wwPDB X-ray Structure Validation Summary Report (i)

Sep 2, 2026 – 08:23 PM EDT

PDB ID	:	9Q6R / pdb_00009q6r
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with pleuromutilin-27 triazole derivative and protein Y at 2.85A resolution
Authors	:	Killam, B.Y.; Kopec, I.; Breiner, L.M.; Hoernig, M.; LoPresti, M.; Abdelsattar, A.S.; Abouelkhair, A.A.; Briganti, A.J.; Slowinski, R.P.; Vogelaar, N.J.; Seleem, M.N.; Brown, A.M.; Lowell, A.N.; Polikanov, Y.S.
Deposited on	:	2025-08-22
Resolution	:	2.85 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

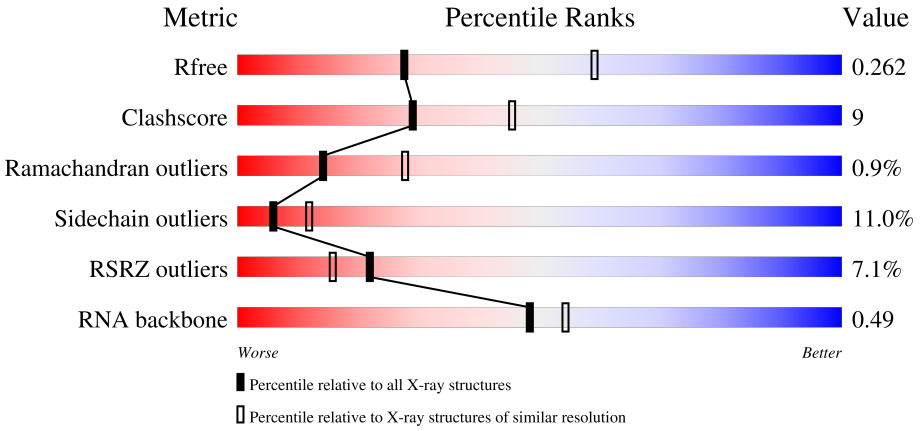
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)
RNA backbone	3983	1009 (3.06-2.66)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	5% 65% 28% 6%
1	2A	2915	6% 60% 32% 7%
2	1B	121	% 72% 26%
2	2B	121	3% 50% 41% 8%

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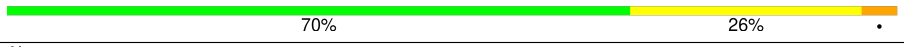
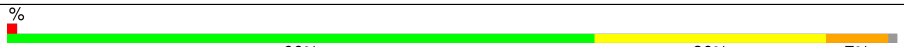
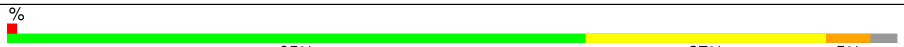
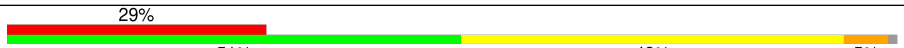
Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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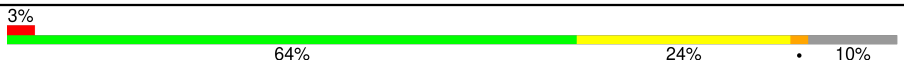
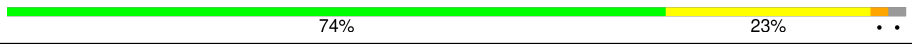
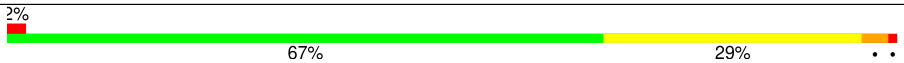
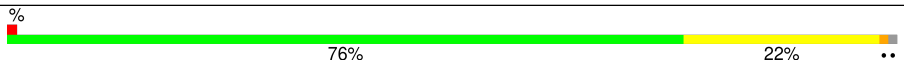
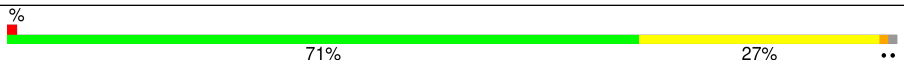
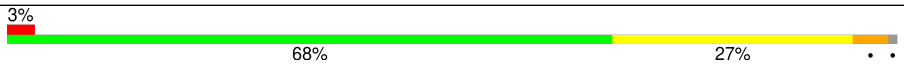
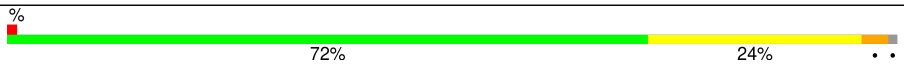
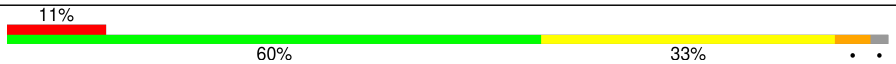
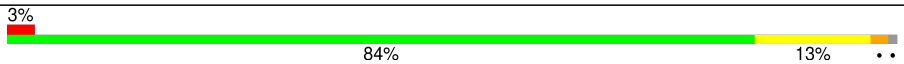
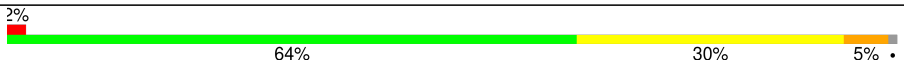
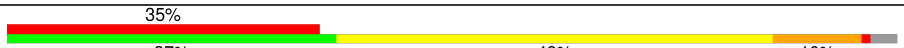
Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	

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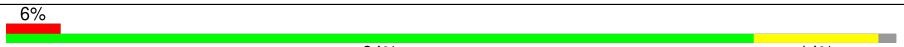
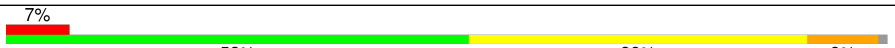
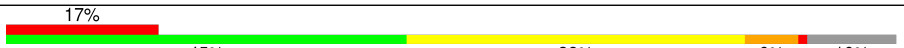
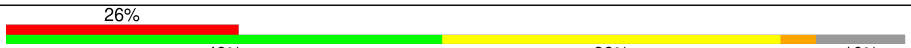
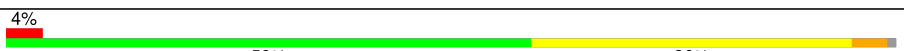
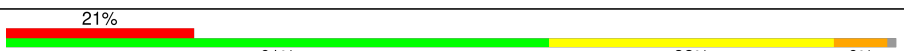
Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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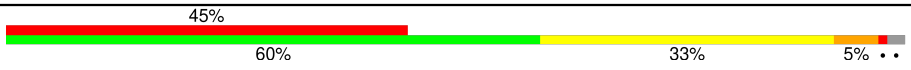
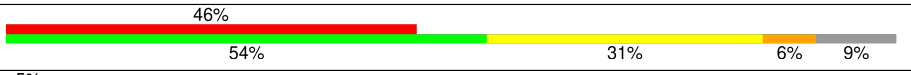
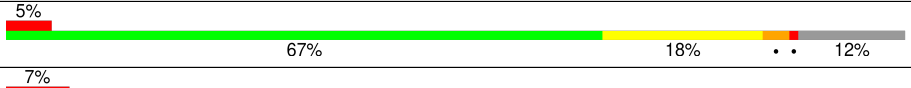
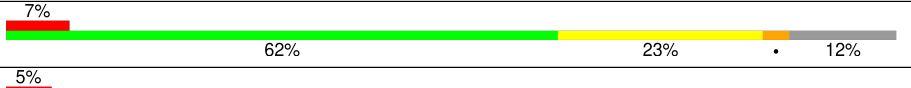
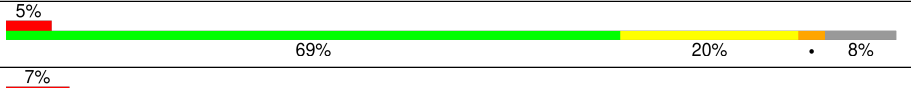
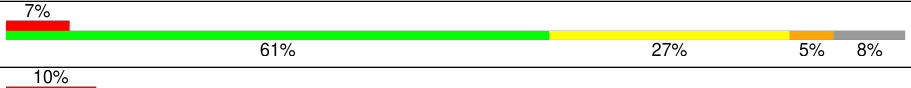
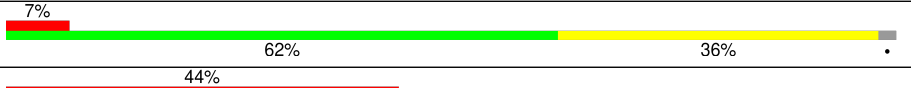
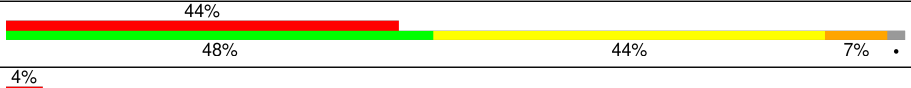
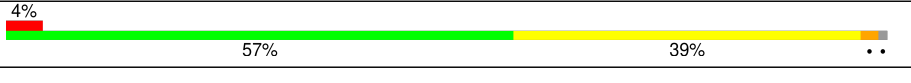
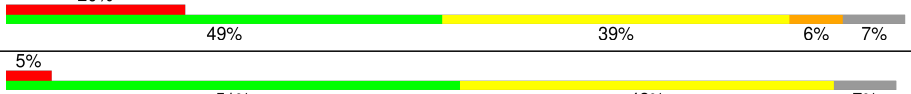
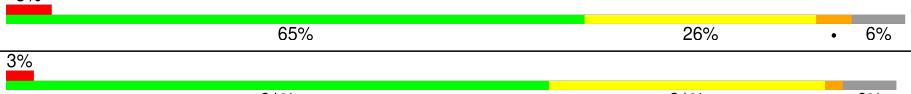
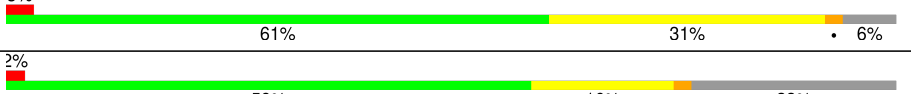
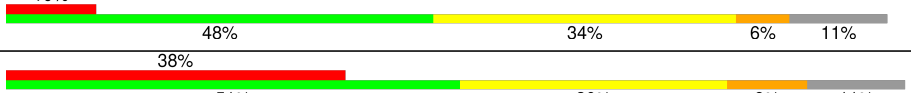
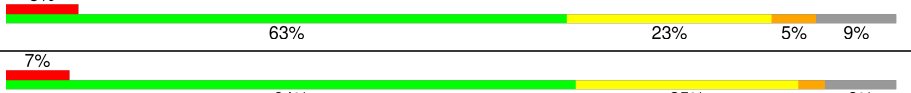
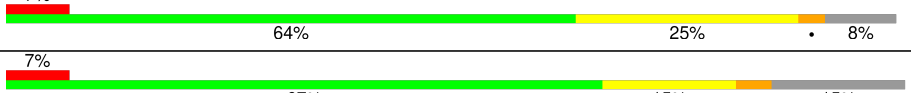
Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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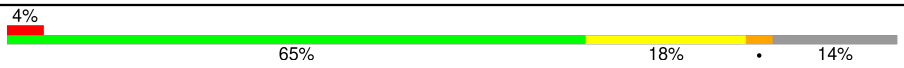
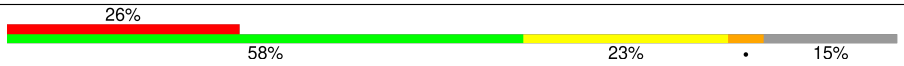
Mol	Chain	Length	Quality of chain
53	1y	113	
53	2y	113	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	1A	3283	-	-	-	X
54	MG	1A	3630	-	-	-	X
54	MG	2A	3697	-	-	-	X
54	MG	2a	3164	-	-	-	X
59	SF4	2d	501	-	-	X	-

