	3040	1/1	0.88	0.13	37,37,37,37	0
57	MG	1A	3666	1/1	0.88	0.16	21,21,21,21	0
57	MG	1A	3288	1/1	0.88	0.13	50,50,50,50	0
57	MG	1a	3179	1/1	0.88	0.07	65,65,65,65	0
57	MG	1A	3155	1/1	0.88	0.28	40,40,40,40	0
57	MG	2A	3072	1/1	0.88	0.43	49,49,49,49	0
57	MG	2A	3599	1/1	0.88	0.25	49,49,49,49	0
57	MG	2A	3602	1/1	0.88	0.08	54,54,54,54	0
57	MG	2A	3074	1/1	0.88	0.18	48,48,48,48	0
57	MG	2a	3019	1/1	0.88	0.11	86,86,86,86	0
57	MG	2A	3604	1/1	0.88	0.11	41,41,41,41	0
57	MG	1A	3321	1/1	0.88	0.33	66,66,66,66	0
57	MG	2A	3078	1/1	0.88	0.35	53,53,53,53	0
57	MG	2A	3363	1/1	0.88	0.10	48,48,48,48	0
57	MG	2A	3364	1/1	0.88	0.14	44,44,44,44	0
57	MG	1A	3463	1/1	0.88	0.27	59,59,59,59	0
57	MG	1A	3481	1/1	0.88	0.21	25,25,25,25	0
57	MG	1A	3158	1/1	0.88	0.27	27,27,27,27	0
57	MG	1A	3556	1/1	0.88	0.13	39,39,39,39	0
57	MG	2A	3626	1/1	0.88	0.19	61,61,61,61	0
57	MG	1a	3078	1/1	0.88	0.27	65,65,65,65	0
57	MG	1A	3825	1/1	0.88	0.15	26,26,26,26	0
57	MG	2a	3047	1/1	0.88	0.17	69,69,69,69	0
57	MG	2a	3048	1/1	0.88	0.24	63,63,63,63	0
57	MG	1G	202	1/1	0.88	0.13	42,42,42,42	0
57	MG	2A	3631	1/1	0.88	0.08	58,58,58,58	0
57	MG	2a	3052	1/1	0.88	0.10	59,59,59,59	0
57	MG	1A	3027	1/1	0.88	0.09	65,65,65,65	0
57	MG	1A	3967	1/1	0.88	0.18	39,39,39,39	0
57	MG	1A	3969	1/1	0.88	0.28	59,59,59,59	0
57	MG	1a	3213	1/1	0.88	0.06	54,54,54,54	0
57	MG	2A	3424	1/1	0.88	0.12	54,54,54,54	0
57	MG	2a	3066	1/1	0.88	0.07	68,68,68,68	0
57	MG	1A	3706	1/1	0.88	0.26	57,57,57,57	0
57	MG	2A	3430	1/1	0.88	0.16	64,64,64,64	0
57	MG	2a	3077	1/1	0.88	0.17	60,60,60,60	0
57	MG	1a	3217	1/1	0.88	0.07	66,66,66,66	0
57	MG	2a	3083	1/1	0.88	0.23	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3651	1/1	0.88	0.12	37,37,37,37	0
57	MG	2a	3089	1/1	0.88	0.12	60,60,60,60	0
57	MG	2A	3655	1/1	0.88	0.04	69,69,69,69	0
57	MG	1A	3347	1/1	0.88	0.09	46,46,46,46	0
57	MG	2A	3451	1/1	0.88	0.22	53,53,53,53	0
57	MG	1A	3709	1/1	0.88	0.14	53,53,53,53	0
57	MG	1A	3976	1/1	0.88	0.14	55,55,55,55	0
57	MG	2A	3152	1/1	0.88	0.14	46,46,46,46	0
57	MG	1a	3098	1/1	0.88	0.11	57,57,57,57	0
57	MG	1A	3853	1/1	0.88	0.14	27,27,27,27	0
57	MG	1A	3715	1/1	0.88	0.14	35,35,35,35	0
57	MG	2a	3137	1/1	0.88	0.13	55,55,55,55	0
57	MG	1A	3071	1/1	0.88	0.18	40,40,40,40	0
57	MG	2A	3682	1/1	0.88	0.08	53,53,53,53	0
57	MG	1a	3236	1/1	0.88	0.10	65,65,65,65	0
57	MG	1A	3718	1/1	0.88	0.42	38,38,38,38	0
57	MG	2A	3489	1/1	0.88	0.13	67,67,67,67	0
57	MG	2A	3176	1/1	0.88	0.21	57,57,57,57	0
57	MG	1l	104	1/1	0.88	0.27	48,48,48,48	0
57	MG	1a	3253	1/1	0.88	0.10	51,51,51,51	0
57	MG	2A	3708	1/1	0.88	0.22	59,59,59,59	0
57	MG	1A	3720	1/1	0.88	0.12	35,35,35,35	0
57	MG	2A	3500	1/1	0.88	0.13	42,42,42,42	0
57	MG	1a	3258	1/1	0.88	0.21	68,68,68,68	0
57	MG	2A	3510	1/1	0.88	0.06	58,58,58,58	0
57	MG	2A	3193	1/1	0.88	0.28	58,58,58,58	0
57	MG	1A	3228	1/1	0.88	0.17	38,38,38,38	0
57	MG	1a	3001	1/1	0.88	0.21	68,68,68,68	0
57	MG	1A	3505	1/1	0.88	0.09	42,42,42,42	0
57	MG	2A	3524	1/1	0.88	0.09	35,35,35,35	0
57	MG	2B	201	1/1	0.88	0.12	64,64,64,64	0
59	ARG	1F	317	12/12	0.88	0.14	48,60,72,73	0
57	MG	1A	3748	1/1	0.88	0.11	49,49,49,49	0
57	MG	1F	314	1/1	0.89	0.11	41,41,41,41	0
57	MG	1A	3372	1/1	0.89	0.12	65,65,65,65	0
57	MG	1a	3216	1/1	0.89	0.07	74,74,74,74	0
57	MG	1A	3441	1/1	0.89	0.15	48,48,48,48	0
57	MG	1A	3309	1/1	0.89	0.33	25,25,25,25	0
57	MG	1A	3378	1/1	0.89	0.25	60,60,60,60	0
57	MG	1A	3313	1/1	0.89	0.30	39,39,39,39	0
57	MG	1a	3089	1/1	0.89	0.16	55,55,55,55	0
57	MG	1a	3229	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
57	MG	2B	213	1/1	0.89	0.12	69,69,69,69	0
57	MG	2A	3520	1/1	0.89	0.23	57,57,57,57	0
57	MG	2A	3522	1/1	0.89	0.15	35,35,35,35	0
57	MG	2B	217	1/1	0.89	0.11	62,62,62,62	0
57	MG	2A	3180	1/1	0.89	0.19	56,56,56,56	0
57	MG	1A	3255	1/1	0.89	0.23	36,36,36,36	0
57	MG	2A	3188	1/1	0.89	0.11	60,60,60,60	0
57	MG	1P	204	1/1	0.89	0.07	69,69,69,69	0
57	MG	1Q	206	1/1	0.89	0.11	41,41,41,41	0
57	MG	1a	3097	1/1	0.89	0.15	60,60,60,60	0
57	MG	2A	3532	1/1	0.89	0.07	62,62,62,62	0
57	MG	1A	3547	1/1	0.89	0.15	44,44,44,44	0
57	MG	1A	3980	1/1	0.89	0.10	48,48,48,48	0
57	MG	1a	3245	1/1	0.89	0.12	46,46,46,46	0
57	MG	2A	3203	1/1	0.89	0.11	52,52,52,52	0
57	MG	1A	3268	1/1	0.89	0.18	31,31,31,31	0
57	MG	1A	3465	1/1	0.89	0.10	55,55,55,55	0
57	MG	1A	3873	1/1	0.89	0.20	30,30,30,30	0
57	MG	2U	201	1/1	0.89	0.16	64,64,64,64	0
57	MG	1A	3468	1/1	0.89	0.12	50,50,50,50	0
57	MG	1a	3108	1/1	0.89	0.09	56,56,56,56	0
57	MG	2A	3221	1/1	0.89	0.10	53,53,53,53	0
57	MG	10	104	1/1	0.89	0.22	60,60,60,60	0
57	MG	1a	3111	1/1	0.89	0.05	56,56,56,56	0
57	MG	1A	3471	1/1	0.89	0.16	26,26,26,26	0
57	MG	2A	3578	1/1	0.89	0.05	50,50,50,50	0
57	MG	1l	102	1/1	0.89	0.34	48,48,48,48	0
57	MG	2A	3580	1/1	0.89	0.09	43,43,43,43	0
57	MG	1e	201	1/1	0.89	0.19	63,63,63,63	0
57	MG	1A	3769	1/1	0.89	0.17	51,51,51,51	0
57	MG	1A	3646	1/1	0.89	0.38	52,52,52,52	0
57	MG	1A	3998	1/1	0.89	0.20	47,47,47,47	0
57	MG	1m	201	1/1	0.89	0.12	62,62,62,62	0
57	MG	1A	3480	1/1	0.89	0.13	27,27,27,27	0
57	MG	2A	3263	1/1	0.89	0.15	51,51,51,51	0
57	MG	1A	3392	1/1	0.89	0.16	35,35,35,35	0
57	MG	1A	3041	1/1	0.89	0.40	58,58,58,58	0
57	MG	1A	3486	1/1	0.89	0.17	18,18,18,18	0
57	MG	1A	4009	1/1	0.89	0.17	45,45,45,45	0
57	MG	2A	3298	1/1	0.89	0.36	56,56,56,56	0
57	MG	2A	3306	1/1	0.89	0.20	43,43,43,43	0
57	MG	1a	3144	1/1	0.89	0.16	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4010	1/1	0.89	0.19	36,36,36,36	0
57	MG	1A	3902	1/1	0.89	0.20	20,20,20,20	0
57	MG	2A	3618	1/1	0.89	0.12	44,44,44,44	0
57	MG	2A	3034	1/1	0.89	0.10	63,63,63,63	0
57	MG	2A	3035	1/1	0.89	0.13	45,45,45,45	0
57	MG	2A	3041	1/1	0.89	0.21	44,44,44,44	0
57	MG	1A	3784	1/1	0.89	0.10	29,29,29,29	0
57	MG	2A	3347	1/1	0.89	0.36	47,47,47,47	0
57	MG	2A	3046	1/1	0.89	0.15	63,63,63,63	0
57	MG	2a	3059	1/1	0.89	0.09	71,71,71,71	0
57	MG	2A	3351	1/1	0.89	0.18	38,38,38,38	0
57	MG	1A	4020	1/1	0.89	0.20	59,59,59,59	0
57	MG	1a	3157	1/1	0.89	0.10	58,58,58,58	0
57	MG	2A	3054	1/1	0.89	0.10	60,60,60,60	0
57	MG	2a	3069	1/1	0.89	0.20	57,57,57,57	0
57	MG	1A	3585	1/1	0.89	0.12	36,36,36,36	0
57	MG	1a	3159	1/1	0.89	0.11	56,56,56,56	0
57	MG	2A	3374	1/1	0.89	0.14	46,46,46,46	0
57	MG	1a	3025	1/1	0.89	0.14	60,60,60,60	0
57	MG	1a	3027	1/1	0.89	0.19	56,56,56,56	0
57	MG	1A	3919	1/1	0.89	0.11	47,47,47,47	0
57	MG	2a	3095	1/1	0.89	0.10	53,53,53,53	0
57	MG	2A	3649	1/1	0.89	0.11	46,46,46,46	0
57	MG	1B	211	1/1	0.89	0.12	71,71,71,71	0
57	MG	1A	3790	1/1	0.89	0.19	47,47,47,47	0
57	MG	2A	3657	1/1	0.89	0.08	58,58,58,58	0
57	MG	2A	3658	1/1	0.89	0.10	66,66,66,66	0
57	MG	1A	3078	1/1	0.89	0.18	44,44,44,44	0
57	MG	1A	3186	1/1	0.89	0.18	38,38,38,38	0
57	MG	2A	3403	1/1	0.89	0.16	34,34,34,34	0
57	MG	1A	3416	1/1	0.89	0.12	38,38,38,38	0
57	MG	2A	3407	1/1	0.89	0.24	45,45,45,45	0
57	MG	1A	3802	1/1	0.89	0.14	26,26,26,26	0
57	MG	1A	3282	1/1	0.89	0.20	33,33,33,33	0
57	MG	1a	3190	1/1	0.89	0.14	55,55,55,55	0
57	MG	1A	3060	1/1	0.89	0.24	36,36,36,36	0
57	MG	2A	3437	1/1	0.89	0.51	49,49,49,49	0
57	MG	1A	3290	1/1	0.89	0.07	67,67,67,67	0
57	MG	1D	307	1/1	0.89	0.19	47,47,47,47	0
57	MG	1A	3600	1/1	0.89	0.16	33,33,33,33	0
57	MG	2A	3110	1/1	0.89	0.45	56,56,56,56	0
57	MG	1A	3702	1/1	0.89	0.14	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1E	308	1/1	0.89	0.14	44,44,44,44	0
57	MG	2A	3702	1/1	0.89	0.08	62,62,62,62	0
57	MG	2A	3122	1/1	0.89	0.13	48,48,48,48	0
57	MG	2A	3123	1/1	0.89	0.19	38,38,38,38	0
57	MG	2a	3178	1/1	0.89	0.08	74,74,74,74	0
57	MG	2A	3719	1/1	0.89	0.10	47,47,47,47	0
57	MG	2A	3124	1/1	0.89	0.10	38,38,38,38	0
57	MG	1A	3368	1/1	0.89	0.14	39,39,39,39	0
57	MG	1a	3206	1/1	0.89	0.14	56,56,56,56	0
57	MG	1A	3608	1/1	0.89	0.11	70,70,70,70	0
57	MG	1a	3210	1/1	0.89	0.15	65,65,65,65	0
57	MG	1a	3212	1/1	0.89	0.09	69,69,69,69	0
60	ZN	29	501	1/1	0.89	0.09	78,78,78,78	0
57	MG	1B	207	1/1	0.90	0.25	53,53,53,53	0
57	MG	1B	209	1/1	0.90	0.14	38,38,38,38	0
57	MG	1A	3929	1/1	0.90	0.07	42,42,42,42	0
57	MG	1A	3461	1/1	0.90	0.20	16,16,16,16	0
57	MG	1B	217	1/1	0.90	0.10	54,54,54,54	0
57	MG	1l	203	1/1	0.90	0.07	63,63,63,63	0
57	MG	2A	3540	1/1	0.90	0.14	53,53,53,53	0
57	MG	2A	3222	1/1	0.90	0.12	43,43,43,43	0
57	MG	1a	3151	1/1	0.90	0.09	64,64,64,64	0
57	MG	1n	102	1/1	0.90	0.09	53,53,53,53	0
57	MG	2A	3548	1/1	0.90	0.07	51,51,51,51	0
57	MG	2A	3225	1/1	0.90	0.23	55,55,55,55	0
57	MG	1A	3567	1/1	0.90	0.13	55,55,55,55	0
57	MG	2A	3553	1/1	0.90	0.13	53,53,53,53	0
57	MG	2A	3554	1/1	0.90	0.06	69,69,69,69	0
57	MG	1y	204	1/1	0.90	0.14	63,63,63,63	0
57	MG	1A	3711	1/1	0.90	0.12	33,33,33,33	0
57	MG	1A	3940	1/1	0.90	0.11	39,39,39,39	0
57	MG	1A	3401	1/1	0.90	0.19	19,19,19,19	0
57	MG	1A	3836	1/1	0.90	0.09	36,36,36,36	0
57	MG	2W	202	1/1	0.90	0.37	52,52,52,52	0
57	MG	2l	101	1/1	0.90	0.22	66,66,66,66	0
57	MG	2A	3249	1/1	0.90	0.31	49,49,49,49	0
57	MG	2a	3001	1/1	0.90	0.19	50,50,50,50	0
57	MG	1A	3322	1/1	0.90	0.40	59,59,59,59	0
57	MG	1a	3161	1/1	0.90	0.09	65,65,65,65	0
57	MG	1a	3165	1/1	0.90	0.18	70,70,70,70	0
57	MG	1A	3633	1/1	0.90	0.14	57,57,57,57	0
57	MG	1a	3169	1/1	0.90	0.08	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3039	1/1	0.90	0.25	58,58,58,58	0
57	MG	2A	3278	1/1	0.90	0.23	45,45,45,45	0
57	MG	2A	3281	1/1	0.90	0.10	66,66,66,66	0
57	MG	1A	3850	1/1	0.90	0.14	63,63,63,63	0
57	MG	2A	3292	1/1	0.90	0.13	64,64,64,64	0
57	MG	1D	309	1/1	0.90	0.81	48,48,48,48	0
57	MG	2A	3302	1/1	0.90	0.19	44,44,44,44	0
57	MG	1A	3719	1/1	0.90	0.20	33,33,33,33	0
57	MG	1A	3374	1/1	0.90	0.12	46,46,46,46	0
57	MG	1a	3064	1/1	0.90	0.11	58,58,58,58	0
57	MG	1a	3066	1/1	0.90	0.44	63,63,63,63	0
57	MG	2A	3056	1/1	0.90	0.17	60,60,60,60	0
57	MG	1A	3971	1/1	0.90	0.10	27,27,27,27	0
57	MG	2A	3340	1/1	0.90	0.15	68,68,68,68	0
57	MG	1A	3516	1/1	0.90	0.09	52,52,52,52	0
57	MG	1E	312	1/1	0.90	0.13	59,59,59,59	0
57	MG	1A	3202	1/1	0.90	0.10	40,40,40,40	0
57	MG	2a	3040	1/1	0.90	0.12	66,66,66,66	0
57	MG	1A	3126	1/1	0.90	0.10	62,62,62,62	0
57	MG	2A	3069	1/1	0.90	0.11	50,50,50,50	0
57	MG	1A	3649	1/1	0.90	0.19	49,49,49,49	0
57	MG	2A	3361	1/1	0.90	0.18	55,55,55,55	0
57	MG	1a	3080	1/1	0.90	0.50	65,65,65,65	0
57	MG	1A	3759	1/1	0.90	0.14	35,35,35,35	0
57	MG	2a	3053	1/1	0.90	0.14	56,56,56,56	0
57	MG	2A	3365	1/1	0.90	0.11	34,34,34,34	0
57	MG	1A	3869	1/1	0.90	0.11	52,52,52,52	0
57	MG	1A	3264	1/1	0.90	0.17	34,34,34,34	0
57	MG	1a	3205	1/1	0.90	0.08	77,77,77,77	0
57	MG	1A	3524	1/1	0.90	0.11	36,36,36,36	0
57	MG	1a	3207	1/1	0.90	0.05	69,69,69,69	0
57	MG	1A	3986	1/1	0.90	0.46	46,46,46,46	0
57	MG	2A	3382	1/1	0.90	0.17	58,58,58,58	0
57	MG	1A	3874	1/1	0.90	0.17	46,46,46,46	0
57	MG	1a	3088	1/1	0.90	0.18	58,58,58,58	0
57	MG	2a	3076	1/1	0.90	0.19	61,61,61,61	0
57	MG	1A	3594	1/1	0.90	0.11	50,50,50,50	0
57	MG	2A	3394	1/1	0.90	0.08	58,58,58,58	0
57	MG	1a	3092	1/1	0.90	0.15	52,52,52,52	0
57	MG	1A	3382	1/1	0.90	0.09	43,43,43,43	0
57	MG	2a	3086	1/1	0.90	0.15	54,54,54,54	0
57	MG	2a	3087	1/1	0.90	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3530	1/1	0.90	0.11	56,56,56,56	0
