



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 2, 2026 – 08:53 PM EDT

PDB ID : 9Q6S / pdb_00009q6s
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with pleuromutilin-30 triazole derivative and protein Y at 2.90Å resolution
Authors : Killam, B.Y.; Kopec, I.; Breiner, L.M.; Hoernig, M.; LoPresti, M.; Abdelsattar, A.S.; Abouelkhair, A.A.; Briganti, A.J.; Slowinski, R.P.; Vogelaar, N.J.; Seleem, M.N.; Brown, A.M.; Lowell, A.N.; Polikanov, Y.S.
Deposited on : 2025-08-22
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

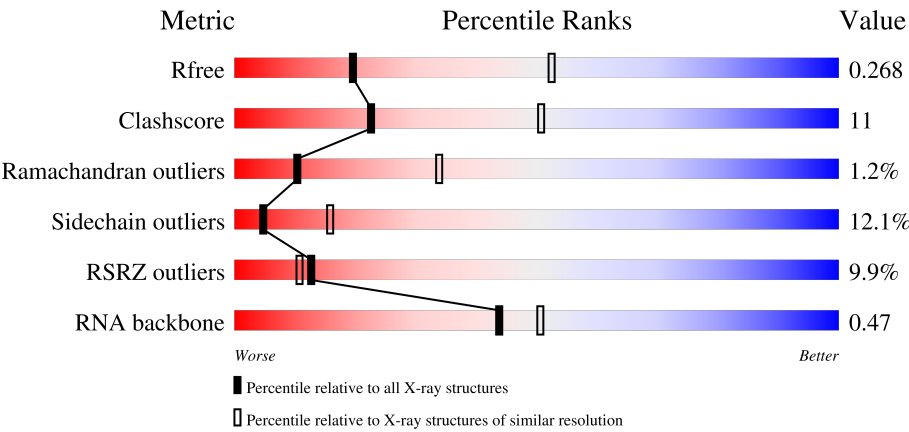
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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.



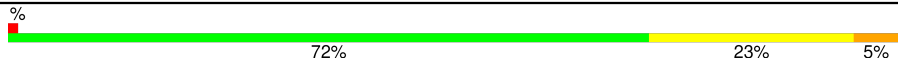
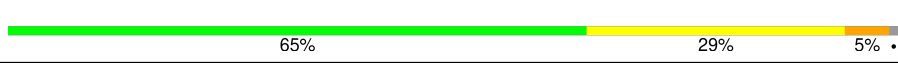
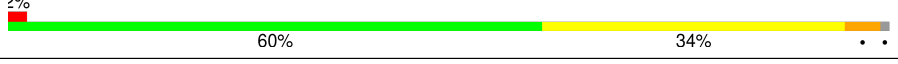
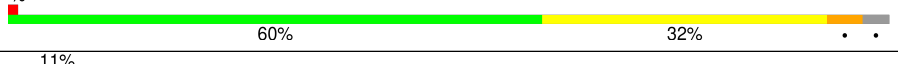
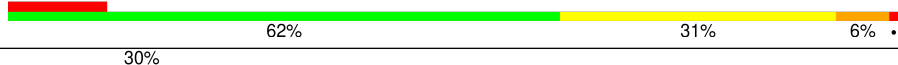
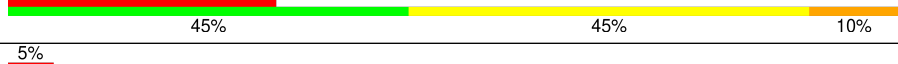
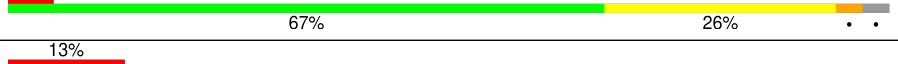
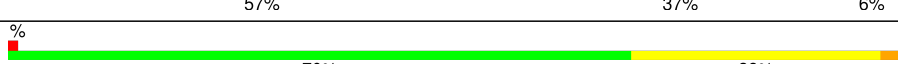
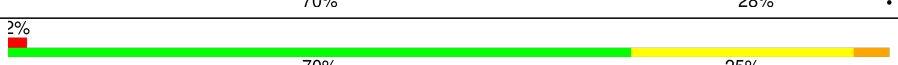
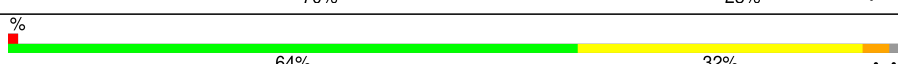
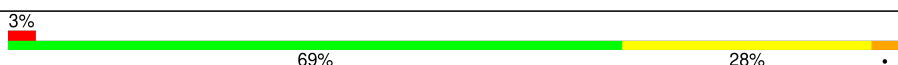
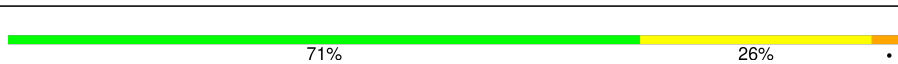
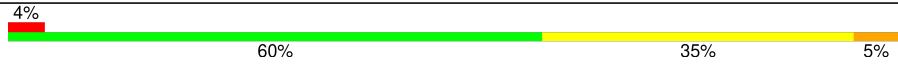
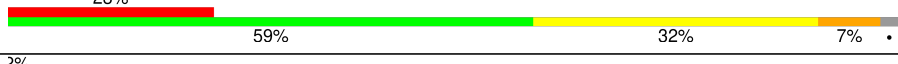
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	5% 58% 33% 8% .
1	2A	2915	6% 53% 37% 8% .
2	1B	121	% 64% 32% . .
2	2B	121	16% 56% 36% 7% .

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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
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	

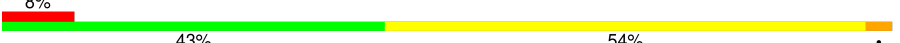
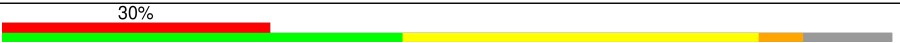
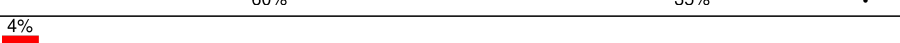
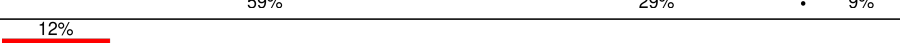
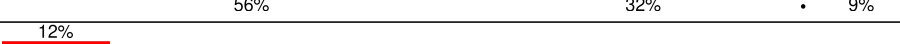
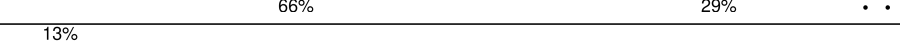
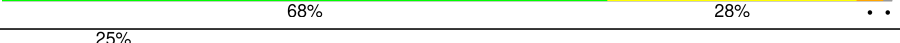
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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	1A	3991	-	-	-	X
54	MG	2a	1712	-	-	-	X
57	MPD	1a	1870	-	-	X	-

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 297211 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	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1010	Total	Mg	0	0
			1010	1010		
54	1B	31	Total	Mg	0	0
			31	31		
54	1D	18	Total	Mg	0	0
			18	18		
54	1E	9	Total	Mg	0	0
			9	9		
54	1F	18	Total	Mg	0	0
			18	18		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	2	Total	Mg	0	0
			2	2		
54	1N	5	Total	Mg	0	0
			5	5		
54	1O	2	Total	Mg	0	0
			2	2		
54	1P	8	Total	Mg	0	0
			8	8		
54	1Q	7	Total	Mg	0	0
			7	7		
54	1R	5	Total	Mg	0	0
			5	5		
54	1S	1	Total	Mg	0	0
			1	1		
54	1T	5	Total	Mg	0	0
			5	5		
54	1U	6	Total	Mg	0	0
			6	6		
54	1V	6	Total	Mg	0	0
			6	6		
54	1W	4	Total	Mg	0	0
			4	4		
54	1X	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1Y	1	Total 1	Mg 1	0	0
54	1Z	1	Total 1	Mg 1	0	0
54	10	10	Total 10	Mg 10	0	0
54	11	5	Total 5	Mg 5	0	0
54	13	4	Total 4	Mg 4	0	0
54	15	6	Total 6	Mg 6	0	0
54	17	4	Total 4	Mg 4	0	0
54	18	1	Total 1	Mg 1	0	0
54	19	2	Total 2	Mg 2	0	0
54	1a	269	Total 269	Mg 269	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	5	Total 5	Mg 5	0	0
54	1e	3	Total 3	Mg 3	0	0
54	1f	2	Total 2	Mg 2	0	0
54	1g	3	Total 3	Mg 3	0	0
54	1h	1	Total 1	Mg 1	0	0
54	1i	1	Total 1	Mg 1	0	0
54	1k	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0
54	1m	1	Total 1	Mg 1	0	0
54	1n	2	Total 2	Mg 2	0	0

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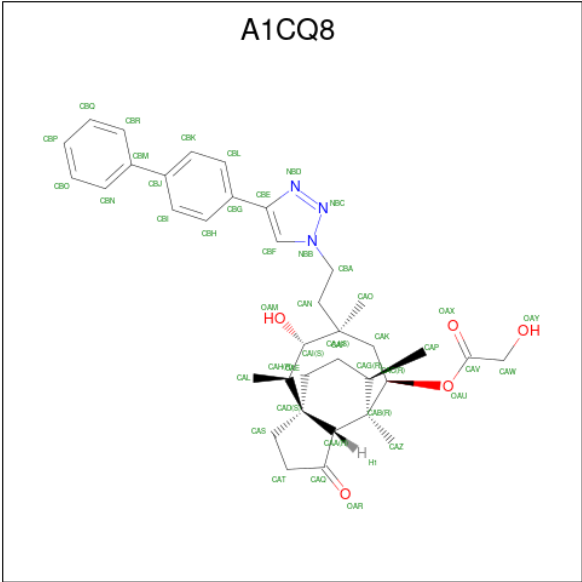
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1o	1	Total 1	Mg 1	0	0
54	1p	1	Total 1	Mg 1	0	0
54	1q	1	Total 1	Mg 1	0	0
54	1t	2	Total 2	Mg 2	0	0
54	1y	4	Total 4	Mg 4	0	0
54	2A	724	Total 724	Mg 724	0	0
54	2B	18	Total 18	Mg 18	0	0
54	2D	8	Total 8	Mg 8	0	0
54	2E	9	Total 9	Mg 9	0	0
54	2F	4	Total 4	Mg 4	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2I	1	Total 1	Mg 1	0	0
54	2N	1	Total 1	Mg 1	0	0
54	2P	3	Total 3	Mg 3	0	0
54	2Q	2	Total 2	Mg 2	0	0
54	2R	2	Total 2	Mg 2	0	0
54	2T	5	Total 5	Mg 5	0	0
54	2V	3	Total 3	Mg 3	0	0
54	2W	3	Total 3	Mg 3	0	0
54	2X	2	Total 2	Mg 2	0	0
54	2Y	1	Total 1	Mg 1	0	0

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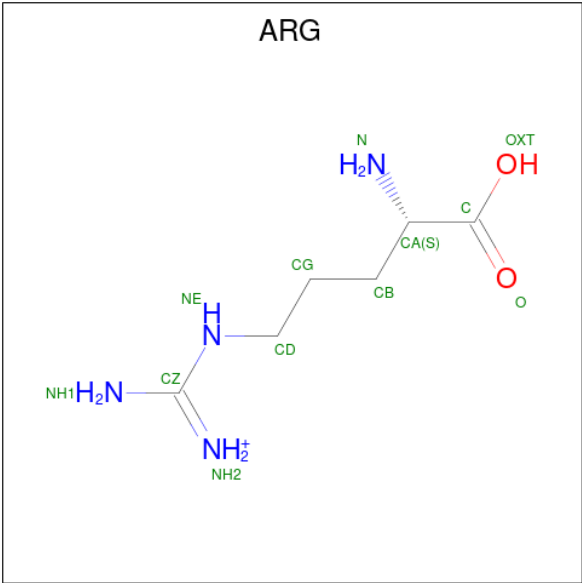
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	20	2	Total 2	Mg 2	0	0
54	21	3	Total 3	Mg 3	0	0
54	23	1	Total 1	Mg 1	0	0
54	25	2	Total 2	Mg 2	0	0
54	26	1	Total 1	Mg 1	0	0
54	27	1	Total 1	Mg 1	0	0
54	28	1	Total 1	Mg 1	0	0
54	2a	177	Total 177	Mg 177	0	0
54	2e	2	Total 2	Mg 2	0	0
54	2f	1	Total 1	Mg 1	0	0
54	2j	1	Total 1	Mg 1	0	0
54	2n	1	Total 1	Mg 1	0	0
54	2r	1	Total 1	Mg 1	0	0
54	2t	1	Total 1	Mg 1	0	0

- Molecule 55 is (3aS,4R,5S,6S,8R,9R,9aR,10R)-6-{2-[4-([1,1'-biphenyl]-4-yl)-1H-1,2,3-triazol-1-yl]ethyl}-5-hydroxy-4,6,9,10-tetramethyl-1-oxodecahydro-3a,9-propanocyclopenta[8]annulen-8-yl hydroxyacetate (CCD ID: A1CQ8) (formula: C₃₆H₄₅N₃O₅) (labeled as "Ligand of Interest" by depositor).



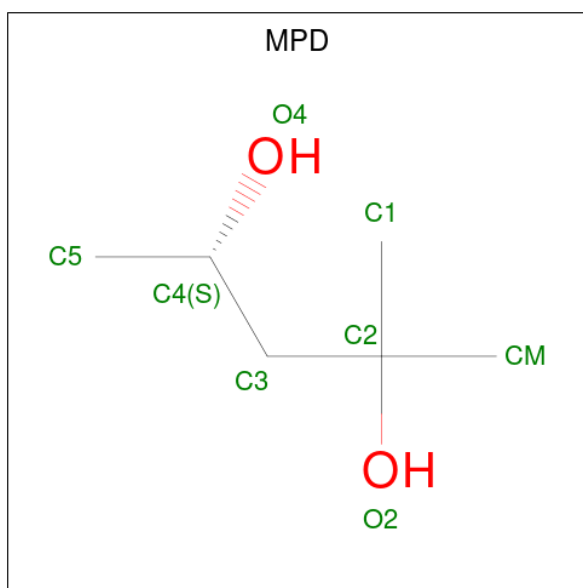
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	1A	1	Total	C	N	O	0	0
			44	36	3	5		
55	2A	1	Total	C	N	O	0	0
			44	36	3	5		

- Molecule 56 is ARGinine (CCD ID: ARG) (formula: C₆H₁₅N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	1A	1	Total	C	N	O	0	0
			12	6	4	2		
56	1B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

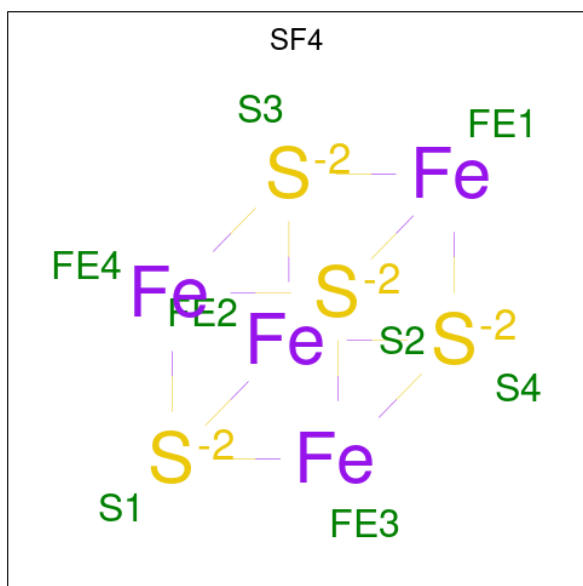
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	19	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	2Y	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		
58	29	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	1d	1	Total	Fe	S	0	0
			8	4	4		
59	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3708	Total 3708	O 3708	0	0
60	1B	95	Total 95	O 95	0	0
60	1D	105	Total 105	O 105	0	0
60	1E	72	Total 72	O 72	0	0
60	1F	59	Total 59	O 59	0	0
60	1G	13	Total 13	O 13	0	0
60	1H	15	Total 15	O 15	0	0
60	1I	8	Total 8	O 8	0	0
60	1N	55	Total 55	O 55	0	0
60	1O	26	Total 26	O 26	0	0
60	1P	64	Total 64	O 64	0	0
60	1Q	42	Total 42	O 42	0	0
60	1R	28	Total 28	O 28	0	0
60	1S	10	Total 10	O 10	0	0
60	1T	35	Total 35	O 35	0	0
60	1U	42	Total 42	O 42	0	0
60	1V	35	Total 35	O 35	0	0
60	1W	27	Total 27	O 27	0	0
60	1X	26	Total 26	O 26	0	0
60	1Y	13	Total 13	O 13	0	0
60	1Z	12	Total 12	O 12	0	0
60	10	27	Total 27	O 27	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	11	27	Total 27	O 27	0	0
60	12	14	Total 14	O 14	0	0
60	13	22	Total 22	O 22	0	0
60	14	3	Total 3	O 3	0	0
60	15	22	Total 22	O 22	0	0
60	16	21	Total 21	O 21	0	0
60	17	13	Total 13	O 13	0	0
60	18	25	Total 25	O 25	0	0
60	19	10	Total 10	O 10	0	0
60	1a	503	Total 503	O 503	0	0
60	1b	1	Total 1	O 1	0	0
60	1c	1	Total 1	O 1	0	0
60	1d	7	Total 7	O 7	0	0
60	1e	5	Total 5	O 5	0	0
60	1f	3	Total 3	O 3	0	0
60	1i	1	Total 1	O 1	0	0
60	1j	1	Total 1	O 1	0	0
60	1l	5	Total 5	O 5	0	0
60	1m	2	Total 2	O 2	0	0
60	1o	2	Total 2	O 2	0	0
60	1p	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1q	1	Total 1	O 1	0	0
60	1t	2	Total 2	O 2	0	0
60	1u	1	Total 1	O 1	0	0
60	1y	3	Total 3	O 3	0	0
60	2A	2290	Total 2290	O 2290	0	0
60	2B	59	Total 59	O 59	0	0
60	2D	46	Total 46	O 46	0	0
60	2E	29	Total 29	O 29	0	0
60	2F	17	Total 17	O 17	0	0
60	2G	5	Total 5	O 5	0	0
60	2H	3	Total 3	O 3	0	0
60	2I	4	Total 4	O 4	0	0
60	2N	6	Total 6	O 6	0	0
60	2O	13	Total 13	O 13	0	0
60	2P	26	Total 26	O 26	0	0
60	2Q	19	Total 19	O 19	0	0
60	2R	23	Total 23	O 23	0	0
60	2S	5	Total 5	O 5	0	0
60	2T	11	Total 11	O 11	0	0
60	2U	12	Total 12	O 12	0	0
60	2V	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2W	24	Total 24	O 24	0	0
60	2X	10	Total 10	O 10	0	0
60	2Y	6	Total 6	O 6	0	0
60	2Z	11	Total 11	O 11	0	0
60	20	10	Total 10	O 10	0	0
60	21	23	Total 23	O 23	0	0
60	22	5	Total 5	O 5	0	0
60	23	3	Total 3	O 3	0	0
60	24	1	Total 1	O 1	0	0
60	25	9	Total 9	O 9	0	0
60	26	4	Total 4	O 4	0	0
60	27	13	Total 13	O 13	0	0
60	28	12	Total 12	O 12	0	0
60	2a	250	Total 250	O 250	0	0
60	2d	4	Total 4	O 4	0	0
60	2e	2	Total 2	O 2	0	0
60	2f	4	Total 4	O 4	0	0
60	2j	1	Total 1	O 1	0	0
60	2l	2	Total 2	O 2	0	0
60	2o	1	Total 1	O 1	0	0
60	2p	2	Total 2	O 2	0	0

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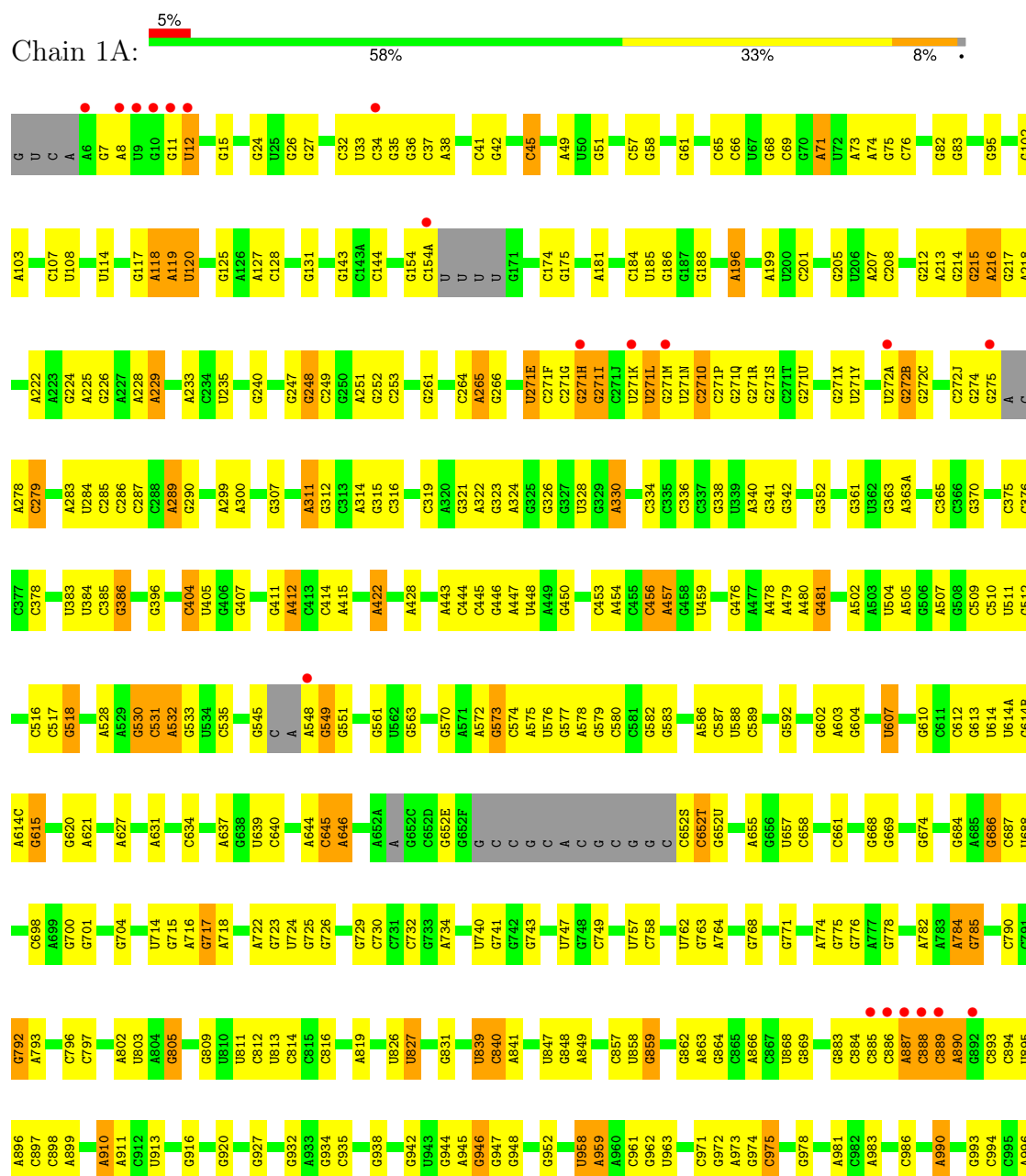
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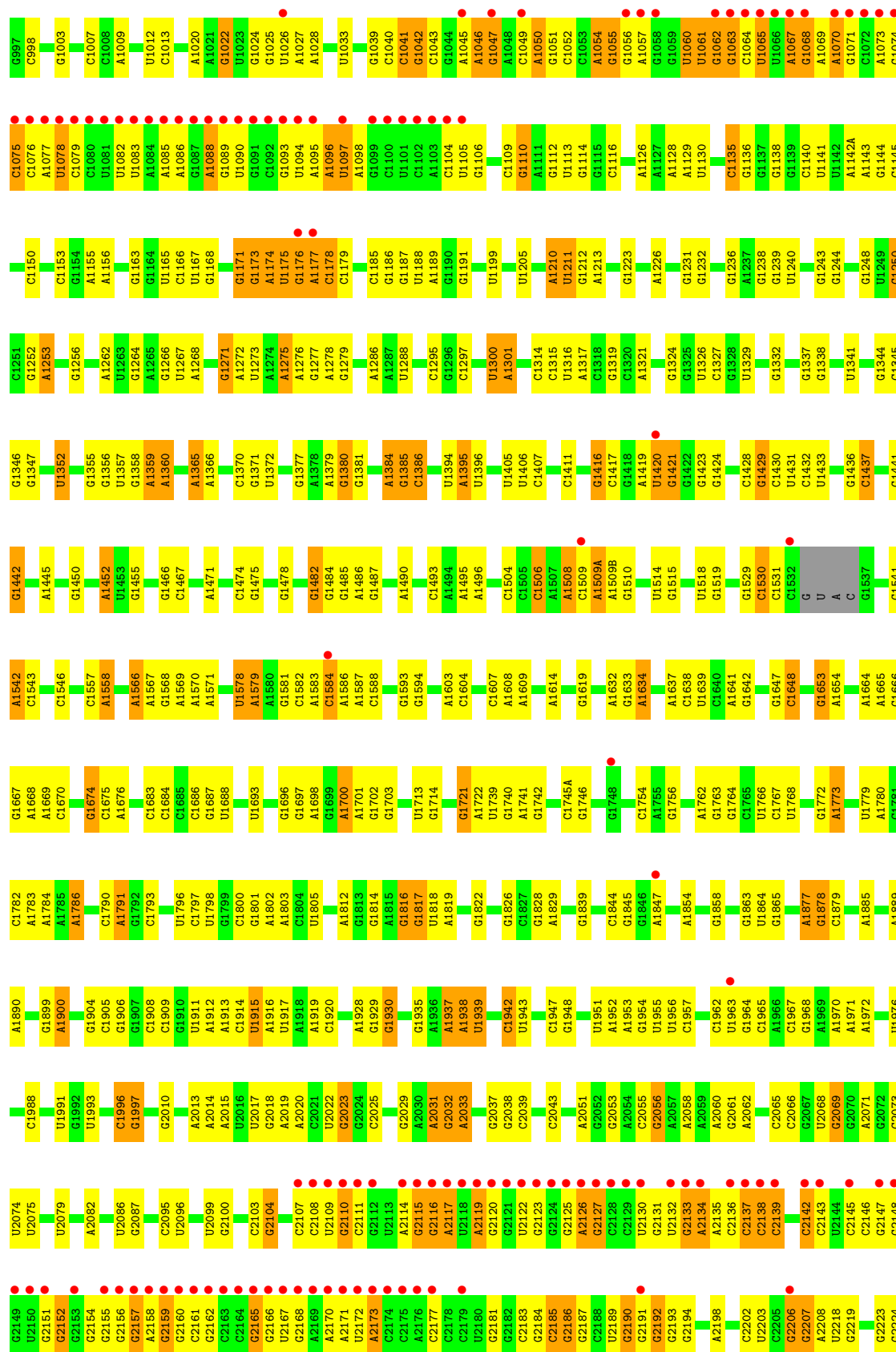
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2q	1	Total	O	0	0
			1	1		
60	2r	2	Total	O	0	0
			2	2		
60	2t	4	Total	O	0	0
			4	4		
60	2y	2	Total	O	0	0
			2	2		

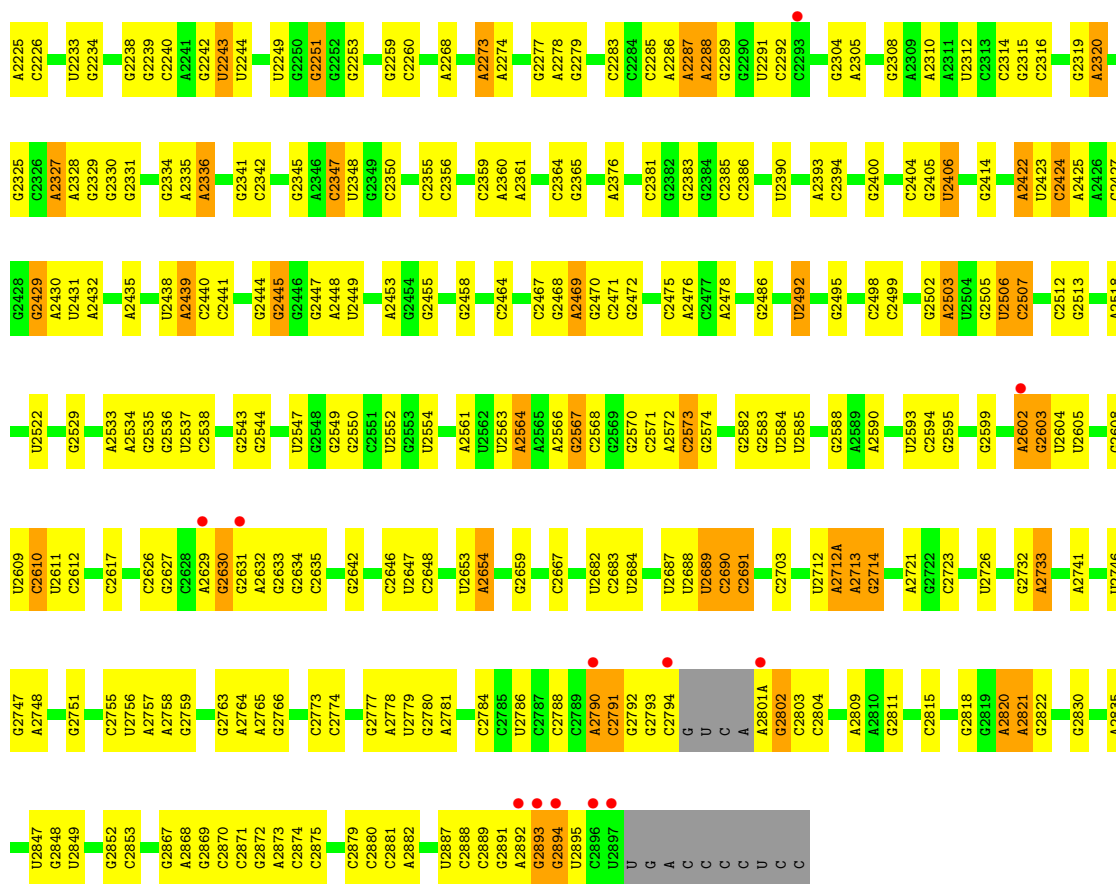
3 Residue-property plots [i](#)

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

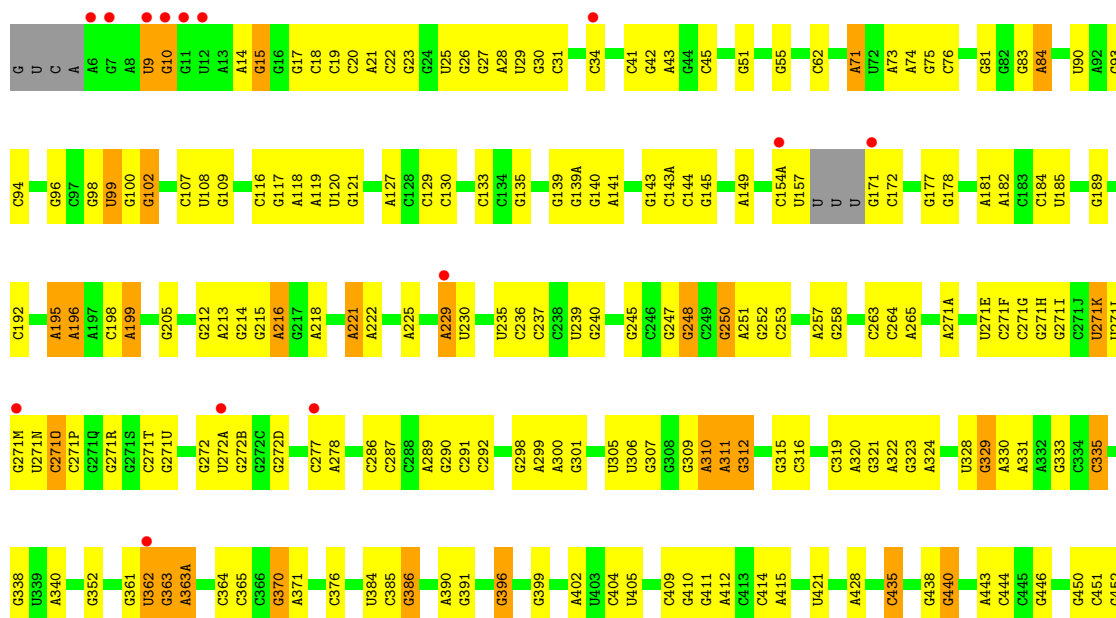
• Molecule 1: 23S Ribosomal RNA







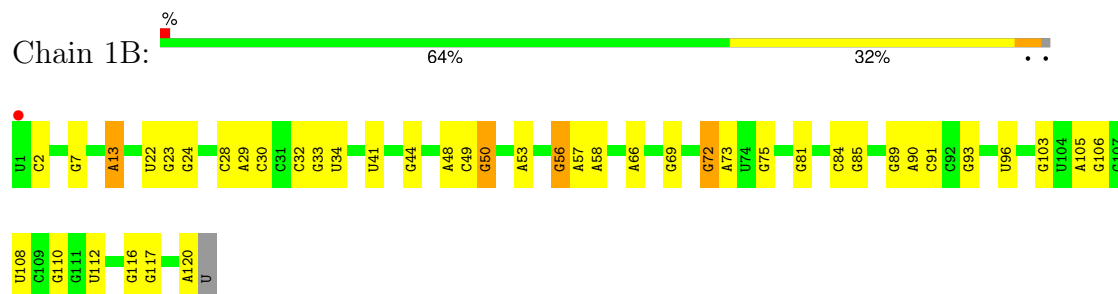
• Molecule 1: 23S Ribosomal RNA



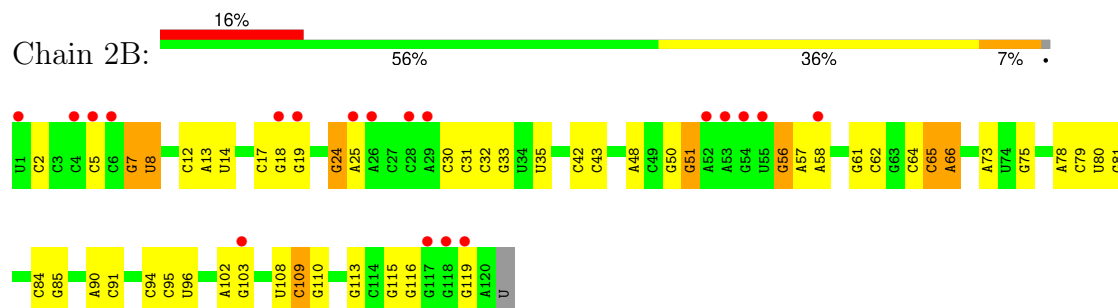


A2873	C2874	C2875	G2876	C2879	A2882	A2883	G2891	A2892	C2893	C2894	C2895	C2896	U2897	U	G	G	A	C	C	C	C	C	U	C	C																																	
C2773	A2776	C2777	A2778	A2781	U2782	U2788	C2785	U2786	C2787	C2788	C2789	C	C	C	C	C	C	C	C	C	C	C	C	C	C																																	
C2680	C2681	U2682	C2683	U2684	U2687	U2688	U2689	C2690	A2693	C2694	C2695	U2696	C2697	U2698	C2699	C2700	C2703	C2704	A2705	G2708	C2711	C2712	A2712A	A2713	C2714	C2723	U2726	G2727	U2728	C2729	C2732	A2733	C2742	A2835	U2836	C2837	G2838	C2839	C2840	C2841	G2842	U2849	A2868	C2869	C2870	C2871	G2872											
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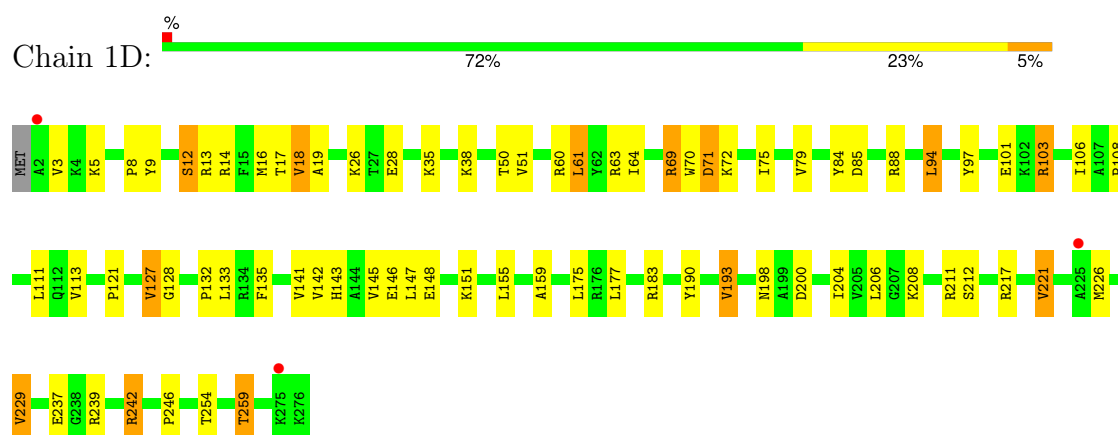
- Molecule 2: 5S Ribosomal RNA



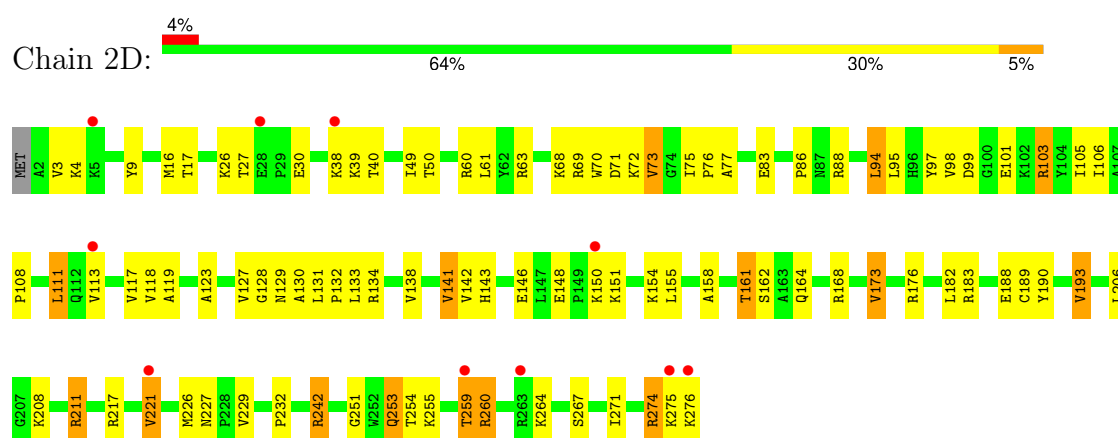
- Molecule 2: 5S Ribosomal RNA



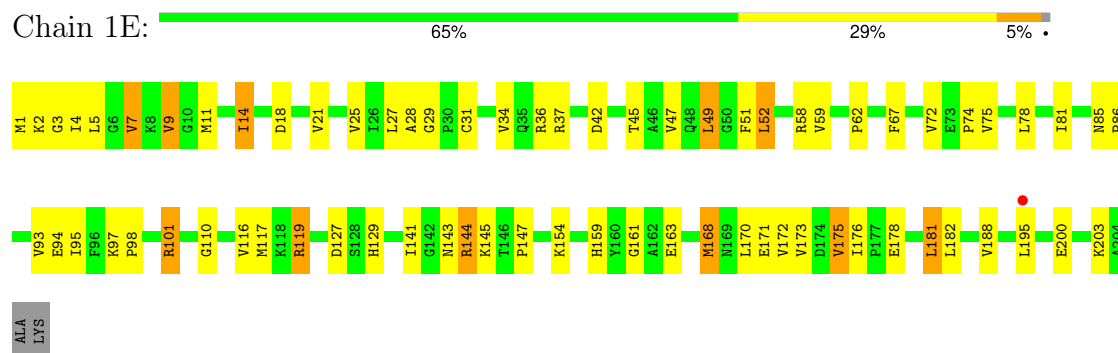
- Molecule 3: 50S ribosomal protein L2



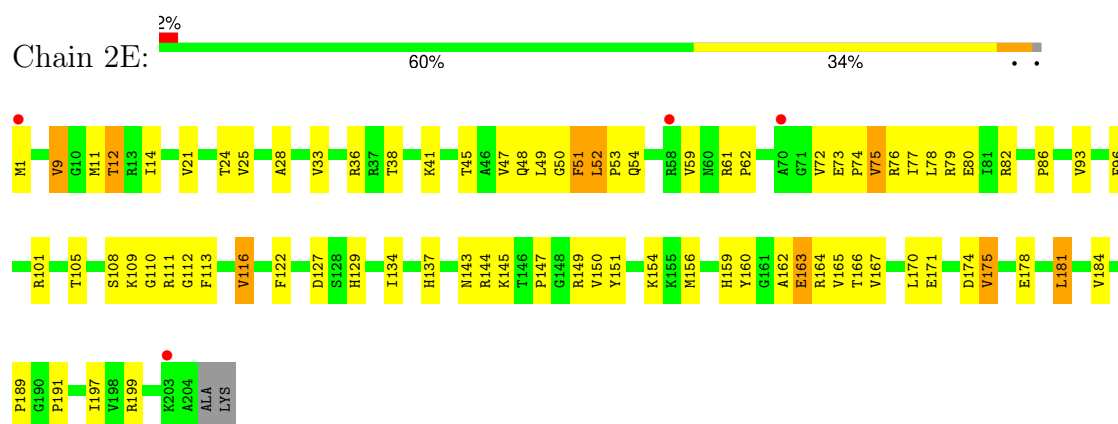
- Molecule 3: 50S ribosomal protein L2



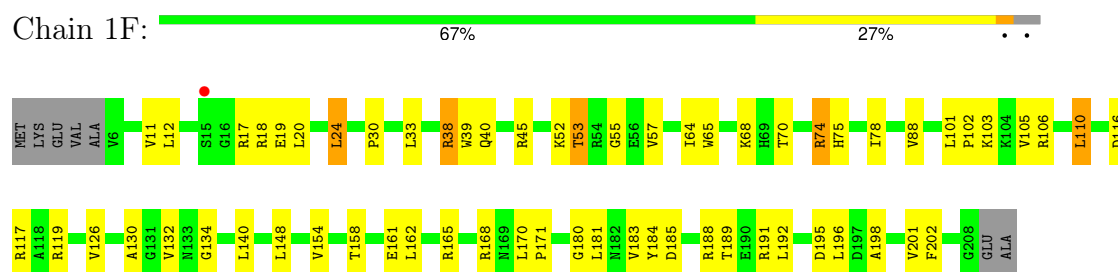
- Molecule 4: 50S ribosomal protein L3



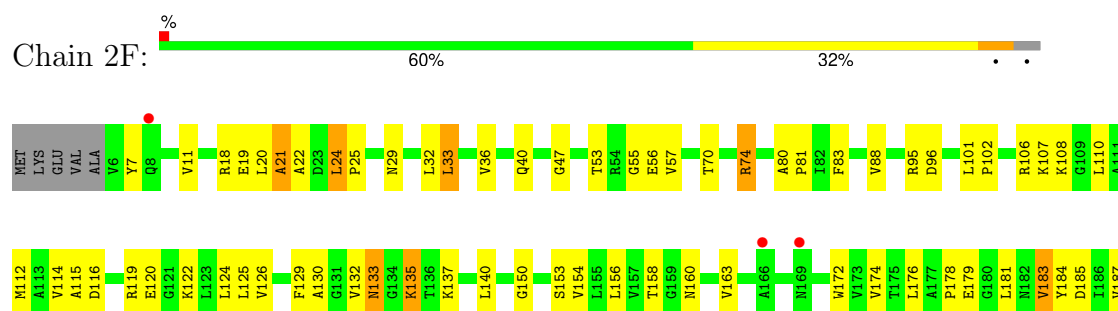
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4