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 297568 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1010	Total 1010	Mg 1010	0	0
54	1B	31	Total 31	Mg 31	0	0
54	1D	18	Total 18	Mg 18	0	0
54	1E	9	Total 9	Mg 9	0	0
54	1F	17	Total 17	Mg 17	0	0
54	1G	4	Total 4	Mg 4	0	0
54	1H	2	Total 2	Mg 2	0	0
54	1N	4	Total 4	Mg 4	0	0
54	1O	1	Total 1	Mg 1	0	0
54	1P	7	Total 7	Mg 7	0	0
54	1Q	5	Total 5	Mg 5	0	0
54	1R	9	Total 9	Mg 9	0	0
54	1T	4	Total 4	Mg 4	0	0
54	1U	6	Total 6	Mg 6	0	0
54	1V	7	Total 7	Mg 7	0	0
54	1W	3	Total 3	Mg 3	0	0
54	1Y	1	Total 1	Mg 1	0	0
54	1Z	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	10	7	Total Mg 7 7	0	0
54	11	5	Total Mg 5 5	0	0
54	13	4	Total Mg 4 4	0	0
54	14	1	Total Mg 1 1	0	0
54	15	8	Total Mg 8 8	0	0
54	17	5	Total Mg 5 5	0	0
54	18	3	Total Mg 3 3	0	0
54	19	3	Total Mg 3 3	0	0
54	1a	277	Total Mg 277 277	0	0
54	1b	1	Total Mg 1 1	0	0
54	1d	5	Total Mg 5 5	0	0
54	1e	2	Total Mg 2 2	0	0
54	1f	2	Total Mg 2 2	0	0
54	1g	3	Total Mg 3 3	0	0
54	1h	2	Total Mg 2 2	0	0
54	1i	1	Total Mg 1 1	0	0
54	1k	1	Total Mg 1 1	0	0
54	1l	3	Total Mg 3 3	0	0
54	1m	1	Total Mg 1 1	0	0
54	1n	2	Total Mg 2 2	0	0
54	1o	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1t	2	Total Mg 2 2	0	0
54	1y	3	Total Mg 3 3	0	0
54	2A	740	Total Mg 740 740	0	0
54	2B	20	Total Mg 20 20	0	0
54	2D	6	Total Mg 6 6	0	0
54	2E	7	Total Mg 7 7	0	0
54	2F	4	Total Mg 4 4	0	0
54	2G	3	Total Mg 3 3	0	0
54	2I	1	Total Mg 1 1	0	0
54	2O	1	Total Mg 1 1	0	0
54	2P	3	Total Mg 3 3	0	0
54	2Q	4	Total Mg 4 4	0	0
54	2R	2	Total Mg 2 2	0	0
54	2T	4	Total Mg 4 4	0	0
54	2U	1	Total Mg 1 1	0	0
54	2V	3	Total Mg 3 3	0	0
54	2W	3	Total Mg 3 3	0	0
54	2X	1	Total Mg 1 1	0	0
54	2Y	1	Total Mg 1 1	0	0
54	20	2	Total Mg 2 2	0	0
54	21	3	Total Mg 3 3	0	0

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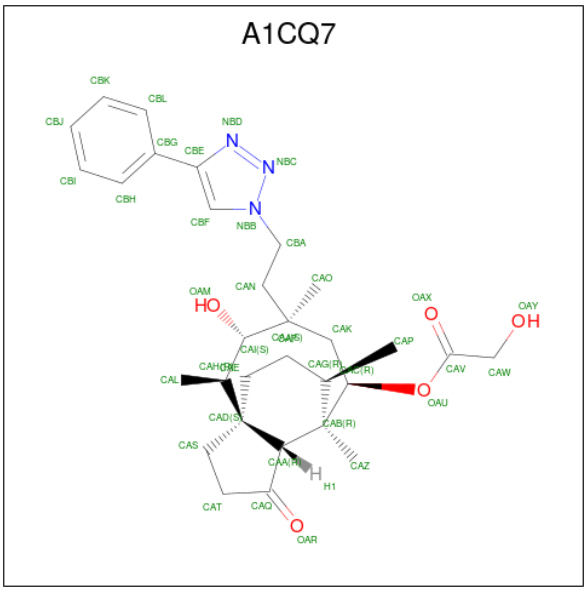
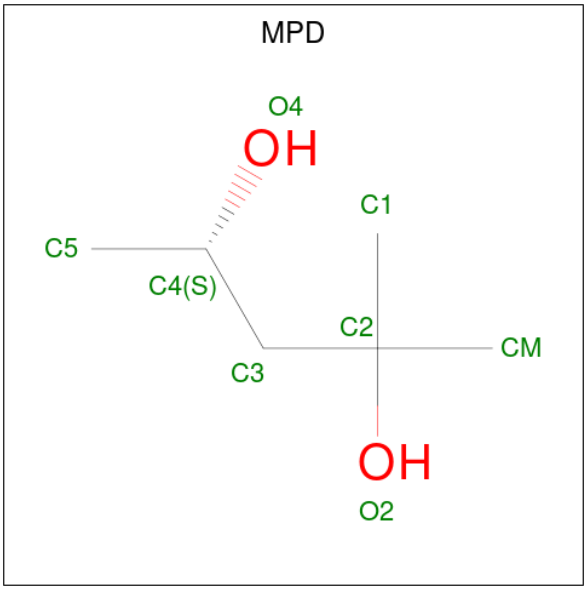
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	23	1	Total Mg 1 1	0	0
54	25	1	Total Mg 1 1	0	0
54	26	2	Total Mg 2 2	0	0
54	28	1	Total Mg 1 1	0	0
54	29	1	Total Mg 1 1	0	0
54	2a	187	Total Mg 187 187	0	0
54	2e	1	Total Mg 1 1	0	0
54	2f	1	Total Mg 1 1	0	0
54	2h	1	Total Mg 1 1	0	0
54	2j	1	Total Mg 1 1	0	0
54	2k	2	Total Mg 2 2	0	0
54	2l	1	Total Mg 1 1	0	0
54	2n	1	Total Mg 1 1	0	0
54	2p	1	Total Mg 1 1	0	0
54	2t	1	Total Mg 1 1	0	0

- Molecule 55 is (3aS,4R,5S,6S,8R,9R,9aR,10R)-5-hydroxy-4,6,9,10-tetramethyl-1-oxo-6-[2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethyl]decahydro-3a,9-propanocyclopenta[8]annulen-8-yl hydroxyacetate (CCD ID: A1CQ7) (formula: $C_{30}H_{41}N_3O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1A	1	Total C N O 38 30 3 5	0	0
55	2A	1	Total C N O 38 30 3 5	0	0

- Molecule 56 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1A	1	Total C O 8 6 2	0	0
56	1T	1	Total C O 8 6 2	0	0

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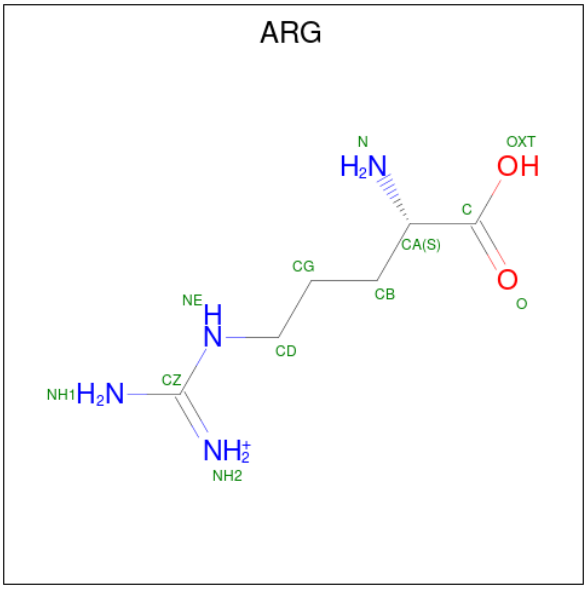
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	18	1	Total C O 8 6 2	0	0
56	1a	1	Total C O 8 6 2	0	0
56	2A	1	Total C O 8 6 2	0	0
56	2A	1	Total C O 8 6 2	0	0
56	2B	1	Total C O 8 6 2	0	0