57	MG	2A	3116	1/1	0.90	0.15	51,51,51,51	0
57	MG	1A	3352	1/1	0.90	0.14	26,26,26,26	0
57	MG	1A	3995	1/1	0.90	0.15	57,57,57,57	0
57	MG	1a	3221	1/1	0.90	0.09	62,62,62,62	0
57	MG	1a	3223	1/1	0.90	0.08	61,61,61,61	0
57	MG	1A	3536	1/1	0.90	0.12	50,50,50,50	0
57	MG	1A	3601	1/1	0.90	0.14	50,50,50,50	0
57	MG	2A	3133	1/1	0.90	0.15	64,64,64,64	0
57	MG	2A	3450	1/1	0.90	0.10	51,51,51,51	0
57	MG	2A	3134	1/1	0.90	0.14	56,56,56,56	0
57	MG	1Y	201	1/1	0.90	0.15	53,53,53,53	0
57	MG	1A	3207	1/1	0.90	0.11	58,58,58,58	0
57	MG	1A	3889	1/1	0.90	0.12	56,56,56,56	0
57	MG	10	108	1/1	0.90	0.07	47,47,47,47	0
57	MG	1A	3895	1/1	0.90	0.12	28,28,28,28	0
57	MG	1A	3685	1/1	0.90	0.17	28,28,28,28	0
57	MG	2A	3165	1/1	0.90	0.16	59,59,59,59	0
57	MG	1A	3487	1/1	0.90	0.09	53,53,53,53	0
57	MG	1A	3690	1/1	0.90	0.14	37,37,37,37	0
57	MG	1a	3248	1/1	0.90	0.08	54,54,54,54	0
57	MG	2A	3490	1/1	0.90	0.09	56,56,56,56	0
57	MG	1a	3250	1/1	0.90	0.09	57,57,57,57	0
57	MG	1A	3552	1/1	0.90	0.10	40,40,40,40	0
57	MG	1a	3002	1/1	0.90	0.21	60,60,60,60	0
57	MG	1A	3063	1/1	0.90	0.10	35,35,35,35	0
57	MG	1a	3261	1/1	0.90	0.08	51,51,51,51	0
57	MG	1a	3264	1/1	0.90	0.07	77,77,77,77	0
57	MG	2a	3183	1/1	0.90	0.17	66,66,66,66	0
57	MG	1a	3128	1/1	0.90	0.09	64,64,64,64	0
57	MG	2a	3185	1/1	0.90	0.10	77,77,77,77	0
57	MG	1A	3701	1/1	0.90	0.14	34,34,34,34	0
57	MG	2f	201	1/1	0.90	0.11	60,60,60,60	0
57	MG	2p	101	1/1	0.90	0.16	60,60,60,60	0
57	MG	1A	3184	1/1	0.90	0.10	43,43,43,43	0
57	MG	1A	3082	1/1	0.90	0.28	47,47,47,47	0
57	MG	1B	203	1/1	0.90	0.24	64,64,64,64	0
57	MG	1d	305	1/1	0.90	0.12	55,55,55,55	0
57	MG	2A	3207	1/1	0.90	0.09	52,52,52,52	0
57	MG	2A	3213	1/1	0.91	0.16	56,56,56,56	0
57	MG	2A	3491	1/1	0.91	0.30	56,56,56,56	0
57	MG	1A	3801	1/1	0.91	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3024	1/1	0.91	0.16	50,50,50,50	0
57	MG	2B	202	1/1	0.91	0.12	62,62,62,62	0
57	MG	1A	3898	1/1	0.91	0.12	56,56,56,56	0
57	MG	1a	3188	1/1	0.91	0.26	80,80,80,80	0
57	MG	1A	3412	1/1	0.91	0.19	48,48,48,48	0
57	MG	1A	3148	1/1	0.91	0.08	40,40,40,40	0
57	MG	1A	3474	1/1	0.91	0.10	59,59,59,59	0
57	MG	1A	3915	1/1	0.91	0.05	47,47,47,47	0
57	MG	1A	3916	1/1	0.91	0.06	47,47,47,47	0
57	MG	2A	3518	1/1	0.91	0.17	59,59,59,59	0
57	MG	2A	3231	1/1	0.91	0.29	59,59,59,59	0
57	MG	1V	204	1/1	0.91	0.18	43,43,43,43	0
57	MG	1A	3477	1/1	0.91	0.17	18,18,18,18	0
57	MG	2A	3236	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3257	1/1	0.91	0.22	39,39,39,39	0
57	MG	2D	309	1/1	0.91	0.11	46,46,46,46	0
57	MG	2A	3242	1/1	0.91	0.39	37,37,37,37	0
57	MG	2A	3245	1/1	0.91	0.18	55,55,55,55	0
57	MG	1A	3022	1/1	0.91	0.15	47,47,47,47	0
57	MG	2A	3055	1/1	0.91	0.11	56,56,56,56	0
57	MG	1A	3833	1/1	0.91	0.05	41,41,41,41	0
57	MG	2A	3533	1/1	0.91	0.32	71,71,71,71	0
57	MG	2P	201	1/1	0.91	0.21	60,60,60,60	0
57	MG	2A	3534	1/1	0.91	0.13	70,70,70,70	0
57	MG	2A	3535	1/1	0.91	0.11	60,60,60,60	0
57	MG	1a	3093	1/1	0.91	0.14	47,47,47,47	0
57	MG	2A	3251	1/1	0.91	0.22	53,53,53,53	0
57	MG	2A	3058	1/1	0.91	0.15	32,32,32,32	0
57	MG	1A	3726	1/1	0.91	0.12	42,42,42,42	0
57	MG	2A	3258	1/1	0.91	0.13	48,48,48,48	0
57	MG	20	102	1/1	0.91	0.07	56,56,56,56	0
57	MG	1A	3727	1/1	0.91	0.17	42,42,42,42	0
57	MG	27	101	1/1	0.91	0.49	49,49,49,49	0
57	MG	10	109	1/1	0.91	0.13	58,58,58,58	0
57	MG	2A	3066	1/1	0.91	0.10	44,44,44,44	0
57	MG	2A	3273	1/1	0.91	0.16	42,42,42,42	0
57	MG	1A	3734	1/1	0.91	0.12	41,41,41,41	0
57	MG	1A	3187	1/1	0.91	0.10	42,42,42,42	0
57	MG	15	3107	1/1	0.91	0.17	25,25,25,25	0
57	MG	1A	3847	1/1	0.91	0.10	36,36,36,36	0
57	MG	1A	3098	1/1	0.91	0.24	49,49,49,49	0
57	MG	2A	3295	1/1	0.91	0.21	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3103	1/1	0.91	0.10	67,67,67,67	0
57	MG	18	101	1/1	0.91	0.14	43,43,43,43	0
57	MG	2A	3304	1/1	0.91	0.11	54,54,54,54	0
57	MG	2a	3018	1/1	0.91	0.14	54,54,54,54	0
57	MG	1A	3668	1/1	0.91	0.12	49,49,49,49	0
57	MG	2A	3308	1/1	0.91	0.17	51,51,51,51	0
57	MG	2A	3311	1/1	0.91	0.09	43,43,43,43	0
57	MG	1A	3218	1/1	0.91	0.18	64,64,64,64	0
57	MG	1A	3854	1/1	0.91	0.08	50,50,50,50	0
57	MG	2A	3585	1/1	0.91	0.15	55,55,55,55	0
57	MG	2a	3030	1/1	0.91	0.18	57,57,57,57	0
57	MG	2A	3322	1/1	0.91	0.11	52,52,52,52	0
57	MG	1A	3603	1/1	0.91	0.11	30,30,30,30	0
57	MG	1A	3157	1/1	0.91	0.24	44,44,44,44	0
57	MG	1B	221	1/1	0.91	0.17	34,34,34,34	0
57	MG	1A	3111	1/1	0.91	0.21	37,37,37,37	0
57	MG	2A	3106	1/1	0.91	0.12	39,39,39,39	0
57	MG	1A	3968	1/1	0.91	0.49	56,56,56,56	0
57	MG	2a	3043	1/1	0.91	0.10	70,70,70,70	0
57	MG	1A	3077	1/1	0.91	0.20	27,27,27,27	0
57	MG	1A	3683	1/1	0.91	0.05	66,66,66,66	0
57	MG	2A	3115	1/1	0.91	0.25	54,54,54,54	0
57	MG	2A	3353	1/1	0.91	0.14	41,41,41,41	0
57	MG	2A	3612	1/1	0.91	0.11	59,59,59,59	0
57	MG	1a	3242	1/1	0.91	0.36	64,64,64,64	0
57	MG	1A	3617	1/1	0.91	0.20	34,34,34,34	0
57	MG	2A	3617	1/1	0.91	0.14	75,75,75,75	0
57	MG	1A	3240	1/1	0.91	0.35	32,32,32,32	0
57	MG	1A	3562	1/1	0.91	0.07	57,57,57,57	0
57	MG	1A	3501	1/1	0.91	0.11	45,45,45,45	0
57	MG	2A	3366	1/1	0.91	0.13	40,40,40,40	0
57	MG	1a	3137	1/1	0.91	0.12	51,51,51,51	0
57	MG	2A	3627	1/1	0.91	0.13	38,38,38,38	0
57	MG	1a	3140	1/1	0.91	0.14	58,58,58,58	0
57	MG	1A	3977	1/1	0.91	0.12	64,64,64,64	0
57	MG	2a	3071	1/1	0.91	0.10	64,64,64,64	0
57	MG	1a	3036	1/1	0.91	0.19	52,52,52,52	0
57	MG	1A	3782	1/1	0.91	0.15	44,44,44,44	0
57	MG	2A	3633	1/1	0.91	0.27	61,61,61,61	0
57	MG	1a	3269	1/1	0.91	0.23	75,75,75,75	0
57	MG	2A	3138	1/1	0.91	0.12	44,44,44,44	0
57	MG	1a	3147	1/1	0.91	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3641	1/1	0.91	0.07	43,43,43,43	0
57	MG	2A	3642	1/1	0.91	0.15	45,45,45,45	0
57	MG	1E	304	1/1	0.91	0.15	26,26,26,26	0
57	MG	2a	3091	1/1	0.91	0.12	64,64,64,64	0
57	MG	2A	3386	1/1	0.91	0.14	62,62,62,62	0
57	MG	1a	3044	1/1	0.91	0.17	57,57,57,57	0
57	MG	2a	3102	1/1	0.91	0.18	51,51,51,51	0
57	MG	1d	302	1/1	0.91	0.17	63,63,63,63	0
57	MG	2A	3395	1/1	0.91	0.20	60,60,60,60	0
57	MG	1E	306	1/1	0.91	0.16	42,42,42,42	0
57	MG	1A	3502	1/1	0.91	0.15	50,50,50,50	0
57	MG	1A	3878	1/1	0.91	0.17	39,39,39,39	0
57	MG	2a	3130	1/1	0.91	0.10	65,65,65,65	0
57	MG	2A	3170	1/1	0.91	0.21	44,44,44,44	0
57	MG	1A	3396	1/1	0.91	0.21	27,27,27,27	0
57	MG	2A	3419	1/1	0.91	0.10	51,51,51,51	0
57	MG	1F	307	1/1	0.91	0.15	28,28,28,28	0
57	MG	2a	3138	1/1	0.91	0.09	67,67,67,67	0
57	MG	1A	3984	1/1	0.91	0.10	47,47,47,47	0
57	MG	2a	3141	1/1	0.91	0.08	68,68,68,68	0
57	MG	1a	3061	1/1	0.91	0.24	60,60,60,60	0
57	MG	2a	3150	1/1	0.91	0.11	49,49,49,49	0
57	MG	1a	3062	1/1	0.91	0.12	57,57,57,57	0
57	MG	2A	3439	1/1	0.91	0.24	52,52,52,52	0
57	MG	2A	3186	1/1	0.91	0.10	49,49,49,49	0
57	MG	2a	3156	1/1	0.91	0.18	72,72,72,72	0
57	MG	1A	3397	1/1	0.91	0.10	35,35,35,35	0
57	MG	1A	3792	1/1	0.91	0.08	49,49,49,49	0
57	MG	1a	3171	1/1	0.91	0.07	61,61,61,61	0
57	MG	1A	3299	1/1	0.91	0.14	44,44,44,44	0
57	MG	2A	3689	1/1	0.91	0.11	55,55,55,55	0
57	MG	1A	3253	1/1	0.91	0.22	37,37,37,37	0
57	MG	1a	3177	1/1	0.91	0.12	59,59,59,59	0
57	MG	2A	3462	1/1	0.91	0.12	53,53,53,53	0
57	MG	2A	3197	1/1	0.91	0.21	59,59,59,59	0
57	MG	2A	3198	1/1	0.91	0.19	61,61,61,61	0
57	MG	1A	3411	1/1	0.91	0.09	33,33,33,33	0
57	MG	2A	3705	1/1	0.91	0.12	56,56,56,56	0
57	MG	2A	3470	1/1	0.91	0.23	61,61,61,61	0
57	MG	2A	3717	1/1	0.91	0.17	63,63,63,63	0
57	MG	2A	3472	1/1	0.91	0.07	66,66,66,66	0
57	MG	1a	3070	1/1	0.91	0.12	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3206	1/1	0.91	0.19	41,41,41,41	0
57	MG	2A	3724	1/1	0.91	0.19	66,66,66,66	0
57	MG	1A	3993	1/1	0.91	0.17	24,24,24,24	0
57	MG	2A	3484	1/1	0.91	0.13	28,28,28,28	0
57	MG	2A	3485	1/1	0.91	0.13	61,61,61,61	0
57	MG	2A	3009	1/1	0.91	0.23	45,45,45,45	0
57	MG	2A	3483	1/1	0.92	0.10	64,64,64,64	0
57	MG	1A	3705	1/1	0.92	0.70	57,57,57,57	0
57	MG	1A	3813	1/1	0.92	0.09	37,37,37,37	0
57	MG	1A	3939	1/1	0.92	0.16	44,44,44,44	0
57	MG	1A	3616	1/1	0.92	0.34	38,38,38,38	0
57	MG	2A	3217	1/1	0.92	0.22	65,65,65,65	0
57	MG	1a	3174	1/1	0.92	0.15	76,76,76,76	0
57	MG	1A	3824	1/1	0.92	0.42	26,26,26,26	0
57	MG	2A	3019	1/1	0.92	0.65	53,53,53,53	0
57	MG	2A	3497	1/1	0.92	0.12	63,63,63,63	0
57	MG	1A	3209	1/1	0.92	0.27	42,42,42,42	0
57	MG	1A	3830	1/1	0.92	0.15	45,45,45,45	0
57	MG	1A	3831	1/1	0.92	0.15	46,46,46,46	0
57	MG	2A	3229	1/1	0.92	0.14	50,50,50,50	0
57	MG	2A	3514	1/1	0.92	0.06	62,62,62,62	0
57	MG	1D	315	1/1	0.92	0.28	48,48,48,48	0
57	MG	1A	3952	1/1	0.92	0.09	58,58,58,58	0
57	MG	2D	302	1/1	0.92	0.20	49,49,49,49	0
57	MG	2D	304	1/1	0.92	0.19	34,34,34,34	0
57	MG	1a	3182	1/1	0.92	0.11	59,59,59,59	0
57	MG	2A	3040	1/1	0.92	0.14	44,44,44,44	0
57	MG	1a	3065	1/1	0.92	0.19	58,58,58,58	0
57	MG	2E	304	1/1	0.92	0.12	38,38,38,38	0
57	MG	1a	3186	1/1	0.92	0.15	50,50,50,50	0
57	MG	2A	3044	1/1	0.92	0.12	53,53,53,53	0
57	MG	1E	305	1/1	0.92	0.23	47,47,47,47	0
57	MG	1A	3619	1/1	0.92	0.08	57,57,57,57	0
57	MG	2I	201	1/1	0.92	0.20	64,64,64,64	0
57	MG	1A	3961	1/1	0.92	0.17	47,47,47,47	0
57	MG	1A	3962	1/1	0.92	0.11	46,46,46,46	0
57	MG	2P	202	1/1	0.92	0.27	64,64,64,64	0
57	MG	1E	311	1/1	0.92	0.10	38,38,38,38	0
57	MG	1a	3071	1/1	0.92	0.14	62,62,62,62	0
57	MG	1A	3545	1/1	0.92	0.19	41,41,41,41	0
57	MG	2R	201	1/1	0.92	0.40	59,59,59,59	0
57	MG	1a	3195	1/1	0.92	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3262	1/1	0.92	0.19	33,33,33,33	0
57	MG	2A	3539	1/1	0.92	0.29	67,67,67,67	0
57	MG	1A	3267	1/1	0.92	0.14	28,28,28,28	0
57	MG	1A	3548	1/1	0.92	0.14	41,41,41,41	0
57	MG	1A	3549	1/1	0.92	0.08	43,43,43,43	0
57	MG	2A	3271	1/1	0.92	0.18	50,50,50,50	0
57	MG	2A	3272	1/1	0.92	0.14	38,38,38,38	0
57	MG	1A	3231	1/1	0.92	0.28	32,32,32,32	0
57	MG	1A	3485	1/1	0.92	0.19	29,29,29,29	0
57	MG	2a	3004	1/1	0.92	0.14	59,59,59,59	0
57	MG	2A	3068	1/1	0.92	0.21	48,48,48,48	0
57	MG	1A	3724	1/1	0.92	0.10	35,35,35,35	0
57	MG	1A	3418	1/1	0.92	0.22	26,26,26,26	0
57	MG	1H	202	1/1	0.92	0.11	49,49,49,49	0
57	MG	2A	3294	1/1	0.92	0.14	50,50,50,50	0
57	MG	1A	3233	1/1	0.92	0.13	44,44,44,44	0
57	MG	1A	3112	1/1	0.92	0.16	32,32,32,32	0
57	MG	2A	3569	1/1	0.92	0.15	45,45,45,45	0
57	MG	2A	3299	1/1	0.92	0.19	53,53,53,53	0
57	MG	2A	3573	1/1	0.92	0.09	49,49,49,49	0
57	MG	2A	3300	1/1	0.92	0.30	64,64,64,64	0
57	MG	2A	3301	1/1	0.92	0.20	64,64,64,64	0
57	MG	2A	3080	1/1	0.92	0.14	56,56,56,56	0
57	MG	1A	3858	1/1	0.92	0.13	40,40,40,40	0
57	MG	1A	3379	1/1	0.92	0.09	33,33,33,33	0
57	MG	2A	3087	1/1	0.92	0.22	45,45,45,45	0
57	MG	2A	3582	1/1	0.92	0.17	50,50,50,50	0
57	MG	2a	3032	1/1	0.92	0.19	57,57,57,57	0
57	MG	2A	3310	1/1	0.92	0.16	58,58,58,58	0
57	MG	1A	3737	1/1	0.92	0.28	44,44,44,44	0
57	MG	1A	3244	1/1	0.92	0.35	51,51,51,51	0
57	MG	2A	3316	1/1	0.92	0.14	40,40,40,40	0
57	MG	1A	3747	1/1	0.92	0.06	61,61,61,61	0
57	MG	2A	3097	1/1	0.92	0.09	48,48,48,48	0
57	MG	2A	3324	1/1	0.92	0.19	26,26,26,26	0
57	MG	1a	3219	1/1	0.92	0.11	63,63,63,63	0
57	MG	2a	3044	1/1	0.92	0.13	57,57,57,57	0
57	MG	1A	3987	1/1	0.92	0.18	32,32,32,32	0
57	MG	1A	3328	1/1	0.92	0.19	51,51,51,51	0
57	MG	2A	3105	1/1	0.92	0.17	56,56,56,56	0
57	MG	2A	3605	1/1	0.92	0.15	34,34,34,34	0