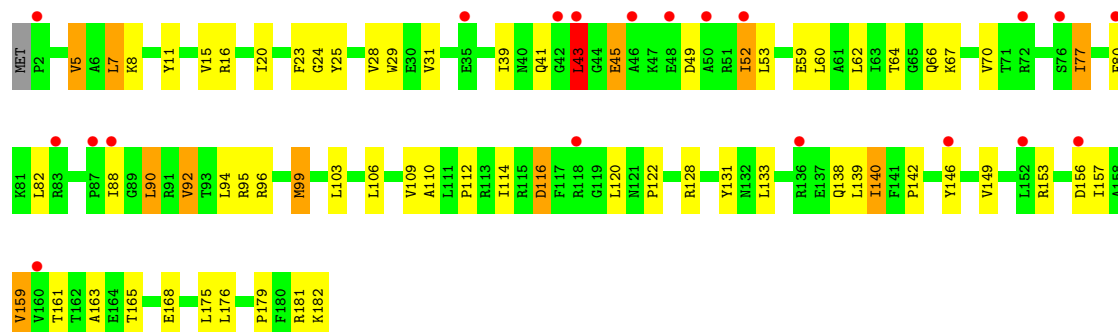


- Molecule 5: 50S ribosomal protein L4

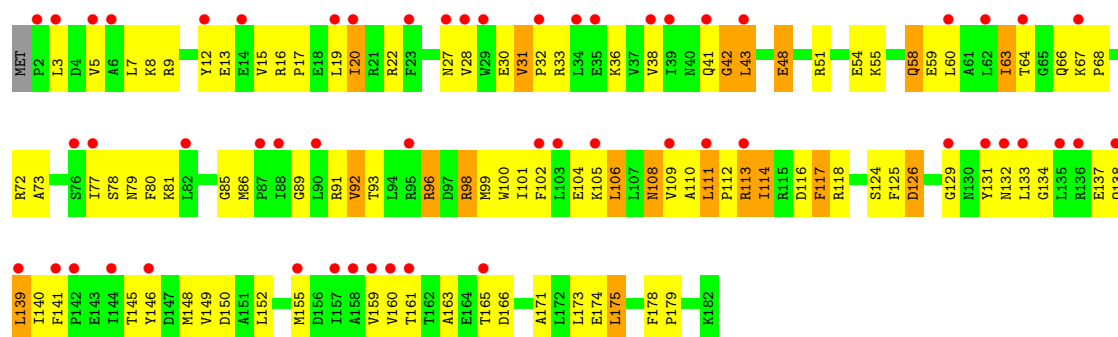
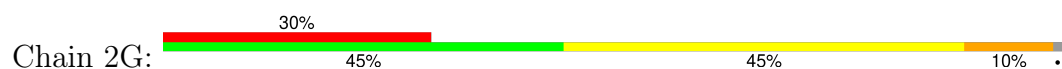




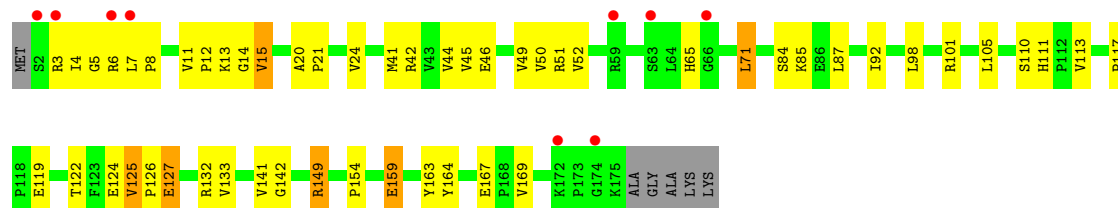
• Molecule 6: 50S ribosomal protein L5



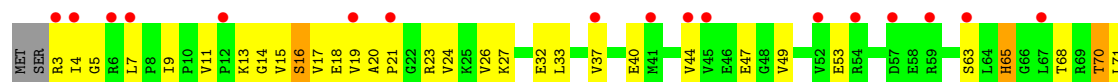
• Molecule 6: 50S ribosomal protein L5

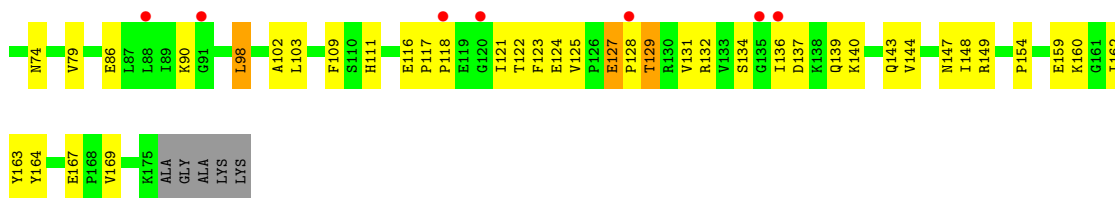


• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6





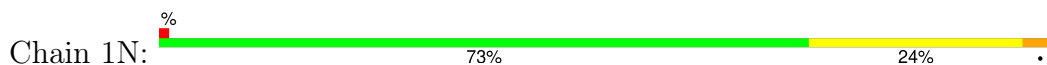
• Molecule 8: 50S ribosomal protein L9



• Molecule 8: 50S ribosomal protein L9



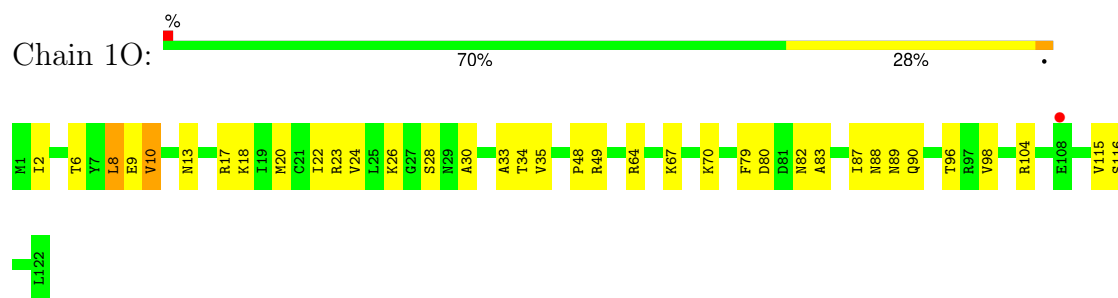
• Molecule 9: 50S ribosomal protein L13



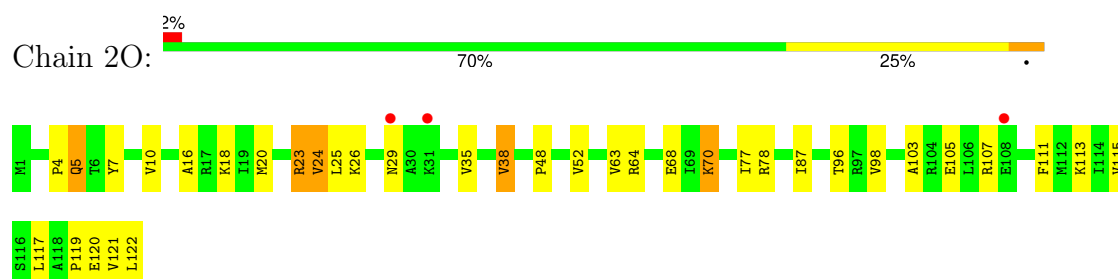
• Molecule 9: 50S ribosomal protein L13



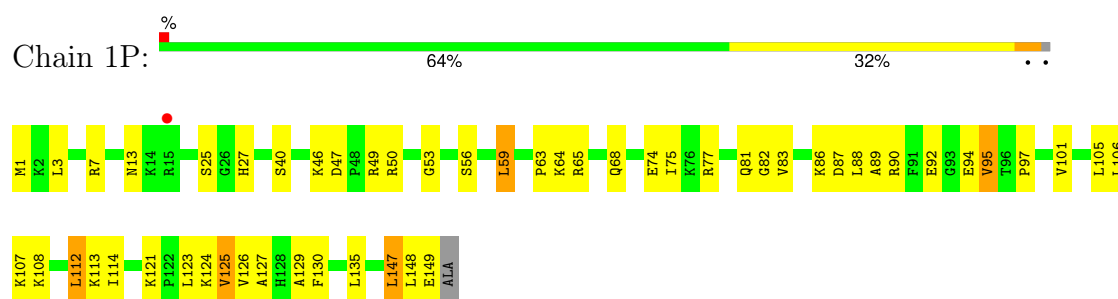
- Molecule 10: 50S ribosomal protein L14



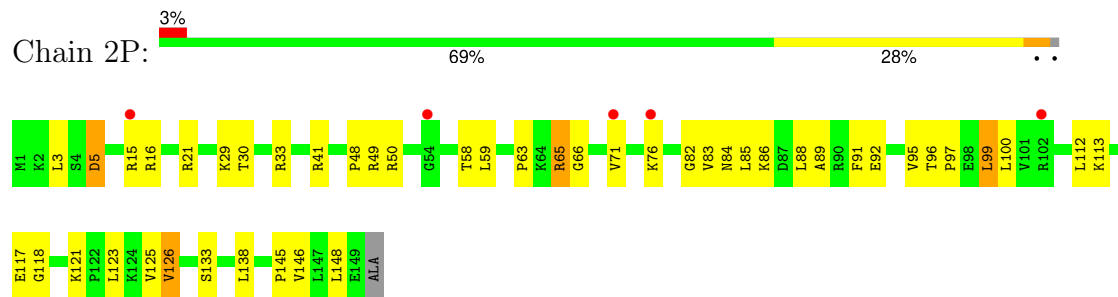
- Molecule 10: 50S ribosomal protein L14



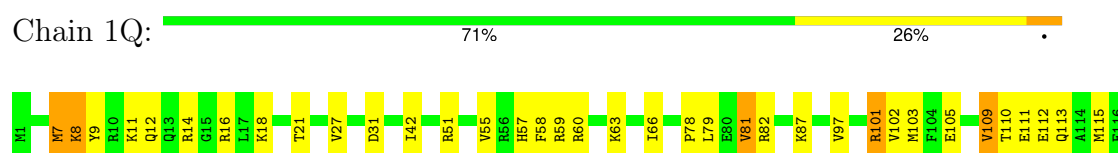
- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16

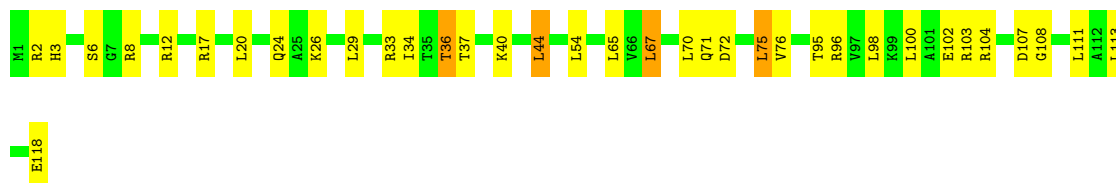




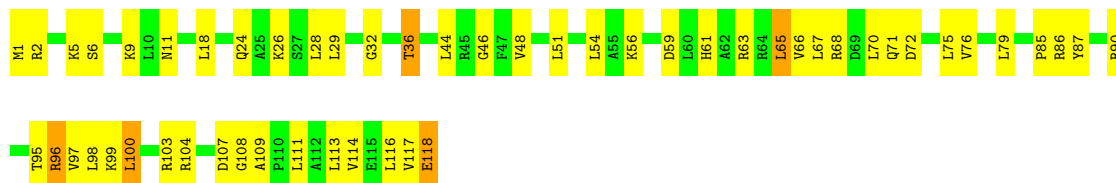
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



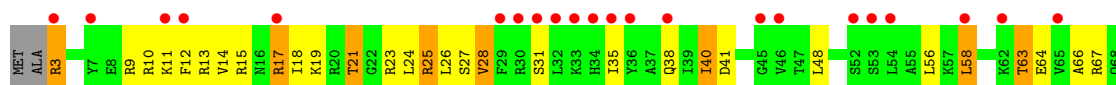
- Molecule 13: 50S ribosomal protein L17

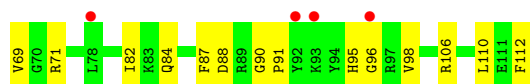


- Molecule 14: 50S ribosomal protein L18

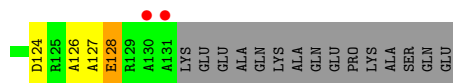


- Molecule 14: 50S ribosomal protein L18

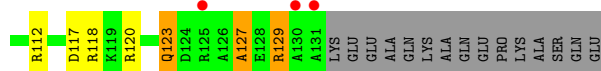




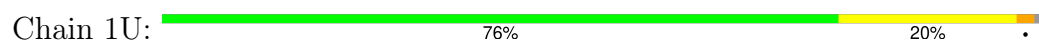
- Molecule 15: 50S ribosomal protein L19



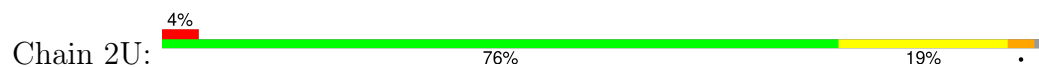
- Molecule 15: 50S ribosomal protein L19



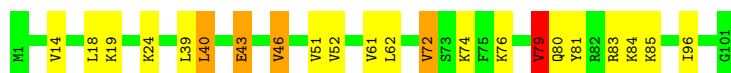
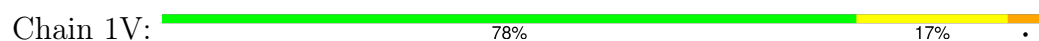
- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21

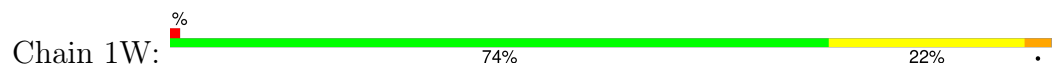


- Molecule 17: 50S ribosomal protein L21





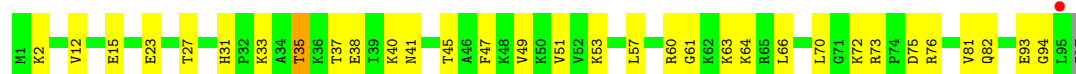
- Molecule 18: 50S ribosomal protein L22



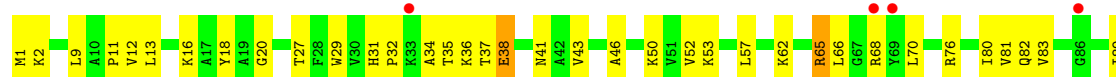
- Molecule 18: 50S ribosomal protein L22

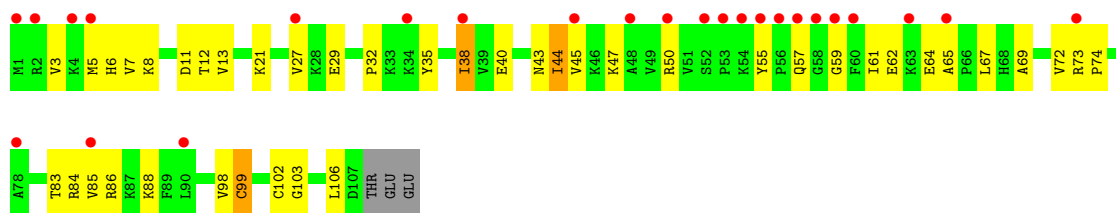


- Molecule 19: 50S ribosomal protein L23

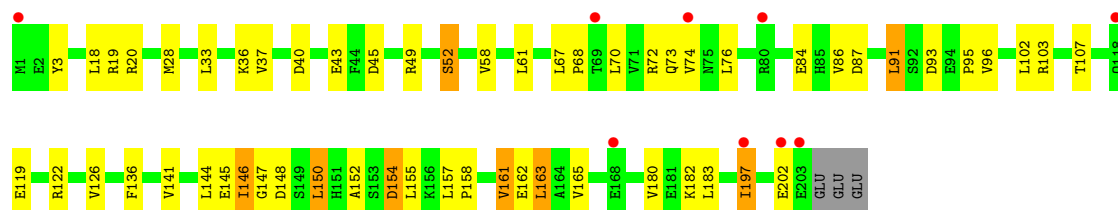


- Molecule 19: 50S ribosomal protein L23

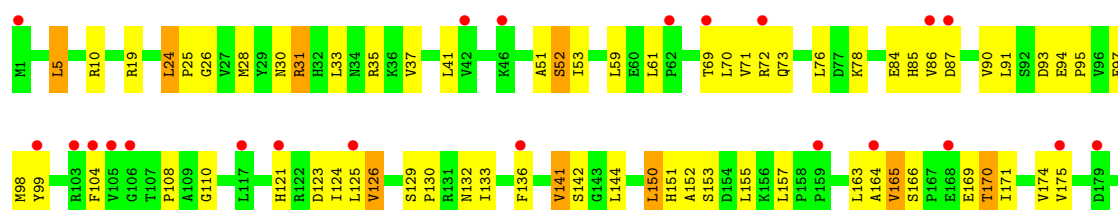




- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25



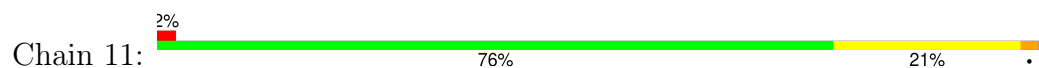
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28





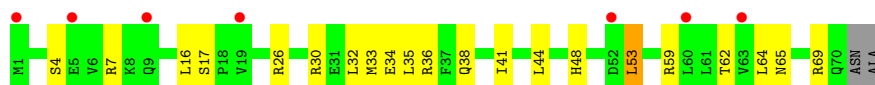
- Molecule 23: 50S ribosomal protein L28



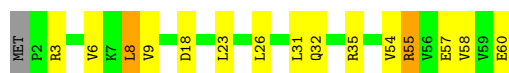
- Molecule 24: 50S ribosomal protein L29



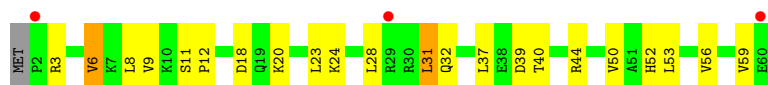
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30

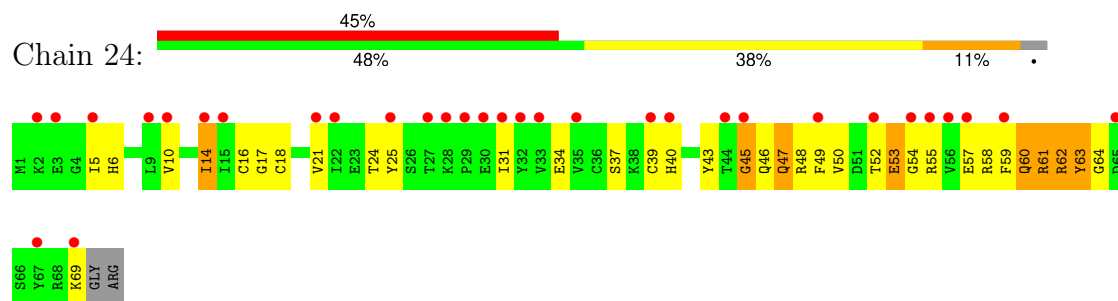


- Molecule 26: 50S ribosomal protein L31

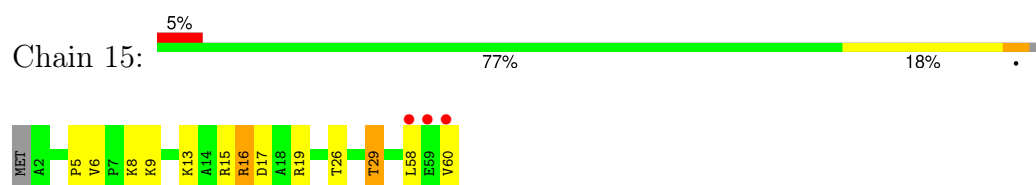


GLY
ARG

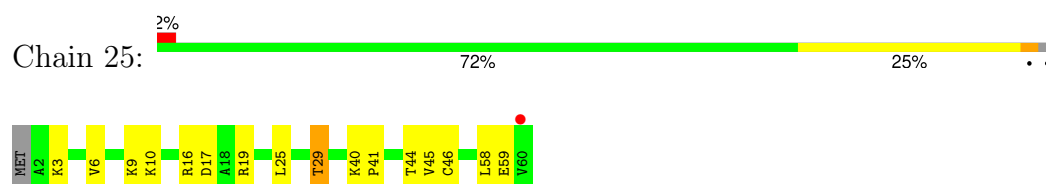
• Molecule 26: 50S ribosomal protein L31



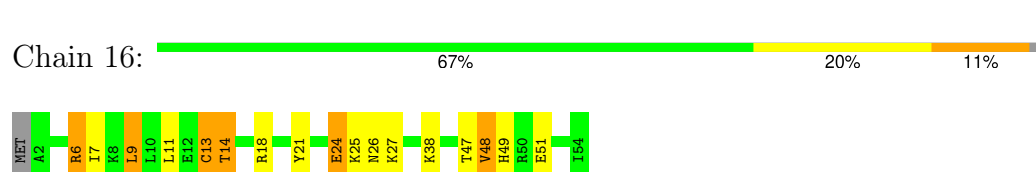
• Molecule 27: 50S ribosomal protein L32



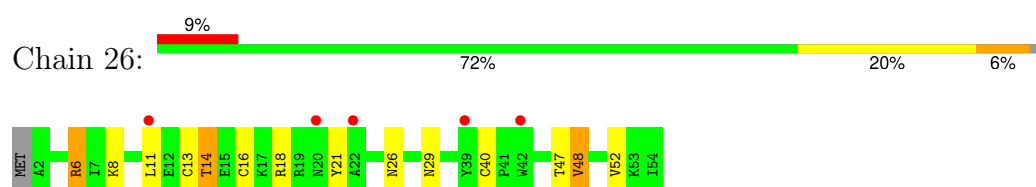
• Molecule 27: 50S ribosomal protein L32



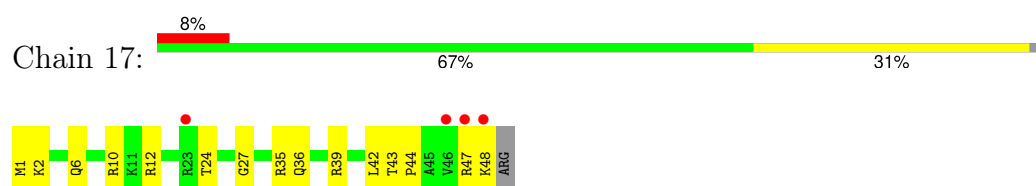
• Molecule 28: 50S ribosomal protein L33



• Molecule 28: 50S ribosomal protein L33



• Molecule 29: 50S ribosomal protein L34



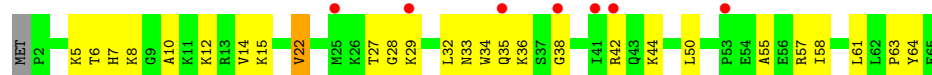
• Molecule 29: 50S ribosomal protein L34



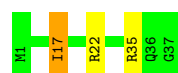
- Molecule 30: 50S ribosomal protein L35



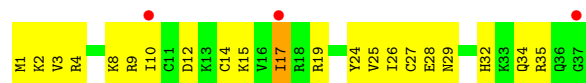
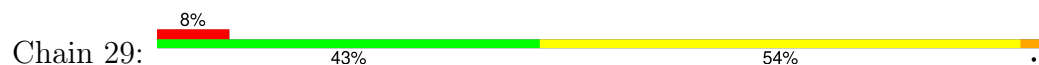
- Molecule 30: 50S ribosomal protein L35



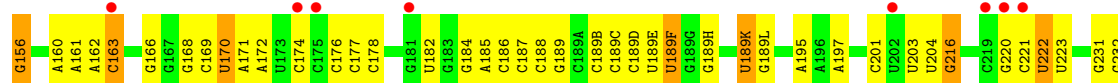
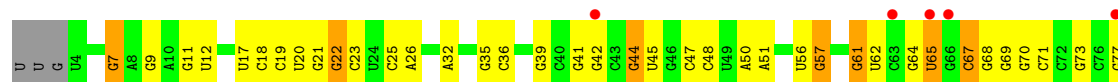
- Molecule 31: 50S ribosomal protein L36



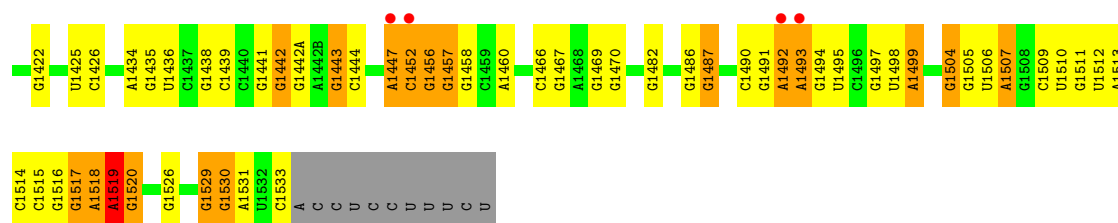
- Molecule 31: 50S ribosomal protein L36



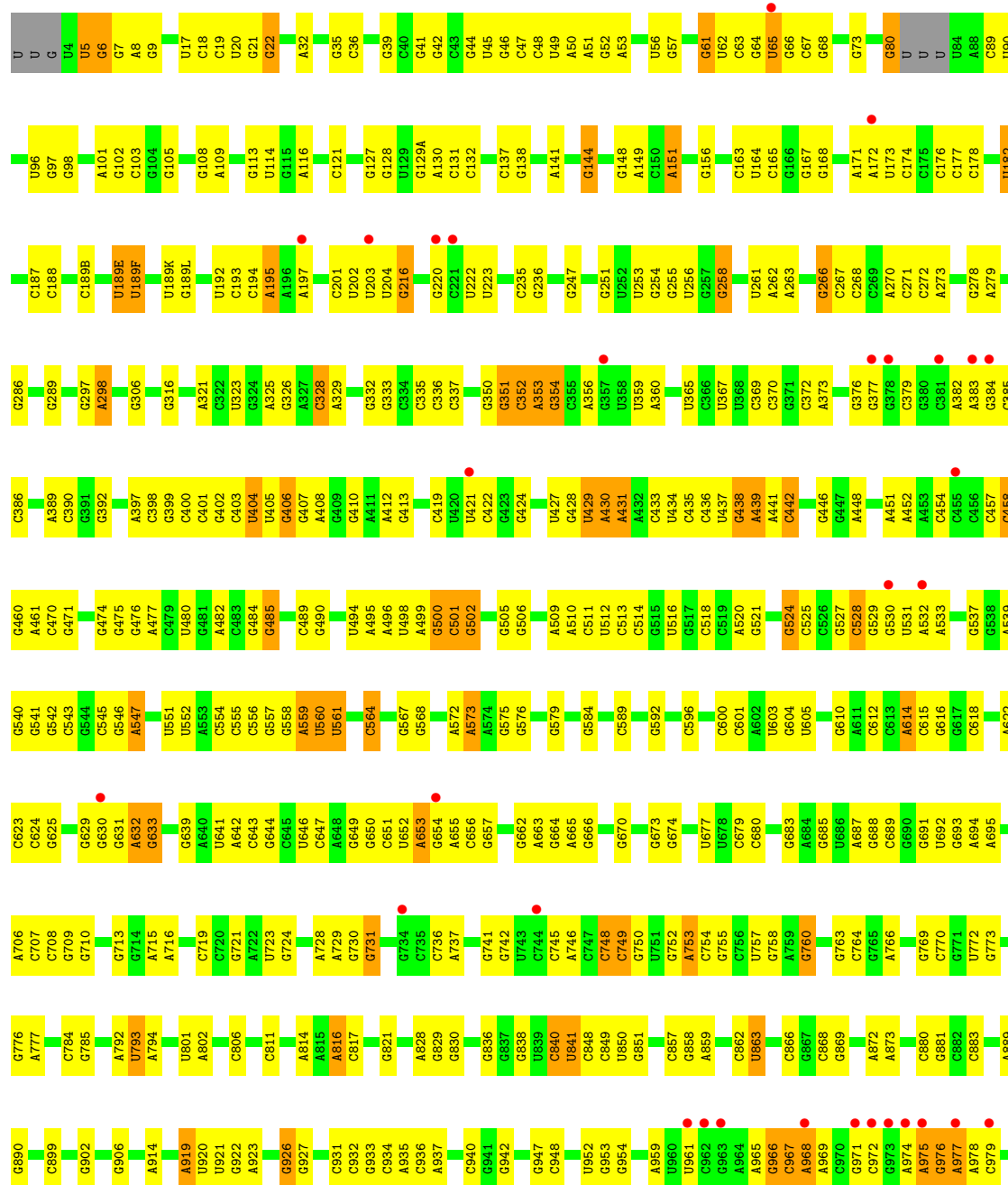
- Molecule 32: 16S Ribosomal RNA

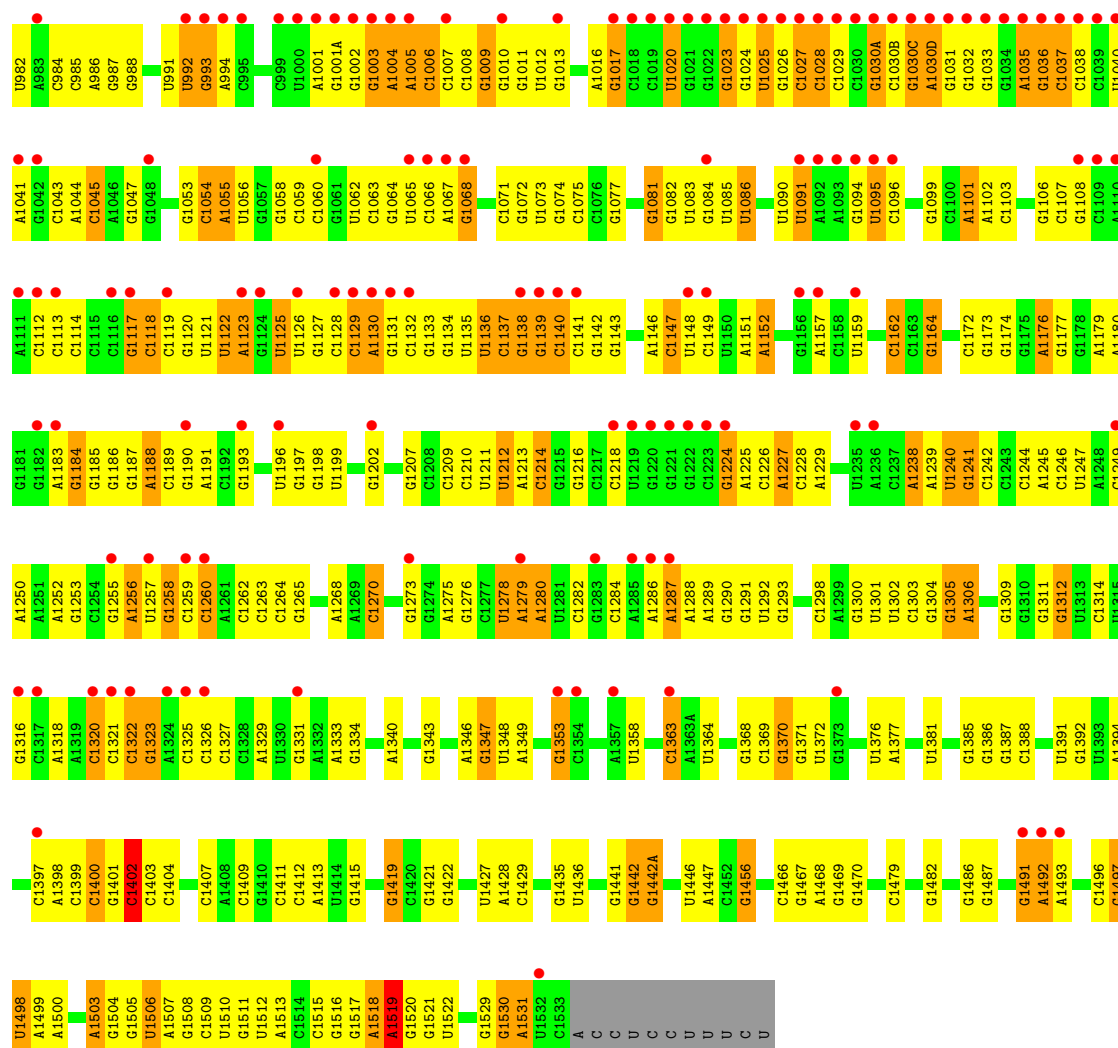




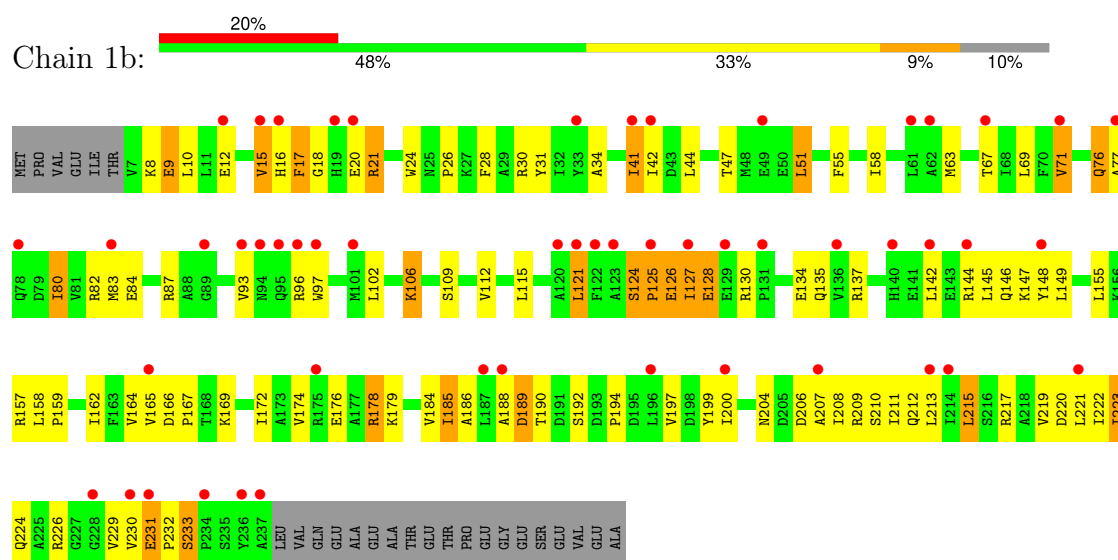


• Molecule 32: 16S Ribosomal RNA



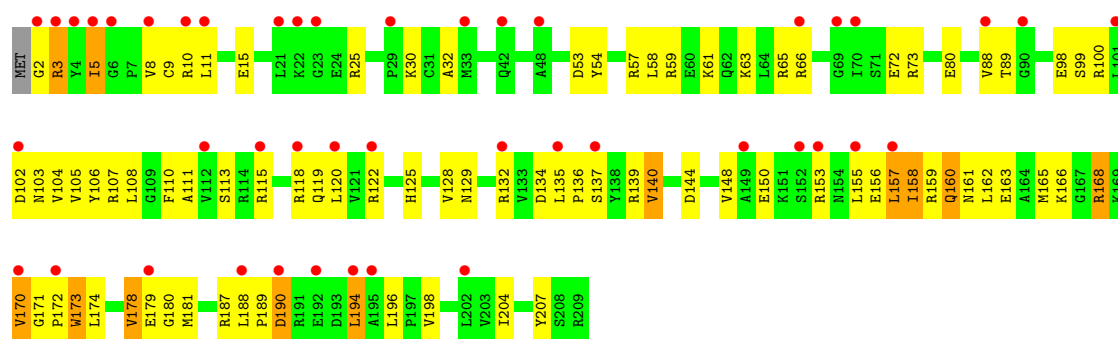


• Molecule 33: 30S ribosomal protein S2



• Molecule 33: 30S ribosomal protein S2

Chain 1d: 



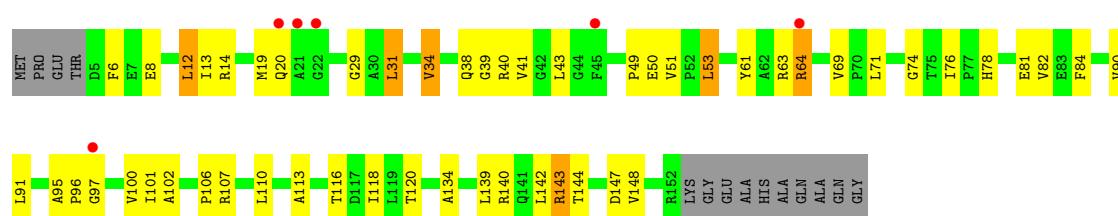
• Molecule 35: 30S ribosomal protein S4

Chain 2d: 



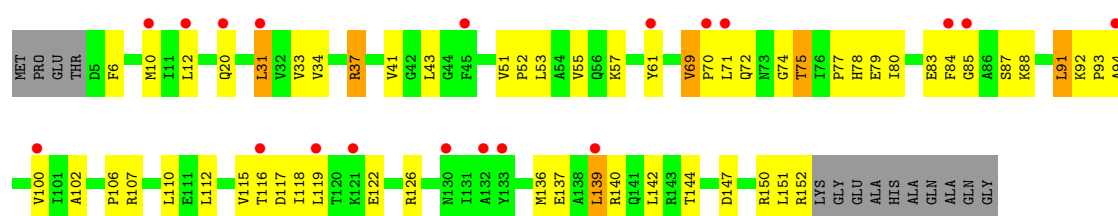
• Molecule 36: 30S ribosomal protein S5

Chain 1e: 

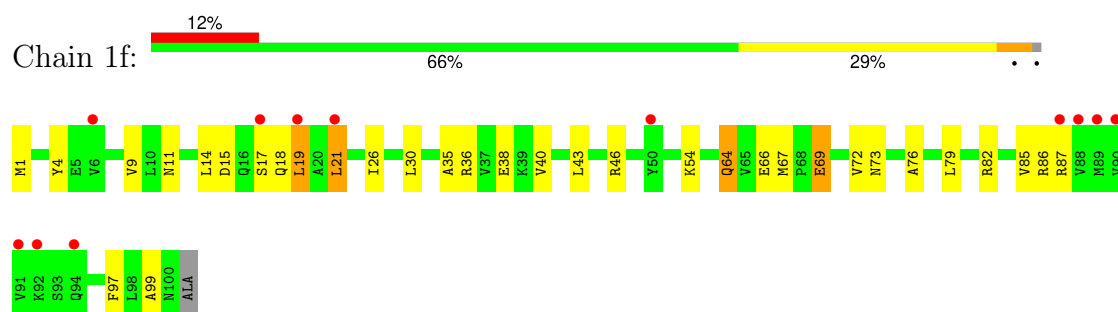


• Molecule 36: 30S ribosomal protein S5

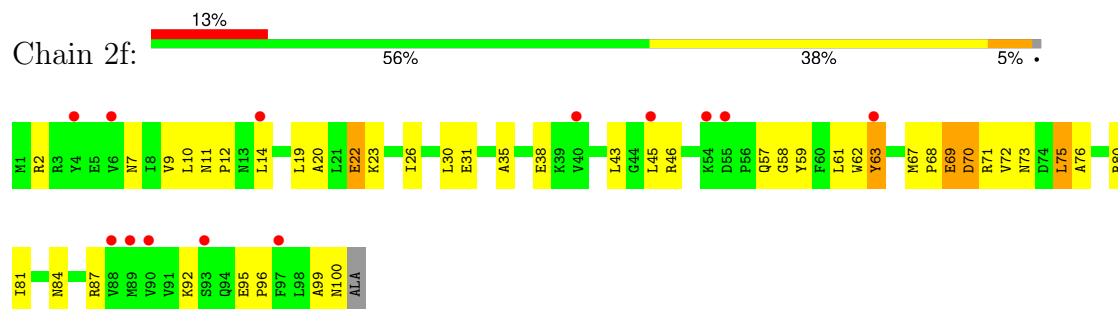
Chain 2e: 



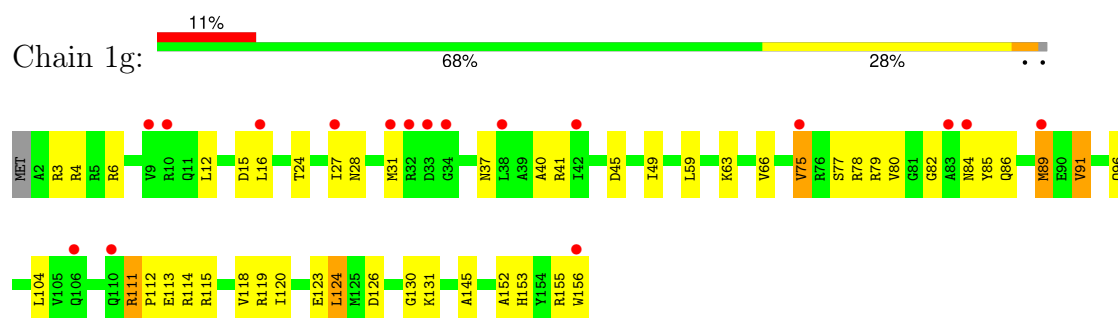
• Molecule 37: 30S ribosomal protein S6



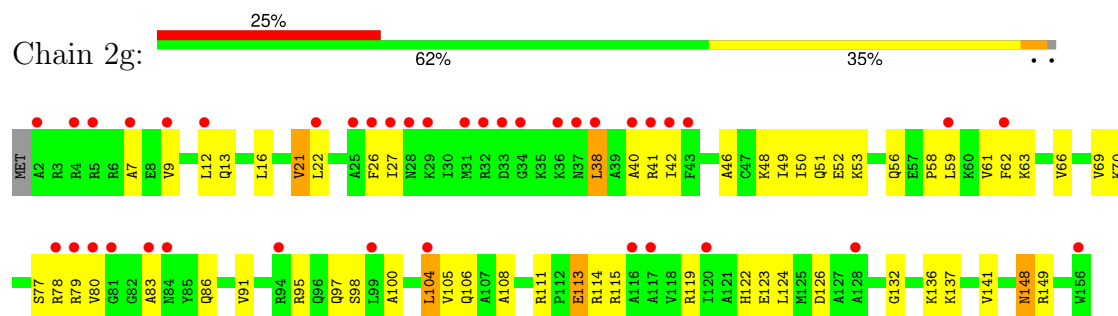
- Molecule 37: 30S ribosomal protein S6



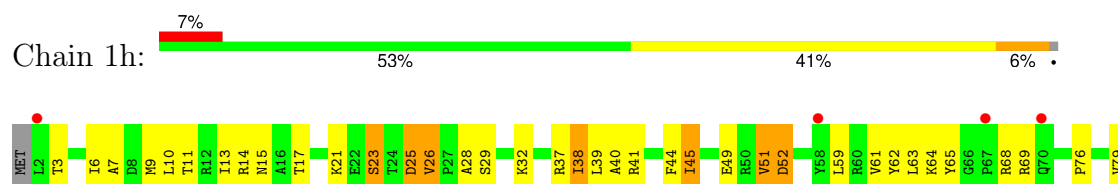
- Molecule 38: 30S ribosomal protein S7

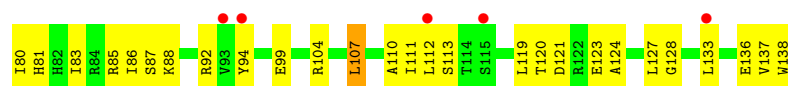


- Molecule 38: 30S ribosomal protein S7

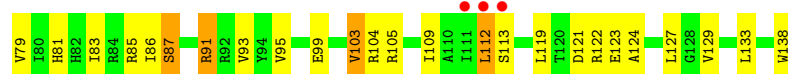
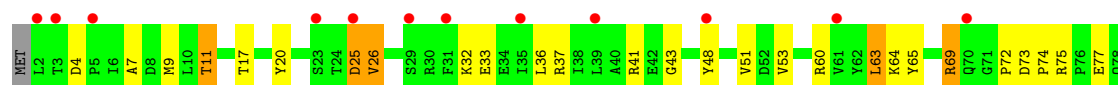


- Molecule 39: 30S ribosomal protein S8

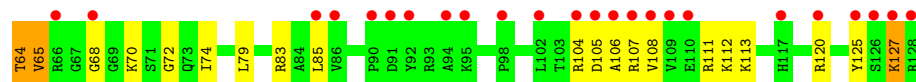
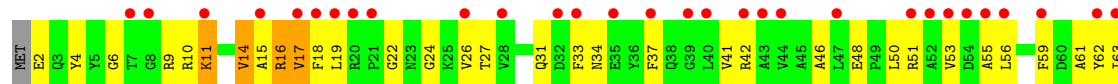
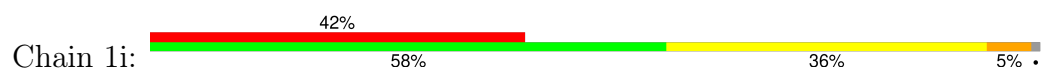




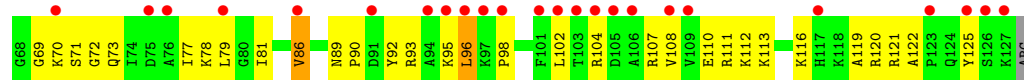
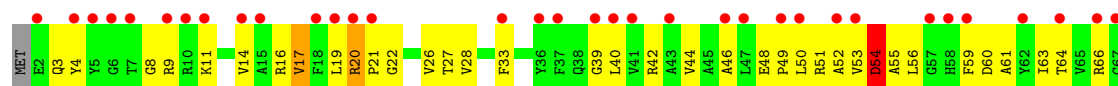
- Molecule 39: 30S ribosomal protein S8



