



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 01:14 AM EDT

PDB ID : 6CZR / pdb_00006czt
Title : The structure of amicitin bound to the 70S ribosome
Authors : Eiler, D.R.; Steitz, T.A.; Looper, R.E.; Serrano, C.M.; Kannareddy, H.R.;
Koch, M.R.; Barrows, L.R.; Testa, C.A.; Sebahar, P.R.
Deposited on : 2018-04-09
Resolution : 3.14 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 ⓘ](#)) 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

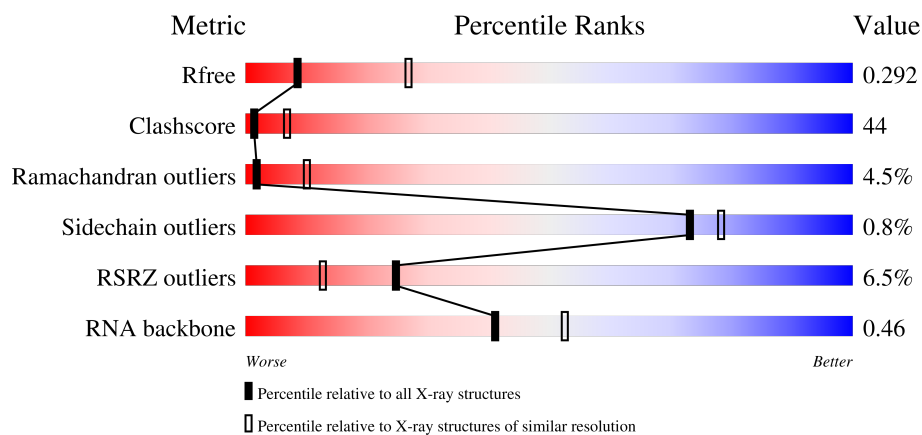
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)
RNA backbone	3983	1040 (3.38-2.90)

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	3% 22% 63% 14%
1	2A	2915	4% 17% 67% 15%
2	1B	120	36% 59% 5%
2	2B	120	8% 23% 66% 11%

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Mol	Chain	Length	Quality of chain
3	1D	275	
3	2D	275	
4	1E	204	
4	2E	204	
5	1F	203	
5	2F	203	
6	1G	181	
6	2G	181	
7	1H	174	
7	2H	174	
8	1I	147	
8	2I	147	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	149	
11	2P	149	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	110	
14	2S	110	
15	1T	131	

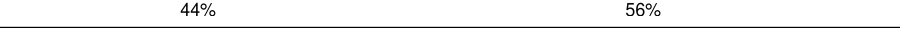
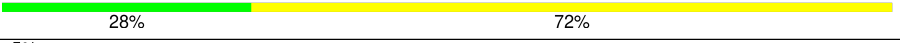
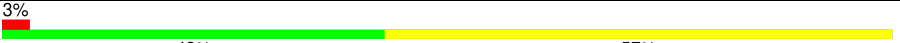
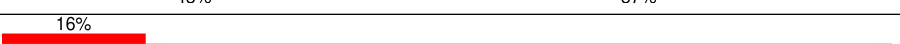
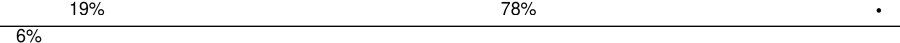
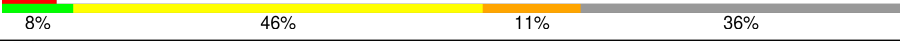
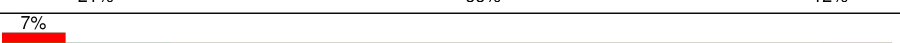
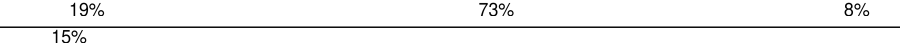
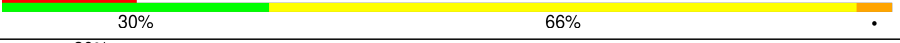
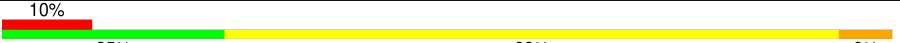
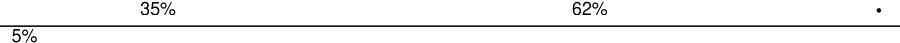
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Mol	Chain	Length	Quality of chain
15	2T	131	
16	1U	116	
16	2U	116	
17	1V	101	
17	2V	101	
18	1W	112	
18	2W	112	
19	1X	95	
19	2X	95	
20	1Y	107	
20	2Y	107	
21	1Z	203	
21	2Z	203	
22	10	77	
22	20	77	
23	11	97	
23	21	97	
24	12	70	
24	22	70	
25	13	59	
25	23	59	
26	14	69	
26	24	69	
27	15	59	
27	25	59	

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Mol	Chain	Length	Quality of chain
28	16	53	
28	26	53	
29	17	48	
29	27	48	
30	18	64	
30	28	64	
31	19	37	
31	29	37	
32	1a	2331	
32	2a	2331	
33	1b	231	
33	2b	231	
34	1c	206	
34	2c	206	
35	1d	208	
35	2d	208	
36	1e	148	
36	2e	148	
37	1f	100	
37	2f	100	
38	1g	155	
38	2g	155	
39	1h	137	
39	2h	137	
40	1i	127	

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Mol	Chain	Length	Quality of chain
40	2i	127	
41	1j	97	
41	2j	97	
42	1k	114	
42	2k	114	
43	1l	122	
43	2l	122	
44	1m	116	
44	2m	116	
45	1n	60	
45	2n	60	
46	1o	88	
46	2o	88	
47	1p	82	
47	2p	82	
48	1q	99	
48	2q	99	
49	1r	68	
49	2r	68	
50	1s	83	
50	2s	83	
51	1t	98	
51	2t	98	
52	1u	23	
52	2u	23	

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
1	OMC	2A	1941	-	-	X	-
32	MA6	1a	1497	-	-	X	-
32	MA6	2a	1496	-	-	X	-
43	0TD	1l	92	-	-	X	-
53	MG	18	102	-	-	-	X
53	MG	1A	3018	-	-	-	X
53	MG	1A	3040	-	-	-	X
53	MG	1A	3044	-	-	-	X
53	MG	1A	3059	-	-	-	X
53	MG	1A	3130	-	-	-	X
53	MG	1A	3541	-	-	-	X
53	MG	1A	3634	-	-	-	X
53	MG	1A	3686	-	-	-	X
53	MG	1Q	202	-	-	-	X
53	MG	1a	1776	-	-	-	X
53	MG	1a	1843	-	-	-	X
53	MG	1a	1851	-	-	-	X
53	MG	2A	3173	-	-	-	X
53	MG	2A	3194	-	-	-	X
53	MG	2A	3265	-	-	-	X
53	MG	2A	3290	-	-	-	X
53	MG	2A	3293	-	-	-	X
53	MG	2A	3375	-	-	-	X
53	MG	2A	3417	-	-	-	X
53	MG	2A	3424	-	-	-	X
53	MG	2A	3446	-	-	-	X
53	MG	2A	3459	-	-	-	X
53	MG	2a	1727	-	-	-	X
53	MG	2a	1829	-	-	-	X
53	MG	2r	101	-	-	-	X
55	MPD	18	104	-	-	X	-
55	MPD	1a	1900	-	-	X	-
58	SF4	1d	501	-	-	X	-
58	SF4	2d	501	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 290633 atoms, of which 88 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
			61868	27540	11574	19883	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
			1080	690	187	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	1A	837	Total Mg 837 837	0	0
53	1B	24	Total Mg 24 24	0	0
53	1D	15	Total Mg 15 15	0	0
53	1E	9	Total Mg 9 9	0	0
53	1F	9	Total Mg 9 9	0	0
53	1G	3	Total Mg 3 3	0	0
53	1H	3	Total Mg 3 3	0	0
53	1N	4	Total Mg 4 4	0	0
53	1O	1	Total Mg 1 1	0	0
53	1P	3	Total Mg 3 3	0	0
53	1Q	3	Total Mg 3 3	0	0
53	1R	3	Total Mg 3 3	0	0
53	1S	1	Total Mg 1 1	0	0
53	1T	3	Total Mg 3 3	0	0
53	1U	1	Total Mg 1 1	0	0
53	1V	3	Total Mg 3 3	0	0
53	1W	2	Total Mg 2 2	0	0
53	1X	1	Total Mg 1 1	0	0
53	1Y	1	Total Mg 1 1	0	0
53	1Z	2	Total Mg 2 2	0	0
53	10	6	Total Mg 6 6	0	0
53	11	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	13	1	Total 1	Mg 1	0	0
53	15	1	Total 1	Mg 1	0	0
53	17	3	Total 3	Mg 3	0	0
53	18	3	Total 3	Mg 3	0	0
53	19	2	Total 2	Mg 2	0	0
53	1a	203	Total 203	Mg 203	0	0
53	1b	1	Total 1	Mg 1	0	0
53	1d	2	Total 2	Mg 2	0	0
53	1e	1	Total 1	Mg 1	0	0
53	1f	2	Total 2	Mg 2	0	0
53	1h	1	Total 1	Mg 1	0	0
53	1l	2	Total 2	Mg 2	0	0
53	1m	1	Total 1	Mg 1	0	0
53	1o	1	Total 1	Mg 1	0	0
53	1s	1	Total 1	Mg 1	0	0
53	1t	1	Total 1	Mg 1	0	0
53	2A	561	Total 561	Mg 561	0	0
53	2B	9	Total 9	Mg 9	0	0
53	2D	7	Total 7	Mg 7	0	0
53	2E	5	Total 5	Mg 5	0	0
53	2F	4	Total 4	Mg 4	0	0

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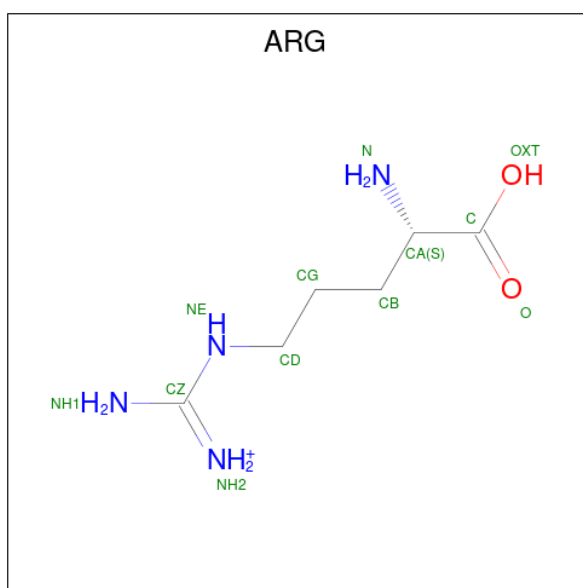
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	2G	1	Total 1	Mg 1	0	0
53	2I	2	Total 2	Mg 2	0	0
53	2O	2	Total 2	Mg 2	0	0
53	2P	3	Total 3	Mg 3	0	0
53	2Q	1	Total 1	Mg 1	0	0
53	2R	2	Total 2	Mg 2	0	0
53	2T	3	Total 3	Mg 3	0	0
53	2U	2	Total 2	Mg 2	0	0
53	2V	1	Total 1	Mg 1	0	0
53	2W	2	Total 2	Mg 2	0	0
53	2X	1	Total 1	Mg 1	0	0
53	2Y	1	Total 1	Mg 1	0	0
53	2Z	1	Total 1	Mg 1	0	0
53	20	1	Total 1	Mg 1	0	0
53	21	1	Total 1	Mg 1	0	0
53	25	1	Total 1	Mg 1	0	0
53	27	1	Total 1	Mg 1	0	0
53	28	4	Total 4	Mg 4	0	0
53	2a	144	Total 144	Mg 144	0	0
53	2e	1	Total 1	Mg 1	0	0
53	2f	2	Total 2	Mg 2	0	0

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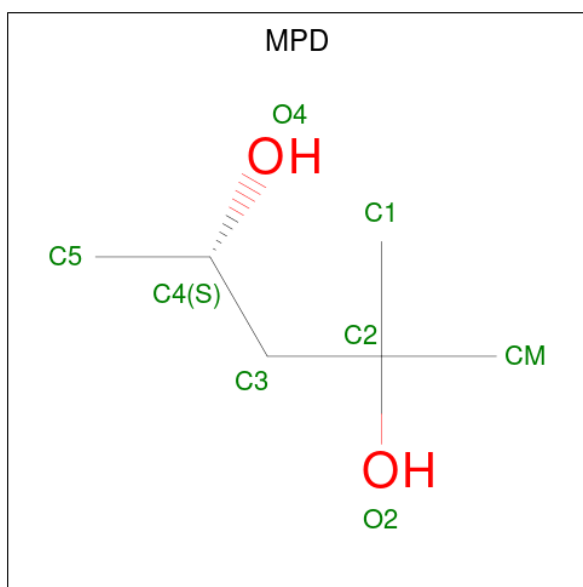
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	2h	1	Total	Mg	0	0
			1	1		
53	2l	2	Total	Mg	0	0
			2	2		
53	2n	1	Total	Mg	0	0
			1	1		
53	2r	2	Total	Mg	0	0
			2	2		
53	2t	1	Total	Mg	0	0
			1	1		

- Molecule 54 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



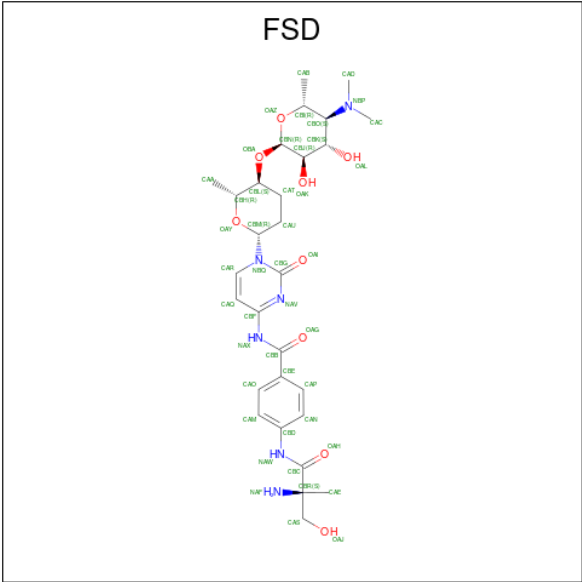
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
54	1A	1	Total	C	N	O	0	0
			12	6	4	2		
54	1B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 55 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
55	1A	1	Total	C	O	0	0
			8	6	2		
55	1T	1	Total	C	O	0	0
			8	6	2		
55	18	1	Total	C	O	0	0
			8	6	2		
55	1a	1	Total	C	O	0	0
			8	6	2		
55	2A	1	Total	C	O	0	0
			8	6	2		
55	2A	1	Total	C	O	0	0
			8	6	2		
55	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 56 is amicetin (CCD ID: FSD) (formula: C₂₉H₄₂N₆O₉).

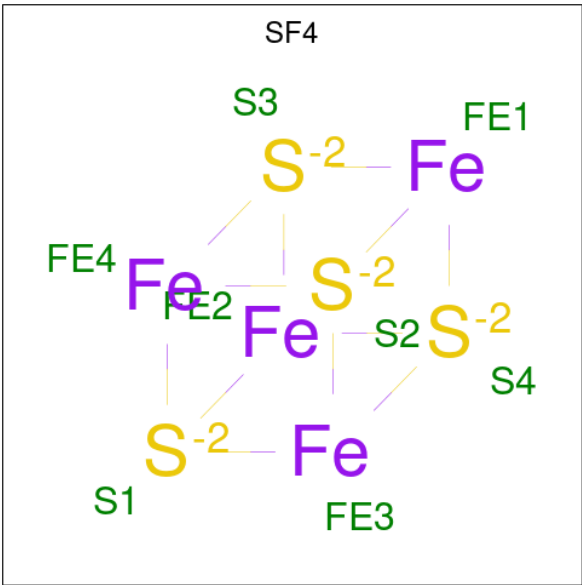


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
56	1A	1	Total	C	H	N	O	0	0
			88	29	44	6	9		
56	2A	1	Total	C	H	N	O	0	0
			88	29	44	6	9		

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total	Zn	0	0
			1	1		
57	15	1	Total	Zn	0	0
			1	1		
57	16	1	Total	Zn	0	0
			1	1		
57	19	1	Total	Zn	0	0
			1	1		
57	2Y	1	Total	Zn	0	0
			1	1		
57	25	1	Total	Zn	0	0
			1	1		
57	26	1	Total	Zn	0	0
			1	1		
57	29	1	Total	Zn	0	0
			1	1		
57	2n	1	Total	Zn	0	0
			1	1		

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1d	1	Total	Fe	S	0	0
			8	4	4		
58	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	1757	Total	O	0	0
			1757	1757		
59	1B	40	Total	O	0	0
			40	40		
59	1D	49	Total	O	0	0
			49	49		
59	1E	31	Total	O	0	0
			31	31		
59	1F	32	Total	O	0	0
			32	32		
59	1G	6	Total	O	0	0
			6	6		
59	1H	10	Total	O	0	0
			10	10		
59	1I	2	Total	O	0	0
			2	2		
59	1N	34	Total	O	0	0
			34	34		
59	1O	10	Total	O	0	0
			10	10		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1P	28	Total 28	O 28	0	0
59	1Q	19	Total 19	O 19	0	0
59	1R	18	Total 18	O 18	0	0
59	1S	3	Total 3	O 3	0	0
59	1T	14	Total 14	O 14	0	0
59	1U	24	Total 24	O 24	0	0
59	1V	33	Total 33	O 33	0	0
59	1W	21	Total 21	O 21	0	0
59	1X	5	Total 5	O 5	0	0
59	1Y	7	Total 7	O 7	0	0
59	1Z	6	Total 6	O 6	0	0
59	10	16	Total 16	O 16	0	0
59	11	13	Total 13	O 13	0	0
59	12	5	Total 5	O 5	0	0
59	13	8	Total 8	O 8	0	0
59	15	6	Total 6	O 6	0	0
59	16	5	Total 5	O 5	0	0
59	17	3	Total 3	O 3	0	0
59	18	18	Total 18	O 18	0	0
59	19	9	Total 9	O 9	0	0
59	1a	235	Total 235	O 235	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1c	1	Total 1	O 1	0	0
59	1d	4	Total 4	O 4	0	0
59	1e	1	Total 1	O 1	0	0
59	1h	2	Total 2	O 2	0	0
59	1i	1	Total 1	O 1	0	0
59	1l	2	Total 2	O 2	0	0
59	1m	1	Total 1	O 1	0	0
59	1o	2	Total 2	O 2	0	0
59	1q	1	Total 1	O 1	0	0
59	2A	859	Total 859	O 859	0	0
59	2B	5	Total 5	O 5	0	0
59	2D	12	Total 12	O 12	0	0
59	2E	11	Total 11	O 11	0	0
59	2F	6	Total 6	O 6	0	0
59	2G	4	Total 4	O 4	0	0
59	2I	1	Total 1	O 1	0	0
59	2O	6	Total 6	O 6	0	0
59	2P	7	Total 7	O 7	0	0
59	2Q	5	Total 5	O 5	0	0
59	2R	5	Total 5	O 5	0	0
59	2S	1	Total 1	O 1	0	0

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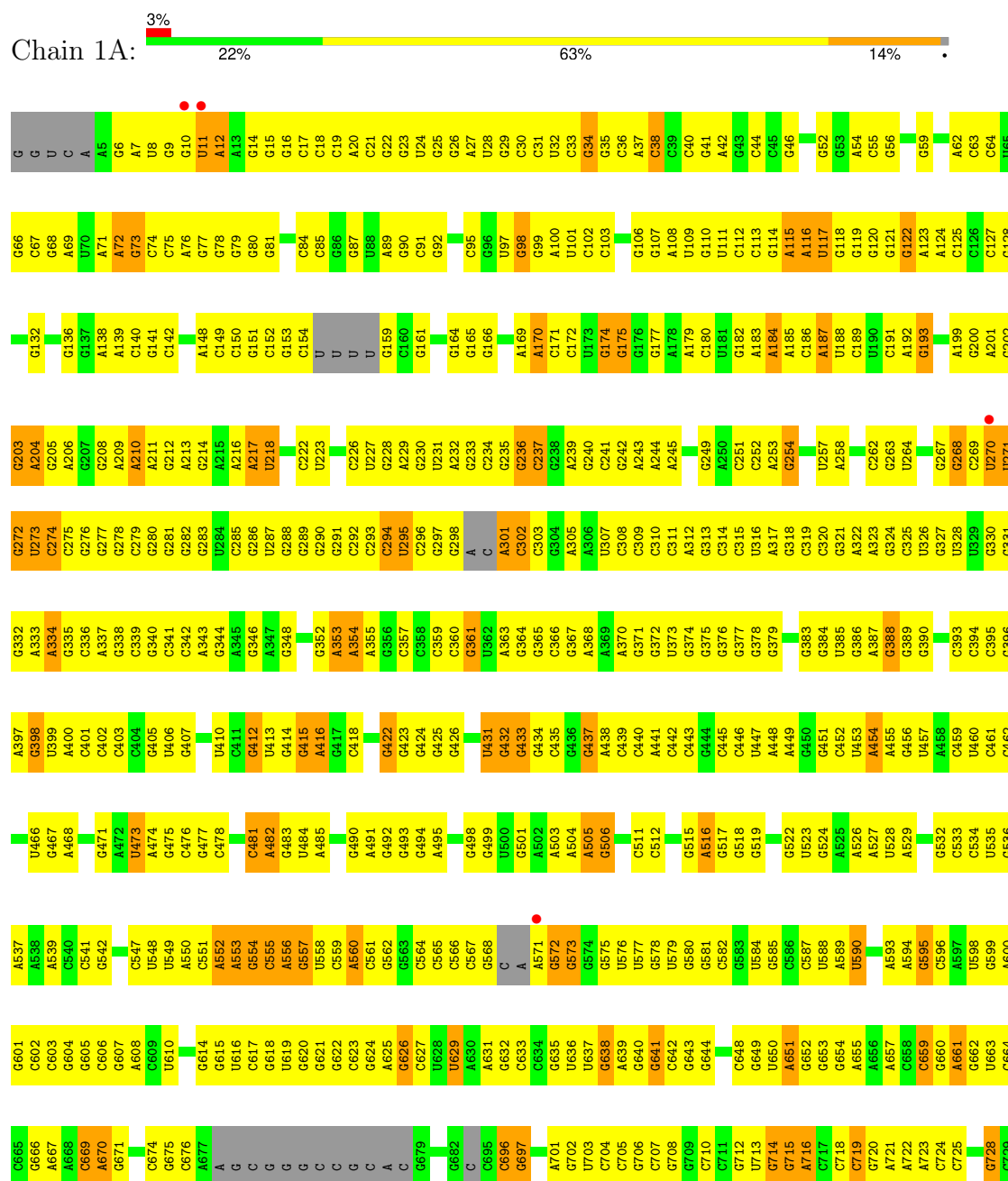
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2T	4	Total 4	O 4	0	0
59	2U	5	Total 5	O 5	0	0
59	2V	3	Total 3	O 3	0	0
59	2W	4	Total 4	O 4	0	0
59	2X	5	Total 5	O 5	0	0
59	2Y	2	Total 2	O 2	0	0
59	20	5	Total 5	O 5	0	0
59	21	4	Total 4	O 4	0	0
59	22	1	Total 1	O 1	0	0
59	23	2	Total 2	O 2	0	0
59	25	1	Total 1	O 1	0	0
59	26	2	Total 2	O 2	0	0
59	27	5	Total 5	O 5	0	0
59	28	5	Total 5	O 5	0	0
59	2a	113	Total 113	O 113	0	0
59	2f	1	Total 1	O 1	0	0
59	2o	1	Total 1	O 1	0	0
59	2q	1	Total 1	O 1	0	0

3 Residue-property plots

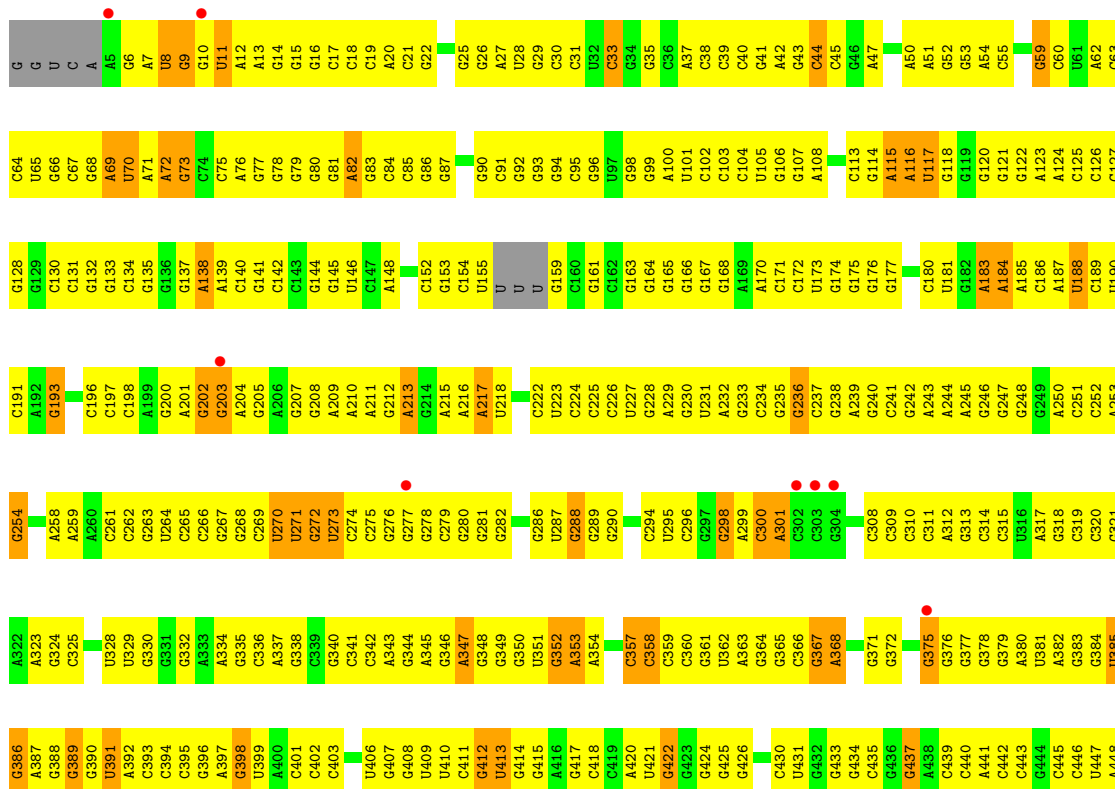
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S Ribosomal RNA



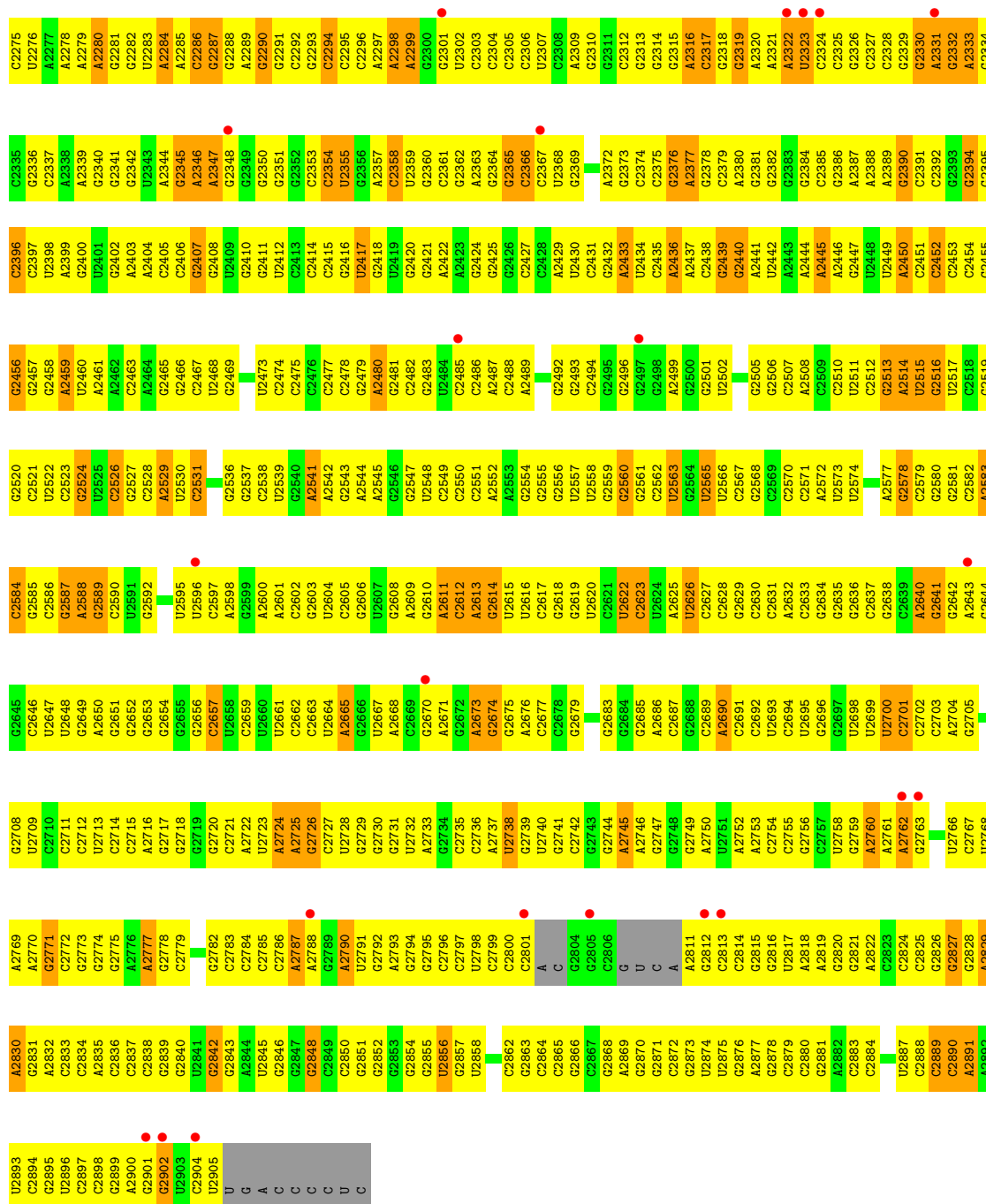
G1570	G1571	G1572	A1573	A1574	A1575	C1576	C1577	C1578	G	U	A	C	G1583	G1584	G1585	G1586	G1587	A1588	C1589	A1590	A1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1603	A1604	A1608	G1609	C1610	C1611	A1612	A1613	G1614	A1615	A1618	G1619	C1620	C1621	U1622	C1623	U1624	A1625	A1626	C1627	C1628	A1629	C1630	A1631	A1632	C1633	C1634			
A1503	C1504	G1505	A1506	G1507	C1508	G1511	G1512	C1513	C1514	A1515	G1516	A1517	G1518	G1519	C1522	G1523	G1524	G1525	G1528	G1529	A1530	G1531	G1532	G1533	G1536	G1537	C1538	A1539	A1540	A1541	U1542	C1543	C1544	A1545	C1546	C1547	U1548	C1549	C1550	A1551	A1552	A1553	C1554	A1555	A1556	U1559	C1560	U1561	G1562	C1563	G1564	U1565	C1566	G1567				
U1439	A1440	U1441	A1442	C1443	G1444	G1445	G1446	C1449	A1450	U1451	C1452	C1453	C1456	A1457	G1458	G1461	C1462	G1463	A1464	U1465	G1466	G1467	G1468	G1469	G1470	G1471	A1472	C1473	C1474	C1475	U1476	U1477	U1478	A1479	G1480	U1483	A1484	G1485	G1486	G1487	G1488	G1489	A1490	G1493	A1494	A1495	G1496	C1497	A1498	A1499	U1500	C1501	G1502					
U1371	C1372	U1373	U1374	A1375	A1376	G1377	C1378	G1379	G1383	A1384	U1385	U1386	A1387	G1388	C1389	C1390	G1391	G1392	C1393	A1394	C1395	A1396	U1397	A1398	U1399	G1400	G1401	U1402	G1403	A1404	A1405	C1408	A1409	A1410	A1411	A1412	G1413	G1414	C1415	G1416	U1417	A1418	C1421	G1422	A1423	A1424	G1425	G1426	G1427	G1428	A1429	G1430	C1431	C1432	G1433	G1434		
A1307	U1308	G1309	A1310	G1311	U1312	A1313	C1314	C1315	C1316	A1317	U1318	A1319	A1320	A1321	G1322	A1323	G1324	G1325	G1326	U1327	G1328	A1329	G1330	A1331	A1332	C1336	C1337	C1338	U1339	C1340	G1341	C1342	U1345	A1346	A1347	G1348	C1349	C1350	A1351	A1352	A1353	G1354	G1355	G1356	U1357	U1358	C1359	C1360	U1361	A1362	A1366	A1367	U1368	G1370				
C1245	C1246	U1247	A1248	U1249	G1250	C1251	C1252	G1253	A1254	U1255	G1256	A1257	A1258	G1259	C1260	C1261	G1262	G1263	A1264	C1265	C1266	C1267	G1268	C1269	G1270	A1271	G1272	G1273	G1276	C1277	C1278	U1279	G1280	G1281	A1282	G1283	G1284	U1285	A1286	G1287	G1288	G1289	G1290	G1293	U1294	G1295	C1296	C1297	A1298	U1299	U1300	G1301	C1302	G1303	G1304	G1305	C1306	
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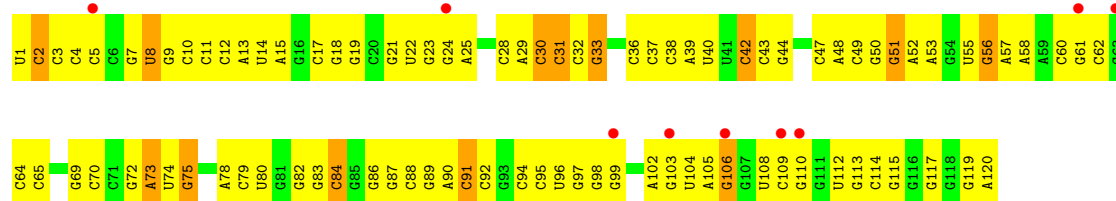


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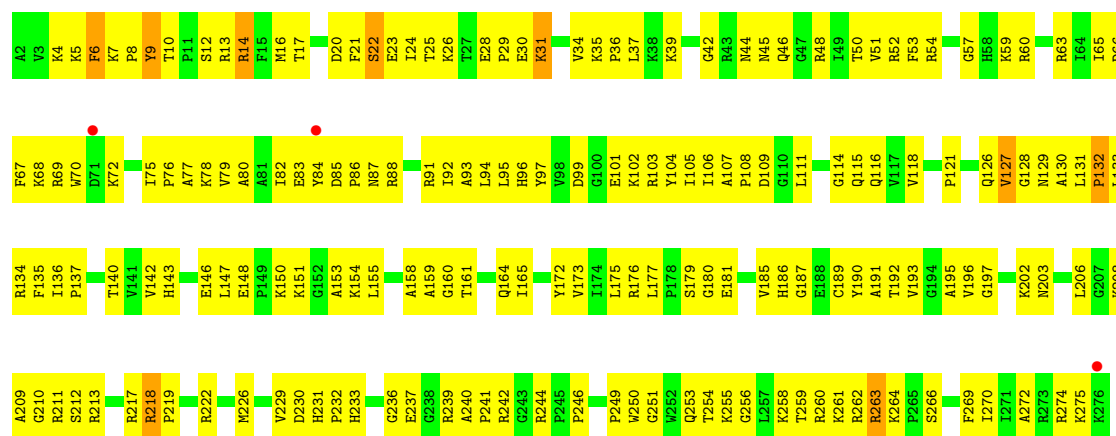
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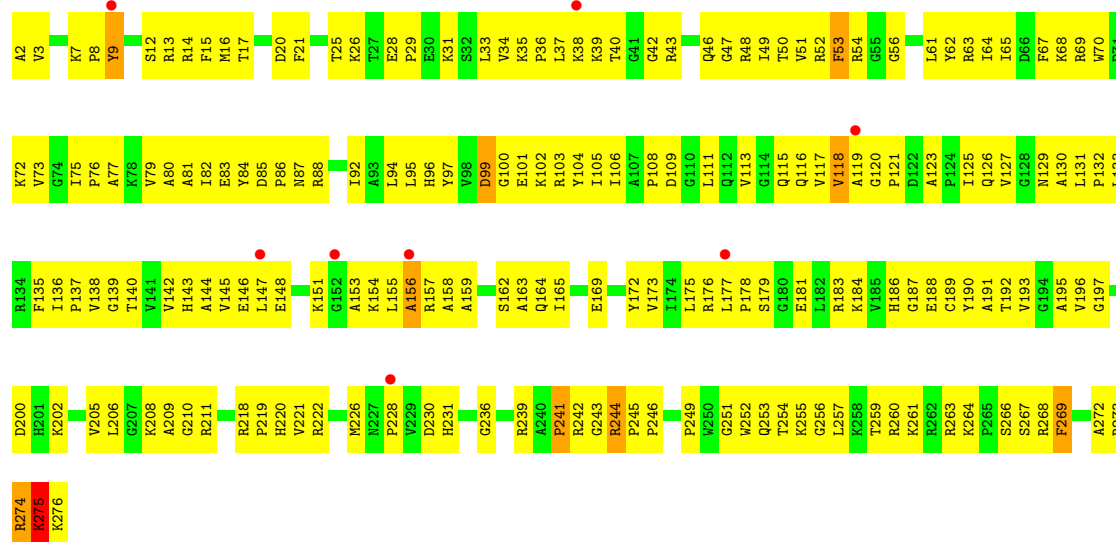
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