57	MG	1A	3648	1/1	0.92	0.16	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3384	1/1	0.92	0.36	56,56,56,56	0
57	MG	1A	3573	1/1	0.92	0.20	43,43,43,43	0
57	MG	2A	3348	1/1	0.92	0.10	54,54,54,54	0
57	MG	2A	3113	1/1	0.92	0.14	52,52,52,52	0
57	MG	1Z	301	1/1	0.92	0.14	61,61,61,61	0
57	MG	1A	3992	1/1	0.92	0.28	37,37,37,37	0
57	MG	2a	3061	1/1	0.92	0.20	67,67,67,67	0
57	MG	2A	3354	1/1	0.92	0.15	38,38,38,38	0
57	MG	2A	3356	1/1	0.92	0.08	40,40,40,40	0
57	MG	1A	3762	1/1	0.92	0.18	48,48,48,48	0
57	MG	2a	3067	1/1	0.92	0.09	69,69,69,69	0
57	MG	1A	3388	1/1	0.92	0.15	27,27,27,27	0
57	MG	1A	3503	1/1	0.92	0.12	37,37,37,37	0
57	MG	1A	3504	1/1	0.92	0.15	42,42,42,42	0
57	MG	1A	3189	1/1	0.92	0.14	66,66,66,66	0
57	MG	1A	3336	1/1	0.92	0.19	30,30,30,30	0
57	MG	1A	3345	1/1	0.92	0.15	48,48,48,48	0
57	MG	1a	3246	1/1	0.92	0.07	50,50,50,50	0
57	MG	2A	3371	1/1	0.92	0.08	43,43,43,43	0
57	MG	1A	3777	1/1	0.92	0.16	41,41,41,41	0
57	MG	1A	3286	1/1	0.92	0.28	32,32,32,32	0
57	MG	1a	3252	1/1	0.92	0.15	54,54,54,54	0
57	MG	1a	3127	1/1	0.92	0.12	32,32,32,32	0
57	MG	2A	3139	1/1	0.92	0.13	36,36,36,36	0
57	MG	2a	3093	1/1	0.92	0.10	65,65,65,65	0
57	MG	2a	3094	1/1	0.92	0.13	55,55,55,55	0
57	MG	2A	3141	1/1	0.92	0.20	60,60,60,60	0
57	MG	1a	3255	1/1	0.92	0.10	48,48,48,48	0
57	MG	2A	3146	1/1	0.92	0.10	61,61,61,61	0
57	MG	18	103	1/1	0.92	0.09	50,50,50,50	0
57	MG	2A	3647	1/1	0.92	0.11	46,46,46,46	0
57	MG	2a	3116	1/1	0.92	0.14	49,49,49,49	0
57	MG	1A	3893	1/1	0.92	0.14	54,54,54,54	0
57	MG	1A	3679	1/1	0.92	0.16	66,66,66,66	0
57	MG	1a	3262	1/1	0.92	0.07	57,57,57,57	0
57	MG	2A	3402	1/1	0.92	0.11	45,45,45,45	0
57	MG	2A	3656	1/1	0.92	0.10	38,38,38,38	0
57	MG	1a	3263	1/1	0.92	0.11	55,55,55,55	0
57	MG	2A	3168	1/1	0.92	0.10	48,48,48,48	0
57	MG	1A	3351	1/1	0.92	0.08	51,51,51,51	0
57	MG	1A	3464	1/1	0.92	0.13	52,52,52,52	0
57	MG	1A	3598	1/1	0.92	0.13	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3903	1/1	0.92	0.15	30,30,30,30	0
57	MG	1A	3519	1/1	0.92	0.16	25,25,25,25	0
57	MG	2a	3148	1/1	0.92	0.08	67,67,67,67	0
57	MG	2A	3178	1/1	0.92	0.37	46,46,46,46	0
57	MG	2A	3673	1/1	0.92	0.07	49,49,49,49	0
57	MG	2A	3432	1/1	0.92	0.14	56,56,56,56	0
57	MG	1A	3163	1/1	0.92	0.17	50,50,50,50	0
57	MG	1A	3289	1/1	0.92	0.17	45,45,45,45	0
57	MG	1A	3917	1/1	0.92	0.16	21,21,21,21	0
57	MG	1A	3069	1/1	0.92	0.61	29,29,29,29	0
57	MG	2a	3160	1/1	0.92	0.14	74,74,74,74	0
57	MG	1a	3148	1/1	0.92	0.09	56,56,56,56	0
57	MG	2A	3693	1/1	0.92	0.12	58,58,58,58	0
57	MG	1a	3024	1/1	0.92	0.09	50,50,50,50	0
57	MG	2A	3453	1/1	0.92	0.12	58,58,58,58	0
57	MG	1A	3800	1/1	0.92	0.15	48,48,48,48	0
57	MG	2a	3171	1/1	0.92	0.06	66,66,66,66	0
57	MG	1A	3408	1/1	0.92	0.16	28,28,28,28	0
57	MG	2A	3194	1/1	0.92	0.16	40,40,40,40	0
57	MG	2a	3175	1/1	0.92	0.15	55,55,55,55	0
57	MG	2A	3460	1/1	0.92	0.12	63,63,63,63	0
57	MG	2A	3704	1/1	0.92	0.13	40,40,40,40	0
57	MG	1B	218	1/1	0.92	0.12	46,46,46,46	0
57	MG	1A	3698	1/1	0.92	0.14	48,48,48,48	0
57	MG	2A	3464	1/1	0.92	0.12	58,58,58,58	0
57	MG	1A	3259	1/1	0.92	0.13	57,57,57,57	0
57	MG	1A	3809	1/1	0.92	0.14	24,24,24,24	0
57	MG	2j	201	1/1	0.92	0.22	71,71,71,71	0
57	MG	1o	101	1/1	0.92	0.14	58,58,58,58	0
57	MG	2A	3204	1/1	0.92	0.06	64,64,64,64	0
57	MG	1a	3041	1/1	0.92	0.18	64,64,64,64	0
57	MG	1A	3479	1/1	0.92	0.10	28,28,28,28	0
60	ZN	2Y	202	1/1	0.92	0.14	82,82,82,82	0
57	MG	1w	101	1/1	0.92	0.13	52,52,52,52	0
57	MG	2A	3482	1/1	0.92	0.13	45,45,45,45	0
57	MG	2A	3511	1/1	0.93	0.17	73,73,73,73	0
57	MG	1A	3375	1/1	0.93	0.10	36,36,36,36	0
57	MG	1A	3238	1/1	0.93	0.20	33,33,33,33	0
57	MG	1A	3035	1/1	0.93	0.25	42,42,42,42	0
57	MG	1A	3755	1/1	0.93	0.21	48,48,48,48	0
57	MG	1A	3670	1/1	0.93	0.12	38,38,38,38	0
57	MG	2A	3284	1/1	0.93	0.15	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3266	1/1	0.93	0.14	61,61,61,61	0
57	MG	2A	3288	1/1	0.93	0.17	57,57,57,57	0
57	MG	2A	3291	1/1	0.93	0.11	62,62,62,62	0
57	MG	1A	3191	1/1	0.93	0.32	34,34,34,34	0
57	MG	2D	305	1/1	0.93	0.21	44,44,44,44	0
57	MG	2A	3526	1/1	0.93	0.57	52,52,52,52	0
57	MG	2D	308	1/1	0.93	0.22	59,59,59,59	0
57	MG	2A	3293	1/1	0.93	0.15	57,57,57,57	0
57	MG	1A	4013	1/1	0.93	0.15	47,47,47,47	0
57	MG	2A	3529	1/1	0.93	0.18	62,62,62,62	0
57	MG	1A	3329	1/1	0.93	0.19	29,29,29,29	0
57	MG	2A	3297	1/1	0.93	0.26	52,52,52,52	0
57	MG	2F	303	1/1	0.93	0.24	57,57,57,57	0
57	MG	1T	204	1/1	0.93	0.14	64,64,64,64	0
57	MG	2A	3121	1/1	0.93	0.15	60,60,60,60	0
57	MG	1U	201	1/1	0.93	0.27	33,33,33,33	0
57	MG	2O	201	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3602	1/1	0.93	0.09	33,33,33,33	0
57	MG	1A	4021	1/1	0.93	0.43	57,57,57,57	0
57	MG	1W	202	1/1	0.93	0.12	38,38,38,38	0
57	MG	2Q	201	1/1	0.93	0.07	56,56,56,56	0
57	MG	1A	3192	1/1	0.93	0.28	45,45,45,45	0
57	MG	2A	3130	1/1	0.93	0.19	47,47,47,47	0
57	MG	2A	3547	1/1	0.93	0.09	32,32,32,32	0
57	MG	1A	3604	1/1	0.93	0.14	54,54,54,54	0
57	MG	1e	203	1/1	0.93	0.19	59,59,59,59	0
57	MG	1f	202	1/1	0.93	0.14	40,40,40,40	0
57	MG	2A	3315	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3946	1/1	0.93	0.12	23,23,23,23	0
57	MG	2W	203	1/1	0.93	0.10	61,61,61,61	0
57	MG	2O	101	1/1	0.93	0.30	54,54,54,54	0
57	MG	1A	3436	1/1	0.93	0.11	51,51,51,51	0
57	MG	2A	3557	1/1	0.93	0.08	60,60,60,60	0
57	MG	2A	3320	1/1	0.93	0.16	45,45,45,45	0
57	MG	2A	3560	1/1	0.93	0.14	30,30,30,30	0
57	MG	1a	3183	1/1	0.93	0.10	66,66,66,66	0
57	MG	1l	202	1/1	0.93	0.21	56,56,56,56	0
57	MG	1A	3859	1/1	0.93	0.05	38,38,38,38	0
57	MG	1a	3085	1/1	0.93	0.12	64,64,64,64	0
57	MG	2a	3006	1/1	0.93	0.15	50,50,50,50	0
57	MG	2A	3331	1/1	0.93	0.09	41,41,41,41	0
57	MG	2A	3571	1/1	0.93	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3333	1/1	0.93	0.07	31,31,31,31	0
57	MG	1A	3488	1/1	0.93	0.11	27,27,27,27	0
57	MG	2A	3335	1/1	0.93	0.11	63,63,63,63	0
57	MG	2A	3148	1/1	0.93	0.15	55,55,55,55	0
57	MG	2A	3149	1/1	0.93	0.24	56,56,56,56	0
57	MG	1A	3437	1/1	0.93	0.08	44,44,44,44	0
57	MG	2a	3017	1/1	0.93	0.09	55,55,55,55	0
57	MG	2A	3154	1/1	0.93	0.11	47,47,47,47	0
57	MG	1o	102	1/1	0.93	0.10	56,56,56,56	0
57	MG	2A	3158	1/1	0.93	0.11	63,63,63,63	0
57	MG	1A	3331	1/1	0.93	0.17	21,21,21,21	0
57	MG	2a	3022	1/1	0.93	0.09	50,50,50,50	0
57	MG	2A	3162	1/1	0.93	0.32	41,41,41,41	0
57	MG	2a	3024	1/1	0.93	0.18	70,70,70,70	0
57	MG	1y	201	1/1	0.93	0.19	66,66,66,66	0
57	MG	1A	3867	1/1	0.93	0.10	38,38,38,38	0
57	MG	2A	3592	1/1	0.93	0.04	57,57,57,57	0
57	MG	1a	3090	1/1	0.93	0.18	47,47,47,47	0
57	MG	13	101	1/1	0.93	0.21	43,43,43,43	0
57	MG	1A	3106	1/1	0.93	0.23	43,43,43,43	0
57	MG	2A	3171	1/1	0.93	0.09	42,42,42,42	0
57	MG	1A	3618	1/1	0.93	0.15	30,30,30,30	0
57	MG	15	3109	1/1	0.93	0.20	51,51,51,51	0
57	MG	1A	3195	1/1	0.93	0.17	51,51,51,51	0
57	MG	1a	3202	1/1	0.93	0.07	70,70,70,70	0
57	MG	2a	3041	1/1	0.93	0.18	56,56,56,56	0
57	MG	17	106	1/1	0.93	0.21	40,40,40,40	0
57	MG	1A	3696	1/1	0.93	0.39	39,39,39,39	0
57	MG	2A	3025	1/1	0.93	0.13	34,34,34,34	0
57	MG	2a	3046	1/1	0.93	0.25	62,62,62,62	0
57	MG	2A	3613	1/1	0.93	0.15	43,43,43,43	0
57	MG	2A	3026	1/1	0.93	0.27	55,55,55,55	0
57	MG	2A	3378	1/1	0.93	0.14	66,66,66,66	0
57	MG	2A	3616	1/1	0.93	0.19	49,49,49,49	0
57	MG	1A	3558	1/1	0.93	0.29	51,51,51,51	0
57	MG	1B	226	1/1	0.93	0.11	32,32,32,32	0
57	MG	1A	3700	1/1	0.93	0.71	53,53,53,53	0
57	MG	2A	3192	1/1	0.93	0.30	55,55,55,55	0
57	MG	1A	3447	1/1	0.93	0.10	55,55,55,55	0
57	MG	2A	3389	1/1	0.93	0.13	37,37,37,37	0
57	MG	2A	3037	1/1	0.93	0.14	62,62,62,62	0
57	MG	2A	3195	1/1	0.93	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3038	1/1	0.93	0.17	43,43,43,43	0
57	MG	1B	229	1/1	0.93	0.12	56,56,56,56	0
57	MG	2A	3400	1/1	0.93	0.14	55,55,55,55	0
57	MG	1a	3008	1/1	0.93	0.17	55,55,55,55	0
57	MG	2A	3199	1/1	0.93	0.09	51,51,51,51	0
57	MG	2A	3200	1/1	0.93	0.13	41,41,41,41	0
57	MG	1A	3449	1/1	0.93	0.13	58,58,58,58	0
57	MG	2A	3202	1/1	0.93	0.13	46,46,46,46	0
57	MG	2A	3412	1/1	0.93	0.09	59,59,59,59	0
57	MG	2A	3418	1/1	0.93	0.15	35,35,35,35	0
57	MG	1D	305	1/1	0.93	0.32	42,42,42,42	0
57	MG	2A	3420	1/1	0.93	0.11	30,30,30,30	0
57	MG	1a	3110	1/1	0.93	0.14	53,53,53,53	0
57	MG	1A	3795	1/1	0.93	0.23	47,47,47,47	0
57	MG	2a	3088	1/1	0.93	0.11	67,67,67,67	0
57	MG	2A	3048	1/1	0.93	0.17	53,53,53,53	0
57	MG	1a	3112	1/1	0.93	0.07	72,72,72,72	0
57	MG	2A	3650	1/1	0.93	0.13	30,30,30,30	0
57	MG	2A	3433	1/1	0.93	0.14	49,49,49,49	0
57	MG	1A	3565	1/1	0.93	0.15	49,49,49,49	0
57	MG	2A	3438	1/1	0.93	0.33	60,60,60,60	0
57	MG	1A	3797	1/1	0.93	0.07	39,39,39,39	0
57	MG	1A	3021	1/1	0.93	0.22	39,39,39,39	0
57	MG	2a	3113	1/1	0.93	0.28	53,53,53,53	0
57	MG	1A	3260	1/1	0.93	0.23	39,39,39,39	0
57	MG	1E	301	1/1	0.93	0.15	28,28,28,28	0
57	MG	1A	3297	1/1	0.93	0.16	34,34,34,34	0
57	MG	2A	3059	1/1	0.93	0.34	46,46,46,46	0
57	MG	1a	3026	1/1	0.93	0.08	49,49,49,49	0
57	MG	2a	3126	1/1	0.93	0.12	61,61,61,61	0
57	MG	2A	3455	1/1	0.93	0.12	57,57,57,57	0
57	MG	2A	3456	1/1	0.93	0.10	39,39,39,39	0
57	MG	1A	3263	1/1	0.93	0.09	59,59,59,59	0
57	MG	1a	3028	1/1	0.93	0.19	59,59,59,59	0
57	MG	1A	3635	1/1	0.93	0.15	44,44,44,44	0
57	MG	2A	3226	1/1	0.93	0.10	59,59,59,59	0
57	MG	2A	3683	1/1	0.93	0.11	38,38,38,38	0
57	MG	2A	3686	1/1	0.93	0.13	47,47,47,47	0
57	MG	1A	3306	1/1	0.93	0.15	70,70,70,70	0
57	MG	1A	3133	1/1	0.93	0.22	32,32,32,32	0
57	MG	1a	3238	1/1	0.93	0.10	56,56,56,56	0
57	MG	1a	3241	1/1	0.93	0.27	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3469	1/1	0.93	0.11	67,67,67,67	0
57	MG	2A	3235	1/1	0.93	0.24	58,58,58,58	0
57	MG	1A	3362	1/1	0.93	0.15	37,37,37,37	0
57	MG	2A	3075	1/1	0.93	0.09	64,64,64,64	0
57	MG	2A	3701	1/1	0.93	0.08	50,50,50,50	0
57	MG	2a	3159	1/1	0.93	0.09	62,62,62,62	0
57	MG	2A	3477	1/1	0.93	0.12	39,39,39,39	0
57	MG	1A	3466	1/1	0.93	0.11	62,62,62,62	0
57	MG	2A	3243	1/1	0.93	0.76	47,47,47,47	0
57	MG	2A	3480	1/1	0.93	0.10	48,48,48,48	0
57	MG	2a	3165	1/1	0.93	0.11	49,49,49,49	0
57	MG	2a	3167	1/1	0.93	0.32	67,67,67,67	0
57	MG	2A	3716	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3481	1/1	0.93	0.07	67,67,67,67	0
57	MG	1A	3365	1/1	0.93	0.18	22,22,22,22	0
57	MG	2A	3079	1/1	0.93	0.06	43,43,43,43	0
57	MG	2A	3722	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	3818	1/1	0.93	0.20	37,37,37,37	0
57	MG	2A	3082	1/1	0.93	0.15	53,53,53,53	0
57	MG	1a	3247	1/1	0.93	0.10	51,51,51,51	0
57	MG	1A	3134	1/1	0.93	0.13	37,37,37,37	0
57	MG	1A	3064	1/1	0.93	0.15	59,59,59,59	0
57	MG	1A	3652	1/1	0.93	0.19	35,35,35,35	0
57	MG	1A	3997	1/1	0.93	0.24	55,55,55,55	0
57	MG	2a	3190	1/1	0.93	0.20	64,64,64,64	0
57	MG	2A	3094	1/1	0.93	0.24	52,52,52,52	0
57	MG	1a	3254	1/1	0.93	0.17	49,49,49,49	0
57	MG	2A	3266	1/1	0.93	0.09	63,63,63,63	0
57	MG	2x	101	1/1	0.93	0.11	50,50,50,50	0
58	MPD	1A	4023	8/8	0.93	0.15	41,51,57,57	0
58	MPD	18	104	8/8	0.93	0.31	31,40,43,44	0
57	MG	1A	3654	1/1	0.93	0.12	37,37,37,37	0
58	MPD	2A	3734	8/8	0.93	0.25	38,49,52,57	0
57	MG	2A	3507	1/1	0.93	0.11	56,56,56,56	0
57	MG	2B	204	1/1	0.93	0.17	56,56,56,56	0
57	MG	2B	205	1/1	0.93	0.23	54,54,54,54	0