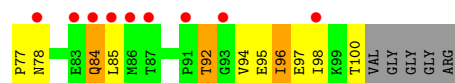
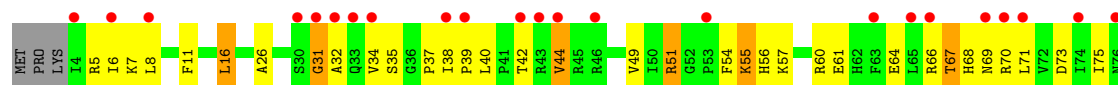
- Molecule 40: 30S ribosomal protein S9



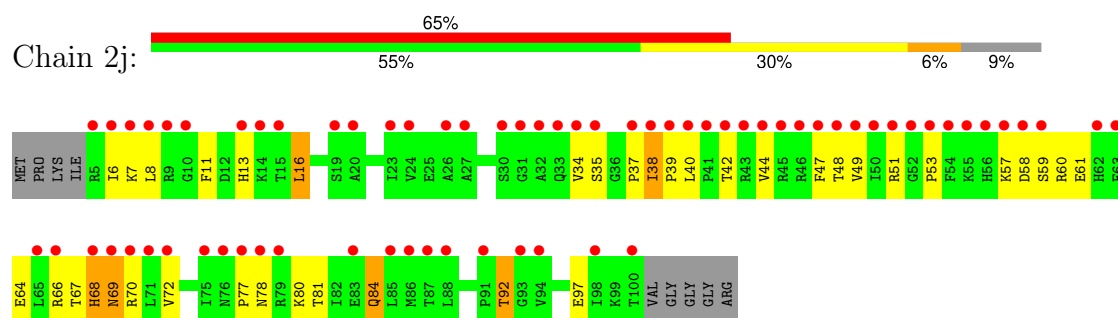
- Molecule 40: 30S ribosomal protein S9



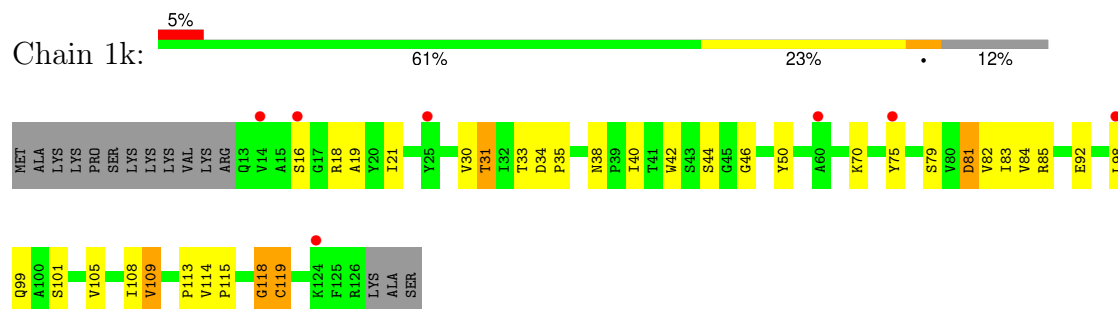
- Molecule 41: 30S ribosomal protein S10



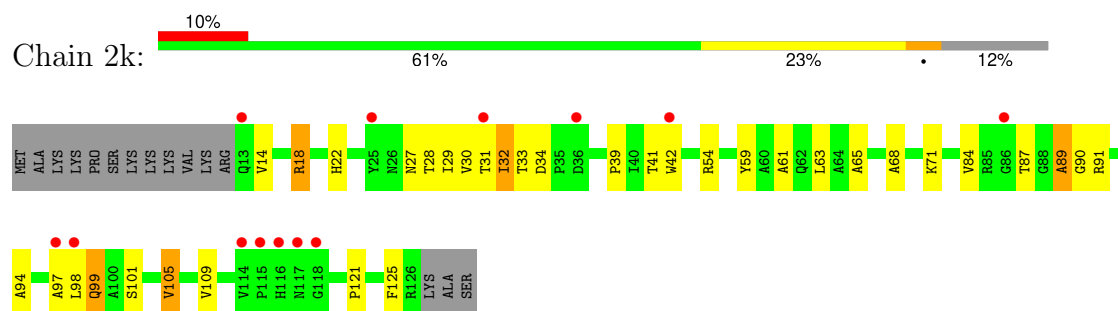
- Molecule 41: 30S ribosomal protein S10



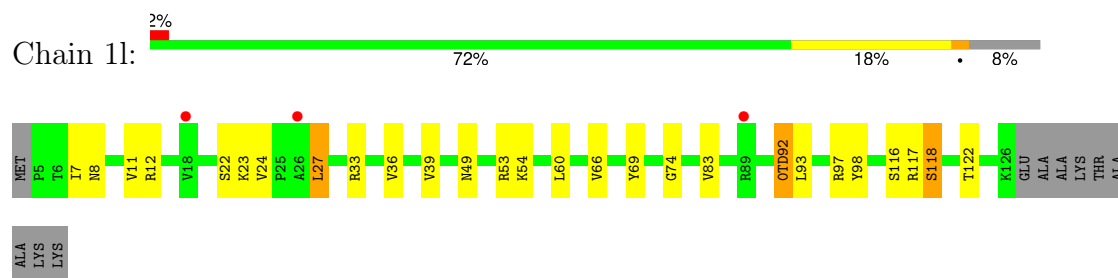
• Molecule 42: 30S ribosomal protein S11



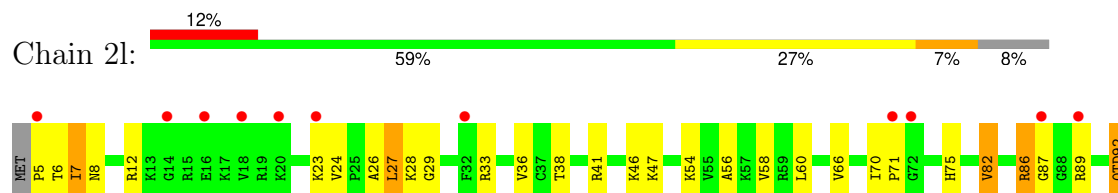
• Molecule 42: 30S ribosomal protein S11

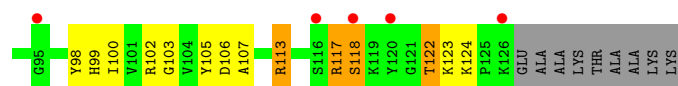


• Molecule 43: 30S ribosomal protein S12

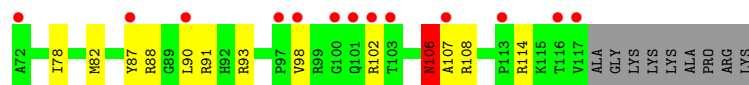
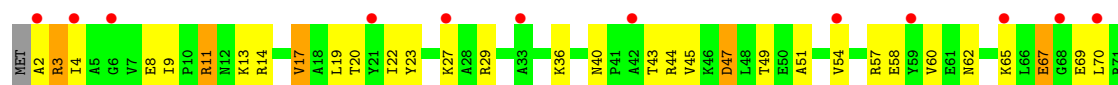


• Molecule 43: 30S ribosomal protein S12

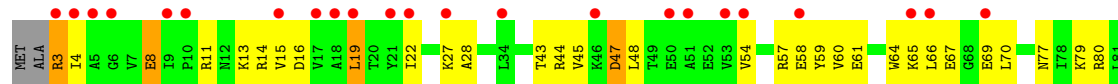




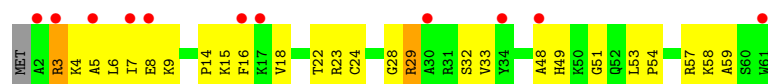
- Molecule 44: 30S ribosomal protein S13



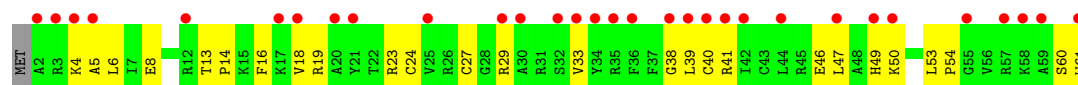
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



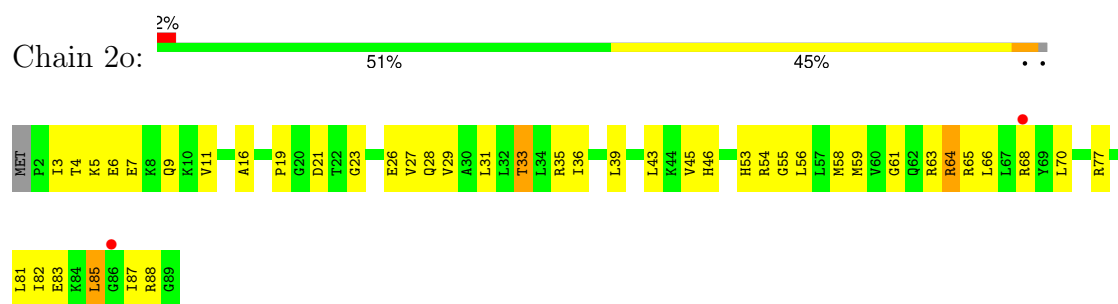
- Molecule 45: 30S ribosomal protein S14 type Z



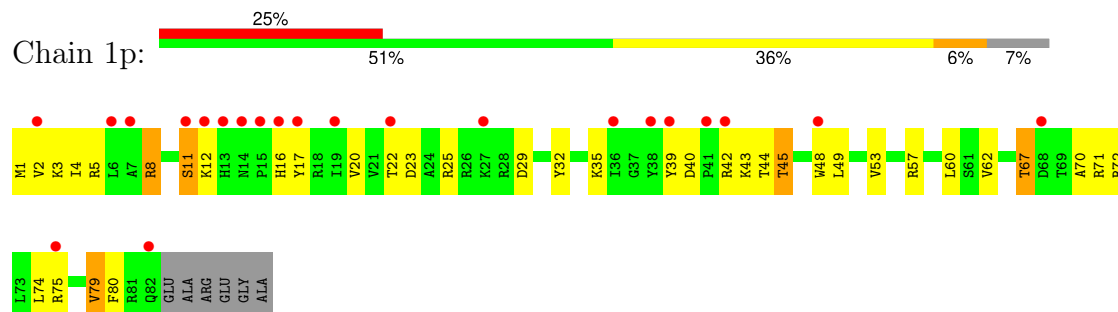
- Molecule 46: 30S ribosomal protein S15



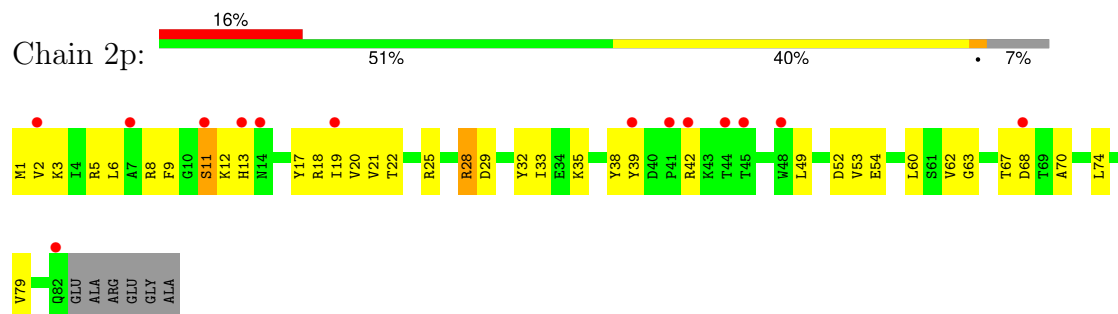
- Molecule 46: 30S ribosomal protein S15



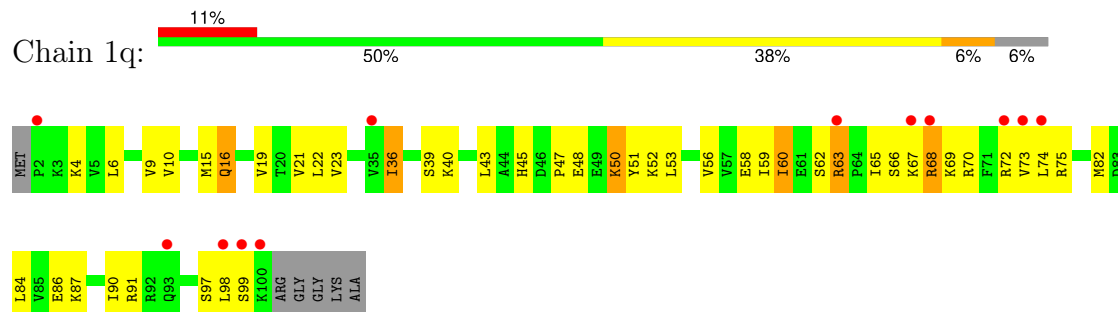
• Molecule 47: 30S ribosomal protein S16



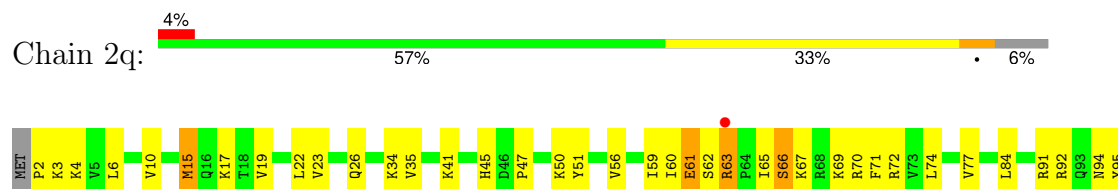
• Molecule 47: 30S ribosomal protein S16

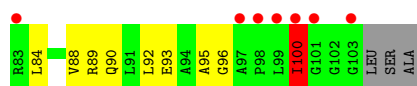


• Molecule 48: 30S ribosomal protein S17

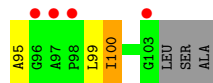


• Molecule 48: 30S ribosomal protein S17





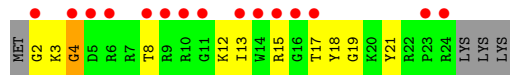
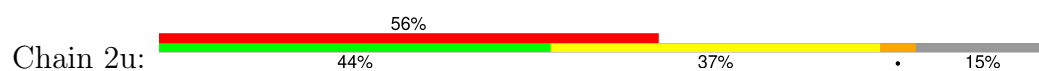
- Molecule 51: 30S ribosomal protein S20



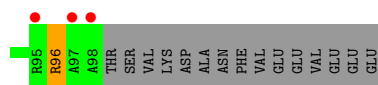
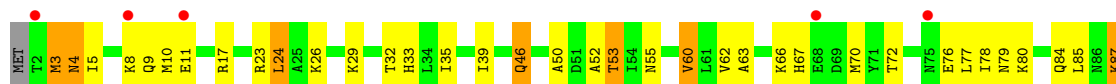
- Molecule 52: 30S ribosomal protein Thx



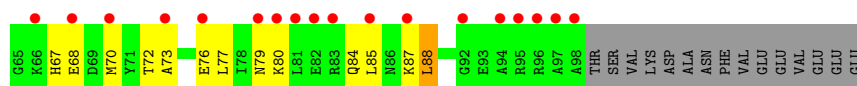
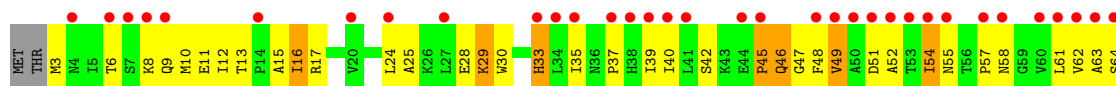
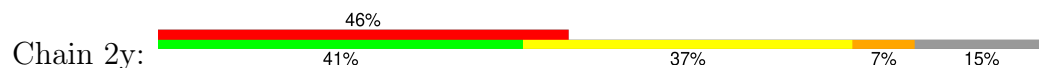
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A



- Molecule 53: Ribosome-associated inhibitor A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.66Å 450.37Å 619.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	255.35 – 2.90 255.35 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (255.35-2.90) 99.6 (255.35-2.90)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.217 , 0.271 0.216 , 0.268	Depositor DCC
R_{free} test set	63932 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 308.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	297211	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 1.53% 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: MG, SF4, 5MU, 4OC, ZN, 2MA, A1CQ8, MPD, 0TD, MA6, OMC, 2MG, M2G, 5MC, OMU, UR3, PSU, OMG, G7M

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	0.29	0/69031	0.45	0/107754
1	2A	0.23	1/68903 (0.0%)	0.41	1/107552 (0.0%)
2	1B	0.22	0/2876	0.39	0/4486
2	2B	0.20	0/2878	0.37	0/4490
3	1D	0.29	0/2181	0.52	0/2940
3	2D	0.24	0/2186	0.49	0/2944
4	1E	0.28	0/1592	0.50	0/2149
4	2E	0.24	0/1592	0.48	0/2149
5	1F	0.27	0/1619	0.48	0/2193
5	2F	0.22	0/1615	0.48	2/2188 (0.1%)
6	1G	0.22	0/1451	0.45	0/1961
6	2G	0.22	0/1449	0.48	0/1957
7	1H	0.22	0/1356	0.45	0/1834
7	2H	0.21	0/1350	0.44	0/1826
8	1I	0.20	0/1109	0.45	0/1512
8	2I	0.20	0/1091	0.42	0/1490
9	1N	0.26	0/1148	0.44	0/1547
9	2N	0.21	0/1144	0.43	0/1543
10	1O	0.28	0/943	0.49	0/1269
10	2O	0.24	0/943	0.47	0/1269
11	1P	0.27	0/1152	0.52	0/1533
11	2P	0.23	0/1152	0.46	0/1533
12	1Q	0.25	0/1143	0.48	0/1527
12	2Q	0.24	0/1143	0.43	0/1527
13	1R	0.27	0/982	0.48	0/1312
13	2R	0.24	0/982	0.49	0/1312
14	1S	0.21	0/887	0.49	0/1180
14	2S	0.20	0/880	0.45	0/1172
15	1T	0.27	0/1105	0.53	0/1477
15	2T	0.23	0/1097	0.44	0/1468
16	1U	0.28	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.23	0/977	0.43	0/1301
17	1V	0.25	0/786	0.45	0/1053
17	2V	0.20	0/782	0.43	0/1049
18	1W	0.27	0/897	0.49	0/1205
18	2W	0.23	0/897	0.42	0/1205
19	1X	0.27	0/764	0.45	0/1025
19	2X	0.23	0/764	0.46	0/1025
20	1Y	0.26	0/823	0.52	0/1099
20	2Y	0.22	0/823	0.44	0/1100
21	1Z	0.22	0/1620	0.44	0/2200
21	2Z	0.21	0/1590	0.45	0/2162
22	10	0.26	0/616	0.50	0/821
22	20	0.27	0/616	0.58	2/821 (0.2%)
23	11	0.25	0/761	0.44	0/1013
23	21	0.24	0/766	0.43	0/1018
24	12	0.24	0/590	0.45	0/781
24	22	0.21	0/594	0.39	0/785
25	13	0.26	0/474	0.54	0/635
25	23	0.18	0/469	0.40	0/630
26	14	0.26	0/559	0.54	0/754
26	24	0.28	0/549	0.68	0/741
27	15	0.27	0/473	0.50	0/639
27	25	0.24	0/469	0.49	0/635
28	16	0.27	0/460	0.49	0/613
28	26	0.21	0/456	0.42	0/608
29	17	0.32	0/426	0.53	0/561
29	27	0.25	0/426	0.47	0/561
30	18	0.29	0/525	0.49	0/691
30	28	0.22	0/525	0.39	0/691
31	19	0.24	0/310	0.46	0/407
31	29	0.18	0/310	0.46	0/407
32	1a	0.21	1/35795 (0.0%)	0.39	1/55864 (0.0%)
32	2a	0.20	0/35890	0.37	0/56012
33	1b	0.25	0/1876	0.54	0/2533
33	2b	0.23	0/1860	0.50	0/2518
34	1c	0.20	0/1582	0.41	0/2137
34	2c	0.21	0/1566	0.42	0/2119
35	1d	0.23	0/1695	0.46	0/2274
35	2d	0.20	0/1698	0.44	0/2277
36	1e	0.22	0/1149	0.47	0/1548
36	2e	0.21	0/1149	0.43	0/1548
37	1f	0.21	0/827	0.45	0/1120
37	2f	0.20	0/829	0.44	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1254	0.41	0/1683
38	2g	0.21	0/1248	0.44	0/1676
39	1h	0.20	0/1118	0.44	0/1506
39	2h	0.19	0/1108	0.44	0/1494
40	1i	0.21	0/1005	0.46	0/1351
40	2i	0.24	0/985	0.50	0/1329
41	1j	0.22	0/732	0.44	0/993
41	2j	0.23	0/723	0.47	0/984
42	1k	0.19	0/849	0.41	0/1150
42	2k	0.19	0/848	0.46	0/1149
43	1l	0.20	0/937	0.45	0/1260
43	2l	0.20	0/937	0.47	0/1260
44	1m	0.20	0/924	0.45	0/1242
44	2m	0.21	0/905	0.47	0/1217
45	1n	0.19	0/501	0.43	0/664
45	2n	0.23	0/501	0.46	0/664
46	1o	0.20	0/739	0.40	0/985
46	2o	0.22	0/739	0.45	0/985
47	1p	0.23	0/697	0.50	0/939
47	2p	0.21	0/693	0.46	0/935
48	1q	0.22	0/836	0.48	0/1117
48	2q	0.19	0/836	0.43	0/1117
49	1r	0.19	0/560	0.49	0/746
49	2r	0.20	0/560	0.40	0/746
50	1s	0.20	0/663	0.47	0/895
50	2s	0.20	0/660	0.39	0/893
51	1t	0.22	0/734	0.50	0/969
51	2t	0.20	0/736	0.43	0/976
52	1u	0.22	0/203	0.43	0/266
52	2u	0.22	0/203	0.47	0/266
53	1y	0.20	0/776	0.36	0/1048
53	2y	0.21	0/761	0.40	0/1030
All	All	0.24	2/309941 (0.0%)	0.43	6/463239 (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
19	1X	0	1
26	24	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	1
43	2l	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	O3'-P	5.12	1.61	1.56
32	1a	1498	UR3	O3'-P	5.08	1.61	1.56

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	20	12	ASN	CB-CA-C	-6.03	108.39	117.07
22	20	12	ASN	N-CA-C	5.46	113.26	108.78
5	2F	21	ALA	CA-C-N	5.24	131.13	121.70
5	2F	21	ALA	C-N-CA	5.24	131.13	121.70
1	2A	1992	G	C2'-C3'-O3'	5.23	117.35	109.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	1X	93	GLU	Peptide
33	1b	231	GLU	Peptide
26	24	18	CYS	Peptide
43	2l	86	ARG	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61869	0	31201	802	0
1	2A	61758	0	31152	866	0
2	1B	2572	0	1305	26	0
2	2B	2573	0	1306	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1D	2131	0	2207	61	0
3	2D	2136	0	2218	68	0
4	1E	1559	0	1616	55	0
4	2E	1559	0	1618	56	0
5	1F	1584	0	1625	34	0
5	2F	1580	0	1619	52	0
6	1G	1426	0	1445	44	0
6	2G	1424	0	1441	66	0
7	1H	1330	0	1407	33	0
7	2H	1324	0	1402	38	0
8	1I	1094	0	1127	24	0
8	2I	1076	0	1094	29	0
9	1N	1121	0	1194	19	0
9	2N	1117	0	1184	36	0
10	1O	933	0	996	27	0
10	2O	933	0	996	24	0
11	1P	1135	0	1212	35	0
11	2P	1135	0	1212	39	0
12	1Q	1122	0	1179	28	0
12	2Q	1122	0	1179	34	0
13	1R	968	0	1033	19	0
13	2R	968	0	1033	36	0
14	1S	877	0	938	25	0
14	2S	870	0	923	27	0
15	1T	1091	0	1151	30	0
15	2T	1083	0	1136	33	0
16	1U	959	0	1019	16	0
16	2U	959	0	1019	14	0
17	1V	775	0	841	14	0
17	2V	771	0	830	20	0
18	1W	886	0	940	15	0
18	2W	886	0	940	19	0
19	1X	750	0	814	18	0
19	2X	750	0	814	22	0
20	1Y	810	0	892	23	0
20	2Y	810	0	887	26	0
21	1Z	1587	0	1598	27	0
21	2Z	1557	0	1564	43	0
22	10	608	0	622	13	0
22	20	608	0	622	15	0
23	11	754	0	823	13	0
23	21	759	0	837	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	12	588	0	643	13	0
24	22	592	0	654	9	0
25	13	469	0	518	8	0
25	23	464	0	514	9	0
26	14	546	0	522	26	0
26	24	536	0	514	25	0
27	15	459	0	476	14	0
27	25	455	0	465	10	0
28	16	453	0	473	14	0
28	26	449	0	469	9	0
29	17	418	0	467	12	0
29	27	418	0	467	9	0
30	18	517	0	582	21	0
30	28	517	0	582	26	0
31	19	307	0	335	2	0
31	29	307	0	335	11	0
32	1a	32246	0	16295	531	0
32	2a	32331	0	16338	526	0
33	1b	1842	0	1862	65	0
33	2b	1825	0	1828	75	0
34	1c	1558	0	1557	50	0
34	2c	1542	0	1517	56	0
35	1d	1665	0	1687	58	0
35	2d	1668	0	1703	59	0
36	1e	1133	0	1191	38	0
36	2e	1133	0	1191	41	0
37	1f	814	0	808	25	0
37	2f	816	0	808	26	0
38	1g	1235	0	1249	30	0
38	2g	1229	0	1238	34	0
39	1h	1098	0	1143	41	0
39	2h	1088	0	1126	35	0
40	1i	986	0	990	37	0
40	2i	966	0	953	49	0
41	1j	719	0	672	29	0
41	2j	710	0	661	25	0
42	1k	834	0	838	20	0
42	2k	833	0	836	20	0
43	1l	932	0	981	19	0
43	2l	932	0	981	30	0
44	1m	914	0	954	31	0
44	2m	895	0	920	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	1n	492	0	529	18	0
45	2n	492	0	529	22	0
46	1o	728	0	760	15	0
46	2o	728	0	760	32	0
47	1p	681	0	697	28	0
47	2p	677	0	686	21	0
48	1q	823	0	891	32	0
48	2q	823	0	891	31	0
49	1r	555	0	618	12	0
49	2r	555	0	618	19	0
50	1s	648	0	658	22	0
50	2s	645	0	635	22	0
51	1t	732	0	809	23	0
51	2t	733	0	795	24	0
52	1u	199	0	208	5	0
52	2u	199	0	208	7	0
53	1y	764	0	786	29	0
53	2y	749	0	757	33	0
54	10	10	0	0	0	0
54	11	5	0	0	0	0
54	13	4	0	0	0	0
54	15	6	0	0	0	0
54	17	4	0	0	0	0
54	18	1	0	0	0	0
54	19	2	0	0	0	0
54	1A	1010	0	0	1	0
54	1B	31	0	0	0	0
54	1D	18	0	0	0	0
54	1E	9	0	0	0	0
54	1F	18	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	5	0	0	0	0
54	1O	2	0	0	0	0
54	1P	8	0	0	0	0
54	1Q	7	0	0	0	0
54	1R	5	0	0	0	0
54	1S	1	0	0	0	0
54	1T	5	0	0	0	0
54	1U	6	0	0	0	0
54	1V	6	0	0	0	0
54	1W	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1X	2	0	0	0	0
54	1Y	1	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	269	0	0	0	0
54	1b	1	0	0	0	0
54	1d	5	0	0	0	0
54	1e	3	0	0	0	0
54	1f	2	0	0	0	0
54	1g	3	0	0	0	0
54	1h	1	0	0	0	0
54	1i	1	0	0	0	0
54	1k	1	0	0	0	0
54	1l	2	0	0	0	0
54	1m	1	0	0	0	0
54	1n	2	0	0	0	0
54	1o	1	0	0	0	0
54	1p	1	0	0	0	0
54	1q	1	0	0	0	0
54	1t	2	0	0	0	0
54	1y	4	0	0	0	0
54	20	2	0	0	0	0
54	21	3	0	0	0	0
54	23	1	0	0	0	0
54	25	2	0	0	0	0
54	26	1	0	0	0	0
54	27	1	0	0	0	0
54	28	1	0	0	0	0
54	2A	724	0	0	0	0
54	2B	18	0	0	0	0
54	2D	8	0	0	0	0
54	2E	9	0	0	0	0
54	2F	4	0	0	0	0
54	2G	3	0	0	0	0
54	2I	1	0	0	0	0
54	2N	1	0	0	0	0
54	2P	3	0	0	0	0
54	2Q	2	0	0	0	0
54	2R	2	0	0	0	0
54	2T	5	0	0	0	0
54	2V	3	0	0	0	0
54	2W	3	0	0	0	0
54	2X	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2Y	1	0	0	0	0
54	2a	177	0	0	0	0
54	2e	2	0	0	0	0
54	2f	1	0	0	0	0
54	2j	1	0	0	0	0
54	2n	1	0	0	0	0
54	2r	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	44	0	0	1	0
55	2A	44	0	0	0	0
56	1A	12	0	12	1	0
56	1B	12	0	12	3	0
57	18	8	0	14	3	0
57	1A	8	0	14	0	0
57	1T	8	0	14	0	0
57	1a	8	0	14	6	0
57	2A	16	0	28	3	0
57	2B	8	0	14	0	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	1	0
59	2d	8	0	0	1	0
60	10	27	0	0	1	0
60	11	27	0	0	1	0
60	12	14	0	0	0	0
60	13	22	0	0	2	0
60	14	3	0	0	0	0
60	15	22	0	0	3	0
60	16	21	0	0	1	0
60	17	13	0	0	0	0
60	18	25	0	0	3	0
60	19	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1A	3708	0	0	198	0
60	1B	95	0	0	5	0
60	1D	105	0	0	5	0
60	1E	72	0	0	5	0
60	1F	59	0	0	1	0
60	1G	13	0	0	1	0
60	1H	15	0	0	0	0
60	1I	8	0	0	1	0
60	1N	55	0	0	1	0
60	1O	26	0	0	1	0
60	1P	64	0	0	4	0
60	1Q	42	0	0	3	0
60	1R	28	0	0	4	0
60	1S	10	0	0	1	0
60	1T	35	0	0	3	0
60	1U	42	0	0	2	0
60	1V	35	0	0	1	0
60	1W	27	0	0	0	0
60	1X	26	0	0	1	0
60	1Y	13	0	0	2	0
60	1Z	12	0	0	2	0
60	1a	503	0	0	35	0
60	1b	1	0	0	0	0
60	1c	1	0	0	0	0
60	1d	7	0	0	0	0
60	1e	5	0	0	0	0
60	1f	3	0	0	0	0
60	1i	1	0	0	0	0
60	1j	1	0	0	0	0
60	1l	5	0	0	1	0
60	1m	2	0	0	0	0
60	1o	2	0	0	0	0
60	1p	2	0	0	0	0
60	1q	1	0	0	0	0
60	1t	2	0	0	0	0
60	1u	1	0	0	1	0
60	1y	3	0	0	0	0
60	20	10	0	0	0	0
60	21	23	0	0	1	0
60	22	5	0	0	0	0
60	23	3	0	0	0	0
60	24	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	25	9	0	0	0	0
60	26	4	0	0	0	0
60	27	13	0	0	1	0
60	28	12	0	0	2	0
60	2A	2290	0	0	177	0
60	2B	59	0	0	6	0
60	2D	46	0	0	3	0
60	2E	29	0	0	3	0
60	2F	17	0	0	1	0
60	2G	5	0	0	0	0
60	2H	3	0	0	0	0
60	2I	4	0	0	1	0
60	2N	6	0	0	1	0
60	2O	13	0	0	1	0
60	2P	26	0	0	3	0
60	2Q	19	0	0	1	0
60	2R	23	0	0	2	0
60	2S	5	0	0	0	0
60	2T	11	0	0	3	0
60	2U	12	0	0	0	0
60	2V	5	0	0	0	0
60	2W	24	0	0	1	0
60	2X	10	0	0	1	0
60	2Y	6	0	0	0	0
60	2Z	11	0	0	1	0
60	2a	250	0	0	19	0
60	2d	4	0	0	1	0
60	2e	2	0	0	0	0
60	2f	4	0	0	0	0
60	2j	1	0	0	0	0
60	2l	2	0	0	0	0
60	2o	1	0	0	0	0
60	2p	2	0	0	0	0
60	2q	1	0	0	0	0
60	2r	2	0	0	0	0
60	2t	4	0	0	0	0
60	2y	2	0	0	0	0
All	All	297211	0	194511	4941	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 4941 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.34	1.24
32:2a:1003:G:H2'	32:2a:1004:A:H4'	1.37	1.04
32:2a:1162:C:H42	32:2a:1174:G:H1	1.09	0.96
1:1A:1082:U:O4	1:1A:1086:A:N1	1.98	0.95
1:1A:792:G:O6	60:1A:4108:HOH:O	1.86	0.92

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	255 (93%)	17 (6%)	1 (0%)	30	59
3	2D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
4	1E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	24	54
4	2E	202/206 (98%)	184 (91%)	17 (8%)	1 (0%)	24	54
5	1F	201/210 (96%)	190 (94%)	10 (5%)	1 (0%)	24	54
5	2F	201/210 (96%)	189 (94%)	11 (6%)	1 (0%)	24	54
6	1G	179/182 (98%)	159 (89%)	18 (10%)	2 (1%)	11	36
6	2G	179/182 (98%)	155 (87%)	17 (10%)	7 (4%)	2	10
7	1H	172/180 (96%)	158 (92%)	11 (6%)	3 (2%)	7	26
7	2H	171/180 (95%)	154 (90%)	15 (9%)	2 (1%)	10	34
8	1I	145/148 (98%)	121 (83%)	21 (14%)	3 (2%)	5	21
8	2I	144/148 (97%)	122 (85%)	17 (12%)	5 (4%)	3	12
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	18	48
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
11	2P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	18	48
12	1Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	18	48
12	2Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
13	1R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
13	2R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
14	1S	108/112 (96%)	94 (87%)	12 (11%)	2 (2%)	6	23
14	2S	108/112 (96%)	99 (92%)	6 (6%)	3 (3%)	4	15
15	1T	129/146 (88%)	120 (93%)	7 (5%)	2 (2%)	7	27
15	2T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	44
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	39
17	2V	99/101 (98%)	90 (91%)	7 (7%)	2 (2%)	6	22
18	1W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
18	2W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11	36
19	2X	93/96 (97%)	83 (89%)	9 (10%)	1 (1%)	11	36
20	1Y	105/110 (96%)	92 (88%)	10 (10%)	3 (3%)	3	15
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	201/206 (98%)	186 (92%)	13 (6%)	2 (1%)	12	39
21	2Z	199/206 (97%)	177 (89%)	20 (10%)	2 (1%)	12	39
22	10	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
22	20	75/85 (88%)	66 (88%)	8 (11%)	1 (1%)	9	32
23	11	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
23	21	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11	36
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
25	23	57/60 (95%)	55 (96%)	1 (2%)	1 (2%)	6	25
26	14	67/71 (94%)	55 (82%)	9 (13%)	3 (4%)	2	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/71 (94%)	49 (73%)	11 (16%)	7 (10%)	0	1
27	15	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	25	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	187 (82%)	32 (14%)	10 (4%)	2	8
33	2b	229/256 (90%)	195 (85%)	27 (12%)	7 (3%)	3	14
34	1c	204/239 (85%)	183 (90%)	20 (10%)	1 (0%)	24	54
34	2c	204/239 (85%)	176 (86%)	26 (13%)	2 (1%)	12	39
35	1d	206/209 (99%)	183 (89%)	22 (11%)	1 (0%)	24	54
35	2d	206/209 (99%)	184 (89%)	22 (11%)	0	100	100
36	1e	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
36	2e	146/162 (90%)	134 (92%)	11 (8%)	1 (1%)	18	48
37	1f	98/101 (97%)	88 (90%)	8 (8%)	2 (2%)	6	22
37	2f	98/101 (97%)	90 (92%)	7 (7%)	1 (1%)	12	39
38	1g	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	9	32
38	2g	153/156 (98%)	140 (92%)	12 (8%)	1 (1%)	18	48
39	1h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
39	2h	135/138 (98%)	122 (90%)	13 (10%)	0	100	100
40	1i	125/128 (98%)	105 (84%)	18 (14%)	2 (2%)	7	27
40	2i	124/128 (97%)	107 (86%)	10 (8%)	7 (6%)	1	4
41	1j	95/105 (90%)	76 (80%)	14 (15%)	5 (5%)	1	5
41	2j	94/105 (90%)	79 (84%)	12 (13%)	3 (3%)	3	13
42	1k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	14	41
42	2k	112/129 (87%)	98 (88%)	11 (10%)	3 (3%)	4	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	105 (88%)	13 (11%)	1 (1%)	16	44
43	2l	119/132 (90%)	106 (89%)	12 (10%)	1 (1%)	16	44
44	1m	114/126 (90%)	102 (90%)	8 (7%)	4 (4%)	3	12
44	2m	112/126 (89%)	98 (88%)	12 (11%)	2 (2%)	6	25
45	1n	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	26
45	2n	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	26
46	1o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
46	2o	86/89 (97%)	74 (86%)	11 (13%)	1 (1%)	10	34
47	1p	80/88 (91%)	67 (84%)	13 (16%)	0	100	100
47	2p	80/88 (91%)	72 (90%)	6 (8%)	2 (2%)	4	17
48	1q	97/105 (92%)	86 (89%)	10 (10%)	1 (1%)	12	39
48	2q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
50	2s	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	4	17
51	1t	94/106 (89%)	85 (90%)	7 (7%)	2 (2%)	5	21
51	2t	96/106 (91%)	87 (91%)	7 (7%)	2 (2%)	5	21
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	17 (81%)	2 (10%)	2 (10%)	0	1
53	1y	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
53	2y	94/113 (83%)	81 (86%)	11 (12%)	2 (2%)	5	21
All	All	11629/12354 (94%)	10577 (91%)	915 (8%)	137 (1%)	10	34

5 of 137 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	43	LEU
7	1H	92	ILE
15	1T	128	GLU
20	1Y	80	GLY

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%)	192 (90%)	22 (10%)	7	23
3	2D	215/218 (99%)	187 (87%)	28 (13%)	4	13
4	1E	164/166 (99%)	140 (85%)	24 (15%)	3	10
4	2E	164/166 (99%)	144 (88%)	20 (12%)	5	16
5	1F	160/166 (96%)	138 (86%)	22 (14%)	3	12
5	2F	159/166 (96%)	137 (86%)	22 (14%)	3	12
6	1G	144/156 (92%)	126 (88%)	18 (12%)	4	15
6	2G	142/156 (91%)	117 (82%)	25 (18%)	2	6
7	1H	144/148 (97%)	129 (90%)	15 (10%)	7	23
7	2H	143/148 (97%)	121 (85%)	22 (15%)	2	9
8	1I	111/124 (90%)	90 (81%)	21 (19%)	1	5
8	2I	108/124 (87%)	88 (82%)	20 (18%)	1	5
9	1N	119/119 (100%)	102 (86%)	17 (14%)	3	11
9	2N	118/119 (99%)	100 (85%)	18 (15%)	3	9
10	1O	100/100 (100%)	92 (92%)	8 (8%)	11	34
10	2O	100/100 (100%)	92 (92%)	8 (8%)	11	34
11	1P	115/116 (99%)	99 (86%)	16 (14%)	3	11
11	2P	115/116 (99%)	101 (88%)	14 (12%)	5	16
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	13	39
12	2Q	111/111 (100%)	97 (87%)	14 (13%)	4	14
13	1R	101/101 (100%)	86 (85%)	15 (15%)	3	10
13	2R	101/101 (100%)	87 (86%)	14 (14%)	3	11
14	1S	87/88 (99%)	75 (86%)	12 (14%)	3	12
14	2S	85/88 (97%)	72 (85%)	13 (15%)	3	9
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	40
15	2T	113/127 (89%)	103 (91%)	10 (9%)	9	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	30
16	2U	93/94 (99%)	83 (89%)	10 (11%)	6	21
17	1V	81/82 (99%)	72 (89%)	9 (11%)	6	20
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	24
18	1W	90/92 (98%)	80 (89%)	10 (11%)	6	20
18	2W	90/92 (98%)	79 (88%)	11 (12%)	5	16
19	1X	77/78 (99%)	71 (92%)	6 (8%)	11	35
19	2X	77/78 (99%)	69 (90%)	8 (10%)	7	23
20	1Y	86/91 (94%)	78 (91%)	8 (9%)	8	27
20	2Y	86/91 (94%)	74 (86%)	12 (14%)	3	11
21	1Z	169/179 (94%)	143 (85%)	26 (15%)	2	9
21	2Z	165/179 (92%)	142 (86%)	23 (14%)	3	11
22	10	61/67 (91%)	57 (93%)	4 (7%)	15	43
22	20	61/67 (91%)	58 (95%)	3 (5%)	22	54
23	11	79/83 (95%)	72 (91%)	7 (9%)	9	28
23	21	81/83 (98%)	71 (88%)	10 (12%)	4	15
24	12	65/67 (97%)	62 (95%)	3 (5%)	24	57
24	22	66/67 (98%)	57 (86%)	9 (14%)	3	12
25	13	51/52 (98%)	45 (88%)	6 (12%)	5	17
25	23	50/52 (96%)	43 (86%)	7 (14%)	3	11
26	14	58/63 (92%)	51 (88%)	7 (12%)	5	16
26	24	54/63 (86%)	46 (85%)	8 (15%)	3	10
27	15	51/52 (98%)	47 (92%)	4 (8%)	11	35
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	34
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	17
28	26	50/52 (96%)	44 (88%)	6 (12%)	5	16
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	54
29	27	41/42 (98%)	39 (95%)	2 (5%)	22	54
30	18	54/55 (98%)	48 (89%)	6 (11%)	6	20
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	64
31	19	34/34 (100%)	32 (94%)	2 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	29 (85%)	5 (15%)	3	10
33	1b	191/220 (87%)	158 (83%)	33 (17%)	2	7
33	2b	187/220 (85%)	164 (88%)	23 (12%)	4	15
34	1c	144/188 (77%)	124 (86%)	20 (14%)	3	11
34	2c	140/188 (74%)	125 (89%)	15 (11%)	6	22
35	1d	171/181 (94%)	148 (86%)	23 (14%)	4	12
35	2d	172/181 (95%)	152 (88%)	20 (12%)	5	18
36	1e	114/123 (93%)	102 (90%)	12 (10%)	6	22
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	26
37	1f	85/90 (94%)	78 (92%)	7 (8%)	10	32
37	2f	85/90 (94%)	75 (88%)	10 (12%)	5	17
38	1g	120/127 (94%)	109 (91%)	11 (9%)	8	27
38	2g	119/127 (94%)	106 (89%)	13 (11%)	6	20
39	1h	116/119 (98%)	103 (89%)	13 (11%)	6	19
39	2h	114/119 (96%)	98 (86%)	16 (14%)	3	11
40	1i	91/99 (92%)	81 (89%)	10 (11%)	6	20
40	2i	88/99 (89%)	79 (90%)	9 (10%)	7	23
41	1j	68/92 (74%)	57 (84%)	11 (16%)	2	8
41	2j	68/92 (74%)	54 (79%)	14 (21%)	1	4
42	1k	83/99 (84%)	73 (88%)	10 (12%)	5	16
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	26
43	1l	96/108 (89%)	89 (93%)	7 (7%)	13	38
43	2l	96/108 (89%)	82 (85%)	14 (15%)	3	10
44	1m	90/101 (89%)	81 (90%)	9 (10%)	7	24
44	2m	87/101 (86%)	75 (86%)	12 (14%)	3	12
45	1n	49/50 (98%)	40 (82%)	9 (18%)	1	6
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	23
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21	53
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16	44
47	1p	69/74 (93%)	59 (86%)	10 (14%)	3	10
47	2p	68/74 (92%)	58 (85%)	10 (15%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	83 (88%)	11 (12%)	5	17
48	2q	94/97 (97%)	85 (90%)	9 (10%)	8	26
49	1r	59/77 (77%)	51 (86%)	8 (14%)	3	12
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	12
50	1s	68/80 (85%)	59 (87%)	9 (13%)	4	13
50	2s	67/80 (84%)	56 (84%)	11 (16%)	2	8
51	1t	71/82 (87%)	62 (87%)	9 (13%)	4	14
51	2t	70/82 (85%)	59 (84%)	11 (16%)	2	9
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	50
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	20
53	1y	82/98 (84%)	72 (88%)	10 (12%)	5	16
53	2y	79/98 (81%)	67 (85%)	12 (15%)	3	9
All	All	9524/10260 (93%)	8373 (88%)	1151 (12%)	5	16

5 of 1151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	2b	136	VAL
53	2y	49	VAL
35	2d	49	ARG
33	2b	135	GLN
41	2j	69	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
35	2d	125	HIS
37	2f	94	GLN
44	2m	92	HIS
38	1g	86	GLN
37	1f	100	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	465 (16%)	29 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2A	2858/2915 (98%)	527 (18%)	32 (1%)
2	1B	119/121 (98%)	19 (15%)	0
2	2B	119/121 (98%)	22 (18%)	0
32	1a	1497/1521 (98%)	279 (18%)	0
32	2a	1501/1521 (98%)	322 (21%)	0
All	All	8959/9114 (98%)	1634 (18%)	61 (0%)

5 of 1634 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	61	G

5 of 61 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2893	G
1	2A	2406	U
1	2A	827	U
1	2A	2321	G
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	2.01	10 (30%)
32	UR3	2a	1498	32	19,22,23	0.95	0	26,32,35	1.79	3 (11%)
1	5MU	1A	1915	1	19,22,23	1.39	6 (31%)	27,32,35	2.29	9 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1A	1962	1,54	19,22,23	1.51	3 (15%)	26,32,35	1.27	4 (15%)
1	OMG	1A	2251	1,54	23,26,27	1.27	3 (13%)	32,38,41	2.14	6 (18%)
1	5MC	1A	1942	1	19,22,23	1.63	3 (15%)	26,32,35	1.14	2 (7%)
32	5MC	1a	1404	32	19,22,23	1.80	3 (15%)	26,32,35	1.21	3 (11%)
1	OMG	2A	2251	1,54	23,26,27	1.23	3 (13%)	32,38,41	2.01	6 (18%)
1	5MC	2A	1962	1,54	19,22,23	1.60	3 (15%)	26,32,35	1.25	3 (11%)
32	5MC	2a	967	32	19,22,23	1.82	3 (15%)	26,32,35	1.16	2 (7%)
32	2MG	2a	1207	32	23,26,27	1.24	4 (17%)	33,38,41	2.10	8 (24%)
1	OMC	1A	1920	1	19,22,23	0.82	0	25,31,34	0.97	1 (4%)
1	PSU	1A	2605	1	18,21,22	1.29	3 (16%)	21,30,33	1.86	5 (23%)
1	5MC	2A	1942	1	19,22,23	1.59	3 (15%)	26,32,35	1.14	2 (7%)
32	5MC	1a	1407	32	19,22,23	1.82	2 (10%)	26,32,35	1.12	3 (11%)
32	M2G	2a	966	32,54	24,27,28	1.30	3 (12%)	33,40,43	1.85	6 (18%)
1	PSU	1A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	2.06	3 (14%)
1	2MA	1A	2503	1,54	22,25,26	1.44	4 (18%)	32,37,40	2.50	8 (25%)
32	5MC	2a	1404	32	19,22,23	1.60	3 (15%)	26,32,35	1.13	2 (7%)
32	M2G	1a	966	32	24,27,28	1.26	4 (16%)	33,40,43	1.77	6 (18%)
32	4OC	1a	1402	32	20,23,24	0.79	0	25,32,35	0.94	1 (4%)
32	2MG	1a	1207	32	23,26,27	1.26	3 (13%)	33,38,41	2.36	8 (24%)
32	5MC	1a	967	32	19,22,23	1.58	3 (15%)	26,32,35	1.06	2 (7%)
1	5MU	2A	1939	1,54	19,22,23	1.44	5 (26%)	27,32,35	2.26	6 (22%)
1	PSU	2A	2605	1	18,21,22	1.39	2 (11%)	21,30,33	1.89	4 (19%)
32	MA6	1a	1519	32	23,26,27	0.42	0	33,38,41	2.02	9 (27%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.13	4 (19%)
1	2MA	2A	2503	1,54	22,25,26	1.47	5 (22%)	32,37,40	2.34	9 (28%)
32	MA6	2a	1518	32	23,26,27	0.39	0	33,38,41	2.05	9 (27%)
1	OMU	1A	2552	1,54	19,22,23	1.24	2 (10%)	25,31,34	1.83	5 (20%)
32	G7M	2a	527	32,54	23,26,27	1.44	3 (13%)	34,39,42	1.72	5 (14%)
32	5MC	2a	1407	32	19,22,23	1.66	3 (15%)	26,32,35	1.15	2 (7%)
1	5MU	1A	1939	1	19,22,23	1.40	5 (26%)	27,32,35	2.11	6 (22%)
1	5MU	2A	1915	1	19,22,23	1.46	4 (21%)	27,32,35	2.26	9 (33%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	1.94	3 (14%)
32	PSU	1a	516	32,54	18,21,22	1.40	2 (11%)	21,30,33	1.99	4 (19%)
43	0TD	1l	92	43	8,9,10	4.49	1 (12%)	6,11,13	1.51	1 (16%)
32	G7M	1a	527	32,54	23,26,27	1.59	3 (13%)	34,39,42	1.77	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	1400	32	19,22,23	1.73	3 (15%)	26,32,35	1.20	2 (7%)
43	0TD	2l	92	43	8,9,10	4.46	1 (12%)	6,11,13	3.48	3 (50%)
32	4OC	2a	1402	32	20,23,24	0.75	0	25,32,35	0.96	1 (4%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	1.99	4 (19%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.11	8 (24%)
32	5MC	1a	1400	32	19,22,23	1.68	3 (15%)	26,32,35	1.22	3 (11%)
1	OMU	2A	2552	1,54	19,22,23	1.19	2 (10%)	25,31,34	1.94	5 (20%)
32	PSU	2a	516	32,54	18,21,22	1.36	2 (11%)	21,30,33	1.95	5 (23%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.91	1 (4%)
32	UR3	1a	1498	32	19,22,23	0.99	2 (10%)	26,32,35	1.72	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	5MC	1A	1962	1,54	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,54	-	1/9/27/28	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,54	-	1/9/27/28	0/3/3/3
1	5MC	2A	1962	1,54	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	OMC	1A	1920	1	-	2/9/27/28	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32,54	-	0/11/29/30	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,54	-	2/7/25/26	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	2A	1939	1,54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,54	-	2/7/25/26	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	OMU	1A	2552	1,54	-	0/9/27/28	0/2/2/2
32	G7M	2a	527	32,54	-	1/7/25/26	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	4/7/12/14	-
32	G7M	1a	527	32,54	-	2/7/25/26	0/3/3/3
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
1	OMU	2A	2552	1,54	-	0/9/27/28	0/2/2/2
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.31	1.69	1.82
43	2l	92	0TD	CB-SB	-12.25	1.69	1.82
32	2a	967	5MC	C5-C4	6.85	1.49	1.44
32	1a	1407	5MC	C5-C4	6.80	1.49	1.44
32	1a	1404	5MC	C5-C4	6.65	1.49	1.44

The worst 5 of 219 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2503	2MA	C5-C4-N3	-9.40	117.28	127.18
1	2A	2503	2MA	C5-C4-N3	-8.64	118.08	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1498	UR3	C4-N3-C2	-7.35	118.66	124.58
43	2l	92	0TD	CSB-SB-CB	-7.24	89.34	102.36
32	1a	1207	2MG	C2-N3-C4	7.24	121.05	112.00

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CG-CB-SB-CSB

There are no ring outliers.