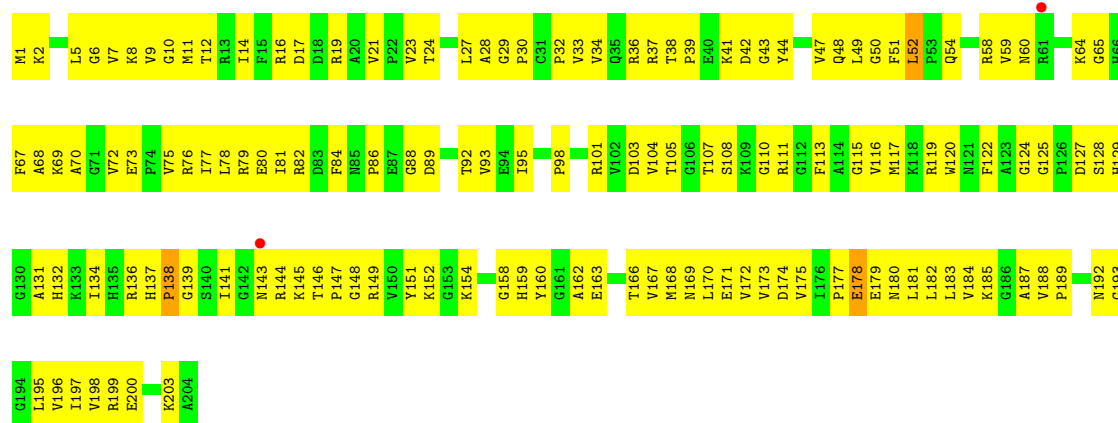


• Molecule 3: 50S ribosomal protein L2

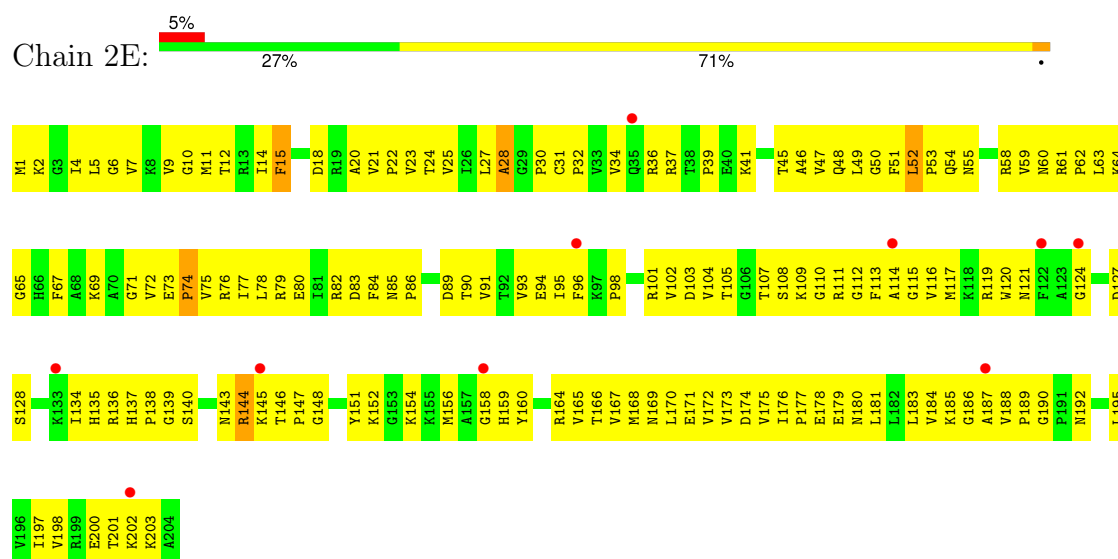


• Molecule 4: 50S ribosomal protein L3





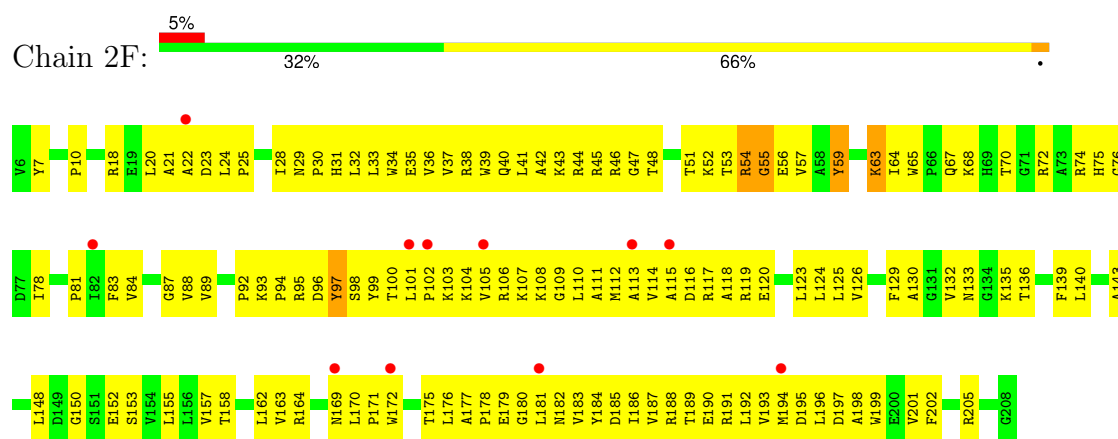
• Molecule 4: 50S ribosomal protein L3



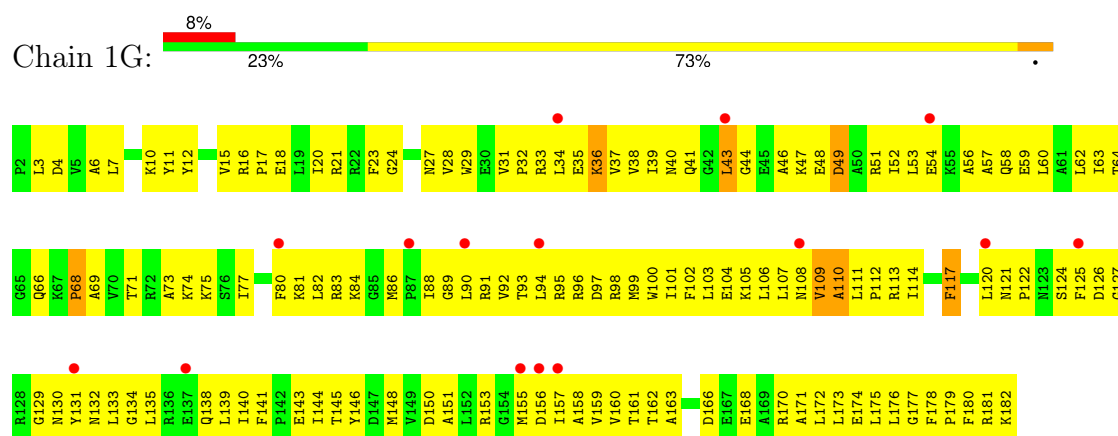
• Molecule 5: 50S ribosomal protein L4



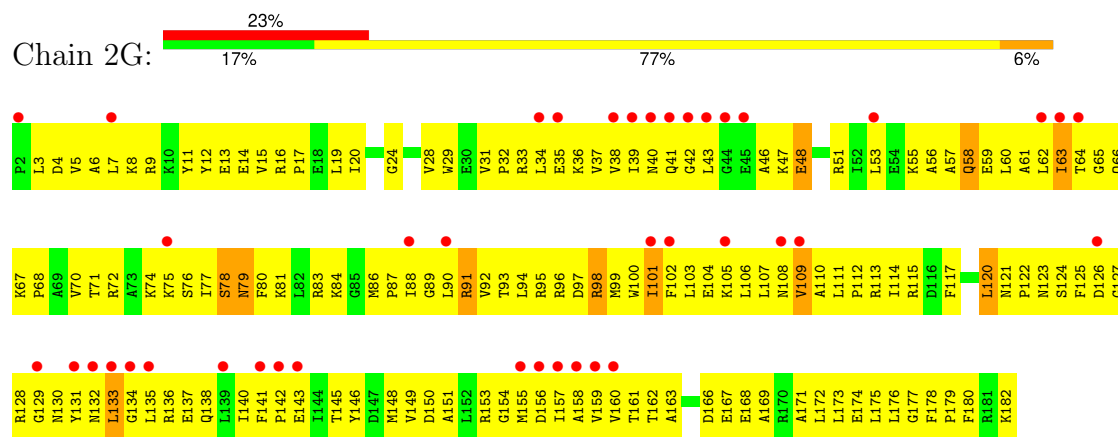
• Molecule 5: 50S ribosomal protein L4



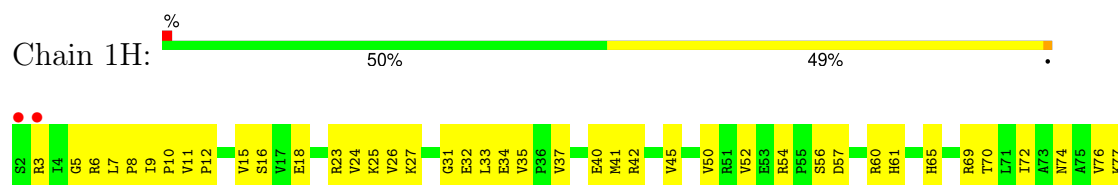
- Molecule 6: 50S ribosomal protein L5

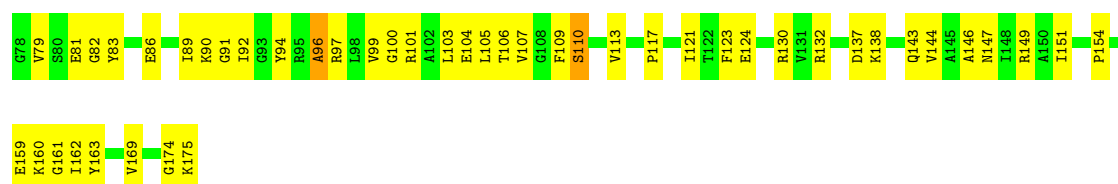


- Molecule 6: 50S ribosomal protein L5

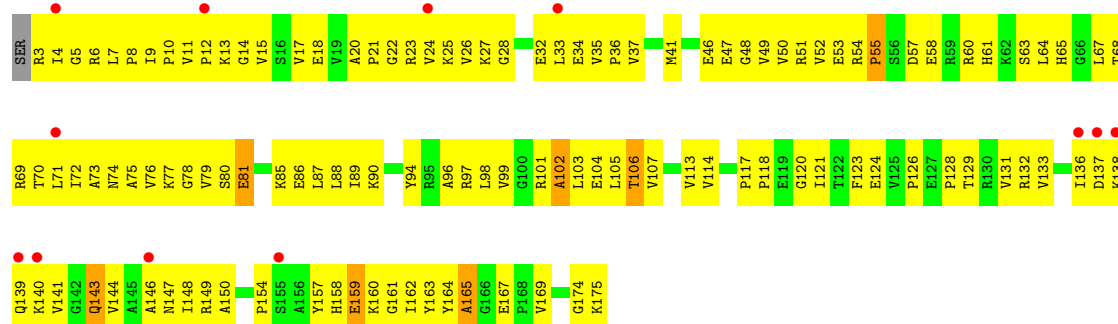


- Molecule 7: 50S ribosomal protein L6

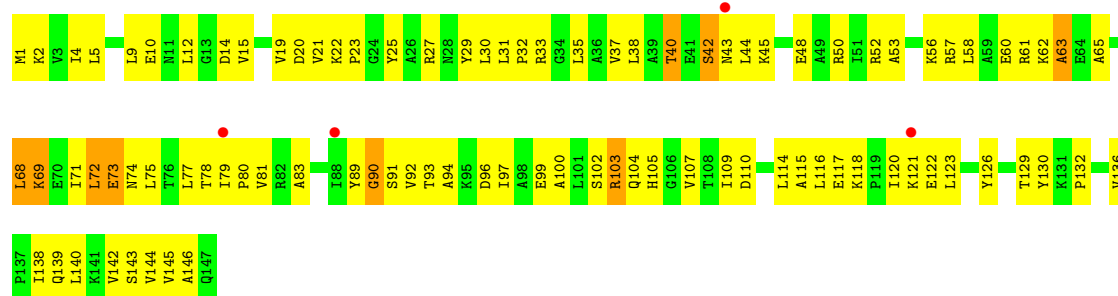




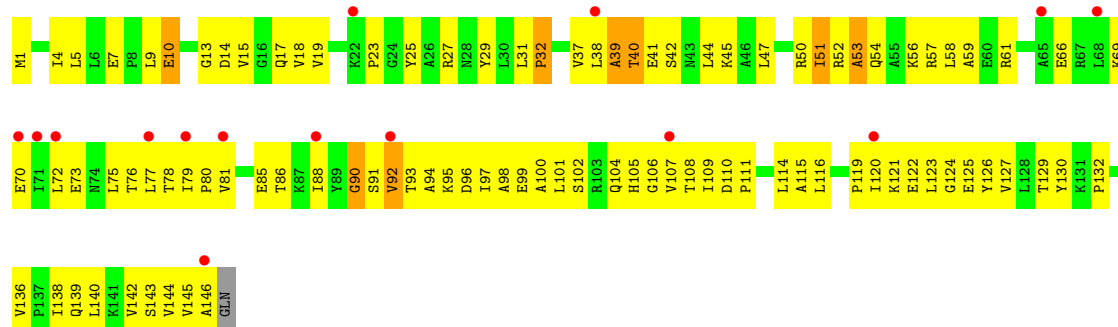
• Molecule 7: 50S ribosomal protein L6



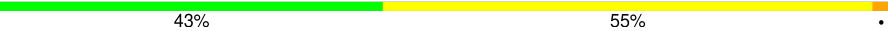
• Molecule 8: 50S ribosomal protein L9

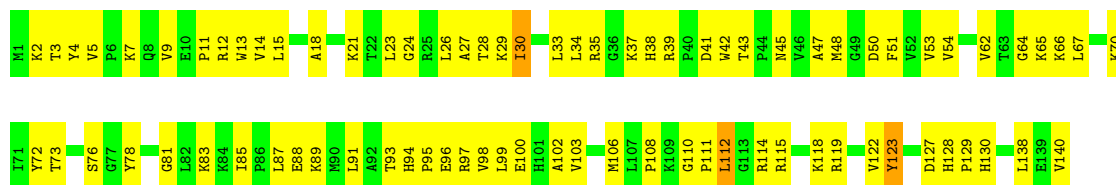


• Molecule 8: 50S ribosomal protein L9



• Molecule 9: 50S ribosomal protein L13

Chain 1N:  43% 55%

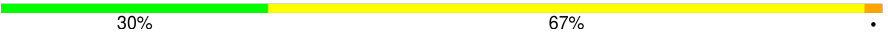


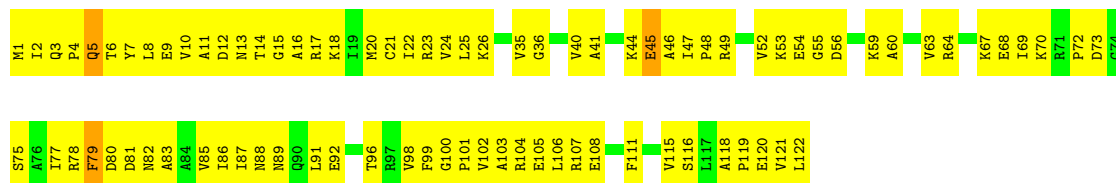
• Molecule 9: 50S ribosomal protein L13

Chain 2N:  3% 32% 62% 6%



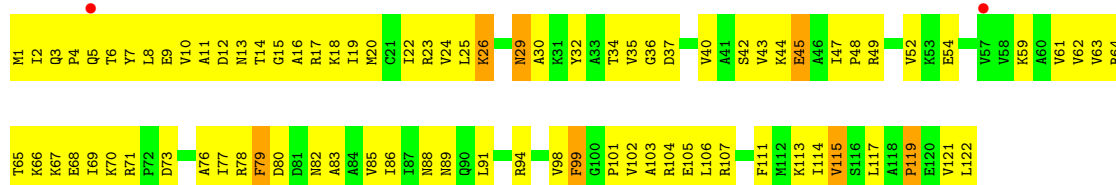
• Molecule 10: 50S ribosomal protein L14

Chain 1O:  30% 67%



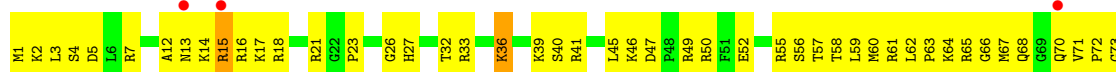
• Molecule 10: 50S ribosomal protein L14

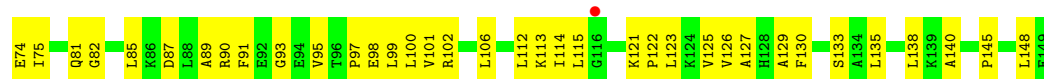
Chain 2O:  2% 30% 64% 6%



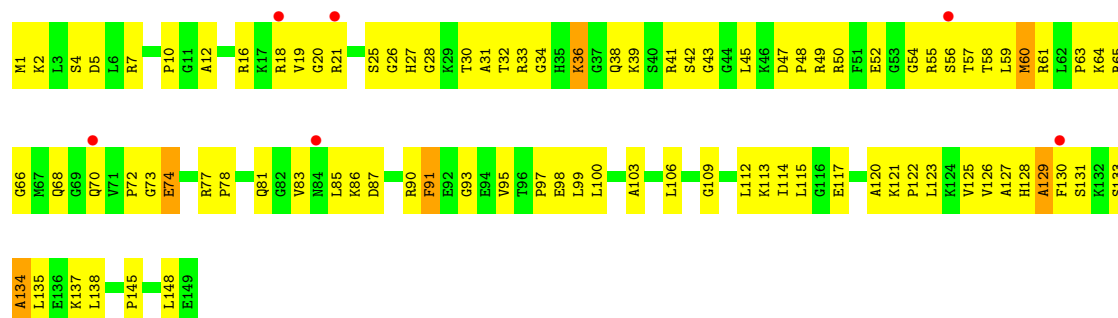
• Molecule 11: 50S ribosomal protein L15

Chain 1P:  3% 44% 54%

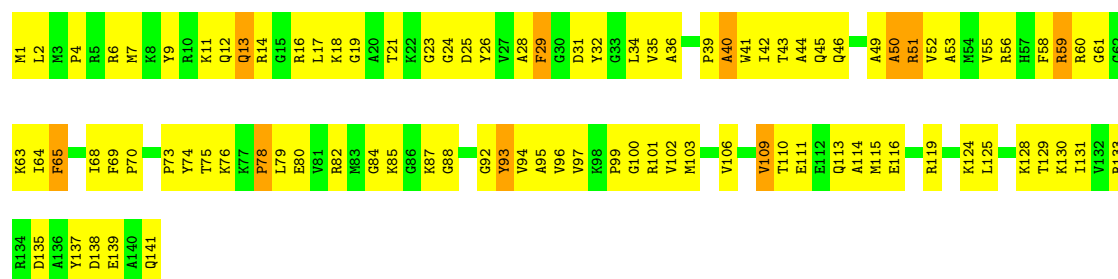




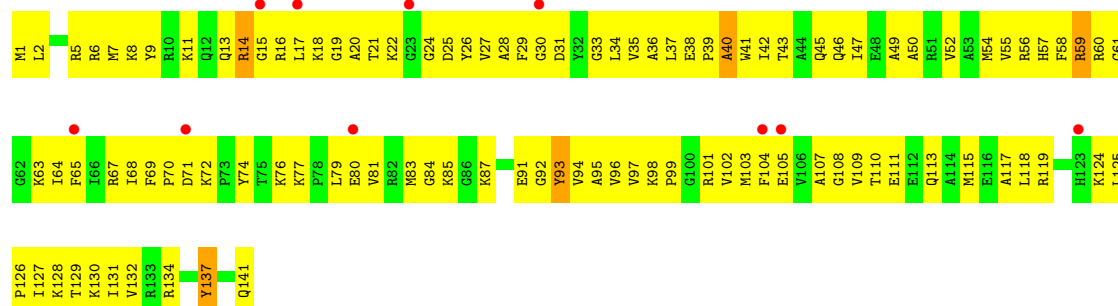
• Molecule 11: 50S ribosomal protein L15



• Molecule 12: 50S ribosomal protein L16

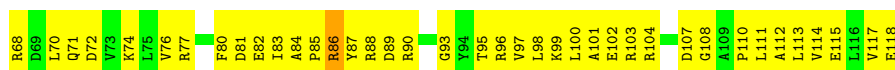


• Molecule 12: 50S ribosomal protein L16

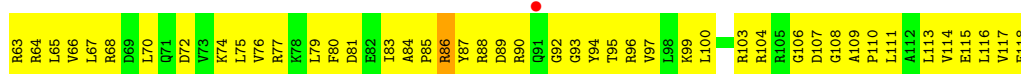


• Molecule 13: 50S ribosomal protein L17





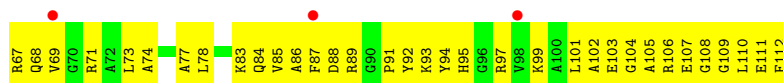
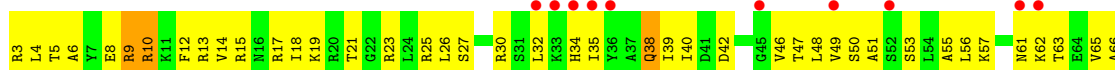
• Molecule 13: 50S ribosomal protein L17



• Molecule 14: 50S ribosomal protein L18



• Molecule 14: 50S ribosomal protein L18



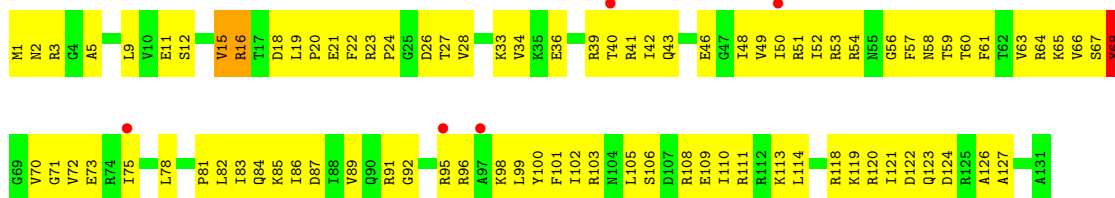
• Molecule 15: 50S ribosomal protein L19



A131

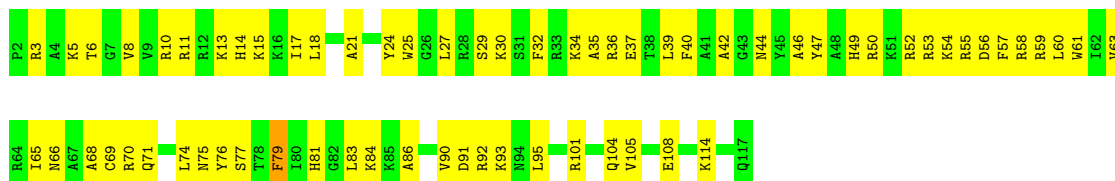
- Molecule 15: 50S ribosomal protein L19

Chain 2T: 



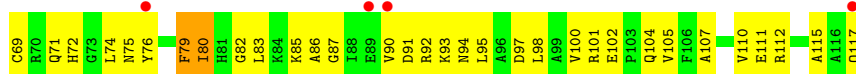
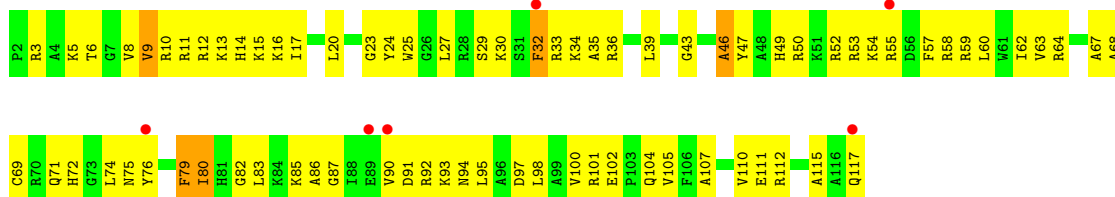
- Molecule 16: 50S ribosomal protein L20

Chain 1U: 



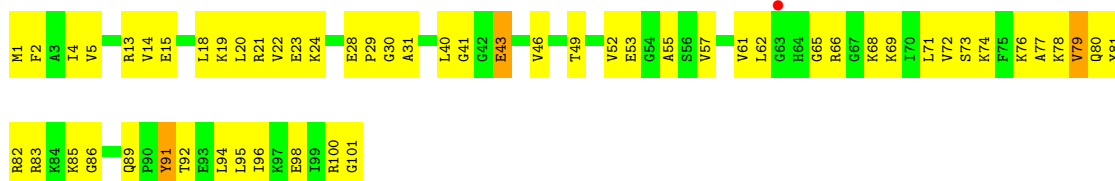
- Molecule 16: 50S ribosomal protein L20

Chain 2U: 



- Molecule 17: 50S ribosomal protein L21

Chain 1V: 



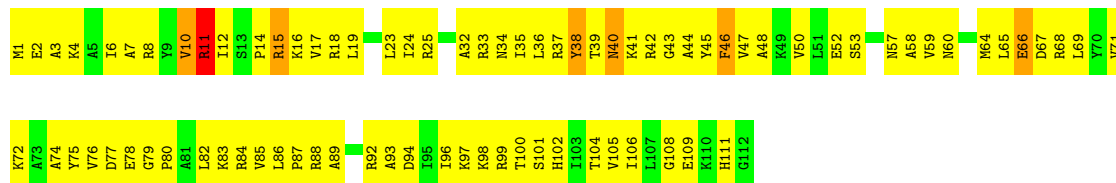
- Molecule 17: 50S ribosomal protein L21

Chain 2V: 



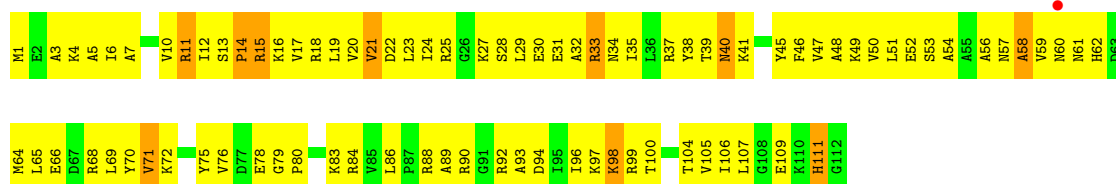
• Molecule 18: 50S ribosomal protein L22

Chain 1W: 27% 67% 5%



• Molecule 18: 50S ribosomal protein L22

Chain 2W: 23% 68% 9%



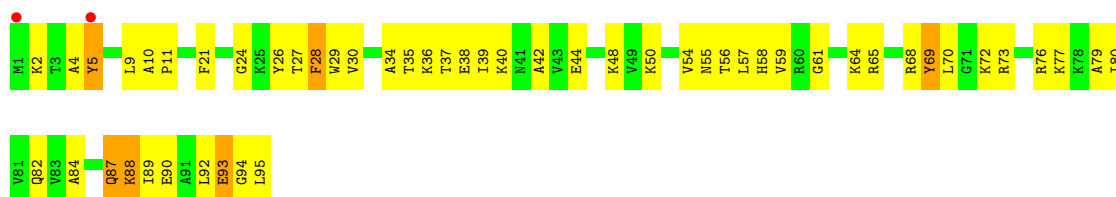
• Molecule 19: 50S ribosomal protein L23

Chain 1X: 39% 59%

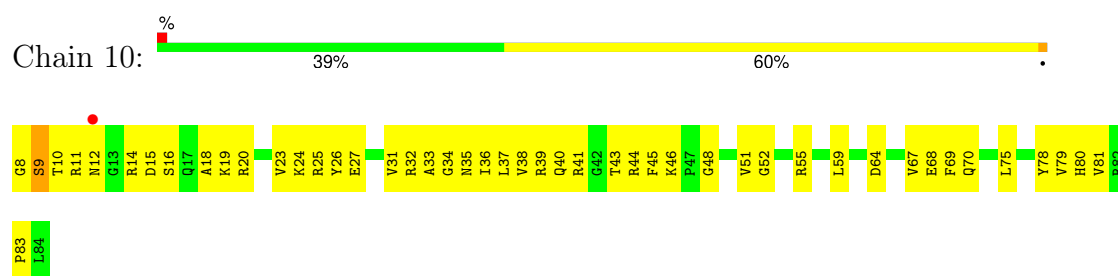


• Molecule 19: 50S ribosomal protein L23

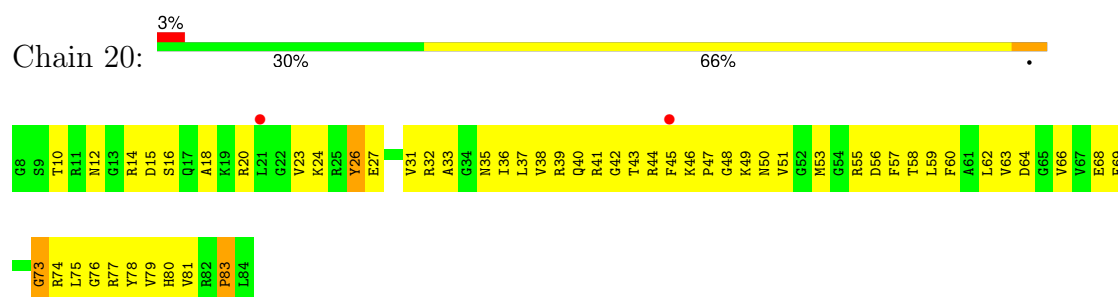
Chain 2X: 2% 45% 48% 6%



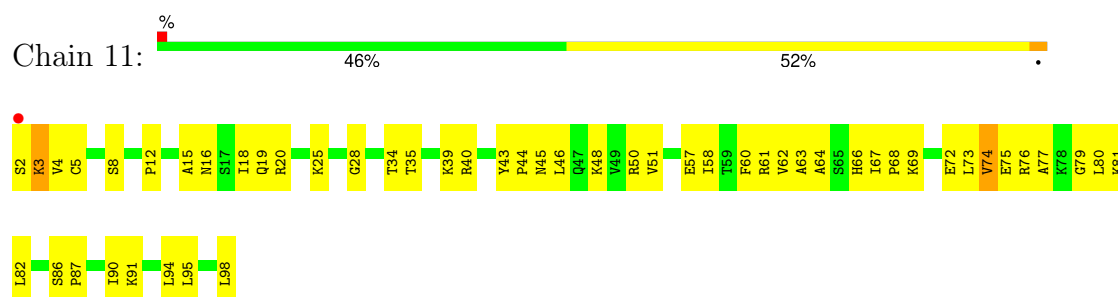
• Molecule 20: 50S ribosomal protein L24



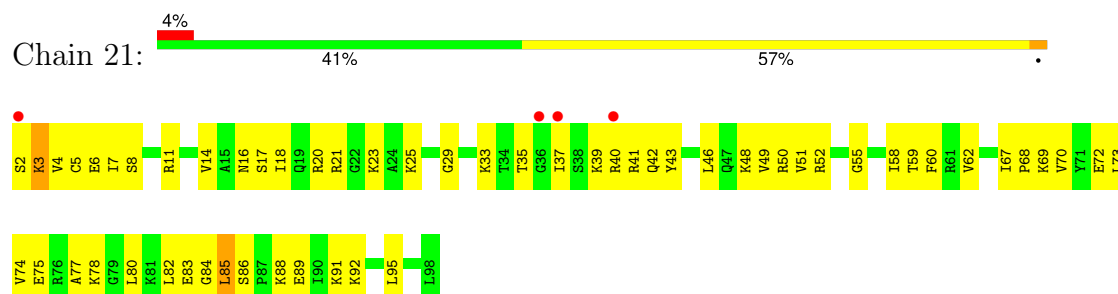
- Molecule 22: 50S ribosomal protein L27



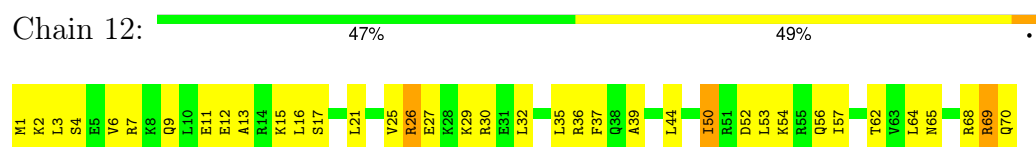
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29

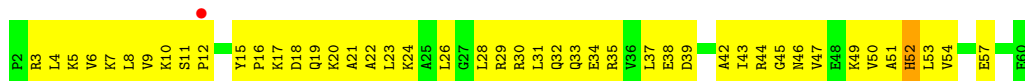




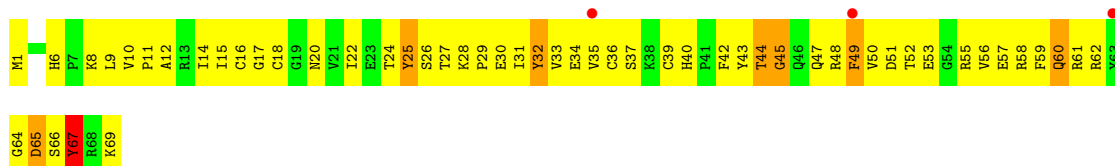
- Molecule 25: 50S ribosomal protein L30



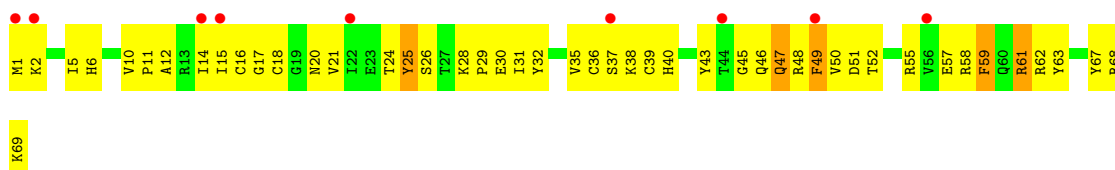
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31

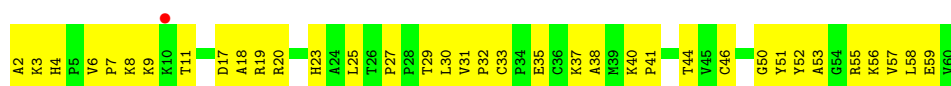


- Molecule 27: 50S ribosomal protein L32

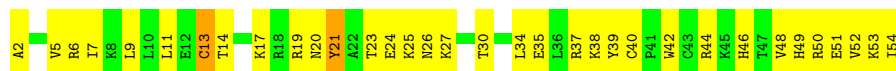


- Molecule 27: 50S ribosomal protein L32

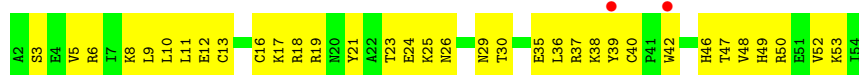




- Molecule 28: 50S ribosomal protein L33



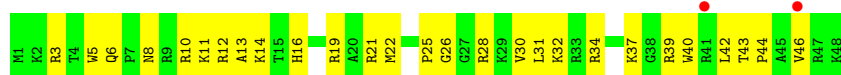
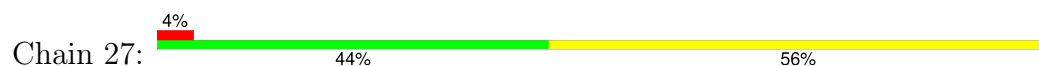
- Molecule 28: 50S ribosomal protein L33



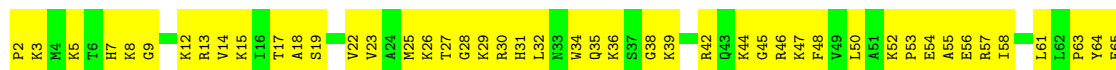
- Molecule 29: 50S ribosomal protein L34



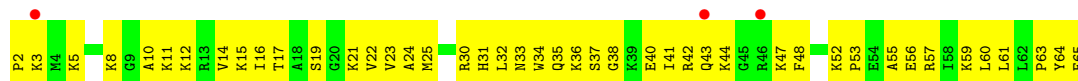
- Molecule 29: 50S ribosomal protein L34



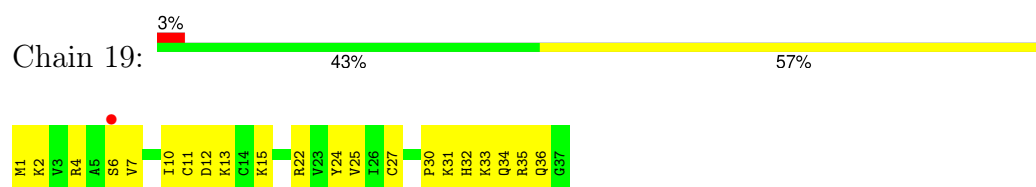
- Molecule 30: 50S ribosomal protein L35



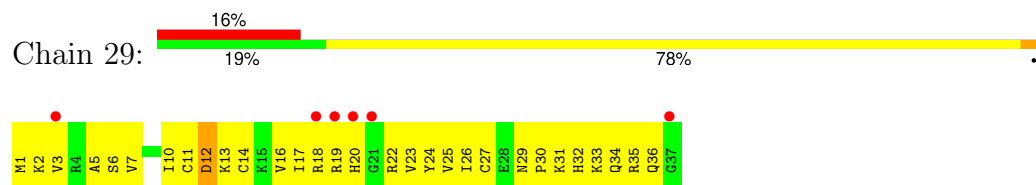
- Molecule 30: 50S ribosomal protein L35



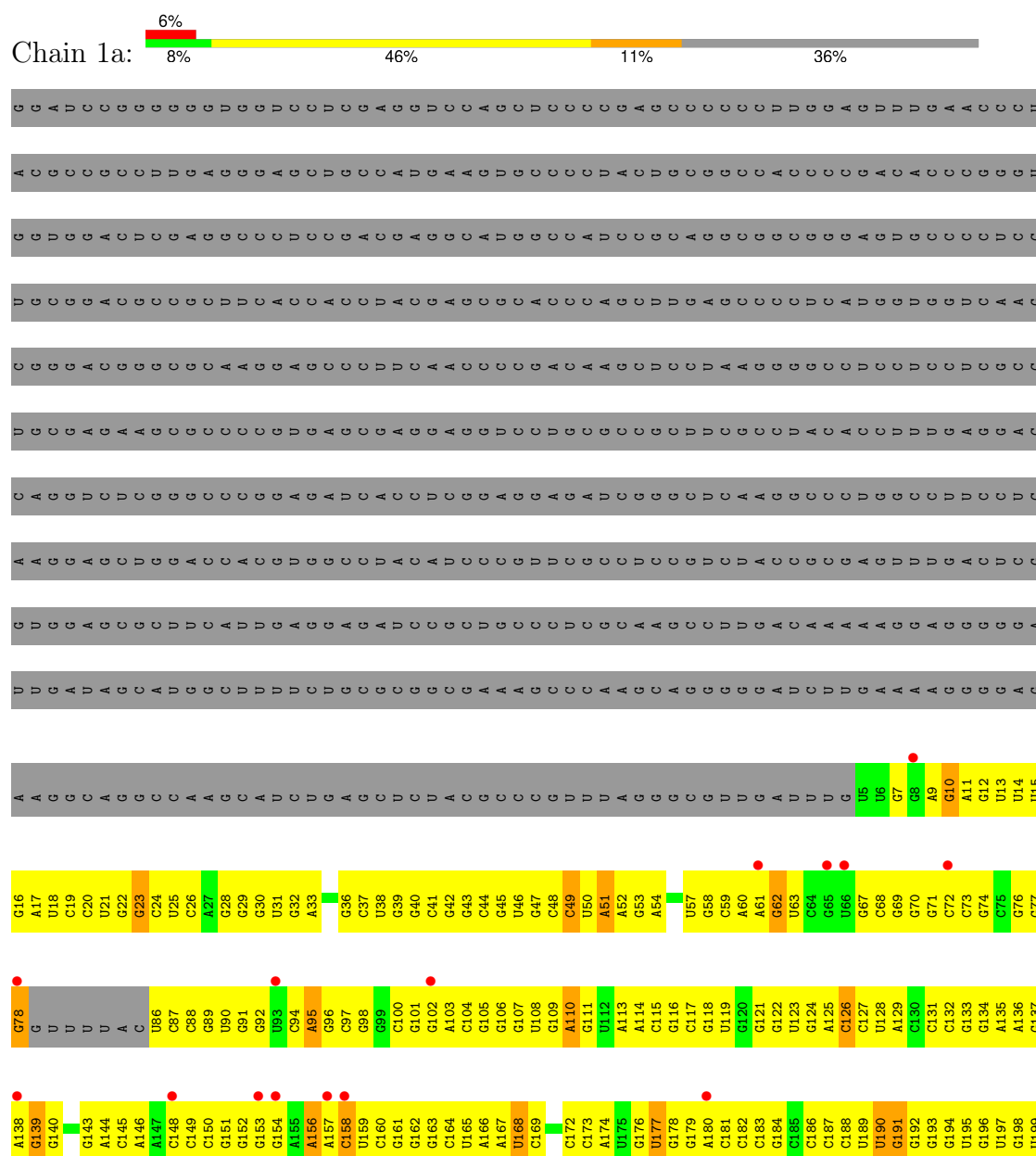
- Molecule 31: 50S ribosomal protein L36



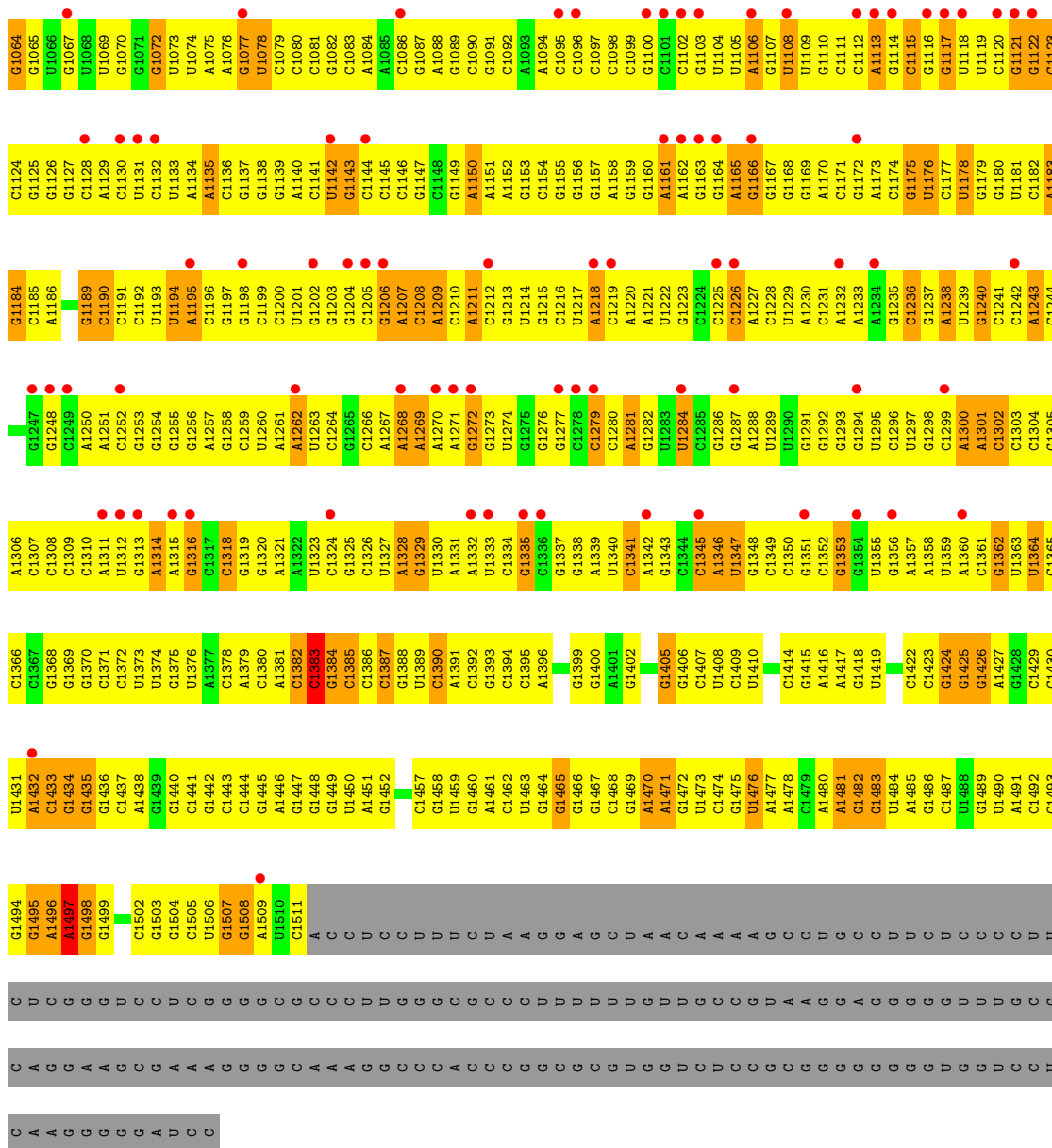
- Molecule 31: 50S ribosomal protein L36



- Molecule 32: 16S Ribosomal RNA



G1003	A943	U883	G820	C754	G694	U630	G565	A504	G442	C382	A321	G261	C200
U1004	G944	G884	G821	G755	G695	C831	U566	G505	G445	U883	G322	G262	C201
G1005	A885	A886	G822	U756	A696	A632	A567	C506	A446	A385	A323	C263	A202
C1006	A946	A886	U823	G757	G697	G633	A568	A507	A446	A385	C324	C264	A203
C1007	A947	A887	G824	G758	G698	G634	G569	G508	A447	C386	A325	C265	A204
C1008	C948	C888	U825	G759	A699	C635	C570	C509	A448	C387	C326	A266	G205
C1009	G949	U889	C826	G760	A700	U636	G571	C510	C449	G388	G327	C267	G206
G1010	C950	C890	C827	A761	C701	A637	G572	G511	C450	A389	G328	C268	G207
C1011	G951	A891	U828	G762	G702	G638	C573	C512	C451	A390	G329	A269	C208
G1012	A952	A892	G829	C763	C703	A639	U574	G513	C452	C391	C330	A270	U209
A1013	G953	A893	G830	G764	C704	C640	U575	G514	C453	G392	C331	G271	U210
G1014	G954	G894	G831	A766	G705	G641	U576	U515	C454	A393	G334	G272	U211
G1015	A955	G895	G832	C767	A706	G642	G577	A516	C455	C394	G335	G273	G212
G1016	A956	A896	G833	C768	U707	U643	G578	A517	C456	G395	C336	G274	C213
A1017	C957	A897	C834	G769	G708	G644	U579	U518	G457	C396	U336	A275	C214
A1018	C958	U898	C835	G770	G709	G645	C580	A519	A458	C397	U337	G276	C215
G1019	U959	U899	G836	U771	C710	G646	G581	C520	G459	G398	C338	G277	G216
C1020	U960	G900	A837	U773	G711	A647	U582	C521	G460	G399	U339	A278	G217
C1021	A961	A901	A838	A774	A712	G648	C583	G522	G461	U400	A340	G279	U218
C1022	C962	C902	G839	G775	A713	A649	C584	A523	G462	U401	C341	G280	U219
U1023	G963	G903	C840	A776	G714	G650	C585	G524	A463	G402	G342	G281	C220
A1024	A964	G904	U841	U777	C715	G651	A586	G525	C464	G403	G343	G282	C221
G1025	G965	G905	A842	A778	C716	G652	U587	G526	U465	A404	G344	G283	G222
C1026	G966	G906	A843	U779	G717	U653	C588	C527	G465	G405	A345	G284	G223
A1027	C967	G907	C844	C781	G718	G654	U589	G528	C468	G406	G346	A284	G224
C1028	C968	C908	G845	G782	C719	G655	G590	C529	G469	A407	G347	C286	U225
A1029	U969	C909	G846	G783	C720	U656	A591	G530	G470	A408	C348	C287	G226
G1030	G970	C910	U847	G784	A721	U657	A592	A531	U471	G409	A349	C288	G227
G1031	G971	G911	U849	U785	C722	G658	C593	G532	A472	G410	G350	G289	G230
C1032	A972	C912	A850	G787	C723	A659	C594	G533	C473	A411	C351	U290	C231
U1033	C973	A913	A851	U788	U724	G660	C595	G534	G474	G412	A352	C291	C232
G1035	A974	C914	C852	C789	G725	U662	C596	U535	G475	C413	G353	U292	C233
U1036	U975	A915	C853	G790	G726	C663	G600	U536	G476	C414	U355	G293	C234
C1037	G976	A916	G854	U791	U727	C664	G601	C537	G477	C415	U356	A294	U235
A1038	C977	G917	C855	G792	C728	G665	C602	U545	G478	U416	G357	G295	U236
U1039	U978	C918	G856	G793	C729	G666	U603	C546	U479	U417	G358	G296	C237
G1040	A979	G919	C857	C794	A730	G667	C604	A547	A480	C418	A359	G297	C238
G1041	G980	G920	C858	C795	C731	A668	A605	G541	A481	G419	A360	U298	A239
C1042	G981	U921	G859	C796	C732	G669	A606	G542	U482	G420	A361	A299	U240
G1043	G982	G922	C860	U797	C733	U670	C607	A543	A483	G421	U362	U300	U241
G1044	A983	G923	C861	A798	G734	A671	C608	U544	G484	G422	C363	G301	A242
U1045	A984	U924	U862	A799	U735	G672	G609	C546	C485	U423	U364	C302	G243
C1046	C985	G925	G863	A800	U736	C673	U610	A547	C486	G424	C365	C303	G244
G1047	G986	C926	G864	C801	A737	G674	G611	C548	C487	U425	C366	C304	U245
U1048	C987	A927	G865	G802	C738	G675	G612	U549	C488	A426	G367	G305	A246
C1049	G988	U928	G866	A803	G739	U676	G613	G550	G489	A427	C368	G306	A247
A1050	G989	G929	U867	U804	C740	G677	G614	G551	G490	A428	C369	C307	G248
G1051	G990	U930	G868	G805	U741	A678	G615	C552	C491	C429	A370	C308	U249
C1052	U991	G931	U869	C906	G742	G679	A616	C553	C492	U430	U371	C310	G250
U1053	G992	G932	A870	G807	A743	U680	G617	G554	A493	C431	G372	A311	G251
C1054	A993	U933	C871	C808	G744	U681	G621	U555	A494	C432	G373	G312	U252
G1055	A994	U934	G872	G809	G745	C685	U622	A556	C495	U433	G374	G313	G253
U1056	A995	U935	G873	C810	C746	G686	G623	A557	U496	G434	C375	G314	G254
G1057	G996	A936	C874	U811	G747	A686	G624	A558	C497	A435	G376	G315	G255
C1058	C997	A937	C875	G812	C748	G687	U625	G559	C498	A436	G377	G316	G256
G1059	C998	U938	G876	A813	G749	U688	A626	G560	G499	C437	C378	A317	U257
G1060	U999	U939	A879	C814	A750	A690	A626	G561	U500	C438	A378	G318	A258
U1061	G1000	C940	G880	U815	A751	C891	C627	G562	G501	C439	G379	U319	A259
G1062	G881	G941	G882	C816	A752	C892	G628	G563	C502	G440	G380	G320	U260
A1063	G1002	A942	C882	G753	G753	G693	C629	U564	C503	G441	C381		