57	MG	1A	3270	1/1	0.93	0.21	65,65,65,65	0
57	MG	2A	3099	1/1	0.93	0.08	48,48,48,48	0
57	MG	2A	3183	1/1	0.94	0.09	61,61,61,61	0
57	MG	2A	3185	1/1	0.94	0.31	55,55,55,55	0
57	MG	2A	3445	1/1	0.94	0.13	71,71,71,71	0
57	MG	1a	3268	1/1	0.94	0.15	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3924	1/1	0.94	0.18	56,56,56,56	0
57	MG	1a	3272	1/1	0.94	0.10	58,58,58,58	0
57	MG	1A	3099	1/1	0.94	0.42	38,38,38,38	0
57	MG	1A	3292	1/1	0.94	0.08	67,67,67,67	0
57	MG	1A	3773	1/1	0.94	0.15	26,26,26,26	0
57	MG	1A	3639	1/1	0.94	0.31	30,30,30,30	0
57	MG	1A	3641	1/1	0.94	0.23	32,32,32,32	0
57	MG	1F	315	1/1	0.94	0.12	53,53,53,53	0
57	MG	1A	3934	1/1	0.94	0.15	38,38,38,38	0
57	MG	1A	3643	1/1	0.94	0.27	58,58,58,58	0
57	MG	1A	3293	1/1	0.94	0.09	62,62,62,62	0
57	MG	1A	3780	1/1	0.94	0.10	43,43,43,43	0
57	MG	1a	3105	1/1	0.94	0.16	46,46,46,46	0
57	MG	1H	201	1/1	0.94	0.23	40,40,40,40	0
57	MG	2B	208	1/1	0.94	0.26	55,55,55,55	0
57	MG	1A	3645	1/1	0.94	0.33	37,37,37,37	0
57	MG	1A	3944	1/1	0.94	0.07	35,35,35,35	0
57	MG	1A	3055	1/1	0.94	0.23	38,38,38,38	0
57	MG	1A	3298	1/1	0.94	0.35	63,63,63,63	0
57	MG	2A	3476	1/1	0.94	0.22	63,63,63,63	0
57	MG	1Q	201	1/1	0.94	0.32	35,35,35,35	0
57	MG	1n	101	1/1	0.94	0.15	66,66,66,66	0
57	MG	2A	3211	1/1	0.94	0.09	52,52,52,52	0
57	MG	1Q	204	1/1	0.94	0.14	30,30,30,30	0
57	MG	1a	3118	1/1	0.94	0.09	42,42,42,42	0
57	MG	1A	3245	1/1	0.94	0.18	49,49,49,49	0
57	MG	1A	3249	1/1	0.94	0.24	42,42,42,42	0
57	MG	1A	3953	1/1	0.94	0.11	50,50,50,50	0
57	MG	1y	202	1/1	0.94	0.15	56,56,56,56	0
57	MG	2A	3488	1/1	0.94	0.13	64,64,64,64	0
57	MG	2A	3220	1/1	0.94	0.11	44,44,44,44	0
57	MG	2E	303	1/1	0.94	0.17	49,49,49,49	0
57	MG	1a	3124	1/1	0.94	0.11	73,73,73,73	0
57	MG	1A	3958	1/1	0.94	0.08	37,37,37,37	0
57	MG	2F	301	1/1	0.94	0.42	40,40,40,40	0
57	MG	1T	201	1/1	0.94	0.08	42,42,42,42	0
57	MG	1A	3651	1/1	0.94	0.20	34,34,34,34	0
57	MG	2A	3002	1/1	0.94	0.12	41,41,41,41	0
57	MG	1A	3108	1/1	0.94	0.17	51,51,51,51	0
57	MG	2A	3498	1/1	0.94	0.17	64,64,64,64	0
57	MG	1A	3467	1/1	0.94	0.12	32,32,32,32	0
57	MG	1U	203	1/1	0.94	0.16	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3015	1/1	0.94	0.19	50,50,50,50	0
57	MG	1A	3059	1/1	0.94	0.30	47,47,47,47	0
57	MG	1V	206	1/1	0.94	0.47	48,48,48,48	0
57	MG	1A	3798	1/1	0.94	0.13	31,31,31,31	0
57	MG	2A	3513	1/1	0.94	0.12	42,42,42,42	0
57	MG	1A	3660	1/1	0.94	0.27	52,52,52,52	0
57	MG	1A	3663	1/1	0.94	0.16	24,24,24,24	0
57	MG	1A	3470	1/1	0.94	0.10	31,31,31,31	0
57	MG	2A	3031	1/1	0.94	0.11	59,59,59,59	0
57	MG	1A	3387	1/1	0.94	0.20	24,24,24,24	0
57	MG	2V	203	1/1	0.94	0.18	59,59,59,59	0
57	MG	10	101	1/1	0.94	0.28	45,45,45,45	0
57	MG	1a	3149	1/1	0.94	0.19	48,48,48,48	0
57	MG	1A	3153	1/1	0.94	0.17	31,31,31,31	0
57	MG	10	106	1/1	0.94	0.09	47,47,47,47	0
57	MG	1A	3805	1/1	0.94	0.12	34,34,34,34	0
57	MG	2A	3253	1/1	0.94	0.18	55,55,55,55	0
57	MG	1A	3669	1/1	0.94	0.09	46,46,46,46	0
57	MG	1A	3810	1/1	0.94	0.11	38,38,38,38	0
57	MG	1A	3154	1/1	0.94	0.09	48,48,48,48	0
57	MG	2a	3003	1/1	0.94	0.07	46,46,46,46	0
57	MG	1A	3569	1/1	0.94	0.14	19,19,19,19	0
57	MG	2A	3531	1/1	0.94	0.10	63,63,63,63	0
57	MG	1A	3673	1/1	0.94	0.12	56,56,56,56	0
57	MG	1A	3478	1/1	0.94	0.14	29,29,29,29	0
57	MG	1a	3164	1/1	0.94	0.17	79,79,79,79	0
57	MG	1A	3002	1/1	0.94	0.14	44,44,44,44	0
57	MG	2A	3538	1/1	0.94	0.18	59,59,59,59	0
57	MG	1A	3678	1/1	0.94	0.08	55,55,55,55	0
57	MG	17	103	1/1	0.94	0.18	32,32,32,32	0
57	MG	2A	3275	1/1	0.94	0.30	38,38,38,38	0
57	MG	1A	3323	1/1	0.94	0.14	27,27,27,27	0
57	MG	1A	3829	1/1	0.94	0.11	45,45,45,45	0
57	MG	2A	3280	1/1	0.94	0.31	56,56,56,56	0
57	MG	1A	3574	1/1	0.94	0.08	34,34,34,34	0
57	MG	2A	3549	1/1	0.94	0.09	45,45,45,45	0
57	MG	2A	3550	1/1	0.94	0.11	62,62,62,62	0
57	MG	2A	3282	1/1	0.94	0.11	55,55,55,55	0
57	MG	2A	3283	1/1	0.94	0.12	75,75,75,75	0
57	MG	18	102	1/1	0.94	0.26	36,36,36,36	0
57	MG	2a	3025	1/1	0.94	0.17	52,52,52,52	0
57	MG	2a	3026	1/1	0.94	0.21	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3156	1/1	0.94	0.40	39,39,39,39	0
57	MG	1A	3578	1/1	0.94	0.11	40,40,40,40	0
57	MG	1A	3582	1/1	0.94	0.52	40,40,40,40	0
57	MG	2a	3031	1/1	0.94	0.18	65,65,65,65	0
57	MG	2A	3065	1/1	0.94	0.07	54,54,54,54	0
57	MG	1A	3395	1/1	0.94	0.19	18,18,18,18	0
57	MG	1A	3484	1/1	0.94	0.17	29,29,29,29	0
57	MG	1A	3325	1/1	0.94	0.18	29,29,29,29	0
57	MG	2A	3565	1/1	0.94	0.09	51,51,51,51	0
57	MG	2A	3567	1/1	0.94	0.17	50,50,50,50	0
57	MG	1A	3327	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3114	1/1	0.94	0.18	39,39,39,39	0
57	MG	1a	3013	1/1	0.94	0.09	54,54,54,54	0
57	MG	1A	3697	1/1	0.94	0.25	39,39,39,39	0
57	MG	1a	3016	1/1	0.94	0.08	60,60,60,60	0
57	MG	1A	3591	1/1	0.94	0.08	56,56,56,56	0
57	MG	2A	3303	1/1	0.94	0.22	45,45,45,45	0
57	MG	1A	3266	1/1	0.94	0.20	37,37,37,37	0
57	MG	1a	3021	1/1	0.94	0.12	48,48,48,48	0
57	MG	2A	3307	1/1	0.94	0.22	70,70,70,70	0
57	MG	1A	4006	1/1	0.94	0.19	42,42,42,42	0
57	MG	2a	3051	1/1	0.94	0.16	54,54,54,54	0
57	MG	1A	3489	1/1	0.94	0.15	23,23,23,23	0
57	MG	1A	3062	1/1	0.94	0.21	46,46,46,46	0
57	MG	1a	3200	1/1	0.94	0.15	66,66,66,66	0
57	MG	2A	3314	1/1	0.94	0.17	37,37,37,37	0
57	MG	2A	3089	1/1	0.94	0.31	45,45,45,45	0
57	MG	2A	3589	1/1	0.94	0.11	42,42,42,42	0
57	MG	2a	3060	1/1	0.94	0.08	76,76,76,76	0
57	MG	1A	3124	1/1	0.94	0.14	40,40,40,40	0
57	MG	1A	3211	1/1	0.94	0.21	40,40,40,40	0
57	MG	1A	3861	1/1	0.94	0.14	49,49,49,49	0
57	MG	1A	4016	1/1	0.94	0.14	47,47,47,47	0
57	MG	1a	3030	1/1	0.94	0.09	46,46,46,46	0
57	MG	2A	3325	1/1	0.94	0.12	50,50,50,50	0
57	MG	1A	3340	1/1	0.94	0.20	53,53,53,53	0
57	MG	2a	3070	1/1	0.94	0.08	51,51,51,51	0
57	MG	1a	3033	1/1	0.94	0.12	28,28,28,28	0
57	MG	2A	3329	1/1	0.94	0.06	38,38,38,38	0
57	MG	2A	3330	1/1	0.94	0.09	38,38,38,38	0
57	MG	2A	3101	1/1	0.94	0.15	43,43,43,43	0
57	MG	2a	3080	1/1	0.94	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3081	1/1	0.94	0.23	51,51,51,51	0
57	MG	1a	3034	1/1	0.94	0.11	48,48,48,48	0
57	MG	1A	3167	1/1	0.94	0.11	27,27,27,27	0
57	MG	1A	3346	1/1	0.94	0.16	41,41,41,41	0
57	MG	2a	3085	1/1	0.94	0.13	60,60,60,60	0
57	MG	2A	3339	1/1	0.94	0.15	53,53,53,53	0
57	MG	1A	3274	1/1	0.94	0.23	49,49,49,49	0
57	MG	1A	3348	1/1	0.94	0.23	52,52,52,52	0
57	MG	1B	202	1/1	0.94	0.16	52,52,52,52	0
57	MG	1A	3046	1/1	0.94	0.31	54,54,54,54	0
57	MG	1a	3047	1/1	0.94	0.16	56,56,56,56	0
57	MG	2A	3349	1/1	0.94	0.13	52,52,52,52	0
57	MG	1B	204	1/1	0.94	0.11	45,45,45,45	0
57	MG	2a	3099	1/1	0.94	0.31	45,45,45,45	0
57	MG	1A	3606	1/1	0.94	0.12	27,27,27,27	0
57	MG	1A	3607	1/1	0.94	0.28	30,30,30,30	0
57	MG	2a	3105	1/1	0.94	0.10	48,48,48,48	0
57	MG	2a	3108	1/1	0.94	0.20	51,51,51,51	0
57	MG	1a	3222	1/1	0.94	0.15	49,49,49,49	0
57	MG	2a	3111	1/1	0.94	0.13	64,64,64,64	0
57	MG	2a	3112	1/1	0.94	0.22	65,65,65,65	0
57	MG	1A	3721	1/1	0.94	0.14	22,22,22,22	0
57	MG	1a	3224	1/1	0.94	0.09	46,46,46,46	0
57	MG	2a	3115	1/1	0.94	0.12	65,65,65,65	0
57	MG	2A	3359	1/1	0.94	0.16	35,35,35,35	0
57	MG	2a	3117	1/1	0.94	0.06	68,68,68,68	0
57	MG	2a	3118	1/1	0.94	0.14	67,67,67,67	0
57	MG	2A	3632	1/1	0.94	0.07	70,70,70,70	0
57	MG	2A	3125	1/1	0.94	0.14	48,48,48,48	0
57	MG	2A	3634	1/1	0.94	0.06	40,40,40,40	0
57	MG	2a	3125	1/1	0.94	0.20	56,56,56,56	0
57	MG	1A	3722	1/1	0.94	0.12	43,43,43,43	0
57	MG	1A	3506	1/1	0.94	0.09	29,29,29,29	0
57	MG	1A	3428	1/1	0.94	0.18	20,20,20,20	0
57	MG	2A	3131	1/1	0.94	0.28	63,63,63,63	0
57	MG	1a	3230	1/1	0.94	0.09	64,64,64,64	0
57	MG	1A	3430	1/1	0.94	0.13	15,15,15,15	0
57	MG	1a	3063	1/1	0.94	0.50	68,68,68,68	0
57	MG	2A	3373	1/1	0.94	0.09	74,74,74,74	0
57	MG	1B	220	1/1	0.94	0.14	28,28,28,28	0
57	MG	2a	3143	1/1	0.94	0.10	64,64,64,64	0
57	MG	2a	3144	1/1	0.94	0.22	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3730	1/1	0.94	0.10	52,52,52,52	0
57	MG	2A	3376	1/1	0.94	0.13	69,69,69,69	0
57	MG	1A	3009	1/1	0.94	0.14	26,26,26,26	0
57	MG	2a	3152	1/1	0.94	0.10	65,65,65,65	0
57	MG	1A	3435	1/1	0.94	0.09	44,44,44,44	0
57	MG	1A	3092	1/1	0.94	0.21	26,26,26,26	0
57	MG	1A	3283	1/1	0.94	0.34	51,51,51,51	0
57	MG	2A	3145	1/1	0.94	0.33	46,46,46,46	0
57	MG	1A	3741	1/1	0.94	0.12	48,48,48,48	0
57	MG	1A	3746	1/1	0.94	0.20	63,63,63,63	0
57	MG	2A	3659	1/1	0.94	0.08	50,50,50,50	0
57	MG	2A	3661	1/1	0.94	0.10	57,57,57,57	0
57	MG	2A	3388	1/1	0.94	0.12	63,63,63,63	0
57	MG	1A	3521	1/1	0.94	0.15	46,46,46,46	0
57	MG	2a	3163	1/1	0.94	0.16	64,64,64,64	0
57	MG	2A	3150	1/1	0.94	0.11	41,41,41,41	0
57	MG	2A	3392	1/1	0.94	0.11	40,40,40,40	0
57	MG	1A	3900	1/1	0.94	0.11	48,48,48,48	0
57	MG	1D	301	1/1	0.94	0.37	33,33,33,33	0
57	MG	1a	3249	1/1	0.94	0.18	68,68,68,68	0
57	MG	1A	3622	1/1	0.94	0.19	23,23,23,23	0
57	MG	1a	3251	1/1	0.94	0.10	61,61,61,61	0
57	MG	1A	3749	1/1	0.94	0.07	26,26,26,26	0
57	MG	1D	308	1/1	0.94	0.31	35,35,35,35	0
57	MG	2a	3177	1/1	0.94	0.10	59,59,59,59	0
57	MG	1A	3911	1/1	0.94	0.16	20,20,20,20	0
57	MG	1A	3754	1/1	0.94	0.17	56,56,56,56	0
57	MG	2A	3409	1/1	0.94	0.13	40,40,40,40	0
57	MG	2A	3411	1/1	0.94	0.24	41,41,41,41	0
57	MG	1A	3438	1/1	0.94	0.09	51,51,51,51	0
57	MG	2A	3417	1/1	0.94	0.12	41,41,41,41	0
57	MG	1a	3257	1/1	0.94	0.11	51,51,51,51	0
57	MG	1A	3065	1/1	0.94	0.08	38,38,38,38	0
57	MG	2A	3172	1/1	0.94	0.11	39,39,39,39	0
57	MG	2A	3173	1/1	0.94	0.12	40,40,40,40	0
57	MG	2A	3425	1/1	0.94	0.12	35,35,35,35	0
57	MG	1A	3287	1/1	0.94	0.31	44,44,44,44	0
57	MG	1A	3364	1/1	0.94	0.13	42,42,42,42	0
57	MG	1A	3138	1/1	0.94	0.12	43,43,43,43	0
57	MG	1A	3533	1/1	0.94	0.14	44,44,44,44	0
58	MPD	2A	3735	8/8	0.94	0.14	53,57,64,68	0
57	MG	2A	3710	1/1	0.94	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
59	ARG	1B	231	12/12	0.94	0.19	29,44,51,55	0
57	MG	2A	3713	1/1	0.94	0.16	24,24,24,24	0
57	MG	2A	3435	1/1	0.94	0.15	56,56,56,56	0
57	MG	1a	3265	1/1	0.94	0.13	64,64,64,64	0
57	MG	1A	3140	1/1	0.94	0.15	32,32,32,32	0
57	MG	1A	3277	1/1	0.95	0.22	34,34,34,34	0
57	MG	1a	3076	1/1	0.95	0.17	47,47,47,47	0
57	MG	2A	3429	1/1	0.95	0.12	44,44,44,44	0
57	MG	1A	3101	1/1	0.95	0.09	45,45,45,45	0
57	MG	2A	3720	1/1	0.95	0.17	46,46,46,46	0
57	MG	2A	3431	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3361	1/1	0.95	0.22	60,60,60,60	0
57	MG	1D	302	1/1	0.95	0.12	42,42,42,42	0
57	MG	1A	3738	1/1	0.95	0.11	32,32,32,32	0
57	MG	2A	3727	1/1	0.95	0.18	56,56,56,56	0
57	MG	1A	3532	1/1	0.95	0.14	25,25,25,25	0
57	MG	1A	3890	1/1	0.95	0.15	21,21,21,21	0
57	MG	2A	3187	1/1	0.95	0.13	63,63,63,63	0
57	MG	1A	3740	1/1	0.95	0.17	24,24,24,24	0
57	MG	2A	3444	1/1	0.95	0.11	41,41,41,41	0
57	MG	1A	3629	1/1	0.95	0.12	42,42,42,42	0
57	MG	1D	312	1/1	0.95	0.23	40,40,40,40	0
57	MG	2A	3449	1/1	0.95	0.28	43,43,43,43	0
57	MG	1a	3271	1/1	0.95	0.17	52,52,52,52	0
57	MG	1A	3896	1/1	0.95	0.13	45,45,45,45	0
57	MG	2A	3452	1/1	0.95	0.16	36,36,36,36	0
57	MG	1D	314	1/1	0.95	0.15	67,67,67,67	0
57	MG	1A	3630	1/1	0.95	0.15	22,22,22,22	0
57	MG	1A	3631	1/1	0.95	0.17	30,30,30,30	0
57	MG	1a	3091	1/1	0.95	0.12	51,51,51,51	0
57	MG	2B	210	1/1	0.95	0.25	66,66,66,66	0
57	MG	1A	3280	1/1	0.95	0.12	33,33,33,33	0