26 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1518	MA6	2	0
32	2a	1498	UR3	1	0
1	1A	1915	5MU	1	0
1	1A	2251	OMG	1	0
1	1A	1942	5MC	1	0
1	2A	2251	OMG	1	0
1	2A	1962	5MC	1	0
32	2a	967	5MC	1	0
1	1A	2503	2MA	1	0
32	1a	966	M2G	1	0
32	1a	1402	4OC	2	0
32	1a	1207	2MG	2	0
1	2A	1939	5MU	1	0
32	1a	1519	MA6	1	0
32	2a	1518	MA6	3	0
1	1A	1939	5MU	2	0
1	2A	1915	5MU	1	0
43	1l	92	0TD	1	0
32	1a	527	G7M	1	0
32	2a	1400	5MC	3	0
43	2l	92	0TD	1	0
32	2a	1402	4OC	2	0
32	2a	1519	MA6	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1400	5MC	1	0
1	2A	2552	OMU	1	0
1	2A	1920	OMC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2486 ligands modelled in this entry, 2473 are monoatomic - leaving 13 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	$\# Z > 2$
57	MPD	1a	1870	-	7,7,7	0.41	0	9,10,10	0.47	0
57	MPD	2A	3727	-	7,7,7	0.32	0	9,10,10	0.28	0
56	ARG	1A	4012	-	10,11,11	0.73	1 (10%)	9,13,13	1.08	1 (11%)
57	MPD	2A	3726	-	7,7,7	0.32	0	9,10,10	0.22	0
55	A1CQ8	1A	4011	-	47,49,49	2.87	13 (27%)	64,75,75	2.44	24 (37%)
57	MPD	1A	4013	-	7,7,7	0.35	0	9,10,10	0.33	0
57	MPD	18	102	-	7,7,7	0.40	0	9,10,10	0.48	0
59	SF4	1d	306	35	0,12,12	-	-	-	-	-
59	SF4	2d	501	35	0,12,12	-	-	-	-	-
57	MPD	2B	219	-	7,7,7	0.32	0	9,10,10	0.21	0
57	MPD	1T	206	-	7,7,7	0.31	0	9,10,10	0.50	0
56	ARG	1B	232	-	10,11,11	0.75	1 (10%)	9,13,13	0.99	1 (11%)
55	A1CQ8	2A	3725	-	47,49,49	2.89	13 (27%)	64,75,75	2.32	21 (32%)

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
57	MPD	1a	1870	-	-	5/5/5/5	-
57	MPD	2A	3727	-	-	4/5/5/5	-
56	ARG	1A	4012	-	-	2/11/11/11	-
57	MPD	2A	3726	-	-	1/5/5/5	-
55	A1CQ8	1A	4011	-	-	0/19/81/81	0/6/6/6
57	MPD	1A	4013	-	-	3/5/5/5	-
57	MPD	18	102	-	-	3/5/5/5	-
59	SF4	1d	306	35	-	-	0/6/5/5
59	SF4	2d	501	35	-	-	0/6/5/5
57	MPD	2B	219	-	-	4/5/5/5	-
57	MPD	1T	206	-	-	5/5/5/5	-
56	ARG	1B	232	-	-	4/11/11/11	-
55	A1CQ8	2A	3725	-	-	0/19/81/81	0/6/6/6

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2A	3725	A1CQ8	CBG-CBE	-10.10	1.32	1.47
55	1A	4011	A1CQ8	CBG-CBE	-9.97	1.32	1.47
55	2A	3725	A1CQ8	CAA-CAQ	-8.81	1.40	1.53
55	2A	3725	A1CQ8	CAT-CAQ	-8.66	1.37	1.51
55	1A	4011	A1CQ8	CAA-CAQ	-8.52	1.40	1.53

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3725	A1CQ8	CAK-CAC-CAB	-8.71	106.93	116.28
55	1A	4011	A1CQ8	CAK-CAC-CAB	-8.66	106.98	116.28
55	1A	4011	A1CQ8	CAZ-CAB-CAC	-5.35	103.34	108.81
55	2A	3725	A1CQ8	CAZ-CAB-CAC	-4.69	104.02	108.81
55	2A	3725	A1CQ8	CAE-CAF-CAG	-4.68	106.34	112.38

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

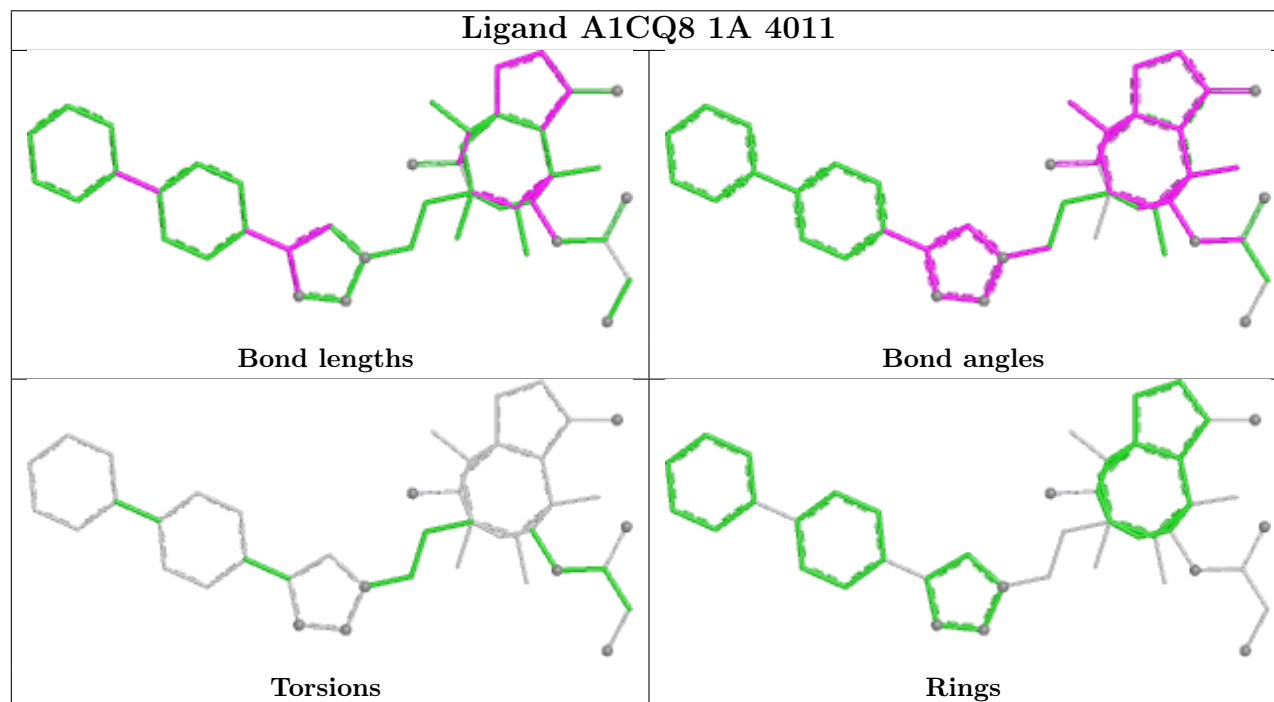
Mol	Chain	Res	Type	Atoms
57	1T	206	MPD	C1-C2-C3-C4
57	1T	206	MPD	O2-C2-C3-C4
57	1a	1870	MPD	C2-C3-C4-O4
57	1a	1870	MPD	C2-C3-C4-C5
57	2B	219	MPD	C2-C3-C4-C5

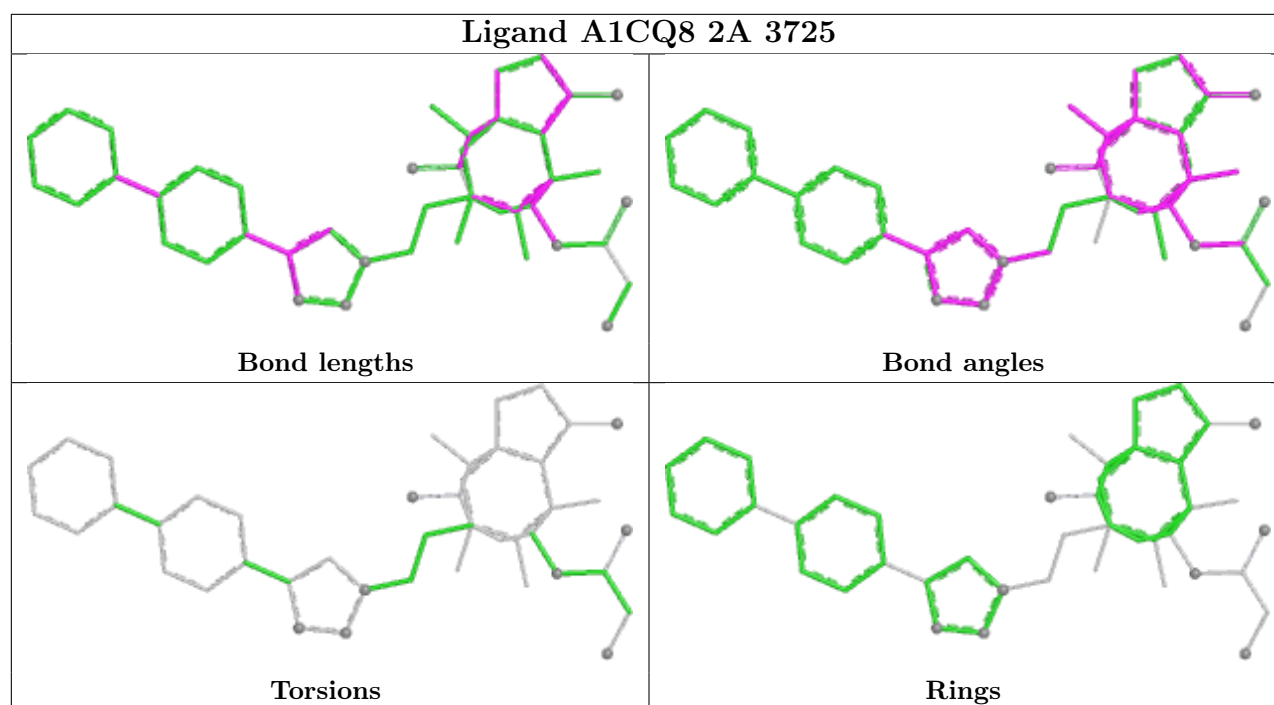
There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1a	1870	MPD	6	0
56	1A	4012	ARG	1	0
57	2A	3726	MPD	3	0
55	1A	4011	A1CQ8	1	0
57	18	102	MPD	3	0
59	1d	306	SF4	1	0
59	2d	501	SF4	1	0
56	1B	232	ARG	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.16	154 (5%) 31 24	14, 32, 94, 111	0
1	2A	2856/2915 (97%)	0.24	175 (6%) 27 21	28, 51, 96, 112	0
2	1B	120/121 (99%)	-0.05	1 (0%) 82 77	27, 49, 65, 78	0
2	2B	120/121 (99%)	1.18	19 (15%) 5 4	54, 79, 88, 89	0
3	1D	275/276 (99%)	-0.03	3 (1%) 78 71	16, 31, 47, 69	0
3	2D	275/276 (99%)	0.35	10 (3%) 46 38	27, 46, 59, 73	0
4	1E	204/206 (99%)	-0.06	1 (0%) 87 83	15, 37, 58, 71	0
4	2E	204/206 (99%)	0.45	4 (1%) 65 56	29, 50, 69, 79	0
5	1F	203/210 (96%)	0.03	1 (0%) 87 83	14, 36, 65, 85	0
5	2F	203/210 (96%)	0.52	3 (1%) 72 64	30, 57, 76, 84	0
6	1G	181/182 (99%)	0.87	20 (11%) 10 9	43, 63, 77, 85	0
6	2G	181/182 (99%)	1.71	55 (30%) 1 1	73, 83, 89, 92	0
7	1H	174/180 (96%)	0.40	9 (5%) 33 26	35, 49, 64, 72	0
7	2H	173/180 (96%)	1.26	24 (13%) 6 5	64, 76, 86, 94	0
8	1I	147/148 (99%)	0.79	8 (5%) 31 24	41, 68, 79, 84	0
8	2I	146/148 (98%)	0.98	14 (9%) 13 11	48, 71, 82, 89	0
9	1N	140/140 (100%)	0.10	2 (1%) 73 65	24, 36, 59, 70	0
9	2N	140/140 (100%)	0.51	3 (2%) 63 54	34, 57, 72, 77	0
10	1O	122/122 (100%)	0.03	1 (0%) 82 77	24, 34, 55, 61	0
10	2O	122/122 (100%)	0.38	3 (2%) 58 48	39, 48, 60, 68	0
11	1P	149/150 (99%)	0.09	1 (0%) 84 79	16, 41, 62, 78	0
11	2P	149/150 (99%)	0.60	5 (3%) 48 39	30, 61, 77, 87	0
12	1Q	141/141 (100%)	-0.04	0 100 100	21, 36, 49, 67	0
12	2Q	141/141 (100%)	0.66	6 (4%) 40 31	38, 57, 68, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.09	0 100 100	21, 32, 50, 60	0
13	2R	118/118 (100%)	0.13	0 100 100	30, 45, 55, 64	0
14	1S	110/112 (98%)	0.44	4 (3%) 46 38	35, 48, 61, 68	0
14	2S	110/112 (98%)	1.62	26 (23%) 2 2	60, 72, 79, 85	0
15	1T	131/146 (89%)	0.15	3 (2%) 61 52	31, 40, 62, 70	0
15	2T	131/146 (89%)	0.44	3 (2%) 61 52	39, 52, 69, 76	0
16	1U	116/118 (98%)	-0.18	0 100 100	18, 28, 45, 62	0
16	2U	116/118 (98%)	0.50	5 (4%) 40 31	34, 53, 67, 75	0
17	1V	101/101 (100%)	-0.13	0 100 100	19, 39, 56, 63	0
17	2V	101/101 (100%)	0.70	6 (5%) 28 22	34, 64, 75, 81	0
18	1W	112/113 (99%)	-0.10	1 (0%) 81 75	19, 28, 48, 76	0
18	2W	112/113 (99%)	0.18	1 (0%) 81 75	28, 42, 61, 92	0
19	1X	95/96 (98%)	-0.09	1 (1%) 78 71	22, 33, 55, 67	0
19	2X	95/96 (98%)	0.67	5 (5%) 32 25	40, 54, 69, 78	0
20	1Y	107/110 (97%)	0.44	3 (2%) 55 46	32, 47, 70, 78	0
20	2Y	107/110 (97%)	1.33	25 (23%) 2 2	51, 65, 81, 87	0
21	1Z	203/206 (98%)	0.62	9 (4%) 39 30	36, 55, 74, 80	0
21	2Z	201/206 (97%)	1.21	28 (13%) 6 5	61, 72, 83, 89	0
22	10	77/85 (90%)	0.17	0 100 100	24, 33, 46, 60	0
22	20	77/85 (90%)	0.79	3 (3%) 43 35	44, 55, 68, 72	0
23	11	97/98 (98%)	0.18	2 (2%) 63 54	22, 37, 64, 75	0
23	21	97/98 (98%)	0.48	4 (4%) 41 33	32, 48, 69, 74	0
24	12	70/72 (97%)	0.19	1 (1%) 73 65	31, 42, 54, 72	0
24	22	70/72 (97%)	1.08	7 (10%) 12 10	52, 64, 73, 76	0
25	13	59/60 (98%)	0.08	0 100 100	24, 32, 56, 65	0
25	23	59/60 (98%)	0.74	3 (5%) 33 26	41, 54, 74, 83	0
26	14	69/71 (97%)	1.25	13 (18%) 3 3	60, 80, 91, 95	0
26	24	69/71 (97%)	2.04	32 (46%) 0 0	79, 90, 98, 102	0
27	15	59/60 (98%)	0.11	3 (5%) 33 26	17, 31, 62, 73	0
27	25	59/60 (98%)	0.46	1 (1%) 69 61	30, 48, 72, 76	0
28	16	53/54 (98%)	0.03	0 100 100	29, 37, 48, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.46	5 (9%) 14 12	46, 56, 64, 74	0
29	17	48/49 (97%)	-0.04	4 (8%) 17 14	16, 22, 54, 62	0
29	27	48/49 (97%)	0.26	4 (8%) 17 14	29, 37, 56, 65	0
30	18	64/65 (98%)	-0.19	0 100 100	20, 28, 36, 44	0
30	28	64/65 (98%)	0.71	7 (10%) 10 9	40, 47, 56, 63	0
31	19	37/37 (100%)	-0.04	0 100 100	28, 37, 53, 60	0
31	29	37/37 (100%)	1.04	3 (8%) 18 15	53, 61, 72, 78	0
32	1a	1488/1521 (97%)	0.72	89 (5%) 27 21	31, 70, 95, 113	0
32	2a	1492/1521 (98%)	0.91	161 (10%) 11 9	38, 75, 97, 111	0
33	1b	231/256 (90%)	1.44	52 (22%) 2 2	66, 78, 89, 95	0
33	2b	231/256 (90%)	1.65	76 (32%) 1 1	68, 83, 92, 98	0
34	1c	206/239 (86%)	1.32	34 (16%) 4 3	63, 76, 86, 89	0
34	2c	206/239 (86%)	1.95	88 (42%) 0 0	70, 84, 91, 95	0
35	1d	208/209 (99%)	1.53	44 (21%) 2 2	52, 71, 81, 85	0
35	2d	208/209 (99%)	1.36	38 (18%) 3 3	56, 71, 80, 85	0
36	1e	148/162 (91%)	0.72	6 (4%) 41 33	42, 65, 73, 78	0
36	2e	148/162 (91%)	1.22	19 (12%) 7 6	60, 72, 80, 89	0
37	1f	100/101 (99%)	1.04	12 (12%) 9 7	56, 67, 77, 79	0
37	2f	100/101 (99%)	1.02	13 (13%) 7 6	59, 70, 79, 82	0
38	1g	155/156 (99%)	1.03	17 (10%) 10 9	61, 72, 81, 91	0
38	2g	155/156 (99%)	1.39	39 (25%) 1 1	72, 80, 86, 91	0
39	1h	137/138 (99%)	0.85	9 (6%) 24 19	53, 66, 74, 80	0
39	2h	137/138 (99%)	1.04	15 (10%) 10 9	62, 71, 78, 86	0
40	1i	127/128 (99%)	1.82	54 (42%) 0 0	64, 80, 87, 89	0
40	2i	126/128 (98%)	2.14	58 (46%) 0 0	75, 86, 92, 95	0
41	1j	97/105 (92%)	1.78	32 (32%) 1 1	65, 80, 90, 93	0
41	2j	96/105 (91%)	2.42	68 (70%) 0 0	77, 85, 94, 97	0
42	1k	114/129 (88%)	0.94	7 (6%) 27 21	38, 61, 74, 79	0
42	2k	114/129 (88%)	1.09	13 (11%) 10 8	54, 70, 79, 84	0
43	1l	121/132 (91%)	0.69	3 (2%) 58 48	47, 56, 69, 75	0
43	2l	121/132 (91%)	1.03	16 (13%) 7 6	55, 65, 73, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	1.39	25 (21%) 2 2	65, 76, 84, 89	0
44	2m	114/126 (90%)	1.59	35 (30%) 1 1	74, 85, 90, 96	0
45	1n	60/61 (98%)	1.45	11 (18%) 3 3	66, 74, 80, 84	0
45	2n	60/61 (98%)	2.18	31 (51%) 0 0	78, 85, 90, 91	0
46	1o	88/89 (98%)	0.97	8 (9%) 15 12	51, 65, 75, 84	0
46	2o	88/89 (98%)	0.77	2 (2%) 61 52	59, 70, 78, 85	0
47	1p	82/88 (93%)	1.60	22 (26%) 1 1	61, 71, 79, 85	0
47	2p	82/88 (93%)	1.23	14 (17%) 4 3	55, 66, 79, 85	0
48	1q	99/105 (94%)	0.99	12 (12%) 8 7	52, 65, 72, 76	0
48	2q	99/105 (94%)	0.76	4 (4%) 42 34	52, 67, 76, 79	0
49	1r	68/88 (77%)	0.99	8 (11%) 9 7	56, 65, 78, 82	0
49	2r	68/88 (77%)	0.96	4 (5%) 28 22	61, 71, 81, 84	0
50	1s	83/93 (89%)	1.39	15 (18%) 3 3	68, 79, 87, 89	0
50	2s	83/93 (89%)	2.20	43 (51%) 0 0	79, 88, 94, 101	0
51	1t	96/106 (90%)	1.60	29 (30%) 1 1	57, 70, 77, 81	0
51	2t	98/106 (92%)	0.98	8 (8%) 17 14	55, 66, 77, 80	0
52	1u	23/27 (85%)	1.60	6 (26%) 1 1	67, 73, 76, 79	0
52	2u	23/27 (85%)	2.41	15 (65%) 0 0	79, 83, 88, 89	0
53	1y	97/113 (85%)	0.84	8 (8%) 17 14	52, 68, 76, 86	0
53	2y	96/113 (84%)	2.15	52 (54%) 0 0	69, 82, 90, 92	0
All	All	20766/21468 (96%)	0.61	2049 (9%) 13 11	14, 60, 89, 113	0

The worst 5 of 2049 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	2174	C	9.3
1	1A	1087	G	8.9
1	1A	1091	G	8.8
1	1A	2173	A	8.7
1	2A	2174	C	8.4