- Molecule 57 is ARGININE (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1B	1	Total C N O 12 6 4 2	0	0
57	1F	1	Total C N O 12 6 4 2	0	0

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

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

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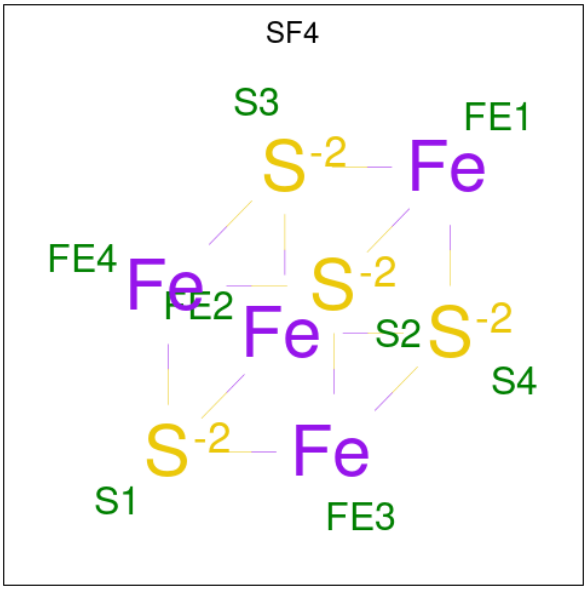
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	15	1	Total Zn 1 1	0	0
58	16	1	Total Zn 1 1	0	0
58	19	1	Total Zn 1 1	0	0
58	1n	1	Total Zn 1 1	0	0
58	2Y	1	Total Zn 1 1	0	0
58	24	1	Total Zn 1 1	0	0
58	25	1	Total Zn 1 1	0	0
58	26	1	Total Zn 1 1	0	0
58	29	1	Total Zn 1 1	0	0
58	2n	1	Total Zn 1 1	0	0

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



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

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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	3924	Total O 3924 3924	0	0
60	1B	103	Total O 103 103	0	0
60	1D	114	Total O 114 114	0	0
60	1E	82	Total O 82 82	0	0
60	1F	72	Total O 72 72	0	0
60	1G	16	Total O 16 16	0	0
60	1H	19	Total O 19 19	0	0
60	1I	8	Total O 8 8	0	0
60	1N	54	Total O 54 54	0	0
60	1O	26	Total O 26 26	0	0
60	1P	63	Total O 63 63	0	0
60	1Q	39	Total O 39 39	0	0
60	1R	32	Total O 32 32	0	0
60	1S	8	Total O 8 8	0	0
60	1T	39	Total O 39 39	0	0
60	1U	47	Total O 47 47	0	0
60	1V	37	Total O 37 37	0	0
60	1W	27	Total O 27 27	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1X	21	Total O 21 21	0	0
60	1Y	19	Total O 19 19	0	0
60	1Z	14	Total O 14 14	0	0
60	10	27	Total O 27 27	0	0
60	11	23	Total O 23 23	0	0
60	12	18	Total O 18 18	0	0
60	13	25	Total O 25 25	0	0
60	14	2	Total O 2 2	0	0
60	15	25	Total O 25 25	0	0
60	16	21	Total O 21 21	0	0
60	17	14	Total O 14 14	0	0
60	18	32	Total O 32 32	0	0
60	19	10	Total O 10 10	0	0
60	1a	576	Total O 576 576	0	0
60	1b	1	Total O 1 1	0	0
60	1d	11	Total O 11 11	0	0
60	1e	10	Total O 10 10	0	0
60	1f	1	Total O 1 1	0	0
60	1j	2	Total O 2 2	0	0
60	1l	5	Total O 5 5	0	0
60	1m	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1o	4	Total O 4 4	0	0
60	1p	4	Total O 4 4	0	0
60	1t	2	Total O 2 2	0	0
60	1y	4	Total O 4 4	0	0
60	2A	2074	Total O 2074 2074	0	0
60	2B	44	Total O 44 44	0	0
60	2D	55	Total O 55 55	0	0
60	2E	37	Total O 37 37	0	0
60	2F	26	Total O 26 26	0	0
60	2G	7	Total O 7 7	0	0
60	2H	3	Total O 3 3	0	0
60	2I	3	Total O 3 3	0	0
60	2N	7	Total O 7 7	0	0
60	2O	19	Total O 19 19	0	0
60	2P	23	Total O 23 23	0	0
60	2Q	19	Total O 19 19	0	0
60	2R	19	Total O 19 19	0	0
60	2S	4	Total O 4 4	0	0
60	2T	9	Total O 9 9	0	0
60	2U	13	Total O 13 13	0	0
60	2V	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2W	18	Total O 18 18	0	0
60	2X	7	Total O 7 7	0	0
60	2Y	3	Total O 3 3	0	0
60	2Z	14	Total O 14 14	0	0
60	20	6	Total O 6 6	0	0
60	21	17	Total O 17 17	0	0
60	22	1	Total O 1 1	0	0
60	23	3	Total O 3 3	0	0
60	24	2	Total O 2 2	0	0
60	25	8	Total O 8 8	0	0
60	26	6	Total O 6 6	0	0
60	27	7	Total O 7 7	0	0
60	28	14	Total O 14 14	0	0
60	29	1	Total O 1 1	0	0
60	2a	438	Total O 438 438	0	0
60	2d	4	Total O 4 4	0	0
60	2e	1	Total O 1 1	0	0
60	2f	1	Total O 1 1	0	0
60	2j	2	Total O 2 2	0	0
60	2l	6	Total O 6 6	0	0
60	2m	1	Total O 1 1	0	0

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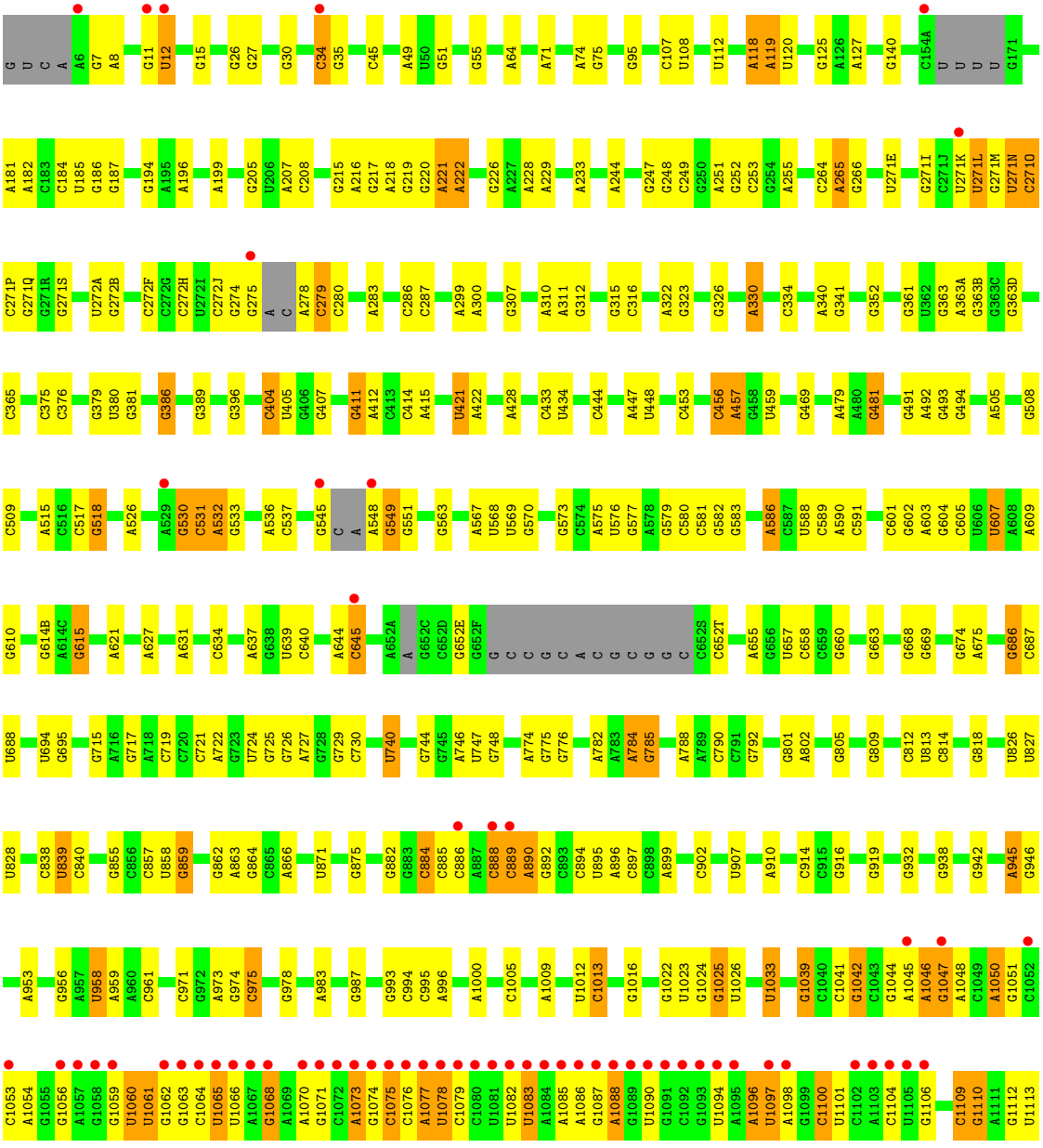
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2n	1	Total O 1 1	0	0
60	2o	3	Total O 3 3	0	0
60	2p	2	Total O 2 2	0	0
60	2q	1	Total O 1 1	0	0
60	2r	4	Total O 4 4	0	0
60	2t	2	Total O 2 2	0	0
60	2y	4	Total O 4 4	0	0