57	MG	1A	3535	1/1	0.95	0.14	49,49,49,49	0
57	MG	1A	3750	1/1	0.95	0.21	29,29,29,29	0
57	MG	2B	214	1/1	0.95	0.14	52,52,52,52	0
57	MG	1E	307	1/1	0.95	0.06	45,45,45,45	0
57	MG	1A	3905	1/1	0.95	0.11	27,27,27,27	0
57	MG	1A	3906	1/1	0.95	0.12	30,30,30,30	0
57	MG	1A	3751	1/1	0.95	0.18	25,25,25,25	0
57	MG	1A	3752	1/1	0.95	0.08	34,34,34,34	0
57	MG	1h	201	1/1	0.95	0.16	49,49,49,49	0
57	MG	1A	3753	1/1	0.95	0.16	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3208	1/1	0.95	0.08	54,54,54,54	0
57	MG	1i	201	1/1	0.95	0.11	51,51,51,51	0
57	MG	2D	307	1/1	0.95	0.14	40,40,40,40	0
57	MG	1A	3105	1/1	0.95	0.19	31,31,31,31	0
57	MG	2A	3212	1/1	0.95	0.11	47,47,47,47	0
57	MG	2D	310	1/1	0.95	0.15	47,47,47,47	0
57	MG	1F	313	1/1	0.95	0.13	31,31,31,31	0
57	MG	1A	3034	1/1	0.95	0.18	51,51,51,51	0
57	MG	1A	3756	1/1	0.95	0.12	40,40,40,40	0
57	MG	1A	3542	1/1	0.95	0.11	29,29,29,29	0
57	MG	1A	3640	1/1	0.95	0.22	34,34,34,34	0
57	MG	1A	3070	1/1	0.95	0.18	28,28,28,28	0
57	MG	2A	3219	1/1	0.95	0.11	63,63,63,63	0
57	MG	1A	3642	1/1	0.95	0.24	63,63,63,63	0
57	MG	2A	3487	1/1	0.95	0.07	62,62,62,62	0
57	MG	2G	203	1/1	0.95	0.13	72,72,72,72	0
57	MG	1A	3767	1/1	0.95	0.08	31,31,31,31	0
57	MG	1A	3056	1/1	0.95	0.16	38,38,38,38	0
57	MG	1A	3373	1/1	0.95	0.15	44,44,44,44	0
57	MG	1y	203	1/1	0.95	0.19	73,73,73,73	0
57	MG	1P	201	1/1	0.95	0.44	31,31,31,31	0
57	MG	1A	3006	1/1	0.95	0.12	25,25,25,25	0
57	MG	2A	3227	1/1	0.95	0.28	44,44,44,44	0
57	MG	1a	3120	1/1	0.95	0.15	63,63,63,63	0
57	MG	1A	3012	1/1	0.95	0.17	30,30,30,30	0
57	MG	2A	3232	1/1	0.95	0.15	52,52,52,52	0
57	MG	2R	202	1/1	0.95	0.16	51,51,51,51	0
57	MG	1A	3224	1/1	0.95	0.21	41,41,41,41	0
57	MG	2A	3501	1/1	0.95	0.10	50,50,50,50	0
57	MG	2A	3502	1/1	0.95	0.15	60,60,60,60	0
57	MG	2V	201	1/1	0.95	0.14	62,62,62,62	0
57	MG	2A	3505	1/1	0.95	0.09	59,59,59,59	0
57	MG	2A	3506	1/1	0.95	0.05	44,44,44,44	0
57	MG	1A	3936	1/1	0.95	0.11	20,20,20,20	0
57	MG	2X	101	1/1	0.95	0.12	51,51,51,51	0
57	MG	1a	3125	1/1	0.95	0.09	50,50,50,50	0
57	MG	2A	3509	1/1	0.95	0.18	64,64,64,64	0
57	MG	2A	3007	1/1	0.95	0.14	42,42,42,42	0
57	MG	25	102	1/1	0.95	0.49	45,45,45,45	0
57	MG	2A	3237	1/1	0.95	0.19	57,57,57,57	0
57	MG	1a	3126	1/1	0.95	0.09	61,61,61,61	0
57	MG	2A	3241	1/1	0.95	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3938	1/1	0.95	0.14	52,52,52,52	0
57	MG	1A	3226	1/1	0.95	0.14	37,37,37,37	0
57	MG	1R	203	1/1	0.95	0.18	45,45,45,45	0
57	MG	2A	3022	1/1	0.95	0.22	51,51,51,51	0
57	MG	2A	3023	1/1	0.95	0.21	54,54,54,54	0
57	MG	1A	3164	1/1	0.95	0.20	51,51,51,51	0
57	MG	1A	3166	1/1	0.95	0.14	42,42,42,42	0
57	MG	2A	3250	1/1	0.95	0.11	57,57,57,57	0
57	MG	1A	3559	1/1	0.95	0.14	61,61,61,61	0
57	MG	1A	3232	1/1	0.95	0.22	31,31,31,31	0
57	MG	1A	3473	1/1	0.95	0.21	47,47,47,47	0
57	MG	2a	3014	1/1	0.95	0.20	55,55,55,55	0
57	MG	1a	3139	1/1	0.95	0.15	66,66,66,66	0
57	MG	2A	3033	1/1	0.95	0.19	52,52,52,52	0
57	MG	2A	3259	1/1	0.95	0.12	24,24,24,24	0
57	MG	2A	3260	1/1	0.95	0.51	40,40,40,40	0
57	MG	2A	3261	1/1	0.95	0.33	55,55,55,55	0
57	MG	1A	3564	1/1	0.95	0.10	45,45,45,45	0
57	MG	1A	3786	1/1	0.95	0.12	45,45,45,45	0
57	MG	2A	3036	1/1	0.95	0.10	46,46,46,46	0
57	MG	1A	3661	1/1	0.95	0.15	21,21,21,21	0
57	MG	2A	3269	1/1	0.95	0.12	45,45,45,45	0
57	MG	1A	3788	1/1	0.95	0.19	39,39,39,39	0
57	MG	1A	3789	1/1	0.95	0.12	20,20,20,20	0
57	MG	1A	3119	1/1	0.95	0.18	32,32,32,32	0
57	MG	1A	3475	1/1	0.95	0.17	20,20,20,20	0
57	MG	2A	3274	1/1	0.95	0.30	55,55,55,55	0
57	MG	1A	3235	1/1	0.95	0.41	34,34,34,34	0
57	MG	1A	3966	1/1	0.95	0.12	52,52,52,52	0
57	MG	1a	3152	1/1	0.95	0.23	65,65,65,65	0
57	MG	2A	3047	1/1	0.95	0.14	44,44,44,44	0
57	MG	1A	3667	1/1	0.95	0.07	46,46,46,46	0
57	MG	1A	3237	1/1	0.95	0.20	26,26,26,26	0
57	MG	10	105	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3311	1/1	0.95	0.12	19,19,19,19	0
57	MG	1A	3170	1/1	0.95	0.17	41,41,41,41	0
57	MG	1A	3239	1/1	0.95	0.19	33,33,33,33	0
57	MG	2A	3559	1/1	0.95	0.10	57,57,57,57	0
57	MG	1A	3575	1/1	0.95	0.08	61,61,61,61	0
57	MG	1a	3162	1/1	0.95	0.18	57,57,57,57	0
57	MG	1A	3482	1/1	0.95	0.12	45,45,45,45	0
57	MG	2A	3061	1/1	0.95	0.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3121	1/1	0.95	0.14	31,31,31,31	0
57	MG	1a	3167	1/1	0.95	0.12	39,39,39,39	0
57	MG	1A	3677	1/1	0.95	0.19	55,55,55,55	0
57	MG	13	102	1/1	0.95	0.09	51,51,51,51	0
57	MG	15	3101	1/1	0.95	0.20	26,26,26,26	0
57	MG	2A	3572	1/1	0.95	0.13	47,47,47,47	0
57	MG	2a	3054	1/1	0.95	0.10	60,60,60,60	0
57	MG	1a	3172	1/1	0.95	0.17	58,58,58,58	0
57	MG	1a	3173	1/1	0.95	0.14	68,68,68,68	0
57	MG	2A	3576	1/1	0.95	0.16	50,50,50,50	0
57	MG	1A	3581	1/1	0.95	0.17	47,47,47,47	0
57	MG	1A	3806	1/1	0.95	0.10	48,48,48,48	0
57	MG	1A	3808	1/1	0.95	0.12	70,70,70,70	0
57	MG	17	101	1/1	0.95	0.15	32,32,32,32	0
57	MG	1A	3177	1/1	0.95	0.18	47,47,47,47	0
57	MG	2A	3309	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3178	1/1	0.95	0.27	28,28,28,28	0
57	MG	1A	3026	1/1	0.95	0.23	29,29,29,29	0
57	MG	1A	3185	1/1	0.95	0.20	38,38,38,38	0
57	MG	2A	3586	1/1	0.95	0.07	54,54,54,54	0
57	MG	1A	3684	1/1	0.95	0.07	34,34,34,34	0
57	MG	1A	3814	1/1	0.95	0.10	43,43,43,43	0
57	MG	2a	3074	1/1	0.95	0.17	50,50,50,50	0
57	MG	1a	3185	1/1	0.95	0.09	72,72,72,72	0
57	MG	2A	3086	1/1	0.95	0.51	42,42,42,42	0
57	MG	2A	3319	1/1	0.95	0.14	57,57,57,57	0
57	MG	1A	3815	1/1	0.95	0.14	38,38,38,38	0
57	MG	2A	3598	1/1	0.95	0.14	39,39,39,39	0
57	MG	1A	3084	1/1	0.95	0.31	40,40,40,40	0
57	MG	2A	3600	1/1	0.95	0.06	47,47,47,47	0
57	MG	1a	3003	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3817	1/1	0.95	0.18	21,21,21,21	0
57	MG	1A	3686	1/1	0.95	0.06	39,39,39,39	0
57	MG	2A	3095	1/1	0.95	0.12	73,73,73,73	0
57	MG	2A	3328	1/1	0.95	0.07	50,50,50,50	0
57	MG	2a	3090	1/1	0.95	0.12	66,66,66,66	0
57	MG	1A	3819	1/1	0.95	0.17	33,33,33,33	0
57	MG	2a	3092	1/1	0.95	0.28	52,52,52,52	0
57	MG	1A	3822	1/1	0.95	0.26	55,55,55,55	0
57	MG	1A	3086	1/1	0.95	0.18	44,44,44,44	0
57	MG	1A	3410	1/1	0.95	0.15	18,18,18,18	0
57	MG	2a	3098	1/1	0.95	0.24	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3828	1/1	0.95	0.12	34,34,34,34	0
57	MG	1a	3015	1/1	0.95	0.10	64,64,64,64	0
57	MG	1A	3258	1/1	0.95	0.21	47,47,47,47	0
57	MG	1A	3128	1/1	0.95	0.11	54,54,54,54	0
57	MG	2a	3107	1/1	0.95	0.17	50,50,50,50	0
57	MG	1A	3693	1/1	0.95	0.25	40,40,40,40	0
57	MG	1A	4005	1/1	0.95	0.16	47,47,47,47	0
57	MG	2A	3346	1/1	0.95	0.20	49,49,49,49	0
57	MG	2A	3111	1/1	0.95	0.18	55,55,55,55	0
57	MG	1A	3832	1/1	0.95	0.11	36,36,36,36	0
57	MG	1A	3694	1/1	0.95	0.20	63,63,63,63	0
57	MG	1A	3495	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3087	1/1	0.95	0.33	41,41,41,41	0
57	MG	1A	3838	1/1	0.95	0.13	42,42,42,42	0
57	MG	2A	3117	1/1	0.95	0.13	58,58,58,58	0
57	MG	2a	3119	1/1	0.95	0.14	50,50,50,50	0
57	MG	2A	3119	1/1	0.95	0.26	54,54,54,54	0
57	MG	2A	3120	1/1	0.95	0.41	55,55,55,55	0
57	MG	2A	3358	1/1	0.95	0.14	31,31,31,31	0
57	MG	1a	3211	1/1	0.95	0.12	68,68,68,68	0
57	MG	1A	3500	1/1	0.95	0.15	47,47,47,47	0
57	MG	1A	3332	1/1	0.95	0.18	20,20,20,20	0
57	MG	1a	3029	1/1	0.95	0.19	49,49,49,49	0
57	MG	1A	4017	1/1	0.95	0.19	58,58,58,58	0
57	MG	1a	3031	1/1	0.95	0.11	52,52,52,52	0
57	MG	2A	3127	1/1	0.95	0.20	34,34,34,34	0
57	MG	1A	3333	1/1	0.95	0.30	48,48,48,48	0
57	MG	1A	3848	1/1	0.95	0.13	43,43,43,43	0
57	MG	1A	3088	1/1	0.95	0.22	46,46,46,46	0
57	MG	1A	3703	1/1	0.95	0.18	40,40,40,40	0
57	MG	1A	3420	1/1	0.95	0.14	53,53,53,53	0
57	MG	1a	3038	1/1	0.95	0.20	64,64,64,64	0
57	MG	1A	3338	1/1	0.95	0.15	44,44,44,44	0
57	MG	2A	3654	1/1	0.95	0.12	23,23,23,23	0
57	MG	2a	3151	1/1	0.95	0.25	60,60,60,60	0
57	MG	1a	3225	1/1	0.95	0.06	71,71,71,71	0
57	MG	2A	3379	1/1	0.95	0.14	42,42,42,42	0
57	MG	1A	3424	1/1	0.95	0.16	32,32,32,32	0
57	MG	1A	3008	1/1	0.95	0.15	27,27,27,27	0
57	MG	2A	3383	1/1	0.95	0.10	53,53,53,53	0
57	MG	2A	3660	1/1	0.95	0.12	36,36,36,36	0
57	MG	2A	3140	1/1	0.95	0.20	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1B	206	1/1	0.95	0.09	47,47,47,47	0
57	MG	2A	3142	1/1	0.95	0.13	46,46,46,46	0
57	MG	1a	3045	1/1	0.95	0.18	50,50,50,50	0
57	MG	1a	3046	1/1	0.95	0.19	49,49,49,49	0
57	MG	1A	3509	1/1	0.95	0.06	44,44,44,44	0
57	MG	1a	3048	1/1	0.95	0.20	61,61,61,61	0
57	MG	2A	3671	1/1	0.95	0.06	53,53,53,53	0
57	MG	2a	3166	1/1	0.95	0.12	58,58,58,58	0
57	MG	2A	3393	1/1	0.95	0.23	59,59,59,59	0
57	MG	1A	3713	1/1	0.95	0.12	36,36,36,36	0
57	MG	2A	3676	1/1	0.95	0.10	40,40,40,40	0
57	MG	1B	210	1/1	0.95	0.19	49,49,49,49	0
57	MG	1A	3511	1/1	0.95	0.17	18,18,18,18	0
57	MG	2A	3679	1/1	0.95	0.23	48,48,48,48	0
57	MG	2A	3680	1/1	0.95	0.16	63,63,63,63	0
57	MG	2A	3398	1/1	0.95	0.17	59,59,59,59	0
57	MG	1A	3716	1/1	0.95	0.16	33,33,33,33	0
57	MG	2A	3685	1/1	0.95	0.15	55,55,55,55	0
57	MG	2a	3181	1/1	0.95	0.06	57,57,57,57	0
57	MG	2a	3182	1/1	0.95	0.10	71,71,71,71	0
57	MG	1B	213	1/1	0.95	0.17	34,34,34,34	0
57	MG	1B	215	1/1	0.95	0.08	56,56,56,56	0
57	MG	2A	3405	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3341	1/1	0.95	0.16	34,34,34,34	0
57	MG	1A	3615	1/1	0.95	0.25	35,35,35,35	0
57	MG	1A	3091	1/1	0.95	0.25	31,31,31,31	0
57	MG	1A	3029	1/1	0.95	0.15	32,32,32,32	0
57	MG	2n	101	1/1	0.95	0.15	58,58,58,58	0
57	MG	1A	3096	1/1	0.95	0.17	50,50,50,50	0
57	MG	2t	201	1/1	0.95	0.12	35,35,35,35	0
57	MG	1A	3097	1/1	0.95	0.13	34,34,34,34	0
57	MG	2A	3413	1/1	0.95	0.10	55,55,55,55	0
57	MG	2A	3414	1/1	0.95	0.10	47,47,47,47	0
57	MG	2A	3703	1/1	0.95	0.15	55,55,55,55	0
58	MPD	1a	3276	8/8	0.95	0.23	54,57,61,63	0
57	MG	1A	3723	1/1	0.95	0.12	39,39,39,39	0
57	MG	1A	3520	1/1	0.95	0.43	47,47,47,47	0
57	MG	1A	3200	1/1	0.95	0.10	38,38,38,38	0
57	MG	2A	3709	1/1	0.95	0.11	44,44,44,44	0
57	MG	1A	3051	1/1	0.95	0.35	42,42,42,42	0
57	MG	2A	3712	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3066	1/1	0.95	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3714	1/1	0.95	0.11	49,49,49,49	0
57	MG	1F	308	1/1	0.96	0.13	24,24,24,24	0
57	MG	1u	101	1/1	0.96	0.21	64,64,64,64	0
57	MG	1A	3743	1/1	0.96	0.14	41,41,41,41	0
57	MG	2A	3473	1/1	0.96	0.08	52,52,52,52	0
57	MG	1a	3107	1/1	0.96	0.20	52,52,52,52	0
57	MG	1A	3403	1/1	0.96	0.16	21,21,21,21	0
57	MG	1A	3404	1/1	0.96	0.11	22,22,22,22	0
57	MG	1A	3407	1/1	0.96	0.14	45,45,45,45	0
57	MG	1A	3913	1/1	0.96	0.17	28,28,28,28	0
57	MG	1A	3508	1/1	0.96	0.09	46,46,46,46	0
57	MG	1a	3113	1/1	0.96	0.09	41,41,41,41	0
57	MG	1a	3115	1/1	0.96	0.13	47,47,47,47	0
57	MG	1a	3116	1/1	0.96	0.11	61,61,61,61	0
57	MG	1A	3316	1/1	0.96	0.14	21,21,21,21	0
57	MG	1A	3104	1/1	0.96	0.19	35,35,35,35	0
57	MG	2A	3486	1/1	0.96	0.08	64,64,64,64	0
57	MG	2A	3014	1/1	0.96	0.15	49,49,49,49	0
57	MG	1A	3628	1/1	0.96	0.12	46,46,46,46	0
57	MG	1A	3319	1/1	0.96	0.25	35,35,35,35	0
57	MG	2A	3240	1/1	0.96	0.35	59,59,59,59	0
57	MG	1A	3515	1/1	0.96	0.18	21,21,21,21	0
57	MG	2A	3492	1/1	0.96	0.14	35,35,35,35	0
57	MG	1O	201	1/1	0.96	0.30	48,48,48,48	0
57	MG	1A	3243	1/1	0.96	0.23	57,57,57,57	0
57	MG	1A	3923	1/1	0.96	0.08	46,46,46,46	0
57	MG	1A	3143	1/1	0.96	0.13	34,34,34,34	0