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

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($\text{\AA}^2$)	Q<0.9
32	5MC	2a	967	21/22	0.82	0.19	72,75,84,93	0
32	2MG	2a	1207	24/25	0.82	0.14	84,88,94,97	0
1	5MU	2A	1915	21/22	0.83	0.13	75,81,89,98	0
1	5MU	1A	1915	21/22	0.84	0.14	71,78,88,102	0
32	PSU	2a	516	20/21	0.85	0.12	76,82,90,91	0
32	M2G	2a	966	25/26	0.86	0.19	70,76,86,92	0
32	2MG	1a	1207	24/25	0.88	0.13	73,80,81,93	0
1	PSU	1A	1917	20/21	0.88	0.11	62,73,80,81	0
32	G7M	2a	527	24/25	0.89	0.15	63,69,75,79	0
43	0TD	1l	92	10/11	0.89	0.14	55,59,63,71	0
1	PSU	2A	1917	20/21	0.90	0.10	76,79,85,86	0
1	PSU	2A	1911	20/21	0.90	0.10	67,70,75,77	0
1	PSU	1A	1911	20/21	0.91	0.11	48,62,66,71	0
32	5MC	1a	967	21/22	0.91	0.11	59,65,78,81	0
32	4OC	2a	1402	22/23	0.91	0.12	55,65,68,73	0
32	5MC	2a	1400	21/22	0.92	0.13	63,72,77,81	0
32	PSU	1a	516	20/21	0.92	0.10	62,69,73,73	0
43	0TD	2l	92	10/11	0.92	0.11	59,64,68,82	0
32	4OC	1a	1402	22/23	0.93	0.12	49,53,57,63	0
1	5MC	2A	1942	21/22	0.94	0.12	41,51,57,63	0
32	M2G	1a	966	25/26	0.94	0.11	54,61,68,78	0
32	5MC	1a	1407	21/22	0.94	0.11	45,52,57,59	0
1	OMC	2A	1920	21/22	0.95	0.09	59,66,71,73	0
32	5MC	1a	1400	21/22	0.95	0.11	40,58,63,64	0
32	G7M	1a	527	24/25	0.95	0.09	48,54,57,62	0
1	5MC	1A	1942	21/22	0.95	0.09	25,34,39,44	0
32	5MC	2a	1404	21/22	0.95	0.10	47,57,62,66	0
32	UR3	2a	1498	21/22	0.95	0.09	53,60,63,66	0
32	MA6	2a	1518	24/25	0.95	0.10	51,60,63,65	0
32	UR3	1a	1498	21/22	0.95	0.10	43,48,52,58	0
1	2MA	2A	2503	23/24	0.96	0.10	23,29,35,41	0
32	MA6	1a	1518	24/25	0.96	0.10	42,44,50,54	0
32	MA6	1a	1519	24/25	0.96	0.09	39,45,51,53	0
32	5MC	2a	1407	21/22	0.96	0.09	51,58,63,63	0
1	OMC	1A	1920	21/22	0.96	0.09	42,52,58,61	0
32	5MC	1a	1404	21/22	0.96	0.09	37,44,49,52	0
32	MA6	2a	1519	24/25	0.96	0.13	53,60,66,68	0
1	OMG	2A	2251	24/25	0.96	0.08	31,34,39,40	0
1	PSU	1A	2605	20/21	0.97	0.09	17,22,27,33	0
1	5MC	2A	1962	21/22	0.97	0.08	36,44,49,57	0
1	5MU	1A	1939	21/22	0.97	0.09	17,27,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	2MA	1A	2503	23/24	0.97	0.08	13,17,22,22	0
1	OMU	2A	2552	21/22	0.97	0.08	29,35,38,42	0
1	5MU	2A	1939	21/22	0.97	0.08	32,35,40,43	0
1	5MC	1A	1962	21/22	0.98	0.07	24,34,39,44	0
1	OMU	1A	2552	21/22	0.98	0.07	18,25,31,32	0
1	PSU	2A	2605	20/21	0.98	0.08	27,34,37,39	0
1	OMG	1A	2251	24/25	0.98	0.07	14,19,22,25	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3730	1/1	0.47	0.29	59,59,59,59	0
54	MG	1A	3661	1/1	0.48	0.18	73,73,73,73	0
54	MG	1a	1821	1/1	0.51	0.18	82,82,82,82	0
54	MG	2B	214	1/1	0.51	0.17	82,82,82,82	0
54	MG	2a	1738	1/1	0.52	0.22	84,84,84,84	0
54	MG	1A	3672	1/1	0.54	0.31	59,59,59,59	0
54	MG	2A	3335	1/1	0.55	0.22	69,69,69,69	0
54	MG	1A	3520	1/1	0.56	0.19	33,33,33,33	0
54	MG	1a	1773	1/1	0.57	0.20	85,85,85,85	0
54	MG	1p	101	1/1	0.58	0.18	83,83,83,83	0
54	MG	2a	1735	1/1	0.59	0.13	64,64,64,64	0
54	MG	2a	1712	1/1	0.59	0.42	75,75,75,75	0
54	MG	2a	1729	1/1	0.60	0.27	76,76,76,76	0
54	MG	1a	1632	1/1	0.61	0.23	59,59,59,59	0
54	MG	2a	1601	1/1	0.61	0.24	67,67,67,67	0
54	MG	1a	1764	1/1	0.61	0.18	72,72,72,72	0
54	MG	2A	3045	1/1	0.62	0.20	60,60,60,60	0
54	MG	2A	3459	1/1	0.62	0.18	58,58,58,58	0
54	MG	2a	1745	1/1	0.62	0.25	65,65,65,65	0
54	MG	2A	3506	1/1	0.63	0.25	70,70,70,70	0
54	MG	1h	201	1/1	0.63	0.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1794	1/1	0.64	0.21	65,65,65,65	0
54	MG	2A	3112	1/1	0.64	0.18	79,79,79,79	0
54	MG	1A	3990	1/1	0.65	0.30	89,89,89,89	0
54	MG	1a	1723	1/1	0.66	0.12	90,90,90,90	0
54	MG	1A	3840	1/1	0.66	0.22	70,70,70,70	0
54	MG	1a	1800	1/1	0.66	0.16	64,64,64,64	0
54	MG	2A	3513	1/1	0.67	0.17	76,76,76,76	0
54	MG	2a	1760	1/1	0.67	0.23	66,66,66,66	0
54	MG	1A	3617	1/1	0.68	0.14	54,54,54,54	0
54	MG	2A	3357	1/1	0.69	0.18	72,72,72,72	0
54	MG	15	106	1/1	0.69	0.14	67,67,67,67	0
54	MG	2a	1674	1/1	0.69	0.22	68,68,68,68	0
54	MG	2a	1682	1/1	0.69	0.31	72,72,72,72	0
54	MG	2A	3720	1/1	0.69	0.19	60,60,60,60	0
54	MG	2A	3570	1/1	0.70	0.20	98,98,98,98	0
54	MG	2A	3440	1/1	0.70	0.30	73,73,73,73	0
54	MG	1A	3554	1/1	0.70	0.16	53,53,53,53	0
54	MG	1B	205	1/1	0.71	0.19	55,55,55,55	0
54	MG	1a	1859	1/1	0.71	0.20	76,76,76,76	0
54	MG	1B	227	1/1	0.71	0.15	70,70,70,70	0
54	MG	1A	3608	1/1	0.71	0.17	41,41,41,41	0
54	MG	1A	3876	1/1	0.72	0.28	41,41,41,41	0
54	MG	2A	3410	1/1	0.72	0.17	71,71,71,71	0
54	MG	1a	1817	1/1	0.72	0.17	76,76,76,76	0
54	MG	2A	3120	1/1	0.72	0.32	70,70,70,70	0
54	MG	2A	3166	1/1	0.72	0.19	61,61,61,61	0
54	MG	1F	315	1/1	0.72	0.24	39,39,39,39	0
54	MG	2n	101	1/1	0.72	0.28	69,69,69,69	0
54	MG	2a	1673	1/1	0.73	0.17	60,60,60,60	0
54	MG	2A	3449	1/1	0.73	0.23	62,62,62,62	0
54	MG	1B	210	1/1	0.73	0.22	55,55,55,55	0
54	MG	1A	3360	1/1	0.73	0.15	40,40,40,40	0
54	MG	2A	3039	1/1	0.73	0.10	59,59,59,59	0
54	MG	1F	314	1/1	0.73	0.34	66,66,66,66	0
54	MG	2A	3649	1/1	0.73	0.32	94,94,94,94	0
54	MG	2A	3384	1/1	0.73	0.20	59,59,59,59	0
54	MG	2A	3080	1/1	0.73	0.26	58,58,58,58	0
54	MG	1a	1715	1/1	0.73	0.24	75,75,75,75	0
54	MG	2A	3502	1/1	0.74	0.20	46,46,46,46	0
54	MG	1A	3758	1/1	0.74	0.22	62,62,62,62	0
54	MG	1A	3389	1/1	0.74	0.19	67,67,67,67	0
54	MG	2a	1716	1/1	0.74	0.15	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2B	217	1/1	0.74	0.24	81,81,81,81	0
54	MG	2G	203	1/1	0.74	0.15	66,66,66,66	0
54	MG	2A	3433	1/1	0.74	0.17	68,68,68,68	0
54	MG	2a	1615	1/1	0.74	0.24	82,82,82,82	0
54	MG	2a	1649	1/1	0.74	0.34	75,75,75,75	0
54	MG	2A	3610	1/1	0.74	0.17	79,79,79,79	0
54	MG	1A	3937	1/1	0.75	0.37	75,75,75,75	0
54	MG	1a	1753	1/1	0.75	0.21	70,70,70,70	0
54	MG	2a	1676	1/1	0.75	0.22	65,65,65,65	0
54	MG	1A	3076	1/1	0.75	0.14	52,52,52,52	0
54	MG	1B	217	1/1	0.75	0.20	69,69,69,69	0
54	MG	1a	1831	1/1	0.75	0.20	64,64,64,64	0
54	MG	1g	202	1/1	0.76	0.10	51,51,51,51	0
54	MG	2A	3658	1/1	0.76	0.27	80,80,80,80	0
54	MG	2A	3675	1/1	0.76	0.17	47,47,47,47	0
54	MG	2A	3677	1/1	0.76	0.19	83,83,83,83	0
54	MG	1a	1725	1/1	0.76	0.25	65,65,65,65	0
54	MG	1A	3995	1/1	0.76	0.23	55,55,55,55	0
54	MG	2a	1727	1/1	0.76	0.24	67,67,67,67	0
54	MG	1A	4007	1/1	0.76	0.27	77,77,77,77	0
54	MG	1A	3754	1/1	0.76	0.14	50,50,50,50	0
54	MG	25	102	1/1	0.76	0.18	53,53,53,53	0
54	MG	1A	3930	1/1	0.76	0.14	76,76,76,76	0
54	MG	2a	1758	1/1	0.76	0.28	78,78,78,78	0
54	MG	2A	3083	1/1	0.76	0.28	60,60,60,60	0
54	MG	2a	1768	1/1	0.76	0.16	62,62,62,62	0
54	MG	2e	202	1/1	0.76	0.23	71,71,71,71	0
54	MG	2A	3090	1/1	0.76	0.15	58,58,58,58	0
54	MG	1a	1675	1/1	0.77	0.15	82,82,82,82	0
54	MG	2A	3415	1/1	0.77	0.25	67,67,67,67	0
54	MG	2A	3722	1/1	0.77	0.18	61,61,61,61	0
54	MG	1A	3214	1/1	0.77	0.21	57,57,57,57	0
54	MG	1Z	301	1/1	0.77	0.15	60,60,60,60	0
54	MG	1d	303	1/1	0.77	0.19	68,68,68,68	0
54	MG	2X	102	1/1	0.77	0.28	57,57,57,57	0
54	MG	2a	1775	1/1	0.77	0.20	66,66,66,66	0
54	MG	1A	3663	1/1	0.77	0.15	76,76,76,76	0
54	MG	1A	3272	1/1	0.77	0.17	80,80,80,80	0
57	MPD	1T	206	8/8	0.77	0.25	55,64,66,72	0
57	MPD	2B	219	8/8	0.77	0.33	61,71,75,83	0
54	MG	1a	1692	1/1	0.78	0.23	62,62,62,62	0
54	MG	2B	207	1/1	0.78	0.25	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1f	202	1/1	0.78	0.18	61,61,61,61	0
54	MG	1a	1777	1/1	0.78	0.23	80,80,80,80	0
54	MG	1a	1792	1/1	0.78	0.20	74,74,74,74	0
54	MG	1B	228	1/1	0.78	0.11	73,73,73,73	0
54	MG	2A	3591	1/1	0.78	0.13	58,58,58,58	0
54	MG	1D	315	1/1	0.78	0.22	62,62,62,62	0
54	MG	2a	1610	1/1	0.78	0.13	63,63,63,63	0
54	MG	1A	3734	1/1	0.78	0.35	55,55,55,55	0
54	MG	2a	1762	1/1	0.78	0.18	72,72,72,72	0
54	MG	2a	1630	1/1	0.78	0.16	73,73,73,73	0
54	MG	2a	1771	1/1	0.78	0.15	65,65,65,65	0
54	MG	2A	3056	1/1	0.78	0.23	59,59,59,59	0
54	MG	2a	1652	1/1	0.78	0.32	67,67,67,67	0
54	MG	1a	1733	1/1	0.78	0.15	60,60,60,60	0
54	MG	1A	3688	1/1	0.78	0.26	37,37,37,37	0
54	MG	1a	1687	1/1	0.78	0.25	58,58,58,58	0
58	ZN	14	501	1/1	0.78	0.22	161,161,161,161	0
54	MG	1A	3808	1/1	0.79	0.13	31,31,31,31	0
54	MG	2A	3517	1/1	0.79	0.14	57,57,57,57	0
54	MG	1A	3271	1/1	0.79	0.18	67,67,67,67	0
54	MG	1A	3943	1/1	0.79	0.12	43,43,43,43	0
54	MG	1a	1640	1/1	0.79	0.22	66,66,66,66	0
54	MG	1b	301	1/1	0.79	0.25	66,66,66,66	0
54	MG	1A	3958	1/1	0.79	0.18	30,30,30,30	0
57	MPD	2A	3726	8/8	0.79	0.30	47,52,62,64	0
54	MG	2A	3071	1/1	0.79	0.25	44,44,44,44	0
54	MG	1A	3510	1/1	0.79	0.12	38,38,38,38	0
54	MG	2A	3697	1/1	0.80	0.16	78,78,78,78	0
54	MG	2a	1688	1/1	0.80	0.22	53,53,53,53	0
54	MG	2A	3226	1/1	0.80	0.19	57,57,57,57	0
54	MG	1F	312	1/1	0.80	0.51	43,43,43,43	0
54	MG	2A	3605	1/1	0.80	0.18	55,55,55,55	0
54	MG	1a	1868	1/1	0.80	0.34	69,69,69,69	0
54	MG	1A	3991	1/1	0.80	0.48	48,48,48,48	0
54	MG	1A	3542	1/1	0.80	0.13	57,57,57,57	0
54	MG	1G	202	1/1	0.80	0.14	68,68,68,68	0
54	MG	2a	1750	1/1	0.80	0.28	71,71,71,71	0
54	MG	1A	3636	1/1	0.80	0.20	45,45,45,45	0
54	MG	1A	3190	1/1	0.81	0.10	57,57,57,57	0
54	MG	2A	3708	1/1	0.81	0.13	67,67,67,67	0
54	MG	2A	3718	1/1	0.81	0.12	54,54,54,54	0
54	MG	2A	3331	1/1	0.81	0.14	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1786	1/1	0.81	0.21	61,61,61,61	0
54	MG	2A	3343	1/1	0.81	0.20	65,65,65,65	0
54	MG	1A	3863	1/1	0.81	0.40	29,29,29,29	0
54	MG	1a	1603	1/1	0.81	0.20	74,74,74,74	0
54	MG	1y	203	1/1	0.81	0.16	73,73,73,73	0
54	MG	2A	3093	1/1	0.81	0.16	61,61,61,61	0
54	MG	2A	3096	1/1	0.81	0.15	50,50,50,50	0
54	MG	1A	3947	1/1	0.81	0.34	79,79,79,79	0
54	MG	1P	207	1/1	0.81	0.17	48,48,48,48	0
54	MG	2A	3050	1/1	0.81	0.16	54,54,54,54	0
54	MG	1a	1673	1/1	0.82	0.10	48,48,48,48	0
54	MG	2a	1709	1/1	0.82	0.16	68,68,68,68	0
54	MG	2A	3201	1/1	0.82	0.12	53,53,53,53	0
54	MG	1A	3740	1/1	0.82	0.17	56,56,56,56	0
54	MG	2A	3227	1/1	0.82	0.13	59,59,59,59	0
54	MG	1B	203	1/1	0.82	0.15	43,43,43,43	0
54	MG	2E	305	1/1	0.82	0.13	43,43,43,43	0
54	MG	1A	3456	1/1	0.82	0.11	23,23,23,23	0
54	MG	2N	201	1/1	0.82	0.10	67,67,67,67	0
54	MG	1a	1695	1/1	0.82	0.23	60,60,60,60	0
54	MG	1d	305	1/1	0.82	0.11	84,84,84,84	0
54	MG	1F	317	1/1	0.82	0.15	50,50,50,50	0
54	MG	1a	1722	1/1	0.82	0.15	61,61,61,61	0
54	MG	1a	1607	1/1	0.82	0.13	77,77,77,77	0
54	MG	1A	3514	1/1	0.82	0.15	53,53,53,53	0
54	MG	1y	201	1/1	0.82	0.16	70,70,70,70	0
54	MG	2A	3444	1/1	0.82	0.14	37,37,37,37	0
54	MG	2a	1653	1/1	0.82	0.15	77,77,77,77	0
54	MG	2A	3702	1/1	0.82	0.38	53,53,53,53	0
54	MG	2A	3707	1/1	0.82	0.14	55,55,55,55	0
54	MG	1N	203	1/1	0.82	0.15	56,56,56,56	0
54	MG	2A	3458	1/1	0.82	0.11	57,57,57,57	0
54	MG	1T	204	1/1	0.83	0.14	61,61,61,61	0
54	MG	2A	3295	1/1	0.83	0.10	26,26,26,26	0
54	MG	2a	1672	1/1	0.83	0.16	56,56,56,56	0
54	MG	1Y	201	1/1	0.83	0.30	61,61,61,61	0
54	MG	2A	3001	1/1	0.83	0.20	52,52,52,52	0
54	MG	2A	3026	1/1	0.83	0.17	53,53,53,53	0
54	MG	1F	302	1/1	0.83	0.35	33,33,33,33	0
54	MG	1a	1712	1/1	0.83	0.15	52,52,52,52	0
54	MG	2a	1707	1/1	0.83	0.13	74,74,74,74	0
54	MG	10	110	1/1	0.83	0.17	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3889	1/1	0.83	0.59	44,44,44,44	0
54	MG	2a	1715	1/1	0.83	0.16	49,49,49,49	0
54	MG	2A	3716	1/1	0.83	0.23	56,56,56,56	0
54	MG	2A	3432	1/1	0.83	0.19	57,57,57,57	0
54	MG	1a	1846	1/1	0.83	0.13	59,59,59,59	0
54	MG	2A	3076	1/1	0.83	0.18	51,51,51,51	0
54	MG	1A	3912	1/1	0.83	0.10	50,50,50,50	0
54	MG	2a	1739	1/1	0.83	0.13	82,82,82,82	0
54	MG	1a	1867	1/1	0.83	0.13	72,72,72,72	0
54	MG	1A	3668	1/1	0.83	0.13	57,57,57,57	0
54	MG	2a	1752	1/1	0.83	0.22	59,59,59,59	0
54	MG	1a	1612	1/1	0.83	0.13	64,64,64,64	0
54	MG	2A	3499	1/1	0.83	0.16	55,55,55,55	0
54	MG	1A	3124	1/1	0.83	0.17	46,46,46,46	0
54	MG	2a	1765	1/1	0.83	0.10	58,58,58,58	0
54	MG	2V	201	1/1	0.83	0.24	64,64,64,64	0
54	MG	1A	3504	1/1	0.83	0.18	46,46,46,46	0
54	MG	2A	3507	1/1	0.83	0.19	50,50,50,50	0
54	MG	2A	3114	1/1	0.83	0.18	51,51,51,51	0
54	MG	1a	1663	1/1	0.83	0.19	51,51,51,51	0
54	MG	1D	303	1/1	0.83	0.17	52,52,52,52	0
54	MG	1a	1783	1/1	0.83	0.26	79,79,79,79	0
54	MG	1A	3881	1/1	0.83	0.14	41,41,41,41	0
54	MG	2a	1650	1/1	0.83	0.13	78,78,78,78	0
54	MG	1A	3577	1/1	0.84	0.36	39,39,39,39	0
54	MG	2a	1625	1/1	0.84	0.12	50,50,50,50	0
54	MG	1A	3402	1/1	0.84	0.12	24,24,24,24	0
54	MG	2A	3095	1/1	0.84	0.26	56,56,56,56	0
54	MG	1A	3359	1/1	0.84	0.17	48,48,48,48	0
54	MG	2A	3510	1/1	0.84	0.15	69,69,69,69	0
54	MG	1A	3796	1/1	0.84	0.14	58,58,58,58	0
54	MG	1A	4001	1/1	0.84	0.14	43,43,43,43	0
54	MG	2A	3557	1/1	0.84	0.13	64,64,64,64	0
54	MG	1A	3925	1/1	0.84	0.12	17,17,17,17	0
54	MG	1a	1608	1/1	0.84	0.19	60,60,60,60	0
54	MG	2A	3198	1/1	0.84	0.17	58,58,58,58	0
54	MG	1A	3798	1/1	0.84	0.26	33,33,33,33	0
54	MG	2a	1695	1/1	0.84	0.25	76,76,76,76	0
54	MG	2A	3204	1/1	0.84	0.18	67,67,67,67	0
54	MG	1a	1617	1/1	0.84	0.21	72,72,72,72	0
54	MG	1a	1734	1/1	0.84	0.12	63,63,63,63	0
54	MG	2A	3254	1/1	0.84	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3258	1/1	0.84	0.13	36,36,36,36	0
54	MG	2A	3700	1/1	0.84	0.12	54,54,54,54	0
54	MG	1A	3933	1/1	0.84	0.20	75,75,75,75	0
54	MG	2a	1732	1/1	0.84	0.28	58,58,58,58	0
54	MG	1A	3547	1/1	0.84	0.15	56,56,56,56	0
54	MG	1a	1641	1/1	0.84	0.16	63,63,63,63	0
54	MG	1a	1650	1/1	0.84	0.22	55,55,55,55	0
54	MG	1a	1656	1/1	0.84	0.34	74,74,74,74	0
54	MG	2A	3719	1/1	0.84	0.23	59,59,59,59	0
54	MG	2A	3378	1/1	0.84	0.16	29,29,29,29	0
54	MG	1a	1784	1/1	0.84	0.14	68,68,68,68	0
54	MG	1a	1661	1/1	0.84	0.18	61,61,61,61	0
54	MG	1a	1787	1/1	0.84	0.15	73,73,73,73	0
54	MG	1A	3655	1/1	0.84	0.13	54,54,54,54	0
54	MG	1B	224	1/1	0.84	0.11	37,37,37,37	0
54	MG	1a	1674	1/1	0.84	0.28	56,56,56,56	0
54	MG	2A	3075	1/1	0.84	0.46	45,45,45,45	0
54	MG	1A	3484	1/1	0.84	0.15	78,78,78,78	0
54	MG	2A	3450	1/1	0.84	0.21	80,80,80,80	0
56	ARG	1A	4012	12/12	0.84	0.17	48,62,68,73	0
54	MG	1a	1818	1/1	0.84	0.20	74,74,74,74	0
54	MG	1a	1679	1/1	0.84	0.29	62,62,62,62	0
54	MG	2a	1609	1/1	0.84	0.17	69,69,69,69	0
54	MG	2A	3498	1/1	0.84	0.16	31,31,31,31	0
58	ZN	24	501	1/1	0.84	0.20	159,159,159,159	0
54	MG	2a	1642	1/1	0.85	0.18	37,37,37,37	0
54	MG	2A	3207	1/1	0.85	0.18	50,50,50,50	0
54	MG	2A	3564	1/1	0.85	0.15	68,68,68,68	0
54	MG	2a	1651	1/1	0.85	0.30	69,69,69,69	0
54	MG	1A	3893	1/1	0.85	0.14	31,31,31,31	0
54	MG	1A	3061	1/1	0.85	0.22	56,56,56,56	0
54	MG	2A	3602	1/1	0.85	0.13	33,33,33,33	0
54	MG	1A	3571	1/1	0.85	0.13	52,52,52,52	0
54	MG	1A	3828	1/1	0.85	0.15	60,60,60,60	0
54	MG	2A	3290	1/1	0.85	0.12	59,59,59,59	0
54	MG	1a	1686	1/1	0.85	0.11	33,33,33,33	0
54	MG	2A	3313	1/1	0.85	0.11	38,38,38,38	0
54	MG	2A	3027	1/1	0.85	0.20	49,49,49,49	0
54	MG	1A	4003	1/1	0.85	0.13	59,59,59,59	0
54	MG	1A	3931	1/1	0.85	0.12	48,48,48,48	0
54	MG	1a	1795	1/1	0.85	0.14	59,59,59,59	0
54	MG	1A	3163	1/1	0.85	0.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1700	1/1	0.85	0.14	67,67,67,67	0
54	MG	2A	3402	1/1	0.85	0.28	66,66,66,66	0
54	MG	1A	3581	1/1	0.85	0.11	50,50,50,50	0
54	MG	2a	1730	1/1	0.85	0.12	54,54,54,54	0
54	MG	2A	3414	1/1	0.85	0.12	65,65,65,65	0
54	MG	1H	201	1/1	0.85	0.13	71,71,71,71	0
54	MG	1A	3658	1/1	0.85	0.13	22,22,22,22	0
54	MG	2B	201	1/1	0.85	0.11	73,73,73,73	0
54	MG	2B	205	1/1	0.85	0.10	50,50,50,50	0
54	MG	1A	3781	1/1	0.85	0.12	70,70,70,70	0
54	MG	1a	1651	1/1	0.85	0.17	51,51,51,51	0
54	MG	2a	1754	1/1	0.85	0.12	63,63,63,63	0
54	MG	1a	1866	1/1	0.85	0.08	51,51,51,51	0
54	MG	1a	1653	1/1	0.85	0.25	58,58,58,58	0
54	MG	1A	3711	1/1	0.85	0.19	47,47,47,47	0
54	MG	2I	201	1/1	0.85	0.11	72,72,72,72	0
54	MG	1a	1744	1/1	0.85	0.14	57,57,57,57	0
54	MG	1a	1752	1/1	0.85	0.12	67,67,67,67	0
54	MG	2A	3117	1/1	0.85	0.16	53,53,53,53	0
54	MG	1a	1657	1/1	0.85	0.21	61,61,61,61	0
54	MG	2A	3125	1/1	0.85	0.18	64,64,64,64	0
54	MG	1e	201	1/1	0.85	0.27	47,47,47,47	0
54	MG	2A	3175	1/1	0.85	0.16	50,50,50,50	0
54	MG	2a	1612	1/1	0.85	0.24	58,58,58,58	0
54	MG	1A	3963	1/1	0.85	0.13	53,53,53,53	0
54	MG	1a	1765	1/1	0.85	0.38	66,66,66,66	0
54	MG	1A	3976	1/1	0.85	0.13	54,54,54,54	0
54	MG	1A	3679	1/1	0.86	0.13	48,48,48,48	0
54	MG	2a	1623	1/1	0.86	0.29	64,64,64,64	0
54	MG	1A	3751	1/1	0.86	0.10	19,19,19,19	0
54	MG	2A	3587	1/1	0.86	0.12	43,43,43,43	0
54	MG	1a	1844	1/1	0.86	0.21	77,77,77,77	0
54	MG	2A	3594	1/1	0.86	0.21	56,56,56,56	0
54	MG	2A	3600	1/1	0.86	0.12	37,37,37,37	0
54	MG	1a	1740	1/1	0.86	0.17	49,49,49,49	0
54	MG	1A	3860	1/1	0.86	0.20	52,52,52,52	0
54	MG	2A	3608	1/1	0.86	0.15	37,37,37,37	0
54	MG	2a	1656	1/1	0.86	0.12	64,64,64,64	0
54	MG	1a	1746	1/1	0.86	0.10	57,57,57,57	0
54	MG	2A	3644	1/1	0.86	0.16	66,66,66,66	0
54	MG	2A	3089	1/1	0.86	0.19	62,62,62,62	0
54	MG	1A	3624	1/1	0.86	0.12	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3371	1/1	0.86	0.21	68,68,68,68	0
54	MG	2A	3373	1/1	0.86	0.18	42,42,42,42	0
54	MG	2A	3689	1/1	0.86	0.20	69,69,69,69	0
54	MG	2A	3695	1/1	0.86	0.12	54,54,54,54	0
54	MG	1A	3690	1/1	0.86	0.38	31,31,31,31	0
54	MG	1a	1756	1/1	0.86	0.18	68,68,68,68	0
54	MG	1A	3691	1/1	0.86	0.20	38,38,38,38	0
54	MG	2A	3098	1/1	0.86	0.12	57,57,57,57	0
54	MG	1a	1681	1/1	0.86	0.17	48,48,48,48	0
54	MG	1a	1623	1/1	0.86	0.15	50,50,50,50	0
54	MG	1A	3786	1/1	0.86	0.13	43,43,43,43	0
54	MG	1a	1689	1/1	0.86	0.18	58,58,58,58	0
54	MG	1A	3972	1/1	0.86	0.09	68,68,68,68	0
54	MG	2A	3139	1/1	0.86	0.16	69,69,69,69	0
54	MG	2A	3723	1/1	0.86	0.14	61,61,61,61	0
54	MG	1A	3506	1/1	0.86	0.18	41,41,41,41	0
54	MG	2a	1747	1/1	0.86	0.17	51,51,51,51	0
54	MG	2A	3167	1/1	0.86	0.11	93,93,93,93	0
54	MG	1A	3250	1/1	0.86	0.38	47,47,47,47	0
54	MG	2B	213	1/1	0.86	0.12	57,57,57,57	0
54	MG	1a	1704	1/1	0.86	0.19	65,65,65,65	0
54	MG	2A	3480	1/1	0.86	0.13	54,54,54,54	0
54	MG	2D	308	1/1	0.86	0.16	63,63,63,63	0
54	MG	1V	204	1/1	0.86	0.24	46,46,46,46	0
54	MG	1A	3058	1/1	0.86	0.09	57,57,57,57	0
54	MG	1A	3817	1/1	0.86	0.12	53,53,53,53	0
54	MG	2A	3504	1/1	0.86	0.19	53,53,53,53	0
54	MG	2A	3224	1/1	0.86	0.15	46,46,46,46	0
54	MG	2W	203	1/1	0.86	0.15	65,65,65,65	0
54	MG	1a	1804	1/1	0.86	0.22	65,65,65,65	0
57	MPD	1A	4013	8/8	0.86	0.30	48,54,61,62	0
54	MG	1D	318	1/1	0.86	0.10	61,61,61,61	0
54	MG	2A	3234	1/1	0.86	0.15	55,55,55,55	0
54	MG	2A	3235	1/1	0.86	0.26	51,51,51,51	0
54	MG	2A	3553	1/1	0.86	0.14	44,44,44,44	0
54	MG	1a	1659	1/1	0.86	0.20	64,64,64,64	0
54	MG	2A	3074	1/1	0.87	0.16	54,54,54,54	0
54	MG	1A	3694	1/1	0.87	0.13	46,46,46,46	0
54	MG	1A	3438	1/1	0.87	0.15	55,55,55,55	0
54	MG	13	102	1/1	0.87	0.12	35,35,35,35	0
54	MG	1a	1799	1/1	0.87	0.18	61,61,61,61	0
54	MG	15	104	1/1	0.87	0.34	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1803	1/1	0.87	0.11	72,72,72,72	0
54	MG	1A	3165	1/1	0.87	0.13	48,48,48,48	0
54	MG	1B	211	1/1	0.87	0.11	55,55,55,55	0
54	MG	26	101	1/1	0.87	0.14	57,57,57,57	0
54	MG	2A	3494	1/1	0.87	0.10	58,58,58,58	0
54	MG	1a	1696	1/1	0.87	0.19	47,47,47,47	0
54	MG	1A	3462	1/1	0.87	0.11	20,20,20,20	0
54	MG	2A	3500	1/1	0.87	0.15	58,58,58,58	0
54	MG	1a	1823	1/1	0.87	0.10	55,55,55,55	0
54	MG	1a	1828	1/1	0.87	0.17	71,71,71,71	0
54	MG	1A	3612	1/1	0.87	0.19	54,54,54,54	0
54	MG	1a	1836	1/1	0.87	0.08	65,65,65,65	0
54	MG	2a	1634	1/1	0.87	0.27	62,62,62,62	0
54	MG	2A	3122	1/1	0.87	0.23	42,42,42,42	0
54	MG	2a	1647	1/1	0.87	0.12	68,68,68,68	0
54	MG	1A	3746	1/1	0.87	0.16	49,49,49,49	0
54	MG	1a	1614	1/1	0.87	0.20	59,59,59,59	0
54	MG	2A	3529	1/1	0.87	0.12	84,84,84,84	0
54	MG	2A	3545	1/1	0.87	0.13	65,65,65,65	0
54	MG	2A	3550	1/1	0.87	0.18	40,40,40,40	0
54	MG	1a	1852	1/1	0.87	0.23	66,66,66,66	0
54	MG	2a	1662	1/1	0.87	0.21	53,53,53,53	0
54	MG	2a	1665	1/1	0.87	0.22	51,51,51,51	0
54	MG	1A	3469	1/1	0.87	0.11	26,26,26,26	0
54	MG	1A	3179	1/1	0.87	0.22	30,30,30,30	0
54	MG	2A	3565	1/1	0.87	0.11	36,36,36,36	0
54	MG	1a	1626	1/1	0.87	0.17	60,60,60,60	0
54	MG	1A	3289	1/1	0.87	0.16	69,69,69,69	0
54	MG	2a	1684	1/1	0.87	0.15	71,71,71,71	0
54	MG	2a	1685	1/1	0.87	0.17	58,58,58,58	0
54	MG	2A	3589	1/1	0.87	0.23	75,75,75,75	0
54	MG	1A	3769	1/1	0.87	0.12	50,50,50,50	0
54	MG	2a	1702	1/1	0.87	0.18	70,70,70,70	0
54	MG	1A	3780	1/1	0.87	0.11	48,48,48,48	0
54	MG	2A	3220	1/1	0.87	0.15	48,48,48,48	0
54	MG	1A	3295	1/1	0.87	0.26	52,52,52,52	0
54	MG	1A	3311	1/1	0.87	0.10	13,13,13,13	0
54	MG	1e	202	1/1	0.87	0.24	57,57,57,57	0
54	MG	2a	1725	1/1	0.87	0.18	58,58,58,58	0
54	MG	1f	201	1/1	0.87	0.20	63,63,63,63	0
54	MG	2A	3611	1/1	0.87	0.14	76,76,76,76	0
54	MG	2A	3640	1/1	0.87	0.13	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1748	1/1	0.87	0.15	68,68,68,68	0
54	MG	2A	3244	1/1	0.87	0.17	48,48,48,48	0
54	MG	2A	3250	1/1	0.87	0.26	54,54,54,54	0
54	MG	2A	3669	1/1	0.87	0.10	65,65,65,65	0
54	MG	1A	3056	1/1	0.87	0.12	37,37,37,37	0
54	MG	1a	1654	1/1	0.87	0.14	63,63,63,63	0
54	MG	2A	3265	1/1	0.87	0.22	54,54,54,54	0
54	MG	1A	3027	1/1	0.87	0.24	47,47,47,47	0
54	MG	2A	3292	1/1	0.87	0.10	48,48,48,48	0
54	MG	1A	3237	1/1	0.87	0.15	57,57,57,57	0
54	MG	2A	3298	1/1	0.87	0.27	61,61,61,61	0
54	MG	1G	204	1/1	0.87	0.07	51,51,51,51	0
54	MG	1a	1767	1/1	0.87	0.17	55,55,55,55	0
54	MG	2A	3024	1/1	0.87	0.30	65,65,65,65	0
54	MG	2a	1770	1/1	0.87	0.33	76,76,76,76	0
54	MG	1A	3034	1/1	0.87	0.14	47,47,47,47	0
54	MG	1A	3408	1/1	0.87	0.12	22,22,22,22	0
54	MG	2A	3035	1/1	0.87	0.20	44,44,44,44	0
54	MG	2j	201	1/1	0.87	0.12	68,68,68,68	0
54	MG	1A	3838	1/1	0.87	0.10	49,49,49,49	0
54	MG	2t	201	1/1	0.87	0.11	55,55,55,55	0
54	MG	2A	3374	1/1	0.87	0.13	32,32,32,32	0
54	MG	1A	3558	1/1	0.87	0.16	27,27,27,27	0
54	MG	1A	3564	1/1	0.87	0.14	47,47,47,47	0
54	MG	2A	3055	1/1	0.87	0.23	65,65,65,65	0
57	MPD	2A	3727	8/8	0.87	0.23	64,70,73,73	0
54	MG	1A	3431	1/1	0.87	0.10	44,44,44,44	0
54	MG	2A	3058	1/1	0.87	0.11	51,51,51,51	0
54	MG	1a	1789	1/1	0.87	0.10	61,61,61,61	0
54	MG	1a	1774	1/1	0.88	0.15	70,70,70,70	0
54	MG	2A	3215	1/1	0.88	0.32	65,65,65,65	0
54	MG	1A	3490	1/1	0.88	0.10	14,14,14,14	0
54	MG	2a	1614	1/1	0.88	0.13	55,55,55,55	0
54	MG	2A	3539	1/1	0.88	0.21	72,72,72,72	0
54	MG	1a	1778	1/1	0.88	0.09	76,76,76,76	0
54	MG	10	105	1/1	0.88	0.10	44,44,44,44	0
54	MG	1A	3701	1/1	0.88	0.17	36,36,36,36	0
54	MG	2A	3554	1/1	0.88	0.12	38,38,38,38	0
54	MG	2a	1638	1/1	0.88	0.21	52,52,52,52	0
54	MG	1A	3590	1/1	0.88	0.20	42,42,42,42	0
54	MG	1A	3724	1/1	0.88	0.30	46,46,46,46	0
54	MG	1A	3592	1/1	0.88	0.24	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3596	1/1	0.88	0.14	15,15,15,15	0
54	MG	2A	3573	1/1	0.88	0.14	53,53,53,53	0
54	MG	2A	3030	1/1	0.88	0.15	44,44,44,44	0
54	MG	1a	1690	1/1	0.88	0.10	58,58,58,58	0
54	MG	1A	3012	1/1	0.88	0.13	33,33,33,33	0
54	MG	2a	1661	1/1	0.88	0.08	66,66,66,66	0
54	MG	2A	3270	1/1	0.88	0.14	56,56,56,56	0
54	MG	2A	3282	1/1	0.88	0.18	55,55,55,55	0
54	MG	2a	1668	1/1	0.88	0.28	63,63,63,63	0
54	MG	2A	3040	1/1	0.88	0.16	54,54,54,54	0
54	MG	1A	3126	1/1	0.88	0.19	45,45,45,45	0
54	MG	1A	3395	1/1	0.88	0.09	57,57,57,57	0
54	MG	1B	230	1/1	0.88	0.10	42,42,42,42	0
54	MG	1a	1702	1/1	0.88	0.18	55,55,55,55	0
54	MG	1a	1813	1/1	0.88	0.12	66,66,66,66	0
54	MG	2A	3060	1/1	0.88	0.13	50,50,50,50	0
54	MG	1a	1814	1/1	0.88	0.09	57,57,57,57	0
54	MG	2A	3651	1/1	0.88	0.12	32,32,32,32	0
54	MG	2A	3344	1/1	0.88	0.27	47,47,47,47	0
54	MG	1A	3209	1/1	0.88	0.14	53,53,53,53	0
54	MG	2A	3370	1/1	0.88	0.14	50,50,50,50	0
54	MG	1A	3627	1/1	0.88	0.24	48,48,48,48	0
54	MG	1A	3102	1/1	0.88	0.32	37,37,37,37	0
54	MG	2A	3077	1/1	0.88	0.16	45,45,45,45	0
54	MG	1A	3532	1/1	0.88	0.13	42,42,42,42	0
54	MG	1a	1824	1/1	0.88	0.17	53,53,53,53	0
54	MG	2A	3399	1/1	0.88	0.13	49,49,49,49	0
54	MG	2A	3084	1/1	0.88	0.26	46,46,46,46	0
54	MG	2A	3407	1/1	0.88	0.19	70,70,70,70	0
54	MG	2a	1733	1/1	0.88	0.14	62,62,62,62	0
54	MG	1a	1639	1/1	0.88	0.23	81,81,81,81	0
54	MG	1A	3534	1/1	0.88	0.18	42,42,42,42	0
54	MG	1A	3953	1/1	0.88	0.13	53,53,53,53	0
54	MG	1a	1649	1/1	0.88	0.17	50,50,50,50	0
54	MG	2a	1746	1/1	0.88	0.22	47,47,47,47	0
54	MG	1A	3215	1/1	0.88	0.11	51,51,51,51	0
54	MG	2A	3437	1/1	0.88	0.14	57,57,57,57	0
54	MG	1A	3116	1/1	0.88	0.13	34,34,34,34	0
54	MG	1A	3967	1/1	0.88	0.13	28,28,28,28	0
54	MG	1a	1862	1/1	0.88	0.12	68,68,68,68	0
54	MG	1A	3321	1/1	0.88	0.16	48,48,48,48	0
54	MG	1A	3459	1/1	0.88	0.10	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3334	1/1	0.88	0.11	18,18,18,18	0
54	MG	2D	303	1/1	0.88	0.27	44,44,44,44	0
54	MG	1a	1869	1/1	0.88	0.21	81,81,81,81	0
54	MG	2A	3483	1/1	0.88	0.24	67,67,67,67	0
54	MG	2G	201	1/1	0.88	0.13	83,83,83,83	0
54	MG	2A	3131	1/1	0.88	0.17	44,44,44,44	0
54	MG	1a	1755	1/1	0.88	0.12	54,54,54,54	0
54	MG	1A	3824	1/1	0.88	0.12	57,57,57,57	0
54	MG	1A	3336	1/1	0.88	0.14	53,53,53,53	0
54	MG	1A	3576	1/1	0.88	0.18	65,65,65,65	0
54	MG	2A	3184	1/1	0.88	0.12	52,52,52,52	0
54	MG	2I	102	1/1	0.88	0.11	50,50,50,50	0
54	MG	25	101	1/1	0.88	0.43	44,44,44,44	0
54	MG	1a	1670	1/1	0.88	0.19	70,70,70,70	0
54	MG	1a	1772	1/1	0.88	0.12	68,68,68,68	0
54	MG	1A	3245	1/1	0.88	0.21	29,29,29,29	0
54	MG	2a	1608	1/1	0.88	0.12	63,63,63,63	0
54	MG	2B	203	1/1	0.89	0.30	72,72,72,72	0
54	MG	1A	3533	1/1	0.89	0.10	49,49,49,49	0
54	MG	1A	3191	1/1	0.89	0.12	49,49,49,49	0
54	MG	2A	3375	1/1	0.89	0.08	52,52,52,52	0
54	MG	2A	3377	1/1	0.89	0.12	45,45,45,45	0
54	MG	2B	216	1/1	0.89	0.11	77,77,77,77	0
54	MG	1A	3704	1/1	0.89	0.20	28,28,28,28	0
54	MG	1A	3705	1/1	0.89	0.21	56,56,56,56	0
54	MG	2D	306	1/1	0.89	0.19	48,48,48,48	0
54	MG	2A	3386	1/1	0.89	0.16	36,36,36,36	0
54	MG	2E	302	1/1	0.89	0.13	43,43,43,43	0
54	MG	2A	3390	1/1	0.89	0.10	56,56,56,56	0
54	MG	2A	3062	1/1	0.89	0.14	48,48,48,48	0
54	MG	2A	3067	1/1	0.89	0.35	43,43,43,43	0
54	MG	2A	3068	1/1	0.89	0.19	45,45,45,45	0
54	MG	1A	3862	1/1	0.89	0.23	38,38,38,38	0
54	MG	1A	3707	1/1	0.89	0.19	32,32,32,32	0
54	MG	1B	229	1/1	0.89	0.16	63,63,63,63	0
54	MG	2A	3417	1/1	0.89	0.21	53,53,53,53	0
54	MG	2A	3425	1/1	0.89	0.10	51,51,51,51	0
54	MG	1A	3868	1/1	0.89	0.12	51,51,51,51	0
54	MG	1A	3125	1/1	0.89	0.18	47,47,47,47	0
54	MG	2A	3436	1/1	0.89	0.12	50,50,50,50	0
54	MG	1a	1662	1/1	0.89	0.14	58,58,58,58	0
54	MG	1A	3721	1/1	0.89	0.13	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1665	1/1	0.89	0.22	58,58,58,58	0
54	MG	1A	3544	1/1	0.89	0.20	36,36,36,36	0
54	MG	1A	3621	1/1	0.89	0.17	50,50,50,50	0
54	MG	1A	3911	1/1	0.89	0.22	60,60,60,60	0
54	MG	2A	3094	1/1	0.89	0.12	58,58,58,58	0
54	MG	2a	1617	1/1	0.89	0.17	52,52,52,52	0
54	MG	2A	3469	1/1	0.89	0.19	51,51,51,51	0
54	MG	2a	1624	1/1	0.89	0.19	72,72,72,72	0
54	MG	1A	3343	1/1	0.89	0.11	39,39,39,39	0
54	MG	1A	3916	1/1	0.89	0.15	45,45,45,45	0
54	MG	2a	1631	1/1	0.89	0.19	53,53,53,53	0
54	MG	1A	3167	1/1	0.89	0.11	32,32,32,32	0
54	MG	2A	3496	1/1	0.89	0.24	63,63,63,63	0
54	MG	1A	3742	1/1	0.89	0.10	22,22,22,22	0
54	MG	2A	3113	1/1	0.89	0.09	56,56,56,56	0
54	MG	1A	3745	1/1	0.89	0.14	44,44,44,44	0
54	MG	1A	3279	1/1	0.89	0.12	40,40,40,40	0
54	MG	2A	3503	1/1	0.89	0.43	50,50,50,50	0
54	MG	1H	202	1/1	0.89	0.08	46,46,46,46	0
54	MG	1A	3384	1/1	0.89	0.18	54,54,54,54	0
54	MG	1a	1837	1/1	0.89	0.11	65,65,65,65	0
54	MG	2a	1657	1/1	0.89	0.29	64,64,64,64	0
54	MG	1A	3569	1/1	0.89	0.14	22,22,22,22	0
54	MG	1T	202	1/1	0.89	0.10	45,45,45,45	0
54	MG	2A	3514	1/1	0.89	0.09	59,59,59,59	0
54	MG	1A	3570	1/1	0.89	0.14	28,28,28,28	0
54	MG	2A	3520	1/1	0.89	0.11	57,57,57,57	0
54	MG	2A	3521	1/1	0.89	0.11	38,38,38,38	0
54	MG	1a	1701	1/1	0.89	0.14	59,59,59,59	0
54	MG	2A	3532	1/1	0.89	0.10	60,60,60,60	0
54	MG	2a	1677	1/1	0.89	0.31	60,60,60,60	0
54	MG	2a	1681	1/1	0.89	0.26	50,50,50,50	0
54	MG	1A	3761	1/1	0.89	0.18	53,53,53,53	0
54	MG	1a	1864	1/1	0.89	0.19	56,56,56,56	0
54	MG	2A	3193	1/1	0.89	0.14	49,49,49,49	0
54	MG	1A	3956	1/1	0.89	0.15	43,43,43,43	0
54	MG	2a	1691	1/1	0.89	0.40	74,74,74,74	0
54	MG	2a	1692	1/1	0.89	0.14	90,90,90,90	0
54	MG	1A	3284	1/1	0.89	0.29	30,30,30,30	0
54	MG	10	104	1/1	0.89	0.12	39,39,39,39	0
54	MG	1A	3050	1/1	0.89	0.49	33,33,33,33	0
54	MG	10	106	1/1	0.89	0.39	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3965	1/1	0.89	0.39	44,44,44,44	0
54	MG	1A	3671	1/1	0.89	0.28	53,53,53,53	0
54	MG	1A	3968	1/1	0.89	0.19	34,34,34,34	0
54	MG	1A	3236	1/1	0.89	0.11	59,59,59,59	0
54	MG	2A	3228	1/1	0.89	0.20	57,57,57,57	0
54	MG	2A	3593	1/1	0.89	0.10	36,36,36,36	0
54	MG	1e	203	1/1	0.89	0.19	46,46,46,46	0
54	MG	1a	1602	1/1	0.89	0.17	62,62,62,62	0
54	MG	2A	3238	1/1	0.89	0.09	45,45,45,45	0
54	MG	2A	3242	1/1	0.89	0.13	56,56,56,56	0
54	MG	1A	3975	1/1	0.89	0.13	63,63,63,63	0
54	MG	2A	3609	1/1	0.89	0.10	42,42,42,42	0
54	MG	2a	1740	1/1	0.89	0.12	73,73,73,73	0
54	MG	1a	1747	1/1	0.89	0.14	60,60,60,60	0
54	MG	1a	1604	1/1	0.89	0.30	64,64,64,64	0