Chain 1b:

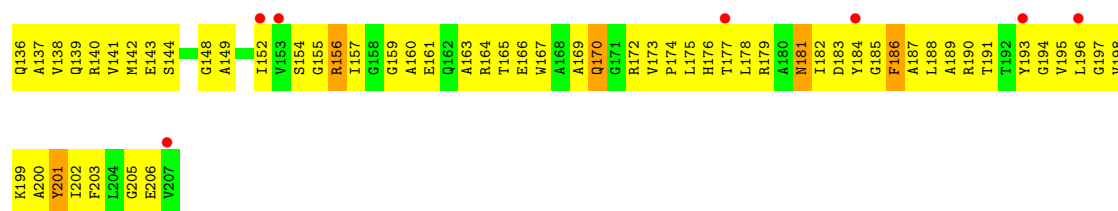
Sample	Sample	Sample	Sample
V7	L69	K133	D195
K8	F70	K134	L196
E9	V71	Q135	V197
L10	G72	Q136	D198
L11	T73	R137	V199
E12	K74	L138	I200
G13	Q75	E141	P201
A14	A77	L142	G202
H15	D79	E143	N203
H16	L80	L144	D205
F17	H81	L145	D206
G18	R82	Y148	I208
H19	M83	L149	R209
E20	E84	S150	S210
R21	A85	G151	I211
K22	E86	F152	Q212
R23	R87	L153	L213
W24	A88	L154	I214
N25	G89	L155	L215
P26	M90	K156	S216
K27	P91	R157	R217
F28	Y92	L158	A218
A29	V93	P159	V219
R30	M94	D160	D220
F31	Q95	A161	L221
I32	R96	I162	I222
Y33	W97	F163	I223
A34	L98	V164	Q224
E35	G99	V165	A225
G38	I100	L166	R226
I39	M101	P167	V229
H40	L102	T168	V230
I41	T103	K169	E231
I42	M104	E170	P232
P43	I108	I172	S233
L44	S109	A173	P234
Q45	Q110	V174	S235
K46	R111	R176	Y236
T47	V112	E176	A237
M48	H113	A177	
E49	R114	K178	
E50	L115	L180	
L51	E116	P183	
E52	F117	V184	
R53	L118	I185	
T54	E119	L186	
F55	A120	L187	
R56	L121	A188	
F57	F122	T189	
L58	A123	D190	
E59	S124	I191	
D60	P125	S192	
L61	E126	P193	
R64	I127	D194	
G65	E128		
G66	F129		
T67	L130		
F68			

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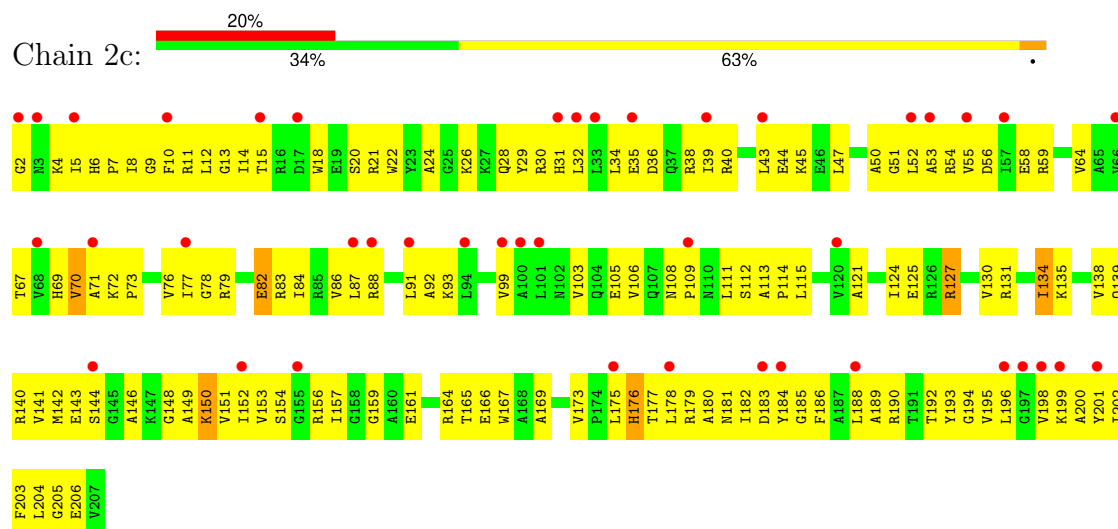
Chain 1c:

15% 30% 66%

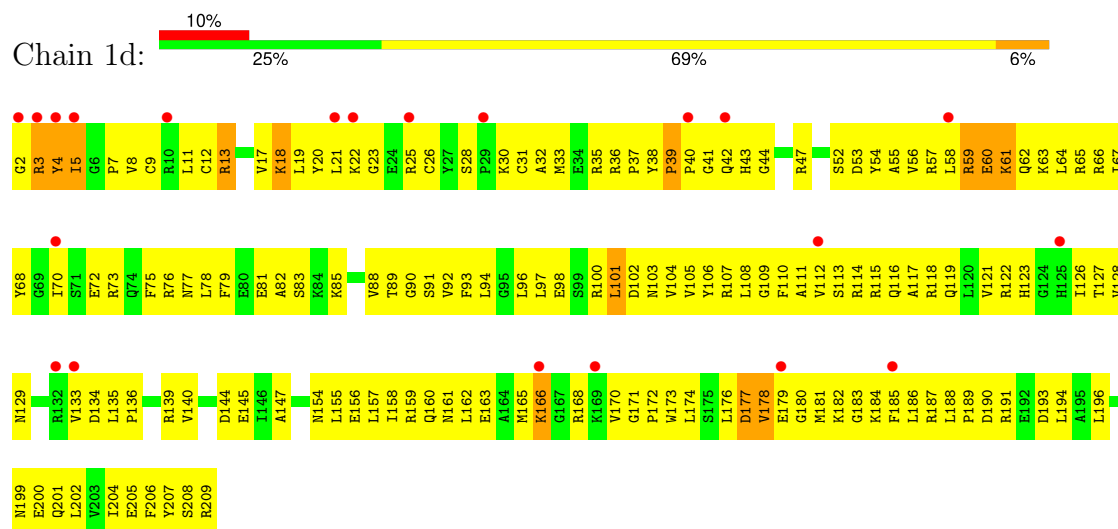
G2 G3 G4 G5 G6 G7 G8 G9 G10 G11 G12 G13 G14 G15 G16 G17 G18 G19 G20 G21 G22 G23 G24 G25 G26 G27 G28 G29 G30 G31 G32 G33 G34 G35 G36 G37 G38 G39 G40 G41 G42 G43 G44 G45 G46 G47 G48 G49 G50 G51 G52 G53 G54 G55 G56 G57 G58 G59 G60 G61 G62 G63 G64 G65 G66 G67 G68 G69 G70 G71 G72 G73 G74 G75 G76 G77 G78 G79 G80 G81 G82 G83 G84 G85 G86 G87 G88 G89 G90 G91 G92 G93 G94 G95 G96 G97 G98 G99 G100 G101 G102 G103 G104 G105 G106 G107 G108 G109 G110 G111 G112 G113 G114 G115 G116 G117 G118 G119 G120 G121 G122 G123 G124 G125 G126



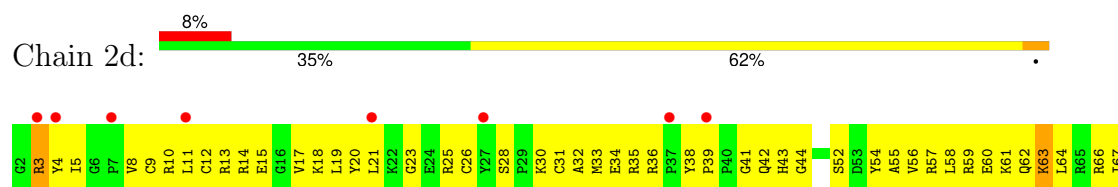
● Molecule 34: 30S ribosomal protein S3

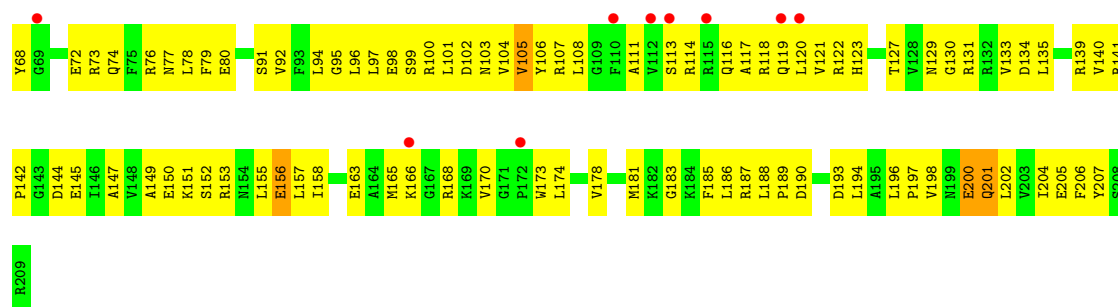


● Molecule 35: 30S ribosomal protein S4

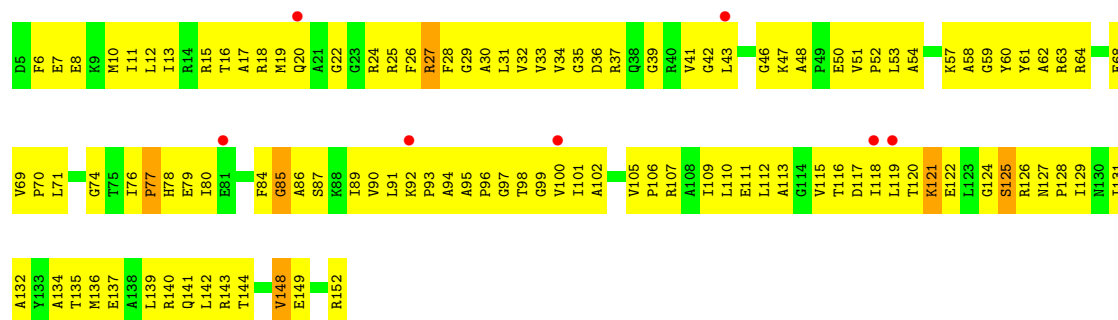


● Molecule 35: 30S ribosomal protein S4

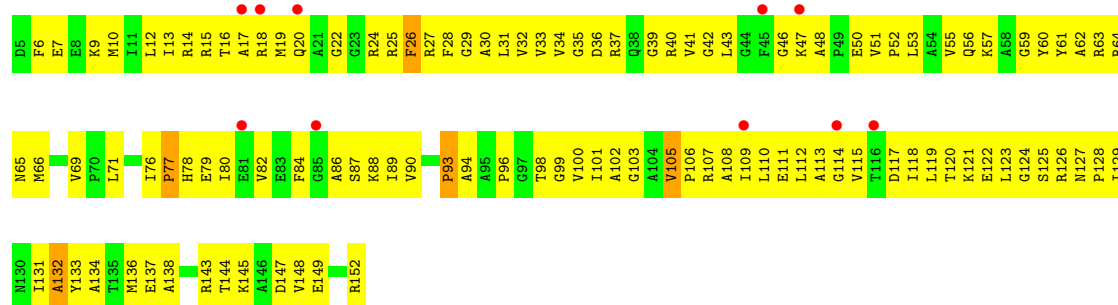




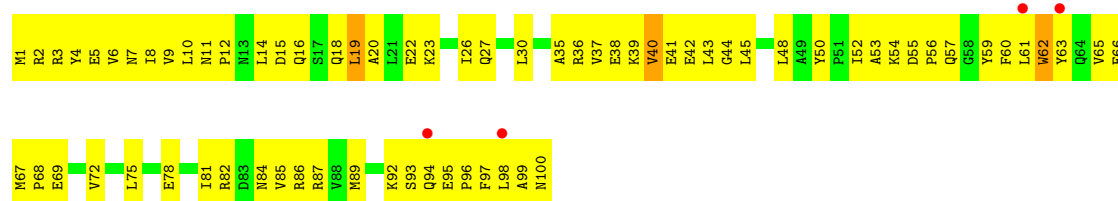
• Molecule 36: 30S ribosomal protein S5



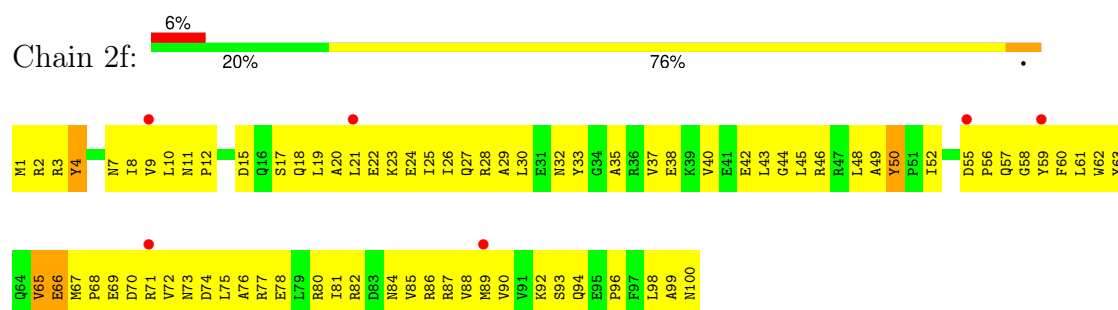
• Molecule 36: 30S ribosomal protein S5



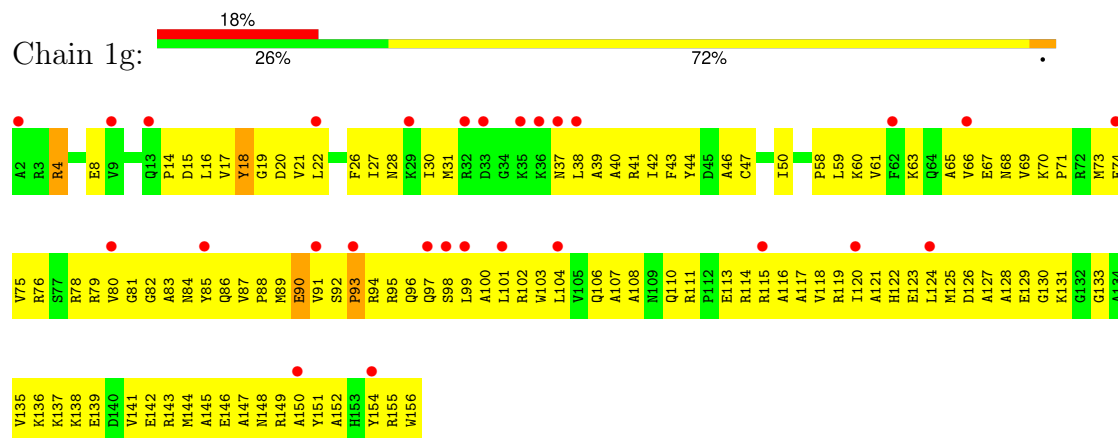
• Molecule 37: 30S ribosomal protein S6



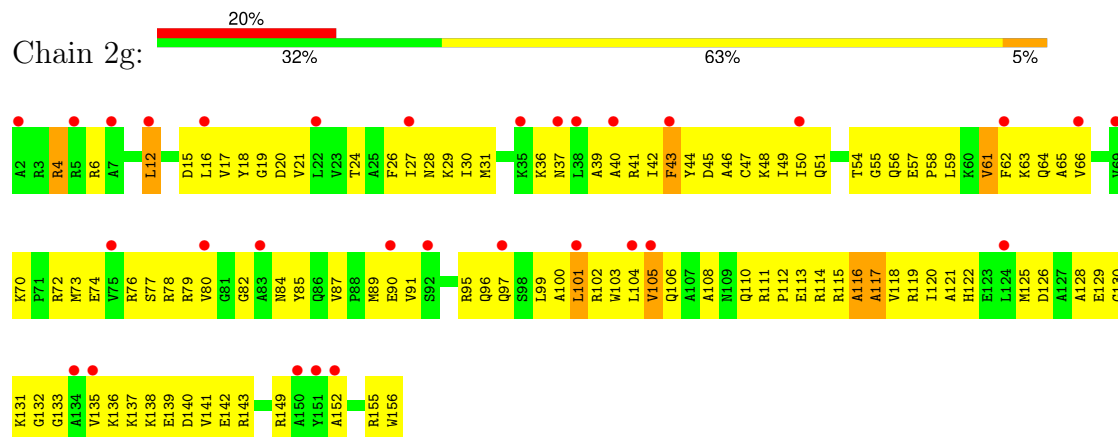
• Molecule 37: 30S ribosomal protein S6



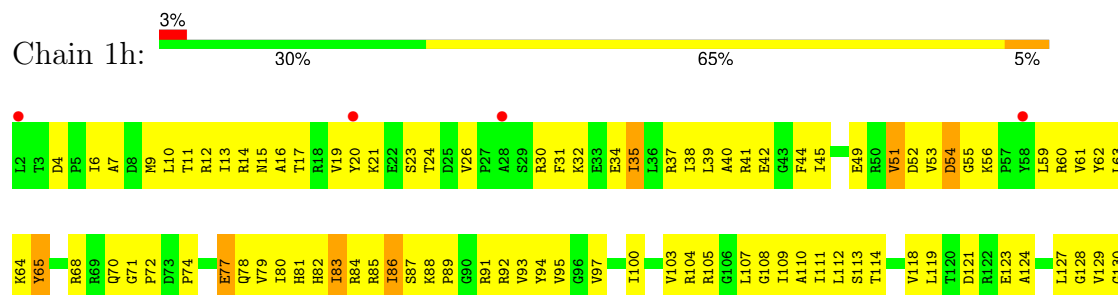
• Molecule 38: 30S ribosomal protein S7



• Molecule 38: 30S ribosomal protein S7



• Molecule 39: 30S ribosomal protein S8



G131
E132
L133
I134
C135
E136
V137
W138

• Molecule 39: 30S ribosomal protein S8

Chain 2h: 6% 18% 73% 9%

L3 T3 D4 P5 I6 A7 D8 N9 L10 T11 R12 R13 I14 T17 T18 R19 Y20 I21 E22 S23 T24 D25 P26 V27 P28 A28 S29 R30 F31 K32 V33 E34 I35 L36 R37 P38 L39 A40 R41 E42 Q43 F44 I109 I45 I46 G47 Y48 E49 V51 R50 D52 K56 P57 Y58 L59 R60 V61 V62 L63 K64

Y65 G66 P67 R68 R69 P72 D73 P74 R75 P76 P77 Q78 V79 I80 H81 R82 I83 R84 R85 S86 K88 P89 G90 R91 R92 V93 F94 V95 G96 V97 R98 I99 E99 I100 P101 R102 I103 R104 R105 I109 I110 I111 L112 S113 T114 S115 K116 G117 V118 L119 T120 D121 L122 E123 A124 R125 K126 L127

G128 V129 G130 E132 L133 I134 C135 E136 V137 W138

• Molecule 40: 30S ribosomal protein S9

Chain 1i: 32% 20% 75% 5%

E2 Q3 Y4 V5 G6 T7 C8 R9 R10 K11 E12 A13 V14 I15 R16 R17 F18 I19 R20 R21 G22 N23 G24 K25 V26 T27 V28 R29 G30 Q31 L32 F33 Y36 F37 Q38 G39 L40 V41 R42 A43 V44 A45 A46 L47 E48 P49 L50 R51 A52 L56 F59 D60 A61 V62 T63 V64 V65

R66 G67 G68 S70 T71 G72 Q73 I74 A76 K78 L79 G80 I81 A82 R83 R84 L85 V86 Q87 Y88 N89 Y92 R93 A94 K95 L96 Q97 P98 L99 G100 F101 L102 T103 R104 D105 R107 V108 V109 E110 R111 K112 K113 G115 K116 H117 K118 A119 R120 R121 A122 P123 Q124 T125 S126

K127 R128

• Molecule 40: 30S ribosomal protein S9

Chain 2i: 28% 19% 76% 5%

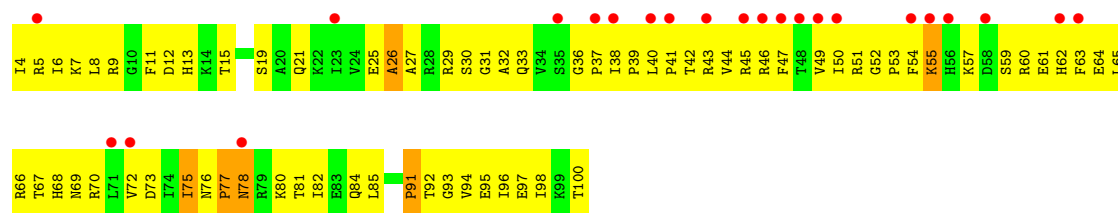
E2 Q3 V4 Y5 G6 T7 C8 R9 R10 K11 E12 A13 V14 I15 R16 R17 F18 I19 R20 R21 G22 N23 G24 K25 V26 T27 V28 R29 G30 Q31 L32 F33 R34 E35 Q38 G39 L40 V41 R42 A43 V44 A45 A46 L47 E48 P49 L50 R51 A52 V53 D54 A55 L56 F59 D60 A61 V62 T63

T64 V65 R66 G68 G69 K70 S71 G72 Q73 I74 D75 A76 I77 K78 L79 G80 I81 A82 R83 A84 L85 V86 Y88 R89 P90 D91 R92 R93 A94 K95 L96 K97 P98 L99 G100 F101 L102 T103 R104 D105 V106 R107 V108 E109 E110 K112 K113 Y114 G115 K116 H117 K118 A119 R120 R121 A122 P123

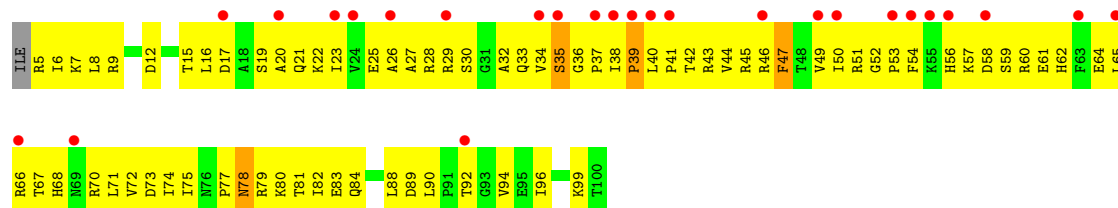
Q124 Y125 S126 K127 ARG

• Molecule 41: 30S ribosomal protein S10

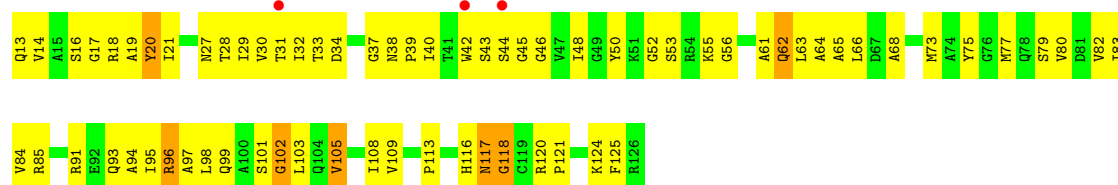
Chain 1j: 24% 26% 68% 6%



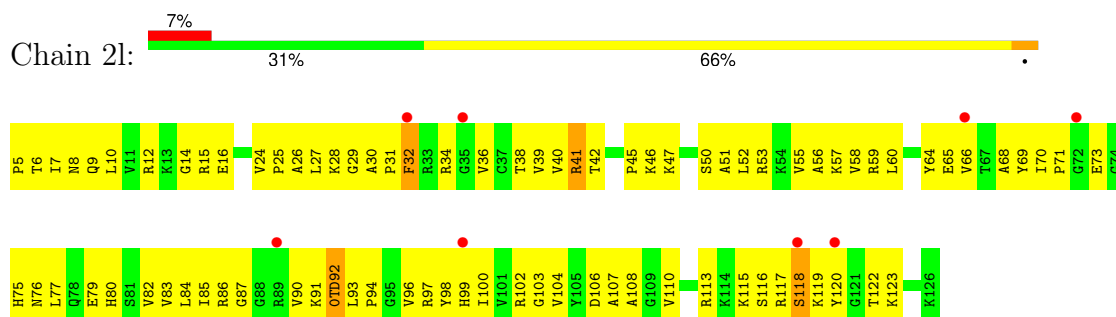
● Molecule 41: 30S ribosomal protein S10



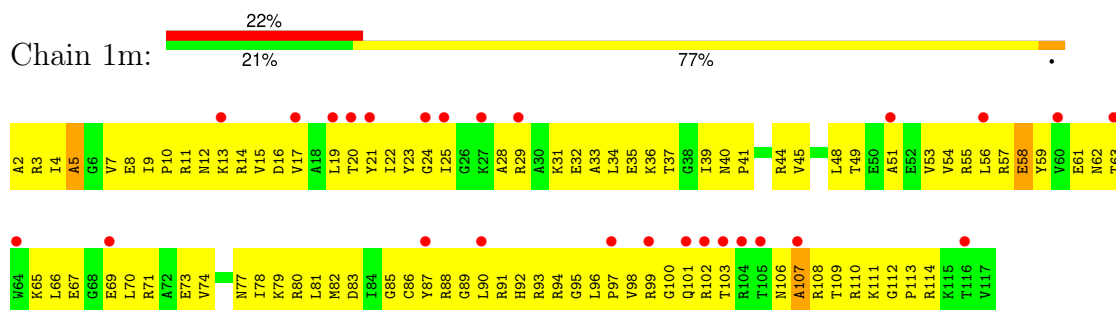
● Molecule 42: 30S ribosomal protein S11



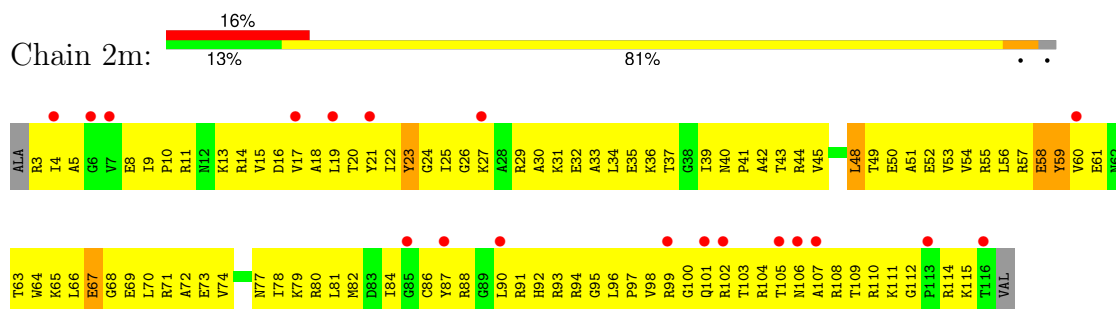
- Molecule 43: 30S ribosomal protein S12



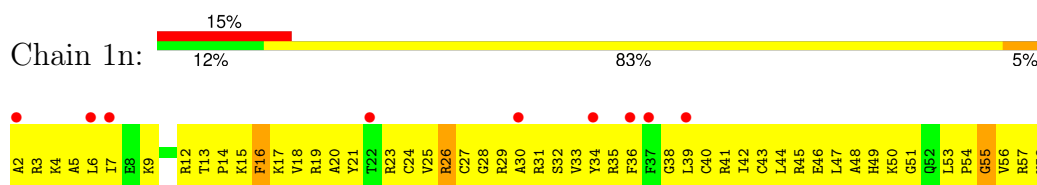
- Molecule 44: 30S ribosomal protein S13



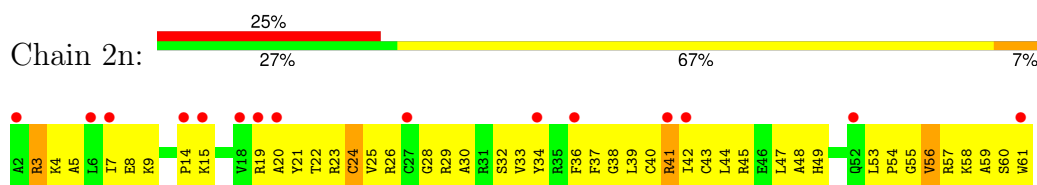
- Molecule 44: 30S ribosomal protein S13



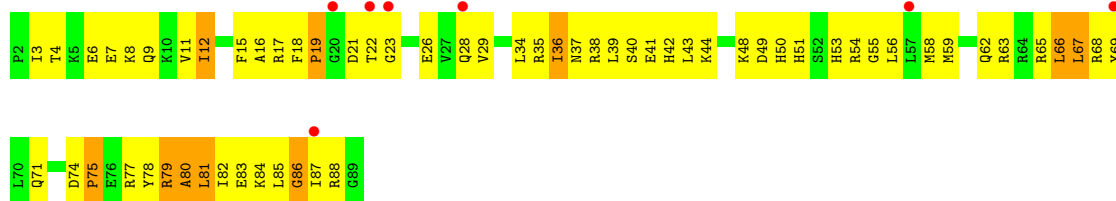
- Molecule 45: 30S ribosomal protein S14 type Z



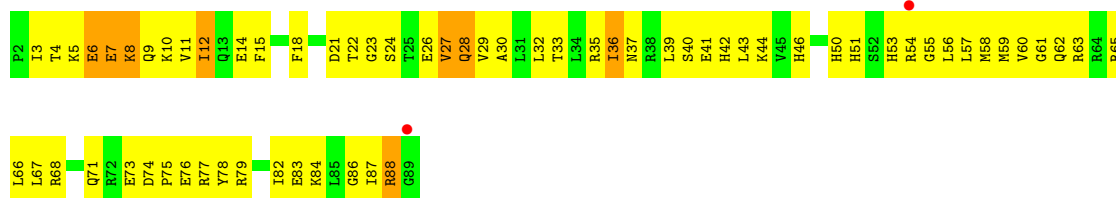
- Molecule 45: 30S ribosomal protein S14 type Z



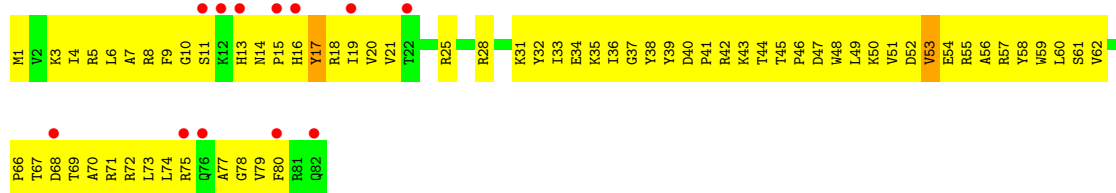
- Molecule 46: 30S ribosomal protein S15



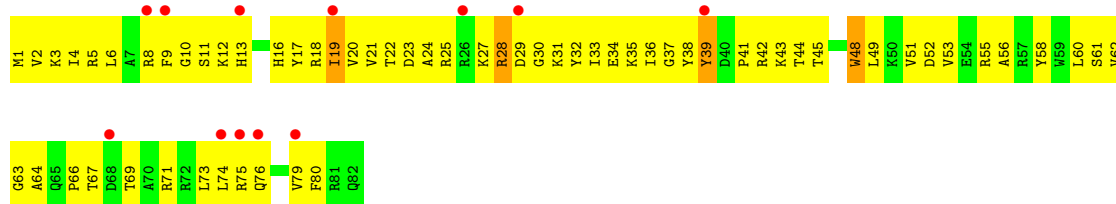
• Molecule 46: 30S ribosomal protein S15



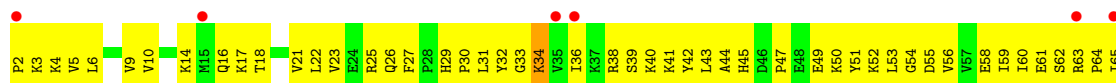
• Molecule 47: 30S ribosomal protein S16

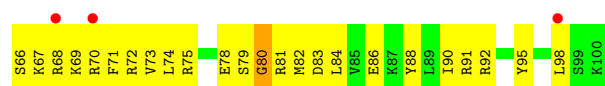


• Molecule 47: 30S ribosomal protein S16



• Molecule 48: 30S ribosomal protein S17

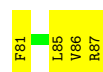




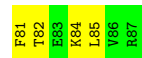
• Molecule 48: 30S ribosomal protein S17



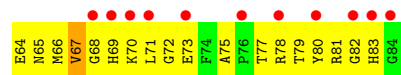
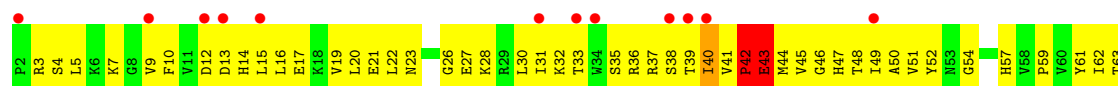
• Molecule 49: 30S ribosomal protein S18



• Molecule 49: 30S ribosomal protein S18

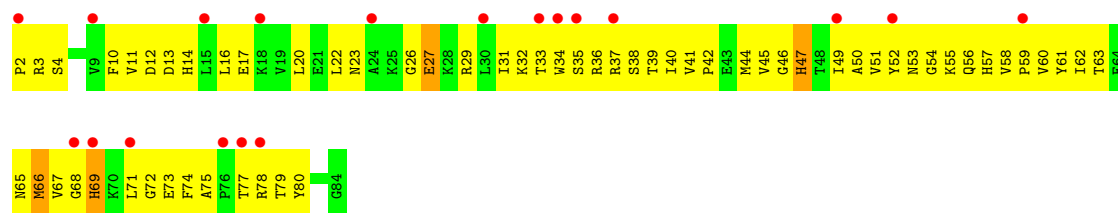


• Molecule 50: 30S ribosomal protein S19

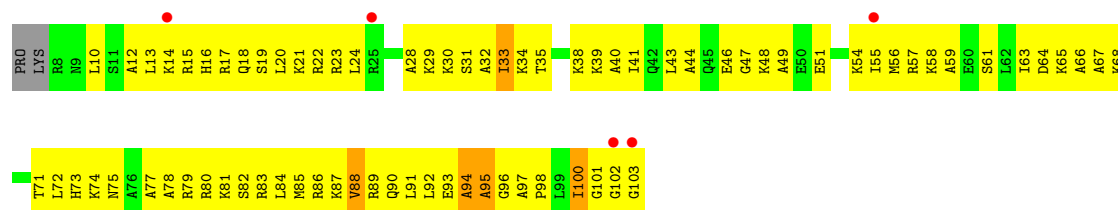


• Molecule 50: 30S ribosomal protein S19

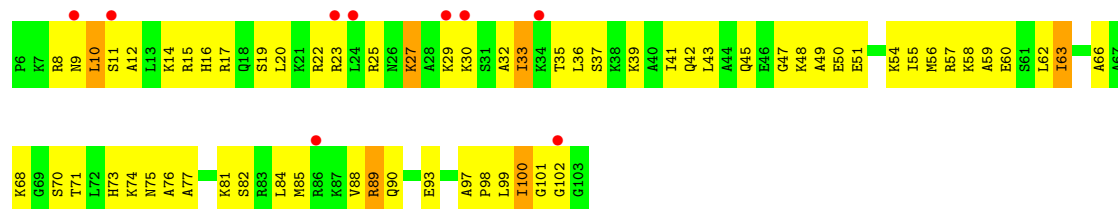




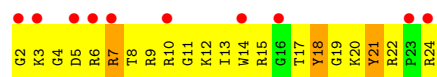
• Molecule 51: 30S ribosomal protein S20



• Molecule 51: 30S ribosomal protein S20



• Molecule 52: 30S ribosomal protein Thx



• Molecule 52: 30S ribosomal protein Thx



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.04Å 449.52Å 624.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 3.14 49.92 – 3.14	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.92-3.14) 97.9 (49.92-3.14)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.238 , 0.292 0.238 , 0.292	Depositor DCC
R_{free} test set	49960 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 217.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	290633	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.08	0/69029	0.24	0/107749
1	2A	0.08	0/68903	0.23	0/107552
2	1B	0.08	0/2876	0.23	0/4486
2	2B	0.08	0/2878	0.22	0/4490
3	1D	0.14	0/2181	0.46	0/2940
3	2D	0.28	1/2186 (0.0%)	0.50	4/2944 (0.1%)
4	1E	0.14	0/1592	0.44	0/2149
4	2E	0.14	0/1592	0.43	0/2149
5	1F	0.13	0/1619	0.38	0/2193
5	2F	0.12	0/1615	0.38	0/2188
6	1G	0.12	0/1451	0.40	0/1961
6	2G	0.11	0/1449	0.43	0/1957
7	1H	0.12	0/1356	0.37	0/1834
7	2H	0.12	0/1350	0.42	2/1826 (0.1%)
8	1I	0.12	0/1109	0.39	0/1512
8	2I	0.12	0/1095	0.36	0/1494
9	1N	0.11	0/1148	0.37	0/1547
9	2N	0.11	0/1144	0.40	0/1543
10	1O	0.11	0/943	0.38	0/1269
10	2O	0.15	0/943	0.40	0/1269
11	1P	0.15	0/1152	0.42	0/1533
11	2P	0.13	0/1152	0.48	1/1533 (0.1%)
12	1Q	0.13	0/1143	0.43	0/1527
12	2Q	0.12	0/1143	0.39	0/1527
13	1R	0.16	0/982	0.46	0/1312
13	2R	0.12	0/982	0.41	0/1312
14	1S	0.12	0/887	0.40	0/1180
14	2S	0.13	0/880	0.41	0/1172
15	1T	0.36	1/1105 (0.1%)	0.61	3/1477 (0.2%)
15	2T	0.22	0/1097	0.55	4/1468 (0.3%)
16	1U	0.15	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.12	0/977	0.40	0/1301
17	1V	0.12	0/786	0.40	0/1053
17	2V	0.16	0/782	0.46	0/1049
18	1W	0.47	2/897 (0.2%)	0.75	7/1205 (0.6%)
18	2W	0.12	0/897	0.44	0/1205
19	1X	0.09	0/764	0.36	0/1025
19	2X	0.13	0/764	0.36	0/1025
20	1Y	0.12	0/823	0.36	0/1099
20	2Y	0.13	0/823	0.39	0/1100
21	1Z	0.12	0/1620	0.38	0/2200
21	2Z	0.18	0/1590	0.50	1/2162 (0.0%)
22	10	0.12	0/616	0.39	0/821
22	20	0.13	0/616	0.44	0/821
23	11	0.14	0/761	0.42	0/1013
23	21	0.12	0/766	0.38	0/1018
24	12	0.11	0/590	0.39	0/781
24	22	0.16	0/594	0.51	0/785
25	13	0.12	0/474	0.38	0/635
25	23	0.14	0/469	0.47	0/630
26	14	0.21	0/559	0.62	1/754 (0.1%)
26	24	0.13	0/549	0.44	0/741
27	15	0.14	0/473	0.45	0/639
27	25	0.12	0/469	0.35	0/635
28	16	0.11	0/460	0.43	0/613
28	26	0.13	0/456	0.40	0/608
29	17	0.13	0/426	0.45	0/561
29	27	0.15	0/426	0.47	0/561
30	18	0.13	0/525	0.35	0/691
30	28	0.11	0/525	0.39	0/691
31	19	0.29	0/310	0.47	0/407
31	29	0.12	0/310	0.45	0/407
32	1a	0.09	0/35795	0.24	0/55864
32	2a	0.09	0/35890	0.24	0/56012
33	1b	0.16	0/1876	0.50	0/2533
33	2b	0.18	0/1860	0.47	0/2518
34	1c	0.13	0/1582	0.40	0/2137
34	2c	0.31	1/1566 (0.1%)	0.42	0/2119
35	1d	0.22	1/1695 (0.1%)	0.52	1/2274 (0.0%)
35	2d	0.14	0/1698	0.46	0/2277
36	1e	0.12	0/1149	0.41	0/1548
36	2e	0.13	0/1149	0.46	0/1548
37	1f	0.12	0/827	0.39	0/1120
37	2f	0.19	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.12	0/1254	0.41	0/1683
38	2g	0.13	0/1248	0.43	0/1676
39	1h	0.13	0/1118	0.45	0/1506
39	2h	0.15	0/1108	0.42	0/1494
40	1i	0.16	0/1005	0.44	0/1351
40	2i	0.12	0/985	0.39	0/1329
41	1j	0.12	0/732	0.41	0/993
41	2j	0.12	0/723	0.36	0/984
42	1k	0.11	0/849	0.37	0/1150
42	2k	0.27	0/848	0.52	2/1149 (0.2%)
43	1l	0.13	0/937	0.44	0/1260
43	2l	0.12	0/937	0.43	0/1260
44	1m	0.13	0/924	0.45	0/1242
44	2m	0.13	0/905	0.45	0/1217
45	1n	0.16	0/501	0.48	0/664
45	2n	0.14	0/501	0.42	0/664
46	1o	0.12	0/739	0.47	0/985
46	2o	0.11	0/739	0.43	0/985
47	1p	0.12	0/697	0.41	0/939
47	2p	0.13	0/693	0.47	0/935
48	1q	0.11	0/836	0.41	0/1117
48	2q	0.12	0/836	0.39	0/1117
49	1r	0.23	0/560	0.52	0/746
49	2r	0.18	0/560	0.48	0/746
50	1s	0.45	1/663 (0.2%)	0.88	8/895 (0.9%)
50	2s	0.14	0/660	0.47	0/893
51	1t	0.12	0/734	0.42	0/969
51	2t	0.16	0/736	0.42	0/976
52	1u	0.21	0/203	0.55	0/266
52	2u	0.14	0/203	0.49	0/266
All	All	0.12	7/308406 (0.0%)	0.31	34/461160 (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
3	2D	0	1
26	14	0	1
26	24	0	1
33	1b	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	2k	0	1
50	1s	0	2
All	All	0	7