57	MG	1A	3925	1/1	0.96	0.08	27,27,27,27	0
57	MG	1A	3004	1/1	0.96	0.25	37,37,37,37	0
57	MG	1A	3190	1/1	0.96	0.17	28,28,28,28	0
57	MG	1a	3131	1/1	0.96	0.11	57,57,57,57	0
57	MG	1A	3930	1/1	0.96	0.16	55,55,55,55	0
57	MG	1A	3252	1/1	0.96	0.51	38,38,38,38	0
57	MG	1A	3326	1/1	0.96	0.14	41,41,41,41	0
57	MG	1A	3765	1/1	0.96	0.09	38,38,38,38	0
57	MG	1A	3083	1/1	0.96	0.36	28,28,28,28	0
57	MG	1A	3049	1/1	0.96	0.18	35,35,35,35	0
57	MG	1A	3525	1/1	0.96	0.14	25,25,25,25	0
57	MG	1A	3770	1/1	0.96	0.12	26,26,26,26	0
57	MG	2A	3512	1/1	0.96	0.12	67,67,67,67	0
57	MG	1a	3142	1/1	0.96	0.16	58,58,58,58	0
57	MG	2A	3042	1/1	0.96	0.08	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3143	1/1	0.96	0.13	65,65,65,65	0
57	MG	1A	3526	1/1	0.96	0.26	26,26,26,26	0
57	MG	1U	204	1/1	0.96	0.28	32,32,32,32	0
57	MG	1V	202	1/1	0.96	0.29	23,23,23,23	0
57	MG	1A	3033	1/1	0.96	0.11	36,36,36,36	0
57	MG	1A	3426	1/1	0.96	0.21	37,37,37,37	0
57	MG	2A	3051	1/1	0.96	0.10	53,53,53,53	0
57	MG	1V	207	1/1	0.96	0.15	45,45,45,45	0
57	MG	1A	3194	1/1	0.96	0.15	45,45,45,45	0
57	MG	1A	3945	1/1	0.96	0.10	23,23,23,23	0
57	MG	1A	3647	1/1	0.96	0.17	36,36,36,36	0
57	MG	1A	3948	1/1	0.96	0.17	39,39,39,39	0
57	MG	1A	3429	1/1	0.96	0.17	27,27,27,27	0
57	MG	1A	3950	1/1	0.96	0.12	43,43,43,43	0
57	MG	2Y	201	1/1	0.96	0.20	53,53,53,53	0
57	MG	2A	3060	1/1	0.96	0.09	43,43,43,43	0
57	MG	10	102	1/1	0.96	0.15	27,27,27,27	0
57	MG	2A	3285	1/1	0.96	0.16	37,37,37,37	0
57	MG	2A	3286	1/1	0.96	0.22	44,44,44,44	0
57	MG	25	103	1/1	0.96	0.11	57,57,57,57	0
57	MG	1A	3016	1/1	0.96	0.18	28,28,28,28	0
57	MG	2A	3536	1/1	0.96	0.11	69,69,69,69	0
57	MG	1A	3053	1/1	0.96	0.24	23,23,23,23	0
57	MG	2A	3289	1/1	0.96	0.17	42,42,42,42	0
57	MG	1A	3262	1/1	0.96	0.12	44,44,44,44	0
57	MG	1A	3954	1/1	0.96	0.13	55,55,55,55	0
57	MG	1A	3956	1/1	0.96	0.07	51,51,51,51	0
57	MG	1A	3334	1/1	0.96	0.16	25,25,25,25	0
57	MG	2A	3545	1/1	0.96	0.10	41,41,41,41	0
57	MG	1A	3785	1/1	0.96	0.09	48,48,48,48	0
57	MG	11	103	1/1	0.96	0.17	36,36,36,36	0
57	MG	1A	3960	1/1	0.96	0.10	38,38,38,38	0
57	MG	2A	3073	1/1	0.96	0.13	24,24,24,24	0
57	MG	11	105	1/1	0.96	0.07	26,26,26,26	0
57	MG	1A	3653	1/1	0.96	0.52	44,44,44,44	0
57	MG	1A	3540	1/1	0.96	0.12	22,22,22,22	0
57	MG	1A	3655	1/1	0.96	0.17	44,44,44,44	0
57	MG	2A	3555	1/1	0.96	0.41	48,48,48,48	0
57	MG	15	3103	1/1	0.96	0.17	22,22,22,22	0
57	MG	2A	3305	1/1	0.96	0.24	46,46,46,46	0
57	MG	15	3105	1/1	0.96	0.14	33,33,33,33	0
57	MG	1A	3656	1/1	0.96	0.32	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3117	1/1	0.96	0.25	27,27,27,27	0
57	MG	1A	3118	1/1	0.96	0.18	21,21,21,21	0
57	MG	2A	3085	1/1	0.96	0.18	41,41,41,41	0
57	MG	1A	3265	1/1	0.96	0.17	46,46,46,46	0
57	MG	2A	3566	1/1	0.96	0.06	68,68,68,68	0
57	MG	1A	3662	1/1	0.96	0.15	49,49,49,49	0
57	MG	1A	3054	1/1	0.96	0.10	23,23,23,23	0
57	MG	2a	3029	1/1	0.96	0.12	53,53,53,53	0
57	MG	1A	3344	1/1	0.96	0.15	25,25,25,25	0
57	MG	1A	3665	1/1	0.96	0.16	45,45,45,45	0
57	MG	2A	3092	1/1	0.96	0.17	42,42,42,42	0
57	MG	2A	3093	1/1	0.96	0.18	45,45,45,45	0
57	MG	2a	3034	1/1	0.96	0.13	45,45,45,45	0
57	MG	1A	3446	1/1	0.96	0.25	31,31,31,31	0
57	MG	1A	3017	1/1	0.96	0.24	27,27,27,27	0
57	MG	19	101	1/1	0.96	0.24	46,46,46,46	0
57	MG	1A	3448	1/1	0.96	0.15	61,61,61,61	0
57	MG	1A	3204	1/1	0.96	0.10	50,50,50,50	0
57	MG	1A	3450	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3804	1/1	0.96	0.14	39,39,39,39	0
57	MG	2a	3042	1/1	0.96	0.20	63,63,63,63	0
57	MG	1a	3005	1/1	0.96	0.14	54,54,54,54	0
57	MG	1a	3197	1/1	0.96	0.24	64,64,64,64	0
57	MG	1a	3198	1/1	0.96	0.12	46,46,46,46	0
57	MG	2A	3332	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3453	1/1	0.96	0.14	21,21,21,21	0
57	MG	1A	3672	1/1	0.96	0.12	44,44,44,44	0
57	MG	2A	3587	1/1	0.96	0.11	54,54,54,54	0
57	MG	1A	3560	1/1	0.96	0.08	38,38,38,38	0
57	MG	2A	3336	1/1	0.96	0.23	54,54,54,54	0
57	MG	1A	3674	1/1	0.96	0.18	31,31,31,31	0
57	MG	1A	3454	1/1	0.96	0.28	56,56,56,56	0
57	MG	2A	3594	1/1	0.96	0.07	67,67,67,67	0
57	MG	2A	3342	1/1	0.96	0.18	45,45,45,45	0
57	MG	1A	3455	1/1	0.96	0.10	51,51,51,51	0
57	MG	2A	3344	1/1	0.96	0.24	53,53,53,53	0
57	MG	1A	3269	1/1	0.96	0.12	48,48,48,48	0
57	MG	1A	3458	1/1	0.96	0.17	46,46,46,46	0
57	MG	2A	3601	1/1	0.96	0.04	62,62,62,62	0
57	MG	1a	3017	1/1	0.96	0.12	57,57,57,57	0
57	MG	2a	3063	1/1	0.96	0.12	66,66,66,66	0
57	MG	1a	3208	1/1	0.96	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3159	1/1	0.96	0.21	22,22,22,22	0
57	MG	1A	3680	1/1	0.96	0.23	58,58,58,58	0
57	MG	1A	3568	1/1	0.96	0.20	34,34,34,34	0
57	MG	2A	3607	1/1	0.96	0.07	43,43,43,43	0
57	MG	2A	3352	1/1	0.96	0.15	44,44,44,44	0
57	MG	1A	3349	1/1	0.96	0.22	31,31,31,31	0
57	MG	1A	3208	1/1	0.96	0.23	39,39,39,39	0
57	MG	2A	3355	1/1	0.96	0.14	65,65,65,65	0
57	MG	2a	3075	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3272	1/1	0.96	0.20	31,31,31,31	0
57	MG	1A	3162	1/1	0.96	0.27	33,33,33,33	0
57	MG	2a	3078	1/1	0.96	0.16	69,69,69,69	0
57	MG	1A	3039	1/1	0.96	0.12	38,38,38,38	0
57	MG	2A	3128	1/1	0.96	0.15	33,33,33,33	0
57	MG	2A	3360	1/1	0.96	0.21	33,33,33,33	0
57	MG	1A	3276	1/1	0.96	0.12	43,43,43,43	0
57	MG	1A	3827	1/1	0.96	0.10	45,45,45,45	0
57	MG	1A	3688	1/1	0.96	0.17	53,53,53,53	0
57	MG	2A	3623	1/1	0.96	0.05	71,71,71,71	0
57	MG	2A	3625	1/1	0.96	0.08	44,44,44,44	0
57	MG	1A	4008	1/1	0.96	0.17	43,43,43,43	0
57	MG	1A	3689	1/1	0.96	0.11	56,56,56,56	0
57	MG	1A	3576	1/1	0.96	0.08	57,57,57,57	0
57	MG	2A	3135	1/1	0.96	0.16	27,27,27,27	0
57	MG	2A	3370	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3072	1/1	0.96	0.19	31,31,31,31	0
57	MG	1A	3213	1/1	0.96	0.36	37,37,37,37	0
57	MG	1A	3579	1/1	0.96	0.18	21,21,21,21	0
57	MG	1A	3834	1/1	0.96	0.17	26,26,26,26	0
57	MG	1A	3279	1/1	0.96	0.12	41,41,41,41	0
57	MG	1a	3039	1/1	0.96	0.22	64,64,64,64	0
57	MG	2A	3639	1/1	0.96	0.11	55,55,55,55	0
57	MG	1A	3695	1/1	0.96	0.21	49,49,49,49	0
57	MG	2a	3106	1/1	0.96	0.20	54,54,54,54	0
57	MG	1A	3837	1/1	0.96	0.18	38,38,38,38	0
57	MG	2A	3144	1/1	0.96	0.30	28,28,28,28	0
57	MG	1A	3165	1/1	0.96	0.13	24,24,24,24	0
57	MG	2a	3110	1/1	0.96	0.24	51,51,51,51	0
57	MG	1a	3235	1/1	0.96	0.07	61,61,61,61	0
57	MG	1a	3043	1/1	0.96	0.08	54,54,54,54	0
57	MG	1A	3840	1/1	0.96	0.13	44,44,44,44	0
57	MG	1A	3366	1/1	0.96	0.12	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3075	1/1	0.96	0.23	40,40,40,40	0
57	MG	1A	3846	1/1	0.96	0.15	31,31,31,31	0
57	MG	2A	3156	1/1	0.96	0.35	55,55,55,55	0
57	MG	1A	3699	1/1	0.96	0.33	45,45,45,45	0
57	MG	2A	3652	1/1	0.96	0.13	36,36,36,36	0
57	MG	1a	3244	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	3586	1/1	0.96	0.15	38,38,38,38	0
57	MG	1A	3076	1/1	0.96	0.21	30,30,30,30	0
57	MG	1A	3223	1/1	0.96	0.30	34,34,34,34	0
57	MG	1a	3054	1/1	0.96	0.13	40,40,40,40	0
57	MG	1A	3168	1/1	0.96	0.12	45,45,45,45	0
57	MG	2A	3401	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	3590	1/1	0.96	0.17	54,54,54,54	0
57	MG	1A	3225	1/1	0.96	0.35	28,28,28,28	0
57	MG	2a	3136	1/1	0.96	0.13	71,71,71,71	0
57	MG	2A	3404	1/1	0.96	0.14	32,32,32,32	0
57	MG	2A	3664	1/1	0.96	0.08	47,47,47,47	0
57	MG	1B	214	1/1	0.96	0.12	37,37,37,37	0
57	MG	2a	3140	1/1	0.96	0.14	69,69,69,69	0
57	MG	1A	3019	1/1	0.96	0.18	23,23,23,23	0
57	MG	1B	216	1/1	0.96	0.27	43,43,43,43	0
57	MG	1A	3130	1/1	0.96	0.43	37,37,37,37	0
57	MG	2a	3145	1/1	0.96	0.15	66,66,66,66	0
57	MG	2A	3669	1/1	0.96	0.13	75,75,75,75	0
57	MG	1A	3710	1/1	0.96	0.09	37,37,37,37	0
57	MG	2a	3149	1/1	0.96	0.09	54,54,54,54	0
57	MG	2A	3672	1/1	0.96	0.11	33,33,33,33	0
57	MG	1A	3291	1/1	0.96	0.15	31,31,31,31	0
57	MG	1A	3862	1/1	0.96	0.12	54,54,54,54	0
57	MG	1a	3260	1/1	0.96	0.14	55,55,55,55	0
57	MG	1A	3712	1/1	0.96	0.10	32,32,32,32	0
57	MG	1A	3380	1/1	0.96	0.10	50,50,50,50	0
57	MG	1A	3714	1/1	0.96	0.34	30,30,30,30	0
57	MG	1A	3230	1/1	0.96	0.19	33,33,33,33	0
57	MG	1A	3173	1/1	0.96	0.10	22,22,22,22	0
57	MG	2A	3422	1/1	0.96	0.12	31,31,31,31	0
57	MG	2A	3423	1/1	0.96	0.14	37,37,37,37	0
57	MG	1A	3132	1/1	0.96	0.25	33,33,33,33	0
57	MG	1a	3267	1/1	0.96	0.10	55,55,55,55	0
57	MG	1A	3100	1/1	0.96	0.19	27,27,27,27	0
57	MG	2A	3691	1/1	0.96	0.10	51,51,51,51	0
57	MG	2A	3428	1/1	0.96	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3694	1/1	0.96	0.16	49,49,49,49	0
57	MG	1A	3183	1/1	0.96	0.47	32,32,32,32	0
57	MG	1a	3270	1/1	0.96	0.08	56,56,56,56	0
57	MG	2a	3169	1/1	0.96	0.09	56,56,56,56	0
57	MG	1a	3079	1/1	0.96	0.22	43,43,43,43	0
57	MG	1A	3300	1/1	0.96	0.21	31,31,31,31	0
57	MG	2a	3172	1/1	0.96	0.08	55,55,55,55	0
57	MG	1A	3302	1/1	0.96	0.13	46,46,46,46	0
57	MG	1A	3303	1/1	0.96	0.22	30,30,30,30	0
57	MG	2A	3436	1/1	0.96	0.15	48,48,48,48	0
57	MG	1A	3879	1/1	0.96	0.12	28,28,28,28	0
57	MG	1A	3304	1/1	0.96	0.20	33,33,33,33	0
57	MG	1A	3882	1/1	0.96	0.12	27,27,27,27	0
57	MG	1A	3394	1/1	0.96	0.17	22,22,22,22	0
57	MG	1A	3609	1/1	0.96	0.19	45,45,45,45	0
57	MG	1A	3613	1/1	0.96	0.17	29,29,29,29	0
57	MG	2A	3711	1/1	0.96	0.11	49,49,49,49	0
57	MG	2A	3446	1/1	0.96	0.10	57,57,57,57	0
57	MG	1A	3728	1/1	0.96	0.17	50,50,50,50	0
57	MG	2a	3188	1/1	0.96	0.08	58,58,58,58	0
57	MG	2A	3448	1/1	0.96	0.12	54,54,54,54	0
57	MG	2e	201	1/1	0.96	0.27	61,61,61,61	0
57	MG	1A	3496	1/1	0.96	0.19	53,53,53,53	0
57	MG	2A	3205	1/1	0.96	0.08	50,50,50,50	0
57	MG	1A	3731	1/1	0.96	0.06	26,26,26,26	0
57	MG	1A	3892	1/1	0.96	0.17	32,32,32,32	0
57	MG	1E	302	1/1	0.96	0.29	35,35,35,35	0
57	MG	1A	3733	1/1	0.96	0.14	46,46,46,46	0
57	MG	2A	3210	1/1	0.96	0.16	59,59,59,59	0
57	MG	1A	3894	1/1	0.96	0.14	36,36,36,36	0
57	MG	2A	3725	1/1	0.96	0.18	45,45,45,45	0
57	MG	1A	3497	1/1	0.96	0.19	22,22,22,22	0
57	MG	1A	3236	1/1	0.96	0.29	35,35,35,35	0
57	MG	2A	3459	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3308	1/1	0.96	0.20	49,49,49,49	0
57	MG	1A	3028	1/1	0.96	0.35	26,26,26,26	0
57	MG	1E	310	1/1	0.96	0.05	58,58,58,58	0
60	ZN	14	501	1/1	0.96	0.06	105,105,105,105	0
57	MG	1A	3137	1/1	0.96	0.16	45,45,45,45	0
57	MG	1A	3102	1/1	0.96	0.14	30,30,30,30	0
57	MG	1A	3402	1/1	0.96	0.21	14,14,14,14	0
57	MG	1A	3409	1/1	0.97	0.08	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3537	1/1	0.97	0.16	47,47,47,47	0
57	MG	1A	3965	1/1	0.97	0.09	35,35,35,35	0
57	MG	2A	3321	1/1	0.97	0.14	37,37,37,37	0
57	MG	1P	205	1/1	0.97	0.09	27,27,27,27	0
57	MG	2A	3323	1/1	0.97	0.08	57,57,57,57	0
57	MG	1A	3839	1/1	0.97	0.28	42,42,42,42	0
57	MG	1Q	203	1/1	0.97	0.13	29,29,29,29	0
57	MG	1A	3216	1/1	0.97	0.24	48,48,48,48	0
57	MG	2A	3546	1/1	0.97	0.18	36,36,36,36	0
57	MG	1A	3015	1/1	0.97	0.14	26,26,26,26	0
57	MG	1Q	207	1/1	0.97	0.18	45,45,45,45	0
57	MG	1A	3570	1/1	0.97	0.09	34,34,34,34	0
57	MG	1A	3970	1/1	0.97	0.13	22,22,22,22	0
57	MG	1A	3844	1/1	0.97	0.09	38,38,38,38	0
57	MG	1A	3845	1/1	0.97	0.11	42,42,42,42	0
57	MG	1A	3220	1/1	0.97	0.16	17,17,17,17	0
57	MG	2T	202	1/1	0.97	0.20	51,51,51,51	0
57	MG	1T	202	1/1	0.97	0.22	41,41,41,41	0
57	MG	1A	3745	1/1	0.97	0.10	58,58,58,58	0
57	MG	2V	202	1/1	0.97	0.47	54,54,54,54	0
57	MG	1A	3414	1/1	0.97	0.16	46,46,46,46	0