54	MG	2A	3256	1/1	0.89	0.21	42,42,42,42	0
54	MG	1i	201	1/1	0.89	0.14	49,49,49,49	0
54	MG	2A	3263	1/1	0.89	0.15	43,43,43,43	0
54	MG	1n	101	1/1	0.89	0.27	61,61,61,61	0
54	MG	2a	1755	1/1	0.89	0.14	67,67,67,67	0
54	MG	2a	1757	1/1	0.89	0.22	59,59,59,59	0
54	MG	2A	3655	1/1	0.89	0.10	25,25,25,25	0
54	MG	2A	3266	1/1	0.89	0.17	49,49,49,49	0
54	MG	1a	1751	1/1	0.89	0.11	76,76,76,76	0
54	MG	1A	3187	1/1	0.89	0.11	57,57,57,57	0
54	MG	1A	3686	1/1	0.89	0.54	32,32,32,32	0
54	MG	1y	204	1/1	0.89	0.13	69,69,69,69	0
54	MG	2A	3690	1/1	0.89	0.10	49,49,49,49	0
54	MG	1A	3803	1/1	0.89	0.18	58,58,58,58	0
54	MG	1A	3806	1/1	0.89	0.10	44,44,44,44	0
54	MG	2f	201	1/1	0.89	0.12	58,58,58,58	0
54	MG	2A	3308	1/1	0.89	0.11	35,35,35,35	0
54	MG	1A	3588	1/1	0.89	0.24	51,51,51,51	0
54	MG	2A	3318	1/1	0.89	0.10	52,52,52,52	0
54	MG	1A	4002	1/1	0.89	0.11	52,52,52,52	0
54	MG	1A	3809	1/1	0.89	0.11	50,50,50,50	0
54	MG	1a	1771	1/1	0.89	0.12	62,62,62,62	0
54	MG	1A	3315	1/1	0.89	0.16	21,21,21,21	0
54	MG	2A	3349	1/1	0.89	0.10	67,67,67,67	0
54	MG	1A	4009	1/1	0.89	0.20	59,59,59,59	0
54	MG	1A	3105	1/1	0.89	0.11	29,29,29,29	0
54	MG	1A	3827	1/1	0.89	0.12	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3299	1/1	0.90	0.12	49,49,49,49	0
54	MG	1A	3819	1/1	0.90	0.22	52,52,52,52	0
54	MG	2A	3709	1/1	0.90	0.11	57,57,57,57	0
54	MG	2A	3712	1/1	0.90	0.21	50,50,50,50	0
54	MG	10	108	1/1	0.90	0.09	40,40,40,40	0
54	MG	1A	3610	1/1	0.90	0.09	46,46,46,46	0
54	MG	1A	3994	1/1	0.90	0.10	60,60,60,60	0
54	MG	2A	3003	1/1	0.90	0.15	54,54,54,54	0
54	MG	2A	3007	1/1	0.90	0.10	56,56,56,56	0
54	MG	13	104	1/1	0.90	0.28	38,38,38,38	0
54	MG	1A	3337	1/1	0.90	0.09	43,43,43,43	0
54	MG	2B	202	1/1	0.90	0.20	49,49,49,49	0
54	MG	2A	3352	1/1	0.90	0.08	57,57,57,57	0
54	MG	1A	3997	1/1	0.90	0.12	47,47,47,47	0
54	MG	2A	3028	1/1	0.90	0.35	49,49,49,49	0
54	MG	18	101	1/1	0.90	0.33	35,35,35,35	0
54	MG	2A	3372	1/1	0.90	0.12	32,32,32,32	0
54	MG	1A	4000	1/1	0.90	0.10	35,35,35,35	0
54	MG	1A	3112	1/1	0.90	0.17	44,44,44,44	0
54	MG	1A	3709	1/1	0.90	0.25	44,44,44,44	0
54	MG	1A	3421	1/1	0.90	0.12	37,37,37,37	0
54	MG	1A	3841	1/1	0.90	0.07	31,31,31,31	0
54	MG	2A	3054	1/1	0.90	0.27	54,54,54,54	0
54	MG	2E	303	1/1	0.90	0.33	41,41,41,41	0
54	MG	1a	1759	1/1	0.90	0.12	59,59,59,59	0
54	MG	2A	3388	1/1	0.90	0.08	47,47,47,47	0
54	MG	1a	1761	1/1	0.90	0.12	64,64,64,64	0
54	MG	2A	3057	1/1	0.90	0.16	55,55,55,55	0
54	MG	1A	4008	1/1	0.90	0.08	48,48,48,48	0
54	MG	2P	201	1/1	0.90	0.14	49,49,49,49	0
54	MG	2T	203	1/1	0.90	0.10	63,63,63,63	0
54	MG	1a	1613	1/1	0.90	0.13	19,19,19,19	0
54	MG	1A	3552	1/1	0.90	0.09	60,60,60,60	0
54	MG	2A	3063	1/1	0.90	0.13	52,52,52,52	0
54	MG	2A	3065	1/1	0.90	0.10	40,40,40,40	0
54	MG	1a	1615	1/1	0.90	0.09	49,49,49,49	0
54	MG	1A	3494	1/1	0.90	0.14	53,53,53,53	0
54	MG	2A	3070	1/1	0.90	0.30	42,42,42,42	0
54	MG	1A	3429	1/1	0.90	0.08	49,49,49,49	0
54	MG	2a	1604	1/1	0.90	0.18	60,60,60,60	0
54	MG	1A	3639	1/1	0.90	0.17	69,69,69,69	0
54	MG	1A	3875	1/1	0.90	0.13	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1633	1/1	0.90	0.13	68,68,68,68	0
54	MG	1B	214	1/1	0.90	0.10	66,66,66,66	0
54	MG	2A	3445	1/1	0.90	0.10	54,54,54,54	0
54	MG	2A	3447	1/1	0.90	0.08	56,56,56,56	0
54	MG	1A	3738	1/1	0.90	0.09	32,32,32,32	0
54	MG	2a	1622	1/1	0.90	0.15	66,66,66,66	0
54	MG	1A	3641	1/1	0.90	0.10	56,56,56,56	0
54	MG	1a	1643	1/1	0.90	0.18	56,56,56,56	0
54	MG	2A	3086	1/1	0.90	0.26	52,52,52,52	0
54	MG	2A	3463	1/1	0.90	0.12	30,30,30,30	0
54	MG	1A	3643	1/1	0.90	0.11	54,54,54,54	0
54	MG	2A	3471	1/1	0.90	0.09	54,54,54,54	0
54	MG	2A	3472	1/1	0.90	0.10	56,56,56,56	0
54	MG	1a	1790	1/1	0.90	0.17	53,53,53,53	0
54	MG	2a	1644	1/1	0.90	0.20	68,68,68,68	0
54	MG	2a	1646	1/1	0.90	0.12	59,59,59,59	0
54	MG	1A	3079	1/1	0.90	0.38	33,33,33,33	0
54	MG	1A	3898	1/1	0.90	0.10	51,51,51,51	0
54	MG	1A	3910	1/1	0.90	0.10	45,45,45,45	0
54	MG	1a	1798	1/1	0.90	0.10	62,62,62,62	0
54	MG	1A	3509	1/1	0.90	0.11	22,22,22,22	0
54	MG	1A	3316	1/1	0.90	0.09	34,34,34,34	0
54	MG	1A	3662	1/1	0.90	0.14	55,55,55,55	0
54	MG	1a	1658	1/1	0.90	0.15	56,56,56,56	0
54	MG	1A	3755	1/1	0.90	0.21	29,29,29,29	0
54	MG	2A	3505	1/1	0.90	0.13	57,57,57,57	0
54	MG	1F	303	1/1	0.90	0.19	27,27,27,27	0
54	MG	1a	1816	1/1	0.90	0.09	61,61,61,61	0
54	MG	1F	304	1/1	0.90	0.31	44,44,44,44	0
54	MG	2A	3511	1/1	0.90	0.10	51,51,51,51	0
54	MG	1A	3513	1/1	0.90	0.13	43,43,43,43	0
54	MG	1F	313	1/1	0.90	0.10	37,37,37,37	0
54	MG	2A	3143	1/1	0.90	0.10	35,35,35,35	0
54	MG	2A	3518	1/1	0.90	0.09	39,39,39,39	0
54	MG	2A	3158	1/1	0.90	0.10	52,52,52,52	0
54	MG	1a	1667	1/1	0.90	0.17	44,44,44,44	0
54	MG	2A	3524	1/1	0.90	0.14	28,28,28,28	0
54	MG	2A	3526	1/1	0.90	0.14	54,54,54,54	0
54	MG	1A	3760	1/1	0.90	0.14	53,53,53,53	0
54	MG	1a	1672	1/1	0.90	0.26	57,57,57,57	0
54	MG	2A	3176	1/1	0.90	0.22	49,49,49,49	0
54	MG	2A	3540	1/1	0.90	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	1705	1/1	0.90	0.11	59,59,59,59	0
54	MG	1a	1830	1/1	0.90	0.15	74,74,74,74	0
54	MG	2A	3546	1/1	0.90	0.09	66,66,66,66	0
54	MG	2A	3188	1/1	0.90	0.12	55,55,55,55	0
54	MG	1A	3439	1/1	0.90	0.09	51,51,51,51	0
54	MG	1F	316	1/1	0.90	0.17	48,48,48,48	0
54	MG	1A	3518	1/1	0.90	0.14	34,34,34,34	0
54	MG	2A	3558	1/1	0.90	0.13	47,47,47,47	0
54	MG	1A	3940	1/1	0.90	0.18	68,68,68,68	0
54	MG	1A	3771	1/1	0.90	0.13	48,48,48,48	0
54	MG	1a	1848	1/1	0.90	0.12	50,50,50,50	0
54	MG	1A	3454	1/1	0.90	0.12	33,33,33,33	0
54	MG	2A	3581	1/1	0.90	0.10	61,61,61,61	0
54	MG	1A	3586	1/1	0.90	0.26	27,27,27,27	0
54	MG	1A	3133	1/1	0.90	0.39	35,35,35,35	0
54	MG	1P	204	1/1	0.90	0.29	29,29,29,29	0
54	MG	1A	3790	1/1	0.90	0.11	58,58,58,58	0
54	MG	1a	1694	1/1	0.90	0.19	68,68,68,68	0
54	MG	1A	3181	1/1	0.90	0.10	55,55,55,55	0
54	MG	1A	3108	1/1	0.90	0.51	48,48,48,48	0
54	MG	2A	3239	1/1	0.90	0.10	54,54,54,54	0
54	MG	1a	1698	1/1	0.90	0.22	60,60,60,60	0
54	MG	1a	1699	1/1	0.90	0.10	46,46,46,46	0
54	MG	1U	203	1/1	0.90	0.13	46,46,46,46	0
54	MG	2A	3251	1/1	0.90	0.24	46,46,46,46	0
54	MG	2A	3621	1/1	0.90	0.09	61,61,61,61	0
54	MG	2A	3638	1/1	0.90	0.21	60,60,60,60	0
54	MG	1A	3540	1/1	0.90	0.09	40,40,40,40	0
54	MG	2a	1766	1/1	0.90	0.15	60,60,60,60	0
54	MG	1V	206	1/1	0.90	0.10	47,47,47,47	0
54	MG	1W	204	1/1	0.90	0.11	58,58,58,58	0
54	MG	1a	1705	1/1	0.90	0.10	59,59,59,59	0
54	MG	1a	1706	1/1	0.90	0.13	45,45,45,45	0
54	MG	1A	3541	1/1	0.90	0.09	45,45,45,45	0
54	MG	2A	3659	1/1	0.90	0.11	64,64,64,64	0
54	MG	1A	3698	1/1	0.90	0.12	24,24,24,24	0
54	MG	2A	3670	1/1	0.90	0.13	43,43,43,43	0
54	MG	2r	101	1/1	0.90	0.12	67,67,67,67	0
54	MG	2A	3277	1/1	0.90	0.10	43,43,43,43	0
54	MG	1a	1720	1/1	0.90	0.12	73,73,73,73	0
54	MG	2A	3283	1/1	0.90	0.27	48,48,48,48	0
54	MG	1A	3700	1/1	0.90	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3291	1/1	0.90	0.12	39,39,39,39	0
54	MG	1A	3609	1/1	0.90	0.15	28,28,28,28	0
54	MG	1q	201	1/1	0.90	0.20	51,51,51,51	0
54	MG	1t	202	1/1	0.90	0.09	56,56,56,56	0
54	MG	2A	3705	1/1	0.90	0.11	69,69,69,69	0
54	MG	1A	3545	1/1	0.91	0.09	16,16,16,16	0
54	MG	2B	204	1/1	0.91	0.11	47,47,47,47	0
54	MG	1A	3763	1/1	0.91	0.09	34,34,34,34	0
54	MG	1A	3287	1/1	0.91	0.15	65,65,65,65	0
54	MG	1A	3141	1/1	0.91	0.10	50,50,50,50	0
54	MG	2A	3426	1/1	0.91	0.10	50,50,50,50	0
54	MG	2A	3427	1/1	0.91	0.11	49,49,49,49	0
54	MG	1P	206	1/1	0.91	0.12	73,73,73,73	0
54	MG	1a	1822	1/1	0.91	0.10	59,59,59,59	0
54	MG	1A	3471	1/1	0.91	0.13	34,34,34,34	0
54	MG	2D	307	1/1	0.91	0.11	35,35,35,35	0
54	MG	1R	204	1/1	0.91	0.14	33,33,33,33	0
54	MG	1a	1684	1/1	0.91	0.12	63,63,63,63	0
54	MG	1A	3477	1/1	0.91	0.07	34,34,34,34	0
54	MG	1A	3782	1/1	0.91	0.20	27,27,27,27	0
54	MG	2E	306	1/1	0.91	0.11	27,27,27,27	0
54	MG	2A	3446	1/1	0.91	0.09	72,72,72,72	0
54	MG	1a	1688	1/1	0.91	0.31	68,68,68,68	0
54	MG	1A	3180	1/1	0.91	0.22	40,40,40,40	0
54	MG	1A	3300	1/1	0.91	0.09	30,30,30,30	0
54	MG	2A	3453	1/1	0.91	0.09	52,52,52,52	0
54	MG	2P	203	1/1	0.91	0.20	60,60,60,60	0
54	MG	1a	1691	1/1	0.91	0.19	60,60,60,60	0
54	MG	1V	205	1/1	0.91	0.11	48,48,48,48	0
54	MG	2W	202	1/1	0.91	0.23	51,51,51,51	0
54	MG	2A	3145	1/1	0.91	0.19	47,47,47,47	0
54	MG	2A	3151	1/1	0.91	0.09	60,60,60,60	0
54	MG	1a	1693	1/1	0.91	0.13	53,53,53,53	0
54	MG	1A	3974	1/1	0.91	0.19	55,55,55,55	0
54	MG	2A	3473	1/1	0.91	0.09	52,52,52,52	0
54	MG	2A	3478	1/1	0.91	0.12	45,45,45,45	0
54	MG	1A	3492	1/1	0.91	0.07	40,40,40,40	0
54	MG	2A	3168	1/1	0.91	0.15	45,45,45,45	0
54	MG	1A	3797	1/1	0.91	0.11	18,18,18,18	0
54	MG	1A	3985	1/1	0.91	0.08	29,29,29,29	0
54	MG	1A	3393	1/1	0.91	0.11	18,18,18,18	0
54	MG	1A	3681	1/1	0.91	0.19	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3191	1/1	0.91	0.22	56,56,56,56	0
54	MG	1A	3683	1/1	0.91	0.15	24,24,24,24	0
54	MG	1A	3685	1/1	0.91	0.27	49,49,49,49	0
54	MG	2a	1618	1/1	0.91	0.12	49,49,49,49	0
54	MG	1d	302	1/1	0.91	0.13	60,60,60,60	0
54	MG	2A	3202	1/1	0.91	0.14	54,54,54,54	0
54	MG	1A	3497	1/1	0.91	0.08	31,31,31,31	0
54	MG	1l	105	1/1	0.91	0.12	39,39,39,39	0
54	MG	2a	1627	1/1	0.91	0.10	46,46,46,46	0
54	MG	2A	3208	1/1	0.91	0.17	52,52,52,52	0
54	MG	1A	3147	1/1	0.91	0.11	40,40,40,40	0
54	MG	1a	1710	1/1	0.91	0.12	53,53,53,53	0
54	MG	1A	3580	1/1	0.91	0.14	39,39,39,39	0
54	MG	2a	1639	1/1	0.91	0.14	73,73,73,73	0
54	MG	2a	1641	1/1	0.91	0.12	47,47,47,47	0
54	MG	2A	3516	1/1	0.91	0.10	62,62,62,62	0
54	MG	1A	3820	1/1	0.91	0.13	23,23,23,23	0
54	MG	1A	3159	1/1	0.91	0.23	27,27,27,27	0
54	MG	1A	3131	1/1	0.91	0.17	36,36,36,36	0
54	MG	2a	1648	1/1	0.91	0.10	41,41,41,41	0
54	MG	1A	3047	1/1	0.91	0.13	37,37,37,37	0
54	MG	1A	3193	1/1	0.91	0.14	36,36,36,36	0
54	MG	2A	3236	1/1	0.91	0.16	50,50,50,50	0
54	MG	1A	3591	1/1	0.91	0.11	53,53,53,53	0
54	MG	1n	102	1/1	0.91	0.11	66,66,66,66	0
54	MG	2a	1655	1/1	0.91	0.08	61,61,61,61	0
54	MG	2A	3536	1/1	0.91	0.30	41,41,41,41	0
54	MG	1A	3195	1/1	0.91	0.07	29,29,29,29	0
54	MG	1A	3843	1/1	0.91	0.09	62,62,62,62	0
54	MG	2A	3245	1/1	0.91	0.14	50,50,50,50	0
54	MG	2a	1663	1/1	0.91	0.19	57,57,57,57	0
54	MG	1a	1609	1/1	0.91	0.19	64,64,64,64	0
54	MG	1a	1611	1/1	0.91	0.11	46,46,46,46	0
54	MG	2a	1670	1/1	0.91	0.14	61,61,61,61	0
54	MG	2A	3551	1/1	0.91	0.12	27,27,27,27	0
54	MG	1y	202	1/1	0.91	0.11	64,64,64,64	0
54	MG	1A	3515	1/1	0.91	0.13	39,39,39,39	0
54	MG	2a	1675	1/1	0.91	0.23	52,52,52,52	0
54	MG	1A	3600	1/1	0.91	0.11	52,52,52,52	0
54	MG	1A	3708	1/1	0.91	0.11	37,37,37,37	0
54	MG	2a	1680	1/1	0.91	0.19	55,55,55,55	0
54	MG	2A	3562	1/1	0.91	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1B	218	1/1	0.91	0.12	51,51,51,51	0
54	MG	2A	3004	1/1	0.91	0.22	54,54,54,54	0
54	MG	2A	3267	1/1	0.91	0.09	38,38,38,38	0
54	MG	1A	3139	1/1	0.91	0.12	47,47,47,47	0
54	MG	2a	1689	1/1	0.91	0.18	48,48,48,48	0
54	MG	2A	3579	1/1	0.91	0.10	59,59,59,59	0
54	MG	2A	3275	1/1	0.91	0.19	41,41,41,41	0
54	MG	1a	1618	1/1	0.91	0.19	58,58,58,58	0
54	MG	2A	3025	1/1	0.91	0.12	53,53,53,53	0
54	MG	1a	1621	1/1	0.91	0.17	60,60,60,60	0
54	MG	2a	1706	1/1	0.91	0.13	54,54,54,54	0
54	MG	1B	225	1/1	0.91	0.12	42,42,42,42	0
54	MG	1A	3519	1/1	0.91	0.11	25,25,25,25	0
54	MG	1A	3716	1/1	0.91	0.08	48,48,48,48	0
54	MG	2A	3293	1/1	0.91	0.19	52,52,52,52	0
54	MG	1A	3340	1/1	0.91	0.15	25,25,25,25	0
54	MG	1a	1638	1/1	0.91	0.11	60,60,60,60	0
54	MG	1a	1769	1/1	0.91	0.11	69,69,69,69	0
54	MG	2A	3301	1/1	0.91	0.14	49,49,49,49	0
54	MG	1A	3528	1/1	0.91	0.08	30,30,30,30	0
54	MG	2A	3614	1/1	0.91	0.12	83,83,83,83	0
54	MG	1A	3531	1/1	0.91	0.21	46,46,46,46	0
54	MG	2A	3053	1/1	0.91	0.16	44,44,44,44	0
54	MG	2A	3639	1/1	0.91	0.09	46,46,46,46	0
54	MG	1D	313	1/1	0.91	0.11	32,32,32,32	0
54	MG	1A	3620	1/1	0.91	0.17	57,57,57,57	0
54	MG	2A	3342	1/1	0.91	0.12	40,40,40,40	0
54	MG	1a	1648	1/1	0.91	0.08	39,39,39,39	0
54	MG	1D	316	1/1	0.91	0.11	44,44,44,44	0
54	MG	2a	1748	1/1	0.91	0.09	66,66,66,66	0
54	MG	1a	1780	1/1	0.91	0.10	71,71,71,71	0
54	MG	1a	1782	1/1	0.91	0.19	69,69,69,69	0
54	MG	2A	3355	1/1	0.91	0.09	58,58,58,58	0
54	MG	1A	3440	1/1	0.91	0.13	40,40,40,40	0
54	MG	2A	3358	1/1	0.91	0.15	48,48,48,48	0
54	MG	2A	3361	1/1	0.91	0.17	52,52,52,52	0
54	MG	2A	3683	1/1	0.91	0.10	47,47,47,47	0
54	MG	2A	3684	1/1	0.91	0.26	73,73,73,73	0
54	MG	2a	1764	1/1	0.91	0.09	61,61,61,61	0
54	MG	1A	3623	1/1	0.91	0.09	46,46,46,46	0
54	MG	1A	3445	1/1	0.91	0.12	57,57,57,57	0
54	MG	1A	3448	1/1	0.91	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3635	1/1	0.91	0.09	18,18,18,18	0
54	MG	2A	3069	1/1	0.91	0.28	45,45,45,45	0
54	MG	1A	3449	1/1	0.91	0.10	31,31,31,31	0
54	MG	2e	201	1/1	0.91	0.19	55,55,55,55	0
54	MG	1a	1791	1/1	0.91	0.19	60,60,60,60	0
54	MG	1A	3211	1/1	0.91	0.12	51,51,51,51	0
54	MG	2A	3380	1/1	0.91	0.13	53,53,53,53	0
54	MG	2A	3383	1/1	0.91	0.10	32,32,32,32	0
54	MG	1A	3932	1/1	0.91	0.09	66,66,66,66	0
54	MG	1a	1660	1/1	0.91	0.13	62,62,62,62	0
54	MG	1A	3351	1/1	0.91	0.13	40,40,40,40	0
54	MG	1A	3353	1/1	0.91	0.15	60,60,60,60	0
54	MG	2A	3395	1/1	0.91	0.10	33,33,33,33	0
57	MPD	1a	1870	8/8	0.91	0.15	55,64,73,74	0
54	MG	1G	201	1/1	0.91	0.13	65,65,65,65	0
54	MG	1A	3759	1/1	0.91	0.10	41,41,41,41	0
54	MG	2A	3724	1/1	0.91	0.13	53,53,53,53	0
54	MG	1a	1666	1/1	0.91	0.11	51,51,51,51	0
54	MG	1A	3644	1/1	0.91	0.10	36,36,36,36	0
54	MG	1A	3258	1/1	0.92	0.06	43,43,43,43	0
54	MG	2A	3701	1/1	0.92	0.11	44,44,44,44	0
54	MG	1A	3846	1/1	0.92	0.41	34,34,34,34	0
54	MG	1A	3848	1/1	0.92	0.25	50,50,50,50	0
54	MG	1A	3268	1/1	0.92	0.35	42,42,42,42	0
54	MG	1B	220	1/1	0.92	0.09	30,30,30,30	0
54	MG	2A	3367	1/1	0.92	0.12	56,56,56,56	0
54	MG	2A	3369	1/1	0.92	0.14	26,26,26,26	0
54	MG	1a	1776	1/1	0.92	0.18	67,67,67,67	0
54	MG	1A	3717	1/1	0.92	0.07	54,54,54,54	0
54	MG	1A	3031	1/1	0.92	0.13	22,22,22,22	0
54	MG	1A	3460	1/1	0.92	0.10	28,28,28,28	0
54	MG	1A	3630	1/1	0.92	0.28	54,54,54,54	0
54	MG	1A	3347	1/1	0.92	0.09	35,35,35,35	0
54	MG	1A	3879	1/1	0.92	0.14	29,29,29,29	0
54	MG	1A	3196	1/1	0.92	0.14	47,47,47,47	0
54	MG	1A	3885	1/1	0.92	0.10	18,18,18,18	0
54	MG	2A	3382	1/1	0.92	0.08	36,36,36,36	0
54	MG	1a	1788	1/1	0.92	0.12	59,59,59,59	0
54	MG	1A	3886	1/1	0.92	0.17	36,36,36,36	0
54	MG	2B	206	1/1	0.92	0.12	38,38,38,38	0
54	MG	1A	3197	1/1	0.92	0.09	40,40,40,40	0
54	MG	2B	210	1/1	0.92	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	1A	3890	1/1	0.92	0.34	38,38,38,38	0
54	MG	1E	305	1/1	0.92	0.17	49,49,49,49	0
54	MG	1E	308	1/1	0.92	0.08	27,27,27,27	0
54	MG	2A	3398	1/1	0.92	0.13	44,44,44,44	0
54	MG	1A	3640	1/1	0.92	0.09	55,55,55,55	0
54	MG	2D	304	1/1	0.92	0.18	42,42,42,42	0
54	MG	1A	3897	1/1	0.92	0.25	59,59,59,59	0
54	MG	2A	3405	1/1	0.92	0.09	54,54,54,54	0
54	MG	1A	3281	1/1	0.92	0.10	47,47,47,47	0
54	MG	1F	309	1/1	0.92	0.18	41,41,41,41	0
54	MG	1A	3483	1/1	0.92	0.08	16,16,16,16	0
54	MG	2E	304	1/1	0.92	0.20	37,37,37,37	0
54	MG	1A	3199	1/1	0.92	0.26	56,56,56,56	0
54	MG	1a	1805	1/1	0.92	0.13	63,63,63,63	0
54	MG	1A	3651	1/1	0.92	0.08	51,51,51,51	0
54	MG	2G	202	1/1	0.92	0.20	67,67,67,67	0
54	MG	2A	3111	1/1	0.92	0.13	61,61,61,61	0
54	MG	1A	3915	1/1	0.92	0.08	31,31,31,31	0
54	MG	2A	3431	1/1	0.92	0.10	57,57,57,57	0
54	MG	1a	1669	1/1	0.92	0.22	52,52,52,52	0
54	MG	1A	3652	1/1	0.92	0.17	45,45,45,45	0
54	MG	1a	1671	1/1	0.92	0.11	48,48,48,48	0
54	MG	2A	3119	1/1	0.92	0.13	41,41,41,41	0
54	MG	2V	202	1/1	0.92	0.23	46,46,46,46	0
54	MG	1A	3489	1/1	0.92	0.09	18,18,18,18	0
54	MG	2A	3442	1/1	0.92	0.09	75,75,75,75	0
54	MG	2A	3443	1/1	0.92	0.09	59,59,59,59	0
54	MG	1A	3567	1/1	0.92	0.15	68,68,68,68	0
54	MG	2A	3124	1/1	0.92	0.15	43,43,43,43	0
54	MG	1A	3367	1/1	0.92	0.09	20,20,20,20	0
54	MG	2A	3127	1/1	0.92	0.22	35,35,35,35	0
54	MG	28	101	1/1	0.92	0.13	46,46,46,46	0
54	MG	1A	3033	1/1	0.92	0.31	48,48,48,48	0
54	MG	2a	1602	1/1	0.92	0.17	51,51,51,51	0
54	MG	1a	1825	1/1	0.92	0.16	49,49,49,49	0
54	MG	2a	1607	1/1	0.92	0.21	53,53,53,53	0
54	MG	2A	3141	1/1	0.92	0.11	53,53,53,53	0
54	MG	2A	3457	1/1	0.92	0.11	55,55,55,55	0
54	MG	1a	1678	1/1	0.92	0.12	59,59,59,59	0
54	MG	1A	3055	1/1	0.92	0.28	30,30,30,30	0
54	MG	1A	3391	1/1	0.92	0.12	26,26,26,26	0
54	MG	2A	3467	1/1	0.92	0.12	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	2A	3157	1/1	0.92	0.07	35,35,35,35	0
54	MG	1A	3669	1/1	0.92	0.30	29,29,29,29	0
54	MG	2A	3165	1/1	0.92	0.19	55,55,55,55	0
54	MG	1O	201	1/1	0.92	0.08	40,40,40,40	0
54	MG	2A	3475	1/1	0.92	0.18	68,68,68,68	0
54	MG	1O	202	1/1	0.92	0.18	41,41,41,41	0
54	MG	1a	1845	1/1	0.92	0.08	43,43,43,43	0
54	MG	2A	3169	1/1	0.92	0.06	48,48,48,48	0
54	MG	2A	3484	1/1	0.92	0.09	55,55,55,55	0
54	MG	2a	1633	1/1	0.92	0.14	54,54,54,54	0
54	MG	2A	3491	1/1	0.92	0.09	47,47,47,47	0
54	MG	2a	1636	1/1	0.92	0.16	73,73,73,73	0
54	MG	2A	3492	1/1	0.92	0.09	55,55,55,55	0
54	MG	2A	3493	1/1	0.92	0.26	50,50,50,50	0
54	MG	2a	1640	1/1	0.92	0.13	61,61,61,61	0
54	MG	1A	3773	1/1	0.92	0.22	54,54,54,54	0
54	MG	1A	3776	1/1	0.92	0.27	45,45,45,45	0
54	MG	2A	3178	1/1	0.92	0.10	45,45,45,45	0
54	MG	1a	1850	1/1	0.92	0.12	51,51,51,51	0
54	MG	2A	3186	1/1	0.92	0.11	58,58,58,58	0
54	MG	2A	3187	1/1	0.92	0.68	41,41,41,41	0
54	MG	1A	3778	1/1	0.92	0.11	46,46,46,46	0
54	MG	1a	1854	1/1	0.92	0.18	86,86,86,86	0
54	MG	1a	1855	1/1	0.92	0.12	55,55,55,55	0
54	MG	2A	3195	1/1	0.92	0.18	42,42,42,42	0
54	MG	1a	1857	1/1	0.92	0.12	88,88,88,88	0
54	MG	2A	3199	1/1	0.92	0.09	46,46,46,46	0
54	MG	1A	3150	1/1	0.92	0.07	41,41,41,41	0
54	MG	1A	3183	1/1	0.92	0.35	57,57,57,57	0
54	MG	1A	3961	1/1	0.92	0.18	36,36,36,36	0
54	MG	1A	3962	1/1	0.92	0.08	58,58,58,58	0
54	MG	1A	3675	1/1	0.92	0.21	32,32,32,32	0
54	MG	2A	3212	1/1	0.92	0.08	43,43,43,43	0
54	MG	2A	3213	1/1	0.92	0.13	56,56,56,56	0
54	MG	1A	3302	1/1	0.92	0.16	46,46,46,46	0
54	MG	1a	1697	1/1	0.92	0.42	71,71,71,71	0
54	MG	2A	3223	1/1	0.92	0.08	44,44,44,44	0
54	MG	2A	3527	1/1	0.92	0.15	81,81,81,81	0
54	MG	1A	3583	1/1	0.92	0.19	35,35,35,35	0
54	MG	2A	3530	1/1	0.92	0.08	59,59,59,59	0
54	MG	1A	3792	1/1	0.92	0.21	30,30,30,30	0
54	MG	2a	1678	1/1	0.92	0.17	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3535	1/1	0.92	0.11	79,79,79,79	0
54	MG	1A	3307	1/1	0.92	0.14	33,33,33,33	0
54	MG	1A	3511	1/1	0.92	0.10	44,44,44,44	0
54	MG	2a	1683	1/1	0.92	0.23	49,49,49,49	0
54	MG	2A	3233	1/1	0.92	0.10	57,57,57,57	0
54	MG	1A	3414	1/1	0.92	0.17	47,47,47,47	0
54	MG	1A	3801	1/1	0.92	0.15	38,38,38,38	0
54	MG	1A	3977	1/1	0.92	0.18	57,57,57,57	0
54	MG	2a	1690	1/1	0.92	0.21	40,40,40,40	0
54	MG	2A	3237	1/1	0.92	0.09	45,45,45,45	0
54	MG	1A	3983	1/1	0.92	0.26	33,33,33,33	0
54	MG	2a	1694	1/1	0.92	0.10	49,49,49,49	0
54	MG	1a	1709	1/1	0.92	0.10	48,48,48,48	0
54	MG	2a	1696	1/1	0.92	0.14	48,48,48,48	0
54	MG	1A	3802	1/1	0.92	0.23	43,43,43,43	0
54	MG	2a	1704	1/1	0.92	0.12	60,60,60,60	0
54	MG	11	102	1/1	0.92	0.19	45,45,45,45	0
54	MG	1A	3986	1/1	0.92	0.09	21,21,21,21	0
54	MG	1a	1719	1/1	0.92	0.13	45,45,45,45	0
54	MG	1A	3130	1/1	0.92	0.09	31,31,31,31	0
54	MG	2A	3566	1/1	0.92	0.12	63,63,63,63	0
54	MG	2A	3569	1/1	0.92	0.09	55,55,55,55	0
54	MG	1o	101	1/1	0.92	0.07	41,41,41,41	0
54	MG	2a	1717	1/1	0.92	0.18	71,71,71,71	0
54	MG	2a	1722	1/1	0.92	0.11	64,64,64,64	0
54	MG	2a	1724	1/1	0.92	0.09	58,58,58,58	0
54	MG	1A	3804	1/1	0.92	0.09	44,44,44,44	0
54	MG	2A	3575	1/1	0.92	0.08	32,32,32,32	0
54	MG	1A	3313	1/1	0.92	0.10	33,33,33,33	0
54	MG	1t	201	1/1	0.92	0.10	52,52,52,52	0
54	MG	1A	3161	1/1	0.92	0.16	50,50,50,50	0
54	MG	1a	1731	1/1	0.92	0.08	45,45,45,45	0
54	MG	2a	1734	1/1	0.92	0.14	71,71,71,71	0
54	MG	1A	3996	1/1	0.92	0.17	49,49,49,49	0
54	MG	2A	3269	1/1	0.92	0.10	36,36,36,36	0
54	MG	1A	3692	1/1	0.92	0.09	21,21,21,21	0
54	MG	1A	3241	1/1	0.92	0.51	28,28,28,28	0
54	MG	1a	1741	1/1	0.92	0.10	45,45,45,45	0
54	MG	2A	3278	1/1	0.92	0.19	45,45,45,45	0
54	MG	2A	3607	1/1	0.92	0.13	45,45,45,45	0
54	MG	2A	3002	1/1	0.92	0.24	62,62,62,62	0
54	MG	1A	3604	1/1	0.92	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3286	1/1	0.92	0.10	33,33,33,33	0
54	MG	1a	1606	1/1	0.92	0.10	49,49,49,49	0
54	MG	2A	3612	1/1	0.92	0.10	63,63,63,63	0
54	MG	1A	3320	1/1	0.92	0.20	41,41,41,41	0
54	MG	2A	3618	1/1	0.92	0.31	49,49,49,49	0
54	MG	2A	3619	1/1	0.92	0.09	79,79,79,79	0
54	MG	2a	1761	1/1	0.92	0.15	59,59,59,59	0
54	MG	2A	3023	1/1	0.92	0.24	44,44,44,44	0
54	MG	2A	3631	1/1	0.92	0.09	80,80,80,80	0
54	MG	1A	3527	1/1	0.92	0.19	32,32,32,32	0
54	MG	1a	1750	1/1	0.92	0.09	50,50,50,50	0
54	MG	2A	3296	1/1	0.92	0.09	47,47,47,47	0
54	MG	2A	3297	1/1	0.92	0.13	51,51,51,51	0
54	MG	1A	4006	1/1	0.92	0.15	44,44,44,44	0
54	MG	1a	1610	1/1	0.92	0.09	49,49,49,49	0
54	MG	1A	3028	1/1	0.92	0.32	31,31,31,31	0
54	MG	1A	3328	1/1	0.92	0.12	57,57,57,57	0
54	MG	2A	3034	1/1	0.92	0.19	53,53,53,53	0
54	MG	1A	3831	1/1	0.92	0.09	61,61,61,61	0
54	MG	1a	1758	1/1	0.92	0.09	66,66,66,66	0
54	MG	1A	4010	1/1	0.92	0.12	51,51,51,51	0
54	MG	2A	3336	1/1	0.92	0.07	43,43,43,43	0
54	MG	2A	3337	1/1	0.92	0.12	46,46,46,46	0
54	MG	2A	3341	1/1	0.92	0.07	30,30,30,30	0
54	MG	1B	202	1/1	0.92	0.11	50,50,50,50	0
54	MG	1A	3616	1/1	0.92	0.13	48,48,48,48	0
54	MG	2A	3693	1/1	0.92	0.13	60,60,60,60	0
54	MG	1A	3094	1/1	0.92	0.45	28,28,28,28	0
54	MG	1A	3256	1/1	0.92	0.36	30,30,30,30	0
54	MG	2A	3698	1/1	0.92	0.15	61,61,61,61	0
54	MG	2A	3699	1/1	0.92	0.14	43,43,43,43	0
54	MG	15	103	1/1	0.93	0.25	38,38,38,38	0
54	MG	2A	3721	1/1	0.93	0.09	53,53,53,53	0
54	MG	2A	3411	1/1	0.93	0.08	44,44,44,44	0
54	MG	1A	3157	1/1	0.93	0.30	31,31,31,31	0
54	MG	1A	3348	1/1	0.93	0.12	49,49,49,49	0
54	MG	2A	3148	1/1	0.93	0.09	48,48,48,48	0
54	MG	2A	3421	1/1	0.93	0.23	38,38,38,38	0
54	MG	1A	3349	1/1	0.93	0.09	28,28,28,28	0
54	MG	1A	3010	1/1	0.93	0.07	24,24,24,24	0
54	MG	1A	3650	1/1	0.93	0.09	57,57,57,57	0
54	MG	2A	3164	1/1	0.93	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1708	1/1	0.93	0.08	50,50,50,50	0
54	MG	1a	1860	1/1	0.93	0.09	57,57,57,57	0
54	MG	1A	3160	1/1	0.93	0.15	30,30,30,30	0
54	MG	1B	216	1/1	0.93	0.13	57,57,57,57	0
54	MG	1a	1865	1/1	0.93	0.08	51,51,51,51	0
54	MG	2A	3174	1/1	0.93	0.14	46,46,46,46	0
54	MG	1A	3555	1/1	0.93	0.10	26,26,26,26	0
54	MG	1A	3654	1/1	0.93	0.07	75,75,75,75	0
54	MG	1A	3478	1/1	0.93	0.13	50,50,50,50	0
54	MG	2A	3179	1/1	0.93	0.13	38,38,38,38	0
54	MG	1A	3762	1/1	0.93	0.18	34,34,34,34	0
54	MG	2A	3448	1/1	0.93	0.19	66,66,66,66	0
54	MG	2A	3185	1/1	0.93	0.13	58,58,58,58	0
54	MG	1a	1721	1/1	0.93	0.07	46,46,46,46	0
54	MG	2A	3451	1/1	0.93	0.13	56,56,56,56	0
54	MG	1d	301	1/1	0.93	0.12	59,59,59,59	0
54	MG	2F	302	1/1	0.93	0.12	34,34,34,34	0
54	MG	2A	3454	1/1	0.93	0.14	56,56,56,56	0
54	MG	1A	3909	1/1	0.93	0.20	34,34,34,34	0
54	MG	1A	3562	1/1	0.93	0.16	45,45,45,45	0
54	MG	1A	3563	1/1	0.93	0.06	25,25,25,25	0
54	MG	1a	1727	1/1	0.93	0.10	56,56,56,56	0
54	MG	2A	3196	1/1	0.93	0.09	39,39,39,39	0
54	MG	2A	3197	1/1	0.93	0.13	38,38,38,38	0
54	MG	2Q	202	1/1	0.93	0.10	59,59,59,59	0
54	MG	1A	3083	1/1	0.93	0.20	35,35,35,35	0
54	MG	2T	204	1/1	0.93	0.11	52,52,52,52	0
54	MG	1A	3088	1/1	0.93	0.15	49,49,49,49	0
54	MG	1A	3203	1/1	0.93	0.09	34,34,34,34	0
54	MG	1a	1735	1/1	0.93	0.11	73,73,73,73	0
54	MG	1a	1736	1/1	0.93	0.15	43,43,43,43	0
54	MG	1A	3923	1/1	0.93	0.10	34,34,34,34	0
54	MG	1a	1619	1/1	0.93	0.08	70,70,70,70	0
54	MG	2I	103	1/1	0.93	0.08	73,73,73,73	0
54	MG	2A	3211	1/1	0.93	0.17	45,45,45,45	0
54	MG	2A	3486	1/1	0.93	0.14	72,72,72,72	0
54	MG	2A	3487	1/1	0.93	0.16	49,49,49,49	0
54	MG	2A	3489	1/1	0.93	0.08	58,58,58,58	0
54	MG	1I	3101	1/1	0.93	0.13	43,43,43,43	0
54	MG	1m	201	1/1	0.93	0.06	65,65,65,65	0
54	MG	2a	1603	1/1	0.93	0.08	43,43,43,43	0
54	MG	1a	1620	1/1	0.93	0.07	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	1606	1/1	0.93	0.15	67,67,67,67	0
54	MG	1A	3372	1/1	0.93	0.08	29,29,29,29	0
54	MG	1A	3670	1/1	0.93	0.11	48,48,48,48	0
54	MG	1A	3491	1/1	0.93	0.10	39,39,39,39	0
54	MG	1a	1627	1/1	0.93	0.14	54,54,54,54	0
54	MG	1a	1629	1/1	0.93	0.13	59,59,59,59	0
54	MG	2A	3501	1/1	0.93	0.12	22,22,22,22	0
54	MG	1A	3375	1/1	0.93	0.11	12,12,12,12	0
54	MG	1A	3673	1/1	0.93	0.17	34,34,34,34	0
54	MG	1a	1754	1/1	0.93	0.16	49,49,49,49	0
54	MG	1A	3286	1/1	0.93	0.16	54,54,54,54	0
54	MG	1A	3938	1/1	0.93	0.10	36,36,36,36	0
54	MG	1A	3204	1/1	0.93	0.22	34,34,34,34	0
54	MG	2A	3508	1/1	0.93	0.08	51,51,51,51	0
54	MG	1F	306	1/1	0.93	0.08	31,31,31,31	0
54	MG	2a	1629	1/1	0.93	0.10	65,65,65,65	0
54	MG	1A	3501	1/1	0.93	0.11	49,49,49,49	0
54	MG	1a	1762	1/1	0.93	0.11	58,58,58,58	0
54	MG	1a	1644	1/1	0.93	0.13	62,62,62,62	0
54	MG	2A	3013	1/1	0.93	0.19	52,52,52,52	0
54	MG	2a	1635	1/1	0.93	0.14	73,73,73,73	0
54	MG	2A	3246	1/1	0.93	0.08	45,45,45,45	0
54	MG	2A	3249	1/1	0.93	0.14	48,48,48,48	0
54	MG	2A	3017	1/1	0.93	0.10	65,65,65,65	0
54	MG	2A	3019	1/1	0.93	0.63	50,50,50,50	0
54	MG	2A	3252	1/1	0.93	0.09	49,49,49,49	0
54	MG	2A	3253	1/1	0.93	0.19	53,53,53,53	0
54	MG	1A	3129	1/1	0.93	0.06	60,60,60,60	0
54	MG	2A	3528	1/1	0.93	0.07	58,58,58,58	0
54	MG	1A	3948	1/1	0.93	0.16	42,42,42,42	0
54	MG	1a	1768	1/1	0.93	0.11	45,45,45,45	0
54	MG	1A	3003	1/1	0.93	0.09	23,23,23,23	0
54	MG	2A	3264	1/1	0.93	0.14	53,53,53,53	0
54	MG	1A	3213	1/1	0.93	0.44	26,26,26,26	0
54	MG	2A	3538	1/1	0.93	0.10	56,56,56,56	0
54	MG	1A	3401	1/1	0.93	0.12	42,42,42,42	0
54	MG	1A	3172	1/1	0.93	0.13	43,43,43,43	0
54	MG	1a	1655	1/1	0.93	0.11	69,69,69,69	0
54	MG	1A	3177	1/1	0.93	0.20	27,27,27,27	0
54	MG	2a	1659	1/1	0.93	0.14	70,70,70,70	0
54	MG	2A	3547	1/1	0.93	0.08	54,54,54,54	0
54	MG	2A	3548	1/1	0.93	0.09	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3216	1/1	0.93	0.09	36,36,36,36	0
54	MG	1A	3219	1/1	0.93	0.08	40,40,40,40	0
54	MG	2a	1666	1/1	0.93	0.18	64,64,64,64	0
54	MG	2A	3552	1/1	0.93	0.10	69,69,69,69	0
54	MG	2a	1669	1/1	0.93	0.17	56,56,56,56	0
54	MG	2A	3042	1/1	0.93	0.20	41,41,41,41	0
54	MG	2a	1671	1/1	0.93	0.23	43,43,43,43	0
54	MG	1A	3695	1/1	0.93	0.11	24,24,24,24	0
54	MG	2A	3049	1/1	0.93	0.08	55,55,55,55	0
54	MG	1A	3516	1/1	0.93	0.07	20,20,20,20	0
54	MG	2A	3560	1/1	0.93	0.17	69,69,69,69	0
54	MG	1N	202	1/1	0.93	0.20	38,38,38,38	0
54	MG	1A	3970	1/1	0.93	0.08	33,33,33,33	0
54	MG	1A	3059	1/1	0.93	0.20	21,21,21,21	0
54	MG	1a	1664	1/1	0.93	0.11	50,50,50,50	0
54	MG	2A	3294	1/1	0.93	0.07	31,31,31,31	0
54	MG	1A	3060	1/1	0.93	0.09	49,49,49,49	0
54	MG	1A	3433	1/1	0.93	0.15	57,57,57,57	0
54	MG	1A	3826	1/1	0.93	0.27	33,33,33,33	0
54	MG	1A	3523	1/1	0.93	0.21	35,35,35,35	0
54	MG	1A	3613	1/1	0.93	0.29	22,22,22,22	0
54	MG	1S	201	1/1	0.93	0.23	49,49,49,49	0
54	MG	2A	3304	1/1	0.93	0.15	46,46,46,46	0
54	MG	1T	201	1/1	0.93	0.11	47,47,47,47	0
54	MG	2A	3311	1/1	0.93	0.08	46,46,46,46	0
54	MG	2a	1693	1/1	0.93	0.08	75,75,75,75	0
54	MG	1A	3829	1/1	0.93	0.17	32,32,32,32	0
54	MG	1A	3524	1/1	0.93	0.17	33,33,33,33	0
54	MG	2A	3319	1/1	0.93	0.09	32,32,32,32	0
54	MG	2A	3603	1/1	0.93	0.09	48,48,48,48	0
54	MG	1T	205	1/1	0.93	0.17	39,39,39,39	0
54	MG	2A	3606	1/1	0.93	0.13	79,79,79,79	0
54	MG	1a	1802	1/1	0.93	0.14	80,80,80,80	0
54	MG	1a	1676	1/1	0.93	0.10	40,40,40,40	0
54	MG	1A	3134	1/1	0.93	0.20	28,28,28,28	0
54	MG	2A	3339	1/1	0.93	0.13	56,56,56,56	0
54	MG	1A	3242	1/1	0.93	0.11	36,36,36,36	0
54	MG	1a	1811	1/1	0.93	0.11	93,93,93,93	0
54	MG	2A	3078	1/1	0.93	0.11	38,38,38,38	0
54	MG	2A	3079	1/1	0.93	0.33	47,47,47,47	0
54	MG	2A	3345	1/1	0.93	0.08	39,39,39,39	0
54	MG	1a	1812	1/1	0.93	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3630	1/1	0.93	0.07	68,68,68,68	0
54	MG	1A	3015	1/1	0.93	0.16	28,28,28,28	0
54	MG	2A	3353	1/1	0.93	0.12	31,31,31,31	0
54	MG	1a	1682	1/1	0.93	0.17	58,58,58,58	0
54	MG	1a	1683	1/1	0.93	0.10	56,56,56,56	0
54	MG	2A	3643	1/1	0.93	0.17	65,65,65,65	0
54	MG	1A	3110	1/1	0.93	0.20	32,32,32,32	0
54	MG	2A	3648	1/1	0.93	0.08	44,44,44,44	0
54	MG	2A	3359	1/1	0.93	0.07	21,21,21,21	0
54	MG	1W	201	1/1	0.93	0.09	22,22,22,22	0
54	MG	2A	3363	1/1	0.93	0.12	57,57,57,57	0
54	MG	2A	3364	1/1	0.93	0.08	61,61,61,61	0
54	MG	2A	3091	1/1	0.93	0.09	36,36,36,36	0
54	MG	1A	3072	1/1	0.93	0.47	33,33,33,33	0
54	MG	1A	3025	1/1	0.93	0.24	38,38,38,38	0
54	MG	2A	3672	1/1	0.93	0.10	66,66,66,66	0
54	MG	1A	3998	1/1	0.93	0.09	44,44,44,44	0
54	MG	1A	3850	1/1	0.93	0.08	29,29,29,29	0
54	MG	2A	3678	1/1	0.93	0.14	81,81,81,81	0
54	MG	2A	3679	1/1	0.93	0.10	43,43,43,43	0
54	MG	2a	1759	1/1	0.93	0.08	61,61,61,61	0
54	MG	2A	3682	1/1	0.93	0.14	60,60,60,60	0