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1W	11	ARG	CZ-NH1	9.79	1.46	1.32
34	2c	127	ARG	CG-CD	7.68	1.75	1.52
3	2D	275	LYS	CE-NZ	7.17	1.70	1.49
50	1s	43	GLU	CB-CG	7.05	1.73	1.52
15	1T	74	ARG	CB-CG	6.58	1.72	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1W	11	ARG	NE-CZ-NH2	-14.08	106.53	119.20
50	1s	43	GLU	CB-CG-CD	-10.30	95.08	112.60
15	1T	74	ARG	CG-CD-NE	8.50	130.71	112.00
42	2k	54	ARG	CB-CG-CD	-7.31	94.48	111.30
42	2k	54	ARG	CG-CD-NE	7.10	127.61	112.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	67	TYR	Peptide
33	1b	124	SER	Peptide
50	1s	42	PRO	Peptide
50	1s	43	GLU	Sidechain
3	2D	275	LYS	Peptide

5.2 Too-close contacts ⓘ

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	61868	0	31189	3056	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2A	61758	0	31145	3530	2
2	1B	2572	0	1305	94	0
2	2B	2573	0	1306	139	0
3	1D	2131	0	2206	286	0
3	2D	2136	0	2218	268	0
4	1E	1559	0	1618	220	0
4	2E	1559	0	1618	247	0
5	1F	1584	0	1625	194	0
5	2F	1580	0	1618	196	0
6	1G	1426	0	1445	228	0
6	2G	1424	0	1441	272	0
7	1H	1330	0	1407	84	0
7	2H	1324	0	1402	154	0
8	1I	1094	0	1127	118	1
8	2I	1080	0	1103	110	1
9	1N	1121	0	1194	109	0
9	2N	1117	0	1184	151	0
10	1O	933	0	996	119	0
10	2O	933	0	996	111	0
11	1P	1135	0	1211	131	0
11	2P	1135	0	1212	144	0
12	1Q	1122	0	1178	134	0
12	2Q	1122	0	1179	146	0
13	1R	968	0	1032	111	0
13	2R	968	0	1033	147	0
14	1S	877	0	938	82	0
14	2S	870	0	923	126	0
15	1T	1091	0	1151	114	0
15	2T	1083	0	1136	127	0
16	1U	959	0	1019	116	0
16	2U	959	0	1019	115	0
17	1V	775	0	841	78	0
17	2V	771	0	830	112	0
18	1W	886	0	940	126	0
18	2W	886	0	939	122	0
19	1X	750	0	814	65	0
19	2X	750	0	814	86	0
20	1Y	810	0	892	79	0
20	2Y	810	0	887	95	0
21	1Z	1587	0	1598	171	0
21	2Z	1557	0	1564	217	0
22	10	608	0	622	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	608	0	622	75	0
23	11	754	0	823	52	0
23	21	759	0	837	68	0
24	12	588	0	643	43	0
24	22	592	0	654	69	0
25	13	469	0	518	43	0
25	23	464	0	514	65	0
26	14	546	0	526	109	0
26	24	536	0	518	80	0
27	15	459	0	476	56	0
27	25	455	0	465	53	0
28	16	453	0	473	44	0
28	26	449	0	469	40	0
29	17	418	0	467	40	0
29	27	418	0	467	37	0
30	18	517	0	582	81	0
30	28	517	0	581	70	0
31	19	307	0	335	23	0
31	29	307	0	335	50	0
32	1a	32246	0	16289	2121	1
32	2a	32331	0	16338	2083	3
33	1b	1842	0	1862	284	0
33	2b	1825	0	1828	280	0
34	1c	1558	0	1557	189	0
34	2c	1542	0	1517	201	0
35	1d	1665	0	1687	273	0
35	2d	1668	0	1702	206	0
36	1e	1133	0	1191	153	0
36	2e	1133	0	1191	151	0
37	1f	814	0	808	122	0
37	2f	816	0	808	137	0
38	1g	1235	0	1249	183	0
38	2g	1229	0	1238	156	0
39	1h	1098	0	1143	148	0
39	2h	1088	0	1126	179	0
40	1i	986	0	990	185	0
40	2i	966	0	953	175	0
41	1j	719	0	672	127	0
41	2j	710	0	661	144	0
42	1k	834	0	838	88	0
42	2k	833	0	836	123	0
43	1l	932	0	978	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	980	122	0
44	1m	914	0	954	169	0
44	2m	895	0	920	191	0
45	1n	492	0	533	122	0
45	2n	492	0	529	69	0
46	1o	728	0	760	78	0
46	2o	728	0	760	90	0
47	1p	681	0	697	116	0
47	2p	677	0	686	94	0
48	1q	823	0	891	116	0
48	2q	823	0	891	115	0
49	1r	555	0	618	84	0
49	2r	555	0	618	103	0
50	1s	648	0	658	151	0
50	2s	645	0	635	122	0
51	1t	732	0	809	101	0
51	2t	733	0	795	77	0
52	1u	199	0	208	51	0
52	2u	199	0	208	47	0
53	10	6	0	0	0	0
53	11	3	0	0	0	0
53	13	1	0	0	0	0
53	15	1	0	0	0	0
53	17	3	0	0	0	0
53	18	3	0	0	0	0
53	19	2	0	0	0	0
53	1A	837	0	0	0	0
53	1B	24	0	0	0	0
53	1D	15	0	0	0	0
53	1E	9	0	0	0	0
53	1F	9	0	0	0	0
53	1G	3	0	0	0	0
53	1H	3	0	0	0	0
53	1N	4	0	0	0	0
53	1O	1	0	0	0	0
53	1P	3	0	0	0	0
53	1Q	3	0	0	0	0
53	1R	3	0	0	0	0
53	1S	1	0	0	0	0
53	1T	3	0	0	0	0
53	1U	1	0	0	0	0
53	1V	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	1W	2	0	0	0	0
53	1X	1	0	0	0	0
53	1Y	1	0	0	0	0
53	1Z	2	0	0	0	0
53	1a	203	0	0	0	0
53	1b	1	0	0	0	0
53	1d	2	0	0	0	0
53	1e	1	0	0	0	0
53	1f	2	0	0	0	0
53	1h	1	0	0	0	0
53	1l	2	0	0	0	0
53	1m	1	0	0	0	0
53	1o	1	0	0	0	0
53	1s	1	0	0	0	0
53	1t	1	0	0	0	0
53	20	1	0	0	0	0
53	21	1	0	0	0	0
53	25	1	0	0	0	0
53	27	1	0	0	0	0
53	28	4	0	0	0	0
53	2A	561	0	0	0	0
53	2B	9	0	0	0	0
53	2D	7	0	0	0	0
53	2E	5	0	0	0	0
53	2F	4	0	0	0	0
53	2G	1	0	0	0	0
53	2I	2	0	0	0	0
53	2O	2	0	0	0	0
53	2P	3	0	0	0	0
53	2Q	1	0	0	0	0
53	2R	2	0	0	0	0
53	2T	3	0	0	0	0
53	2U	2	0	0	0	0
53	2V	1	0	0	0	0
53	2W	2	0	0	0	0
53	2X	1	0	0	0	0
53	2Y	1	0	0	0	0
53	2Z	1	0	0	0	0
53	2a	144	0	0	0	0
53	2e	1	0	0	0	0
53	2f	2	0	0	0	0
53	2h	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	2l	2	0	0	0	0
53	2n	1	0	0	0	0
53	2r	2	0	0	0	0
53	2t	1	0	0	0	0
54	1A	12	0	12	2	0
54	1B	12	0	12	1	0
55	18	8	0	14	8	0
55	1A	8	0	14	2	0
55	1T	8	0	14	0	0
55	1a	8	0	14	12	0
55	2A	16	0	27	3	0
55	2B	8	0	14	1	0
56	1A	44	44	0	1	0
56	2A	44	44	0	10	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	3	0
58	2d	8	0	0	4	0
59	10	16	0	0	6	0
59	11	13	0	0	1	0
59	12	5	0	0	5	0
59	13	8	0	0	5	0
59	15	6	0	0	3	0
59	16	5	0	0	0	0
59	17	3	0	0	0	0
59	18	18	0	0	9	0
59	19	9	0	0	2	0
59	1A	1757	0	0	580	1
59	1B	40	0	0	13	0
59	1D	49	0	0	24	0
59	1E	31	0	0	14	0
59	1F	32	0	0	16	0
59	1G	6	0	0	3	0
59	1H	10	0	0	2	0
59	1I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1N	34	0	0	13	0
59	1O	10	0	0	6	0
59	1P	28	0	0	12	0
59	1Q	19	0	0	12	0
59	1R	18	0	0	14	0
59	1S	3	0	0	4	0
59	1T	14	0	0	3	0
59	1U	24	0	0	9	0
59	1V	33	0	0	19	1
59	1W	21	0	0	16	0
59	1X	5	0	0	1	0
59	1Y	7	0	0	4	0
59	1Z	6	0	0	5	0
59	1a	235	0	0	86	0
59	1c	1	0	0	0	0
59	1d	4	0	0	4	0
59	1e	1	0	0	1	0
59	1h	2	0	0	3	0
59	1i	1	0	0	0	0
59	1l	2	0	0	0	0
59	1m	1	0	0	0	0
59	1o	2	0	0	0	0
59	1q	1	0	0	0	0
59	20	5	0	0	2	0
59	21	4	0	0	2	0
59	22	1	0	0	2	0
59	23	2	0	0	0	0
59	25	1	0	0	1	0
59	26	2	0	0	3	0
59	27	5	0	0	2	0
59	28	5	0	0	2	0
59	2A	859	0	0	367	0
59	2B	5	0	0	5	0
59	2D	12	0	0	5	0
59	2E	11	0	0	9	0
59	2F	6	0	0	5	0
59	2G	4	0	0	4	0
59	2I	1	0	0	1	0
59	2O	6	0	0	4	0
59	2P	7	0	0	6	0
59	2Q	5	0	0	1	0
59	2R	5	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2S	1	0	0	1	0
59	2T	4	0	0	0	0
59	2U	5	0	0	2	0
59	2V	3	0	0	1	0
59	2W	4	0	0	2	0
59	2X	5	0	0	2	0
59	2Y	2	0	0	1	0
59	2a	113	0	0	49	0
59	2f	1	0	0	0	0
59	2o	1	0	0	0	0
59	2q	1	0	0	1	0
All	All	290545	88	192953	20570	5

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 44.

The worst 5 of 20570 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)
34:2c:127:ARG:CG	34:2c:127:ARG:CD	1.75	1.55
3:2D:275:LYS:CE	3:2D:275:LYS:NZ	1.70	1.51
1:2A:2612:C:OP1	56:2A:3553:FSD:CAC	1.86	1.24
1:1A:1109:C:H3'	1:1A:1110:U:H5''	1.23	1.19
36:1e:11:ILE:HB	36:1e:31:LEU:HD12	1.23	1.17

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:91:SER:OG	32:2a:364:U:OP1[3_654]	2.01	0.19
1:2A:384:G:O2'	32:2a:83:U:O4[3_754]	2.05	0.15
59:1A:5615:HOH:O	59:1V:322:HOH:O[4_445]	2.08	0.12
32:1a:364:U:OP1	8:2I:91:SER:OG[2_655]	2.08	0.12
1:2A:384:G:N2	32:2a:83:U:O2[3_754]	2.10	0.10

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	273/275 (99%)	222 (81%)	39 (14%)	12 (4%)	2	10
3	2D	273/275 (99%)	222 (81%)	46 (17%)	5 (2%)	6	25
4	1E	202/204 (99%)	170 (84%)	29 (14%)	3 (2%)	8	29
4	2E	202/204 (99%)	166 (82%)	31 (15%)	5 (2%)	4	19
5	1F	201/203 (99%)	173 (86%)	23 (11%)	5 (2%)	4	19
5	2F	201/203 (99%)	163 (81%)	33 (16%)	5 (2%)	4	19
6	1G	179/181 (99%)	137 (76%)	34 (19%)	8 (4%)	2	10
6	2G	179/181 (99%)	124 (69%)	43 (24%)	12 (7%)	1	5
7	1H	172/174 (99%)	144 (84%)	23 (13%)	5 (3%)	3	17
7	2H	171/174 (98%)	134 (78%)	27 (16%)	10 (6%)	1	7
8	1I	145/147 (99%)	119 (82%)	15 (10%)	11 (8%)	1	4
8	2I	144/147 (98%)	110 (76%)	24 (17%)	10 (7%)	1	5
9	1N	138/140 (99%)	118 (86%)	17 (12%)	3 (2%)	5	21
9	2N	138/140 (99%)	116 (84%)	15 (11%)	7 (5%)	1	9
10	1O	120/122 (98%)	98 (82%)	19 (16%)	3 (2%)	4	19
10	2O	120/122 (98%)	92 (77%)	22 (18%)	6 (5%)	1	9
11	1P	147/149 (99%)	129 (88%)	15 (10%)	3 (2%)	6	23
11	2P	147/149 (99%)	113 (77%)	28 (19%)	6 (4%)	2	11
12	1Q	139/141 (99%)	114 (82%)	17 (12%)	8 (6%)	1	7
12	2Q	139/141 (99%)	114 (82%)	22 (16%)	3 (2%)	5	21
13	1R	116/118 (98%)	95 (82%)	17 (15%)	4 (3%)	3	14
13	2R	116/118 (98%)	87 (75%)	20 (17%)	9 (8%)	1	3
14	1S	108/110 (98%)	85 (79%)	20 (18%)	3 (3%)	4	17
14	2S	108/110 (98%)	85 (79%)	20 (18%)	3 (3%)	4	17
15	1T	129/131 (98%)	99 (77%)	24 (19%)	6 (5%)	2	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/131 (98%)	104 (81%)	23 (18%)	2 (2%)	7	28
16	1U	114/116 (98%)	99 (87%)	15 (13%)	0	100	100
16	2U	114/116 (98%)	89 (78%)	21 (18%)	4 (4%)	3	14
17	1V	99/101 (98%)	84 (85%)	12 (12%)	3 (3%)	3	16
17	2V	99/101 (98%)	80 (81%)	17 (17%)	2 (2%)	6	23
18	1W	110/112 (98%)	96 (87%)	11 (10%)	3 (3%)	4	18
18	2W	110/112 (98%)	80 (73%)	18 (16%)	12 (11%)	0	2
19	1X	93/95 (98%)	77 (83%)	13 (14%)	3 (3%)	3	15
19	2X	93/95 (98%)	80 (86%)	9 (10%)	4 (4%)	2	10
20	1Y	105/107 (98%)	95 (90%)	6 (6%)	4 (4%)	2	13
20	2Y	105/107 (98%)	85 (81%)	17 (16%)	3 (3%)	3	17
21	1Z	201/203 (99%)	161 (80%)	28 (14%)	12 (6%)	1	6
21	2Z	199/203 (98%)	148 (74%)	38 (19%)	13 (6%)	1	5
22	10	75/77 (97%)	61 (81%)	11 (15%)	3 (4%)	2	11
22	20	75/77 (97%)	58 (77%)	15 (20%)	2 (3%)	4	18
23	11	95/97 (98%)	80 (84%)	13 (14%)	2 (2%)	5	22
23	21	95/97 (98%)	84 (88%)	9 (10%)	2 (2%)	5	22
24	12	68/70 (97%)	55 (81%)	10 (15%)	3 (4%)	2	10
24	22	68/70 (97%)	51 (75%)	13 (19%)	4 (6%)	1	7
25	13	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	6	25
25	23	57/59 (97%)	47 (82%)	9 (16%)	1 (2%)	6	25
26	14	67/69 (97%)	48 (72%)	14 (21%)	5 (8%)	1	4
26	24	67/69 (97%)	45 (67%)	18 (27%)	4 (6%)	1	6
27	15	57/59 (97%)	49 (86%)	8 (14%)	0	100	100
27	25	57/59 (97%)	47 (82%)	10 (18%)	0	100	100
28	16	51/53 (96%)	41 (80%)	8 (16%)	2 (4%)	2	12
28	26	51/53 (96%)	44 (86%)	7 (14%)	0	100	100
29	17	46/48 (96%)	37 (80%)	7 (15%)	2 (4%)	2	10
29	27	46/48 (96%)	33 (72%)	13 (28%)	0	100	100
30	18	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	7	28
30	28	62/64 (97%)	54 (87%)	8 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
31	29	35/37 (95%)	27 (77%)	7 (20%)	1 (3%)	3	17
33	1b	229/231 (99%)	164 (72%)	35 (15%)	30 (13%)	0	1
33	2b	229/231 (99%)	162 (71%)	48 (21%)	19 (8%)	0	3
34	1c	204/206 (99%)	161 (79%)	34 (17%)	9 (4%)	2	10
34	2c	204/206 (99%)	153 (75%)	40 (20%)	11 (5%)	1	8
35	1d	206/208 (99%)	157 (76%)	38 (18%)	11 (5%)	1	8
35	2d	206/208 (99%)	161 (78%)	39 (19%)	6 (3%)	3	17
36	1e	146/148 (99%)	121 (83%)	17 (12%)	8 (6%)	1	7
36	2e	146/148 (99%)	116 (80%)	24 (16%)	6 (4%)	2	11
37	1f	98/100 (98%)	75 (76%)	20 (20%)	3 (3%)	3	16
37	2f	98/100 (98%)	75 (76%)	21 (21%)	2 (2%)	6	23
38	1g	153/155 (99%)	120 (78%)	29 (19%)	4 (3%)	4	18
38	2g	153/155 (99%)	121 (79%)	23 (15%)	9 (6%)	1	7
39	1h	135/137 (98%)	104 (77%)	23 (17%)	8 (6%)	1	7
39	2h	135/137 (98%)	102 (76%)	23 (17%)	10 (7%)	1	4
40	1i	125/127 (98%)	92 (74%)	29 (23%)	4 (3%)	3	15
40	2i	124/127 (98%)	95 (77%)	21 (17%)	8 (6%)	1	5
41	1j	95/97 (98%)	72 (76%)	16 (17%)	7 (7%)	1	4
41	2j	94/97 (97%)	74 (79%)	15 (16%)	5 (5%)	1	8
42	1k	112/114 (98%)	86 (77%)	20 (18%)	6 (5%)	1	8
42	2k	112/114 (98%)	82 (73%)	24 (21%)	6 (5%)	1	8
43	1l	119/122 (98%)	92 (77%)	20 (17%)	7 (6%)	1	7
43	2l	119/122 (98%)	94 (79%)	22 (18%)	3 (2%)	4	19
44	1m	114/116 (98%)	89 (78%)	21 (18%)	4 (4%)	3	14
44	2m	112/116 (97%)	82 (73%)	24 (21%)	6 (5%)	1	8
45	1n	58/60 (97%)	45 (78%)	11 (19%)	2 (3%)	3	14
45	2n	58/60 (97%)	43 (74%)	9 (16%)	6 (10%)	0	2
46	1o	86/88 (98%)	57 (66%)	18 (21%)	11 (13%)	0	1
46	2o	86/88 (98%)	56 (65%)	22 (26%)	8 (9%)	0	2
47	1p	80/82 (98%)	66 (82%)	12 (15%)	2 (2%)	4	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/82 (98%)	64 (80%)	12 (15%)	4 (5%)	1	9
48	1q	97/99 (98%)	75 (77%)	19 (20%)	3 (3%)	3	16
48	2q	97/99 (98%)	85 (88%)	9 (9%)	3 (3%)	3	16
49	1r	66/68 (97%)	49 (74%)	11 (17%)	6 (9%)	0	2
49	2r	66/68 (97%)	50 (76%)	11 (17%)	5 (8%)	1	4
50	1s	81/83 (98%)	58 (72%)	22 (27%)	1 (1%)	10	34
50	2s	81/83 (98%)	64 (79%)	12 (15%)	5 (6%)	1	6
51	1t	94/98 (96%)	76 (81%)	13 (14%)	5 (5%)	1	8
51	2t	96/98 (98%)	68 (71%)	18 (19%)	10 (10%)	0	2
52	1u	21/23 (91%)	19 (90%)	1 (5%)	1 (5%)	2	10
52	2u	21/23 (91%)	15 (71%)	4 (19%)	2 (10%)	0	2
All	All	11440/11648 (98%)	9049 (79%)	1872 (16%)	519 (4%)	2	10

5 of 519 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1D	22	SER
3	1D	127	VAL
6	1G	49	ASP
6	1G	52	ILE
6	1G	110	ALA

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	214/217 (99%)	212 (99%)	2 (1%)	70	77
3	2D	215/217 (99%)	213 (99%)	2 (1%)	70	77
4	1E	164/165 (99%)	164 (100%)	0	100	100
4	2E	164/165 (99%)	163 (99%)	1 (1%)	78	80
5	1F	160/161 (99%)	160 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/161 (99%)	157 (99%)	2 (1%)	61	73
6	1G	144/155 (93%)	144 (100%)	0	100	100
6	2G	142/155 (92%)	142 (100%)	0	100	100
7	1H	144/145 (99%)	144 (100%)	0	100	100
7	2H	143/145 (99%)	143 (100%)	0	100	100
8	1I	111/123 (90%)	111 (100%)	0	100	100
8	2I	109/123 (89%)	109 (100%)	0	100	100
9	1N	119/119 (100%)	118 (99%)	1 (1%)	73	78
9	2N	118/119 (99%)	117 (99%)	1 (1%)	73	78
10	1O	100/100 (100%)	99 (99%)	1 (1%)	68	76
10	2O	100/100 (100%)	98 (98%)	2 (2%)	48	68
11	1P	115/116 (99%)	115 (100%)	0	100	100
11	2P	115/116 (99%)	114 (99%)	1 (1%)	70	77
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	39	63
12	2Q	111/111 (100%)	109 (98%)	2 (2%)	51	69
13	1R	101/101 (100%)	101 (100%)	0	100	100
13	2R	101/101 (100%)	101 (100%)	0	100	100
14	1S	87/87 (100%)	86 (99%)	1 (1%)	65	75
14	2S	85/87 (98%)	85 (100%)	0	100	100
15	1T	115/115 (100%)	113 (98%)	2 (2%)	53	70
15	2T	113/115 (98%)	112 (99%)	1 (1%)	70	77
16	1U	93/93 (100%)	92 (99%)	1 (1%)	65	75
16	2U	93/93 (100%)	92 (99%)	1 (1%)	65	75
17	1V	81/82 (99%)	80 (99%)	1 (1%)	63	74
17	2V	80/82 (98%)	78 (98%)	2 (2%)	42	64
18	1W	90/91 (99%)	87 (97%)	3 (3%)	33	59
18	2W	90/91 (99%)	90 (100%)	0	100	100
19	1X	77/77 (100%)	76 (99%)	1 (1%)	61	73
19	2X	77/77 (100%)	74 (96%)	3 (4%)	28	56
20	1Y	86/88 (98%)	85 (99%)	1 (1%)	63	74
20	2Y	86/88 (98%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	169/176 (96%)	166 (98%)	3 (2%)	51	69
21	2Z	165/176 (94%)	162 (98%)	3 (2%)	51	69
22	10	61/62 (98%)	61 (100%)	0	100	100
22	20	61/62 (98%)	60 (98%)	1 (2%)	55	71
23	11	79/82 (96%)	79 (100%)	0	100	100
23	21	81/82 (99%)	81 (100%)	0	100	100
24	12	65/66 (98%)	65 (100%)	0	100	100
24	22	66/66 (100%)	66 (100%)	0	100	100
25	13	51/51 (100%)	51 (100%)	0	100	100
25	23	50/51 (98%)	50 (100%)	0	100	100
26	14	58/62 (94%)	55 (95%)	3 (5%)	21	48
26	24	54/62 (87%)	53 (98%)	1 (2%)	50	69
27	15	51/51 (100%)	50 (98%)	1 (2%)	48	68
27	25	50/51 (98%)	50 (100%)	0	100	100
28	16	51/51 (100%)	50 (98%)	1 (2%)	48	68
28	26	50/51 (98%)	50 (100%)	0	100	100
29	17	41/41 (100%)	41 (100%)	0	100	100
29	27	41/41 (100%)	41 (100%)	0	100	100
30	18	54/54 (100%)	54 (100%)	0	100	100
30	28	54/54 (100%)	54 (100%)	0	100	100
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	191/199 (96%)	190 (100%)	1 (0%)	81	82
33	2b	187/199 (94%)	186 (100%)	1 (0%)	81	82
34	1c	144/160 (90%)	142 (99%)	2 (1%)	59	72
34	2c	140/160 (88%)	140 (100%)	0	100	100
35	1d	171/180 (95%)	171 (100%)	0	100	100
35	2d	172/180 (96%)	171 (99%)	1 (1%)	78	80
36	1e	114/114 (100%)	114 (100%)	0	100	100
36	2e	114/114 (100%)	113 (99%)	1 (1%)	70	77
37	1f	85/90 (94%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	83 (98%)	2 (2%)	43	65
38	1g	120/126 (95%)	119 (99%)	1 (1%)	73	78
38	2g	119/126 (94%)	119 (100%)	0	100	100
39	1h	116/118 (98%)	115 (99%)	1 (1%)	70	77
39	2h	114/118 (97%)	112 (98%)	2 (2%)	51	69
40	1i	91/98 (93%)	88 (97%)	3 (3%)	33	59
40	2i	88/98 (90%)	88 (100%)	0	100	100
41	1j	68/87 (78%)	68 (100%)	0	100	100
41	2j	68/87 (78%)	67 (98%)	1 (2%)	57	71
42	1k	83/86 (96%)	82 (99%)	1 (1%)	63	74
42	2k	83/86 (96%)	83 (100%)	0	100	100
43	1l	96/102 (94%)	95 (99%)	1 (1%)	68	76
43	2l	96/102 (94%)	95 (99%)	1 (1%)	68	76
44	1m	90/94 (96%)	90 (100%)	0	100	100
44	2m	87/94 (93%)	87 (100%)	0	100	100
45	1n	49/49 (100%)	48 (98%)	1 (2%)	48	68
45	2n	49/49 (100%)	49 (100%)	0	100	100
46	1o	78/79 (99%)	78 (100%)	0	100	100
46	2o	78/79 (99%)	78 (100%)	0	100	100
47	1p	69/71 (97%)	68 (99%)	1 (1%)	59	72
47	2p	68/71 (96%)	67 (98%)	1 (2%)	57	71
48	1q	94/94 (100%)	94 (100%)	0	100	100
48	2q	94/94 (100%)	94 (100%)	0	100	100
49	1r	59/59 (100%)	57 (97%)	2 (3%)	32	58
49	2r	59/59 (100%)	58 (98%)	1 (2%)	53	70
50	1s	68/72 (94%)	67 (98%)	1 (2%)	57	71
50	2s	67/72 (93%)	67 (100%)	0	100	100
51	1t	71/76 (93%)	71 (100%)	0	100	100
51	2t	70/76 (92%)	70 (100%)	0	100	100
52	1u	18/18 (100%)	16 (89%)	2 (11%)	6	21
52	2u	18/18 (100%)	17 (94%)	1 (6%)	19	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9364/9696 (97%)	9287 (99%)	77 (1%)	73 78

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	2X	5	TYR
39	2h	65	TYR
19	2X	69	TYR
33	2b	199	TYR
49	2r	43	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 155 such sidechains are listed below:

Mol	Chain	Res	Type
27	25	22	HIS
46	2o	50	HIS
31	29	36	GLN
37	2f	64	GLN
49	2r	63	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	484 (16%)	22 (0%)
1	2A	2858/2915 (98%)	519 (18%)	38 (1%)
2	1B	119/120 (99%)	13 (10%)	0
2	2B	119/120 (99%)	17 (14%)	0
32	1a	1497/2331 (64%)	279 (18%)	0
32	2a	1501/2331 (64%)	273 (18%)	0
All	All	8959/10732 (83%)	1585 (17%)	60 (0%)

5 of 1585 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	12	A
1	1A	34	G
1	1A	38	C
1	1A	44	C

5 of 60 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	367	G
1	2A	2193	U
1	2A	1039	C
1	2A	2192	A
1	2A	2700	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	$\# Z > 2$
1	5MC	2A	1983	1	19,22,23	1.69	3 (15%)	26,32,35	1.11	2 (7%)
32	5MC	2a	1387	32	19,22,23	1.61	3 (15%)	26,32,35	1.17	2 (7%)
43	0TD	1l	92	43	8,9,10	4.69	2 (25%)	6,11,13	10.16	2 (33%)
1	5MU	2A	1960	1,53	19,22,23	1.42	6 (31%)	27,32,35	2.11	6 (22%)
1	PSU	2A	2616	1	18,21,22	1.34	2 (11%)	21,30,33	2.06	4 (19%)
32	PSU	1a	500	32,53	18,21,22	1.35	2 (11%)	21,30,33	2.05	5 (23%)
32	G7M	1a	511	32,53	23,26,27	2.40	5 (21%)	34,39,42	3.04	10 (29%)
1	OMG	2A	2262	1,53	23,26,27	1.18	3 (13%)	32,38,41	1.99	7 (21%)
1	2MA	2A	2514	1,53	22,25,26	1.51	4 (18%)	32,37,40	2.27	9 (28%)
32	PSU	2a	500	32,53	18,21,22	1.37	2 (11%)	21,30,33	2.02	5 (23%)
32	G7M	2a	511	32,53	23,26,27	2.38	5 (21%)	34,39,42	3.08	10 (29%)
32	UR3	2a	1476	32	19,22,23	1.00	2 (10%)	26,32,35	1.72	2 (7%)
32	MA6	1a	1496	32	23,26,27	1.51	4 (17%)	33,38,41	2.41	13 (39%)
32	5MC	1a	1387	32	19,22,23	1.70	3 (15%)	26,32,35	1.12	2 (7%)
1	PSU	1A	2616	1	18,21,22	1.35	2 (11%)	21,30,33	2.06	4 (19%)
32	5MC	1a	945	32	19,22,23	1.68	3 (15%)	26,32,35	1.13	2 (7%)
32	5MC	2a	945	32	19,22,23	1.67	3 (15%)	26,32,35	1.12	2 (7%)
32	MA6	2a	1496	32	23,26,27	1.53	4 (17%)	33,38,41	2.35	13 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	2A	1936	1	19,22,23	1.41	6 (31%)	27,32,35	2.09	7 (25%)
1	5MC	1A	1983	1	19,22,23	1.68	3 (15%)	26,32,35	1.12	2 (7%)
1	5MC	1A	1963	1	19,22,23	1.67	3 (15%)	26,32,35	1.12	2 (7%)
1	PSU	1A	1932	1	18,21,22	1.35	2 (11%)	21,30,33	2.04	5 (23%)
32	M2G	2a	944	32	24,27,28	1.30	4 (16%)	33,40,43	1.87	6 (18%)
32	5MC	1a	1390	32	19,22,23	1.67	3 (15%)	26,32,35	1.12	2 (7%)
1	OMG	1A	2262	1,53	23,26,27	1.19	3 (13%)	32,38,41	1.94	6 (18%)
32	UR3	1a	1476	32	19,22,23	1.01	1 (5%)	26,32,35	1.73	2 (7%)
1	OMU	1A	2563	1,53	19,22,23	1.28	4 (21%)	25,31,34	1.88	6 (24%)
1	5MC	2A	1963	1	19,22,23	1.66	3 (15%)	26,32,35	1.10	2 (7%)
1	OMC	1A	1941	1	19,22,23	0.77	0	25,31,34	0.83	0
1	PSU	1A	1938	1	18,21,22	1.37	2 (11%)	21,30,33	2.04	4 (19%)
1	5MU	1A	1936	1	19,22,23	1.41	6 (31%)	27,32,35	2.08	7 (25%)
32	5MC	1a	1383	32	19,22,23	1.68	3 (15%)	26,32,35	1.11	2 (7%)
1	PSU	2A	1932	1	18,21,22	1.35	2 (11%)	21,30,33	2.05	4 (19%)
32	2MG	1a	1189	32,53	23,26,27	1.23	3 (13%)	33,38,41	2.25	8 (24%)
32	5MC	2a	1383	32	19,22,23	1.68	3 (15%)	26,32,35	1.12	2 (7%)
32	4OC	1a	1385	32	20,23,24	0.77	0	25,32,35	0.95	1 (4%)
32	2MG	2a	1189	32	23,26,27	1.26	4 (17%)	33,38,41	2.15	5 (15%)
32	MA6	1a	1497	32	23,26,27	1.51	4 (17%)	33,38,41	2.46	12 (36%)
32	MA6	2a	1497	32	23,26,27	1.50	4 (17%)	33,38,41	2.47	14 (42%)
32	4OC	2a	1385	32	20,23,24	0.77	0	25,32,35	0.91	1 (4%)
1	OMU	2A	2563	1,53	19,22,23	1.27	4 (21%)	25,31,34	1.92	6 (24%)
1	2MA	1A	2514	1,53	22,25,26	1.52	4 (18%)	32,37,40	2.27	9 (28%)
1	5MU	1A	1960	1	19,22,23	1.44	6 (31%)	27,32,35	2.13	6 (22%)
32	M2G	1a	944	32	24,27,28	1.30	4 (16%)	33,40,43	1.87	6 (18%)
1	OMC	2A	1941	1	19,22,23	0.79	0	25,31,34	0.85	0
1	PSU	2A	1938	1	18,21,22	1.36	2 (11%)	21,30,33	2.03	4 (19%)
43	0TD	2l	92	43	8,9,10	4.42	1 (12%)	6,11,13	7.14	2 (33%)
32	5MC	2a	1390	32	19,22,23	1.69	3 (15%)	26,32,35	1.12	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	2A	1983	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1387	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
1	5MU	2A	1960	1,53	-	0/7/25/26	0/2/2/2
1	PSU	2A	2616	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	500	32,53	-	2/7/25/26	0/2/2/2
32	G7M	1a	511	32,53	-	2/7/25/26	0/3/3/3
1	OMG	2A	2262	1,53	-	0/9/27/28	0/3/3/3
1	2MA	2A	2514	1,53	-	2/7/25/26	0/3/3/3
32	PSU	2a	500	32,53	-	1/7/25/26	0/2/2/2
32	G7M	2a	511	32,53	-	2/7/25/26	0/3/3/3
32	UR3	2a	1476	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1496	32	-	1/11/29/30	0/3/3/3
32	5MC	1a	1387	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2616	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	945	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	945	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1496	32	-	3/11/29/30	0/3/3/3
1	5MU	2A	1936	1	-	2/7/25/26	0/2/2/2
1	5MC	1A	1983	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1963	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1932	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	944	32	-	4/11/29/30	0/3/3/3
32	5MC	1a	1390	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2262	1,53	-	0/9/27/28	0/3/3/3
32	UR3	1a	1476	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2563	1,53	-	1/9/27/28	0/2/2/2
1	5MC	2A	1963	1	-	2/7/25/26	0/2/2/2
1	OMC	1A	1941	1	-	2/9/27/28	0/2/2/2
1	PSU	1A	1938	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1936	1	-	2/7/25/26	0/2/2/2
32	5MC	1a	1383	32	-	2/7/25/26	0/2/2/2
1	PSU	2A	1932	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1189	32,53	-	0/9/27/28	0/3/3/3
32	5MC	2a	1383	32	-	2/7/25/26	0/2/2/2
32	4OC	1a	1385	32	-	0/9/29/30	0/2/2/2
32	2MG	2a	1189	32	-	0/9/27/28	0/3/3/3
32	MA6	1a	1497	32	-	3/11/29/30	0/3/3/3
32	MA6	2a	1497	32	-	6/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	2a	1385	32	-	2/9/29/30	0/2/2/2
1	OMU	2A	2563	1,53	-	0/9/27/28	0/2/2/2
1	2MA	1A	2514	1,53	-	2/7/25/26	0/3/3/3
1	5MU	1A	1960	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	944	32	-	0/11/29/30	0/3/3/3
1	OMC	2A	1941	1	-	2/9/27/28	0/2/2/2
1	PSU	2A	1938	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
32	5MC	2a	1390	32	-	0/7/25/26	0/2/2/2

The worst 5 of 145 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.40	1.69	1.82
43	2l	92	0TD	CB-SB	-12.09	1.70	1.82
32	1a	511	G7M	C8-N7	7.86	1.46	1.33
32	2a	511	G7M	C8-N7	7.72	1.46	1.33
32	1a	1387	5MC	C5-C4	6.18	1.48	1.44

The worst 5 of 235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-24.62	58.11	102.36
43	2l	92	0TD	CSB-SB-CB	-17.13	71.57	102.36
1	1A	2514	2MA	C5-C4-N3	-7.94	118.82	127.18
1	2A	2514	2MA	C5-C4-N3	-7.89	118.86	127.18
32	2a	511	G7M	CN7-N7-C8	-7.85	112.91	124.79

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	CG-CB-SB-CSB
1	1A	1936	5MU	O4'-C1'-N1-C2
1	1A	1936	5MU	O4'-C1'-N1-C6
1	2A	1936	5MU	O4'-C1'-N1-C2
1	2A	1936	5MU	O4'-C1'-N1-C6

There are no ring outliers.

44 monomers are involved in 143 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1983	5MC	2	0
32	2a	1387	5MC	5	0
43	1l	92	0TD	6	0
1	2A	1960	5MU	1	0
32	1a	500	PSU	2	0
1	2A	2262	OMG	6	0
1	2A	2514	2MA	4	0
32	2a	500	PSU	1	0
32	2a	511	G7M	1	0
32	1a	1496	MA6	5	0
32	1a	1387	5MC	2	0
1	1A	2616	PSU	3	0
32	1a	945	5MC	1	0
32	2a	945	5MC	4	0
32	2a	1496	MA6	9	0
1	2A	1936	5MU	2	0
1	1A	1983	5MC	3	0
1	1A	1963	5MC	1	0
1	1A	1932	PSU	1	0
32	2a	944	M2G	3	0
32	1a	1390	5MC	3	0
1	1A	2262	OMG	3	0
32	1a	1476	UR3	1	0
1	1A	2563	OMU	1	0
1	2A	1963	5MC	4	0
1	1A	1941	OMC	5	0
1	1A	1938	PSU	2	0
1	1A	1936	5MU	3	0
32	1a	1383	5MC	3	0
1	2A	1932	PSU	1	0
32	1a	1189	2MG	5	0
32	2a	1383	5MC	3	0
32	1a	1385	4OC	3	0
32	2a	1189	2MG	7	0
32	1a	1497	MA6	11	0
32	2a	1497	MA6	5	0
32	2a	1385	4OC	7	0
1	2A	2563	OMU	2	0
1	1A	2514	2MA	4	0
1	1A	1960	5MU	3	0
32	1a	944	M2G	3	0
1	2A	1941	OMC	7	0
1	2A	1938	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	2l	92	0TD	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1955 ligands modelled in this entry, 1942 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	$\# Z > 2$
55	MPD	1A	3800	53	7,7,7	0.31	0	9,10,10	0.24	0
55	MPD	2A	3551	1	7,7,7	0.31	0	9,10,10	0.21	0
58	SF4	1d	501	35	0,12,12	-	-	-	-	-
54	ARG	1A	3799	-	10,11,11	0.76	1 (10%)	9,13,13	0.91	1 (11%)
55	MPD	2A	3552	-	7,7,7	0.31	0	9,10,10	0.22	0
55	MPD	1a	1900	-	7,7,7	0.33	0	9,10,10	0.23	0
56	FSD	1A	3801	-	44,47,47	1.17	6 (13%)	57,69,69	1.52	7 (12%)
55	MPD	18	104	-	7,7,7	0.32	0	9,10,10	0.25	0
55	MPD	2B	210	-	7,7,7	0.29	0	9,10,10	0.20	0
58	SF4	2d	501	35	0,12,12	-	-	-	-	-
56	FSD	2A	3553	-	44,47,47	1.49	6 (13%)	57,69,69	2.33	20 (35%)
55	MPD	1T	8004	-	7,7,7	0.31	0	9,10,10	0.30	0
54	ARG	1B	223	53	10,11,11	0.76	1 (10%)	9,13,13	0.91	1 (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
55	MPD	1A	3800	53	-	3/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	MPD	2A	3551	1	-	4/5/5/5	-
58	SF4	1d	501	35	-	-	0/6/5/5
54	ARG	1A	3799	-	-	0/11/11/11	-
55	MPD	2A	3552	-	-	4/5/5/5	-
55	MPD	1a	1900	-	-	4/5/5/5	-
56	FSD	1A	3801	-	-	6/31/66/66	0/4/4/4
55	MPD	18	104	-	-	3/5/5/5	-
55	MPD	2B	210	-	-	1/5/5/5	-
58	SF4	2d	501	35	-	-	0/6/5/5
56	FSD	2A	3553	-	-	12/31/66/66	0/4/4/4
55	MPD	1T	8004	-	-	4/5/5/5	-
54	ARG	1B	223	53	-	1/11/11/11	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2A	3553	FSD	OAY-CBM	-3.79	1.37	1.42
56	2A	3553	FSD	CBF-NAX	-3.75	1.34	1.39
56	2A	3553	FSD	CBF-NAV	-3.57	1.26	1.32
56	1A	3801	FSD	CBG-NAV	2.87	1.42	1.36
56	2A	3553	FSD	CBO-NBP	2.74	1.57	1.48

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	3801	FSD	OAY-CBM-NBQ	7.03	113.40	105.77
56	2A	3553	FSD	CBM-NBQ-CBG	6.83	129.55	117.83
56	2A	3553	FSD	OAH-CBC-CBR	-6.77	112.35	120.24
56	2A	3553	FSD	CBH-OAY-CBM	5.10	119.98	113.00
56	2A	3553	FSD	CBM-NBQ-CAR	-4.64	112.40	121.53

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	1A	3800	MPD	O2-C2-C3-C4
55	1A	3800	MPD	CM-C2-C3-C4
55	1T	8004	MPD	C1-C2-C3-C4
55	1T	8004	MPD	O2-C2-C3-C4
55	1a	1900	MPD	C2-C3-C4-O4

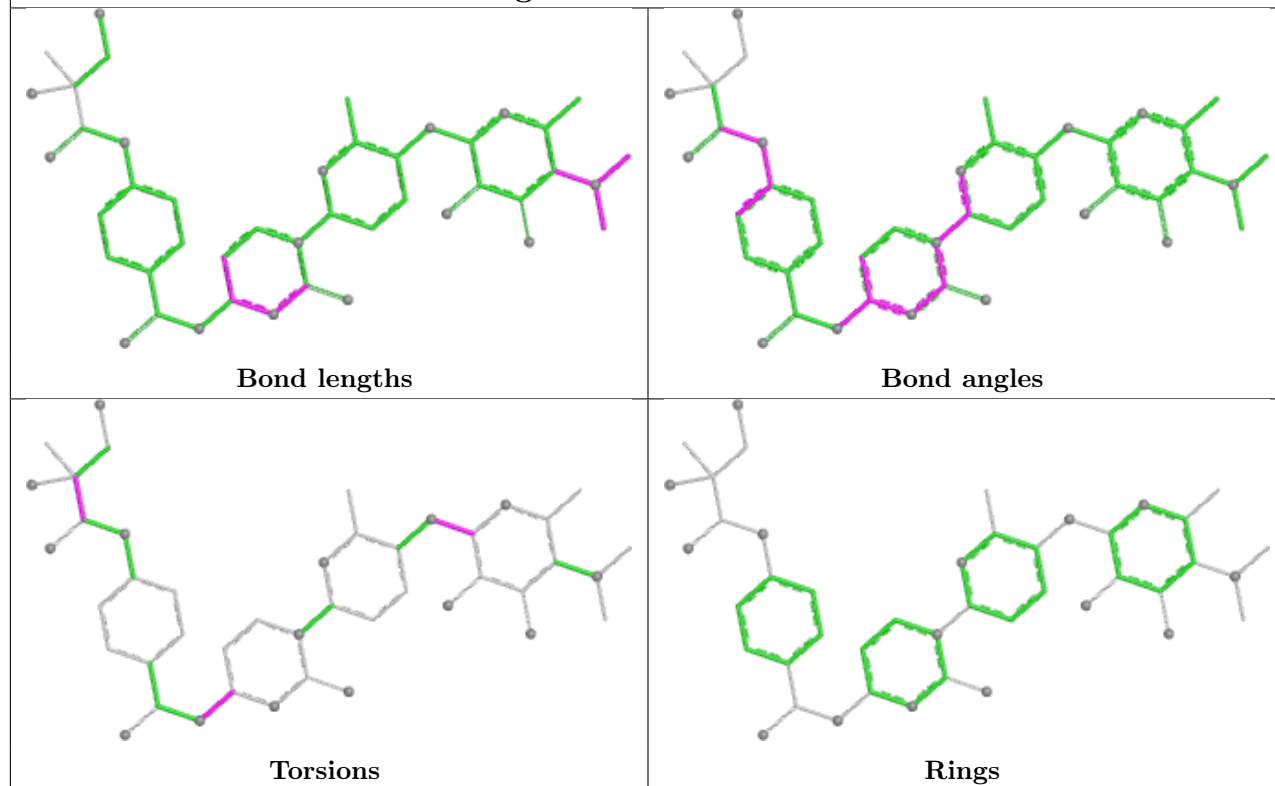
There are no ring outliers.