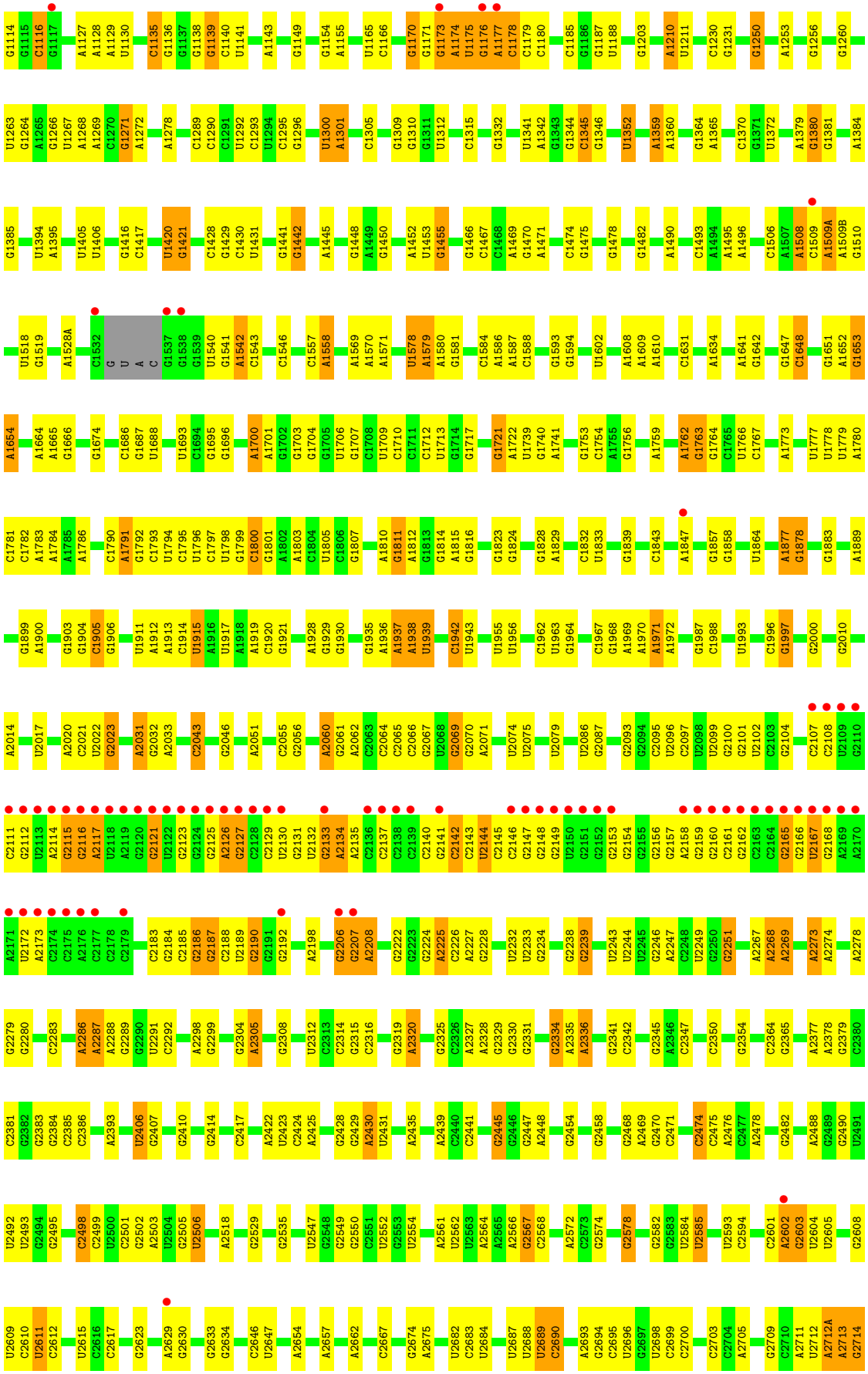
3 Residue-property plots (i)

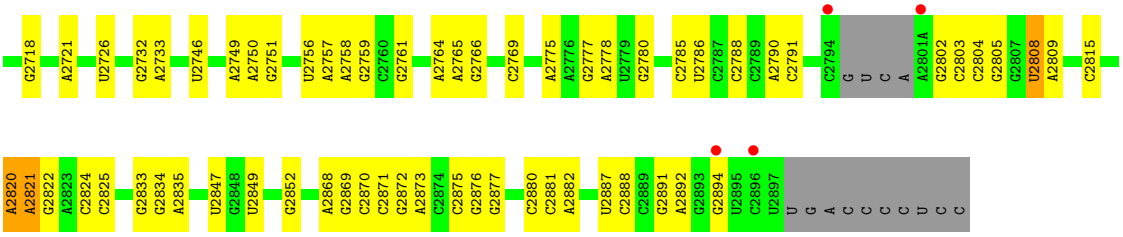
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S Ribosomal RNA

Chain 1A:

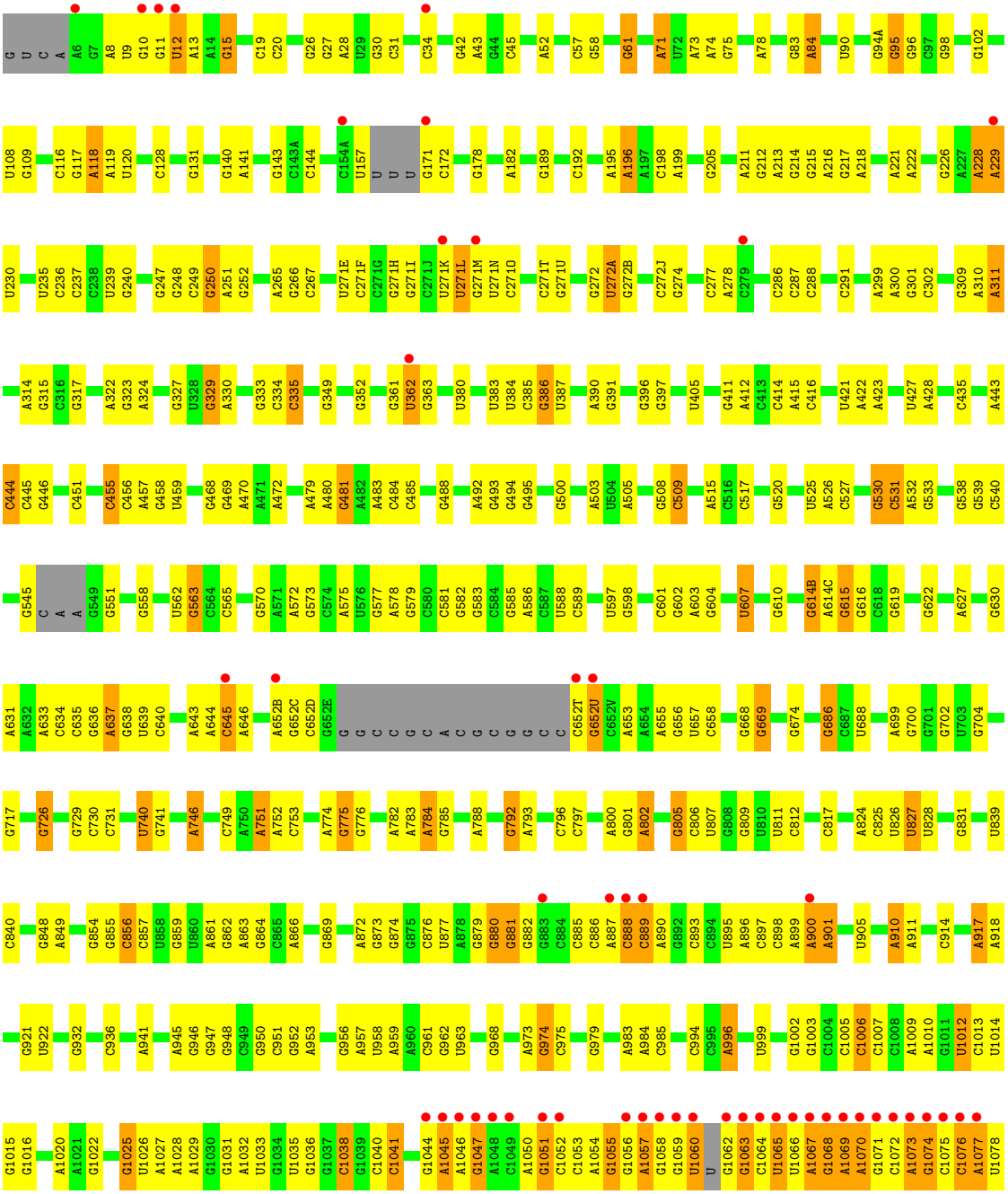


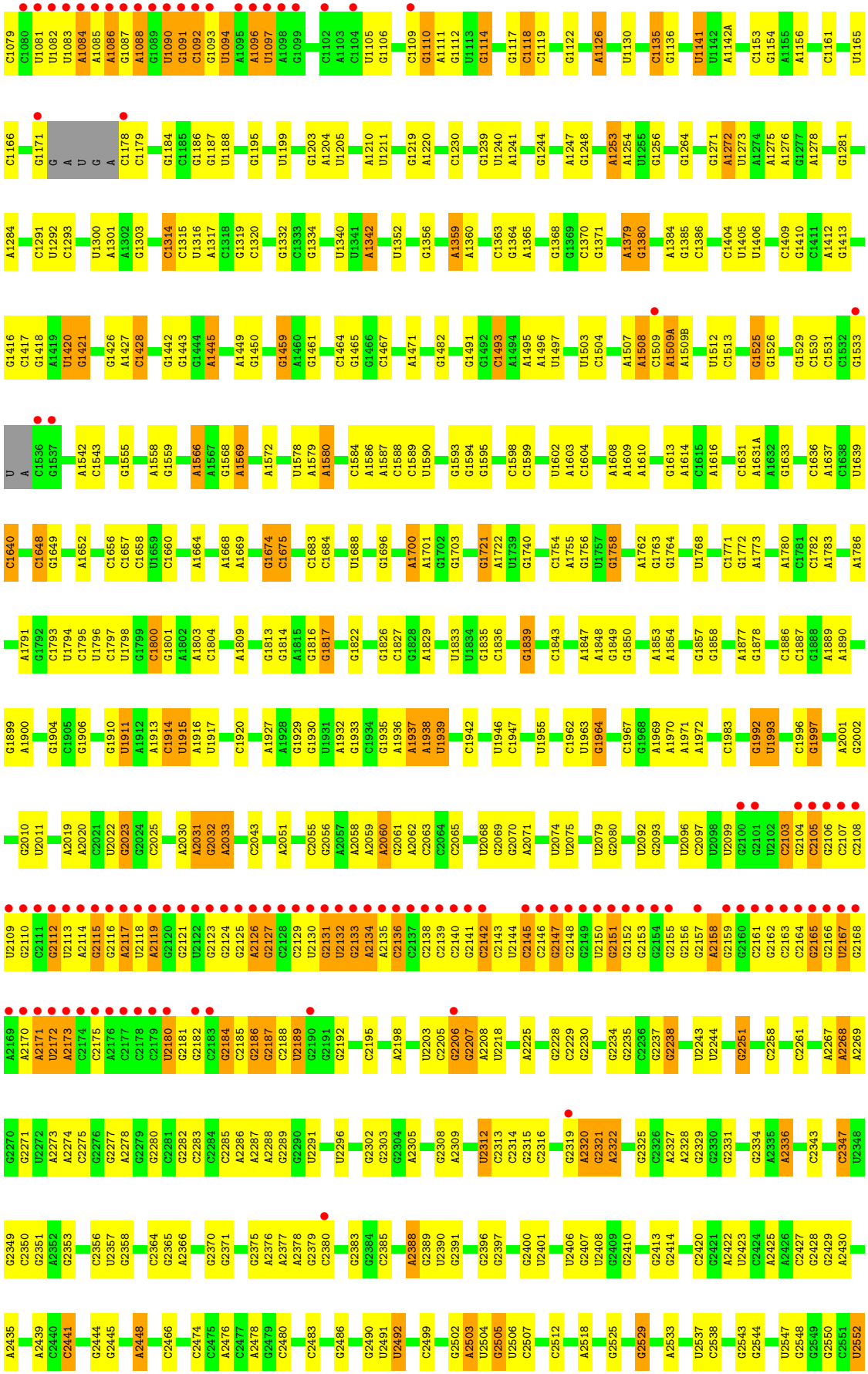


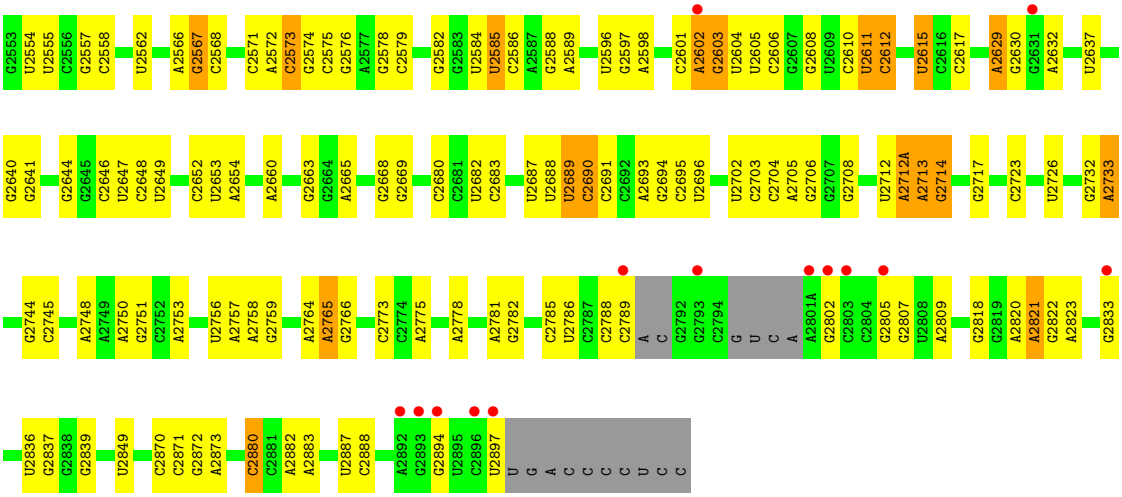


• Molecule 1: 23S Ribosomal RNA

Chain 2A:

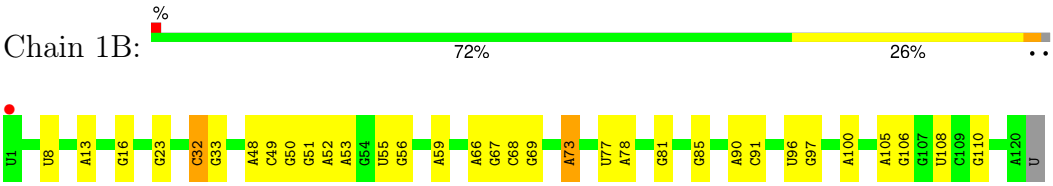



C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1102 A1103 C1104 U1105 G1106 C1109 G1110 A1111 G1112 U1113 G1114 G1117 C1118 C1119 G1122 A1126 U1130 C1135 G1136 U1141 U1142 A1142A C1153 G1154 A1155 A1156 C1161 U1165
C1166 G1171 G A U G A C1178 C1179 G1184 C1185 G1186 G1187 U1188 G1195 U1199 G1203 A1204 U1205 A1210 U1211 G1219 A1220 C1230 G1239 U1240 A1241 G1244 A1247 G1248 A1253 A1254 U1255 G1256 G1264 G1271 A1272 U1273 A1274 A1275 A1276 G1277 A1278 G1281
A1284 C1291 U1292 C1293 U1300 A1301 A1302 G1303 C1314 C1315 U1316 A1317 C1318 G1319 C1320 G1332 C1333 G1334 U1340 U1341 A1342 U1352 G1356 A1359 A1360 C1363 G1364 A1365 G1368 G1369 C1370 G1371 A1379 G1380 A1384 G1385 C1386 C1404 U1405 U1406 C1409 G1410 C1411 A1412 G1413
G1416 C1417 G1418 A1419 U1420 G1421 G1426 A1427 C1428 G1442 G1443 G1444 A1445 A1449 G1450 G1459 A1460 G1461 C1464 G1465 G1466 C1467 A1471 G1482 G1491 G1492 C1493 A1494 A1495 A1496 U1497 U1503 C1504 A1507 A1508 C1509 A1509A A1509B U1512 C1513 G1525 G1526 G1529 C1530 C1531 C1532 G1533
U A C1536 G1537 A1542 C1543 G1555 A1558 G1559 A1566 A1567 G1568 A1569 A1572 U1578 A1579 A1580 C1584 A1586 A1587 C1588 C1589 U1590 G1593 G1594 G1595 C1598 C1599 U1602 A1603 C1604 A1608 A1609 A1610 G1613 A1614 C1615 A1616 C1631 A1631A A1632 G1633 C1636 A1637 C1638 U1639
C1640 C1648 G1649 A1652 C1656 C1657 C1658 U1659 C1660 A1664 A1668 A1669 G1674 C1675 C1683 C1684 U1688 G1696 A1700 A1701 G1702 G1703 G1721 A1722 U1739 G1740 C1754 A1755 G1756 U1757 G1758 A1762 G1763 G1764 U1768 C1771 G1772 A1773 A1780 C1781 C1782 A1783 A1786
A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 A1809 G1813 G1814 A1815 G1816 G1817 G1822 G1826 C1827 G1828 A1829 U1833 U1834 G1835 C1836 G1839 C1843 A1847 A1848 G1849 G1850 A1853 A1854 G1857 G1858 A1877 G1878 C1886 C1887 G1888 A1889 A1890
G1899 A1900 G1904 C1905 G1906 G1910 U1911 A1912 A1913 C1914 U1915 A1916 U1917 C1920 A1927 A1928 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 C1942 U1946 C1947 U1955 C1962 U1963 G1964 C1967 G1968 A1969 A1970 A1971 A1972 C1983 G1992 U1993 C1996 G1997 A2001 G2002
G2010 U2011 A2019 A2020 C2021 U2022 G2023 G2024 C2025 A2030 A2031 G2032 A2033 C2043 A2051 C2055 G2056 A2057 A2058 A2059 A2060 G2061 A2062 C2063 C2064 C2065 U2068 G2069 G2070 A2071 U2074 U2075 U2079 G2080 U2092 G2093 U2096 C2097 U2098 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108
U2109 G2110 C2111 G2112 U2113 A2114 G2115 C2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168
A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 C2192 C2195 A2198 U2203 C2205 G2206 G2207 A2208 U2218 A2225 G2228 C2229 G2230 G2234 G2235 C2236 G2237 G2238 U2243 U2244 G2251 C2258 C2261 A2267 A2268 A2269
G2270 G2271 U2272 A2273 A2274 C2275 G2276 G2277 A2278 G2279 G2280 C2281 G2282 C2283 C2284 C2285 A2286 A2287 A2288 G2289 G2290 U2291 U2296 G2302 G2303 G2304 A2305 G2308 A2309 U2312 C2313 C2314 G2315 C2316 G2319 A2320 G2321 A2322 G2325 C2326 A2327 A2328 G2329 G2330 G2331 G2334 A2335 A2336 C2343 C2347 U2348
G2349 C2350 C2351 A2352 G2353 C2356 U2357 C2358 C2364 G2365 A2366 G2370 G2371 C2375 A2376 A2377 A2378 G2379 C2380 G2383 G2384 C2385 A2388 G2389 U2390 G2391 G2396 G2397 G2400 U2401 U2406 G2407 U2408 G2409 G2410 G2413 G2414 C2420 G2421 A2422 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430
A2435 A2439 C2440 C2441 G2444 G2445 A2448 C2466 C2474 C2475 A2476 C2477 A2478 G2479 C2480 C2483 G2486 G2490 U2491 U2492 C2499 G2502 A2503 U2504 G2505 U2506 C2507 C2512 A2518 G2525 G2529 A2533 U2537 C2538 G2543 G2544 U2547 G2548 G2549 G2550 C2551 U2552