54	MG	1A	3855	1/1	0.93	0.12	71,71,71,71	0
54	MG	2A	3100	1/1	0.93	0.18	31,31,31,31	0
54	MG	2A	3103	1/1	0.93	0.06	42,42,42,42	0
54	MG	1A	3857	1/1	0.93	0.11	43,43,43,43	0
54	MG	2A	3691	1/1	0.93	0.17	52,52,52,52	0
54	MG	2A	3692	1/1	0.93	0.11	75,75,75,75	0
54	MG	1a	1829	1/1	0.93	0.10	66,66,66,66	0
54	MG	1A	3538	1/1	0.93	0.17	42,42,42,42	0
54	MG	2a	1773	1/1	0.93	0.11	57,57,57,57	0
54	MG	2a	1774	1/1	0.93	0.15	62,62,62,62	0
54	MG	1A	3633	1/1	0.93	0.09	13,13,13,13	0
54	MG	1a	1833	1/1	0.93	0.12	61,61,61,61	0
54	MG	1a	1834	1/1	0.93	0.21	53,53,53,53	0
54	MG	1a	1835	1/1	0.93	0.10	44,44,44,44	0
54	MG	1A	3259	1/1	0.93	0.11	50,50,50,50	0
54	MG	2A	3123	1/1	0.93	0.11	36,36,36,36	0
54	MG	1A	3341	1/1	0.93	0.08	11,11,11,11	0
54	MG	1A	3869	1/1	0.93	0.10	49,49,49,49	0
54	MG	1A	3266	1/1	0.93	0.14	38,38,38,38	0
54	MG	15	102	1/1	0.93	0.31	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3711	1/1	0.93	0.25	67,67,67,67	0
57	MPD	18	102	8/8	0.93	0.14	21,29,33,34	0
54	MG	2A	3132	1/1	0.93	0.15	56,56,56,56	0
54	MG	2A	3715	1/1	0.93	0.18	54,54,54,54	0
54	MG	2A	3406	1/1	0.93	0.32	39,39,39,39	0
54	MG	2A	3717	1/1	0.93	0.13	43,43,43,43	0
54	MG	1a	1847	1/1	0.93	0.08	51,51,51,51	0
58	ZN	2Y	202	1/1	0.93	0.11	136,136,136,136	0
54	MG	2A	3408	1/1	0.93	0.17	49,49,49,49	0
54	MG	2B	209	1/1	0.94	0.08	37,37,37,37	0
54	MG	1A	3364	1/1	0.94	0.06	18,18,18,18	0
54	MG	1A	3723	1/1	0.94	0.09	18,18,18,18	0
54	MG	1A	3901	1/1	0.94	0.22	50,50,50,50	0
54	MG	2A	3189	1/1	0.94	0.08	42,42,42,42	0
54	MG	1A	3907	1/1	0.94	0.08	39,39,39,39	0
54	MG	1A	3603	1/1	0.94	0.12	40,40,40,40	0
54	MG	2A	3194	1/1	0.94	0.15	49,49,49,49	0
54	MG	1A	3143	1/1	0.94	0.19	14,14,14,14	0
54	MG	2A	3460	1/1	0.94	0.12	42,42,42,42	0
54	MG	2A	3461	1/1	0.94	0.08	48,48,48,48	0
54	MG	1A	3732	1/1	0.94	0.14	42,42,42,42	0
54	MG	1A	3275	1/1	0.94	0.09	24,24,24,24	0
54	MG	1P	202	1/1	0.94	0.16	23,23,23,23	0
54	MG	1A	3914	1/1	0.94	0.09	45,45,45,45	0
54	MG	1P	205	1/1	0.94	0.10	38,38,38,38	0
54	MG	1A	3737	1/1	0.94	0.09	55,55,55,55	0
54	MG	1A	3099	1/1	0.94	0.13	52,52,52,52	0
54	MG	1Q	202	1/1	0.94	0.12	34,34,34,34	0
54	MG	1Q	206	1/1	0.94	0.09	33,33,33,33	0
54	MG	2A	3209	1/1	0.94	0.10	46,46,46,46	0
54	MG	2A	3210	1/1	0.94	0.09	49,49,49,49	0
54	MG	1A	3919	1/1	0.94	0.12	48,48,48,48	0
54	MG	1g	201	1/1	0.94	0.16	49,49,49,49	0
54	MG	1A	3739	1/1	0.94	0.09	27,27,27,27	0
54	MG	1A	3101	1/1	0.94	0.25	36,36,36,36	0
54	MG	1A	3152	1/1	0.94	0.18	35,35,35,35	0
54	MG	1A	3744	1/1	0.94	0.08	27,27,27,27	0
54	MG	1A	3200	1/1	0.94	0.13	26,26,26,26	0
54	MG	1A	3002	1/1	0.94	0.11	44,44,44,44	0
54	MG	1U	206	1/1	0.94	0.19	41,41,41,41	0
54	MG	1A	3288	1/1	0.94	0.17	45,45,45,45	0
54	MG	20	101	1/1	0.94	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3230	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	3619	1/1	0.94	0.21	28,28,28,28	0
54	MG	1A	3021	1/1	0.94	0.20	32,32,32,32	0
54	MG	1A	3290	1/1	0.94	0.09	29,29,29,29	0
54	MG	1A	3944	1/1	0.94	0.12	52,52,52,52	0
54	MG	1A	3037	1/1	0.94	0.13	37,37,37,37	0
54	MG	1a	1730	1/1	0.94	0.09	67,67,67,67	0
54	MG	1A	3409	1/1	0.94	0.10	32,32,32,32	0
54	MG	1A	3951	1/1	0.94	0.10	41,41,41,41	0
54	MG	1A	3410	1/1	0.94	0.15	44,44,44,44	0
54	MG	1A	3955	1/1	0.94	0.18	53,53,53,53	0
54	MG	10	107	1/1	0.94	0.09	49,49,49,49	0
54	MG	2A	3247	1/1	0.94	0.09	45,45,45,45	0
54	MG	1A	3629	1/1	0.94	0.14	56,56,56,56	0
54	MG	1A	3038	1/1	0.94	0.20	42,42,42,42	0
54	MG	11	101	1/1	0.94	0.26	43,43,43,43	0
54	MG	1A	3960	1/1	0.94	0.09	65,65,65,65	0
54	MG	1A	3042	1/1	0.94	0.05	30,30,30,30	0
54	MG	2A	3020	1/1	0.94	0.40	43,43,43,43	0
54	MG	1A	3770	1/1	0.94	0.08	82,82,82,82	0
54	MG	13	103	1/1	0.94	0.12	54,54,54,54	0
54	MG	2A	3261	1/1	0.94	0.15	46,46,46,46	0
54	MG	1A	3423	1/1	0.94	0.14	63,63,63,63	0
54	MG	1A	3964	1/1	0.94	0.08	23,23,23,23	0
54	MG	2A	3531	1/1	0.94	0.10	52,52,52,52	0
54	MG	1A	3425	1/1	0.94	0.10	32,32,32,32	0
54	MG	1A	3774	1/1	0.94	0.09	40,40,40,40	0
54	MG	1A	3775	1/1	0.94	0.11	41,41,41,41	0
54	MG	2A	3032	1/1	0.94	0.15	21,21,21,21	0
54	MG	2A	3033	1/1	0.94	0.05	34,34,34,34	0
54	MG	1A	3303	1/1	0.94	0.10	26,26,26,26	0
54	MG	19	102	1/1	0.94	0.09	62,62,62,62	0
54	MG	2A	3036	1/1	0.94	0.12	43,43,43,43	0
54	MG	2A	3279	1/1	0.94	0.17	60,60,60,60	0
54	MG	1A	3064	1/1	0.94	0.12	40,40,40,40	0
54	MG	1a	1760	1/1	0.94	0.14	42,42,42,42	0
54	MG	2A	3041	1/1	0.94	0.12	57,57,57,57	0
54	MG	1A	3071	1/1	0.94	0.46	30,30,30,30	0
54	MG	1A	3043	1/1	0.94	0.14	7,7,7,7	0
54	MG	1A	3314	1/1	0.94	0.14	37,37,37,37	0
54	MG	1A	3645	1/1	0.94	0.14	39,39,39,39	0
54	MG	1a	1766	1/1	0.94	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3646	1/1	0.94	0.28	32,32,32,32	0
54	MG	1A	3649	1/1	0.94	0.11	46,46,46,46	0
54	MG	1A	3795	1/1	0.94	0.38	30,30,30,30	0
54	MG	1A	3073	1/1	0.94	0.08	36,36,36,36	0
54	MG	1A	3442	1/1	0.94	0.07	40,40,40,40	0
54	MG	1A	3992	1/1	0.94	0.10	62,62,62,62	0
54	MG	1A	3228	1/1	0.94	0.43	32,32,32,32	0
54	MG	1a	1775	1/1	0.94	0.09	66,66,66,66	0
54	MG	2a	1660	1/1	0.94	0.19	58,58,58,58	0
54	MG	2A	3064	1/1	0.94	0.07	33,33,33,33	0
54	MG	2A	3578	1/1	0.94	0.08	38,38,38,38	0
54	MG	1A	3800	1/1	0.94	0.08	20,20,20,20	0
54	MG	2a	1664	1/1	0.94	0.21	38,38,38,38	0
54	MG	1A	3230	1/1	0.94	0.77	34,34,34,34	0
54	MG	2A	3585	1/1	0.94	0.12	51,51,51,51	0
54	MG	1A	3178	1/1	0.94	0.25	29,29,29,29	0
54	MG	2A	3320	1/1	0.94	0.09	32,32,32,32	0
54	MG	1A	3550	1/1	0.94	0.14	45,45,45,45	0
54	MG	1A	3551	1/1	0.94	0.07	55,55,55,55	0
54	MG	1A	3326	1/1	0.94	0.06	19,19,19,19	0
54	MG	1A	3022	1/1	0.94	0.14	31,31,31,31	0
54	MG	1a	1624	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3340	1/1	0.94	0.07	28,28,28,28	0
54	MG	1A	3238	1/1	0.94	0.28	34,34,34,34	0
54	MG	1A	4005	1/1	0.94	0.12	45,45,45,45	0
54	MG	1A	3816	1/1	0.94	0.10	38,38,38,38	0
54	MG	1A	3240	1/1	0.94	0.08	26,26,26,26	0
54	MG	1A	3559	1/1	0.94	0.22	42,42,42,42	0
54	MG	2A	3347	1/1	0.94	0.06	53,53,53,53	0
54	MG	1a	1634	1/1	0.94	0.12	48,48,48,48	0
54	MG	1a	1793	1/1	0.94	0.09	40,40,40,40	0
54	MG	1A	3030	1/1	0.94	0.12	22,22,22,22	0
54	MG	2A	3087	1/1	0.94	0.12	38,38,38,38	0
54	MG	2A	3356	1/1	0.94	0.11	58,58,58,58	0
54	MG	1A	3822	1/1	0.94	0.17	32,32,32,32	0
54	MG	2A	3625	1/1	0.94	0.09	43,43,43,43	0
54	MG	2A	3627	1/1	0.94	0.11	75,75,75,75	0
54	MG	1A	3823	1/1	0.94	0.10	46,46,46,46	0
54	MG	1A	3464	1/1	0.94	0.09	54,54,54,54	0
54	MG	2A	3092	1/1	0.94	0.25	44,44,44,44	0
54	MG	1A	3468	1/1	0.94	0.09	69,69,69,69	0
54	MG	2a	1698	1/1	0.94	0.24	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1B	206	1/1	0.94	0.08	45,45,45,45	0
54	MG	2A	3641	1/1	0.94	0.08	54,54,54,54	0
54	MG	1B	209	1/1	0.94	0.27	50,50,50,50	0
54	MG	2A	3368	1/1	0.94	0.10	27,27,27,27	0
54	MG	1A	3566	1/1	0.94	0.17	52,52,52,52	0
54	MG	1A	3677	1/1	0.94	0.27	51,51,51,51	0
54	MG	2a	1710	1/1	0.94	0.11	56,56,56,56	0
54	MG	1a	1806	1/1	0.94	0.09	41,41,41,41	0
54	MG	2a	1713	1/1	0.94	0.10	67,67,67,67	0
54	MG	2A	3652	1/1	0.94	0.10	22,22,22,22	0
54	MG	2A	3653	1/1	0.94	0.10	44,44,44,44	0
54	MG	1A	3052	1/1	0.94	0.34	34,34,34,34	0
54	MG	2a	1721	1/1	0.94	0.06	57,57,57,57	0
54	MG	2A	3657	1/1	0.94	0.12	59,59,59,59	0
54	MG	1A	3680	1/1	0.94	0.09	38,38,38,38	0
54	MG	1A	3835	1/1	0.94	0.09	33,33,33,33	0
54	MG	2A	3664	1/1	0.94	0.10	70,70,70,70	0
54	MG	1A	3568	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3376	1/1	0.94	0.10	29,29,29,29	0
54	MG	1B	219	1/1	0.94	0.09	37,37,37,37	0
54	MG	1A	3839	1/1	0.94	0.11	44,44,44,44	0
54	MG	1A	3243	1/1	0.94	0.27	35,35,35,35	0
54	MG	2A	3381	1/1	0.94	0.17	62,62,62,62	0
54	MG	2a	1736	1/1	0.94	0.12	77,77,77,77	0
54	MG	1A	3472	1/1	0.94	0.19	46,46,46,46	0
54	MG	1A	3182	1/1	0.94	0.08	37,37,37,37	0
54	MG	1A	3844	1/1	0.94	0.07	26,26,26,26	0
54	MG	2a	1741	1/1	0.94	0.20	49,49,49,49	0
54	MG	2a	1743	1/1	0.94	0.21	58,58,58,58	0
54	MG	1A	3344	1/1	0.94	0.07	26,26,26,26	0
54	MG	2A	3685	1/1	0.94	0.08	51,51,51,51	0
54	MG	2A	3688	1/1	0.94	0.12	45,45,45,45	0
54	MG	1A	3053	1/1	0.94	0.19	28,28,28,28	0
54	MG	2a	1749	1/1	0.94	0.28	39,39,39,39	0
54	MG	2A	3126	1/1	0.94	0.31	41,41,41,41	0
54	MG	2A	3394	1/1	0.94	0.10	63,63,63,63	0
54	MG	1A	3579	1/1	0.94	0.07	25,25,25,25	0
54	MG	2A	3130	1/1	0.94	0.25	71,71,71,71	0
54	MG	2a	1756	1/1	0.94	0.14	47,47,47,47	0
54	MG	1A	3854	1/1	0.94	0.07	13,13,13,13	0
54	MG	1A	3185	1/1	0.94	0.18	31,31,31,31	0
54	MG	2A	3135	1/1	0.94	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3137	1/1	0.94	0.12	47,47,47,47	0
54	MG	1A	3091	1/1	0.94	0.13	32,32,32,32	0
54	MG	1A	3582	1/1	0.94	0.12	57,57,57,57	0
54	MG	1A	3136	1/1	0.94	0.07	26,26,26,26	0
54	MG	2A	3704	1/1	0.94	0.13	62,62,62,62	0
54	MG	1A	3352	1/1	0.94	0.10	59,59,59,59	0
54	MG	2A	3706	1/1	0.94	0.14	69,69,69,69	0
54	MG	1E	309	1/1	0.94	0.10	51,51,51,51	0
54	MG	1A	3587	1/1	0.94	0.30	25,25,25,25	0
54	MG	1a	1841	1/1	0.94	0.07	63,63,63,63	0
54	MG	1A	3023	1/1	0.94	0.20	26,26,26,26	0
54	MG	1A	3589	1/1	0.94	0.23	30,30,30,30	0
54	MG	1A	3493	1/1	0.94	0.09	18,18,18,18	0
54	MG	1a	1677	1/1	0.94	0.09	49,49,49,49	0
54	MG	2A	3430	1/1	0.94	0.09	47,47,47,47	0
54	MG	1A	3192	1/1	0.94	0.10	31,31,31,31	0
54	MG	1A	3098	1/1	0.94	0.09	41,41,41,41	0
54	MG	1A	3883	1/1	0.94	0.10	16,16,16,16	0
54	MG	2A	3172	1/1	0.94	0.10	40,40,40,40	0
54	MG	1A	3593	1/1	0.94	0.13	34,34,34,34	0
54	MG	2A	3439	1/1	0.94	0.06	50,50,50,50	0
54	MG	1A	3712	1/1	0.94	0.07	21,21,21,21	0
54	MG	1A	3595	1/1	0.94	0.10	51,51,51,51	0
54	MG	1A	3499	1/1	0.94	0.11	54,54,54,54	0
54	MG	1F	318	1/1	0.94	0.07	44,44,44,44	0
54	MG	2A	3181	1/1	0.94	0.20	45,45,45,45	0
54	MG	2A	3183	1/1	0.94	0.21	51,51,51,51	0
58	ZN	1Y	202	1/1	0.94	0.11	109,109,109,109	0
54	MG	1a	1861	1/1	0.94	0.08	78,78,78,78	0
54	MG	1A	3719	1/1	0.94	0.13	45,45,45,45	0
54	MG	2B	208	1/1	0.94	0.15	62,62,62,62	0
54	MG	2A	3073	1/1	0.95	0.09	33,33,33,33	0
54	MG	1A	3842	1/1	0.95	0.08	30,30,30,30	0
54	MG	1A	3999	1/1	0.95	0.27	32,32,32,32	0
54	MG	1A	3715	1/1	0.95	0.12	32,32,32,32	0
54	MG	1A	3155	1/1	0.95	0.10	35,35,35,35	0
54	MG	1A	3611	1/1	0.95	0.19	26,26,26,26	0
54	MG	1A	3070	1/1	0.95	0.29	40,40,40,40	0
54	MG	1A	3026	1/1	0.95	0.42	31,31,31,31	0
54	MG	2A	3081	1/1	0.95	0.06	42,42,42,42	0
54	MG	2A	3082	1/1	0.95	0.09	38,38,38,38	0
54	MG	1a	1779	1/1	0.95	0.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3852	1/1	0.95	0.10	36,36,36,36	0
54	MG	1A	3615	1/1	0.95	0.48	27,27,27,27	0
54	MG	1A	3417	1/1	0.95	0.09	28,28,28,28	0
54	MG	2A	3088	1/1	0.95	0.11	28,28,28,28	0
54	MG	1A	3521	1/1	0.95	0.10	36,36,36,36	0
54	MG	1a	1785	1/1	0.95	0.09	72,72,72,72	0
54	MG	1A	3324	1/1	0.95	0.10	25,25,25,25	0
54	MG	1A	3861	1/1	0.95	0.16	47,47,47,47	0
54	MG	1A	3422	1/1	0.95	0.12	47,47,47,47	0
54	MG	1A	3263	1/1	0.95	0.08	45,45,45,45	0
54	MG	1A	3264	1/1	0.95	0.19	49,49,49,49	0
54	MG	1A	3426	1/1	0.95	0.08	38,38,38,38	0
54	MG	1a	1622	1/1	0.95	0.14	42,42,42,42	0
54	MG	2A	3385	1/1	0.95	0.11	35,35,35,35	0
54	MG	1A	3873	1/1	0.95	0.10	49,49,49,49	0
54	MG	1A	3331	1/1	0.95	0.07	17,17,17,17	0
54	MG	2A	3105	1/1	0.95	0.28	38,38,38,38	0
54	MG	2A	3392	1/1	0.95	0.09	48,48,48,48	0
54	MG	2A	3108	1/1	0.95	0.20	44,44,44,44	0
54	MG	2A	3110	1/1	0.95	0.15	42,42,42,42	0
54	MG	2A	3396	1/1	0.95	0.07	35,35,35,35	0
54	MG	1A	3186	1/1	0.95	0.20	31,31,31,31	0
54	MG	1a	1797	1/1	0.95	0.12	60,60,60,60	0
54	MG	2A	3400	1/1	0.95	0.10	43,43,43,43	0
54	MG	2A	3401	1/1	0.95	0.07	42,42,42,42	0
54	MG	1A	3877	1/1	0.95	0.10	14,14,14,14	0
54	MG	1a	1628	1/1	0.95	0.22	41,41,41,41	0
54	MG	2A	3115	1/1	0.95	0.09	35,35,35,35	0
54	MG	1A	3335	1/1	0.95	0.09	37,37,37,37	0
54	MG	2B	211	1/1	0.95	0.08	46,46,46,46	0
54	MG	2A	3118	1/1	0.95	0.07	42,42,42,42	0
54	MG	1a	1801	1/1	0.95	0.11	53,53,53,53	0
54	MG	2B	215	1/1	0.95	0.08	53,53,53,53	0
54	MG	1a	1630	1/1	0.95	0.12	43,43,43,43	0
54	MG	2A	3412	1/1	0.95	0.06	27,27,27,27	0
54	MG	1A	3267	1/1	0.95	0.12	56,56,56,56	0
54	MG	1A	3115	1/1	0.95	0.11	42,42,42,42	0
54	MG	1A	3884	1/1	0.95	0.12	33,33,33,33	0
54	MG	2A	3418	1/1	0.95	0.11	32,32,32,32	0
54	MG	2A	3419	1/1	0.95	0.14	44,44,44,44	0
54	MG	2A	3420	1/1	0.95	0.07	40,40,40,40	0
54	MG	1a	1637	1/1	0.95	0.30	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1808	1/1	0.95	0.06	69,69,69,69	0
54	MG	1A	3189	1/1	0.95	0.07	34,34,34,34	0
54	MG	2A	3128	1/1	0.95	0.06	58,58,58,58	0
54	MG	2E	307	1/1	0.95	0.09	67,67,67,67	0
54	MG	2E	309	1/1	0.95	0.16	44,44,44,44	0
54	MG	2F	301	1/1	0.95	0.10	34,34,34,34	0
54	MG	2A	3429	1/1	0.95	0.10	51,51,51,51	0
54	MG	2F	303	1/1	0.95	0.06	50,50,50,50	0
54	MG	1A	3752	1/1	0.95	0.12	36,36,36,36	0
54	MG	1B	226	1/1	0.95	0.09	48,48,48,48	0
54	MG	1A	3013	1/1	0.95	0.12	20,20,20,20	0
54	MG	1A	3444	1/1	0.95	0.08	37,37,37,37	0
54	MG	2A	3434	1/1	0.95	0.13	58,58,58,58	0
54	MG	2A	3435	1/1	0.95	0.11	48,48,48,48	0
54	MG	2A	3136	1/1	0.95	0.07	63,63,63,63	0
54	MG	1A	3220	1/1	0.95	0.07	35,35,35,35	0
54	MG	2R	201	1/1	0.95	0.10	42,42,42,42	0
54	MG	2T	201	1/1	0.95	0.10	51,51,51,51	0
54	MG	2T	202	1/1	0.95	0.08	37,37,37,37	0
54	MG	2A	3438	1/1	0.95	0.23	43,43,43,43	0
54	MG	1a	1647	1/1	0.95	0.07	60,60,60,60	0
54	MG	1a	1820	1/1	0.95	0.05	46,46,46,46	0
54	MG	2A	3441	1/1	0.95	0.10	28,28,28,28	0
54	MG	2W	201	1/1	0.95	0.27	36,36,36,36	0
54	MG	1A	3222	1/1	0.95	0.34	27,27,27,27	0
54	MG	1B	231	1/1	0.95	0.07	64,64,64,64	0
54	MG	1A	3345	1/1	0.95	0.11	35,35,35,35	0
54	MG	2A	3150	1/1	0.95	0.14	40,40,40,40	0
54	MG	2I	101	1/1	0.95	0.08	42,42,42,42	0
54	MG	1D	306	1/1	0.95	0.18	20,20,20,20	0
54	MG	2A	3153	1/1	0.95	0.14	33,33,33,33	0
54	MG	2A	3156	1/1	0.95	0.07	39,39,39,39	0
54	MG	1D	307	1/1	0.95	0.11	43,43,43,43	0
54	MG	1a	1826	1/1	0.95	0.07	57,57,57,57	0
54	MG	27	101	1/1	0.95	0.14	46,46,46,46	0
54	MG	2A	3161	1/1	0.95	0.29	48,48,48,48	0
54	MG	1a	1827	1/1	0.95	0.09	61,61,61,61	0
54	MG	1D	308	1/1	0.95	0.08	34,34,34,34	0
54	MG	1D	311	1/1	0.95	0.08	37,37,37,37	0
54	MG	1D	312	1/1	0.95	0.10	26,26,26,26	0
54	MG	1A	3346	1/1	0.95	0.07	31,31,31,31	0
54	MG	1a	1832	1/1	0.95	0.07	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3170	1/1	0.95	0.14	36,36,36,36	0
54	MG	1D	314	1/1	0.95	0.10	49,49,49,49	0
54	MG	1A	3904	1/1	0.95	0.12	64,64,64,64	0
54	MG	1A	3225	1/1	0.95	0.28	38,38,38,38	0
54	MG	1D	317	1/1	0.95	0.09	39,39,39,39	0
54	MG	1A	3283	1/1	0.95	0.10	39,39,39,39	0
54	MG	1A	3764	1/1	0.95	0.06	40,40,40,40	0
54	MG	2A	3180	1/1	0.95	0.13	49,49,49,49	0
54	MG	2a	1620	1/1	0.95	0.24	53,53,53,53	0
54	MG	2a	1621	1/1	0.95	0.17	57,57,57,57	0
54	MG	1a	1842	1/1	0.95	0.08	58,58,58,58	0
54	MG	1A	3766	1/1	0.95	0.13	48,48,48,48	0
54	MG	1A	3768	1/1	0.95	0.12	54,54,54,54	0
54	MG	1A	3913	1/1	0.95	0.09	55,55,55,55	0
54	MG	2a	1626	1/1	0.95	0.14	47,47,47,47	0
54	MG	2A	3485	1/1	0.95	0.22	57,57,57,57	0
54	MG	1A	3137	1/1	0.95	0.08	39,39,39,39	0
54	MG	1A	3556	1/1	0.95	0.14	38,38,38,38	0
54	MG	2A	3488	1/1	0.95	0.08	47,47,47,47	0
54	MG	2a	1632	1/1	0.95	0.07	68,68,68,68	0
54	MG	1A	3461	1/1	0.95	0.06	29,29,29,29	0
54	MG	1F	307	1/1	0.95	0.14	20,20,20,20	0
54	MG	2A	3190	1/1	0.95	0.08	50,50,50,50	0
54	MG	1A	3350	1/1	0.95	0.11	29,29,29,29	0
54	MG	2A	3192	1/1	0.95	0.06	29,29,29,29	0
54	MG	1A	3921	1/1	0.95	0.13	69,69,69,69	0
54	MG	1A	3463	1/1	0.95	0.10	15,15,15,15	0
54	MG	1A	3138	1/1	0.95	0.40	32,32,32,32	0
54	MG	1A	3928	1/1	0.95	0.11	49,49,49,49	0
54	MG	2a	1643	1/1	0.95	0.07	35,35,35,35	0
54	MG	1A	3231	1/1	0.95	0.14	35,35,35,35	0
54	MG	2a	1645	1/1	0.95	0.10	52,52,52,52	0
54	MG	1A	3014	1/1	0.95	0.06	31,31,31,31	0
54	MG	1A	3779	1/1	0.95	0.15	45,45,45,45	0
54	MG	1a	1680	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3355	1/1	0.95	0.10	50,50,50,50	0
54	MG	1A	3935	1/1	0.95	0.09	38,38,38,38	0
54	MG	1A	3936	1/1	0.95	0.08	31,31,31,31	0
54	MG	1A	3665	1/1	0.95	0.10	49,49,49,49	0
54	MG	1A	3358	1/1	0.95	0.09	32,32,32,32	0
54	MG	1N	201	1/1	0.95	0.10	40,40,40,40	0
54	MG	2A	3512	1/1	0.95	0.08	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	1A	3939	1/1	0.95	0.10	44,44,44,44	0
54	MG	1A	3168	1/1	0.95	0.07	23,23,23,23	0
54	MG	1A	3941	1/1	0.95	0.37	43,43,43,43	0
54	MG	2A	3214	1/1	0.95	0.10	62,62,62,62	0
54	MG	1A	3942	1/1	0.95	0.07	26,26,26,26	0
54	MG	2A	3519	1/1	0.95	0.06	40,40,40,40	0
54	MG	1A	3005	1/1	0.95	0.04	14,14,14,14	0
54	MG	1P	203	1/1	0.95	0.26	23,23,23,23	0
54	MG	1A	3479	1/1	0.95	0.06	35,35,35,35	0
54	MG	2A	3225	1/1	0.95	0.14	47,47,47,47	0
54	MG	1A	3946	1/1	0.95	0.15	27,27,27,27	0
54	MG	1A	3575	1/1	0.95	0.13	55,55,55,55	0
54	MG	1A	3362	1/1	0.95	0.07	23,23,23,23	0
54	MG	1g	203	1/1	0.95	0.24	55,55,55,55	0
54	MG	1P	208	1/1	0.95	0.09	47,47,47,47	0
54	MG	1Q	201	1/1	0.95	0.29	32,32,32,32	0
54	MG	1k	3100	1/1	0.95	0.11	42,42,42,42	0
54	MG	1A	3949	1/1	0.95	0.11	18,18,18,18	0
54	MG	1l	3102	1/1	0.95	0.07	52,52,52,52	0
54	MG	1Q	203	1/1	0.95	0.09	26,26,26,26	0
54	MG	1A	3291	1/1	0.95	0.19	31,31,31,31	0
54	MG	2A	3541	1/1	0.95	0.08	75,75,75,75	0
54	MG	2A	3543	1/1	0.95	0.06	45,45,45,45	0
54	MG	1a	1703	1/1	0.95	0.07	65,65,65,65	0
54	MG	1Q	207	1/1	0.95	0.08	36,36,36,36	0
54	MG	1R	201	1/1	0.95	0.16	30,30,30,30	0
54	MG	1A	3486	1/1	0.95	0.10	45,45,45,45	0
54	MG	1a	1707	1/1	0.95	0.17	52,52,52,52	0
54	MG	2A	3248	1/1	0.95	0.21	36,36,36,36	0
54	MG	1A	3365	1/1	0.95	0.11	38,38,38,38	0
54	MG	1A	3041	1/1	0.95	0.16	46,46,46,46	0
54	MG	1A	3128	1/1	0.95	0.08	48,48,48,48	0
54	MG	1a	1711	1/1	0.95	0.12	59,59,59,59	0
54	MG	1T	203	1/1	0.95	0.06	49,49,49,49	0
54	MG	1A	3959	1/1	0.95	0.10	35,35,35,35	0
54	MG	2A	3255	1/1	0.95	0.06	47,47,47,47	0
54	MG	1a	1717	1/1	0.95	0.07	37,37,37,37	0
54	MG	2a	1703	1/1	0.95	0.14	70,70,70,70	0
54	MG	1A	3682	1/1	0.95	0.12	40,40,40,40	0
54	MG	1U	201	1/1	0.95	0.09	22,22,22,22	0
54	MG	2A	3262	1/1	0.95	0.19	36,36,36,36	0
54	MG	2A	3005	1/1	0.95	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3017	1/1	0.95	0.24	17,17,17,17	0
54	MG	2A	3009	1/1	0.95	0.11	27,27,27,27	0
54	MG	2a	1711	1/1	0.95	0.09	64,64,64,64	0
54	MG	2A	3010	1/1	0.95	0.10	32,32,32,32	0
54	MG	1A	3381	1/1	0.95	0.08	38,38,38,38	0
54	MG	2a	1714	1/1	0.95	0.10	46,46,46,46	0
54	MG	2A	3268	1/1	0.95	0.09	46,46,46,46	0
54	MG	2A	3584	1/1	0.95	0.07	30,30,30,30	0
54	MG	2A	3015	1/1	0.95	0.11	34,34,34,34	0
54	MG	2a	1718	1/1	0.95	0.11	55,55,55,55	0
54	MG	2a	1719	1/1	0.95	0.07	65,65,65,65	0
54	MG	1V	202	1/1	0.95	0.18	28,28,28,28	0
54	MG	1a	1724	1/1	0.95	0.10	64,64,64,64	0
54	MG	2a	1723	1/1	0.95	0.13	65,65,65,65	0
54	MG	1A	3382	1/1	0.95	0.16	39,39,39,39	0
54	MG	2A	3021	1/1	0.95	0.17	44,44,44,44	0
54	MG	1A	3151	1/1	0.95	0.12	31,31,31,31	0
54	MG	2A	3595	1/1	0.95	0.11	69,69,69,69	0
54	MG	2A	3599	1/1	0.95	0.07	33,33,33,33	0
54	MG	2A	3281	1/1	0.95	0.12	41,41,41,41	0
54	MG	1A	3812	1/1	0.95	0.07	28,28,28,28	0
54	MG	1A	3966	1/1	0.95	0.12	19,19,19,19	0
54	MG	2A	3284	1/1	0.95	0.07	46,46,46,46	0
54	MG	1W	202	1/1	0.95	0.10	35,35,35,35	0
54	MG	2A	3288	1/1	0.95	0.06	32,32,32,32	0
54	MG	1A	3387	1/1	0.95	0.18	35,35,35,35	0
54	MG	1X	102	1/1	0.95	0.09	33,33,33,33	0
54	MG	1A	3304	1/1	0.95	0.12	56,56,56,56	0
54	MG	2a	1742	1/1	0.95	0.16	61,61,61,61	0
54	MG	1a	1738	1/1	0.95	0.12	49,49,49,49	0
54	MG	1a	1739	1/1	0.95	0.17	69,69,69,69	0
54	MG	1A	3502	1/1	0.95	0.06	32,32,32,32	0
54	MG	10	101	1/1	0.95	0.06	35,35,35,35	0
54	MG	1A	3971	1/1	0.95	0.15	31,31,31,31	0
54	MG	2A	3620	1/1	0.95	0.09	69,69,69,69	0
54	MG	1A	3306	1/1	0.95	0.07	17,17,17,17	0
54	MG	2a	1751	1/1	0.95	0.07	52,52,52,52	0
54	MG	2A	3623	1/1	0.95	0.20	78,78,78,78	0
54	MG	1A	3067	1/1	0.95	0.08	33,33,33,33	0
54	MG	1A	3594	1/1	0.95	0.09	58,58,58,58	0
54	MG	2A	3303	1/1	0.95	0.07	39,39,39,39	0
54	MG	1A	3699	1/1	0.95	0.06	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	2A	3637	1/1	0.95	0.09	83,83,83,83	0
54	MG	2A	3307	1/1	0.95	0.10	23,23,23,23	0
54	MG	2A	3044	1/1	0.95	0.14	21,21,21,21	0
54	MG	2A	3310	1/1	0.95	0.08	32,32,32,32	0
54	MG	1A	3507	1/1	0.95	0.13	47,47,47,47	0
54	MG	2A	3642	1/1	0.95	0.06	39,39,39,39	0
54	MG	2A	3048	1/1	0.95	0.16	42,42,42,42	0
54	MG	1A	3978	1/1	0.95	0.12	45,45,45,45	0
54	MG	2a	1767	1/1	0.95	0.07	48,48,48,48	0
54	MG	1A	3246	1/1	0.95	0.18	32,32,32,32	0
54	MG	2A	3052	1/1	0.95	0.14	51,51,51,51	0
54	MG	2A	3323	1/1	0.95	0.11	39,39,39,39	0
54	MG	2a	1772	1/1	0.95	0.11	45,45,45,45	0
54	MG	2A	3324	1/1	0.95	0.12	42,42,42,42	0
54	MG	2A	3325	1/1	0.95	0.09	39,39,39,39	0
54	MG	2A	3654	1/1	0.95	0.08	30,30,30,30	0
54	MG	2a	1776	1/1	0.95	0.09	53,53,53,53	0
54	MG	2a	1777	1/1	0.95	0.24	54,54,54,54	0
54	MG	11	104	1/1	0.95	0.07	39,39,39,39	0
54	MG	2A	3332	1/1	0.95	0.10	62,62,62,62	0
54	MG	1A	3599	1/1	0.95	0.08	23,23,23,23	0
54	MG	1A	3397	1/1	0.95	0.08	58,58,58,58	0
54	MG	1a	1757	1/1	0.95	0.07	50,50,50,50	0
54	MG	2A	3665	1/1	0.95	0.09	54,54,54,54	0
54	MG	2A	3667	1/1	0.95	0.10	35,35,35,35	0
54	MG	1A	3987	1/1	0.95	0.07	32,32,32,32	0
56	ARG	1B	232	12/12	0.95	0.12	31,44,50,55	0
54	MG	1A	3399	1/1	0.95	0.07	28,28,28,28	0
54	MG	15	101	1/1	0.95	0.20	31,31,31,31	0
54	MG	1A	3205	1/1	0.95	0.24	37,37,37,37	0
54	MG	1A	3837	1/1	0.95	0.09	34,34,34,34	0
54	MG	1A	3993	1/1	0.95	0.11	51,51,51,51	0
54	MG	1A	3606	1/1	0.95	0.08	24,24,24,24	0
54	MG	1A	3252	1/1	0.95	0.10	72,72,72,72	0
54	MG	19	101	1/1	0.95	0.07	43,43,43,43	0
54	MG	1A	3255	1/1	0.95	0.11	31,31,31,31	0
54	MG	1a	1601	1/1	0.95	0.07	61,61,61,61	0
54	MG	1A	3713	1/1	0.95	0.06	38,38,38,38	0
54	MG	1A	3557	1/1	0.96	0.10	35,35,35,35	0
54	MG	1a	1645	1/1	0.96	0.20	49,49,49,49	0
54	MG	1A	3435	1/1	0.96	0.12	30,30,30,30	0
54	MG	2A	3140	1/1	0.96	0.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3436	1/1	0.96	0.07	13,13,13,13	0
54	MG	2A	3142	1/1	0.96	0.09	40,40,40,40	0
54	MG	1A	3560	1/1	0.96	0.10	52,52,52,52	0
54	MG	2A	3144	1/1	0.96	0.11	36,36,36,36	0
54	MG	1A	3689	1/1	0.96	0.12	83,83,83,83	0
54	MG	1A	3561	1/1	0.96	0.05	47,47,47,47	0
54	MG	1a	1652	1/1	0.96	0.13	48,48,48,48	0
54	MG	1A	3063	1/1	0.96	0.05	22,22,22,22	0
54	MG	1A	3859	1/1	0.96	0.07	43,43,43,43	0
54	MG	1D	301	1/1	0.96	0.35	33,33,33,33	0
54	MG	1A	3092	1/1	0.96	0.05	38,38,38,38	0
54	MG	1A	3093	1/1	0.96	0.23	30,30,30,30	0
54	MG	2A	3160	1/1	0.96	0.09	51,51,51,51	0
54	MG	1a	1838	1/1	0.96	0.13	78,78,78,78	0
54	MG	2A	3162	1/1	0.96	0.19	50,50,50,50	0
54	MG	2B	212	1/1	0.96	0.10	94,94,94,94	0
54	MG	1A	3029	1/1	0.96	0.08	35,35,35,35	0
54	MG	1A	3024	1/1	0.96	0.08	20,20,20,20	0
54	MG	1D	309	1/1	0.96	0.20	31,31,31,31	0
54	MG	1A	3327	1/1	0.96	0.07	29,29,29,29	0
54	MG	1A	3054	1/1	0.96	0.13	26,26,26,26	0
54	MG	2D	301	1/1	0.96	0.15	38,38,38,38	0
54	MG	2D	302	1/1	0.96	0.38	45,45,45,45	0
54	MG	1A	3019	1/1	0.96	0.19	20,20,20,20	0
54	MG	1A	3453	1/1	0.96	0.07	14,14,14,14	0
54	MG	2D	305	1/1	0.96	0.08	48,48,48,48	0
54	MG	1A	3573	1/1	0.96	0.12	36,36,36,36	0
54	MG	1a	1851	1/1	0.96	0.07	27,27,27,27	0
54	MG	1A	3004	1/1	0.96	0.06	27,27,27,27	0
54	MG	2E	301	1/1	0.96	0.09	41,41,41,41	0
54	MG	1A	3104	1/1	0.96	0.14	46,46,46,46	0
54	MG	1a	1668	1/1	0.96	0.16	42,42,42,42	0
54	MG	1A	3457	1/1	0.96	0.11	23,23,23,23	0
54	MG	1E	301	1/1	0.96	0.20	33,33,33,33	0
54	MG	1E	302	1/1	0.96	0.37	39,39,39,39	0
54	MG	1A	3045	1/1	0.96	0.43	29,29,29,29	0
54	MG	1A	3247	1/1	0.96	0.07	38,38,38,38	0
54	MG	1a	1863	1/1	0.96	0.07	54,54,54,54	0
54	MG	1A	3248	1/1	0.96	0.08	51,51,51,51	0
54	MG	1A	3714	1/1	0.96	0.10	39,39,39,39	0
54	MG	2F	304	1/1	0.96	0.17	46,46,46,46	0
54	MG	1A	3188	1/1	0.96	0.08	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3251	1/1	0.96	0.32	33,33,33,33	0
54	MG	1F	305	1/1	0.96	0.12	31,31,31,31	0
54	MG	1A	3892	1/1	0.96	0.16	59,59,59,59	0
54	MG	1A	3585	1/1	0.96	0.09	41,41,41,41	0
54	MG	2A	3456	1/1	0.96	0.08	21,21,21,21	0
54	MG	1A	3894	1/1	0.96	0.21	37,37,37,37	0
54	MG	1F	311	1/1	0.96	0.24	26,26,26,26	0
54	MG	1A	3895	1/1	0.96	0.07	43,43,43,43	0
54	MG	2R	202	1/1	0.96	0.07	28,28,28,28	0
54	MG	1d	304	1/1	0.96	0.27	53,53,53,53	0
54	MG	1A	3142	1/1	0.96	0.05	27,27,27,27	0
54	MG	2A	3462	1/1	0.96	0.13	50,50,50,50	0
54	MG	1A	3467	1/1	0.96	0.07	33,33,33,33	0
54	MG	2T	205	1/1	0.96	0.07	29,29,29,29	0
54	MG	2A	3466	1/1	0.96	0.06	41,41,41,41	0
54	MG	1A	3899	1/1	0.96	0.05	36,36,36,36	0
54	MG	2V	203	1/1	0.96	0.09	38,38,38,38	0
54	MG	2A	3468	1/1	0.96	0.07	47,47,47,47	0
54	MG	1A	3722	1/1	0.96	0.06	30,30,30,30	0
54	MG	1A	3107	1/1	0.96	0.56	28,28,28,28	0
54	MG	2X	101	1/1	0.96	0.08	49,49,49,49	0
54	MG	2A	3203	1/1	0.96	0.10	46,46,46,46	0
54	MG	1A	3145	1/1	0.96	0.07	24,24,24,24	0
54	MG	20	102	1/1	0.96	0.08	57,57,57,57	0
54	MG	2A	3205	1/1	0.96	0.05	45,45,45,45	0
54	MG	2A	3206	1/1	0.96	0.17	37,37,37,37	0
54	MG	1A	3007	1/1	0.96	0.06	31,31,31,31	0
54	MG	23	101	1/1	0.96	0.10	46,46,46,46	0
54	MG	1A	3731	1/1	0.96	0.05	42,42,42,42	0
54	MG	1A	3149	1/1	0.96	0.36	30,30,30,30	0
54	MG	1A	3475	1/1	0.96	0.10	63,63,63,63	0
54	MG	1A	3735	1/1	0.96	0.06	38,38,38,38	0
54	MG	1A	3736	1/1	0.96	0.11	33,33,33,33	0
54	MG	1A	3260	1/1	0.96	0.07	43,43,43,43	0
54	MG	1A	3194	1/1	0.96	0.14	46,46,46,46	0
54	MG	2A	3490	1/1	0.96	0.04	32,32,32,32	0
54	MG	1N	205	1/1	0.96	0.08	49,49,49,49	0
54	MG	2A	3216	1/1	0.96	0.12	46,46,46,46	0
54	MG	2A	3217	1/1	0.96	0.12	39,39,39,39	0
54	MG	2A	3219	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3077	1/1	0.96	0.46	40,40,40,40	0
54	MG	1A	3265	1/1	0.96	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1P	201	1/1	0.96	0.39	25,25,25,25	0
54	MG	1A	3741	1/1	0.96	0.07	49,49,49,49	0
54	MG	1A	3597	1/1	0.96	0.07	19,19,19,19	0
54	MG	1A	3111	1/1	0.96	0.16	38,38,38,38	0
54	MG	1A	3929	1/1	0.96	0.10	55,55,55,55	0
54	MG	2a	1619	1/1	0.96	0.22	42,42,42,42	0
54	MG	1A	3048	1/1	0.96	0.05	24,24,24,24	0
54	MG	2A	3231	1/1	0.96	0.50	45,45,45,45	0
54	MG	1A	3601	1/1	0.96	0.09	38,38,38,38	0
54	MG	1A	3748	1/1	0.96	0.12	14,14,14,14	0
54	MG	1A	3750	1/1	0.96	0.10	42,42,42,42	0
54	MG	1A	3602	1/1	0.96	0.10	15,15,15,15	0
54	MG	1A	3356	1/1	0.96	0.05	28,28,28,28	0
54	MG	1A	3753	1/1	0.96	0.07	24,24,24,24	0
54	MG	2a	1628	1/1	0.96	0.10	39,39,39,39	0
54	MG	1a	1716	1/1	0.96	0.07	50,50,50,50	0
54	MG	2A	3240	1/1	0.96	0.12	51,51,51,51	0
54	MG	1A	3198	1/1	0.96	0.33	43,43,43,43	0
54	MG	2A	3006	1/1	0.96	0.17	44,44,44,44	0
54	MG	1a	1718	1/1	0.96	0.09	49,49,49,49	0
54	MG	2A	3008	1/1	0.96	0.11	41,41,41,41	0
54	MG	1A	3114	1/1	0.96	0.27	26,26,26,26	0
54	MG	1A	3156	1/1	0.96	0.18	33,33,33,33	0
54	MG	2a	1637	1/1	0.96	0.14	41,41,41,41	0
54	MG	2A	3011	1/1	0.96	0.09	51,51,51,51	0
54	MG	2A	3525	1/1	0.96	0.06	43,43,43,43	0
54	MG	2A	3012	1/1	0.96	0.11	36,36,36,36	0
54	MG	1A	3273	1/1	0.96	0.07	32,32,32,32	0
54	MG	2A	3014	1/1	0.96	0.05	25,25,25,25	0
54	MG	1A	3201	1/1	0.96	0.32	31,31,31,31	0
54	MG	1A	3495	1/1	0.96	0.10	50,50,50,50	0
54	MG	2A	3018	1/1	0.96	0.14	38,38,38,38	0
54	MG	1A	3277	1/1	0.96	0.10	32,32,32,32	0
54	MG	2A	3533	1/1	0.96	0.06	73,73,73,73	0
54	MG	2A	3534	1/1	0.96	0.09	67,67,67,67	0
54	MG	1A	3945	1/1	0.96	0.14	39,39,39,39	0
54	MG	2A	3259	1/1	0.96	0.10	21,21,21,21	0
54	MG	1A	3498	1/1	0.96	0.13	21,21,21,21	0
54	MG	1a	1729	1/1	0.96	0.07	55,55,55,55	0
54	MG	1A	3278	1/1	0.96	0.47	29,29,29,29	0
54	MG	2a	1654	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3765	1/1	0.96	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1U	204	1/1	0.96	0.42	34,34,34,34	0
54	MG	1U	205	1/1	0.96	0.08	37,37,37,37	0
54	MG	1A	3500	1/1	0.96	0.12	19,19,19,19	0
54	MG	1A	3767	1/1	0.96	0.05	88,88,88,88	0
54	MG	1a	1737	1/1	0.96	0.08	48,48,48,48	0
54	MG	1A	3952	1/1	0.96	0.09	41,41,41,41	0
54	MG	2A	3273	1/1	0.96	0.10	18,18,18,18	0
54	MG	1A	3370	1/1	0.96	0.07	13,13,13,13	0
54	MG	1A	3202	1/1	0.96	0.28	38,38,38,38	0
54	MG	1A	3280	1/1	0.96	0.05	30,30,30,30	0
54	MG	2A	3556	1/1	0.96	0.06	27,27,27,27	0
54	MG	2A	3037	1/1	0.96	0.27	54,54,54,54	0
54	MG	2A	3038	1/1	0.96	0.10	52,52,52,52	0
54	MG	2A	3559	1/1	0.96	0.10	46,46,46,46	0
54	MG	1a	1742	1/1	0.96	0.06	43,43,43,43	0
54	MG	1a	1743	1/1	0.96	0.12	52,52,52,52	0
54	MG	2A	3563	1/1	0.96	0.06	48,48,48,48	0
54	MG	1A	3957	1/1	0.96	0.07	48,48,48,48	0
54	MG	1A	3080	1/1	0.96	0.14	48,48,48,48	0
54	MG	1A	3282	1/1	0.96	0.25	33,33,33,33	0
54	MG	2A	3568	1/1	0.96	0.08	57,57,57,57	0
54	MG	2a	1679	1/1	0.96	0.37	52,52,52,52	0
54	MG	2A	3289	1/1	0.96	0.07	30,30,30,30	0
54	MG	1A	3158	1/1	0.96	0.14	28,28,28,28	0
54	MG	2A	3571	1/1	0.96	0.07	65,65,65,65	0
54	MG	2A	3046	1/1	0.96	0.10	47,47,47,47	0
54	MG	2A	3574	1/1	0.96	0.08	40,40,40,40	0