12 monomers are involved in 47 short contacts:

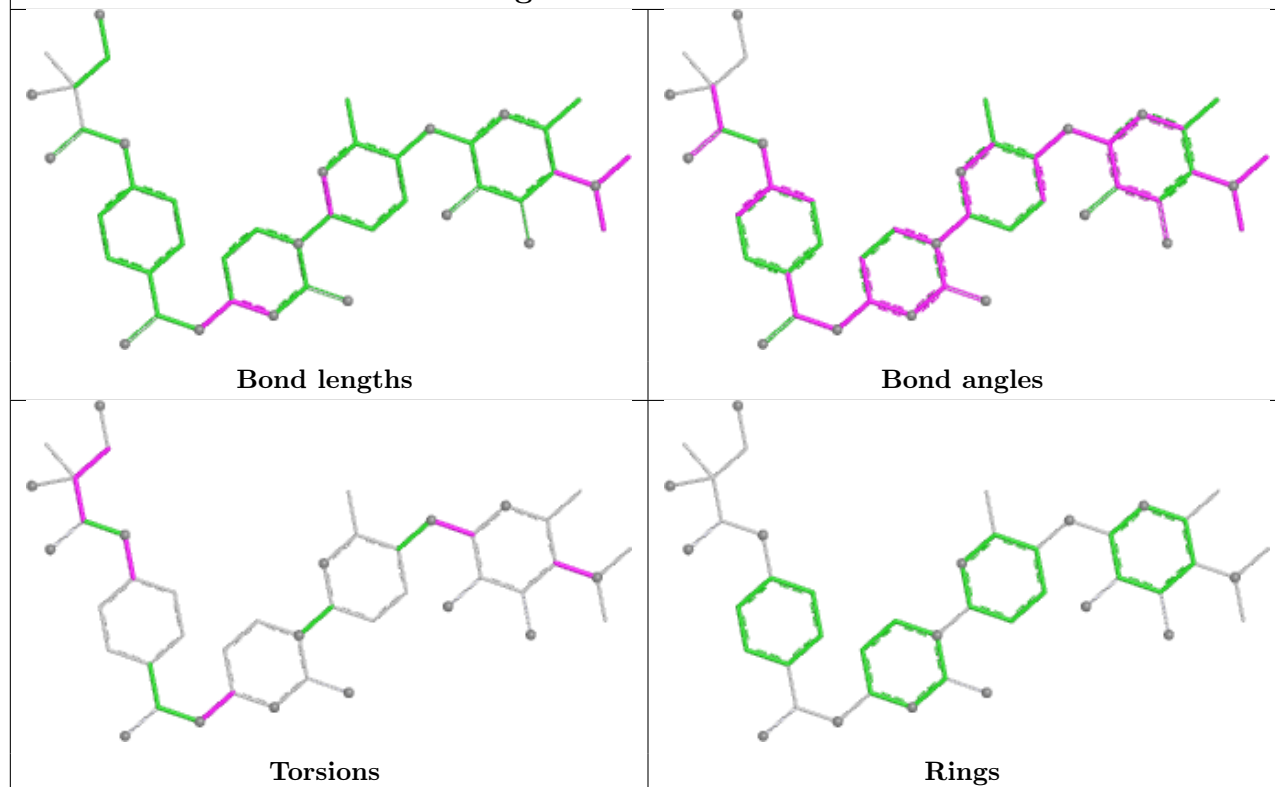
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	1A	3800	MPD	2	0
55	2A	3551	MPD	1	0
58	1d	501	SF4	3	0
54	1A	3799	ARG	2	0
55	2A	3552	MPD	2	0
55	1a	1900	MPD	12	0
56	1A	3801	FSD	1	0
55	18	104	MPD	8	0
55	2B	210	MPD	1	0
58	2d	501	SF4	4	0
56	2A	3553	FSD	10	0
54	1B	223	ARG	1	0

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.

Ligand FSD 1A 3801



Ligand FSD 2A 3553



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%)	0.25	93 (3%)	49	28	26, 55, 217, 326	0
1	2A	2856/2915 (97%)	0.56	110 (3%)	43	23	56, 89, 195, 358	0
2	1B	120/120 (100%)	0.27	0	100	100	35, 70, 93, 122	0
2	2B	120/120 (100%)	0.99	9 (7%)	20	10	83, 134, 160, 179	0
3	1D	275/275 (100%)	0.22	3 (1%)	78	59	29, 54, 74, 105	0
3	2D	275/275 (100%)	0.49	8 (2%)	53	32	53, 78, 100, 112	0
4	1E	204/204 (100%)	0.12	2 (0%)	79	61	26, 54, 75, 100	0
4	2E	204/204 (100%)	0.65	10 (4%)	35	18	60, 96, 131, 142	0
5	1F	203/203 (100%)	0.17	2 (0%)	79	61	26, 59, 96, 165	0
5	2F	203/203 (100%)	0.58	11 (5%)	31	16	57, 91, 124, 143	0
6	1G	181/181 (100%)	0.80	15 (8%)	17	9	67, 120, 158, 180	0
6	2G	181/181 (100%)	1.24	41 (22%)	2	1	124, 175, 205, 217	0
7	1H	174/174 (100%)	0.10	2 (1%)	78	59	39, 69, 88, 101	0
7	2H	173/174 (99%)	0.85	12 (6%)	23	11	104, 144, 172, 178	0
8	1I	147/147 (100%)	0.43	4 (2%)	56	34	60, 113, 135, 160	0
8	2I	146/147 (99%)	0.82	15 (10%)	12	6	83, 132, 152, 162	0
9	1N	140/140 (100%)	0.00	0	100	100	33, 50, 73, 88	0
9	2N	140/140 (100%)	0.54	4 (2%)	53	32	76, 106, 125, 143	0
10	1O	122/122 (100%)	0.05	0	100	100	41, 58, 77, 89	0
10	2O	122/122 (100%)	0.42	2 (1%)	70	49	62, 91, 108, 121	0
11	1P	149/149 (100%)	0.18	4 (2%)	56	34	27, 64, 95, 123	0
11	2P	149/149 (100%)	0.56	6 (4%)	42	22	62, 97, 129, 145	0
12	1Q	141/141 (100%)	0.06	0	100	100	35, 53, 72, 101	0
12	2Q	141/141 (100%)	0.81	10 (7%)	22	11	75, 102, 124, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.10	0 100 100	33, 50, 69, 81	0
13	2R	118/118 (100%)	0.43	2 (1%) 69 48	66, 84, 100, 114	0
14	1S	110/110 (100%)	0.24	1 (0%) 81 63	41, 65, 91, 110	0
14	2S	110/110 (100%)	0.89	13 (11%) 9 4	96, 125, 147, 153	0
15	1T	131/131 (100%)	0.26	4 (3%) 51 30	45, 63, 96, 118	0
15	2T	131/131 (100%)	0.38	5 (3%) 44 24	76, 100, 124, 141	0
16	1U	116/116 (100%)	0.13	0 100 100	27, 45, 63, 90	0
16	2U	116/116 (100%)	0.60	6 (5%) 33 17	61, 99, 125, 131	0
17	1V	101/101 (100%)	-0.11	1 (0%) 79 61	32, 51, 76, 97	0
17	2V	101/101 (100%)	0.37	5 (4%) 34 17	61, 104, 130, 153	0
18	1W	112/112 (100%)	0.17	0 100 100	21, 42, 70, 104	0
18	2W	112/112 (100%)	0.26	1 (0%) 81 63	51, 70, 96, 121	0
19	1X	95/95 (100%)	0.05	0 100 100	33, 53, 76, 97	0
19	2X	95/95 (100%)	0.34	2 (2%) 63 42	60, 79, 104, 132	0
20	1Y	107/107 (100%)	0.12	1 (0%) 81 63	47, 65, 95, 117	0
20	2Y	107/107 (100%)	0.62	6 (5%) 30 15	69, 100, 131, 145	0
21	1Z	203/203 (100%)	0.21	1 (0%) 87 73	47, 72, 102, 115	0
21	2Z	201/203 (99%)	0.79	17 (8%) 16 8	92, 124, 151, 174	0
22	10	77/77 (100%)	0.15	1 (1%) 75 55	34, 51, 73, 121	0
22	20	77/77 (100%)	0.58	2 (2%) 57 35	71, 92, 111, 132	0
23	11	97/97 (100%)	0.22	1 (1%) 79 61	39, 60, 88, 98	0
23	21	97/97 (100%)	0.38	4 (4%) 41 22	58, 85, 116, 127	0
24	12	70/70 (100%)	0.27	0 100 100	40, 63, 82, 100	0
24	22	70/70 (100%)	0.42	4 (5%) 29 15	72, 90, 112, 129	0
25	13	59/59 (100%)	-0.05	0 100 100	31, 48, 71, 105	0
25	23	59/59 (100%)	0.39	1 (1%) 69 48	71, 98, 124, 134	0
26	14	69/69 (100%)	0.86	3 (4%) 40 21	110, 160, 235, 240	0
26	24	69/69 (100%)	1.26	9 (13%) 7 4	157, 208, 229, 241	0
27	15	59/59 (100%)	0.07	0 100 100	29, 46, 72, 76	0
27	25	59/59 (100%)	0.38	1 (1%) 69 48	64, 82, 112, 122	0
28	16	53/53 (100%)	0.16	0 100 100	43, 57, 78, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/53 (100%)	0.52	2 (3%) 44 24	74, 87, 104, 113	0
29	17	48/48 (100%)	0.43	2 (4%) 40 21	30, 44, 79, 97	0
29	27	48/48 (100%)	0.57	2 (4%) 40 21	52, 66, 99, 115	0
30	18	64/64 (100%)	0.09	0 100 100	34, 51, 61, 66	0
30	28	64/64 (100%)	0.57	3 (4%) 36 19	63, 81, 97, 112	0
31	19	37/37 (100%)	0.29	1 (2%) 56 34	41, 53, 72, 92	0
31	29	37/37 (100%)	0.95	6 (16%) 4 2	84, 108, 138, 148	0
32	1a	1488/2331 (63%)	0.92	147 (9%) 13 6	55, 122, 256, 317	0
32	2a	1492/2331 (64%)	0.94	126 (8%) 17 8	75, 132, 247, 372	0
33	1b	231/231 (100%)	0.90	22 (9%) 14 7	112, 142, 168, 180	0
33	2b	231/231 (100%)	0.89	17 (7%) 20 10	127, 163, 187, 203	0
34	1c	206/206 (100%)	1.19	31 (15%) 5 2	139, 173, 194, 208	0
34	2c	206/206 (100%)	1.26	42 (20%) 3 1	139, 173, 189, 203	0
35	1d	208/208 (100%)	0.91	21 (10%) 12 6	100, 129, 150, 161	0
35	2d	208/208 (100%)	0.89	17 (8%) 17 9	100, 126, 148, 158	0
36	1e	148/148 (100%)	0.60	7 (4%) 36 19	81, 113, 139, 161	0
36	2e	148/148 (100%)	0.69	10 (6%) 23 12	102, 121, 140, 158	0
37	1f	100/100 (100%)	0.54	4 (4%) 42 22	81, 108, 126, 136	0
37	2f	100/100 (100%)	0.61	6 (6%) 27 14	106, 127, 142, 157	0
38	1g	155/155 (100%)	1.26	28 (18%) 3 1	150, 188, 208, 223	0
38	2g	155/155 (100%)	1.21	31 (20%) 3 1	153, 183, 197, 210	0
39	1h	137/137 (100%)	0.45	4 (2%) 53 32	85, 107, 123, 141	0
39	2h	137/137 (100%)	0.70	8 (5%) 29 15	100, 125, 144, 157	0
40	1i	127/127 (100%)	1.59	41 (32%) 1 1	157, 206, 220, 229	0
40	2i	126/127 (99%)	1.53	35 (27%) 1 1	167, 203, 221, 233	0
41	1j	97/97 (100%)	1.57	23 (23%) 2 1	173, 205, 220, 230	0
41	2j	96/97 (98%)	1.50	26 (27%) 1 1	156, 193, 215, 222	0
42	1k	114/114 (100%)	0.63	3 (2%) 57 35	69, 107, 127, 144	0
42	2k	114/114 (100%)	0.76	11 (9%) 13 7	98, 129, 145, 156	0
43	1l	121/122 (99%)	0.72	9 (7%) 20 10	62, 102, 120, 133	0
43	2l	121/122 (99%)	0.64	8 (6%) 24 12	83, 111, 125, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/116 (100%)	1.43	26 (22%) 2 1	187, 228, 248, 257	0
44	2m	114/116 (98%)	1.35	19 (16%) 4 2	188, 217, 227, 233	0
45	1n	60/60 (100%)	1.29	9 (15%) 5 2	165, 192, 219, 228	0
45	2n	60/60 (100%)	1.54	15 (25%) 2 1	166, 190, 213, 220	0
46	1o	88/88 (100%)	0.65	7 (7%) 18 9	67, 101, 121, 128	0
46	2o	88/88 (100%)	0.57	2 (2%) 61 39	83, 118, 138, 152	0
47	1p	82/82 (100%)	1.05	12 (14%) 6 3	103, 125, 150, 176	0
47	2p	82/82 (100%)	1.05	12 (14%) 6 3	101, 123, 145, 160	0
48	1q	99/99 (100%)	0.68	9 (9%) 15 7	74, 98, 112, 128	0
48	2q	99/99 (100%)	0.54	3 (3%) 52 31	93, 112, 126, 131	0
49	1r	68/68 (100%)	0.66	4 (5%) 28 14	78, 102, 127, 142	0
49	2r	68/68 (100%)	0.57	1 (1%) 72 51	108, 127, 150, 158	0
50	1s	83/83 (100%)	1.64	23 (27%) 1 1	175, 227, 240, 242	0
50	2s	83/83 (100%)	1.46	19 (22%) 2 1	157, 222, 233, 240	0
51	1t	96/98 (97%)	0.68	5 (5%) 33 17	80, 111, 125, 133	0
51	2t	98/98 (100%)	0.83	9 (9%) 14 7	98, 118, 144, 152	0
52	1u	23/23 (100%)	2.25	10 (43%) 0 0	203, 216, 226, 235	0
52	2u	23/23 (100%)	1.74	10 (43%) 0 0	195, 210, 221, 226	0
All	All	20573/22380 (91%)	0.62	1342 (6%) 25 13	21, 100, 220, 372	0

The worst 5 of 1342 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
41	1j	71	LEU	8.8
40	2i	109	VAL	7.9
35	1d	42	GLN	6.9
40	1i	30	GLY	6.7
23	21	2	SER	6.6