57	MG	2A	3337	1/1	0.97	0.10	42,42,42,42	0
57	MG	1A	3849	1/1	0.97	0.15	40,40,40,40	0
57	MG	1U	202	1/1	0.97	0.29	43,43,43,43	0
57	MG	1A	3657	1/1	0.97	0.27	38,38,38,38	0
57	MG	1A	3135	1/1	0.97	0.28	24,24,24,24	0
57	MG	1A	3852	1/1	0.97	0.21	36,36,36,36	0
57	MG	1A	3981	1/1	0.97	0.06	66,66,66,66	0
57	MG	1V	205	1/1	0.97	0.08	44,44,44,44	0
57	MG	1A	3161	1/1	0.97	0.27	35,35,35,35	0
57	MG	1A	3417	1/1	0.97	0.14	21,21,21,21	0
57	MG	1A	3855	1/1	0.97	0.10	35,35,35,35	0
57	MG	1A	3856	1/1	0.97	0.14	40,40,40,40	0
57	MG	1d	301	1/1	0.97	0.11	67,67,67,67	0
57	MG	2A	3151	1/1	0.97	0.09	56,56,56,56	0
57	MG	1a	3114	1/1	0.97	0.14	30,30,30,30	0
57	MG	2A	3574	1/1	0.97	0.15	31,31,31,31	0
57	MG	2A	3153	1/1	0.97	0.26	58,58,58,58	0
57	MG	1W	203	1/1	0.97	0.17	58,58,58,58	0
57	MG	2A	3155	1/1	0.97	0.11	52,52,52,52	0
57	MG	1A	3024	1/1	0.97	0.14	15,15,15,15	0
57	MG	1A	3354	1/1	0.97	0.13	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3355	1/1	0.97	0.16	23,23,23,23	0
57	MG	2A	3159	1/1	0.97	0.13	38,38,38,38	0
57	MG	1A	3305	1/1	0.97	0.18	45,45,45,45	0
57	MG	1A	3031	1/1	0.97	0.18	14,14,14,14	0
57	MG	2A	3163	1/1	0.97	0.16	47,47,47,47	0
57	MG	2A	3164	1/1	0.97	0.28	48,48,48,48	0
57	MG	1f	201	1/1	0.97	0.27	62,62,62,62	0
57	MG	2A	3166	1/1	0.97	0.12	70,70,70,70	0
57	MG	10	103	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3359	1/1	0.97	0.18	32,32,32,32	0
57	MG	1A	3863	1/1	0.97	0.16	28,28,28,28	0
57	MG	2A	3372	1/1	0.97	0.10	35,35,35,35	0
57	MG	1A	3307	1/1	0.97	0.13	42,42,42,42	0
57	MG	2A	3595	1/1	0.97	0.11	40,40,40,40	0
57	MG	1A	3584	1/1	0.97	0.17	39,39,39,39	0
57	MG	1A	3760	1/1	0.97	0.20	35,35,35,35	0
57	MG	1A	3427	1/1	0.97	0.25	16,16,16,16	0
57	MG	1A	3999	1/1	0.97	0.17	30,30,30,30	0
57	MG	1A	3074	1/1	0.97	0.14	29,29,29,29	0
57	MG	1A	3870	1/1	0.97	0.20	25,25,25,25	0
57	MG	2A	3380	1/1	0.97	0.14	42,42,42,42	0
57	MG	2A	3177	1/1	0.97	0.16	32,32,32,32	0
57	MG	1A	3763	1/1	0.97	0.11	31,31,31,31	0
57	MG	2A	3179	1/1	0.97	0.16	52,52,52,52	0
57	MG	1A	3764	1/1	0.97	0.14	30,30,30,30	0
57	MG	1A	3042	1/1	0.97	0.21	28,28,28,28	0
57	MG	2A	3608	1/1	0.97	0.08	40,40,40,40	0
57	MG	2A	3182	1/1	0.97	0.07	64,64,64,64	0
57	MG	2A	3387	1/1	0.97	0.23	41,41,41,41	0
57	MG	1A	3766	1/1	0.97	0.25	41,41,41,41	0
57	MG	1A	3310	1/1	0.97	0.19	32,32,32,32	0
57	MG	1A	3432	1/1	0.97	0.17	46,46,46,46	0
57	MG	15	3106	1/1	0.97	0.14	40,40,40,40	0
57	MG	1A	3036	1/1	0.97	0.10	27,27,27,27	0
57	MG	1A	3312	1/1	0.97	0.29	26,26,26,26	0
57	MG	1A	4012	1/1	0.97	0.26	33,33,33,33	0
57	MG	2A	3396	1/1	0.97	0.13	59,59,59,59	0
57	MG	1A	3881	1/1	0.97	0.10	29,29,29,29	0
57	MG	1a	3146	1/1	0.97	0.07	52,52,52,52	0
57	MG	17	102	1/1	0.97	0.19	28,28,28,28	0
57	MG	1A	3369	1/1	0.97	0.14	25,25,25,25	0
57	MG	2A	3004	1/1	0.97	0.22	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	17	104	1/1	0.97	0.24	30,30,30,30	0
57	MG	2A	3006	1/1	0.97	0.11	38,38,38,38	0
57	MG	1A	3370	1/1	0.97	0.12	23,23,23,23	0
57	MG	1A	4018	1/1	0.97	0.10	39,39,39,39	0
57	MG	2A	3012	1/1	0.97	0.26	57,57,57,57	0
57	MG	2A	3013	1/1	0.97	0.11	31,31,31,31	0
57	MG	1A	3371	1/1	0.97	0.18	58,58,58,58	0
57	MG	1A	3774	1/1	0.97	0.11	34,34,34,34	0
57	MG	1a	3154	1/1	0.97	0.15	60,60,60,60	0
57	MG	1A	3229	1/1	0.97	0.52	39,39,39,39	0
57	MG	2A	3020	1/1	0.97	0.48	42,42,42,42	0
57	MG	2A	3415	1/1	0.97	0.13	49,49,49,49	0
57	MG	2A	3021	1/1	0.97	0.11	34,34,34,34	0
57	MG	1A	3888	1/1	0.97	0.15	27,27,27,27	0
57	MG	19	102	1/1	0.97	0.07	60,60,60,60	0
57	MG	1A	3314	1/1	0.97	0.15	26,26,26,26	0
57	MG	2A	3421	1/1	0.97	0.18	49,49,49,49	0
57	MG	1A	3443	1/1	0.97	0.17	42,42,42,42	0
57	MG	1A	3125	1/1	0.97	0.23	45,45,45,45	0
57	MG	2A	3027	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3445	1/1	0.97	0.10	22,22,22,22	0
57	MG	2A	3029	1/1	0.97	0.10	39,39,39,39	0
57	MG	2a	3079	1/1	0.97	0.12	59,59,59,59	0
57	MG	2A	3427	1/1	0.97	0.17	40,40,40,40	0
57	MG	2A	3030	1/1	0.97	0.17	26,26,26,26	0
57	MG	1A	3781	1/1	0.97	0.39	49,49,49,49	0
57	MG	1A	3038	1/1	0.97	0.19	26,26,26,26	0
57	MG	1a	3166	1/1	0.97	0.17	51,51,51,51	0
57	MG	1a	3007	1/1	0.97	0.17	47,47,47,47	0
57	MG	1A	3376	1/1	0.97	0.10	30,30,30,30	0
57	MG	1A	3318	1/1	0.97	0.24	21,21,21,21	0
57	MG	1A	3169	1/1	0.97	0.45	35,35,35,35	0
57	MG	1A	3149	1/1	0.97	0.13	32,32,32,32	0
57	MG	1A	3901	1/1	0.97	0.10	26,26,26,26	0
57	MG	1A	3451	1/1	0.97	0.10	35,35,35,35	0
57	MG	2A	3440	1/1	0.97	0.04	75,75,75,75	0
57	MG	1A	3234	1/1	0.97	0.18	34,34,34,34	0
57	MG	2A	3443	1/1	0.97	0.27	51,51,51,51	0
57	MG	1A	3904	1/1	0.97	0.07	49,49,49,49	0
57	MG	2a	3096	1/1	0.97	0.11	51,51,51,51	0
57	MG	2a	3097	1/1	0.97	0.18	55,55,55,55	0
57	MG	2A	3230	1/1	0.97	0.23	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3610	1/1	0.97	0.12	32,32,32,32	0
57	MG	2a	3100	1/1	0.97	0.19	41,41,41,41	0
57	MG	2A	3670	1/1	0.97	0.12	50,50,50,50	0
57	MG	1A	3611	1/1	0.97	0.23	31,31,31,31	0
57	MG	2a	3103	1/1	0.97	0.19	49,49,49,49	0
57	MG	2A	3045	1/1	0.97	0.12	52,52,52,52	0
57	MG	1A	3908	1/1	0.97	0.57	55,55,55,55	0
57	MG	2A	3674	1/1	0.97	0.11	61,61,61,61	0
57	MG	1A	3909	1/1	0.97	0.17	28,28,28,28	0
57	MG	1A	3612	1/1	0.97	0.32	35,35,35,35	0
57	MG	2A	3049	1/1	0.97	0.12	57,57,57,57	0
57	MG	1A	3794	1/1	0.97	0.18	59,59,59,59	0
57	MG	2A	3239	1/1	0.97	0.51	52,52,52,52	0
57	MG	1A	3057	1/1	0.97	0.16	26,26,26,26	0
57	MG	2A	3681	1/1	0.97	0.13	36,36,36,36	0
57	MG	2A	3052	1/1	0.97	0.10	32,32,32,32	0
57	MG	1A	3172	1/1	0.97	0.35	46,46,46,46	0
57	MG	2A	3684	1/1	0.97	0.14	45,45,45,45	0
57	MG	1B	225	1/1	0.97	0.10	54,54,54,54	0
57	MG	2A	3244	1/1	0.97	0.12	53,53,53,53	0
57	MG	1A	3528	1/1	0.97	0.12	39,39,39,39	0
57	MG	2a	3121	1/1	0.97	0.08	58,58,58,58	0
57	MG	2A	3461	1/1	0.97	0.15	61,61,61,61	0
57	MG	2A	3690	1/1	0.97	0.11	56,56,56,56	0
57	MG	1A	3529	1/1	0.97	0.13	23,23,23,23	0
57	MG	1A	3079	1/1	0.97	0.20	37,37,37,37	0
57	MG	1A	3174	1/1	0.97	0.10	30,30,30,30	0
57	MG	1A	3175	1/1	0.97	0.30	32,32,32,32	0
57	MG	1A	3460	1/1	0.97	0.30	43,43,43,43	0
57	MG	2a	3133	1/1	0.97	0.06	66,66,66,66	0
57	MG	2A	3697	1/1	0.97	0.46	39,39,39,39	0
57	MG	2a	3135	1/1	0.97	0.08	46,46,46,46	0
57	MG	1A	3922	1/1	0.97	0.10	52,52,52,52	0
57	MG	1a	3194	1/1	0.97	0.07	51,51,51,51	0
57	MG	2A	3471	1/1	0.97	0.13	36,36,36,36	0
57	MG	1A	3534	1/1	0.97	0.13	38,38,38,38	0
57	MG	1A	3205	1/1	0.97	0.19	40,40,40,40	0
57	MG	2A	3474	1/1	0.97	0.11	40,40,40,40	0
57	MG	2a	3142	1/1	0.97	0.21	60,60,60,60	0
57	MG	2A	3255	1/1	0.97	0.11	49,49,49,49	0
57	MG	1a	3037	1/1	0.97	0.11	36,36,36,36	0
57	MG	2A	3707	1/1	0.97	0.14	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3390	1/1	0.97	0.11	29,29,29,29	0
57	MG	1A	3241	1/1	0.97	0.23	31,31,31,31	0
57	MG	1A	3927	1/1	0.97	0.18	47,47,47,47	0
57	MG	1A	3928	1/1	0.97	0.13	32,32,32,32	0
57	MG	2A	3070	1/1	0.97	0.16	47,47,47,47	0
57	MG	2A	3265	1/1	0.97	0.49	50,50,50,50	0
57	MG	1A	3539	1/1	0.97	0.13	41,41,41,41	0
57	MG	2A	3715	1/1	0.97	0.12	40,40,40,40	0
57	MG	1A	3081	1/1	0.97	0.15	31,31,31,31	0
57	MG	1A	3285	1/1	0.97	0.25	31,31,31,31	0
57	MG	1A	3543	1/1	0.97	0.13	30,30,30,30	0
57	MG	1A	3544	1/1	0.97	0.12	36,36,36,36	0
57	MG	1E	303	1/1	0.97	0.11	28,28,28,28	0
57	MG	2A	3721	1/1	0.97	0.22	49,49,49,49	0
57	MG	1A	3131	1/1	0.97	0.21	30,30,30,30	0
57	MG	1A	3935	1/1	0.97	0.15	58,58,58,58	0
57	MG	1A	3179	1/1	0.97	0.18	42,42,42,42	0
57	MG	1A	3632	1/1	0.97	0.15	24,24,24,24	0
57	MG	1A	3246	1/1	0.97	0.23	32,32,32,32	0
57	MG	1a	3055	1/1	0.97	0.15	44,44,44,44	0
57	MG	1A	3469	1/1	0.97	0.17	40,40,40,40	0
57	MG	1a	3057	1/1	0.97	0.06	58,58,58,58	0
57	MG	2A	3088	1/1	0.97	0.17	60,60,60,60	0
57	MG	1A	3550	1/1	0.97	0.16	46,46,46,46	0
57	MG	1A	3637	1/1	0.97	0.19	41,41,41,41	0
57	MG	1A	3821	1/1	0.97	0.28	26,26,26,26	0
57	MG	1F	305	1/1	0.97	0.13	23,23,23,23	0
57	MG	2A	3503	1/1	0.97	0.20	63,63,63,63	0
57	MG	1A	3335	1/1	0.97	0.18	20,20,20,20	0
57	MG	1A	3554	1/1	0.97	0.13	37,37,37,37	0
57	MG	1F	309	1/1	0.97	0.24	33,33,33,33	0
57	MG	1F	310	1/1	0.97	0.11	41,41,41,41	0
57	MG	1F	311	1/1	0.97	0.15	33,33,33,33	0
57	MG	1A	3182	1/1	0.97	0.13	30,30,30,30	0
57	MG	1A	3400	1/1	0.97	0.17	25,25,25,25	0
57	MG	2A	3296	1/1	0.97	0.16	40,40,40,40	0
57	MG	1A	3725	1/1	0.97	0.09	36,36,36,36	0
57	MG	2A	3102	1/1	0.97	0.13	55,55,55,55	0
57	MG	2a	3187	1/1	0.97	0.25	57,57,57,57	0
57	MG	1A	3250	1/1	0.97	0.32	30,30,30,30	0
57	MG	2a	3189	1/1	0.97	0.19	55,55,55,55	0
57	MG	1a	3072	1/1	0.97	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3517	1/1	0.97	0.05	49,49,49,49	0
57	MG	1F	316	1/1	0.97	0.17	50,50,50,50	0
57	MG	1a	3075	1/1	0.97	0.06	66,66,66,66	0
57	MG	2A	3107	1/1	0.97	0.11	30,30,30,30	0
57	MG	2A	3521	1/1	0.97	0.10	53,53,53,53	0
57	MG	2r	101	1/1	0.97	0.11	63,63,63,63	0
57	MG	2A	3109	1/1	0.97	0.11	50,50,50,50	0
57	MG	1A	3058	1/1	0.97	0.23	42,42,42,42	0
57	MG	1A	3476	1/1	0.97	0.17	42,42,42,42	0
57	MG	1A	3212	1/1	0.97	0.20	39,39,39,39	0
57	MG	1a	3239	1/1	0.97	0.12	58,58,58,58	0
57	MG	1A	3561	1/1	0.97	0.17	38,38,38,38	0
57	MG	1A	3957	1/1	0.97	0.14	49,49,49,49	0
57	MG	1A	3254	1/1	0.97	0.18	34,34,34,34	0
57	MG	2A	3312	1/1	0.97	0.12	55,55,55,55	0
57	MG	2E	302	1/1	0.97	0.24	39,39,39,39	0
57	MG	1N	201	1/1	0.97	0.13	38,38,38,38	0
57	MG	2A	3118	1/1	0.97	0.22	57,57,57,57	0
57	MG	1A	3405	1/1	0.97	0.15	34,34,34,34	0
57	MG	1A	3296	1/1	0.97	0.26	46,46,46,46	0
57	MG	1A	3115	1/1	0.97	0.12	28,28,28,28	0
60	ZN	2n	102	1/1	0.97	0.07	76,76,76,76	0
57	MG	1A	3963	1/1	0.98	0.10	44,44,44,44	0
57	MG	2A	3290	1/1	0.98	0.11	49,49,49,49	0
57	MG	1A	3343	1/1	0.98	0.16	31,31,31,31	0
57	MG	1A	3399	1/1	0.98	0.16	15,15,15,15	0
57	MG	1F	302	1/1	0.98	0.09	25,25,25,25	0
57	MG	1n	103	1/1	0.98	0.15	60,60,60,60	0
57	MG	2A	3637	1/1	0.98	0.15	33,33,33,33	0
57	MG	2A	3638	1/1	0.98	0.17	30,30,30,30	0
57	MG	1F	303	1/1	0.98	0.24	28,28,28,28	0
57	MG	1A	3864	1/1	0.98	0.08	31,31,31,31	0
57	MG	1F	306	1/1	0.98	0.13	35,35,35,35	0
57	MG	1A	3295	1/1	0.98	0.12	15,15,15,15	0
57	MG	1A	3248	1/1	0.98	0.34	39,39,39,39	0
57	MG	2A	3467	1/1	0.98	0.14	53,53,53,53	0
57	MG	1a	3163	1/1	0.98	0.07	57,57,57,57	0
57	MG	1A	3206	1/1	0.98	0.23	41,41,41,41	0
57	MG	1A	3089	1/1	0.98	0.11	36,36,36,36	0
57	MG	2A	3147	1/1	0.98	0.20	54,54,54,54	0
57	MG	1A	3972	1/1	0.98	0.07	56,56,56,56	0
57	MG	1A	3251	1/1	0.98	0.11	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3778	1/1	0.98	0.12	22,22,22,22	0
57	MG	1A	3538	1/1	0.98	0.26	31,31,31,31	0
57	MG	2A	3653	1/1	0.98	0.09	34,34,34,34	0
57	MG	1a	3170	1/1	0.98	0.14	57,57,57,57	0
57	MG	1A	3023	1/1	0.98	0.22	28,28,28,28	0
57	MG	1A	3350	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3541	1/1	0.98	0.13	23,23,23,23	0
57	MG	1A	3783	1/1	0.98	0.17	35,35,35,35	0
57	MG	2A	3008	1/1	0.98	0.14	29,29,29,29	0
57	MG	1A	3877	1/1	0.98	0.17	62,62,62,62	0
57	MG	2A	3011	1/1	0.98	0.12	34,34,34,34	0
57	MG	1A	3139	1/1	0.98	0.26	38,38,38,38	0
57	MG	2A	3161	1/1	0.98	0.19	43,43,43,43	0
57	MG	1A	3113	1/1	0.98	0.16	21,21,21,21	0
57	MG	1A	3141	1/1	0.98	0.15	21,21,21,21	0
57	MG	1A	3985	1/1	0.98	0.13	20,20,20,20	0