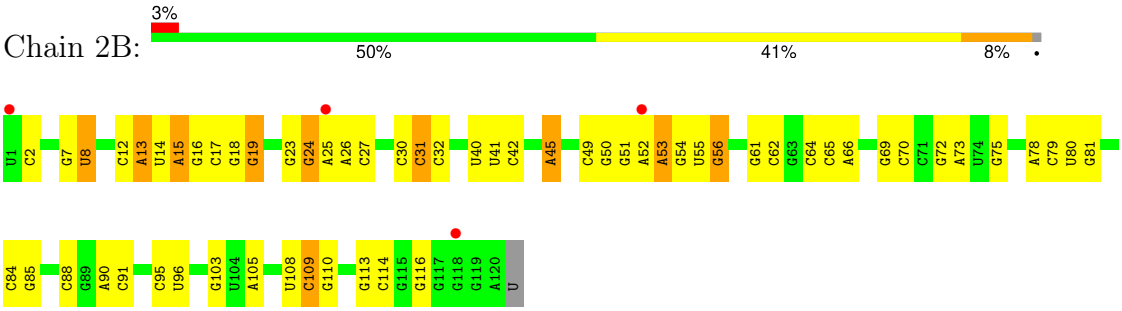
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



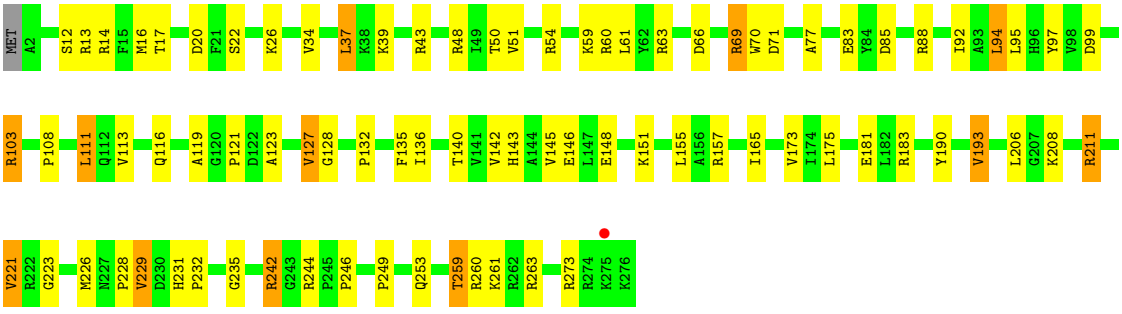
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



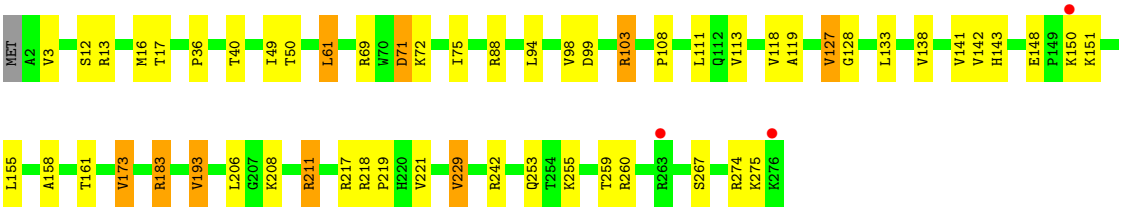
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



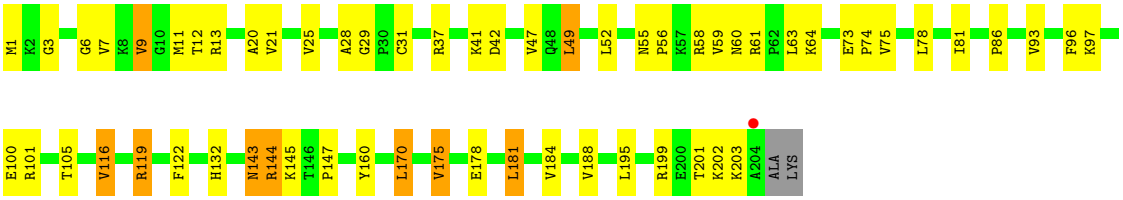
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



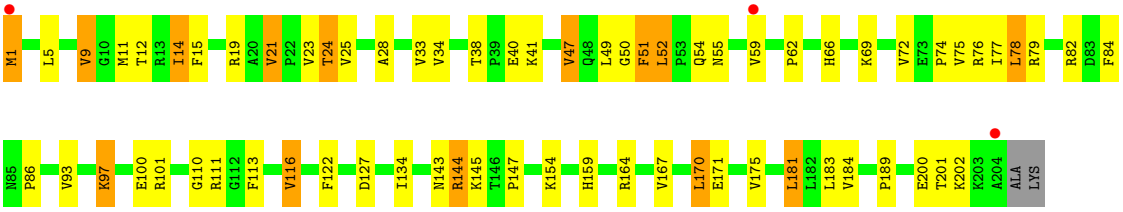
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



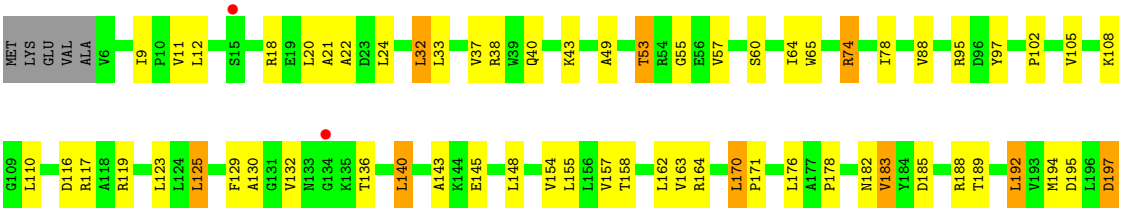
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



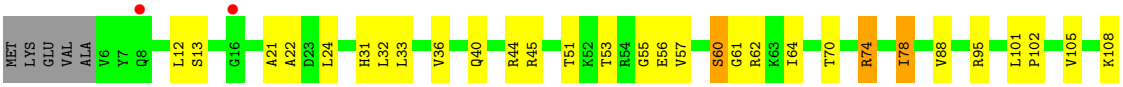
• Molecule 5: 50S ribosomal protein L4

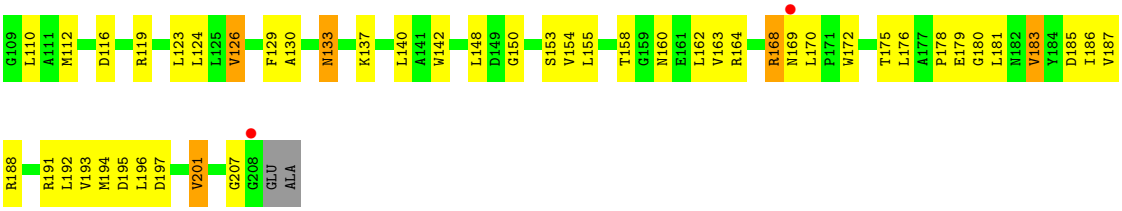
Chain 1F:



• Molecule 5: 50S ribosomal protein L4

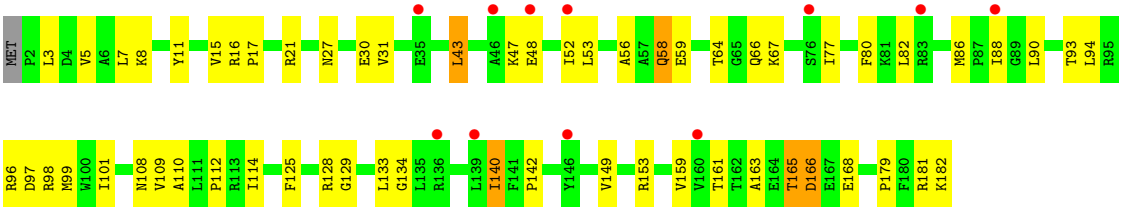
Chain 2F:





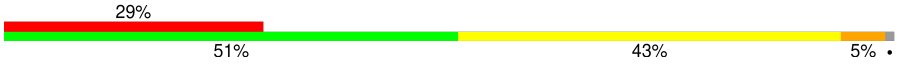
• Molecule 6: 50S ribosomal protein L5

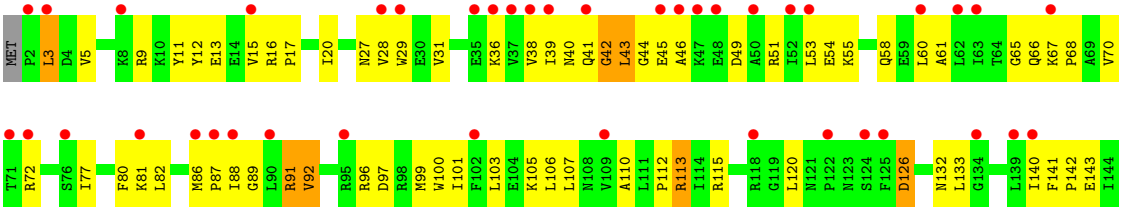
Chain 1G:



• Molecule 6: 50S ribosomal protein L5

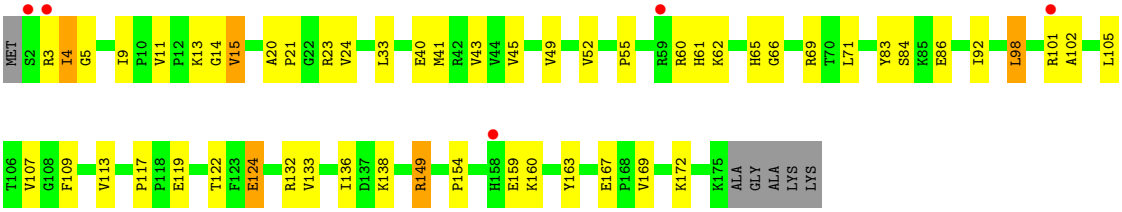
Chain 2G:





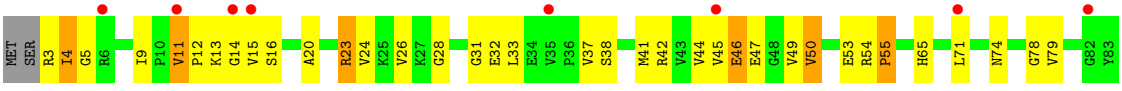
• Molecule 7: 50S ribosomal protein L6

Chain 1H:

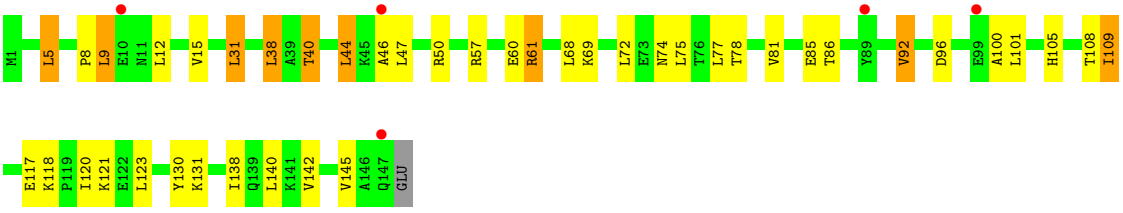


• Molecule 7: 50S ribosomal protein L6

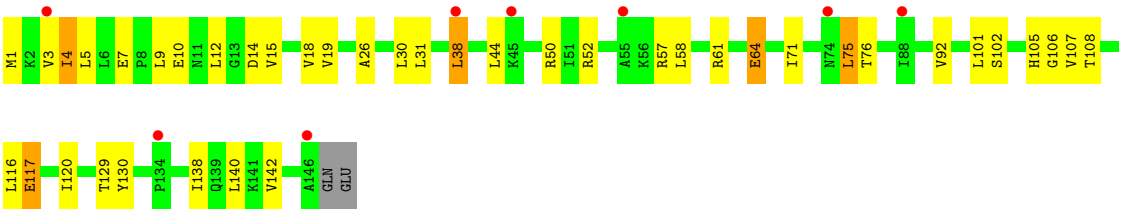
Chain 2H:



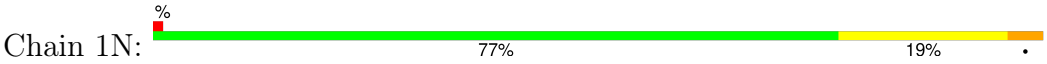
• Molecule 8: 50S ribosomal protein L9



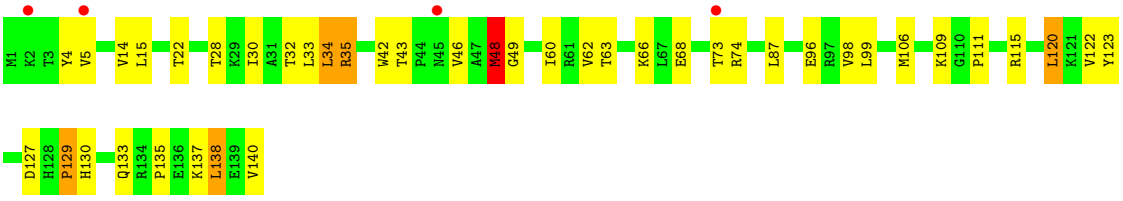
• Molecule 8: 50S ribosomal protein L9



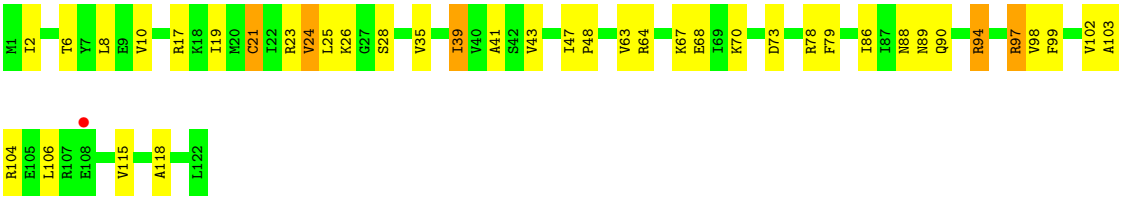
• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13

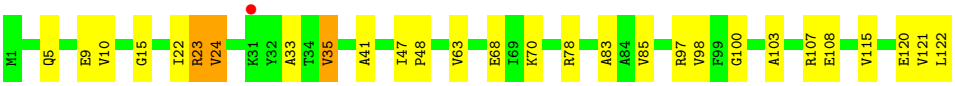


• Molecule 10: 50S ribosomal protein L14



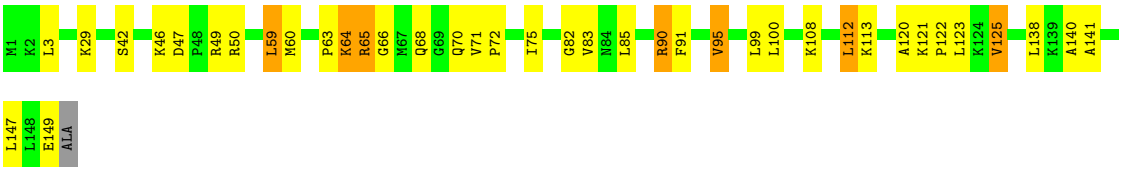
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



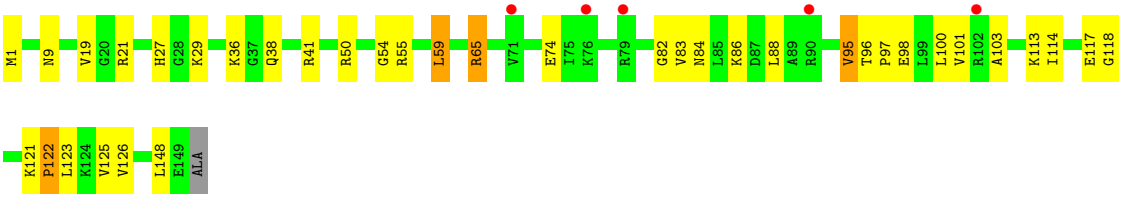
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



• Molecule 11: 50S ribosomal protein L15

Chain 2P:



• Molecule 12: 50S ribosomal protein L16

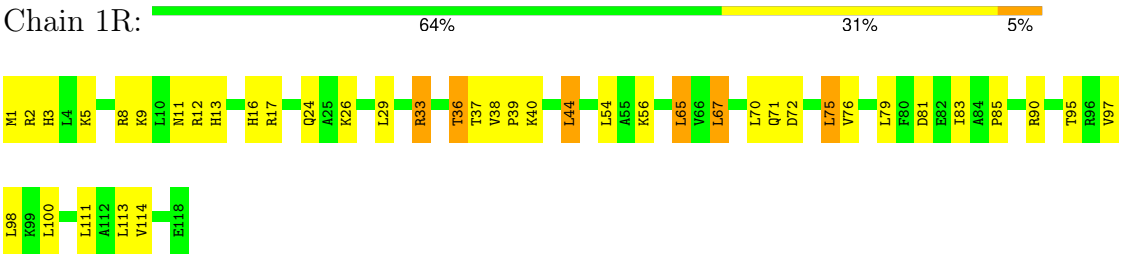
Chain 1Q:

• Molecule 12: 50S ribosomal protein L16

Chain 2Q:

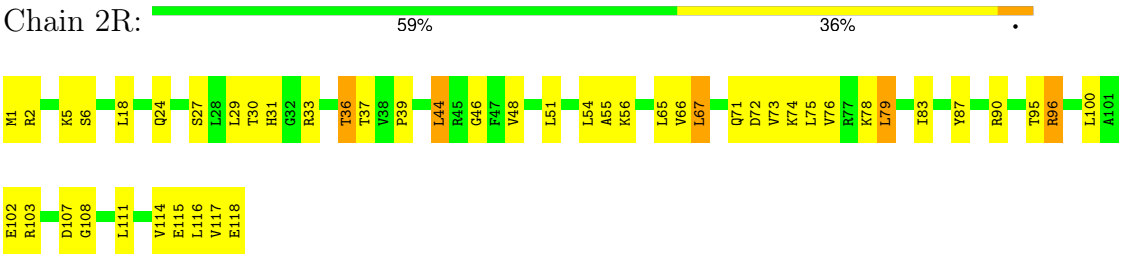
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