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	1a	945	21/22	0.65	0.16	167,190,209,211	0
32	M2G	2a	944	25/26	0.69	0.17	149,173,196,215	0
32	M2G	1a	944	25/26	0.69	0.16	174,190,199,215	0
32	2MG	2a	1189	24/25	0.70	0.16	180,204,208,221	0
32	5MC	2a	945	21/22	0.74	0.12	148,172,188,202	0
32	2MG	1a	1189	24/25	0.74	0.15	211,226,238,245	0
1	5MU	2A	1936	21/22	0.74	0.11	138,161,170,174	0
1	5MU	1A	1936	21/22	0.78	0.12	121,142,154,157	0
32	PSU	1a	500	20/21	0.79	0.14	94,120,144,149	0
1	PSU	2A	1932	20/21	0.80	0.12	119,134,142,160	0
32	PSU	2a	500	20/21	0.84	0.15	120,144,167,167	0
32	5MC	1a	1383	21/22	0.85	0.10	87,107,122,125	0
1	PSU	2A	1938	20/21	0.86	0.10	135,154,172,183	0
1	PSU	1A	1938	20/21	0.86	0.14	110,132,143,150	0
32	5MC	2a	1390	21/22	0.86	0.16	111,129,139,149	0
43	0TD	2l	92	10/11	0.87	0.13	103,114,130,148	0
32	5MC	2a	1383	21/22	0.87	0.13	105,128,143,145	0
32	4OC	1a	1385	22/23	0.87	0.15	72,92,108,122	0
32	G7M	2a	511	24/25	0.87	0.14	94,123,134,141	0
1	OMC	2A	1941	21/22	0.88	0.13	121,133,143,165	0
32	5MC	2a	1387	21/22	0.88	0.11	102,127,139,146	0
1	OMC	1A	1941	21/22	0.88	0.15	95,110,120,128	0
32	4OC	2a	1385	22/23	0.89	0.15	109,124,128,131	0
43	0TD	1l	92	10/11	0.90	0.14	94,117,125,174	0
1	PSU	1A	1932	20/21	0.90	0.14	102,112,120,121	0
32	UR3	1a	1476	21/22	0.90	0.14	80,91,105,107	0
32	UR3	2a	1476	21/22	0.90	0.15	78,115,129,130	0
32	G7M	1a	511	24/25	0.91	0.13	89,108,122,128	0
1	5MC	2A	1983	21/22	0.91	0.10	70,80,88,108	0
1	2MA	2A	2514	23/24	0.92	0.13	49,61,71,80	0
1	5MC	1A	1963	21/22	0.92	0.10	37,53,70,100	0
1	OMG	2A	2262	24/25	0.92	0.16	68,87,96,102	0
32	5MC	1a	1387	21/22	0.92	0.10	60,85,98,106	0
32	MA6	2a	1496	24/25	0.92	0.11	108,121,129,133	0
1	PSU	2A	2616	20/21	0.93	0.10	54,71,80,96	0
1	5MC	1A	1983	21/22	0.93	0.11	26,60,76,94	0
1	5MC	2A	1963	21/22	0.93	0.08	79,95,105,115	0
32	MA6	1a	1496	24/25	0.94	0.10	54,73,87,88	0
1	5MU	1A	1960	21/22	0.94	0.15	40,55,69,75	0
1	2MA	1A	2514	23/24	0.95	0.11	24,40,53,58	0
1	OMG	1A	2262	24/25	0.95	0.11	31,43,50,70	0
32	5MC	1a	1390	21/22	0.95	0.11	77,91,105,108	0
1	OMU	2A	2563	21/22	0.95	0.13	59,75,95,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MA6	1a	1497	24/25	0.95	0.11	63,81,94,96	0
32	MA6	2a	1497	24/25	0.95	0.12	98,115,131,143	0
1	5MU	2A	1960	21/22	0.96	0.11	54,66,78,79	0
1	PSU	1A	2616	20/21	0.96	0.08	30,41,57,57	0
1	OMU	1A	2563	21/22	0.96	0.09	35,43,54,63	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
53	MG	1a	1902	1/1	-0.37	0.23	195,195,195,195	0
53	MG	1a	1858	1/1	-0.23	0.18	152,152,152,152	0
53	MG	1a	1846	1/1	-0.23	0.22	227,227,227,227	0
53	MG	2a	1706	1/1	0.07	0.21	123,123,123,123	0
53	MG	2a	1744	1/1	0.09	0.20	132,132,132,132	0
53	MG	2a	1819	1/1	0.09	0.26	180,180,180,180	0
53	MG	1A	3188	1/1	0.12	0.25	256,256,256,256	0
53	MG	2A	3261	1/1	0.19	0.33	115,115,115,115	0
53	MG	2A	3085	1/1	0.22	0.24	123,123,123,123	0
53	MG	2a	1733	1/1	0.23	0.22	171,171,171,171	0
53	MG	2a	1755	1/1	0.24	0.19	120,120,120,120	0
53	MG	2a	1727	1/1	0.24	0.43	149,149,149,149	0
53	MG	2n	101	1/1	0.26	0.27	169,169,169,169	0
53	MG	2A	3236	1/1	0.27	0.26	110,110,110,110	0
53	MG	2A	3064	1/1	0.27	0.27	91,91,91,91	0
53	MG	1a	1754	1/1	0.27	0.24	95,95,95,95	0
53	MG	1A	3634	1/1	0.28	0.41	52,52,52,52	0
53	MG	1a	1746	1/1	0.32	0.17	167,167,167,167	0
53	MG	2I	3002	1/1	0.33	0.17	129,129,129,129	0
53	MG	20	101	1/1	0.35	0.20	82,82,82,82	0
53	MG	1m	201	1/1	0.35	0.23	192,192,192,192	0
53	MG	2A	3054	1/1	0.35	0.18	142,142,142,142	0
53	MG	2A	3119	1/1	0.35	0.20	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3521	1/1	0.36	0.36	58,58,58,58	0
53	MG	2a	1715	1/1	0.36	0.13	168,168,168,168	0
53	MG	1a	1732	1/1	0.38	0.18	110,110,110,110	0
53	MG	2a	1758	1/1	0.38	0.17	100,100,100,100	0
53	MG	2a	1783	1/1	0.39	0.20	183,183,183,183	0
53	MG	2O	202	1/1	0.41	0.26	115,115,115,115	0
53	MG	1a	1819	1/1	0.41	0.13	124,124,124,124	0
53	MG	2a	1732	1/1	0.42	0.23	188,188,188,188	0
53	MG	2a	1833	1/1	0.42	0.21	85,85,85,85	0
53	MG	2a	1786	1/1	0.42	0.38	91,91,91,91	0
53	MG	2a	1812	1/1	0.44	0.32	86,86,86,86	0
53	MG	2A	3084	1/1	0.44	0.22	109,109,109,109	0
53	MG	2A	3173	1/1	0.45	0.51	78,78,78,78	0
53	MG	1a	1884	1/1	0.45	0.12	104,104,104,104	0
53	MG	2A	3035	1/1	0.46	0.23	90,90,90,90	0
53	MG	2h	201	1/1	0.46	0.15	123,123,123,123	0
53	MG	1A	3144	1/1	0.46	0.15	92,92,92,92	0
53	MG	2A	3290	1/1	0.47	0.48	84,84,84,84	0
53	MG	2a	1762	1/1	0.47	0.21	88,88,88,88	0
53	MG	2A	3367	1/1	0.47	0.29	90,90,90,90	0
53	MG	2A	3024	1/1	0.48	0.21	86,86,86,86	0
53	MG	2a	1806	1/1	0.49	0.37	85,85,85,85	0
53	MG	1a	1703	1/1	0.49	0.23	97,97,97,97	0
53	MG	2a	1757	1/1	0.49	0.20	206,206,206,206	0
53	MG	1A	3087	1/1	0.50	0.19	94,94,94,94	0
53	MG	2a	1738	1/1	0.50	0.18	218,218,218,218	0
53	MG	1a	1867	1/1	0.50	0.16	143,143,143,143	0
53	MG	1A	3093	1/1	0.50	0.25	71,71,71,71	0
53	MG	1A	3086	1/1	0.50	0.18	77,77,77,77	0
53	MG	2A	3010	1/1	0.52	0.26	83,83,83,83	0
53	MG	2A	3138	1/1	0.53	0.16	79,79,79,79	0
53	MG	2A	3446	1/1	0.53	0.46	115,115,115,115	0
53	MG	1a	1735	1/1	0.53	0.27	207,207,207,207	0
53	MG	1a	1851	1/1	0.53	0.49	84,84,84,84	0
53	MG	1a	1854	1/1	0.53	0.20	112,112,112,112	0
53	MG	1A	3153	1/1	0.53	0.18	107,107,107,107	0
53	MG	2A	3474	1/1	0.54	0.33	102,102,102,102	0
53	MG	2A	3061	1/1	0.54	0.35	95,95,95,95	0
53	MG	1a	1745	1/1	0.54	0.36	71,71,71,71	0
53	MG	1a	1868	1/1	0.54	0.25	128,128,128,128	0
53	MG	1A	3600	1/1	0.54	0.32	58,58,58,58	0
53	MG	2a	1713	1/1	0.54	0.33	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1a	1784	1/1	0.55	0.36	96,96,96,96	0
53	MG	1a	1788	1/1	0.56	0.24	83,83,83,83	0
53	MG	2A	3376	1/1	0.56	0.33	108,108,108,108	0
53	MG	2a	1716	1/1	0.56	0.18	112,112,112,112	0
53	MG	2A	3163	1/1	0.56	0.23	75,75,75,75	0
53	MG	1A	3124	1/1	0.56	0.27	82,82,82,82	0
53	MG	2D	307	1/1	0.57	0.17	90,90,90,90	0
53	MG	1A	3486	1/1	0.57	0.25	75,75,75,75	0
53	MG	1a	1770	1/1	0.57	0.16	81,81,81,81	0
53	MG	2A	3450	1/1	0.57	0.26	103,103,103,103	0
53	MG	2a	1823	1/1	0.57	0.21	102,102,102,102	0
53	MG	1a	1718	1/1	0.57	0.22	193,193,193,193	0
53	MG	2a	1769	1/1	0.57	0.19	97,97,97,97	0
53	MG	2A	3485	1/1	0.57	0.18	100,100,100,100	0
53	MG	2a	1729	1/1	0.58	0.19	75,75,75,75	0
53	MG	1A	3525	1/1	0.58	0.24	108,108,108,108	0
53	MG	1a	1726	1/1	0.58	0.18	91,91,91,91	0
53	MG	2a	1764	1/1	0.58	0.18	139,139,139,139	0
53	MG	1a	1881	1/1	0.58	0.18	99,99,99,99	0
53	MG	1A	3019	1/1	0.58	0.27	93,93,93,93	0
53	MG	2a	1728	1/1	0.58	0.14	98,98,98,98	0
53	MG	1B	222	1/1	0.60	0.12	69,69,69,69	0
53	MG	2a	1743	1/1	0.60	0.32	98,98,98,98	0
53	MG	1a	1825	1/1	0.60	0.13	98,98,98,98	0
53	MG	1A	3346	1/1	0.60	0.20	27,27,27,27	0
53	MG	2A	3122	1/1	0.60	0.17	83,83,83,83	0
53	MG	2a	1717	1/1	0.60	0.17	100,100,100,100	0
53	MG	1A	3567	1/1	0.61	0.25	83,83,83,83	0
53	MG	2A	3477	1/1	0.61	0.17	115,115,115,115	0
53	MG	2A	3008	1/1	0.61	0.26	100,100,100,100	0
53	MG	2A	3105	1/1	0.61	0.29	88,88,88,88	0
53	MG	2a	1753	1/1	0.61	0.13	127,127,127,127	0
53	MG	2A	3099	1/1	0.62	0.14	105,105,105,105	0
53	MG	1a	1810	1/1	0.62	0.29	211,211,211,211	0
53	MG	1a	1713	1/1	0.62	0.18	81,81,81,81	0
53	MG	2a	1794	1/1	0.62	0.32	84,84,84,84	0
53	MG	1A	3396	1/1	0.62	0.37	80,80,80,80	0
53	MG	2A	3497	1/1	0.62	0.18	75,75,75,75	0
53	MG	2A	3500	1/1	0.62	0.26	99,99,99,99	0
53	MG	2A	3128	1/1	0.62	0.39	97,97,97,97	0
53	MG	2E	305	1/1	0.62	0.14	83,83,83,83	0
53	MG	1a	1768	1/1	0.62	0.17	172,172,172,172	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1d	503	1/1	0.62	0.15	120,120,120,120	0
53	MG	1A	3130	1/1	0.63	0.45	100,100,100,100	0
53	MG	1a	1817	1/1	0.63	0.15	122,122,122,122	0
53	MG	2A	3070	1/1	0.63	0.34	83,83,83,83	0
53	MG	1B	224	1/1	0.63	0.20	82,82,82,82	0
53	MG	1A	3576	1/1	0.63	0.23	75,75,75,75	0
53	MG	2a	1725	1/1	0.63	0.40	93,93,93,93	0
53	MG	2a	1796	1/1	0.63	0.24	93,93,93,93	0
53	MG	2a	1711	1/1	0.64	0.24	84,84,84,84	0
53	MG	1A	3059	1/1	0.64	0.41	67,67,67,67	0
53	MG	2a	1745	1/1	0.64	0.16	79,79,79,79	0
53	MG	1A	3752	1/1	0.64	0.31	61,61,61,61	0
53	MG	1G	8001	1/1	0.64	0.20	95,95,95,95	0
53	MG	2A	3266	1/1	0.64	0.22	55,55,55,55	0
53	MG	1A	3815	1/1	0.64	0.23	68,68,68,68	0
53	MG	2a	1792	1/1	0.65	0.26	157,157,157,157	0
53	MG	1A	3075	1/1	0.65	0.28	83,83,83,83	0
53	MG	1a	1767	1/1	0.65	0.23	99,99,99,99	0
53	MG	1a	1748	1/1	0.65	0.17	107,107,107,107	0
53	MG	2A	3046	1/1	0.65	0.28	68,68,68,68	0
53	MG	1a	1885	1/1	0.65	0.23	86,86,86,86	0
53	MG	2A	3086	1/1	0.65	0.20	106,106,106,106	0
53	MG	2A	3060	1/1	0.65	0.24	112,112,112,112	0
53	MG	2F	301	1/1	0.65	0.28	72,72,72,72	0
53	MG	2A	3177	1/1	0.65	0.28	70,70,70,70	0
53	MG	2a	1760	1/1	0.66	0.13	81,81,81,81	0
53	MG	2a	1804	1/1	0.66	0.27	151,151,151,151	0
53	MG	1a	1725	1/1	0.66	0.20	55,55,55,55	0
53	MG	2A	3539	1/1	0.66	0.18	78,78,78,78	0
53	MG	2A	3328	1/1	0.66	0.32	89,89,89,89	0
53	MG	2A	3030	1/1	0.66	0.18	104,104,104,104	0
53	MG	1a	1899	1/1	0.66	0.12	102,102,102,102	0
53	MG	2A	3495	1/1	0.66	0.19	69,69,69,69	0
53	MG	1f	8002	1/1	0.66	0.25	110,110,110,110	0
53	MG	1Q	202	1/1	0.67	0.40	80,80,80,80	0
53	MG	1e	3001	1/1	0.67	0.16	89,89,89,89	0
53	MG	1a	1727	1/1	0.67	0.11	92,92,92,92	0
53	MG	2A	3219	1/1	0.67	0.17	100,100,100,100	0
53	MG	2a	1829	1/1	0.67	0.49	99,99,99,99	0
53	MG	1A	3507	1/1	0.67	0.11	118,118,118,118	0
53	MG	1a	1753	1/1	0.67	0.31	184,184,184,184	0
53	MG	1a	1712	1/1	0.67	0.16	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1a	1716	1/1	0.68	0.40	179,179,179,179	0
53	MG	2A	3205	1/1	0.68	0.31	81,81,81,81	0
53	MG	2A	3118	1/1	0.68	0.10	76,76,76,76	0
53	MG	2A	3029	1/1	0.68	0.16	91,91,91,91	0
53	MG	1a	1729	1/1	0.68	0.15	96,96,96,96	0
53	MG	2a	1825	1/1	0.68	0.17	90,90,90,90	0
53	MG	1A	3210	1/1	0.68	0.24	53,53,53,53	0
53	MG	1t	3001	1/1	0.68	0.15	92,92,92,92	0
53	MG	1A	3545	1/1	0.68	0.33	72,72,72,72	0
53	MG	1A	3726	1/1	0.68	0.18	82,82,82,82	0
53	MG	2a	1703	1/1	0.69	0.32	84,84,84,84	0
53	MG	1A	3002	1/1	0.69	0.23	60,60,60,60	0
53	MG	2a	1736	1/1	0.69	0.31	125,125,125,125	0
53	MG	2a	1710	1/1	0.69	0.10	119,119,119,119	0
53	MG	2a	1741	1/1	0.69	0.20	114,114,114,114	0
53	MG	2A	3448	1/1	0.69	0.10	120,120,120,120	0
53	MG	2a	1712	1/1	0.69	0.15	109,109,109,109	0
53	MG	2A	3502	1/1	0.69	0.24	84,84,84,84	0
53	MG	2A	3075	1/1	0.69	0.11	127,127,127,127	0
53	MG	2A	3461	1/1	0.69	0.28	95,95,95,95	0
53	MG	2A	3143	1/1	0.69	0.12	107,107,107,107	0
53	MG	2A	3098	1/1	0.69	0.24	90,90,90,90	0
53	MG	2A	3484	1/1	0.69	0.16	81,81,81,81	0
53	MG	1d	502	1/1	0.69	0.15	66,66,66,66	0
53	MG	2A	3415	1/1	0.69	0.16	81,81,81,81	0
53	MG	2a	1766	1/1	0.69	0.20	119,119,119,119	0
55	MPD	2B	210	8/8	0.69	0.37	114,144,150,162	0
53	MG	1a	1741	1/1	0.70	0.28	79,79,79,79	0
53	MG	1B	211	1/1	0.70	0.18	68,68,68,68	0
53	MG	2A	3188	1/1	0.70	0.14	79,79,79,79	0
53	MG	2A	3194	1/1	0.70	0.42	75,75,75,75	0
53	MG	2A	3463	1/1	0.70	0.27	68,68,68,68	0
53	MG	2A	3518	1/1	0.70	0.22	91,91,91,91	0
53	MG	2A	3535	1/1	0.70	0.15	84,84,84,84	0
53	MG	1s	101	1/1	0.70	0.16	158,158,158,158	0
53	MG	1A	3548	1/1	0.70	0.25	118,118,118,118	0
53	MG	1a	1776	1/1	0.70	0.47	88,88,88,88	0
53	MG	1a	1837	1/1	0.71	0.18	97,97,97,97	0
53	MG	2a	1767	1/1	0.71	0.26	59,59,59,59	0
53	MG	2a	1768	1/1	0.71	0.22	89,89,89,89	0
53	MG	2A	3091	1/1	0.71	0.29	73,73,73,73	0
53	MG	1A	3524	1/1	0.71	0.38	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	2A	3459	1/1	0.71	0.51	92,92,92,92	0
53	MG	1a	1847	1/1	0.71	0.23	90,90,90,90	0
53	MG	1A	3772	1/1	0.71	0.36	98,98,98,98	0
53	MG	2a	1739	1/1	0.71	0.21	164,164,164,164	0
53	MG	1A	3511	1/1	0.71	0.18	77,77,77,77	0
53	MG	1T	8002	1/1	0.71	0.13	94,94,94,94	0
53	MG	1A	3639	1/1	0.71	0.24	85,85,85,85	0
53	MG	2A	3286	1/1	0.71	0.18	79,79,79,79	0
53	MG	1a	1706	1/1	0.71	0.12	105,105,105,105	0
53	MG	1B	220	1/1	0.71	0.12	53,53,53,53	0
53	MG	2A	3358	1/1	0.71	0.27	78,78,78,78	0
53	MG	1a	1820	1/1	0.71	0.19	107,107,107,107	0
53	MG	2a	1840	1/1	0.71	0.17	86,86,86,86	0
53	MG	2a	1843	1/1	0.71	0.15	99,99,99,99	0
53	MG	1A	3024	1/1	0.71	0.24	91,91,91,91	0
53	MG	1a	1896	1/1	0.71	0.27	100,100,100,100	0
53	MG	2A	3424	1/1	0.71	0.45	77,77,77,77	0
53	MG	2A	3207	1/1	0.72	0.30	75,75,75,75	0
53	MG	1A	3385	1/1	0.72	0.28	70,70,70,70	0
53	MG	2A	3066	1/1	0.72	0.14	92,92,92,92	0
53	MG	1a	1848	1/1	0.72	0.11	107,107,107,107	0
53	MG	1A	3510	1/1	0.72	0.17	74,74,74,74	0
53	MG	2A	3276	1/1	0.72	0.22	73,73,73,73	0
53	MG	1A	3300	1/1	0.72	0.14	69,69,69,69	0
53	MG	1A	3425	1/1	0.72	0.20	79,79,79,79	0
53	MG	2a	1708	1/1	0.72	0.19	129,129,129,129	0
53	MG	1a	1834	1/1	0.72	0.21	102,102,102,102	0
53	MG	2A	3338	1/1	0.72	0.12	86,86,86,86	0
53	MG	2a	1754	1/1	0.72	0.36	83,83,83,83	0
53	MG	18	102	1/1	0.72	0.69	75,75,75,75	0
53	MG	1a	1843	1/1	0.72	0.62	208,208,208,208	0
53	MG	1a	1845	1/1	0.72	0.20	106,106,106,106	0
53	MG	2a	1837	1/1	0.72	0.13	78,78,78,78	0
53	MG	2A	3407	1/1	0.72	0.22	76,76,76,76	0
53	MG	2A	3507	1/1	0.72	0.29	92,92,92,92	0
53	MG	1A	3044	1/1	0.72	0.68	88,88,88,88	0
53	MG	2A	3113	1/1	0.72	0.20	96,96,96,96	0
53	MG	2A	3443	1/1	0.72	0.18	91,91,91,91	0
53	MG	1A	3110	1/1	0.73	0.14	109,109,109,109	0
53	MG	2A	3543	1/1	0.73	0.23	91,91,91,91	0
53	MG	1a	1812	1/1	0.73	0.13	93,93,93,93	0
53	MG	2a	1771	1/1	0.73	0.15	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	2a	1773	1/1	0.73	0.14	141,141,141,141	0
53	MG	2A	3291	1/1	0.73	0.18	94,94,94,94	0
53	MG	2A	3309	1/1	0.73	0.25	82,82,82,82	0
53	MG	1A	3402	1/1	0.73	0.14	70,70,70,70	0
53	MG	1a	1744	1/1	0.73	0.25	69,69,69,69	0
53	MG	2U	202	1/1	0.73	0.21	81,81,81,81	0
53	MG	2A	3106	1/1	0.73	0.28	74,74,74,74	0
53	MG	1A	3412	1/1	0.73	0.20	91,91,91,91	0
53	MG	2a	1704	1/1	0.73	0.27	105,105,105,105	0
53	MG	1A	3049	1/1	0.73	0.23	84,84,84,84	0
53	MG	2a	1707	1/1	0.73	0.13	76,76,76,76	0
53	MG	1a	1857	1/1	0.73	0.17	122,122,122,122	0
53	MG	2A	3080	1/1	0.73	0.14	144,144,144,144	0
53	MG	1A	3394	1/1	0.73	0.25	92,92,92,92	0
53	MG	2A	3505	1/1	0.73	0.15	99,99,99,99	0
53	MG	1a	1717	1/1	0.73	0.17	196,196,196,196	0
53	MG	2a	1842	1/1	0.73	0.19	98,98,98,98	0
53	MG	2A	3270	1/1	0.73	0.19	89,89,89,89	0
53	MG	2A	3523	1/1	0.73	0.16	69,69,69,69	0
53	MG	1a	1801	1/1	0.73	0.22	164,164,164,164	0
53	MG	2a	1721	1/1	0.73	0.15	72,72,72,72	0
53	MG	1A	3669	1/1	0.74	0.28	69,69,69,69	0
53	MG	2A	3103	1/1	0.74	0.14	96,96,96,96	0
53	MG	2A	3198	1/1	0.74	0.25	66,66,66,66	0
53	MG	2A	3005	1/1	0.74	0.23	87,87,87,87	0
53	MG	1A	3276	1/1	0.74	0.27	68,68,68,68	0
53	MG	1A	3399	1/1	0.74	0.20	50,50,50,50	0
53	MG	2A	3433	1/1	0.74	0.12	94,94,94,94	0
53	MG	2A	3115	1/1	0.74	0.35	105,105,105,105	0
53	MG	1A	3769	1/1	0.74	0.26	71,71,71,71	0
53	MG	2A	3077	1/1	0.74	0.14	86,86,86,86	0
53	MG	2a	1822	1/1	0.74	0.18	101,101,101,101	0
53	MG	1A	3562	1/1	0.74	0.24	65,65,65,65	0
53	MG	2A	3550	1/1	0.74	0.15	61,61,61,61	0
53	MG	1A	3811	1/1	0.74	0.29	72,72,72,72	0
53	MG	2a	1761	1/1	0.74	0.10	90,90,90,90	0
53	MG	2a	1722	1/1	0.74	0.21	161,161,161,161	0
53	MG	1A	3526	1/1	0.74	0.24	113,113,113,113	0
53	MG	1a	1880	1/1	0.74	0.20	67,67,67,67	0
53	MG	2A	3150	1/1	0.74	0.24	79,79,79,79	0
53	MG	2A	3088	1/1	0.74	0.27	58,58,58,58	0
53	MG	1A	3653	1/1	0.74	0.31	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MPD	1T	8004	8/8	0.74	0.19	85,109,114,114	0
53	MG	1A	3667	1/1	0.74	0.19	40,40,40,40	0
53	MG	1a	1734	1/1	0.75	0.17	86,86,86,86	0
53	MG	1N	201	1/1	0.75	0.22	86,86,86,86	0
53	MG	1A	3679	1/1	0.75	0.39	68,68,68,68	0
53	MG	2A	3342	1/1	0.75	0.12	86,86,86,86	0
53	MG	1a	1839	1/1	0.75	0.26	121,121,121,121	0
53	MG	1A	3029	1/1	0.75	0.18	72,72,72,72	0
53	MG	1a	1720	1/1	0.75	0.15	127,127,127,127	0
53	MG	1A	3731	1/1	0.75	0.10	86,86,86,86	0
53	MG	1A	3577	1/1	0.75	0.19	64,64,64,64	0
53	MG	2A	3026	1/1	0.75	0.21	119,119,119,119	0
53	MG	1A	3755	1/1	0.75	0.16	79,79,79,79	0
53	MG	1A	3541	1/1	0.75	0.54	78,78,78,78	0
53	MG	1a	1852	1/1	0.75	0.16	70,70,70,70	0
53	MG	2A	3148	1/1	0.75	0.16	76,76,76,76	0
53	MG	2A	3284	1/1	0.75	0.28	150,150,150,150	0
53	MG	2A	3546	1/1	0.75	0.39	77,77,77,77	0
53	MG	1a	1756	1/1	0.75	0.36	72,72,72,72	0
53	MG	2A	3160	1/1	0.75	0.17	93,93,93,93	0
53	MG	2E	302	1/1	0.75	0.14	106,106,106,106	0
53	MG	2E	303	1/1	0.75	0.26	79,79,79,79	0
53	MG	2A	3462	1/1	0.75	0.15	88,88,88,88	0
53	MG	2r	102	1/1	0.75	0.10	104,104,104,104	0
53	MG	1A	3421	1/1	0.75	0.18	74,74,74,74	0
53	MG	2a	1731	1/1	0.75	0.17	92,92,92,92	0
53	MG	2A	3456	1/1	0.76	0.36	89,89,89,89	0
53	MG	1a	1814	1/1	0.76	0.14	84,84,84,84	0
53	MG	1A	3095	1/1	0.76	0.27	53,53,53,53	0
53	MG	2A	3315	1/1	0.76	0.33	64,64,64,64	0
53	MG	2A	3114	1/1	0.76	0.22	110,110,110,110	0
53	MG	2A	3467	1/1	0.76	0.27	79,79,79,79	0
53	MG	1A	3630	1/1	0.76	0.39	57,57,57,57	0
53	MG	1A	3203	1/1	0.76	0.28	55,55,55,55	0
53	MG	1A	3114	1/1	0.76	0.13	76,76,76,76	0
53	MG	1A	3233	1/1	0.76	0.12	35,35,35,35	0
53	MG	2A	3125	1/1	0.76	0.15	114,114,114,114	0
53	MG	2A	3401	1/1	0.76	0.24	61,61,61,61	0
53	MG	1A	3238	1/1	0.76	0.12	89,89,89,89	0
53	MG	1A	3166	1/1	0.76	0.10	154,154,154,154	0
53	MG	2A	3417	1/1	0.76	0.40	81,81,81,81	0
53	MG	2A	3139	1/1	0.76	0.10	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	2a	1836	1/1	0.76	0.38	83,83,83,83	0
53	MG	2A	3425	1/1	0.76	0.24	77,77,77,77	0
53	MG	2A	3431	1/1	0.76	0.20	101,101,101,101	0
53	MG	2A	3528	1/1	0.76	0.37	85,85,85,85	0
53	MG	1A	3535	1/1	0.76	0.26	74,74,74,74	0
53	MG	1a	1872	1/1	0.76	0.14	78,78,78,78	0
53	MG	1a	1879	1/1	0.76	0.16	72,72,72,72	0
53	MG	1A	3826	1/1	0.76	0.14	52,52,52,52	0
53	MG	1A	3712	1/1	0.76	0.34	79,79,79,79	0
53	MG	2A	3555	1/1	0.76	0.10	225,225,225,225	0
53	MG	2A	3063	1/1	0.77	0.11	86,86,86,86	0
53	MG	2A	3120	1/1	0.77	0.12	66,66,66,66	0
53	MG	1D	306	1/1	0.77	0.18	49,49,49,49	0
53	MG	1A	3282	1/1	0.77	0.11	52,52,52,52	0
53	MG	1A	3392	1/1	0.77	0.17	56,56,56,56	0
53	MG	2A	3476	1/1	0.77	0.18	132,132,132,132	0
53	MG	2A	3133	1/1	0.77	0.27	84,84,84,84	0
53	MG	2A	3136	1/1	0.77	0.11	75,75,75,75	0
53	MG	2A	3319	1/1	0.77	0.21	99,99,99,99	0
53	MG	1A	3759	1/1	0.77	0.13	79,79,79,79	0
53	MG	1A	3222	1/1	0.77	0.15	46,46,46,46	0
53	MG	13	101	1/1	0.77	0.16	84,84,84,84	0
53	MG	2a	1785	1/1	0.77	0.29	89,89,89,89	0
53	MG	1A	3564	1/1	0.77	0.33	52,52,52,52	0
53	MG	2A	3366	1/1	0.77	0.22	86,86,86,86	0
53	MG	2A	3007	1/1	0.77	0.25	61,61,61,61	0
53	MG	1A	3810	1/1	0.77	0.11	55,55,55,55	0
53	MG	2A	3382	1/1	0.77	0.31	85,85,85,85	0
53	MG	2A	3387	1/1	0.77	0.29	82,82,82,82	0
53	MG	1A	3466	1/1	0.77	0.32	45,45,45,45	0
53	MG	2a	1730	1/1	0.77	0.16	87,87,87,87	0
53	MG	1a	1710	1/1	0.77	0.19	86,86,86,86	0
53	MG	2A	3093	1/1	0.77	0.13	93,93,93,93	0
53	MG	2A	3025	1/1	0.77	0.28	85,85,85,85	0
53	MG	2a	1735	1/1	0.77	0.12	122,122,122,122	0
53	MG	1A	3303	1/1	0.77	0.22	95,95,95,95	0
53	MG	1a	1751	1/1	0.77	0.13	105,105,105,105	0
53	MG	2A	3559	1/1	0.77	0.17	78,78,78,78	0
53	MG	1A	3821	1/1	0.77	0.27	86,86,86,86	0
53	MG	1A	3325	1/1	0.77	0.17	92,92,92,92	0
53	MG	1A	3540	1/1	0.77	0.31	67,67,67,67	0
53	MG	1A	3728	1/1	0.77	0.34	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3066	1/1	0.77	0.14	93,93,93,93	0
53	MG	2A	3262	1/1	0.77	0.23	89,89,89,89	0
53	MG	2A	3117	1/1	0.77	0.16	69,69,69,69	0
53	MG	1A	3736	1/1	0.77	0.11	53,53,53,53	0
53	MG	2A	3181	1/1	0.78	0.20	61,61,61,61	0
53	MG	2A	3184	1/1	0.78	0.18	67,67,67,67	0
53	MG	1A	3476	1/1	0.78	0.28	62,62,62,62	0
53	MG	1A	3047	1/1	0.78	0.23	52,52,52,52	0
53	MG	1A	3223	1/1	0.78	0.22	44,44,44,44	0
53	MG	2a	1776	1/1	0.78	0.18	157,157,157,157	0
53	MG	2B	204	1/1	0.78	0.19	100,100,100,100	0
53	MG	1a	1758	1/1	0.78	0.12	152,152,152,152	0
53	MG	2A	3364	1/1	0.78	0.22	69,69,69,69	0
53	MG	1A	3018	1/1	0.78	0.42	70,70,70,70	0
53	MG	2A	3132	1/1	0.78	0.20	78,78,78,78	0
53	MG	2A	3234	1/1	0.78	0.18	79,79,79,79	0
53	MG	2a	1801	1/1	0.78	0.28	72,72,72,72	0
53	MG	1a	1856	1/1	0.78	0.15	109,109,109,109	0
53	MG	1a	1821	1/1	0.78	0.21	130,130,130,130	0
53	MG	1A	3608	1/1	0.78	0.23	70,70,70,70	0
53	MG	2W	202	1/1	0.78	0.14	80,80,80,80	0
53	MG	2a	1740	1/1	0.78	0.16	85,85,85,85	0
53	MG	2Y	502	1/1	0.78	0.18	90,90,90,90	0
53	MG	2A	3265	1/1	0.78	0.44	72,72,72,72	0
53	MG	2a	1702	1/1	0.78	0.10	104,104,104,104	0
53	MG	1a	1865	1/1	0.78	0.21	78,78,78,78	0
53	MG	1A	3070	1/1	0.78	0.28	45,45,45,45	0
53	MG	1a	1835	1/1	0.78	0.17	131,131,131,131	0
53	MG	1A	3461	1/1	0.78	0.37	87,87,87,87	0
53	MG	1a	1719	1/1	0.78	0.12	224,224,224,224	0
53	MG	2A	3519	1/1	0.78	0.15	87,87,87,87	0
53	MG	2f	3001	1/1	0.78	0.16	87,87,87,87	0
53	MG	1A	3638	1/1	0.78	0.21	65,65,65,65	0
53	MG	1A	3464	1/1	0.78	0.17	90,90,90,90	0
53	MG	2A	3293	1/1	0.78	0.43	68,68,68,68	0
53	MG	1A	3090	1/1	0.78	0.13	66,66,66,66	0
53	MG	2A	3541	1/1	0.78	0.13	57,57,57,57	0
53	MG	1a	1855	1/1	0.79	0.17	71,71,71,71	0
53	MG	2A	3161	1/1	0.79	0.22	97,97,97,97	0
53	MG	2A	3111	1/1	0.79	0.09	138,138,138,138	0
53	MG	1a	1887	1/1	0.79	0.30	60,60,60,60	0
53	MG	1a	1892	1/1	0.79	0.12	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3040	1/1	0.79	0.47	61,61,61,61	0
53	MG	2A	3533	1/1	0.79	0.18	55,55,55,55	0
53	MG	1A	3118	1/1	0.79	0.17	91,91,91,91	0
53	MG	1a	1840	1/1	0.79	0.26	99,99,99,99	0
53	MG	1A	3201	1/1	0.79	0.18	41,41,41,41	0
53	MG	1A	3606	1/1	0.79	0.25	60,60,60,60	0
53	MG	1a	1777	1/1	0.79	0.15	164,164,164,164	0
53	MG	2a	1824	1/1	0.79	0.22	108,108,108,108	0
53	MG	2a	1714	1/1	0.79	0.17	106,106,106,106	0
53	MG	2a	1828	1/1	0.79	0.15	103,103,103,103	0
53	MG	2A	3087	1/1	0.79	0.24	90,90,90,90	0
53	MG	2A	3465	1/1	0.79	0.15	74,74,74,74	0
53	MG	2A	3037	1/1	0.79	0.17	64,64,64,64	0
53	MG	1A	3607	1/1	0.79	0.30	71,71,71,71	0
53	MG	2A	3047	1/1	0.79	0.17	75,75,75,75	0
53	MG	2A	3094	1/1	0.79	0.12	117,117,117,117	0
53	MG	2A	3097	1/1	0.79	0.20	53,53,53,53	0
53	MG	1A	3358	1/1	0.79	0.18	75,75,75,75	0
53	MG	1a	1826	1/1	0.79	0.32	99,99,99,99	0
53	MG	1A	3398	1/1	0.79	0.18	71,71,71,71	0
53	MG	2A	3499	1/1	0.79	0.18	70,70,70,70	0
53	MG	1G	8003	1/1	0.79	0.12	92,92,92,92	0
53	MG	2A	3157	1/1	0.79	0.21	102,102,102,102	0
53	MG	1A	3021	1/1	0.80	0.30	75,75,75,75	0
53	MG	1A	3003	1/1	0.80	0.22	50,50,50,50	0
53	MG	2X	101	1/1	0.80	0.14	70,70,70,70	0
53	MG	1A	3230	1/1	0.80	0.20	28,28,28,28	0
53	MG	1a	1859	1/1	0.80	0.15	105,105,105,105	0
53	MG	28	8002	1/1	0.80	0.20	74,74,74,74	0
53	MG	2A	3306	1/1	0.80	0.34	77,77,77,77	0
53	MG	1a	1714	1/1	0.80	0.28	211,211,211,211	0
53	MG	2A	3310	1/1	0.80	0.14	70,70,70,70	0
53	MG	1a	1866	1/1	0.80	0.34	68,68,68,68	0
53	MG	1A	3072	1/1	0.80	0.35	69,69,69,69	0
53	MG	2A	3323	1/1	0.80	0.25	101,101,101,101	0
53	MG	1A	3401	1/1	0.80	0.25	54,54,54,54	0
53	MG	1A	3336	1/1	0.80	0.18	44,44,44,44	0
53	MG	2a	1781	1/1	0.80	0.14	85,85,85,85	0
53	MG	1a	1874	1/1	0.80	0.13	51,51,51,51	0
53	MG	1F	303	1/1	0.80	0.18	56,56,56,56	0
53	MG	1A	3235	1/1	0.80	0.16	51,51,51,51	0
53	MG	2A	3034	1/1	0.80	0.16	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3419	1/1	0.80	0.19	38,38,38,38	0
53	MG	2A	3375	1/1	0.80	0.46	100,100,100,100	0
53	MG	2a	1799	1/1	0.80	0.34	69,69,69,69	0
53	MG	2A	3036	1/1	0.80	0.11	76,76,76,76	0
53	MG	2A	3109	1/1	0.80	0.17	89,89,89,89	0
53	MG	2A	3197	1/1	0.80	0.16	73,73,73,73	0
53	MG	1A	3660	1/1	0.80	0.23	54,54,54,54	0
53	MG	1A	3207	1/1	0.80	0.17	52,52,52,52	0
53	MG	1A	3781	1/1	0.80	0.19	33,33,33,33	0
53	MG	1A	3253	1/1	0.80	0.23	67,67,67,67	0
53	MG	1A	3670	1/1	0.80	0.22	85,85,85,85	0
53	MG	1A	3102	1/1	0.80	0.15	72,72,72,72	0
53	MG	2A	3248	1/1	0.80	0.11	103,103,103,103	0
53	MG	1a	1738	1/1	0.80	0.21	177,177,177,177	0
53	MG	2A	3560	1/1	0.80	0.29	96,96,96,96	0
53	MG	1a	1904	1/1	0.80	0.13	240,240,240,240	0
53	MG	2D	305	1/1	0.80	0.25	115,115,115,115	0
53	MG	2A	3444	1/1	0.80	0.22	54,54,54,54	0
53	MG	2A	3264	1/1	0.80	0.35	72,72,72,72	0
53	MG	1a	1805	1/1	0.80	0.12	86,86,86,86	0
53	MG	2A	3069	1/1	0.80	0.20	75,75,75,75	0
53	MG	1a	1740	1/1	0.80	0.19	91,91,91,91	0
53	MG	2a	1748	1/1	0.80	0.40	81,81,81,81	0
53	MG	2r	101	1/1	0.80	0.49	95,95,95,95	0
53	MG	2a	1749	1/1	0.80	0.18	75,75,75,75	0
53	MG	1a	1811	1/1	0.80	0.18	61,61,61,61	0
53	MG	1A	3686	1/1	0.80	0.41	96,96,96,96	0
56	FSD	2A	3553	44/44	0.80	0.13	61,91,113,126	0
53	MG	1A	3734	1/1	0.81	0.25	83,83,83,83	0
53	MG	1A	3015	1/1	0.81	0.18	39,39,39,39	0
53	MG	2A	3314	1/1	0.81	0.11	80,80,80,80	0
53	MG	2A	3065	1/1	0.81	0.33	76,76,76,76	0
53	MG	1A	3741	1/1	0.81	0.43	84,84,84,84	0
53	MG	2A	3320	1/1	0.81	0.21	80,80,80,80	0
53	MG	2A	3481	1/1	0.81	0.15	99,99,99,99	0
53	MG	2A	3322	1/1	0.81	0.10	114,114,114,114	0
53	MG	1a	1796	1/1	0.81	0.14	119,119,119,119	0
53	MG	2A	3490	1/1	0.81	0.26	62,62,62,62	0
53	MG	2A	3325	1/1	0.81	0.24	69,69,69,69	0
53	MG	1A	3429	1/1	0.81	0.17	50,50,50,50	0
53	MG	2A	3498	1/1	0.81	0.13	59,59,59,59	0
53	MG	2a	1777	1/1	0.81	0.21	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3542	1/1	0.81	0.27	98,98,98,98	0
53	MG	2A	3200	1/1	0.81	0.28	59,59,59,59	0
53	MG	2A	3203	1/1	0.81	0.15	74,74,74,74	0
53	MG	1A	3387	1/1	0.81	0.21	64,64,64,64	0
53	MG	1A	3463	1/1	0.81	0.20	58,58,58,58	0
53	MG	1A	3629	1/1	0.81	0.24	44,44,44,44	0
53	MG	2a	1718	1/1	0.81	0.13	89,89,89,89	0
53	MG	2A	3227	1/1	0.81	0.22	61,61,61,61	0
53	MG	2A	3228	1/1	0.81	0.13	59,59,59,59	0
53	MG	2A	3027	1/1	0.81	0.13	95,95,95,95	0
53	MG	1A	3069	1/1	0.81	0.19	63,63,63,63	0
53	MG	2A	3400	1/1	0.81	0.22	81,81,81,81	0
53	MG	2a	1815	1/1	0.81	0.12	158,158,158,158	0
53	MG	2a	1818	1/1	0.81	0.37	106,106,106,106	0
53	MG	2A	3243	1/1	0.81	0.18	95,95,95,95	0
53	MG	1A	3805	1/1	0.81	0.10	80,80,80,80	0
53	MG	2A	3249	1/1	0.81	0.20	79,79,79,79	0
53	MG	2A	3031	1/1	0.81	0.17	82,82,82,82	0
53	MG	2A	3090	1/1	0.81	0.16	106,106,106,106	0
53	MG	1a	1898	1/1	0.81	0.27	64,64,64,64	0
53	MG	1T	8001	1/1	0.81	0.13	95,95,95,95	0
53	MG	1A	3696	1/1	0.81	0.22	45,45,45,45	0
53	MG	2A	3439	1/1	0.81	0.16	54,54,54,54	0
53	MG	2A	3095	1/1	0.81	0.19	91,91,91,91	0
53	MG	1A	3155	1/1	0.81	0.19	67,67,67,67	0
53	MG	1A	3635	1/1	0.81	0.30	45,45,45,45	0
53	MG	1A	3295	1/1	0.81	0.15	64,64,64,64	0
53	MG	1a	1831	1/1	0.81	0.17	110,110,110,110	0
53	MG	2a	1746	1/1	0.81	0.16	67,67,67,67	0
53	MG	1a	1771	1/1	0.81	0.10	62,62,62,62	0
53	MG	2A	3165	1/1	0.81	0.16	73,73,73,73	0
53	MG	2a	1751	1/1	0.81	0.15	109,109,109,109	0
53	MG	2A	3304	1/1	0.81	0.25	78,78,78,78	0
53	MG	2Q	8001	1/1	0.81	0.12	72,72,72,72	0
53	MG	1A	3164	1/1	0.81	0.17	77,77,77,77	0
53	MG	2A	3464	1/1	0.82	0.34	90,90,90,90	0
53	MG	2Z	301	1/1	0.82	0.13	99,99,99,99	0
53	MG	1A	3485	1/1	0.82	0.20	80,80,80,80	0
53	MG	1A	3023	1/1	0.82	0.12	72,72,72,72	0
53	MG	1A	3698	1/1	0.82	0.12	78,78,78,78	0
53	MG	1a	1775	1/1	0.82	0.25	74,74,74,74	0
53	MG	2A	3174	1/1	0.82	0.18	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3503	1/1	0.82	0.14	45,45,45,45	0
53	MG	2A	3013	1/1	0.82	0.21	79,79,79,79	0
53	MG	1A	3175	1/1	0.82	0.19	86,86,86,86	0
53	MG	2a	1774	1/1	0.82	0.15	152,152,152,152	0
53	MG	1A	3840	1/1	0.82	0.44	41,41,41,41	0
53	MG	1A	3632	1/1	0.82	0.33	44,44,44,44	0
53	MG	1A	3428	1/1	0.82	0.34	85,85,85,85	0
53	MG	2A	3101	1/1	0.82	0.19	93,93,93,93	0
53	MG	1A	3732	1/1	0.82	0.22	62,62,62,62	0
53	MG	2A	3361	1/1	0.82	0.23	95,95,95,95	0
53	MG	1A	3733	1/1	0.82	0.18	48,48,48,48	0
53	MG	1A	3232	1/1	0.82	0.18	63,63,63,63	0
53	MG	1D	312	1/1	0.82	0.21	57,57,57,57	0
53	MG	2A	3213	1/1	0.82	0.23	71,71,71,71	0
53	MG	1a	1730	1/1	0.82	0.08	81,81,81,81	0
53	MG	2A	3380	1/1	0.82	0.22	65,65,65,65	0
53	MG	2A	3525	1/1	0.82	0.23	106,106,106,106	0
53	MG	1A	3159	1/1	0.82	0.16	88,88,88,88	0
53	MG	1F	306	1/1	0.82	0.40	75,75,75,75	0
53	MG	2a	1816	1/1	0.82	0.23	100,100,100,100	0
53	MG	1A	3293	1/1	0.82	0.20	83,83,83,83	0
53	MG	1A	3749	1/1	0.82	0.19	57,57,57,57	0
53	MG	2A	3403	1/1	0.82	0.14	102,102,102,102	0
53	MG	1A	3571	1/1	0.82	0.18	63,63,63,63	0
53	MG	1A	3013	1/1	0.82	0.12	43,43,43,43	0
53	MG	1a	1742	1/1	0.82	0.12	117,117,117,117	0
53	MG	2A	3062	1/1	0.82	0.11	118,118,118,118	0
53	MG	1a	1895	1/1	0.82	0.19	66,66,66,66	0
53	MG	2a	1832	1/1	0.82	0.10	76,76,76,76	0
53	MG	1A	3237	1/1	0.82	0.32	65,65,65,65	0
53	MG	1A	3764	1/1	0.82	0.18	71,71,71,71	0
53	MG	1A	3594	1/1	0.82	0.30	80,80,80,80	0
53	MG	17	102	1/1	0.82	0.27	56,56,56,56	0
53	MG	2A	3275	1/1	0.82	0.20	81,81,81,81	0
53	MG	1A	3531	1/1	0.82	0.16	61,61,61,61	0
53	MG	19	103	1/1	0.82	0.12	86,86,86,86	0
53	MG	2A	3141	1/1	0.82	0.11	72,72,72,72	0
53	MG	2A	3453	1/1	0.82	0.15	96,96,96,96	0
53	MG	1A	3776	1/1	0.82	0.25	48,48,48,48	0
53	MG	1a	1755	1/1	0.82	0.07	87,87,87,87	0
54	ARG	1A	3799	12/12	0.82	0.21	85,101,112,114	0
53	MG	1A	3302	1/1	0.82	0.21	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1a	1709	1/1	0.82	0.12	209,209,209,209	0
53	MG	1A	3683	1/1	0.82	0.30	62,62,62,62	0
53	MG	1A	3432	1/1	0.83	0.29	79,79,79,79	0
53	MG	2A	3458	1/1	0.83	0.16	73,73,73,73	0
53	MG	1A	3604	1/1	0.83	0.23	81,81,81,81	0
53	MG	1A	3433	1/1	0.83	0.28	94,94,94,94	0
53	MG	1A	3812	1/1	0.83	0.13	61,61,61,61	0
53	MG	2A	3176	1/1	0.83	0.26	70,70,70,70	0
53	MG	2A	3023	1/1	0.83	0.15	73,73,73,73	0
53	MG	1a	1772	1/1	0.83	0.12	88,88,88,88	0
53	MG	2l	101	1/1	0.83	0.17	70,70,70,70	0
53	MG	1A	3437	1/1	0.83	0.17	58,58,58,58	0
53	MG	28	8004	1/1	0.83	0.12	63,63,63,63	0
53	MG	2A	3471	1/1	0.83	0.14	51,51,51,51	0
53	MG	1A	3713	1/1	0.83	0.20	68,68,68,68	0
53	MG	2a	1775	1/1	0.83	0.28	90,90,90,90	0
53	MG	2A	3475	1/1	0.83	0.10	83,83,83,83	0
53	MG	1A	3825	1/1	0.83	0.12	55,55,55,55	0
53	MG	1a	1781	1/1	0.83	0.24	123,123,123,123	0
53	MG	1A	3448	1/1	0.83	0.18	61,61,61,61	0
53	MG	2A	3332	1/1	0.83	0.13	108,108,108,108	0
53	MG	2A	3334	1/1	0.83	0.17	64,64,64,64	0
53	MG	2a	1789	1/1	0.83	0.26	79,79,79,79	0
53	MG	1A	3614	1/1	0.83	0.30	68,68,68,68	0
53	MG	2a	1793	1/1	0.83	0.31	87,87,87,87	0
53	MG	1B	202	1/1	0.83	0.32	63,63,63,63	0
53	MG	2A	3344	1/1	0.83	0.14	93,93,93,93	0
53	MG	2a	1798	1/1	0.83	0.18	98,98,98,98	0
53	MG	1A	3032	1/1	0.83	0.17	65,65,65,65	0
53	MG	1B	213	1/1	0.83	0.18	97,97,97,97	0
53	MG	1A	3177	1/1	0.83	0.22	96,96,96,96	0
53	MG	2A	3215	1/1	0.83	0.19	59,59,59,59	0
53	MG	1A	3182	1/1	0.83	0.13	74,74,74,74	0
53	MG	1A	3315	1/1	0.83	0.17	64,64,64,64	0
53	MG	2a	1724	1/1	0.83	0.20	103,103,103,103	0
53	MG	1A	3270	1/1	0.83	0.16	50,50,50,50	0
53	MG	2A	3230	1/1	0.83	0.13	87,87,87,87	0
53	MG	1A	3737	1/1	0.83	0.12	73,73,73,73	0
53	MG	1A	3330	1/1	0.83	0.15	105,105,105,105	0
53	MG	1A	3747	1/1	0.83	0.10	96,96,96,96	0
53	MG	1F	307	1/1	0.83	0.18	87,87,87,87	0
53	MG	1A	3271	1/1	0.83	0.11	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3648	1/1	0.83	0.10	63,63,63,63	0
53	MG	2a	1830	1/1	0.83	0.13	98,98,98,98	0
53	MG	2a	1831	1/1	0.83	0.31	55,55,55,55	0
53	MG	2A	3412	1/1	0.83	0.16	72,72,72,72	0
53	MG	1A	3753	1/1	0.83	0.29	63,63,63,63	0
53	MG	2A	3134	1/1	0.83	0.17	69,69,69,69	0
53	MG	1A	3273	1/1	0.83	0.18	62,62,62,62	0
53	MG	2a	1839	1/1	0.83	0.37	73,73,73,73	0
53	MG	1A	3565	1/1	0.83	0.10	105,105,105,105	0
53	MG	2A	3429	1/1	0.83	0.27	78,78,78,78	0
53	MG	1A	3050	1/1	0.83	0.09	59,59,59,59	0
53	MG	1A	3054	1/1	0.83	0.15	75,75,75,75	0
53	MG	1A	3770	1/1	0.83	0.12	85,85,85,85	0
53	MG	1A	3142	1/1	0.83	0.26	75,75,75,75	0
53	MG	1A	3512	1/1	0.83	0.34	58,58,58,58	0
53	MG	1A	3777	1/1	0.83	0.24	93,93,93,93	0
53	MG	2t	3001	1/1	0.83	0.09	109,109,109,109	0
53	MG	1A	3079	1/1	0.83	0.10	41,41,41,41	0
53	MG	1a	1766	1/1	0.83	0.24	70,70,70,70	0
53	MG	2I	3001	1/1	0.83	0.10	159,159,159,159	0
53	MG	2A	3299	1/1	0.83	0.15	81,81,81,81	0
53	MG	2A	3011	1/1	0.84	0.23	63,63,63,63	0
53	MG	1a	1702	1/1	0.84	0.11	81,81,81,81	0
53	MG	1A	3820	1/1	0.84	0.14	39,39,39,39	0
53	MG	1A	3193	1/1	0.84	0.20	59,59,59,59	0
53	MG	1A	3555	1/1	0.84	0.22	93,93,93,93	0
53	MG	1A	3498	1/1	0.84	0.21	69,69,69,69	0
53	MG	2A	3232	1/1	0.84	0.24	76,76,76,76	0
53	MG	1A	3097	1/1	0.84	0.28	64,64,64,64	0
53	MG	2A	3414	1/1	0.84	0.11	116,116,116,116	0
53	MG	1A	3431	1/1	0.84	0.13	68,68,68,68	0
53	MG	2A	3241	1/1	0.84	0.19	83,83,83,83	0
53	MG	2A	3422	1/1	0.84	0.24	73,73,73,73	0
53	MG	1A	3643	1/1	0.84	0.15	46,46,46,46	0
53	MG	2A	3247	1/1	0.84	0.11	72,72,72,72	0
53	MG	1B	212	1/1	0.84	0.12	55,55,55,55	0
53	MG	1A	3395	1/1	0.84	0.22	58,58,58,58	0
53	MG	2A	3432	1/1	0.84	0.15	80,80,80,80	0
53	MG	1A	3004	1/1	0.84	0.19	84,84,84,84	0
53	MG	1A	3655	1/1	0.84	0.15	62,62,62,62	0
53	MG	1A	3343	1/1	0.84	0.25	53,53,53,53	0
53	MG	1a	1724	1/1	0.84	0.15	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3438	1/1	0.84	0.19	66,66,66,66	0
53	MG	2A	3267	1/1	0.84	0.30	56,56,56,56	0
53	MG	1a	1798	1/1	0.84	0.35	76,76,76,76	0
53	MG	1A	3756	1/1	0.84	0.17	56,56,56,56	0
53	MG	2A	3455	1/1	0.84	0.36	88,88,88,88	0
53	MG	2a	1787	1/1	0.84	0.16	90,90,90,90	0
53	MG	1a	1804	1/1	0.84	0.16	85,85,85,85	0
53	MG	2A	3277	1/1	0.84	0.20	82,82,82,82	0
53	MG	2A	3283	1/1	0.84	0.15	56,56,56,56	0
53	MG	2A	3137	1/1	0.84	0.19	66,66,66,66	0
53	MG	1A	3580	1/1	0.84	0.09	60,60,60,60	0
53	MG	1A	3588	1/1	0.84	0.08	77,77,77,77	0
53	MG	1A	3593	1/1	0.84	0.17	62,62,62,62	0
53	MG	2a	1709	1/1	0.84	0.13	124,124,124,124	0
53	MG	1A	3439	1/1	0.84	0.12	61,61,61,61	0
53	MG	1a	1733	1/1	0.84	0.31	108,108,108,108	0
53	MG	2A	3149	1/1	0.84	0.21	81,81,81,81	0
53	MG	2A	3068	1/1	0.84	0.12	68,68,68,68	0
53	MG	2A	3151	1/1	0.84	0.10	83,83,83,83	0
53	MG	1A	3129	1/1	0.84	0.18	91,91,91,91	0
53	MG	1A	3455	1/1	0.84	0.14	94,94,94,94	0
53	MG	1a	1897	1/1	0.84	0.29	88,88,88,88	0
53	MG	1A	3052	1/1	0.84	0.22	61,61,61,61	0
53	MG	2a	1720	1/1	0.84	0.08	68,68,68,68	0
53	MG	1S	201	1/1	0.84	0.13	84,84,84,84	0
53	MG	1A	3371	1/1	0.84	0.29	70,70,70,70	0
53	MG	1A	3033	1/1	0.84	0.16	68,68,68,68	0
53	MG	1a	1830	1/1	0.84	0.17	115,115,115,115	0
53	MG	2a	1726	1/1	0.84	0.11	188,188,188,188	0
53	MG	1V	202	1/1	0.84	0.30	77,77,77,77	0
53	MG	1Z	8002	1/1	0.84	0.15	55,55,55,55	0
53	MG	2A	3183	1/1	0.84	0.20	74,74,74,74	0
53	MG	1f	8001	1/1	0.84	0.11	78,78,78,78	0
53	MG	2A	3504	1/1	0.84	0.14	58,58,58,58	0
53	MG	2A	3185	1/1	0.84	0.17	60,60,60,60	0
53	MG	10	103	1/1	0.84	0.15	84,84,84,84	0
53	MG	2A	3511	1/1	0.84	0.13	132,132,132,132	0
53	MG	2A	3516	1/1	0.84	0.19	78,78,78,78	0
53	MG	2f	3002	1/1	0.84	0.19	74,74,74,74	0
53	MG	2a	1737	1/1	0.84	0.16	85,85,85,85	0
53	MG	2A	3347	1/1	0.84	0.13	80,80,80,80	0
53	MG	11	103	1/1	0.84	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3280	1/1	0.84	0.19	53,53,53,53	0
53	MG	1a	1752	1/1	0.84	0.17	118,118,118,118	0
53	MG	1a	1842	1/1	0.84	0.12	76,76,76,76	0
53	MG	1A	3388	1/1	0.84	0.15	72,72,72,72	0
53	MG	1A	3730	1/1	0.84	0.18	84,84,84,84	0
53	MG	1A	3391	1/1	0.84	0.22	77,77,77,77	0
53	MG	1A	3320	1/1	0.85	0.22	73,73,73,73	0
53	MG	1A	3321	1/1	0.85	0.40	55,55,55,55	0
53	MG	2a	1770	1/1	0.85	0.10	141,141,141,141	0
53	MG	2A	3351	1/1	0.85	0.14	88,88,88,88	0
53	MG	2A	3357	1/1	0.85	0.21	107,107,107,107	0
53	MG	1A	3569	1/1	0.85	0.19	69,69,69,69	0
53	MG	1A	3116	1/1	0.85	0.13	85,85,85,85	0
53	MG	2A	3056	1/1	0.85	0.25	92,92,92,92	0
53	MG	1a	1739	1/1	0.85	0.10	80,80,80,80	0
53	MG	1A	3329	1/1	0.85	0.15	64,64,64,64	0
53	MG	1A	3026	1/1	0.85	0.14	71,71,71,71	0
53	MG	2A	3245	1/1	0.85	0.34	68,68,68,68	0
53	MG	1A	3331	1/1	0.85	0.17	49,49,49,49	0
53	MG	1A	3121	1/1	0.85	0.17	65,65,65,65	0
53	MG	1A	3665	1/1	0.85	0.32	74,74,74,74	0
53	MG	2A	3388	1/1	0.85	0.12	63,63,63,63	0
53	MG	1A	3666	1/1	0.85	0.27	91,91,91,91	0
53	MG	1A	3339	1/1	0.85	0.13	70,70,70,70	0
53	MG	1a	1750	1/1	0.85	0.17	118,118,118,118	0
53	MG	2A	3406	1/1	0.85	0.11	83,83,83,83	0
53	MG	1A	3289	1/1	0.85	0.19	61,61,61,61	0
53	MG	2A	3071	1/1	0.85	0.13	70,70,70,70	0
53	MG	1a	1704	1/1	0.85	0.13	193,193,193,193	0
53	MG	1A	3240	1/1	0.85	0.15	101,101,101,101	0
53	MG	1A	3538	1/1	0.85	0.39	61,61,61,61	0
53	MG	1A	3417	1/1	0.85	0.13	96,96,96,96	0
53	MG	2A	3423	1/1	0.85	0.26	96,96,96,96	0
53	MG	1D	304	1/1	0.85	0.14	81,81,81,81	0
53	MG	1A	3123	1/1	0.85	0.13	68,68,68,68	0
53	MG	1a	1763	1/1	0.85	0.17	101,101,101,101	0
53	MG	2A	3285	1/1	0.85	0.18	78,78,78,78	0
53	MG	1A	3687	1/1	0.85	0.19	73,73,73,73	0
53	MG	1D	314	1/1	0.85	0.16	72,72,72,72	0
53	MG	2A	3437	1/1	0.85	0.20	86,86,86,86	0
53	MG	2B	203	1/1	0.85	0.35	85,85,85,85	0
53	MG	1E	306	1/1	0.85	0.14	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1F	302	1/1	0.85	0.25	72,72,72,72	0
53	MG	1A	3265	1/1	0.85	0.20	41,41,41,41	0
53	MG	1a	1850	1/1	0.85	0.08	73,73,73,73	0
53	MG	1A	3037	1/1	0.85	0.13	45,45,45,45	0
53	MG	1A	3427	1/1	0.85	0.25	64,64,64,64	0
53	MG	2A	3451	1/1	0.85	0.15	64,64,64,64	0
53	MG	1A	3493	1/1	0.85	0.24	110,110,110,110	0
53	MG	2a	1750	1/1	0.85	0.16	119,119,119,119	0
53	MG	1A	3780	1/1	0.85	0.27	74,74,74,74	0
53	MG	1a	1778	1/1	0.85	0.21	68,68,68,68	0
53	MG	1a	1779	1/1	0.85	0.14	100,100,100,100	0
53	MG	1A	3113	1/1	0.85	0.16	59,59,59,59	0
53	MG	1Q	201	1/1	0.85	0.22	51,51,51,51	0
53	MG	1a	1785	1/1	0.85	0.16	72,72,72,72	0
53	MG	2A	3112	1/1	0.85	0.10	108,108,108,108	0
53	MG	1A	3727	1/1	0.85	0.12	82,82,82,82	0
53	MG	2A	3212	1/1	0.85	0.21	59,59,59,59	0
53	MG	1a	1792	1/1	0.85	0.14	71,71,71,71	0
53	MG	1a	1731	1/1	0.85	0.16	78,78,78,78	0
53	MG	1A	3084	1/1	0.85	0.13	57,57,57,57	0
53	MG	1a	1782	1/1	0.86	0.13	104,104,104,104	0
53	MG	1a	1783	1/1	0.86	0.56	63,63,63,63	0
53	MG	2D	304	1/1	0.86	0.20	111,111,111,111	0
53	MG	1A	3327	1/1	0.86	0.12	84,84,84,84	0
53	MG	1A	3088	1/1	0.86	0.14	66,66,66,66	0
53	MG	1A	3560	1/1	0.86	0.16	65,65,65,65	0
53	MG	1a	1875	1/1	0.86	0.14	58,58,58,58	0
53	MG	1a	1791	1/1	0.86	0.20	72,72,72,72	0
53	MG	1F	309	1/1	0.86	0.11	92,92,92,92	0
53	MG	2a	1765	1/1	0.86	0.13	95,95,95,95	0
53	MG	1A	3626	1/1	0.86	0.21	57,57,57,57	0
53	MG	1A	3168	1/1	0.86	0.16	88,88,88,88	0
53	MG	1A	3778	1/1	0.86	0.26	82,82,82,82	0
53	MG	2A	3294	1/1	0.86	0.20	103,103,103,103	0
53	MG	2A	3297	1/1	0.86	0.15	70,70,70,70	0
53	MG	1A	3779	1/1	0.86	0.19	71,71,71,71	0
53	MG	2a	1772	1/1	0.86	0.40	70,70,70,70	0
53	MG	1A	3699	1/1	0.86	0.15	71,71,71,71	0
53	MG	1A	3226	1/1	0.86	0.17	68,68,68,68	0
53	MG	1a	1736	1/1	0.86	0.17	87,87,87,87	0
53	MG	1A	3278	1/1	0.86	0.17	64,64,64,64	0
53	MG	1A	3338	1/1	0.86	0.19	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	2A	3460	1/1	0.86	0.25	128,128,128,128	0
53	MG	2A	3180	1/1	0.86	0.25	60,60,60,60	0
53	MG	1A	3309	1/1	0.86	0.13	104,104,104,104	0
53	MG	1A	3636	1/1	0.86	0.10	48,48,48,48	0
53	MG	1A	3227	1/1	0.86	0.14	41,41,41,41	0
53	MG	10	106	1/1	0.86	0.12	72,72,72,72	0
53	MG	11	101	1/1	0.86	0.21	40,40,40,40	0
53	MG	11	102	1/1	0.86	0.20	70,70,70,70	0
53	MG	2A	3329	1/1	0.86	0.22	65,65,65,65	0
53	MG	1a	1829	1/1	0.86	0.13	64,64,64,64	0
53	MG	1A	3430	1/1	0.86	0.18	53,53,53,53	0
53	MG	2A	3199	1/1	0.86	0.24	65,65,65,65	0
53	MG	1A	3530	1/1	0.86	0.30	74,74,74,74	0
53	MG	1A	3172	1/1	0.86	0.17	49,49,49,49	0
53	MG	1A	3585	1/1	0.86	0.17	82,82,82,82	0
53	MG	2a	1807	1/1	0.86	0.38	68,68,68,68	0
53	MG	2a	1811	1/1	0.86	0.23	73,73,73,73	0
53	MG	1A	3156	1/1	0.86	0.36	76,76,76,76	0
53	MG	1a	1838	1/1	0.86	0.13	67,67,67,67	0
53	MG	1A	3590	1/1	0.86	0.19	66,66,66,66	0
53	MG	1A	3664	1/1	0.86	0.12	62,62,62,62	0
53	MG	2A	3363	1/1	0.86	0.14	126,126,126,126	0
53	MG	1A	3745	1/1	0.86	0.19	88,88,88,88	0
53	MG	1A	3746	1/1	0.86	0.12	118,118,118,118	0
53	MG	2A	3017	1/1	0.86	0.11	69,69,69,69	0
53	MG	2A	3229	1/1	0.86	0.18	65,65,65,65	0
53	MG	1a	1761	1/1	0.86	0.23	103,103,103,103	0
53	MG	2A	3378	1/1	0.86	0.09	95,95,95,95	0
53	MG	2A	3514	1/1	0.86	0.20	66,66,66,66	0
53	MG	1B	216	1/1	0.86	0.32	80,80,80,80	0
53	MG	1A	3489	1/1	0.86	0.09	69,69,69,69	0
53	MG	1a	1711	1/1	0.86	0.13	90,90,90,90	0
53	MG	1A	3212	1/1	0.86	0.12	51,51,51,51	0
53	MG	2A	3389	1/1	0.86	0.29	75,75,75,75	0
53	MG	1A	3494	1/1	0.86	0.12	86,86,86,86	0
53	MG	1A	3602	1/1	0.86	0.12	58,58,58,58	0
53	MG	1A	3497	1/1	0.86	0.31	101,101,101,101	0
53	MG	2A	3032	1/1	0.86	0.20	69,69,69,69	0
53	MG	1D	307	1/1	0.86	0.26	53,53,53,53	0
53	MG	1A	3384	1/1	0.86	0.51	70,70,70,70	0
53	MG	2A	3544	1/1	0.86	0.14	59,59,59,59	0
53	MG	1A	3681	1/1	0.86	0.12	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3682	1/1	0.86	0.23	72,72,72,72	0
53	MG	2A	3038	1/1	0.86	0.13	55,55,55,55	0
53	MG	1a	1721	1/1	0.86	0.15	114,114,114,114	0
53	MG	1A	3766	1/1	0.86	0.42	47,47,47,47	0
53	MG	2A	3562	1/1	0.86	0.10	72,72,72,72	0
53	MG	2A	3564	1/1	0.86	0.30	82,82,82,82	0
53	MG	2a	1752	1/1	0.86	0.22	127,127,127,127	0
53	MG	1N	203	1/1	0.87	0.11	56,56,56,56	0
53	MG	2A	3006	1/1	0.87	0.24	73,73,73,73	0
53	MG	1A	3006	1/1	0.87	0.17	59,59,59,59	0
53	MG	2T	3003	1/1	0.87	0.22	78,78,78,78	0
53	MG	1A	3190	1/1	0.87	0.25	85,85,85,85	0
53	MG	1A	3154	1/1	0.87	0.12	76,76,76,76	0
53	MG	1A	3506	1/1	0.87	0.23	81,81,81,81	0
53	MG	1A	3169	1/1	0.87	0.22	88,88,88,88	0
53	MG	1T	8003	1/1	0.87	0.11	89,89,89,89	0
53	MG	1A	3403	1/1	0.87	0.24	55,55,55,55	0
53	MG	1A	3453	1/1	0.87	0.19	66,66,66,66	0
53	MG	25	101	1/1	0.87	0.24	99,99,99,99	0
53	MG	1A	3376	1/1	0.87	0.11	70,70,70,70	0
53	MG	1A	3067	1/1	0.87	0.33	71,71,71,71	0
53	MG	1A	3012	1/1	0.87	0.17	69,69,69,69	0
53	MG	1A	3757	1/1	0.87	0.25	87,87,87,87	0
53	MG	1a	1860	1/1	0.87	0.09	92,92,92,92	0
53	MG	1A	3236	1/1	0.87	0.29	61,61,61,61	0
53	MG	2A	3349	1/1	0.87	0.38	77,77,77,77	0
53	MG	1a	1799	1/1	0.87	0.20	63,63,63,63	0
53	MG	1A	3761	1/1	0.87	0.12	52,52,52,52	0
53	MG	1a	1802	1/1	0.87	0.16	67,67,67,67	0
53	MG	2a	1790	1/1	0.87	0.11	96,96,96,96	0
53	MG	1a	1743	1/1	0.87	0.12	74,74,74,74	0
53	MG	2A	3121	1/1	0.87	0.18	70,70,70,70	0
53	MG	1B	217	1/1	0.87	0.15	60,60,60,60	0
53	MG	1A	3763	1/1	0.87	0.14	69,69,69,69	0
53	MG	1B	221	1/1	0.87	0.15	80,80,80,80	0
53	MG	2A	3242	1/1	0.87	0.13	60,60,60,60	0
53	MG	2A	3130	1/1	0.87	0.10	73,73,73,73	0
53	MG	2A	3244	1/1	0.87	0.12	109,109,109,109	0
53	MG	1A	3122	1/1	0.87	0.22	81,81,81,81	0
53	MG	1a	1813	1/1	0.87	0.14	74,74,74,74	0
53	MG	2a	1809	1/1	0.87	0.28	65,65,65,65	0
53	MG	1A	3705	1/1	0.87	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3468	1/1	0.87	0.14	87,87,87,87	0
53	MG	2A	3255	1/1	0.87	0.17	87,87,87,87	0
53	MG	2A	3257	1/1	0.87	0.11	77,77,77,77	0
53	MG	1a	1886	1/1	0.87	0.25	83,83,83,83	0
53	MG	1A	3390	1/1	0.87	0.15	56,56,56,56	0
53	MG	1A	3477	1/1	0.87	0.14	57,57,57,57	0
53	MG	1A	3652	1/1	0.87	0.22	71,71,71,71	0
53	MG	2A	3411	1/1	0.87	0.16	71,71,71,71	0
53	MG	1a	1822	1/1	0.87	0.14	60,60,60,60	0
53	MG	1A	3181	1/1	0.87	0.14	61,61,61,61	0
53	MG	1D	315	1/1	0.87	0.21	63,63,63,63	0
53	MG	2A	3274	1/1	0.87	0.17	81,81,81,81	0
53	MG	1A	3100	1/1	0.87	0.12	101,101,101,101	0
53	MG	1a	1759	1/1	0.87	0.14	73,73,73,73	0
53	MG	2A	3154	1/1	0.87	0.16	108,108,108,108	0
53	MG	1E	307	1/1	0.87	0.10	38,38,38,38	0
53	MG	2A	3159	1/1	0.87	0.16	84,84,84,84	0
53	MG	1b	3001	1/1	0.87	0.09	132,132,132,132	0
53	MG	1A	3250	1/1	0.87	0.16	74,74,74,74	0
53	MG	2B	201	1/1	0.87	0.08	81,81,81,81	0
53	MG	2A	3288	1/1	0.87	0.15	83,83,83,83	0
53	MG	2e	201	1/1	0.87	0.23	79,79,79,79	0
53	MG	2A	3162	1/1	0.87	0.15	78,78,78,78	0
53	MG	2B	208	1/1	0.87	0.25	68,68,68,68	0
53	MG	1A	3662	1/1	0.87	0.13	72,72,72,72	0
53	MG	1A	3184	1/1	0.87	0.23	41,41,41,41	0
53	MG	2D	306	1/1	0.87	0.24	59,59,59,59	0
53	MG	1A	3793	1/1	0.87	0.19	60,60,60,60	0
53	MG	1A	3796	1/1	0.87	0.17	50,50,50,50	0
53	MG	1h	3001	1/1	0.87	0.11	74,74,74,74	0
53	MG	1A	3263	1/1	0.87	0.12	47,47,47,47	0
55	MPD	2A	3551	8/8	0.87	0.32	57,89,97,104	0
53	MG	1A	3806	1/1	0.87	0.12	49,49,49,49	0
53	MG	1A	3605	1/1	0.87	0.11	86,86,86,86	0
53	MG	1B	210	1/1	0.88	0.23	49,49,49,49	0
53	MG	2A	3009	1/1	0.88	0.18	71,71,71,71	0
53	MG	2A	3368	1/1	0.88	0.13	75,75,75,75	0
53	MG	2a	1747	1/1	0.88	0.15	88,88,88,88	0
53	MG	2A	3370	1/1	0.88	0.22	63,63,63,63	0
53	MG	1A	3366	1/1	0.88	0.12	84,84,84,84	0
53	MG	2A	3540	1/1	0.88	0.31	82,82,82,82	0
53	MG	1A	3301	1/1	0.88	0.27	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3738	1/1	0.88	0.14	40,40,40,40	0
53	MG	1A	3185	1/1	0.88	0.44	61,61,61,61	0
53	MG	2A	3381	1/1	0.88	0.10	67,67,67,67	0
53	MG	1A	3496	1/1	0.88	0.12	69,69,69,69	0
53	MG	2A	3240	1/1	0.88	0.18	60,60,60,60	0
53	MG	2A	3557	1/1	0.88	0.14	58,58,58,58	0
53	MG	1A	3031	1/1	0.88	0.15	60,60,60,60	0
53	MG	1A	3570	1/1	0.88	0.15	40,40,40,40	0
53	MG	2A	3398	1/1	0.88	0.17	89,89,89,89	0
53	MG	1a	1853	1/1	0.88	0.12	86,86,86,86	0
53	MG	1a	1715	1/1	0.88	0.12	236,236,236,236	0
53	MG	2A	3028	1/1	0.88	0.28	51,51,51,51	0
53	MG	1A	3657	1/1	0.88	0.27	63,63,63,63	0
53	MG	1A	3307	1/1	0.88	0.27	66,66,66,66	0
53	MG	2A	3409	1/1	0.88	0.20	59,59,59,59	0
53	MG	2A	3126	1/1	0.88	0.18	107,107,107,107	0
53	MG	1A	3499	1/1	0.88	0.13	66,66,66,66	0