54	MG	1a	1749	1/1	0.96	0.08	52,52,52,52	0
54	MG	2a	1686	1/1	0.96	0.21	47,47,47,47	0
54	MG	2a	1687	1/1	0.96	0.25	41,41,41,41	0
54	MG	2A	3576	1/1	0.96	0.06	43,43,43,43	0
54	MG	1A	3626	1/1	0.96	0.09	46,46,46,46	0
54	MG	1A	3081	1/1	0.96	0.25	34,34,34,34	0
54	MG	1A	3285	1/1	0.96	0.10	24,24,24,24	0
54	MG	1A	3390	1/1	0.96	0.05	31,31,31,31	0
54	MG	1A	3631	1/1	0.96	0.11	33,33,33,33	0
54	MG	1A	3206	1/1	0.96	0.10	35,35,35,35	0
54	MG	1A	3634	1/1	0.96	0.09	42,42,42,42	0
54	MG	2A	3300	1/1	0.96	0.11	43,43,43,43	0
54	MG	10	109	1/1	0.96	0.10	61,61,61,61	0
54	MG	2a	1701	1/1	0.96	0.17	63,63,63,63	0
54	MG	2A	3302	1/1	0.96	0.07	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3783	1/1	0.96	0.14	32,32,32,32	0
54	MG	1A	3969	1/1	0.96	0.07	40,40,40,40	0
54	MG	2A	3305	1/1	0.96	0.09	35,35,35,35	0
54	MG	1A	3785	1/1	0.96	0.13	47,47,47,47	0
54	MG	1A	3392	1/1	0.96	0.06	16,16,16,16	0
54	MG	2A	3309	1/1	0.96	0.05	46,46,46,46	0
54	MG	1A	3788	1/1	0.96	0.10	45,45,45,45	0
54	MG	1A	3973	1/1	0.96	0.12	36,36,36,36	0
54	MG	1A	3789	1/1	0.96	0.09	47,47,47,47	0
54	MG	2A	3314	1/1	0.96	0.07	43,43,43,43	0
54	MG	2A	3317	1/1	0.96	0.14	28,28,28,28	0
54	MG	1A	3207	1/1	0.96	0.26	34,34,34,34	0
54	MG	1A	3637	1/1	0.96	0.10	13,13,13,13	0
54	MG	1A	3794	1/1	0.96	0.12	50,50,50,50	0
54	MG	2A	3615	1/1	0.96	0.09	59,59,59,59	0
54	MG	2A	3322	1/1	0.96	0.07	32,32,32,32	0
54	MG	1A	3394	1/1	0.96	0.07	12,12,12,12	0
54	MG	1A	3981	1/1	0.96	0.08	21,21,21,21	0
54	MG	1A	3118	1/1	0.96	0.06	27,27,27,27	0
54	MG	2A	3327	1/1	0.96	0.06	38,38,38,38	0
54	MG	2A	3328	1/1	0.96	0.11	44,44,44,44	0
54	MG	17	101	1/1	0.96	0.13	31,31,31,31	0
54	MG	2A	3629	1/1	0.96	0.07	48,48,48,48	0
54	MG	17	103	1/1	0.96	0.31	29,29,29,29	0
54	MG	2A	3333	1/1	0.96	0.06	43,43,43,43	0
54	MG	2A	3334	1/1	0.96	0.06	25,25,25,25	0
54	MG	1A	3396	1/1	0.96	0.06	18,18,18,18	0
54	MG	1A	3120	1/1	0.96	0.14	31,31,31,31	0
54	MG	1A	3522	1/1	0.96	0.06	27,27,27,27	0
54	MG	1A	3212	1/1	0.96	0.14	25,25,25,25	0
54	MG	1A	3008	1/1	0.96	0.06	34,34,34,34	0
54	MG	1A	3647	1/1	0.96	0.05	41,41,41,41	0
54	MG	1a	1781	1/1	0.96	0.09	54,54,54,54	0
54	MG	2A	3646	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3526	1/1	0.96	0.11	50,50,50,50	0
54	MG	1a	1605	1/1	0.96	0.07	43,43,43,43	0
54	MG	1A	3805	1/1	0.96	0.07	36,36,36,36	0
54	MG	1A	3164	1/1	0.96	0.05	21,21,21,21	0
54	MG	1A	3405	1/1	0.96	0.05	22,22,22,22	0
54	MG	1A	3529	1/1	0.96	0.09	45,45,45,45	0
54	MG	1A	3810	1/1	0.96	0.08	37,37,37,37	0
54	MG	2A	3354	1/1	0.96	0.05	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3653	1/1	0.96	0.14	61,61,61,61	0
54	MG	2a	1753	1/1	0.96	0.07	75,75,75,75	0
54	MG	1A	3407	1/1	0.96	0.16	50,50,50,50	0
54	MG	2A	3660	1/1	0.96	0.06	68,68,68,68	0
54	MG	1A	3297	1/1	0.96	0.07	37,37,37,37	0
54	MG	1A	3657	1/1	0.96	0.06	38,38,38,38	0
54	MG	1A	3299	1/1	0.96	0.07	33,33,33,33	0
54	MG	2A	3360	1/1	0.96	0.05	54,54,54,54	0
54	MG	1a	1616	1/1	0.96	0.13	52,52,52,52	0
54	MG	2A	3099	1/1	0.96	0.19	47,47,47,47	0
54	MG	1A	4004	1/1	0.96	0.12	42,42,42,42	0
54	MG	2a	1763	1/1	0.96	0.08	72,72,72,72	0
54	MG	2A	3365	1/1	0.96	0.08	52,52,52,52	0
54	MG	2A	3101	1/1	0.96	0.19	49,49,49,49	0
54	MG	2A	3102	1/1	0.96	0.25	57,57,57,57	0
54	MG	2A	3680	1/1	0.96	0.05	30,30,30,30	0
54	MG	2A	3681	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3085	1/1	0.96	0.14	25,25,25,25	0
54	MG	1A	3536	1/1	0.96	0.07	47,47,47,47	0
54	MG	1A	3411	1/1	0.96	0.09	45,45,45,45	0
54	MG	1A	3166	1/1	0.96	0.26	34,34,34,34	0
54	MG	2A	3687	1/1	0.96	0.15	35,35,35,35	0
54	MG	1A	3086	1/1	0.96	0.27	34,34,34,34	0
54	MG	1A	3127	1/1	0.96	0.06	17,17,17,17	0
54	MG	1B	201	1/1	0.96	0.09	37,37,37,37	0
54	MG	1a	1625	1/1	0.96	0.06	50,50,50,50	0
54	MG	1A	3305	1/1	0.96	0.08	18,18,18,18	0
54	MG	2A	3116	1/1	0.96	0.22	44,44,44,44	0
54	MG	1A	3170	1/1	0.96	0.17	33,33,33,33	0
54	MG	1A	3834	1/1	0.96	0.09	26,26,26,26	0
54	MG	1a	1809	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3424	1/1	0.96	0.06	36,36,36,36	0
55	A1CQ8	1A	4011	44/44	0.96	0.10	17,24,31,34	0
55	A1CQ8	2A	3725	44/44	0.96	0.10	29,34,40,43	0
54	MG	1B	208	1/1	0.96	0.09	35,35,35,35	0
54	MG	1A	3836	1/1	0.96	0.06	48,48,48,48	0
54	MG	1A	3224	1/1	0.96	0.21	29,29,29,29	0
54	MG	1A	3062	1/1	0.96	0.10	29,29,29,29	0
54	MG	2A	3389	1/1	0.96	0.10	28,28,28,28	0
54	MG	1A	3173	1/1	0.96	0.09	27,27,27,27	0
54	MG	1A	3678	1/1	0.96	0.10	43,43,43,43	0
54	MG	1A	3553	1/1	0.96	0.09	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3129	1/1	0.96	0.16	43,43,43,43	0
54	MG	1A	3229	1/1	0.96	0.56	30,30,30,30	0
54	MG	1A	3432	1/1	0.96	0.11	35,35,35,35	0
54	MG	1a	1642	1/1	0.96	0.15	40,40,40,40	0
54	MG	1A	3174	1/1	0.96	0.07	42,42,42,42	0
54	MG	1A	3208	1/1	0.97	0.19	31,31,31,31	0
54	MG	1A	3920	1/1	0.97	0.10	49,49,49,49	0
54	MG	2A	3549	1/1	0.97	0.06	60,60,60,60	0
54	MG	1A	3318	1/1	0.97	0.07	19,19,19,19	0
54	MG	1A	3922	1/1	0.97	0.14	24,24,24,24	0
54	MG	1A	3400	1/1	0.97	0.10	27,27,27,27	0
54	MG	1A	3319	1/1	0.97	0.05	37,37,37,37	0
54	MG	1A	3926	1/1	0.97	0.08	43,43,43,43	0
54	MG	1A	3927	1/1	0.97	0.14	42,42,42,42	0
54	MG	1A	3176	1/1	0.97	0.06	25,25,25,25	0
54	MG	1A	3584	1/1	0.97	0.06	61,61,61,61	0
54	MG	1A	3787	1/1	0.97	0.05	35,35,35,35	0
54	MG	1a	1763	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3404	1/1	0.97	0.04	16,16,16,16	0
54	MG	1E	303	1/1	0.97	0.17	29,29,29,29	0
54	MG	1A	3090	1/1	0.97	0.05	37,37,37,37	0
54	MG	1E	307	1/1	0.97	0.05	34,34,34,34	0
54	MG	1A	3113	1/1	0.97	0.20	25,25,25,25	0
54	MG	2A	3567	1/1	0.97	0.13	35,35,35,35	0
54	MG	2A	3366	1/1	0.97	0.07	66,66,66,66	0
54	MG	2A	3182	1/1	0.97	0.06	64,64,64,64	0
54	MG	1A	3934	1/1	0.97	0.06	31,31,31,31	0
54	MG	2a	1605	1/1	0.97	0.05	38,38,38,38	0
54	MG	1a	1770	1/1	0.97	0.13	57,57,57,57	0
54	MG	1a	1631	1/1	0.97	0.09	41,41,41,41	0
54	MG	2A	3016	1/1	0.97	0.12	37,37,37,37	0
54	MG	1A	3684	1/1	0.97	0.05	25,25,25,25	0
54	MG	1A	3793	1/1	0.97	0.09	34,34,34,34	0
54	MG	1A	3074	1/1	0.97	0.29	26,26,26,26	0
54	MG	1a	1635	1/1	0.97	0.05	38,38,38,38	0
54	MG	1a	1636	1/1	0.97	0.09	54,54,54,54	0
54	MG	2a	1616	1/1	0.97	0.06	53,53,53,53	0
54	MG	2A	3022	1/1	0.97	0.08	34,34,34,34	0
54	MG	1A	3144	1/1	0.97	0.11	25,25,25,25	0
54	MG	1A	3075	1/1	0.97	0.21	34,34,34,34	0
54	MG	1A	3505	1/1	0.97	0.08	43,43,43,43	0
54	MG	2A	3590	1/1	0.97	0.06	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	MG	1A	3146	1/1	0.97	0.12	26,26,26,26	0
54	MG	1A	3799	1/1	0.97	0.06	20,20,20,20	0
54	MG	1A	3413	1/1	0.97	0.10	35,35,35,35	0
54	MG	1A	3217	1/1	0.97	0.07	39,39,39,39	0
54	MG	2A	3031	1/1	0.97	0.07	36,36,36,36	0
54	MG	2A	3387	1/1	0.97	0.07	46,46,46,46	0
54	MG	2A	3601	1/1	0.97	0.06	57,57,57,57	0
54	MG	1A	3415	1/1	0.97	0.08	17,17,17,17	0
54	MG	1A	3269	1/1	0.97	0.05	43,43,43,43	0
54	MG	1A	3418	1/1	0.97	0.09	35,35,35,35	0
54	MG	1A	3419	1/1	0.97	0.07	41,41,41,41	0
54	MG	1A	3218	1/1	0.97	0.23	42,42,42,42	0
54	MG	1A	3035	1/1	0.97	0.08	28,28,28,28	0
54	MG	1A	3702	1/1	0.97	0.07	34,34,34,34	0
54	MG	2A	3397	1/1	0.97	0.05	28,28,28,28	0
54	MG	1A	3703	1/1	0.97	0.05	22,22,22,22	0
54	MG	1A	3954	1/1	0.97	0.06	33,33,33,33	0
54	MG	2A	3613	1/1	0.97	0.12	56,56,56,56	0
54	MG	1A	3517	1/1	0.97	0.11	29,29,29,29	0
54	MG	1A	3813	1/1	0.97	0.11	34,34,34,34	0
54	MG	2A	3616	1/1	0.97	0.08	45,45,45,45	0
54	MG	2A	3617	1/1	0.97	0.06	50,50,50,50	0
54	MG	1A	3339	1/1	0.97	0.04	33,33,33,33	0
54	MG	2A	3403	1/1	0.97	0.11	58,58,58,58	0
54	MG	1a	1796	1/1	0.97	0.06	57,57,57,57	0
54	MG	1A	3184	1/1	0.97	0.23	26,26,26,26	0
54	MG	1N	204	1/1	0.97	0.12	61,61,61,61	0
54	MG	1A	3818	1/1	0.97	0.12	35,35,35,35	0
54	MG	2A	3409	1/1	0.97	0.11	54,54,54,54	0
54	MG	2A	3218	1/1	0.97	0.20	53,53,53,53	0
54	MG	1A	3274	1/1	0.97	0.14	45,45,45,45	0
54	MG	1A	3607	1/1	0.97	0.09	59,59,59,59	0
54	MG	2A	3413	1/1	0.97	0.07	40,40,40,40	0
54	MG	1A	3821	1/1	0.97	0.09	21,21,21,21	0
54	MG	1A	3710	1/1	0.97	0.08	22,22,22,22	0
54	MG	1A	3117	1/1	0.97	0.22	26,26,26,26	0
54	MG	1A	3276	1/1	0.97	0.07	12,12,12,12	0
54	MG	1A	3825	1/1	0.97	0.16	47,47,47,47	0
54	MG	1a	1807	1/1	0.97	0.05	85,85,85,85	0
54	MG	2A	3229	1/1	0.97	0.07	41,41,41,41	0
54	MG	2A	3422	1/1	0.97	0.07	52,52,52,52	0
54	MG	2A	3647	1/1	0.97	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3424	1/1	0.97	0.09	59,59,59,59	0
54	MG	1A	3430	1/1	0.97	0.05	46,46,46,46	0
54	MG	2a	1667	1/1	0.97	0.13	56,56,56,56	0
54	MG	2A	3650	1/1	0.97	0.06	45,45,45,45	0
54	MG	1A	3223	1/1	0.97	0.18	34,34,34,34	0
54	MG	2A	3232	1/1	0.97	0.32	51,51,51,51	0
54	MG	1A	3018	1/1	0.97	0.18	27,27,27,27	0
54	MG	1A	3119	1/1	0.97	0.18	31,31,31,31	0
54	MG	1A	3226	1/1	0.97	0.28	25,25,25,25	0
54	MG	2A	3656	1/1	0.97	0.05	71,71,71,71	0
54	MG	1A	3833	1/1	0.97	0.10	51,51,51,51	0
54	MG	1Q	205	1/1	0.97	0.14	34,34,34,34	0
54	MG	1A	3227	1/1	0.97	0.18	55,55,55,55	0
54	MG	1A	3530	1/1	0.97	0.08	31,31,31,31	0
54	MG	2A	3661	1/1	0.97	0.07	56,56,56,56	0
54	MG	1A	3095	1/1	0.97	0.17	32,32,32,32	0
54	MG	1R	202	1/1	0.97	0.09	30,30,30,30	0
54	MG	2A	3243	1/1	0.97	0.16	43,43,43,43	0
54	MG	2A	3668	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3153	1/1	0.97	0.10	25,25,25,25	0
54	MG	1R	205	1/1	0.97	0.13	35,35,35,35	0
54	MG	1A	3122	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3725	1/1	0.97	0.05	42,42,42,42	0
54	MG	1A	3727	1/1	0.97	0.09	19,19,19,19	0
54	MG	1A	3728	1/1	0.97	0.06	31,31,31,31	0
54	MG	1A	3729	1/1	0.97	0.05	39,39,39,39	0
54	MG	1A	3123	1/1	0.97	0.11	32,32,32,32	0
54	MG	1A	3235	1/1	0.97	0.25	33,33,33,33	0
54	MG	1U	202	1/1	0.97	0.55	36,36,36,36	0
54	MG	1A	3988	1/1	0.97	0.04	22,22,22,22	0
54	MG	2A	3085	1/1	0.97	0.23	33,33,33,33	0
54	MG	1A	3537	1/1	0.97	0.07	34,34,34,34	0
54	MG	1A	3097	1/1	0.97	0.07	9,9,9,9	0
54	MG	2a	1699	1/1	0.97	0.04	43,43,43,43	0
54	MG	2a	1700	1/1	0.97	0.12	53,53,53,53	0
54	MG	1A	3628	1/1	0.97	0.05	45,45,45,45	0
54	MG	2A	3455	1/1	0.97	0.16	58,58,58,58	0
54	MG	2A	3260	1/1	0.97	0.08	26,26,26,26	0
54	MG	1A	3066	1/1	0.97	0.06	51,51,51,51	0
54	MG	1V	203	1/1	0.97	0.10	33,33,33,33	0
54	MG	1A	3011	1/1	0.97	0.07	32,32,32,32	0
54	MG	2A	3694	1/1	0.97	0.08	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1840	1/1	0.97	0.06	66,66,66,66	0
54	MG	2A	3696	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3451	1/1	0.97	0.06	10,10,10,10	0
54	MG	1A	3632	1/1	0.97	0.07	29,29,29,29	0
54	MG	1a	1843	1/1	0.97	0.10	62,62,62,62	0
54	MG	2A	3465	1/1	0.97	0.10	45,45,45,45	0
54	MG	1A	3543	1/1	0.97	0.14	38,38,38,38	0
54	MG	1A	3100	1/1	0.97	0.12	24,24,24,24	0
54	MG	2A	3703	1/1	0.97	0.09	63,63,63,63	0
54	MG	1A	3068	1/1	0.97	0.06	10,10,10,10	0
54	MG	2A	3272	1/1	0.97	0.08	41,41,41,41	0
54	MG	1X	101	1/1	0.97	0.08	50,50,50,50	0
54	MG	1A	3294	1/1	0.97	0.30	26,26,26,26	0
54	MG	1A	3549	1/1	0.97	0.07	39,39,39,39	0
54	MG	2A	3474	1/1	0.97	0.06	32,32,32,32	0
54	MG	1A	3082	1/1	0.97	0.24	29,29,29,29	0
54	MG	2A	3477	1/1	0.97	0.08	76,76,76,76	0
54	MG	2A	3713	1/1	0.97	0.12	65,65,65,65	0
54	MG	2A	3104	1/1	0.97	0.07	53,53,53,53	0
54	MG	1A	3747	1/1	0.97	0.05	24,24,24,24	0
54	MG	2A	3106	1/1	0.97	0.07	27,27,27,27	0
54	MG	2A	3107	1/1	0.97	0.10	39,39,39,39	0
54	MG	1A	3458	1/1	0.97	0.04	31,31,31,31	0
54	MG	1A	3749	1/1	0.97	0.14	43,43,43,43	0
54	MG	2a	1737	1/1	0.97	0.06	51,51,51,51	0
54	MG	1A	3296	1/1	0.97	0.20	30,30,30,30	0
54	MG	1a	1858	1/1	0.97	0.09	74,74,74,74	0
54	MG	1A	3368	1/1	0.97	0.05	18,18,18,18	0
54	MG	1A	3039	1/1	0.97	0.05	42,42,42,42	0
54	MG	1A	3371	1/1	0.97	0.09	16,16,16,16	0
54	MG	1A	3882	1/1	0.97	0.05	21,21,21,21	0
54	MG	2a	1744	1/1	0.97	0.08	39,39,39,39	0
54	MG	1A	3298	1/1	0.97	0.06	18,18,18,18	0
54	MG	1A	3374	1/1	0.97	0.09	13,13,13,13	0
54	MG	2A	3495	1/1	0.97	0.06	40,40,40,40	0
54	MG	11	103	1/1	0.97	0.05	32,32,32,32	0
54	MG	1A	3757	1/1	0.97	0.07	34,34,34,34	0
54	MG	1B	204	1/1	0.97	0.08	43,43,43,43	0
54	MG	1A	3648	1/1	0.97	0.06	56,56,56,56	0
54	MG	1A	3466	1/1	0.97	0.07	12,12,12,12	0
54	MG	1A	3244	1/1	0.97	0.32	35,35,35,35	0
54	MG	1A	3379	1/1	0.97	0.05	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3084	1/1	0.97	0.06	24,24,24,24	0
54	MG	1A	3301	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3106	1/1	0.97	0.25	20,20,20,20	0
54	MG	15	105	1/1	0.97	0.08	27,27,27,27	0
54	MG	1A	3386	1/1	0.97	0.04	39,39,39,39	0
54	MG	2B	218	1/1	0.97	0.05	54,54,54,54	0
54	MG	2A	3509	1/1	0.97	0.04	44,44,44,44	0
54	MG	1A	3032	1/1	0.97	0.09	47,47,47,47	0
54	MG	2A	3133	1/1	0.97	0.14	32,32,32,32	0
54	MG	2A	3134	1/1	0.97	0.06	35,35,35,35	0
54	MG	2A	3312	1/1	0.97	0.07	53,53,53,53	0
54	MG	17	102	1/1	0.97	0.14	18,18,18,18	0
54	MG	2A	3515	1/1	0.97	0.07	36,36,36,36	0
54	MG	1A	3135	1/1	0.97	0.23	30,30,30,30	0
54	MG	2A	3316	1/1	0.97	0.10	24,24,24,24	0
54	MG	1A	3020	1/1	0.97	0.17	24,24,24,24	0
54	MG	2A	3138	1/1	0.97	0.13	41,41,41,41	0
54	MG	1A	3903	1/1	0.97	0.12	48,48,48,48	0
54	MG	1B	222	1/1	0.97	0.10	49,49,49,49	0
54	MG	2A	3522	1/1	0.97	0.09	32,32,32,32	0
54	MG	2A	3523	1/1	0.97	0.06	28,28,28,28	0
54	MG	1A	3109	1/1	0.97	0.07	32,32,32,32	0
54	MG	1A	3087	1/1	0.97	0.46	38,38,38,38	0
54	MG	1A	3664	1/1	0.97	0.06	23,23,23,23	0
54	MG	1A	3772	1/1	0.97	0.05	20,20,20,20	0
54	MG	1A	3485	1/1	0.97	0.10	43,43,43,43	0
54	MG	2A	3146	1/1	0.97	0.13	46,46,46,46	0
54	MG	2A	3329	1/1	0.97	0.09	41,41,41,41	0
54	MG	2A	3147	1/1	0.97	0.17	56,56,56,56	0
54	MG	1A	3253	1/1	0.97	0.07	24,24,24,24	0
54	MG	2A	3149	1/1	0.97	0.08	35,35,35,35	0
54	MG	1A	3574	1/1	0.97	0.08	34,34,34,34	0
54	MG	2P	202	1/1	0.97	0.09	62,62,62,62	0
54	MG	1A	3001	1/1	0.97	0.08	26,26,26,26	0
54	MG	2Q	201	1/1	0.97	0.12	46,46,46,46	0
54	MG	2A	3152	1/1	0.97	0.16	48,48,48,48	0
54	MG	2A	3537	1/1	0.97	0.06	51,51,51,51	0
54	MG	1A	3175	1/1	0.97	0.17	30,30,30,30	0
54	MG	2A	3338	1/1	0.97	0.09	28,28,28,28	0
54	MG	2A	3155	1/1	0.97	0.06	40,40,40,40	0
54	MG	1A	3257	1/1	0.97	0.12	33,33,33,33	0
54	MG	1D	304	1/1	0.97	0.15	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3917	1/1	0.97	0.14	50,50,50,50	0
54	MG	1A	3918	1/1	0.97	0.08	31,31,31,31	0
58	ZN	29	501	1/1	0.97	0.05	58,58,58,58	0
54	MG	2A	3097	1/1	0.98	0.07	52,52,52,52	0
54	MG	1D	302	1/1	0.98	0.18	25,25,25,25	0
54	MG	1A	3811	1/1	0.98	0.06	30,30,30,30	0
54	MG	1A	3638	1/1	0.98	0.05	49,49,49,49	0
54	MG	1D	305	1/1	0.98	0.34	26,26,26,26	0
54	MG	1A	3330	1/1	0.98	0.03	19,19,19,19	0
54	MG	2a	1611	1/1	0.98	0.14	45,45,45,45	0
54	MG	1A	3814	1/1	0.98	0.11	31,31,31,31	0
54	MG	2a	1613	1/1	0.98	0.11	45,45,45,45	0
54	MG	1A	3006	1/1	0.98	0.07	16,16,16,16	0
54	MG	2A	3428	1/1	0.98	0.05	35,35,35,35	0
54	MG	1A	3332	1/1	0.98	0.06	9,9,9,9	0
54	MG	2A	3257	1/1	0.98	0.06	35,35,35,35	0
54	MG	1A	3642	1/1	0.98	0.07	34,34,34,34	0
54	MG	1A	3376	1/1	0.98	0.05	11,11,11,11	0
54	MG	1A	3377	1/1	0.98	0.07	16,16,16,16	0
54	MG	2A	3622	1/1	0.98	0.07	56,56,56,56	0
54	MG	1A	3333	1/1	0.98	0.10	21,21,21,21	0
54	MG	2A	3624	1/1	0.98	0.06	64,64,64,64	0
54	MG	1A	3572	1/1	0.98	0.04	28,28,28,28	0
54	MG	1A	3733	1/1	0.98	0.04	38,38,38,38	0
54	MG	2A	3628	1/1	0.98	0.12	45,45,45,45	0
54	MG	1A	3503	1/1	0.98	0.05	24,24,24,24	0
54	MG	1A	3380	1/1	0.98	0.04	28,28,28,28	0
54	MG	1A	3036	1/1	0.98	0.05	22,22,22,22	0
54	MG	2A	3635	1/1	0.98	0.09	56,56,56,56	0
54	MG	2A	3636	1/1	0.98	0.04	34,34,34,34	0
54	MG	1A	3437	1/1	0.98	0.07	33,33,33,33	0
54	MG	1A	3249	1/1	0.98	0.07	24,24,24,24	0
54	MG	1A	3578	1/1	0.98	0.05	33,33,33,33	0
54	MG	1A	3049	1/1	0.98	0.21	37,37,37,37	0
54	MG	2A	3271	1/1	0.98	0.04	23,23,23,23	0
54	MG	1A	3385	1/1	0.98	0.05	18,18,18,18	0
54	MG	1A	3132	1/1	0.98	0.08	29,29,29,29	0
54	MG	2A	3274	1/1	0.98	0.05	60,60,60,60	0
54	MG	1F	301	1/1	0.98	0.17	22,22,22,22	0
54	MG	1A	3656	1/1	0.98	0.05	14,14,14,14	0
54	MG	1A	3950	1/1	0.98	0.04	22,22,22,22	0
54	MG	1A	3512	1/1	0.98	0.08	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3280	1/1	0.98	0.08	28,28,28,28	0
54	MG	1A	3443	1/1	0.98	0.10	43,43,43,43	0
54	MG	1A	3659	1/1	0.98	0.09	33,33,33,33	0
54	MG	1A	3338	1/1	0.98	0.08	17,17,17,17	0
54	MG	1A	3057	1/1	0.98	0.07	30,30,30,30	0
54	MG	1F	310	1/1	0.98	0.05	38,38,38,38	0
54	MG	2A	3287	1/1	0.98	0.09	35,35,35,35	0
54	MG	1A	3446	1/1	0.98	0.07	30,30,30,30	0
54	MG	1A	3148	1/1	0.98	0.08	23,23,23,23	0
54	MG	1A	3254	1/1	0.98	0.05	36,36,36,36	0
54	MG	1A	3667	1/1	0.98	0.09	28,28,28,28	0
54	MG	1A	3342	1/1	0.98	0.07	44,44,44,44	0
54	MG	2A	3662	1/1	0.98	0.06	46,46,46,46	0
54	MG	1A	3232	1/1	0.98	0.19	27,27,27,27	0
54	MG	2a	1658	1/1	0.98	0.15	34,34,34,34	0
54	MG	1A	3756	1/1	0.98	0.14	40,40,40,40	0
54	MG	1A	3851	1/1	0.98	0.05	16,16,16,16	0
54	MG	1A	3234	1/1	0.98	0.25	25,25,25,25	0
54	MG	1A	3065	1/1	0.98	0.08	30,30,30,30	0
54	MG	1G	203	1/1	0.98	0.12	52,52,52,52	0
54	MG	1A	3096	1/1	0.98	0.14	29,29,29,29	0
54	MG	2A	3674	1/1	0.98	0.04	36,36,36,36	0
54	MG	1A	3856	1/1	0.98	0.11	32,32,32,32	0
54	MG	2A	3676	1/1	0.98	0.12	70,70,70,70	0
54	MG	1A	3308	1/1	0.98	0.05	14,14,14,14	0
54	MG	2A	3476	1/1	0.98	0.07	37,37,37,37	0
54	MG	1A	3858	1/1	0.98	0.04	40,40,40,40	0
54	MG	1A	3674	1/1	0.98	0.05	33,33,33,33	0
54	MG	2A	3479	1/1	0.98	0.06	29,29,29,29	0
54	MG	1A	3309	1/1	0.98	0.07	14,14,14,14	0
54	MG	2A	3482	1/1	0.98	0.05	43,43,43,43	0
54	MG	1A	3676	1/1	0.98	0.06	38,38,38,38	0
54	MG	2A	3306	1/1	0.98	0.05	51,51,51,51	0
54	MG	1A	3044	1/1	0.98	0.12	22,22,22,22	0
54	MG	1A	3016	1/1	0.98	0.41	30,30,30,30	0
54	MG	1a	1646	1/1	0.98	0.08	40,40,40,40	0
54	MG	1A	3864	1/1	0.98	0.09	27,27,27,27	0
54	MG	2A	3154	1/1	0.98	0.08	31,31,31,31	0
54	MG	1A	3865	1/1	0.98	0.04	25,25,25,25	0
54	MG	1A	3866	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3261	1/1	0.98	0.10	45,45,45,45	0
54	MG	2A	3315	1/1	0.98	0.11	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3979	1/1	0.98	0.14	7,7,7,7	0
54	MG	2A	3159	1/1	0.98	0.04	31,31,31,31	0
54	MG	1A	3980	1/1	0.98	0.07	32,32,32,32	0
54	MG	1A	3403	1/1	0.98	0.05	20,20,20,20	0
54	MG	1A	3982	1/1	0.98	0.04	28,28,28,28	0
54	MG	2A	3163	1/1	0.98	0.07	44,44,44,44	0
54	MG	1A	3872	1/1	0.98	0.08	50,50,50,50	0
54	MG	1A	3046	1/1	0.98	0.11	14,14,14,14	0
54	MG	1A	3465	1/1	0.98	0.09	15,15,15,15	0
54	MG	2A	3326	1/1	0.98	0.06	27,27,27,27	0
54	MG	1A	3171	1/1	0.98	0.27	20,20,20,20	0
54	MG	2a	1697	1/1	0.98	0.04	46,46,46,46	0
54	MG	1Q	204	1/1	0.98	0.04	23,23,23,23	0
54	MG	1A	3406	1/1	0.98	0.09	28,28,28,28	0
54	MG	1A	3878	1/1	0.98	0.07	12,12,12,12	0
54	MG	2A	3710	1/1	0.98	0.11	29,29,29,29	0
54	MG	2A	3171	1/1	0.98	0.19	42,42,42,42	0
54	MG	1A	3605	1/1	0.98	0.04	24,24,24,24	0
54	MG	2A	3173	1/1	0.98	0.08	43,43,43,43	0
54	MG	2A	3714	1/1	0.98	0.06	37,37,37,37	0
54	MG	1A	3880	1/1	0.98	0.07	47,47,47,47	0
54	MG	1A	3535	1/1	0.98	0.07	34,34,34,34	0
54	MG	2a	1708	1/1	0.98	0.07	38,38,38,38	0
54	MG	2A	3029	1/1	0.98	0.04	23,23,23,23	0
54	MG	2A	3177	1/1	0.98	0.05	54,54,54,54	0
54	MG	1R	203	1/1	0.98	0.05	35,35,35,35	0
54	MG	1A	3687	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3317	1/1	0.98	0.06	22,22,22,22	0
54	MG	1A	3221	1/1	0.98	0.06	32,32,32,32	0
54	MG	1A	3777	1/1	0.98	0.13	54,54,54,54	0
54	MG	1A	3470	1/1	0.98	0.06	17,17,17,17	0
54	MG	1A	3888	1/1	0.98	0.11	53,53,53,53	0
54	MG	1A	3357	1/1	0.98	0.05	37,37,37,37	0
54	MG	2A	3348	1/1	0.98	0.05	47,47,47,47	0
54	MG	1A	3154	1/1	0.98	0.14	42,42,42,42	0
54	MG	2A	3350	1/1	0.98	0.06	31,31,31,31	0
54	MG	1A	3473	1/1	0.98	0.08	42,42,42,42	0
54	MG	1A	3474	1/1	0.98	0.05	11,11,11,11	0
54	MG	1A	3697	1/1	0.98	0.05	62,62,62,62	0
54	MG	1A	3784	1/1	0.98	0.10	22,22,22,22	0
54	MG	2a	1728	1/1	0.98	0.07	67,67,67,67	0
54	MG	2A	3043	1/1	0.98	0.06	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3896	1/1	0.98	0.06	49,49,49,49	0
54	MG	2a	1731	1/1	0.98	0.08	42,42,42,42	0
54	MG	1a	1810	1/1	0.98	0.04	50,50,50,50	0
54	MG	1A	3078	1/1	0.98	0.23	35,35,35,35	0
54	MG	2A	3047	1/1	0.98	0.09	48,48,48,48	0
54	MG	1V	201	1/1	0.98	0.13	19,19,19,19	0
54	MG	1A	3476	1/1	0.98	0.07	28,28,28,28	0
54	MG	1A	3412	1/1	0.98	0.07	37,37,37,37	0
54	MG	1a	1815	1/1	0.98	0.18	59,59,59,59	0
54	MG	2A	3200	1/1	0.98	0.05	40,40,40,40	0
54	MG	1A	3900	1/1	0.98	0.04	39,39,39,39	0
54	MG	2A	3542	1/1	0.98	0.09	25,25,25,25	0
54	MG	1A	3618	1/1	0.98	0.05	32,32,32,32	0
54	MG	1a	1685	1/1	0.98	0.13	32,32,32,32	0
54	MG	1A	3902	1/1	0.98	0.06	30,30,30,30	0
54	MG	1A	3548	1/1	0.98	0.14	19,19,19,19	0
54	MG	1A	3089	1/1	0.98	0.10	34,34,34,34	0
54	MG	2A	3059	1/1	0.98	0.19	30,30,30,30	0
54	MG	1W	203	1/1	0.98	0.10	21,21,21,21	0
54	MG	2A	3061	1/1	0.98	0.06	28,28,28,28	0
54	MG	1A	3905	1/1	0.98	0.08	36,36,36,36	0
54	MG	1A	3906	1/1	0.98	0.07	36,36,36,36	0
54	MG	1B	207	1/1	0.98	0.10	43,43,43,43	0
54	MG	2A	3555	1/1	0.98	0.04	48,48,48,48	0
54	MG	2A	3379	1/1	0.98	0.05	29,29,29,29	0
54	MG	1A	3323	1/1	0.98	0.04	21,21,21,21	0
54	MG	2A	3066	1/1	0.98	0.05	45,45,45,45	0
54	MG	1A	3480	1/1	0.98	0.06	36,36,36,36	0
54	MG	1A	3481	1/1	0.98	0.07	27,27,27,27	0
54	MG	10	102	1/1	0.98	0.15	38,38,38,38	0
54	MG	10	103	1/1	0.98	0.11	40,40,40,40	0
54	MG	1A	3625	1/1	0.98	0.05	30,30,30,30	0
54	MG	2A	3072	1/1	0.98	0.10	31,31,31,31	0
54	MG	2A	3221	1/1	0.98	0.07	38,38,38,38	0
54	MG	2A	3222	1/1	0.98	0.09	45,45,45,45	0
54	MG	1A	3482	1/1	0.98	0.08	36,36,36,36	0
54	MG	1B	215	1/1	0.98	0.07	31,31,31,31	0
54	MG	2A	3393	1/1	0.98	0.05	26,26,26,26	0
54	MG	1A	3363	1/1	0.98	0.09	12,12,12,12	0
54	MG	2a	1769	1/1	0.98	0.10	47,47,47,47	0
54	MG	1A	3416	1/1	0.98	0.12	42,42,42,42	0
54	MG	1A	3292	1/1	0.98	0.19	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3325	1/1	0.98	0.10	38,38,38,38	0
54	MG	1A	3366	1/1	0.98	0.04	34,34,34,34	0
54	MG	1B	221	1/1	0.98	0.09	54,54,54,54	0
54	MG	1A	3420	1/1	0.98	0.04	18,18,18,18	0
54	MG	2A	3580	1/1	0.98	0.10	51,51,51,51	0
54	MG	1B	223	1/1	0.98	0.04	38,38,38,38	0
54	MG	1A	3293	1/1	0.98	0.23	27,27,27,27	0
54	MG	13	101	1/1	0.98	0.11	23,23,23,23	0
54	MG	2A	3586	1/1	0.98	0.06	23,23,23,23	0
54	MG	2A	3404	1/1	0.98	0.20	37,37,37,37	0
54	MG	1A	3069	1/1	0.98	0.06	32,32,32,32	0
54	MG	1A	3718	1/1	0.98	0.12	38,38,38,38	0
54	MG	1a	1714	1/1	0.98	0.07	36,36,36,36	0
54	MG	2Y	201	1/1	0.98	0.14	45,45,45,45	0
54	MG	2A	3592	1/1	0.98	0.04	26,26,26,26	0
54	MG	1a	1849	1/1	0.98	0.06	57,57,57,57	0
54	MG	1A	3369	1/1	0.98	0.06	12,12,12,12	0
54	MG	1A	3807	1/1	0.98	0.04	37,37,37,37	0
54	MG	2A	3596	1/1	0.98	0.07	28,28,28,28	0
54	MG	2A	3597	1/1	0.98	0.04	44,44,44,44	0
54	MG	2A	3241	1/1	0.98	0.21	38,38,38,38	0
54	MG	1A	3924	1/1	0.98	0.18	25,25,25,25	0
54	MG	1a	1853	1/1	0.98	0.05	53,53,53,53	0
54	MG	1A	3720	1/1	0.98	0.06	29,29,29,29	0
54	MG	1A	3270	1/1	0.98	0.08	37,37,37,37	0
54	MG	2A	3604	1/1	0.98	0.10	71,71,71,71	0
54	MG	2A	3416	1/1	0.98	0.07	50,50,50,50	0
54	MG	1a	1856	1/1	0.98	0.10	46,46,46,46	0
54	MG	1A	3329	1/1	0.98	0.04	23,23,23,23	0
58	ZN	2n	102	1/1	0.98	0.07	103,103,103,103	0
59	SF4	1d	306	8/8	0.98	0.04	54,64,67,81	0
59	SF4	2d	501	8/8	0.98	0.05	62,71,77,83	0
54	MG	1A	3373	1/1	0.99	0.04	28,28,28,28	0
54	MG	1A	3310	1/1	0.99	0.07	20,20,20,20	0
54	MG	2A	3577	1/1	0.99	0.07	31,31,31,31	0
54	MG	1A	3539	1/1	0.99	0.03	56,56,56,56	0
54	MG	1A	3262	1/1	0.99	0.20	29,29,29,29	0
54	MG	2A	3686	1/1	0.99	0.04	28,28,28,28	0
54	MG	1E	304	1/1	0.99	0.04	28,28,28,28	0
54	MG	1A	3614	1/1	0.99	0.12	34,34,34,34	0
54	MG	2A	3582	1/1	0.99	0.06	63,63,63,63	0
54	MG	2A	3583	1/1	0.99	0.06	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1E	306	1/1	0.99	0.09	9,9,9,9	0
54	MG	1A	3693	1/1	0.99	0.04	11,11,11,11	0
54	MG	1A	3312	1/1	0.99	0.03	24,24,24,24	0
54	MG	1A	3508	1/1	0.99	0.05	58,58,58,58	0
54	MG	2A	3588	1/1	0.99	0.04	41,41,41,41	0
54	MG	1A	3830	1/1	0.99	0.08	33,33,33,33	0
54	MG	1A	3887	1/1	0.99	0.10	21,21,21,21	0
54	MG	2A	3321	1/1	0.99	0.05	37,37,37,37	0
54	MG	1a	1839	1/1	0.99	0.09	43,43,43,43	0
54	MG	2A	3497	1/1	0.99	0.06	41,41,41,41	0
54	MG	1A	3398	1/1	0.99	0.09	14,14,14,14	0
54	MG	1A	3832	1/1	0.99	0.09	28,28,28,28	0
54	MG	1A	3447	1/1	0.99	0.10	31,31,31,31	0
54	MG	1A	3891	1/1	0.99	0.03	36,36,36,36	0
54	MG	2A	3598	1/1	0.99	0.03	40,40,40,40	0
54	MG	2a	1720	1/1	0.99	0.04	58,58,58,58	0
54	MG	1A	3162	1/1	0.99	0.05	26,26,26,26	0
54	MG	1F	308	1/1	0.99	0.11	26,26,26,26	0
54	MG	1A	3743	1/1	0.99	0.03	23,23,23,23	0
54	MG	2A	3330	1/1	0.99	0.05	31,31,31,31	0
54	MG	1A	3546	1/1	0.99	0.04	23,23,23,23	0
54	MG	2a	1726	1/1	0.99	0.05	52,52,52,52	0
54	MG	1A	3378	1/1	0.99	0.03	14,14,14,14	0
54	MG	1A	3660	1/1	0.99	0.11	46,46,46,46	0
54	MG	1A	3791	1/1	0.99	0.10	14,14,14,14	0
54	MG	1A	3622	1/1	0.99	0.13	34,34,34,34	0
54	MG	1A	3450	1/1	0.99	0.03	38,38,38,38	0
54	MG	1A	3051	1/1	0.99	0.27	30,30,30,30	0
54	MG	2A	3423	1/1	0.99	0.05	45,45,45,45	0
54	MG	1A	3706	1/1	0.99	0.03	35,35,35,35	0
54	MG	1A	3361	1/1	0.99	0.04	23,23,23,23	0
54	MG	1A	3845	1/1	0.99	0.05	42,42,42,42	0
54	MG	1B	212	1/1	0.99	0.05	39,39,39,39	0
54	MG	1B	213	1/1	0.99	0.03	45,45,45,45	0
54	MG	1a	1713	1/1	0.99	0.05	41,41,41,41	0
54	MG	2A	3109	1/1	0.99	0.08	42,42,42,42	0
54	MG	1A	3103	1/1	0.99	0.21	24,24,24,24	0
54	MG	1A	3847	1/1	0.99	0.04	21,21,21,21	0
54	MG	1A	3666	1/1	0.99	0.10	39,39,39,39	0
54	MG	1A	3849	1/1	0.99	0.04	25,25,25,25	0
54	MG	1A	3908	1/1	0.99	0.11	53,53,53,53	0
54	MG	2A	3351	1/1	0.99	0.04	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3455	1/1	0.99	0.07	14,14,14,14	0
54	MG	1A	3140	1/1	0.99	0.04	32,32,32,32	0
54	MG	2A	3626	1/1	0.99	0.04	49,49,49,49	0
54	MG	1A	3427	1/1	0.99	0.05	21,21,21,21	0
54	MG	1A	3853	1/1	0.99	0.03	29,29,29,29	0
54	MG	1A	3487	1/1	0.99	0.06	8,8,8,8	0
54	MG	1A	3428	1/1	0.99	0.04	16,16,16,16	0
54	MG	2A	3121	1/1	0.99	0.15	37,37,37,37	0
54	MG	2A	3632	1/1	0.99	0.13	61,61,61,61	0
54	MG	2A	3633	1/1	0.99	0.03	34,34,34,34	0
54	MG	2A	3276	1/1	0.99	0.06	34,34,34,34	0
54	MG	1A	3383	1/1	0.99	0.03	16,16,16,16	0
54	MG	1a	1726	1/1	0.99	0.04	27,27,27,27	0
54	MG	2A	3362	1/1	0.99	0.05	30,30,30,30	0
54	MG	1A	3233	1/1	0.99	0.15	18,18,18,18	0
54	MG	1a	1728	1/1	0.99	0.05	42,42,42,42	0
54	MG	1A	3009	1/1	0.99	0.15	21,21,21,21	0
54	MG	1A	3525	1/1	0.99	0.04	48,48,48,48	0
54	MG	2A	3452	1/1	0.99	0.07	34,34,34,34	0
54	MG	2A	3051	1/1	0.99	0.25	40,40,40,40	0
54	MG	2A	3645	1/1	0.99	0.03	31,31,31,31	0
54	MG	2A	3544	1/1	0.99	0.04	40,40,40,40	0
54	MG	1A	3121	1/1	0.99	0.07	15,15,15,15	0
54	MG	2A	3285	1/1	0.99	0.04	32,32,32,32	0
54	MG	1a	1732	1/1	0.99	0.03	47,47,47,47	0
54	MG	1A	3040	1/1	0.99	0.10	30,30,30,30	0
54	MG	1A	3434	1/1	0.99	0.05	47,47,47,47	0
54	MG	2E	308	1/1	0.99	0.06	21,21,21,21	0
54	MG	17	104	1/1	0.99	0.05	45,45,45,45	0
54	MG	1A	3496	1/1	0.99	0.04	41,41,41,41	0
54	MG	1A	3565	1/1	0.99	0.06	32,32,32,32	0
54	MG	1A	3388	1/1	0.99	0.04	13,13,13,13	0
54	MG	1A	3169	1/1	0.99	0.14	29,29,29,29	0
54	MG	1A	3984	1/1	0.99	0.07	48,48,48,48	0
54	MG	1A	3867	1/1	0.99	0.05	42,42,42,42	0
54	MG	1A	3815	1/1	0.99	0.03	12,12,12,12	0
54	MG	1A	3726	1/1	0.99	0.04	33,33,33,33	0
54	MG	1A	3871	1/1	0.99	0.03	22,22,22,22	0
54	MG	2A	3470	1/1	0.99	0.03	36,36,36,36	0
54	MG	2A	3663	1/1	0.99	0.03	40,40,40,40	0
54	MG	2A	3561	1/1	0.99	0.04	52,52,52,52	0
54	MG	1a	1745	1/1	0.99	0.04	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3666	1/1	0.99	0.03	60,60,60,60	0
54	MG	1D	310	1/1	0.99	0.08	15,15,15,15	0
54	MG	1a	1819	1/1	0.99	0.04	54,54,54,54	0
54	MG	1A	3989	1/1	0.99	0.11	18,18,18,18	0
54	MG	1A	3322	1/1	0.99	0.06	36,36,36,36	0
54	MG	2A	3671	1/1	0.99	0.04	55,55,55,55	0
54	MG	1A	3210	1/1	0.99	0.15	28,28,28,28	0
54	MG	2A	3673	1/1	0.99	0.06	57,57,57,57	0
54	MG	1A	3874	1/1	0.99	0.08	44,44,44,44	0
58	ZN	15	107	1/1	0.99	0.03	57,57,57,57	0
58	ZN	16	501	1/1	0.99	0.02	38,38,38,38	0
58	ZN	1n	103	1/1	0.99	0.02	72,72,72,72	0
54	MG	1A	3354	1/1	0.99	0.05	15,15,15,15	0
54	MG	2A	3391	1/1	0.99	0.05	45,45,45,45	0
58	ZN	25	103	1/1	0.99	0.04	88,88,88,88	0
58	ZN	26	102	1/1	0.99	0.02	51,51,51,51	0
54	MG	1A	3239	1/1	0.99	0.18	38,38,38,38	0
54	MG	2A	3572	1/1	0.99	0.04	58,58,58,58	0
54	MG	2A	3481	1/1	0.99	0.05	28,28,28,28	0
54	MG	1A	3441	1/1	0.99	0.06	36,36,36,36	0
54	MG	2A	3464	1/1	1.00	0.03	21,21,21,21	0
54	MG	1A	3598	1/1	1.00	0.06	19,19,19,19	0
54	MG	2A	3634	1/1	1.00	0.03	37,37,37,37	0
54	MG	1A	3488	1/1	1.00	0.05	14,14,14,14	0
54	MG	2A	3346	1/1	1.00	0.03	25,25,25,25	0
54	MG	1A	3696	1/1	1.00	0.06	28,28,28,28	0
54	MG	1A	3452	1/1	1.00	0.02	32,32,32,32	0
54	MG	1A	3870	1/1	1.00	0.02	19,19,19,19	0
58	ZN	19	103	1/1	1.00	0.02	39,39,39,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.