57	MG	2A	3016	1/1	0.98	0.29	38,38,38,38	0
57	MG	1a	3180	1/1	0.98	0.10	49,49,49,49	0
57	MG	2A	3018	1/1	0.98	0.44	37,37,37,37	0
57	MG	1A	3142	1/1	0.98	0.08	31,31,31,31	0
57	MG	2A	3493	1/1	0.98	0.20	49,49,49,49	0
57	MG	1N	204	1/1	0.98	0.19	51,51,51,51	0
57	MG	2a	3055	1/1	0.98	0.11	51,51,51,51	0
57	MG	1a	3049	1/1	0.98	0.17	41,41,41,41	0
57	MG	1A	3546	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3176	1/1	0.98	0.13	24,24,24,24	0
57	MG	1P	202	1/1	0.98	0.22	23,23,23,23	0
57	MG	1A	3413	1/1	0.98	0.14	26,26,26,26	0
57	MG	1A	3791	1/1	0.98	0.14	27,27,27,27	0
57	MG	1A	3704	1/1	0.98	0.08	31,31,31,31	0
57	MG	1A	3887	1/1	0.98	0.20	27,27,27,27	0
57	MG	1a	3058	1/1	0.98	0.24	47,47,47,47	0
57	MG	2A	3504	1/1	0.98	0.08	35,35,35,35	0
57	MG	1Q	202	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3214	1/1	0.98	0.17	29,29,29,29	0
57	MG	1A	3047	1/1	0.98	0.14	24,24,24,24	0
57	MG	1Q	205	1/1	0.98	0.18	47,47,47,47	0
57	MG	2A	3687	1/1	0.98	0.11	43,43,43,43	0
57	MG	2A	3341	1/1	0.98	0.20	38,38,38,38	0
57	MG	1a	3196	1/1	0.98	0.09	52,52,52,52	0
57	MG	1A	3551	1/1	0.98	0.21	29,29,29,29	0
57	MG	1A	3891	1/1	0.98	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3692	1/1	0.98	0.14	50,50,50,50	0
57	MG	1A	3217	1/1	0.98	0.23	31,31,31,31	0
57	MG	1A	3553	1/1	0.98	0.10	59,59,59,59	0
57	MG	1A	3360	1/1	0.98	0.10	19,19,19,19	0
57	MG	1A	3048	1/1	0.98	0.10	37,37,37,37	0
57	MG	1A	3219	1/1	0.98	0.18	26,26,26,26	0
57	MG	1A	3897	1/1	0.98	0.05	48,48,48,48	0
57	MG	1A	3363	1/1	0.98	0.17	10,10,10,10	0
57	MG	1A	3116	1/1	0.98	0.19	31,31,31,31	0
57	MG	1a	3073	1/1	0.98	0.12	59,59,59,59	0
57	MG	1T	205	1/1	0.98	0.15	40,40,40,40	0
57	MG	1A	3422	1/1	0.98	0.12	44,44,44,44	0
57	MG	1A	3180	1/1	0.98	0.20	29,29,29,29	0
57	MG	1A	3147	1/1	0.98	0.25	29,29,29,29	0
57	MG	2A	3706	1/1	0.98	0.14	39,39,39,39	0
57	MG	1A	3367	1/1	0.98	0.23	45,45,45,45	0
57	MG	1A	3807	1/1	0.98	0.34	40,40,40,40	0
57	MG	1V	203	1/1	0.98	0.12	34,34,34,34	0
57	MG	1a	3215	1/1	0.98	0.10	62,62,62,62	0
57	MG	2A	3362	1/1	0.98	0.14	27,27,27,27	0
57	MG	1A	3315	1/1	0.98	0.18	29,29,29,29	0
57	MG	1A	3093	1/1	0.98	0.18	31,31,31,31	0
57	MG	1A	4014	1/1	0.98	0.31	37,37,37,37	0
57	MG	1A	4015	1/1	0.98	0.17	36,36,36,36	0
57	MG	2A	3367	1/1	0.98	0.12	63,63,63,63	0
57	MG	1A	3907	1/1	0.98	0.15	14,14,14,14	0
57	MG	1A	3492	1/1	0.98	0.13	25,25,25,25	0
57	MG	2a	3104	1/1	0.98	0.27	50,50,50,50	0
57	MG	1A	3094	1/1	0.98	0.14	14,14,14,14	0
57	MG	1A	3910	1/1	0.98	0.07	37,37,37,37	0
57	MG	1A	3095	1/1	0.98	0.11	45,45,45,45	0
57	MG	1A	3431	1/1	0.98	0.22	32,32,32,32	0
57	MG	1A	3152	1/1	0.98	0.33	31,31,31,31	0
57	MG	1a	3227	1/1	0.98	0.19	45,45,45,45	0
57	MG	2A	3544	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3914	1/1	0.98	0.38	39,39,39,39	0
57	MG	1A	3320	1/1	0.98	0.38	59,59,59,59	0
57	MG	1A	3499	1/1	0.98	0.13	32,32,32,32	0
57	MG	1A	3434	1/1	0.98	0.19	19,19,19,19	0
57	MG	1A	3120	1/1	0.98	0.14	31,31,31,31	0
57	MG	2A	3071	1/1	0.98	0.20	39,39,39,39	0
57	MG	1a	3233	1/1	0.98	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3732	1/1	0.98	0.10	25,25,25,25	0
57	MG	1B	208	1/1	0.98	0.20	50,50,50,50	0
57	MG	1A	3820	1/1	0.98	0.17	28,28,28,28	0
57	MG	2a	3122	1/1	0.98	0.21	62,62,62,62	0
57	MG	2A	3076	1/1	0.98	0.15	35,35,35,35	0
57	MG	1l	101	1/1	0.98	0.26	39,39,39,39	0
57	MG	2A	3228	1/1	0.98	0.16	33,33,33,33	0
57	MG	1A	3020	1/1	0.98	0.49	28,28,28,28	0
57	MG	2a	3128	1/1	0.98	0.09	71,71,71,71	0
57	MG	2a	3129	1/1	0.98	0.13	62,62,62,62	0
57	MG	2A	3390	1/1	0.98	0.09	44,44,44,44	0
57	MG	1a	3102	1/1	0.98	0.22	57,57,57,57	0
57	MG	1a	3240	1/1	0.98	0.16	51,51,51,51	0
57	MG	2A	3562	1/1	0.98	0.08	45,45,45,45	0
57	MG	2A	3563	1/1	0.98	0.10	53,53,53,53	0
57	MG	1A	3122	1/1	0.98	0.18	37,37,37,37	0
57	MG	1A	3735	1/1	0.98	0.12	27,27,27,27	0
57	MG	1A	3037	1/1	0.98	0.10	44,44,44,44	0
57	MG	1A	3030	1/1	0.98	0.15	26,26,26,26	0
57	MG	1A	3440	1/1	0.98	0.13	14,14,14,14	0
57	MG	13	103	1/1	0.98	0.25	34,34,34,34	0
57	MG	2A	3399	1/1	0.98	0.17	56,56,56,56	0
57	MG	1A	3580	1/1	0.98	0.15	34,34,34,34	0
57	MG	2D	301	1/1	0.98	0.81	46,46,46,46	0
57	MG	15	3102	1/1	0.98	0.24	34,34,34,34	0
57	MG	2D	303	1/1	0.98	0.64	39,39,39,39	0
57	MG	2a	3146	1/1	0.98	0.08	49,49,49,49	0
57	MG	1A	3052	1/1	0.98	0.12	27,27,27,27	0
57	MG	1A	3659	1/1	0.98	0.14	19,19,19,19	0
57	MG	1A	3742	1/1	0.98	0.15	41,41,41,41	0
57	MG	1A	3025	1/1	0.98	0.21	33,33,33,33	0
57	MG	1A	3744	1/1	0.98	0.21	51,51,51,51	0
57	MG	1A	3127	1/1	0.98	0.12	24,24,24,24	0
57	MG	1A	3510	1/1	0.98	0.15	16,16,16,16	0
57	MG	1A	3068	1/1	0.98	0.18	29,29,29,29	0
57	MG	2A	3410	1/1	0.98	0.11	38,38,38,38	0
57	MG	1A	3512	1/1	0.98	0.17	17,17,17,17	0
57	MG	1A	3032	1/1	0.98	0.22	40,40,40,40	0
57	MG	2E	306	1/1	0.98	0.12	30,30,30,30	0
57	MG	2A	3100	1/1	0.98	0.22	45,45,45,45	0
57	MG	1A	3514	1/1	0.98	0.12	36,36,36,36	0
57	MG	1a	3122	1/1	0.98	0.11	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3416	1/1	0.98	0.22	50,50,50,50	0
57	MG	2F	304	1/1	0.98	0.36	41,41,41,41	0
57	MG	1A	3385	1/1	0.98	0.18	32,32,32,32	0
57	MG	1A	3386	1/1	0.98	0.16	31,31,31,31	0
57	MG	2A	3590	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3103	1/1	0.98	0.35	27,27,27,27	0
57	MG	2A	3256	1/1	0.98	0.36	44,44,44,44	0
57	MG	2A	3593	1/1	0.98	0.12	54,54,54,54	0
57	MG	2A	3257	1/1	0.98	0.15	36,36,36,36	0
57	MG	1A	3943	1/1	0.98	0.19	23,23,23,23	0
57	MG	1A	3592	1/1	0.98	0.14	52,52,52,52	0
57	MG	1D	303	1/1	0.98	0.17	36,36,36,36	0
57	MG	1D	304	1/1	0.98	0.15	34,34,34,34	0
57	MG	1a	3130	1/1	0.98	0.15	55,55,55,55	0
57	MG	2a	3176	1/1	0.98	0.07	63,63,63,63	0
57	MG	1A	3593	1/1	0.98	0.11	18,18,18,18	0
57	MG	2A	3264	1/1	0.98	0.33	50,50,50,50	0
57	MG	2a	3179	1/1	0.98	0.13	60,60,60,60	0
57	MG	1A	3198	1/1	0.98	0.29	36,36,36,36	0
57	MG	1A	3947	1/1	0.98	0.07	45,45,45,45	0
57	MG	2A	3267	1/1	0.98	0.10	25,25,25,25	0
57	MG	2T	203	1/1	0.98	0.17	60,60,60,60	0
57	MG	1A	3757	1/1	0.98	0.14	31,31,31,31	0
57	MG	1A	3085	1/1	0.98	0.28	38,38,38,38	0
57	MG	2A	3434	1/1	0.98	0.11	50,50,50,50	0
57	MG	1a	3136	1/1	0.98	0.12	34,34,34,34	0
57	MG	2W	201	1/1	0.98	0.21	42,42,42,42	0
57	MG	1A	3596	1/1	0.98	0.13	41,41,41,41	0
57	MG	2A	3610	1/1	0.98	0.08	25,25,25,25	0
57	MG	1a	3138	1/1	0.98	0.10	48,48,48,48	0
57	MG	1A	3452	1/1	0.98	0.19	22,22,22,22	0
57	MG	1a	3009	1/1	0.98	0.21	51,51,51,51	0
57	MG	1A	3201	1/1	0.98	0.22	41,41,41,41	0
57	MG	2A	3441	1/1	0.98	0.13	43,43,43,43	0
57	MG	25	101	1/1	0.98	0.40	39,39,39,39	0
57	MG	2A	3276	1/1	0.98	0.27	29,29,29,29	0
57	MG	1A	3522	1/1	0.98	0.20	24,24,24,24	0
57	MG	1a	3012	1/1	0.98	0.17	27,27,27,27	0
57	MG	28	101	1/1	0.98	0.14	51,51,51,51	0
57	MG	2A	3279	1/1	0.98	0.28	44,44,44,44	0
57	MG	1A	3005	1/1	0.98	0.17	22,22,22,22	0
57	MG	2A	3621	1/1	0.98	0.06	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3955	1/1	0.98	0.13	40,40,40,40	0
57	MG	1A	3003	1/1	0.98	0.18	28,28,28,28	0
57	MG	2A	3624	1/1	0.98	0.15	41,41,41,41	0
57	MG	1A	3456	1/1	0.98	0.09	41,41,41,41	0
60	ZN	1Y	202	1/1	0.98	0.20	53,53,53,53	0
57	MG	1A	3337	1/1	0.98	0.15	14,14,14,14	0
60	ZN	15	3110	1/1	0.98	0.20	43,43,43,43	0
60	ZN	1n	104	1/1	0.98	0.13	65,65,65,65	0
57	MG	1A	3043	1/1	0.98	0.17	21,21,21,21	0
57	MG	1A	3339	1/1	0.98	0.13	36,36,36,36	0
60	ZN	25	104	1/1	0.98	0.20	49,49,49,49	0
57	MG	1A	3109	1/1	0.98	0.27	27,27,27,27	0
57	MG	1A	3247	1/1	0.98	0.15	28,28,28,28	0
61	SF4	1d	307	8/8	0.98	0.13	54,58,64,66	0
61	SF4	2d	501	8/8	0.98	0.12	64,74,77,79	0
57	MG	2a	3065	1/1	0.99	0.07	76,76,76,76	0
57	MG	1A	3150	1/1	0.99	0.10	61,61,61,61	0
57	MG	1A	3442	1/1	0.99	0.19	27,27,27,27	0
57	MG	1N	202	1/1	0.99	0.16	38,38,38,38	0
57	MG	1A	3136	1/1	0.99	0.20	24,24,24,24	0
57	MG	1e	202	1/1	0.99	0.21	51,51,51,51	0
57	MG	1A	4000	1/1	0.99	0.21	15,15,15,15	0
57	MG	2a	3072	1/1	0.99	0.09	59,59,59,59	0
57	MG	2A	3108	1/1	0.99	0.15	51,51,51,51	0
57	MG	27	102	1/1	0.99	0.26	32,32,32,32	0
57	MG	1A	3242	1/1	0.99	0.20	21,21,21,21	0
57	MG	1A	3080	1/1	0.99	0.19	33,33,33,33	0
57	MG	1A	4003	1/1	0.99	0.60	44,44,44,44	0
57	MG	15	3104	1/1	0.99	0.21	30,30,30,30	0
57	MG	1A	3823	1/1	0.99	0.12	12,12,12,12	0
57	MG	1A	3044	1/1	0.99	0.21	25,25,25,25	0
57	MG	2A	3318	1/1	0.99	0.16	17,17,17,17	0
57	MG	1A	3294	1/1	0.99	0.15	20,20,20,20	0
57	MG	1A	3826	1/1	0.99	0.11	24,24,24,24	0
57	MG	2A	3184	1/1	0.99	0.07	41,41,41,41	0
57	MG	1D	306	1/1	0.99	0.15	20,20,20,20	0
57	MG	1A	3045	1/1	0.99	0.22	8,8,8,8	0
57	MG	1a	3050	1/1	0.99	0.13	46,46,46,46	0
57	MG	2a	3012	1/1	0.99	0.17	48,48,48,48	0
57	MG	1A	3383	1/1	0.99	0.13	42,42,42,42	0
57	MG	2A	3466	1/1	0.99	0.18	42,42,42,42	0
57	MG	1A	3872	1/1	0.99	0.14	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1D	310	1/1	0.99	0.14	26,26,26,26	0
57	MG	1A	3073	1/1	0.99	0.14	33,33,33,33	0
57	MG	1R	201	1/1	0.99	0.14	30,30,30,30	0
57	MG	1A	3708	1/1	0.99	0.12	21,21,21,21	0
57	MG	1A	3964	1/1	0.99	0.16	28,28,28,28	0
57	MG	1A	3013	1/1	0.99	0.20	22,22,22,22	0
57	MG	1A	3227	1/1	0.99	0.19	30,30,30,30	0
57	MG	1A	3634	1/1	0.99	0.13	35,35,35,35	0
57	MG	1A	3356	1/1	0.99	0.17	18,18,18,18	0
57	MG	1x	101	1/1	0.99	0.09	46,46,46,46	0
57	MG	1A	3007	1/1	0.99	0.15	33,33,33,33	0
57	MG	2A	3338	1/1	0.99	0.14	33,33,33,33	0
57	MG	1A	3273	1/1	0.99	0.40	37,37,37,37	0
57	MG	1A	3301	1/1	0.99	0.21	32,32,32,32	0
57	MG	1A	3423	1/1	0.99	0.24	20,20,20,20	0
57	MG	2E	305	1/1	0.99	0.08	38,38,38,38	0
57	MG	1A	3493	1/1	0.99	0.15	24,24,24,24	0
57	MG	1A	3566	1/1	0.99	0.17	49,49,49,49	0
57	MG	1A	3841	1/1	0.99	0.13	22,22,22,22	0
57	MG	1V	201	1/1	0.99	0.23	27,27,27,27	0
57	MG	1A	3067	1/1	0.99	0.14	27,27,27,27	0
57	MG	1A	3144	1/1	0.99	0.18	34,34,34,34	0
57	MG	2A	3010	1/1	0.99	0.18	61,61,61,61	0
57	MG	1B	205	1/1	0.99	0.54	39,39,39,39	0
57	MG	1F	301	1/1	0.99	0.20	28,28,28,28	0
57	MG	1A	3160	1/1	0.99	0.29	29,29,29,29	0
57	MG	1A	3107	1/1	0.99	0.20	35,35,35,35	0
57	MG	1F	304	1/1	0.99	0.17	28,28,28,28	0
57	MG	2A	3081	1/1	0.99	0.14	73,73,73,73	0
57	MG	1a	3259	1/1	0.99	0.13	33,33,33,33	0
57	MG	1A	3018	1/1	0.99	0.18	23,23,23,23	0
57	MG	1a	3018	1/1	0.99	0.14	46,46,46,46	0
57	MG	1A	3061	1/1	0.99	0.11	30,30,30,30	0
57	MG	1A	3982	1/1	0.99	0.12	39,39,39,39	0
57	MG	1A	3256	1/1	0.99	0.15	38,38,38,38	0
57	MG	2a	3127	1/1	0.99	0.06	71,71,71,71	0
57	MG	1A	3937	1/1	0.99	0.19	35,35,35,35	0
57	MG	1A	3281	1/1	0.99	0.17	32,32,32,32	0
57	MG	1A	3215	1/1	0.99	0.61	35,35,35,35	0
57	MG	1A	3110	1/1	0.99	0.19	26,26,26,26	0
57	MG	1A	3729	1/1	0.99	0.20	23,23,23,23	0
57	MG	1A	3284	1/1	0.99	0.12	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	ZN	16	501	1/1	0.99	0.21	40,40,40,40	0
60	ZN	19	103	1/1	0.99	0.20	41,41,41,41	0
57	MG	1A	3181	1/1	0.99	0.16	26,26,26,26	0
57	MG	1A	3342	1/1	0.99	0.08	48,48,48,48	0
57	MG	1A	3199	1/1	0.99	0.16	27,27,27,27	0
57	MG	1A	3472	1/1	0.99	0.17	49,49,49,49	0
60	ZN	26	501	1/1	0.99	0.20	59,59,59,59	0
57	MG	1A	3261	1/1	0.99	0.20	26,26,26,26	0
57	MG	1A	3406	1/1	0.99	0.13	57,57,57,57	0
57	MG	1A	3001	1/1	0.99	0.15	26,26,26,26	0
57	MG	1a	3155	1/1	0.99	0.14	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.