53	MG	1A	3663	1/1	0.88	0.16	54,54,54,54	0
53	MG	2A	3033	1/1	0.88	0.06	129,129,129,129	0
53	MG	1A	3501	1/1	0.88	0.12	67,67,67,67	0
53	MG	2A	3421	1/1	0.88	0.14	112,112,112,112	0
53	MG	1A	3042	1/1	0.88	0.58	87,87,87,87	0
53	MG	1A	3017	1/1	0.88	0.14	85,85,85,85	0
53	MG	1A	3101	1/1	0.88	0.17	54,54,54,54	0
53	MG	1A	3234	1/1	0.88	0.21	68,68,68,68	0
53	MG	1A	3277	1/1	0.88	0.10	72,72,72,72	0
53	MG	1a	1794	1/1	0.88	0.23	73,73,73,73	0
53	MG	2A	3053	1/1	0.88	0.09	98,98,98,98	0
53	MG	1A	3058	1/1	0.88	0.12	57,57,57,57	0
53	MG	1A	3515	1/1	0.88	0.11	61,61,61,61	0
53	MG	2A	3281	1/1	0.88	0.14	57,57,57,57	0
53	MG	2A	3058	1/1	0.88	0.25	71,71,71,71	0
53	MG	1A	3441	1/1	0.88	0.20	63,63,63,63	0
53	MG	2A	3153	1/1	0.88	0.16	71,71,71,71	0
53	MG	1A	3205	1/1	0.88	0.23	65,65,65,65	0
53	MG	27	101	1/1	0.88	0.29	83,83,83,83	0
53	MG	1A	3773	1/1	0.88	0.11	67,67,67,67	0
53	MG	2A	3158	1/1	0.88	0.08	80,80,80,80	0
53	MG	1A	3104	1/1	0.88	0.26	69,69,69,69	0
53	MG	1A	3284	1/1	0.88	0.11	66,66,66,66	0
53	MG	1A	3693	1/1	0.88	0.19	79,79,79,79	0
53	MG	1A	3332	1/1	0.88	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3285	1/1	0.88	0.12	27,27,27,27	0
53	MG	2A	3300	1/1	0.88	0.28	51,51,51,51	0
53	MG	1A	3609	1/1	0.88	0.10	51,51,51,51	0
53	MG	1A	3783	1/1	0.88	0.16	65,65,65,65	0
53	MG	1A	3700	1/1	0.88	0.34	54,54,54,54	0
53	MG	1A	3179	1/1	0.88	0.34	62,62,62,62	0
53	MG	2A	3311	1/1	0.88	0.26	63,63,63,63	0
53	MG	1A	3707	1/1	0.88	0.29	75,75,75,75	0
53	MG	1a	1901	1/1	0.88	0.09	91,91,91,91	0
53	MG	1U	201	1/1	0.88	0.23	58,58,58,58	0
53	MG	1a	1903	1/1	0.88	0.18	81,81,81,81	0
53	MG	1A	3708	1/1	0.88	0.27	90,90,90,90	0
53	MG	1A	3620	1/1	0.88	0.17	75,75,75,75	0
53	MG	2A	3187	1/1	0.88	0.10	69,69,69,69	0
53	MG	2A	3483	1/1	0.88	0.11	99,99,99,99	0
53	MG	1A	3010	1/1	0.88	0.25	79,79,79,79	0
53	MG	1a	1827	1/1	0.88	0.13	76,76,76,76	0
53	MG	2A	3196	1/1	0.88	0.13	85,85,85,85	0
53	MG	1A	3127	1/1	0.88	0.09	69,69,69,69	0
53	MG	1A	3415	1/1	0.88	0.15	91,91,91,91	0
53	MG	1A	3631	1/1	0.88	0.28	67,67,67,67	0
53	MG	1A	3298	1/1	0.88	0.16	73,73,73,73	0
53	MG	2A	3201	1/1	0.88	0.46	76,76,76,76	0
53	MG	2A	3348	1/1	0.88	0.33	114,114,114,114	0
53	MG	1A	3482	1/1	0.88	0.14	81,81,81,81	0
53	MG	2A	3350	1/1	0.88	0.20	85,85,85,85	0
53	MG	1A	3030	1/1	0.88	0.14	74,74,74,74	0
53	MG	2A	3355	1/1	0.88	0.23	69,69,69,69	0
53	MG	1A	3837	1/1	0.88	0.29	74,74,74,74	0
53	MG	1A	3364	1/1	0.88	0.12	65,65,65,65	0
54	ARG	1B	223	12/12	0.88	0.18	25,48,89,97	0
53	MG	1A	3487	1/1	0.88	0.09	76,76,76,76	0
53	MG	2A	3104	1/1	0.88	0.10	192,192,192,192	0
53	MG	2a	1742	1/1	0.88	0.16	65,65,65,65	0
53	MG	1B	207	1/1	0.88	0.18	75,75,75,75	0
53	MG	1a	1765	1/1	0.89	0.24	83,83,83,83	0
53	MG	1A	3581	1/1	0.89	0.11	57,57,57,57	0
53	MG	1A	3661	1/1	0.89	0.11	109,109,109,109	0
53	MG	2A	3506	1/1	0.89	0.19	65,65,65,65	0
53	MG	1A	3582	1/1	0.89	0.10	71,71,71,71	0
53	MG	2A	3508	1/1	0.89	0.08	86,86,86,86	0
53	MG	2A	3510	1/1	0.89	0.18	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	2A	3360	1/1	0.89	0.22	53,53,53,53	0
53	MG	1A	3519	1/1	0.89	0.17	98,98,98,98	0
53	MG	1A	3128	1/1	0.89	0.30	87,87,87,87	0
53	MG	2A	3019	1/1	0.89	0.20	77,77,77,77	0
53	MG	2A	3022	1/1	0.89	0.14	59,59,59,59	0
53	MG	2A	3116	1/1	0.89	0.09	68,68,68,68	0
53	MG	1A	3522	1/1	0.89	0.10	58,58,58,58	0
53	MG	2A	3369	1/1	0.89	0.14	79,79,79,79	0
53	MG	1A	3592	1/1	0.89	0.20	74,74,74,74	0
53	MG	2A	3534	1/1	0.89	0.23	61,61,61,61	0
53	MG	1A	3469	1/1	0.89	0.17	59,59,59,59	0
53	MG	2A	3536	1/1	0.89	0.08	90,90,90,90	0
53	MG	1A	3471	1/1	0.89	0.12	29,29,29,29	0
53	MG	1A	3424	1/1	0.89	0.34	69,69,69,69	0
53	MG	1A	3255	1/1	0.89	0.16	34,34,34,34	0
53	MG	2A	3124	1/1	0.89	0.23	69,69,69,69	0
53	MG	1A	3426	1/1	0.89	0.14	69,69,69,69	0
53	MG	2A	3384	1/1	0.89	0.17	97,97,97,97	0
53	MG	1A	3162	1/1	0.89	0.13	55,55,55,55	0
53	MG	1A	3536	1/1	0.89	0.14	70,70,70,70	0
53	MG	1A	3163	1/1	0.89	0.09	75,75,75,75	0
53	MG	2A	3558	1/1	0.89	0.21	81,81,81,81	0
53	MG	2A	3256	1/1	0.89	0.15	58,58,58,58	0
53	MG	1A	3048	1/1	0.89	0.09	82,82,82,82	0
53	MG	2A	3258	1/1	0.89	0.12	71,71,71,71	0
53	MG	1E	303	1/1	0.89	0.12	82,82,82,82	0
53	MG	1a	1790	1/1	0.89	0.15	65,65,65,65	0
53	MG	1A	3165	1/1	0.89	0.21	83,83,83,83	0
53	MG	1a	1869	1/1	0.89	0.13	106,106,106,106	0
53	MG	1A	3025	1/1	0.89	0.48	79,79,79,79	0
53	MG	2B	209	1/1	0.89	0.12	87,87,87,87	0
53	MG	2A	3041	1/1	0.89	0.17	66,66,66,66	0
53	MG	1A	3543	1/1	0.89	0.27	56,56,56,56	0
53	MG	1a	1728	1/1	0.89	0.12	78,78,78,78	0
53	MG	2A	3048	1/1	0.89	0.10	75,75,75,75	0
53	MG	2A	3050	1/1	0.89	0.32	101,101,101,101	0
53	MG	1a	1877	1/1	0.89	0.14	87,87,87,87	0
53	MG	1A	3622	1/1	0.89	0.11	44,44,44,44	0
53	MG	1A	3544	1/1	0.89	0.10	36,36,36,36	0
53	MG	1A	3628	1/1	0.89	0.19	59,59,59,59	0
53	MG	2A	3426	1/1	0.89	0.13	86,86,86,86	0
53	MG	2A	3427	1/1	0.89	0.25	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	2P	202	1/1	0.89	0.18	85,85,85,85	0
53	MG	1a	1882	1/1	0.89	0.13	72,72,72,72	0
53	MG	1F	308	1/1	0.89	0.14	52,52,52,52	0
53	MG	1A	3138	1/1	0.89	0.17	68,68,68,68	0
53	MG	1A	3341	1/1	0.89	0.17	41,41,41,41	0
53	MG	1A	3782	1/1	0.89	0.21	66,66,66,66	0
53	MG	1a	1891	1/1	0.89	0.29	67,67,67,67	0
53	MG	2A	3441	1/1	0.89	0.14	57,57,57,57	0
53	MG	1A	3711	1/1	0.89	0.39	69,69,69,69	0
53	MG	2A	3295	1/1	0.89	0.16	78,78,78,78	0
53	MG	1N	202	1/1	0.89	0.15	67,67,67,67	0
53	MG	2A	3168	1/1	0.89	0.11	71,71,71,71	0
53	MG	1A	3786	1/1	0.89	0.40	63,63,63,63	0
53	MG	1A	3787	1/1	0.89	0.27	86,86,86,86	0
53	MG	1a	1815	1/1	0.89	0.08	78,78,78,78	0
53	MG	2A	3307	1/1	0.89	0.20	107,107,107,107	0
53	MG	1A	3552	1/1	0.89	0.10	36,36,36,36	0
53	MG	1A	3120	1/1	0.89	0.34	74,74,74,74	0
53	MG	1A	3797	1/1	0.89	0.16	60,60,60,60	0
53	MG	2A	3313	1/1	0.89	0.17	91,91,91,91	0
53	MG	1A	3714	1/1	0.89	0.15	61,61,61,61	0
53	MG	1A	3721	1/1	0.89	0.15	84,84,84,84	0
53	MG	2A	3317	1/1	0.89	0.08	105,105,105,105	0
53	MG	1A	3308	1/1	0.89	0.12	80,80,80,80	0
53	MG	2A	3186	1/1	0.89	0.21	105,105,105,105	0
53	MG	2A	3321	1/1	0.89	0.19	67,67,67,67	0
53	MG	2a	1838	1/1	0.89	0.17	69,69,69,69	0
53	MG	1A	3400	1/1	0.89	0.25	68,68,68,68	0
53	MG	1A	3045	1/1	0.89	0.28	70,70,70,70	0
53	MG	1A	3363	1/1	0.89	0.17	67,67,67,67	0
53	MG	1A	3310	1/1	0.89	0.19	86,86,86,86	0
53	MG	1A	3405	1/1	0.89	0.21	73,73,73,73	0
53	MG	2A	3480	1/1	0.89	0.11	61,61,61,61	0
53	MG	1A	3109	1/1	0.89	0.12	50,50,50,50	0
53	MG	1A	3062	1/1	0.89	0.17	58,58,58,58	0
53	MG	1A	3098	1/1	0.89	0.15	45,45,45,45	0
53	MG	1A	3022	1/1	0.89	0.18	76,76,76,76	0
53	MG	2A	3343	1/1	0.89	0.22	80,80,80,80	0
53	MG	2A	3493	1/1	0.89	0.11	84,84,84,84	0
53	MG	2A	3001	1/1	0.89	0.19	98,98,98,98	0
53	MG	2A	3496	1/1	0.89	0.16	77,77,77,77	0
53	MG	2A	3204	1/1	0.89	0.24	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3517	1/1	0.89	0.18	59,59,59,59	0
55	MPD	2A	3552	8/8	0.89	0.31	72,112,120,128	0
53	MG	1B	206	1/1	0.89	0.11	75,75,75,75	0
56	FSD	1A	3801	44/44	0.89	0.13	24,64,94,111	0
53	MG	1A	3658	1/1	0.89	0.15	40,40,40,40	0
53	MG	1A	3518	1/1	0.90	0.11	92,92,92,92	0
53	MG	1a	1849	1/1	0.90	0.10	94,94,94,94	0
53	MG	1A	3224	1/1	0.90	0.23	77,77,77,77	0
53	MG	1A	3281	1/1	0.90	0.23	68,68,68,68	0
53	MG	1A	3407	1/1	0.90	0.19	78,78,78,78	0
53	MG	1A	3241	1/1	0.90	0.09	73,73,73,73	0
53	MG	1A	3414	1/1	0.90	0.16	57,57,57,57	0
53	MG	2A	3520	1/1	0.90	0.10	81,81,81,81	0
53	MG	2A	3522	1/1	0.90	0.27	110,110,110,110	0
53	MG	1A	3367	1/1	0.90	0.16	70,70,70,70	0
53	MG	1A	3596	1/1	0.90	0.22	45,45,45,45	0
53	MG	1A	3527	1/1	0.90	0.15	56,56,56,56	0
53	MG	1A	3370	1/1	0.90	0.09	30,30,30,30	0
53	MG	2A	3127	1/1	0.90	0.11	67,67,67,67	0
53	MG	1A	3225	1/1	0.90	0.36	44,44,44,44	0
53	MG	1A	3375	1/1	0.90	0.24	57,57,57,57	0
53	MG	2A	3131	1/1	0.90	0.12	69,69,69,69	0
53	MG	1A	3194	1/1	0.90	0.10	82,82,82,82	0
53	MG	1A	3483	1/1	0.90	0.27	47,47,47,47	0
53	MG	1A	3287	1/1	0.90	0.17	68,68,68,68	0
53	MG	1a	1786	1/1	0.90	0.11	73,73,73,73	0
53	MG	2A	3408	1/1	0.90	0.10	105,105,105,105	0
53	MG	1A	3685	1/1	0.90	0.13	62,62,62,62	0
53	MG	2a	1759	1/1	0.90	0.14	68,68,68,68	0
53	MG	2A	3410	1/1	0.90	0.14	88,88,88,88	0
53	MG	1A	3254	1/1	0.90	0.17	55,55,55,55	0
53	MG	1A	3613	1/1	0.90	0.10	60,60,60,60	0
53	MG	2A	3044	1/1	0.90	0.13	79,79,79,79	0
53	MG	1E	301	1/1	0.90	0.15	64,64,64,64	0
53	MG	2A	3146	1/1	0.90	0.32	92,92,92,92	0
53	MG	2A	3279	1/1	0.90	0.13	92,92,92,92	0
53	MG	2A	3280	1/1	0.90	0.09	70,70,70,70	0
53	MG	1A	3688	1/1	0.90	0.30	60,60,60,60	0
53	MG	1A	3292	1/1	0.90	0.17	55,55,55,55	0
53	MG	2B	205	1/1	0.90	0.23	62,62,62,62	0
53	MG	2B	206	1/1	0.90	0.13	71,71,71,71	0
53	MG	1A	3615	1/1	0.90	0.14	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1E	309	1/1	0.90	0.09	49,49,49,49	0
53	MG	2D	302	1/1	0.90	0.12	86,86,86,86	0
53	MG	2D	303	1/1	0.90	0.21	77,77,77,77	0
53	MG	1A	3616	1/1	0.90	0.12	73,73,73,73	0
53	MG	1a	1883	1/1	0.90	0.11	65,65,65,65	0
53	MG	1A	3197	1/1	0.90	0.17	70,70,70,70	0
53	MG	2A	3059	1/1	0.90	0.12	84,84,84,84	0
53	MG	1A	3491	1/1	0.90	0.18	72,72,72,72	0
53	MG	1A	3702	1/1	0.90	0.27	83,83,83,83	0
53	MG	1a	1809	1/1	0.90	0.11	94,94,94,94	0
53	MG	1a	1888	1/1	0.90	0.17	68,68,68,68	0
53	MG	1a	1889	1/1	0.90	0.11	63,63,63,63	0
53	MG	1A	3158	1/1	0.90	0.20	70,70,70,70	0
53	MG	2A	3445	1/1	0.90	0.25	83,83,83,83	0
53	MG	2P	201	1/1	0.90	0.10	81,81,81,81	0
53	MG	1A	3627	1/1	0.90	0.17	89,89,89,89	0
53	MG	2A	3447	1/1	0.90	0.15	81,81,81,81	0
53	MG	2T	3002	1/1	0.90	0.07	81,81,81,81	0
53	MG	2A	3169	1/1	0.90	0.19	61,61,61,61	0
53	MG	2A	3449	1/1	0.90	0.21	72,72,72,72	0
53	MG	2A	3171	1/1	0.90	0.17	73,73,73,73	0
53	MG	1A	3007	1/1	0.90	0.09	42,42,42,42	0
53	MG	1A	3710	1/1	0.90	0.09	68,68,68,68	0
53	MG	1A	3550	1/1	0.90	0.16	49,49,49,49	0
53	MG	2a	1813	1/1	0.90	0.20	97,97,97,97	0
53	MG	2A	3312	1/1	0.90	0.08	104,104,104,104	0
53	MG	1A	3795	1/1	0.90	0.20	80,80,80,80	0
53	MG	2A	3072	1/1	0.90	0.15	72,72,72,72	0
53	MG	1A	3299	1/1	0.90	0.12	80,80,80,80	0
53	MG	28	8001	1/1	0.90	0.12	119,119,119,119	0
53	MG	1P	203	1/1	0.90	0.14	59,59,59,59	0
53	MG	28	8003	1/1	0.90	0.12	87,87,87,87	0
53	MG	1A	3393	1/1	0.90	0.27	62,62,62,62	0
53	MG	2A	3081	1/1	0.90	0.11	80,80,80,80	0
53	MG	1A	3160	1/1	0.90	0.62	49,49,49,49	0
53	MG	1R	203	1/1	0.90	0.13	67,67,67,67	0
53	MG	1a	1824	1/1	0.90	0.15	76,76,76,76	0
53	MG	2A	3469	1/1	0.90	0.11	109,109,109,109	0
53	MG	1A	3103	1/1	0.90	0.26	88,88,88,88	0
53	MG	1A	3187	1/1	0.90	0.10	65,65,65,65	0
53	MG	1a	1747	1/1	0.90	0.17	64,64,64,64	0
53	MG	1a	1828	1/1	0.90	0.59	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3065	1/1	0.90	0.20	58,58,58,58	0
53	MG	1A	3125	1/1	0.90	0.21	65,65,65,65	0
53	MG	1A	3442	1/1	0.90	0.16	84,84,84,84	0
53	MG	1A	3509	1/1	0.90	0.12	85,85,85,85	0
53	MG	2a	1844	1/1	0.90	0.15	66,66,66,66	0
53	MG	1Y	502	1/1	0.90	0.15	100,100,100,100	0
53	MG	1A	3447	1/1	0.90	0.20	51,51,51,51	0
53	MG	2A	3488	1/1	0.90	0.16	56,56,56,56	0
53	MG	2A	3003	1/1	0.90	0.12	90,90,90,90	0
53	MG	2I	202	1/1	0.90	0.21	73,73,73,73	0
53	MG	1A	3649	1/1	0.90	0.16	49,49,49,49	0
53	MG	1A	3347	1/1	0.90	0.16	69,69,69,69	0
53	MG	1A	3829	1/1	0.90	0.20	64,64,64,64	0
53	MG	1A	3452	1/1	0.90	0.26	72,72,72,72	0
53	MG	2A	3224	1/1	0.90	0.16	92,92,92,92	0
53	MG	2A	3226	1/1	0.90	0.08	80,80,80,80	0
55	MPD	1A	3800	8/8	0.90	0.32	67,80,94,98	0
53	MG	2A	3108	1/1	0.90	0.10	81,81,81,81	0
55	MPD	18	104	8/8	0.90	0.15	32,49,55,65	0
55	MPD	1a	1900	8/8	0.90	0.15	80,100,105,111	0
53	MG	1A	3352	1/1	0.90	0.13	52,52,52,52	0
53	MG	1A	3105	1/1	0.90	0.24	69,69,69,69	0
53	MG	1B	203	1/1	0.90	0.27	59,59,59,59	0
53	MG	1B	205	1/1	0.90	0.28	76,76,76,76	0
53	MG	2A	3014	1/1	0.90	0.17	88,88,88,88	0
53	MG	2A	3172	1/1	0.91	0.15	45,45,45,45	0
53	MG	1A	3553	1/1	0.91	0.20	86,86,86,86	0
53	MG	2A	3292	1/1	0.91	0.16	78,78,78,78	0
53	MG	2A	3004	1/1	0.91	0.15	72,72,72,72	0
53	MG	1A	3624	1/1	0.91	0.27	74,74,74,74	0
53	MG	2A	3089	1/1	0.91	0.10	101,101,101,101	0
53	MG	2A	3563	1/1	0.91	0.12	63,63,63,63	0
53	MG	2a	1756	1/1	0.91	0.13	92,92,92,92	0
53	MG	1A	3217	1/1	0.91	0.15	69,69,69,69	0
53	MG	1A	3557	1/1	0.91	0.21	64,64,64,64	0
53	MG	2A	3092	1/1	0.91	0.09	72,72,72,72	0
53	MG	1A	3239	1/1	0.91	0.17	55,55,55,55	0
53	MG	2A	3305	1/1	0.91	0.16	84,84,84,84	0
53	MG	1A	3132	1/1	0.91	0.08	52,52,52,52	0
53	MG	1A	3136	1/1	0.91	0.26	93,93,93,93	0
53	MG	1A	3248	1/1	0.91	0.22	63,63,63,63	0
53	MG	1A	3566	1/1	0.91	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3083	1/1	0.91	0.12	58,58,58,58	0
53	MG	1A	3568	1/1	0.91	0.19	44,44,44,44	0
53	MG	2A	3018	1/1	0.91	0.08	139,139,139,139	0
53	MG	1A	3288	1/1	0.91	0.20	72,72,72,72	0
53	MG	1A	3423	1/1	0.91	0.32	62,62,62,62	0
53	MG	1a	1862	1/1	0.91	0.12	87,87,87,87	0
53	MG	1A	3089	1/1	0.91	0.09	45,45,45,45	0
53	MG	1A	3724	1/1	0.91	0.14	44,44,44,44	0
53	MG	2A	3452	1/1	0.91	0.29	79,79,79,79	0
53	MG	2G	8001	1/1	0.91	0.13	112,112,112,112	0
53	MG	1A	3573	1/1	0.91	0.19	67,67,67,67	0
53	MG	1A	3574	1/1	0.91	0.10	56,56,56,56	0
53	MG	2a	1782	1/1	0.91	0.09	78,78,78,78	0
53	MG	2A	3206	1/1	0.91	0.11	80,80,80,80	0
53	MG	2a	1784	1/1	0.91	0.13	68,68,68,68	0
53	MG	1A	3106	1/1	0.91	0.08	84,84,84,84	0
53	MG	2A	3326	1/1	0.91	0.18	105,105,105,105	0
53	MG	1A	3520	1/1	0.91	0.18	47,47,47,47	0
53	MG	1A	3472	1/1	0.91	0.16	76,76,76,76	0
53	MG	2A	3214	1/1	0.91	0.34	66,66,66,66	0
53	MG	2a	1791	1/1	0.91	0.11	114,114,114,114	0
53	MG	1A	3107	1/1	0.91	0.25	34,34,34,34	0
53	MG	2A	3337	1/1	0.91	0.12	79,79,79,79	0
53	MG	1A	3260	1/1	0.91	0.12	50,50,50,50	0
53	MG	2A	3223	1/1	0.91	0.14	56,56,56,56	0
53	MG	1a	1806	1/1	0.91	0.12	119,119,119,119	0
53	MG	1A	3816	1/1	0.91	0.08	31,31,31,31	0
53	MG	2A	3473	1/1	0.91	0.15	79,79,79,79	0
53	MG	1A	3479	1/1	0.91	0.13	63,63,63,63	0
53	MG	2a	1805	1/1	0.91	0.15	105,105,105,105	0
53	MG	1A	3099	1/1	0.91	0.09	37,37,37,37	0
53	MG	1A	3823	1/1	0.91	0.31	70,70,70,70	0
53	MG	1A	3231	1/1	0.91	0.23	76,76,76,76	0
53	MG	2A	3231	1/1	0.91	0.23	53,53,53,53	0
53	MG	2A	3352	1/1	0.91	0.15	86,86,86,86	0
53	MG	2A	3039	1/1	0.91	0.08	59,59,59,59	0
53	MG	1A	3266	1/1	0.91	0.12	28,28,28,28	0
53	MG	1A	3064	1/1	0.91	0.24	57,57,57,57	0
53	MG	1A	3742	1/1	0.91	0.13	53,53,53,53	0
53	MG	1V	203	1/1	0.91	0.15	46,46,46,46	0
53	MG	1A	3344	1/1	0.91	0.16	48,48,48,48	0
53	MG	1A	3111	1/1	0.91	0.13	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	2A	3365	1/1	0.91	0.12	69,69,69,69	0
53	MG	10	101	1/1	0.91	0.13	54,54,54,54	0
53	MG	1A	3537	1/1	0.91	0.15	78,78,78,78	0
53	MG	10	104	1/1	0.91	0.07	70,70,70,70	0
53	MG	1A	3435	1/1	0.91	0.11	66,66,66,66	0
53	MG	1A	3092	1/1	0.91	0.11	51,51,51,51	0
53	MG	2A	3373	1/1	0.91	0.30	95,95,95,95	0
53	MG	2A	3253	1/1	0.91	0.14	78,78,78,78	0
53	MG	1A	3348	1/1	0.91	0.18	72,72,72,72	0
53	MG	1B	209	1/1	0.91	0.11	33,33,33,33	0
53	MG	1a	1757	1/1	0.91	0.07	123,123,123,123	0
53	MG	1A	3676	1/1	0.91	0.11	42,42,42,42	0
53	MG	1A	3351	1/1	0.91	0.20	52,52,52,52	0
53	MG	1A	3304	1/1	0.91	0.19	101,101,101,101	0
53	MG	1a	1836	1/1	0.91	0.06	98,98,98,98	0
53	MG	1A	3758	1/1	0.91	0.15	53,53,53,53	0
53	MG	2A	3152	1/1	0.91	0.11	72,72,72,72	0
53	MG	2A	3395	1/1	0.91	0.09	84,84,84,84	0
53	MG	1A	3046	1/1	0.91	0.14	90,90,90,90	0
53	MG	2A	3399	1/1	0.91	0.17	74,74,74,74	0
53	MG	1A	3445	1/1	0.91	0.14	71,71,71,71	0
53	MG	2A	3527	1/1	0.91	0.27	60,60,60,60	0
53	MG	1A	3546	1/1	0.91	0.16	43,43,43,43	0
53	MG	1A	3039	1/1	0.91	0.19	60,60,60,60	0
53	MG	1l	3002	1/1	0.91	0.09	70,70,70,70	0
53	MG	1A	3765	1/1	0.91	0.15	85,85,85,85	0
53	MG	2A	3078	1/1	0.91	0.18	61,61,61,61	0
53	MG	2A	3537	1/1	0.91	0.18	65,65,65,65	0
53	MG	2A	3079	1/1	0.91	0.14	103,103,103,103	0
53	MG	1o	3001	1/1	0.91	0.09	51,51,51,51	0
53	MG	2A	3164	1/1	0.91	0.07	126,126,126,126	0
53	MG	1A	3549	1/1	0.91	0.15	65,65,65,65	0
53	MG	2A	3082	1/1	0.91	0.10	89,89,89,89	0
53	MG	1A	3117	1/1	0.91	0.33	85,85,85,85	0
53	MG	2A	3547	1/1	0.91	0.16	81,81,81,81	0
53	MG	1A	3505	1/1	0.91	0.15	78,78,78,78	0
53	MG	2A	3083	1/1	0.92	0.14	98,98,98,98	0
53	MG	1A	3449	1/1	0.92	0.20	68,68,68,68	0
53	MG	1A	3451	1/1	0.92	0.08	62,62,62,62	0
53	MG	1A	3835	1/1	0.92	0.11	56,56,56,56	0
53	MG	2A	3545	1/1	0.92	0.08	58,58,58,58	0
53	MG	2A	3416	1/1	0.92	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
53	MG	1A	3671	1/1	0.92	0.20	58,58,58,58	0
53	MG	2A	3418	1/1	0.92	0.19	63,63,63,63	0
53	MG	1A	3839	1/1	0.92	0.52	72,72,72,72	0
53	MG	2A	3002	1/1	0.92	0.11	74,74,74,74	0
53	MG	2A	3296	1/1	0.92	0.19	82,82,82,82	0
53	MG	10	102	1/1	0.92	0.09	48,48,48,48	0
53	MG	1A	3675	1/1	0.92	0.19	35,35,35,35	0
53	MG	1B	201	1/1	0.92	0.09	48,48,48,48	0
53	MG	2A	3303	1/1	0.92	0.16	64,64,64,64	0
53	MG	1a	1760	1/1	0.92	0.10	69,69,69,69	0
53	MG	1A	3161	1/1	0.92	0.11	59,59,59,59	0
53	MG	2B	202	1/1	0.92	0.24	134,134,134,134	0
53	MG	1A	3211	1/1	0.92	0.13	76,76,76,76	0
53	MG	2A	3190	1/1	0.92	0.07	74,74,74,74	0
53	MG	1B	204	1/1	0.92	0.12	68,68,68,68	0
53	MG	1A	3454	1/1	0.92	0.19	64,64,64,64	0
53	MG	1A	3074	1/1	0.92	0.23	80,80,80,80	0
53	MG	1A	3213	1/1	0.92	0.17	54,54,54,54	0
53	MG	18	101	1/1	0.92	0.16	69,69,69,69	0
53	MG	1A	3684	1/1	0.92	0.15	65,65,65,65	0
53	MG	1A	3462	1/1	0.92	0.17	55,55,55,55	0
53	MG	1a	1701	1/1	0.92	0.08	71,71,71,71	0
53	MG	2A	3020	1/1	0.92	0.10	77,77,77,77	0
53	MG	1A	3082	1/1	0.92	0.18	53,53,53,53	0
53	MG	1A	3382	1/1	0.92	0.09	71,71,71,71	0
53	MG	1A	3762	1/1	0.92	0.26	86,86,86,86	0
53	MG	1A	3141	1/1	0.92	0.20	64,64,64,64	0
53	MG	1a	1780	1/1	0.92	0.20	77,77,77,77	0
53	MG	2F	302	1/1	0.92	0.17	75,75,75,75	0
53	MG	2A	3454	1/1	0.92	0.21	69,69,69,69	0
53	MG	1A	3690	1/1	0.92	0.12	40,40,40,40	0
53	MG	1A	3337	1/1	0.92	0.25	53,53,53,53	0
53	MG	2O	201	1/1	0.92	0.07	66,66,66,66	0
53	MG	1A	3028	1/1	0.92	0.09	81,81,81,81	0
53	MG	1A	3768	1/1	0.92	0.08	96,96,96,96	0
53	MG	1A	3143	1/1	0.92	0.08	69,69,69,69	0
53	MG	2A	3225	1/1	0.92	0.10	58,58,58,58	0
53	MG	1D	303	1/1	0.92	0.24	79,79,79,79	0
53	MG	1A	3134	1/1	0.92	0.18	73,73,73,73	0
53	MG	1a	1871	1/1	0.92	0.22	74,74,74,74	0
53	MG	2W	201	1/1	0.92	0.11	64,64,64,64	0
53	MG	2A	3123	1/1	0.92	0.18	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3279	1/1	0.92	0.12	53,53,53,53	0
53	MG	1A	3701	1/1	0.92	0.12	45,45,45,45	0
53	MG	1A	3775	1/1	0.92	0.11	54,54,54,54	0
53	MG	1a	1876	1/1	0.92	0.11	105,105,105,105	0
53	MG	1A	3242	1/1	0.92	0.19	74,74,74,74	0
53	MG	2A	3040	1/1	0.92	0.12	80,80,80,80	0
53	MG	2a	1810	1/1	0.92	0.09	58,58,58,58	0
53	MG	1A	3345	1/1	0.92	0.20	47,47,47,47	0
53	MG	1A	3637	1/1	0.92	0.16	74,74,74,74	0
53	MG	1A	3480	1/1	0.92	0.20	92,92,92,92	0
53	MG	1A	3245	1/1	0.92	0.17	90,90,90,90	0
53	MG	1A	3640	1/1	0.92	0.08	65,65,65,65	0
53	MG	2a	1701	1/1	0.92	0.08	74,74,74,74	0
53	MG	1A	3529	1/1	0.92	0.13	50,50,50,50	0
53	MG	1A	3204	1/1	0.92	0.13	99,99,99,99	0
53	MG	2A	3487	1/1	0.92	0.17	60,60,60,60	0
53	MG	1A	3152	1/1	0.92	0.18	87,87,87,87	0
53	MG	1a	1807	1/1	0.92	0.30	69,69,69,69	0
53	MG	2A	3254	1/1	0.92	0.23	115,115,115,115	0
53	MG	1A	3718	1/1	0.92	0.14	112,112,112,112	0
53	MG	1A	3790	1/1	0.92	0.13	38,38,38,38	0
53	MG	1A	3791	1/1	0.92	0.16	52,52,52,52	0
53	MG	1A	3651	1/1	0.92	0.15	59,59,59,59	0
53	MG	1A	3349	1/1	0.92	0.15	33,33,33,33	0
53	MG	1A	3229	1/1	0.92	0.26	66,66,66,66	0
53	MG	2A	3501	1/1	0.92	0.15	60,60,60,60	0
53	MG	2A	3377	1/1	0.92	0.13	82,82,82,82	0
53	MG	2A	3263	1/1	0.92	0.12	72,72,72,72	0
53	MG	1H	201	1/1	0.92	0.11	76,76,76,76	0
53	MG	1H	202	1/1	0.92	0.09	61,61,61,61	0
53	MG	1A	3488	1/1	0.92	0.21	46,46,46,46	0
53	MG	1A	3317	1/1	0.92	0.09	57,57,57,57	0
53	MG	2A	3386	1/1	0.92	0.13	59,59,59,59	0
53	MG	2A	3269	1/1	0.92	0.10	70,70,70,70	0
53	MG	1A	3490	1/1	0.92	0.09	85,85,85,85	0
53	MG	2A	3271	1/1	0.92	0.16	56,56,56,56	0
53	MG	2A	3392	1/1	0.92	0.30	66,66,66,66	0
53	MG	1A	3206	1/1	0.92	0.11	64,64,64,64	0
53	MG	2A	3396	1/1	0.92	0.11	58,58,58,58	0
53	MG	1A	3360	1/1	0.92	0.13	67,67,67,67	0
53	MG	1A	3171	1/1	0.92	0.12	73,73,73,73	0
53	MG	1A	3495	1/1	0.92	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	2A	3526	1/1	0.92	0.08	78,78,78,78	0
53	MG	1A	3443	1/1	0.92	0.21	90,90,90,90	0
53	MG	1A	3323	1/1	0.92	0.17	66,66,66,66	0
53	MG	2A	3405	1/1	0.92	0.08	77,77,77,77	0
53	MG	1A	3209	1/1	0.92	0.16	81,81,81,81	0
53	MG	1A	3739	1/1	0.92	0.11	37,37,37,37	0
53	MG	1A	3411	1/1	0.92	0.11	68,68,68,68	0
53	MG	2A	3170	1/1	0.92	0.23	70,70,70,70	0
53	MG	2A	3538	1/1	0.92	0.12	75,75,75,75	0
53	MG	1a	1832	1/1	0.92	0.09	65,65,65,65	0
53	MG	1A	3794	1/1	0.93	0.10	66,66,66,66	0
53	MG	1G	8002	1/1	0.93	0.14	92,92,92,92	0
53	MG	2A	3107	1/1	0.93	0.14	99,99,99,99	0
53	MG	2A	3503	1/1	0.93	0.10	76,76,76,76	0
53	MG	1A	3215	1/1	0.93	0.12	80,80,80,80	0
53	MG	1A	3196	1/1	0.93	0.17	34,34,34,34	0
53	MG	2A	3110	1/1	0.93	0.16	59,59,59,59	0
53	MG	2a	1734	1/1	0.93	0.20	78,78,78,78	0
53	MG	1A	3176	1/1	0.93	0.16	89,89,89,89	0
53	MG	1H	203	1/1	0.93	0.20	77,77,77,77	0
53	MG	1A	3198	1/1	0.93	0.17	38,38,38,38	0
53	MG	1A	3601	1/1	0.93	0.24	56,56,56,56	0
53	MG	2A	3371	1/1	0.93	0.21	113,113,113,113	0
53	MG	2A	3372	1/1	0.93	0.09	42,42,42,42	0
53	MG	2A	3517	1/1	0.93	0.14	86,86,86,86	0
53	MG	1A	3014	1/1	0.93	0.30	81,81,81,81	0
53	MG	1P	201	1/1	0.93	0.24	60,60,60,60	0
53	MG	1A	3146	1/1	0.93	0.11	62,62,62,62	0
53	MG	1a	1841	1/1	0.93	0.12	69,69,69,69	0
53	MG	1A	3148	1/1	0.93	0.29	47,47,47,47	0
53	MG	1A	3312	1/1	0.93	0.14	55,55,55,55	0
53	MG	2A	3246	1/1	0.93	0.11	65,65,65,65	0
53	MG	1Q	203	1/1	0.93	0.11	60,60,60,60	0
53	MG	1A	3055	1/1	0.93	0.10	56,56,56,56	0
53	MG	2A	3385	1/1	0.93	0.15	79,79,79,79	0
53	MG	1A	3818	1/1	0.93	0.26	76,76,76,76	0
53	MG	1A	3668	1/1	0.93	0.20	74,74,74,74	0
53	MG	1A	3078	1/1	0.93	0.17	91,91,91,91	0
53	MG	1A	3357	1/1	0.93	0.10	37,37,37,37	0
53	MG	1A	3744	1/1	0.93	0.20	73,73,73,73	0
53	MG	1V	201	1/1	0.93	0.11	60,60,60,60	0
53	MG	1A	3611	1/1	0.93	0.07	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3828	1/1	0.93	0.08	67,67,67,67	0
53	MG	1a	1762	1/1	0.93	0.08	63,63,63,63	0
53	MG	1A	3318	1/1	0.93	0.20	83,83,83,83	0
53	MG	1A	3832	1/1	0.93	0.14	41,41,41,41	0
53	MG	2a	1763	1/1	0.93	0.07	83,83,83,83	0
53	MG	1A	3319	1/1	0.93	0.11	79,79,79,79	0
53	MG	1A	3748	1/1	0.93	0.15	93,93,93,93	0
53	MG	2A	3549	1/1	0.93	0.11	73,73,73,73	0
53	MG	1A	3361	1/1	0.93	0.09	59,59,59,59	0
53	MG	1A	3750	1/1	0.93	0.14	78,78,78,78	0
53	MG	1a	1863	1/1	0.93	0.14	61,61,61,61	0
53	MG	10	105	1/1	0.93	0.12	68,68,68,68	0
53	MG	2A	3144	1/1	0.93	0.18	64,64,64,64	0
53	MG	1A	3751	1/1	0.93	0.12	82,82,82,82	0
53	MG	2A	3147	1/1	0.93	0.26	86,86,86,86	0
53	MG	2A	3413	1/1	0.93	0.19	93,93,93,93	0
53	MG	2A	3042	1/1	0.93	0.09	83,83,83,83	0
53	MG	1A	3680	1/1	0.93	0.08	28,28,28,28	0
53	MG	1A	3362	1/1	0.93	0.13	59,59,59,59	0
53	MG	2a	1778	1/1	0.93	0.15	111,111,111,111	0
53	MG	1A	3457	1/1	0.93	0.65	65,65,65,65	0
53	MG	1A	3459	1/1	0.93	0.16	53,53,53,53	0
53	MG	17	101	1/1	0.93	0.12	65,65,65,65	0
53	MG	2A	3051	1/1	0.93	0.10	97,97,97,97	0
53	MG	2B	207	1/1	0.93	0.09	67,67,67,67	0
53	MG	2A	3155	1/1	0.93	0.30	104,104,104,104	0
53	MG	1A	3460	1/1	0.93	0.14	66,66,66,66	0
53	MG	1A	3625	1/1	0.93	0.15	67,67,67,67	0
53	MG	1A	3251	1/1	0.93	0.08	45,45,45,45	0
53	MG	19	101	1/1	0.93	0.08	40,40,40,40	0
53	MG	2A	3428	1/1	0.93	0.18	66,66,66,66	0
53	MG	1A	3760	1/1	0.93	0.23	81,81,81,81	0
53	MG	1A	3252	1/1	0.93	0.13	48,48,48,48	0
53	MG	1A	3137	1/1	0.93	0.08	66,66,66,66	0
53	MG	2a	1797	1/1	0.93	0.17	79,79,79,79	0
53	MG	1A	3689	1/1	0.93	0.15	69,69,69,69	0
53	MG	1a	1789	1/1	0.93	0.09	85,85,85,85	0
53	MG	2A	3298	1/1	0.93	0.10	87,87,87,87	0
53	MG	2A	3440	1/1	0.93	0.20	73,73,73,73	0
53	MG	1A	3324	1/1	0.93	0.22	68,68,68,68	0
53	MG	1A	3096	1/1	0.93	0.06	87,87,87,87	0
53	MG	1a	1707	1/1	0.93	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
53	MG	2a	1808	1/1	0.93	0.13	103,103,103,103	0
53	MG	2A	3067	1/1	0.93	0.13	80,80,80,80	0
53	MG	1a	1793	1/1	0.93	0.14	81,81,81,81	0
53	MG	1a	1708	1/1	0.93	0.07	164,164,164,164	0
53	MG	1A	3326	1/1	0.93	0.10	73,73,73,73	0
53	MG	1a	1890	1/1	0.93	0.16	67,67,67,67	0
53	MG	2R	202	1/1	0.93	0.05	62,62,62,62	0
53	MG	2T	3001	1/1	0.93	0.08	95,95,95,95	0
53	MG	1A	3139	1/1	0.93	0.06	37,37,37,37	0
53	MG	2A	3179	1/1	0.93	0.09	59,59,59,59	0
53	MG	1A	3633	1/1	0.93	0.11	80,80,80,80	0
53	MG	2A	3076	1/1	0.93	0.09	61,61,61,61	0
53	MG	1A	3256	1/1	0.93	0.12	63,63,63,63	0
53	MG	1B	225	1/1	0.93	0.28	69,69,69,69	0
53	MG	2a	1826	1/1	0.93	0.17	89,89,89,89	0
53	MG	2a	1827	1/1	0.93	0.14	68,68,68,68	0
53	MG	1A	3771	1/1	0.93	0.07	25,25,25,25	0
53	MG	2A	3318	1/1	0.93	0.20	67,67,67,67	0
53	MG	1A	3258	1/1	0.93	0.17	59,59,59,59	0
53	MG	1A	3259	1/1	0.93	0.12	43,43,43,43	0
53	MG	1A	3703	1/1	0.93	0.18	61,61,61,61	0
53	MG	2A	3189	1/1	0.93	0.24	67,67,67,67	0
53	MG	1D	308	1/1	0.93	0.13	79,79,79,79	0
53	MG	1A	3020	1/1	0.93	0.22	58,58,58,58	0
53	MG	1D	313	1/1	0.93	0.07	67,67,67,67	0
53	MG	1A	3478	1/1	0.93	0.20	59,59,59,59	0
53	MG	1A	3335	1/1	0.93	0.13	45,45,45,45	0
53	MG	2A	3331	1/1	0.93	0.23	103,103,103,103	0
53	MG	2A	3472	1/1	0.93	0.20	87,87,87,87	0
53	MG	1A	3108	1/1	0.93	0.15	60,60,60,60	0
53	MG	1E	302	1/1	0.93	0.23	42,42,42,42	0
53	MG	1A	3481	1/1	0.93	0.13	67,67,67,67	0
53	MG	1a	1818	1/1	0.93	0.08	80,80,80,80	0
53	MG	1A	3584	1/1	0.93	0.17	55,55,55,55	0
53	MG	2l	201	1/1	0.93	0.07	89,89,89,89	0
53	MG	1l	3001	1/1	0.93	0.05	78,78,78,78	0
53	MG	1A	3131	1/1	0.93	0.14	89,89,89,89	0
53	MG	2A	3345	1/1	0.93	0.07	52,52,52,52	0
53	MG	1A	3650	1/1	0.93	0.20	62,62,62,62	0
53	MG	2A	3096	1/1	0.93	0.16	50,50,50,50	0
53	MG	2A	3486	1/1	0.93	0.11	73,73,73,73	0
53	MG	1A	3214	1/1	0.93	0.10	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3589	1/1	0.93	0.14	63,63,63,63	0
53	MG	1A	3788	1/1	0.93	0.10	52,52,52,52	0
53	MG	2a	1719	1/1	0.93	0.09	48,48,48,48	0
53	MG	2A	3217	1/1	0.93	0.11	66,66,66,66	0
53	MG	2A	3354	1/1	0.93	0.24	60,60,60,60	0
53	MG	1A	3269	1/1	0.93	0.09	71,71,71,71	0
53	MG	2A	3356	1/1	0.93	0.14	75,75,75,75	0
53	MG	1A	3725	1/1	0.93	0.09	63,63,63,63	0
53	MG	1A	3436	1/1	0.93	0.12	76,76,76,76	0
57	ZN	29	501	1/1	0.93	0.07	136,136,136,136	0
57	ZN	2n	102	1/1	0.93	0.07	205,205,205,205	0
53	MG	1A	3715	1/1	0.94	0.11	52,52,52,52	0
53	MG	1a	1769	1/1	0.94	0.16	129,129,129,129	0
53	MG	1A	3716	1/1	0.94	0.20	83,83,83,83	0
53	MG	1A	3011	1/1	0.94	0.20	78,78,78,78	0
53	MG	1A	3654	1/1	0.94	0.14	55,55,55,55	0
53	MG	1a	1774	1/1	0.94	0.06	111,111,111,111	0
53	MG	2A	3209	1/1	0.94	0.29	71,71,71,71	0
53	MG	1A	3416	1/1	0.94	0.11	80,80,80,80	0
53	MG	1A	3377	1/1	0.94	0.16	79,79,79,79	0
53	MG	1A	3456	1/1	0.94	0.10	52,52,52,52	0
53	MG	2A	3327	1/1	0.94	0.13	82,82,82,82	0
53	MG	1A	3379	1/1	0.94	0.09	53,53,53,53	0
53	MG	1A	3458	1/1	0.94	0.38	78,78,78,78	0
53	MG	1a	1705	1/1	0.94	0.22	82,82,82,82	0
53	MG	1A	3729	1/1	0.94	0.33	71,71,71,71	0
53	MG	1A	3420	1/1	0.94	0.12	66,66,66,66	0
53	MG	1A	3502	1/1	0.94	0.09	43,43,43,43	0
53	MG	1A	3080	1/1	0.94	0.08	26,26,26,26	0
53	MG	2A	3340	1/1	0.94	0.10	64,64,64,64	0
53	MG	1A	3221	1/1	0.94	0.15	32,32,32,32	0
53	MG	1E	305	1/1	0.94	0.17	32,32,32,32	0
53	MG	1A	3554	1/1	0.94	0.08	43,43,43,43	0
53	MG	1A	3735	1/1	0.94	0.17	57,57,57,57	0
53	MG	2E	304	1/1	0.94	0.06	93,93,93,93	0
53	MG	1A	3073	1/1	0.94	0.14	53,53,53,53	0
53	MG	1a	1873	1/1	0.94	0.32	98,98,98,98	0
53	MG	1F	301	1/1	0.94	0.17	73,73,73,73	0
53	MG	2F	304	1/1	0.94	0.12	74,74,74,74	0
53	MG	2A	3235	1/1	0.94	0.11	54,54,54,54	0
53	MG	2A	3129	1/1	0.94	0.12	76,76,76,76	0
53	MG	1A	3803	1/1	0.94	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
53	MG	2A	3353	1/1	0.94	0.09	86,86,86,86	0
53	MG	1A	3804	1/1	0.94	0.09	67,67,67,67	0
53	MG	1F	305	1/1	0.94	0.09	39,39,39,39	0
53	MG	1a	1795	1/1	0.94	0.10	69,69,69,69	0
53	MG	2P	203	1/1	0.94	0.11	81,81,81,81	0
53	MG	1A	3272	1/1	0.94	0.14	46,46,46,46	0
53	MG	1a	1797	1/1	0.94	0.24	112,112,112,112	0
53	MG	2A	3359	1/1	0.94	0.07	78,78,78,78	0
53	MG	1A	3322	1/1	0.94	0.08	80,80,80,80	0
53	MG	1A	3561	1/1	0.94	0.08	68,68,68,68	0
53	MG	2A	3362	1/1	0.94	0.31	82,82,82,82	0
53	MG	1a	1722	1/1	0.94	0.09	114,114,114,114	0
53	MG	1A	3465	1/1	0.94	0.10	89,89,89,89	0
53	MG	1A	3619	1/1	0.94	0.38	82,82,82,82	0
53	MG	2a	1800	1/1	0.94	0.06	79,79,79,79	0
53	MG	1A	3192	1/1	0.94	0.14	59,59,59,59	0
53	MG	2a	1802	1/1	0.94	0.24	86,86,86,86	0
53	MG	1A	3274	1/1	0.94	0.13	56,56,56,56	0
53	MG	1A	3623	1/1	0.94	0.17	97,97,97,97	0
53	MG	1A	3133	1/1	0.94	0.14	65,65,65,65	0
53	MG	1A	3356	1/1	0.94	0.18	68,68,68,68	0
53	MG	1A	3008	1/1	0.94	0.17	57,57,57,57	0
53	MG	1a	1893	1/1	0.94	0.12	82,82,82,82	0
53	MG	1A	3473	1/1	0.94	0.48	62,62,62,62	0
53	MG	2A	3494	1/1	0.94	0.25	79,79,79,79	0
53	MG	2A	3374	1/1	0.94	0.11	59,59,59,59	0
53	MG	1A	3119	1/1	0.94	0.25	87,87,87,87	0
53	MG	1O	8001	1/1	0.94	0.08	75,75,75,75	0
53	MG	1A	3257	1/1	0.94	0.09	40,40,40,40	0
53	MG	2a	1817	1/1	0.94	0.18	81,81,81,81	0
53	MG	1A	3572	1/1	0.94	0.15	56,56,56,56	0
53	MG	1A	3754	1/1	0.94	0.07	54,54,54,54	0
53	MG	1A	3009	1/1	0.94	0.12	55,55,55,55	0
53	MG	2A	3074	1/1	0.94	0.13	101,101,101,101	0
53	MG	2A	3383	1/1	0.94	0.16	78,78,78,78	0
53	MG	1A	3306	1/1	0.94	0.10	73,73,73,73	0
53	MG	1R	202	1/1	0.94	0.15	64,64,64,64	0
53	MG	1A	3170	1/1	0.94	0.21	59,59,59,59	0
53	MG	1a	1823	1/1	0.94	0.23	91,91,91,91	0
53	MG	1A	3199	1/1	0.94	0.18	39,39,39,39	0
53	MG	2A	3166	1/1	0.94	0.11	73,73,73,73	0
53	MG	2A	3167	1/1	0.94	0.10	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	2A	3513	1/1	0.94	0.17	84,84,84,84	0
53	MG	1A	3578	1/1	0.94	0.08	49,49,49,49	0
53	MG	1A	3579	1/1	0.94	0.14	55,55,55,55	0
53	MG	1A	3243	1/1	0.94	0.14	49,49,49,49	0
53	MG	1A	3264	1/1	0.94	0.19	46,46,46,46	0
53	MG	1A	3404	1/1	0.94	0.11	60,60,60,60	0
53	MG	1A	3311	1/1	0.94	0.14	65,65,65,65	0
53	MG	2A	3402	1/1	0.94	0.10	76,76,76,76	0
53	MG	1A	3641	1/1	0.94	0.09	57,57,57,57	0
53	MG	1A	3704	1/1	0.94	0.15	47,47,47,47	0
53	MG	1a	1833	1/1	0.94	0.16	67,67,67,67	0
53	MG	1Z	8001	1/1	0.94	0.05	54,54,54,54	0
53	MG	1A	3406	1/1	0.94	0.10	78,78,78,78	0
53	MG	2A	3529	1/1	0.94	0.20	84,84,84,84	0
53	MG	2A	3530	1/1	0.94	0.31	69,69,69,69	0
53	MG	1A	3644	1/1	0.94	0.13	66,66,66,66	0
53	MG	1A	3645	1/1	0.94	0.09	61,61,61,61	0
53	MG	1A	3286	1/1	0.94	0.12	67,67,67,67	0
53	MG	1B	215	1/1	0.94	0.14	45,45,45,45	0
53	MG	1A	3372	1/1	0.94	0.19	83,83,83,83	0
53	MG	2A	3302	1/1	0.94	0.10	70,70,70,70	0
53	MG	1A	3373	1/1	0.94	0.11	54,54,54,54	0
53	MG	1B	218	1/1	0.94	0.05	27,27,27,27	0
53	MG	1B	219	1/1	0.94	0.15	67,67,67,67	0
53	MG	1a	1844	1/1	0.94	0.10	86,86,86,86	0
53	MG	2A	3419	1/1	0.94	0.14	54,54,54,54	0
53	MG	2A	3191	1/1	0.94	0.08	75,75,75,75	0
53	MG	2A	3100	1/1	0.94	0.09	79,79,79,79	0
53	MG	1A	3774	1/1	0.94	0.18	63,63,63,63	0
53	MG	2A	3102	1/1	0.94	0.17	90,90,90,90	0
53	MG	1A	3413	1/1	0.94	0.29	57,57,57,57	0
53	MG	15	102	1/1	0.94	0.05	50,50,50,50	0
53	MG	1A	3005	1/1	0.94	0.07	59,59,59,59	0
53	MG	1A	3283	1/1	0.95	0.07	35,35,35,35	0
53	MG	1A	3261	1/1	0.95	0.12	71,71,71,71	0
53	MG	1A	3792	1/1	0.95	0.05	61,61,61,61	0
53	MG	1A	3409	1/1	0.95	0.14	78,78,78,78	0
53	MG	1A	3410	1/1	0.95	0.08	58,58,58,58	0
53	MG	1A	3450	1/1	0.95	0.14	41,41,41,41	0
53	MG	1A	3547	1/1	0.95	0.07	58,58,58,58	0
53	MG	1A	3077	1/1	0.95	0.17	83,83,83,83	0
53	MG	1A	3798	1/1	0.95	0.13	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3057	1/1	0.95	0.24	73,73,73,73	0
53	MG	2A	3556	1/1	0.95	0.06	62,62,62,62	0
53	MG	1A	3342	1/1	0.95	0.18	62,62,62,62	0
53	MG	1A	3610	1/1	0.95	0.12	66,66,66,66	0
53	MG	1A	3027	1/1	0.95	0.13	54,54,54,54	0
53	MG	1A	3612	1/1	0.95	0.12	79,79,79,79	0
53	MG	2A	3561	1/1	0.95	0.14	78,78,78,78	0
53	MG	1a	1870	1/1	0.95	0.07	101,101,101,101	0
53	MG	2A	3208	1/1	0.95	0.07	48,48,48,48	0
53	MG	2A	3436	1/1	0.95	0.11	91,91,91,91	0
53	MG	1A	3316	1/1	0.95	0.11	87,87,87,87	0
53	MG	2A	3438	1/1	0.95	0.15	100,100,100,100	0
53	MG	1A	3672	1/1	0.95	0.19	35,35,35,35	0
53	MG	1A	3380	1/1	0.95	0.14	52,52,52,52	0
53	MG	1A	3016	1/1	0.95	0.23	73,73,73,73	0
53	MG	2A	3442	1/1	0.95	0.18	89,89,89,89	0
53	MG	1A	3678	1/1	0.95	0.08	53,53,53,53	0
53	MG	2A	3216	1/1	0.95	0.12	79,79,79,79	0
53	MG	1A	3819	1/1	0.95	0.14	42,42,42,42	0
53	MG	2A	3218	1/1	0.95	0.13	76,76,76,76	0
53	MG	1A	3418	1/1	0.95	0.16	64,64,64,64	0
53	MG	2A	3221	1/1	0.95	0.09	65,65,65,65	0
53	MG	1A	3558	1/1	0.95	0.11	66,66,66,66	0
53	MG	2A	3335	1/1	0.95	0.13	95,95,95,95	0
53	MG	2A	3336	1/1	0.95	0.17	73,73,73,73	0
53	MG	1A	3383	1/1	0.95	0.20	43,43,43,43	0
53	MG	1a	1803	1/1	0.95	0.08	81,81,81,81	0
53	MG	1A	3081	1/1	0.95	0.10	70,70,70,70	0
53	MG	1A	3191	1/1	0.95	0.10	62,62,62,62	0
53	MG	2A	3049	1/1	0.95	0.09	78,78,78,78	0
53	MG	1A	3508	1/1	0.95	0.10	57,57,57,57	0
53	MG	1A	3422	1/1	0.95	0.18	62,62,62,62	0
53	MG	2a	1788	1/1	0.95	0.08	96,96,96,96	0
53	MG	1a	1808	1/1	0.95	0.09	87,87,87,87	0
53	MG	1N	204	1/1	0.95	0.10	37,37,37,37	0
53	MG	2A	3233	1/1	0.95	0.09	56,56,56,56	0
53	MG	2A	3055	1/1	0.95	0.10	78,78,78,78	0
53	MG	2A	3135	1/1	0.95	0.24	109,109,109,109	0
53	MG	1A	3830	1/1	0.95	0.20	62,62,62,62	0
53	MG	2a	1795	1/1	0.95	0.20	114,114,114,114	0
53	MG	2A	3057	1/1	0.95	0.41	87,87,87,87	0
53	MG	2A	3468	1/1	0.95	0.06	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3208	1/1	0.95	0.10	55,55,55,55	0
53	MG	1A	3833	1/1	0.95	0.10	59,59,59,59	0
53	MG	2A	3140	1/1	0.95	0.14	81,81,81,81	0
53	MG	1A	3834	1/1	0.95	0.07	57,57,57,57	0
53	MG	2A	3142	1/1	0.95	0.11	93,93,93,93	0
53	MG	2a	1803	1/1	0.95	0.10	146,146,146,146	0
53	MG	1A	3294	1/1	0.95	0.23	65,65,65,65	0
53	MG	2V	201	1/1	0.95	0.06	63,63,63,63	0
53	MG	1A	3389	1/1	0.95	0.10	76,76,76,76	0
53	MG	1R	201	1/1	0.95	0.16	93,93,93,93	0
53	MG	2A	3479	1/1	0.95	0.10	119,119,119,119	0
53	MG	1A	3838	1/1	0.95	0.26	66,66,66,66	0
53	MG	2A	3250	1/1	0.95	0.09	104,104,104,104	0
53	MG	1A	3145	1/1	0.95	0.15	66,66,66,66	0
53	MG	1A	3041	1/1	0.95	0.27	72,72,72,72	0
53	MG	1A	3354	1/1	0.95	0.20	73,73,73,73	0
53	MG	2a	1814	1/1	0.95	0.09	118,118,118,118	0
53	MG	1A	3038	1/1	0.95	0.08	50,50,50,50	0
53	MG	1A	3697	1/1	0.95	0.10	75,75,75,75	0
53	MG	1A	3275	1/1	0.95	0.08	42,42,42,42	0
53	MG	1A	3195	1/1	0.95	0.12	52,52,52,52	0
53	MG	2A	3492	1/1	0.95	0.05	86,86,86,86	0
53	MG	1A	3575	1/1	0.95	0.16	73,73,73,73	0
53	MG	2A	3156	1/1	0.95	0.11	74,74,74,74	0
53	MG	2A	3073	1/1	0.95	0.23	60,60,60,60	0
53	MG	1A	3475	1/1	0.95	0.09	36,36,36,36	0
53	MG	1W	3001	1/1	0.95	0.11	36,36,36,36	0
53	MG	1W	3002	1/1	0.95	0.12	45,45,45,45	0
53	MG	1X	101	1/1	0.95	0.16	75,75,75,75	0
53	MG	1A	3043	1/1	0.95	0.10	70,70,70,70	0
53	MG	2A	3379	1/1	0.95	0.09	114,114,114,114	0
53	MG	1A	3397	1/1	0.95	0.11	61,61,61,61	0
53	MG	2A	3272	1/1	0.95	0.13	114,114,114,114	0
53	MG	2A	3273	1/1	0.95	0.09	70,70,70,70	0
53	MG	2a	1835	1/1	0.95	0.17	77,77,77,77	0
53	MG	1A	3180	1/1	0.95	0.08	71,71,71,71	0
53	MG	1A	3126	1/1	0.95	0.17	57,57,57,57	0
53	MG	1A	3305	1/1	0.95	0.21	31,31,31,31	0
53	MG	1B	214	1/1	0.95	0.12	82,82,82,82	0
53	MG	2A	3278	1/1	0.95	0.07	73,73,73,73	0
53	MG	1A	3056	1/1	0.95	0.21	78,78,78,78	0
53	MG	1A	3333	1/1	0.95	0.12	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	2A	3391	1/1	0.95	0.07	67,67,67,67	0
53	MG	2A	3515	1/1	0.95	0.06	76,76,76,76	0
53	MG	2a	1723	1/1	0.95	0.20	120,120,120,120	0
53	MG	1A	3532	1/1	0.95	0.14	82,82,82,82	0
53	MG	2A	3282	1/1	0.95	0.09	110,110,110,110	0
53	MG	1A	3647	1/1	0.95	0.08	65,65,65,65	0
53	MG	1a	1764	1/1	0.95	0.10	68,68,68,68	0
53	MG	1A	3440	1/1	0.95	0.09	60,60,60,60	0
53	MG	1A	3484	1/1	0.95	0.17	71,71,71,71	0
53	MG	2A	3287	1/1	0.95	0.18	65,65,65,65	0
53	MG	2A	3175	1/1	0.95	0.09	70,70,70,70	0
53	MG	1A	3219	1/1	0.95	0.13	62,62,62,62	0
53	MG	1A	3591	1/1	0.95	0.08	56,56,56,56	0
53	MG	2A	3178	1/1	0.95	0.29	96,96,96,96	0
53	MG	1A	3717	1/1	0.95	0.06	72,72,72,72	0
53	MG	1A	3369	1/1	0.95	0.15	22,22,22,22	0
53	MG	2A	3532	1/1	0.95	0.12	70,70,70,70	0
53	MG	1A	3539	1/1	0.95	0.14	53,53,53,53	0
53	MG	1A	3722	1/1	0.95	0.13	89,89,89,89	0
53	MG	2A	3012	1/1	0.95	0.13	101,101,101,101	0
53	MG	1A	3723	1/1	0.95	0.09	63,63,63,63	0
53	MG	1A	3200	1/1	0.95	0.17	57,57,57,57	0
53	MG	1A	3595	1/1	0.95	0.15	47,47,47,47	0
53	MG	1A	3444	1/1	0.95	0.12	66,66,66,66	0
53	MG	2A	3457	1/1	0.96	0.18	94,94,94,94	0
53	MG	2a	1705	1/1	0.96	0.06	126,126,126,126	0
53	MG	1A	3563	1/1	0.96	0.13	56,56,56,56	0
53	MG	1A	3216	1/1	0.96	0.08	48,48,48,48	0
53	MG	2A	3316	1/1	0.96	0.06	74,74,74,74	0
53	MG	2A	3542	1/1	0.96	0.23	71,71,71,71	0
53	MG	1A	3533	1/1	0.96	0.17	64,64,64,64	0
53	MG	1P	202	1/1	0.96	0.10	65,65,65,65	0
53	MG	1A	3603	1/1	0.96	0.11	69,69,69,69	0
53	MG	1A	3807	1/1	0.96	0.24	47,47,47,47	0
53	MG	1A	3534	1/1	0.96	0.06	43,43,43,43	0
53	MG	1A	3504	1/1	0.96	0.08	38,38,38,38	0
53	MG	1A	3313	1/1	0.96	0.19	45,45,45,45	0
53	MG	2A	3554	1/1	0.96	0.07	68,68,68,68	0
53	MG	2A	3260	1/1	0.96	0.12	62,62,62,62	0
53	MG	1A	3386	1/1	0.96	0.09	40,40,40,40	0
53	MG	1A	3001	1/1	0.96	0.15	57,57,57,57	0
53	MG	1a	1878	1/1	0.96	0.17	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3817	1/1	0.96	0.24	34,34,34,34	0
53	MG	2A	3330	1/1	0.96	0.39	45,45,45,45	0
53	MG	2A	3195	1/1	0.96	0.26	65,65,65,65	0
53	MG	1D	301	1/1	0.96	0.11	61,61,61,61	0
53	MG	2A	3404	1/1	0.96	0.10	83,83,83,83	0
53	MG	2A	3333	1/1	0.96	0.20	72,72,72,72	0
53	MG	1A	3218	1/1	0.96	0.08	71,71,71,71	0
53	MG	2A	3482	1/1	0.96	0.18	115,115,115,115	0
53	MG	1a	1773	1/1	0.96	0.11	51,51,51,51	0
53	MG	1A	3296	1/1	0.96	0.10	61,61,61,61	0
53	MG	1A	3150	1/1	0.96	0.11	66,66,66,66	0
53	MG	1a	1723	1/1	0.96	0.13	79,79,79,79	0
53	MG	2A	3339	1/1	0.96	0.08	80,80,80,80	0
53	MG	1A	3189	1/1	0.96	0.10	50,50,50,50	0
53	MG	2A	3341	1/1	0.96	0.07	117,117,117,117	0
53	MG	2A	3491	1/1	0.96	0.08	66,66,66,66	0
53	MG	1A	3822	1/1	0.96	0.05	25,25,25,25	0
53	MG	2a	1820	1/1	0.96	0.10	126,126,126,126	0
53	MG	1D	311	1/1	0.96	0.12	71,71,71,71	0
53	MG	1A	3173	1/1	0.96	0.12	79,79,79,79	0
53	MG	2A	3145	1/1	0.96	0.24	89,89,89,89	0
53	MG	1A	3824	1/1	0.96	0.30	65,65,65,65	0
53	MG	1A	3513	1/1	0.96	0.10	99,99,99,99	0
53	MG	2A	3420	1/1	0.96	0.07	65,65,65,65	0
53	MG	1A	3174	1/1	0.96	0.12	78,78,78,78	0
53	MG	1A	3827	1/1	0.96	0.13	72,72,72,72	0
53	MG	1A	3516	1/1	0.96	0.06	70,70,70,70	0
53	MG	1A	3617	1/1	0.96	0.12	77,77,77,77	0
53	MG	2F	303	1/1	0.96	0.09	88,88,88,88	0
53	MG	1a	1787	1/1	0.96	0.16	118,118,118,118	0
53	MG	1A	3140	1/1	0.96	0.18	89,89,89,89	0
53	MG	1A	3091	1/1	0.96	0.09	67,67,67,67	0
53	MG	1A	3621	1/1	0.96	0.10	74,74,74,74	0
53	MG	1A	3068	1/1	0.96	0.08	83,83,83,83	0
53	MG	2A	3430	1/1	0.96	0.06	71,71,71,71	0
53	MG	2A	3289	1/1	0.96	0.20	57,57,57,57	0
53	MG	2a	1841	1/1	0.96	0.23	58,58,58,58	0
53	MG	2A	3043	1/1	0.96	0.10	114,114,114,114	0
53	MG	2A	3512	1/1	0.96	0.10	79,79,79,79	0
53	MG	1A	3112	1/1	0.96	0.10	44,44,44,44	0
53	MG	2R	201	1/1	0.96	0.18	93,93,93,93	0
53	MG	1A	3374	1/1	0.96	0.12	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3785	1/1	0.96	0.12	82,82,82,82	0
53	MG	1F	304	1/1	0.96	0.18	49,49,49,49	0
53	MG	1A	3706	1/1	0.96	0.08	44,44,44,44	0
53	MG	1A	3053	1/1	0.96	0.15	72,72,72,72	0
53	MG	1A	3586	1/1	0.96	0.08	57,57,57,57	0
53	MG	2A	3052	1/1	0.96	0.09	65,65,65,65	0
53	MG	1A	3789	1/1	0.96	0.08	73,73,73,73	0
53	MG	17	103	1/1	0.96	0.14	66,66,66,66	0
53	MG	2A	3524	1/1	0.96	0.09	90,90,90,90	0
53	MG	1A	3470	1/1	0.96	0.10	39,39,39,39	0
53	MG	1A	3249	1/1	0.96	0.11	58,58,58,58	0
53	MG	1A	3556	1/1	0.96	0.11	49,49,49,49	0
53	MG	1A	3328	1/1	0.96	0.15	56,56,56,56	0
53	MG	1A	3167	1/1	0.96	0.12	80,80,80,80	0
53	MG	1A	3559	1/1	0.96	0.08	47,47,47,47	0
53	MG	2A	3308	1/1	0.96	0.12	92,92,92,92	0
53	MG	1A	3157	1/1	0.96	0.07	75,75,75,75	0
53	MG	1A	3034	1/1	0.96	0.09	34,34,34,34	0
53	MG	1a	1864	1/1	0.96	0.13	113,113,113,113	0
53	MG	1A	3051	1/1	0.96	0.07	37,37,37,37	0
53	MG	1A	3802	1/1	0.96	0.16	54,54,54,54	0
53	MG	18	103	1/1	0.97	0.10	73,73,73,73	0
53	MG	1A	3492	1/1	0.97	0.18	69,69,69,69	0
53	MG	1A	3220	1/1	0.97	0.11	46,46,46,46	0
53	MG	2A	3346	1/1	0.97	0.07	76,76,76,76	0
53	MG	1A	3365	1/1	0.97	0.20	42,42,42,42	0
53	MG	2A	3489	1/1	0.97	0.09	74,74,74,74	0
53	MG	1A	3186	1/1	0.97	0.06	70,70,70,70	0
53	MG	2A	3220	1/1	0.97	0.16	76,76,76,76	0
53	MG	1A	3061	1/1	0.97	0.13	56,56,56,56	0
53	MG	2A	3222	1/1	0.97	0.09	65,65,65,65	0
53	MG	1A	3528	1/1	0.97	0.16	56,56,56,56	0
53	MG	1a	1861	1/1	0.97	0.04	99,99,99,99	0
53	MG	1A	3368	1/1	0.97	0.12	32,32,32,32	0
53	MG	2D	301	1/1	0.97	0.13	68,68,68,68	0
53	MG	1A	3268	1/1	0.97	0.07	41,41,41,41	0
53	MG	1A	3149	1/1	0.97	0.10	55,55,55,55	0
53	MG	1A	3036	1/1	0.97	0.08	57,57,57,57	0
53	MG	1A	3808	1/1	0.97	0.08	59,59,59,59	0
53	MG	1A	3597	1/1	0.97	0.06	41,41,41,41	0
53	MG	1A	3674	1/1	0.97	0.06	45,45,45,45	0
53	MG	1A	3598	1/1	0.97	0.11	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3446	1/1	0.97	0.12	64,64,64,64	0
53	MG	1A	3474	1/1	0.97	0.09	52,52,52,52	0
53	MG	1A	3767	1/1	0.97	0.07	55,55,55,55	0
53	MG	2A	3434	1/1	0.97	0.07	55,55,55,55	0
53	MG	2A	3435	1/1	0.97	0.10	60,60,60,60	0
53	MG	2A	3509	1/1	0.97	0.04	67,67,67,67	0
53	MG	1A	3178	1/1	0.97	0.09	71,71,71,71	0
53	MG	2A	3301	1/1	0.97	0.08	66,66,66,66	0
53	MG	2a	1821	1/1	0.97	0.10	115,115,115,115	0
53	MG	2A	3239	1/1	0.97	0.07	74,74,74,74	0
53	MG	1A	3151	1/1	0.97	0.19	58,58,58,58	0
53	MG	1A	3290	1/1	0.97	0.09	51,51,51,51	0
53	MG	1D	305	1/1	0.97	0.13	45,45,45,45	0
53	MG	1A	3350	1/1	0.97	0.05	52,52,52,52	0
53	MG	2A	3015	1/1	0.97	0.11	69,69,69,69	0
53	MG	1A	3035	1/1	0.97	0.11	57,57,57,57	0
53	MG	1A	3094	1/1	0.97	0.06	51,51,51,51	0
53	MG	1D	309	1/1	0.97	0.08	77,77,77,77	0
53	MG	1A	3378	1/1	0.97	0.09	52,52,52,52	0
53	MG	2A	3021	1/1	0.97	0.07	66,66,66,66	0
53	MG	1A	3071	1/1	0.97	0.11	83,83,83,83	0
53	MG	2A	3251	1/1	0.97	0.08	41,41,41,41	0
53	MG	2A	3252	1/1	0.97	0.15	61,61,61,61	0
53	MG	1A	3646	1/1	0.97	0.05	83,83,83,83	0
53	MG	1A	3085	1/1	0.97	0.05	64,64,64,64	0
53	MG	1A	3381	1/1	0.97	0.11	44,44,44,44	0
53	MG	1A	3514	1/1	0.97	0.07	70,70,70,70	0
53	MG	2A	3531	1/1	0.97	0.09	94,94,94,94	0
53	MG	1A	3691	1/1	0.97	0.07	70,70,70,70	0
53	MG	1A	3334	1/1	0.97	0.19	59,59,59,59	0
53	MG	2A	3259	1/1	0.97	0.08	93,93,93,93	0
53	MG	1E	304	1/1	0.97	0.10	60,60,60,60	0
53	MG	2A	3324	1/1	0.97	0.55	78,78,78,78	0
53	MG	2A	3390	1/1	0.97	0.11	87,87,87,87	0
53	MG	1A	3244	1/1	0.97	0.07	68,68,68,68	0
53	MG	1A	3740	1/1	0.97	0.19	33,33,33,33	0
53	MG	2A	3393	1/1	0.97	0.05	65,65,65,65	0
53	MG	1A	3784	1/1	0.97	0.05	39,39,39,39	0
53	MG	1E	308	1/1	0.97	0.06	67,67,67,67	0
53	MG	1a	1737	1/1	0.97	0.07	114,114,114,114	0
53	MG	1A	3836	1/1	0.97	0.07	34,34,34,34	0
53	MG	1A	3147	1/1	0.97	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
53	MG	2a	1779	1/1	0.97	0.09	109,109,109,109	0
53	MG	2A	3268	1/1	0.97	0.09	44,44,44,44	0
53	MG	1A	3434	1/1	0.97	0.07	67,67,67,67	0
53	MG	1A	3246	1/1	0.97	0.12	46,46,46,46	0
53	MG	1A	3618	1/1	0.97	0.10	60,60,60,60	0
53	MG	1A	3656	1/1	0.97	0.06	83,83,83,83	0
53	MG	1A	3551	1/1	0.97	0.10	66,66,66,66	0
53	MG	1A	3583	1/1	0.97	0.11	61,61,61,61	0
53	MG	2A	3210	1/1	0.97	0.08	62,62,62,62	0
53	MG	1A	3659	1/1	0.97	0.14	56,56,56,56	0
53	MG	1A	3262	1/1	0.97	0.07	36,36,36,36	0
53	MG	1A	3247	1/1	0.97	0.14	55,55,55,55	0
58	SF4	1d	501	8/8	0.97	0.07	116,146,171,175	0
58	SF4	2d	501	8/8	0.97	0.06	118,150,171,175	0
53	MG	2A	3237	1/1	0.98	0.13	54,54,54,54	0
53	MG	2A	3045	1/1	0.98	0.08	92,92,92,92	0
53	MG	1A	3709	1/1	0.98	0.05	30,30,30,30	0
53	MG	1A	3202	1/1	0.98	0.13	49,49,49,49	0
53	MG	1A	3063	1/1	0.98	0.14	84,84,84,84	0
53	MG	2A	3548	1/1	0.98	0.04	77,77,77,77	0
53	MG	1A	3642	1/1	0.98	0.06	77,77,77,77	0
53	MG	1a	1894	1/1	0.98	0.05	53,53,53,53	0
53	MG	2A	3202	1/1	0.98	0.09	54,54,54,54	0
53	MG	1A	3228	1/1	0.98	0.15	28,28,28,28	0
53	MG	1A	3340	1/1	0.98	0.05	38,38,38,38	0
53	MG	2A	3016	1/1	0.98	0.11	105,105,105,105	0
53	MG	1A	3353	1/1	0.98	0.11	63,63,63,63	0
53	MG	2a	1834	1/1	0.98	0.15	46,46,46,46	0
53	MG	1A	3297	1/1	0.98	0.10	65,65,65,65	0
53	MG	1A	3743	1/1	0.98	0.07	103,103,103,103	0
53	MG	1A	3355	1/1	0.98	0.04	47,47,47,47	0
53	MG	2A	3466	1/1	0.98	0.07	61,61,61,61	0
53	MG	1A	3692	1/1	0.98	0.04	53,53,53,53	0
53	MG	2A	3211	1/1	0.98	0.10	62,62,62,62	0
53	MG	1A	3719	1/1	0.98	0.04	73,73,73,73	0
53	MG	1a	1800	1/1	0.98	0.08	59,59,59,59	0
53	MG	1A	3831	1/1	0.98	0.10	41,41,41,41	0
53	MG	1A	3587	1/1	0.98	0.10	50,50,50,50	0
53	MG	1A	3183	1/1	0.98	0.08	85,85,85,85	0
53	MG	1A	3135	1/1	0.98	0.16	45,45,45,45	0
53	MG	2A	3521	1/1	0.98	0.12	79,79,79,79	0
53	MG	1A	3500	1/1	0.98	0.07	65,65,65,65	0

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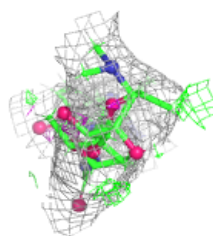
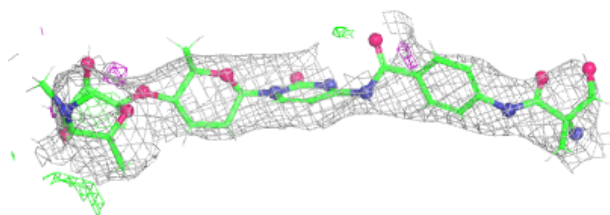
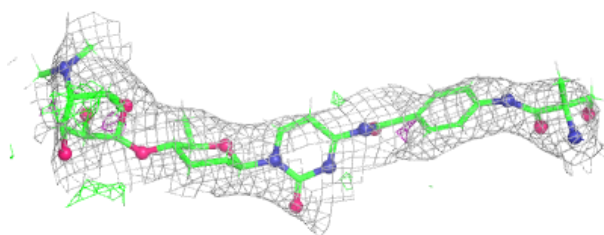
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	MG	1A	3076	1/1	0.98	0.07	78,78,78,78	0
53	MG	2A	3478	1/1	0.98	0.05	81,81,81,81	0
53	MG	1A	3359	1/1	0.98	0.10	65,65,65,65	0
53	MG	1A	3291	1/1	0.98	0.06	37,37,37,37	0
53	MG	1A	3677	1/1	0.98	0.07	42,42,42,42	0
53	MG	1A	3267	1/1	0.98	0.06	25,25,25,25	0
53	MG	1A	3115	1/1	0.98	0.05	45,45,45,45	0
53	MG	2A	3394	1/1	0.98	0.09	105,105,105,105	0
53	MG	2E	301	1/1	0.98	0.07	52,52,52,52	0
53	MG	1A	3813	1/1	0.98	0.11	37,37,37,37	0
53	MG	1D	310	1/1	0.98	0.06	92,92,92,92	0
53	MG	1a	1749	1/1	0.98	0.12	95,95,95,95	0
53	MG	1A	3814	1/1	0.98	0.06	44,44,44,44	0
53	MG	1a	1816	1/1	0.98	0.06	125,125,125,125	0
53	MG	1A	3523	1/1	0.98	0.06	59,59,59,59	0
53	MG	1A	3408	1/1	0.98	0.11	85,85,85,85	0
53	MG	1A	3314	1/1	0.98	0.06	62,62,62,62	0
57	ZN	15	101	1/1	0.98	0.09	74,74,74,74	0
57	ZN	26	501	1/1	0.98	0.07	118,118,118,118	0
53	MG	2A	3192	1/1	0.98	0.14	68,68,68,68	0
53	MG	2A	3193	1/1	0.98	0.05	75,75,75,75	0
53	MG	1A	3599	1/1	0.98	0.14	57,57,57,57	0
53	MG	1B	208	1/1	0.98	0.08	43,43,43,43	0
53	MG	1A	3720	1/1	0.99	0.04	61,61,61,61	0
53	MG	2U	201	1/1	0.99	0.06	79,79,79,79	0
53	MG	1A	3809	1/1	0.99	0.06	47,47,47,47	0
53	MG	2A	3470	1/1	0.99	0.06	73,73,73,73	0
53	MG	1A	3673	1/1	0.99	0.04	48,48,48,48	0
53	MG	2A	3238	1/1	0.99	0.07	74,74,74,74	0
53	MG	2A	3182	1/1	0.99	0.04	86,86,86,86	0
57	ZN	1Y	501	1/1	0.99	0.06	97,97,97,97	0
53	MG	1A	3467	1/1	0.99	0.07	30,30,30,30	0
57	ZN	16	501	1/1	0.99	0.08	68,68,68,68	0
57	ZN	19	102	1/1	0.99	0.10	67,67,67,67	0
57	ZN	2Y	501	1/1	0.99	0.04	143,143,143,143	0
57	ZN	25	102	1/1	0.99	0.11	103,103,103,103	0
53	MG	1D	302	1/1	0.99	0.12	58,58,58,58	0
53	MG	1A	3060	1/1	0.99	0.06	45,45,45,45	0
53	MG	1A	3694	1/1	0.99	0.06	72,72,72,72	0
53	MG	2A	3397	1/1	0.99	0.11	81,81,81,81	0
53	MG	2a	1780	1/1	0.99	0.04	74,74,74,74	0
53	MG	1A	3695	1/1	1.00	0.05	36,36,36,36	0

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

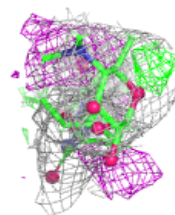
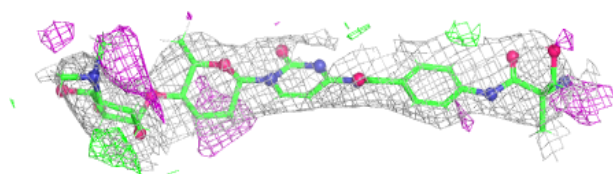
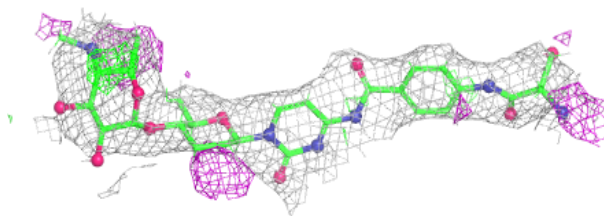
Electron density around FSD 2A 3553:

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



Electron density around FSD 1A 3801:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.