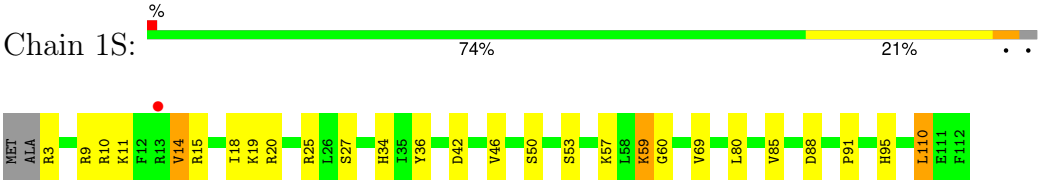
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



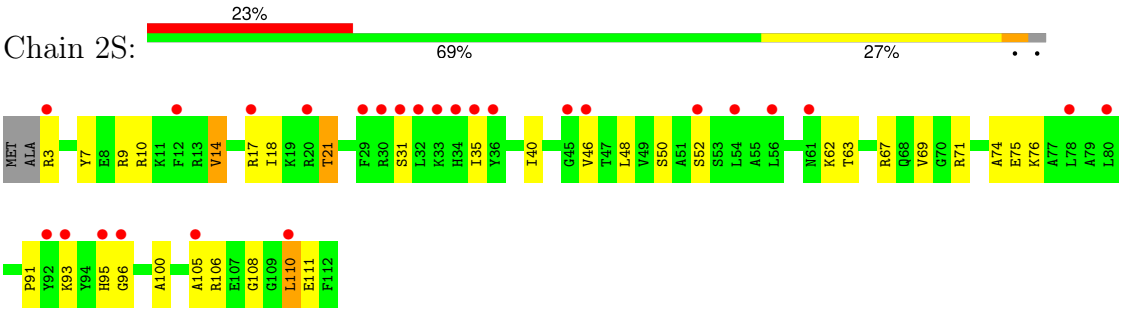
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



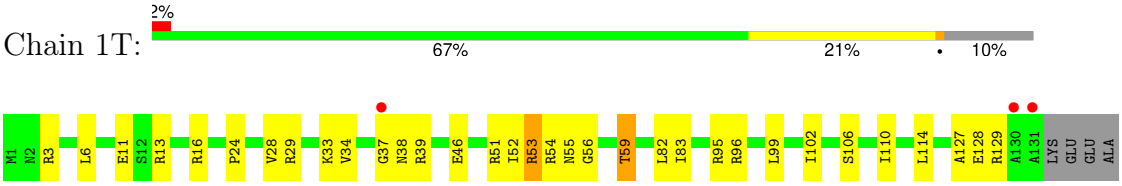
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



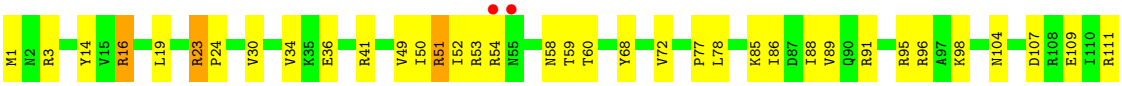
• Molecule 15: 50S ribosomal protein L19

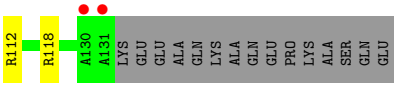
Chain 1T:



• Molecule 15: 50S ribosomal protein L19

Chain 2T:



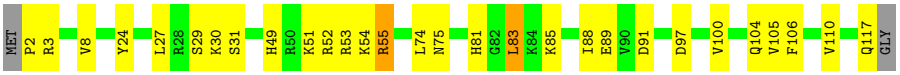


• Molecule 16: 50S ribosomal protein L20

Chain 1U:

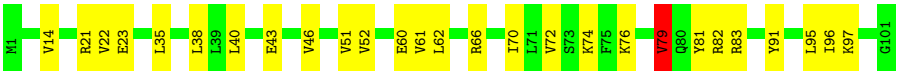
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



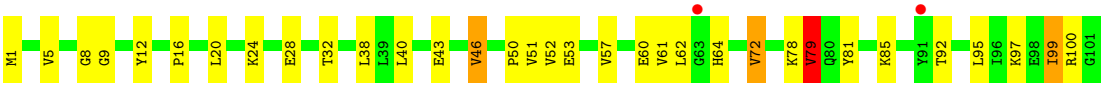
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



• Molecule 17: 50S ribosomal protein L21

Chain 2V:

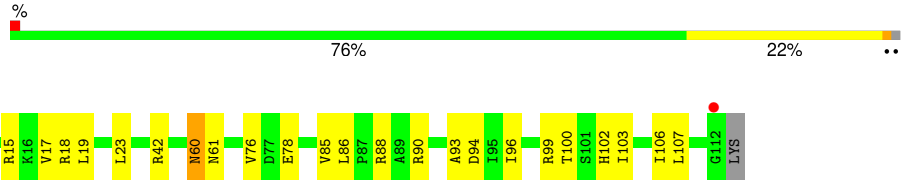


• Molecule 18: 50S ribosomal protein L22

Chain 1W:

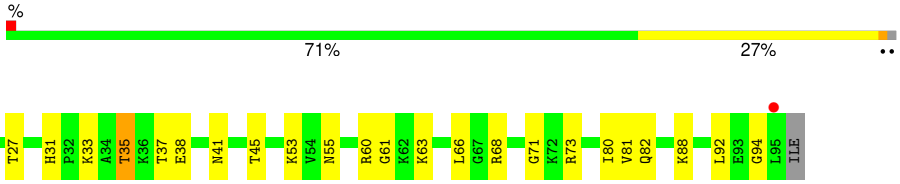
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



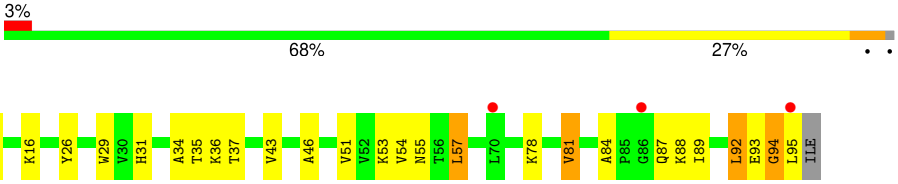
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



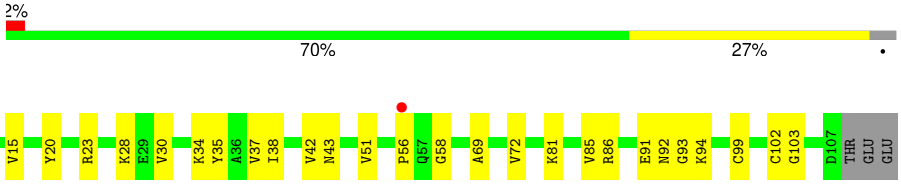
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



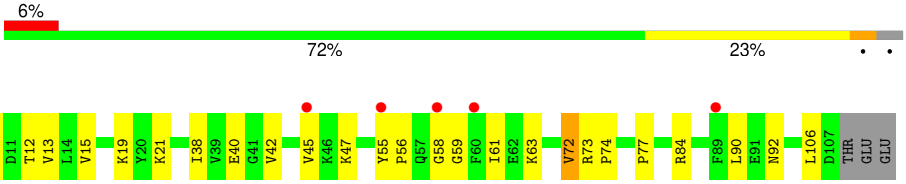
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



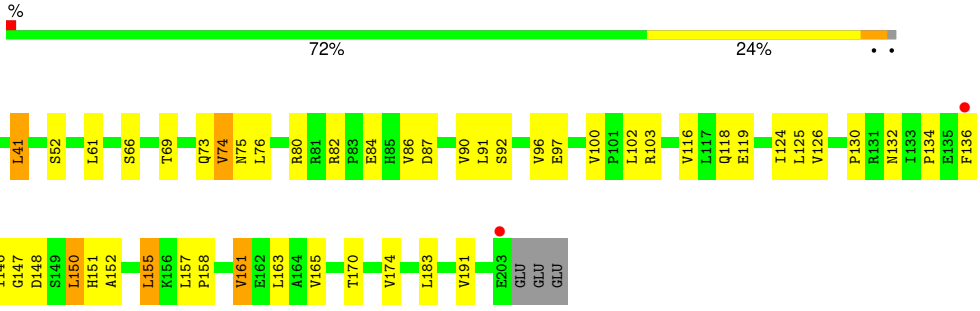
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



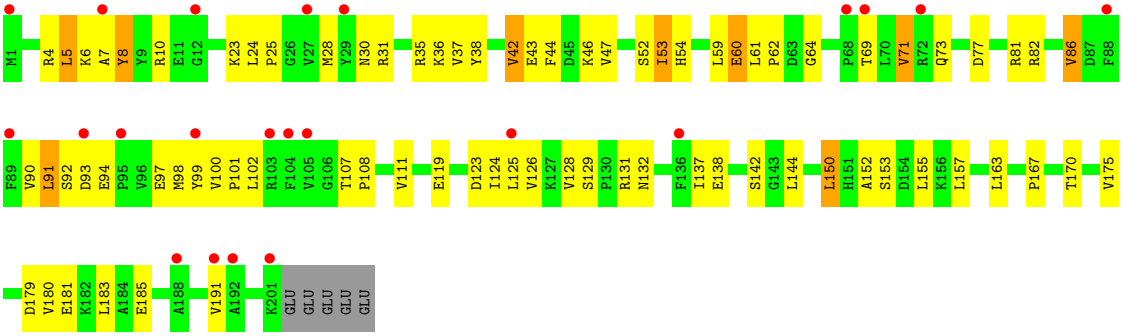
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



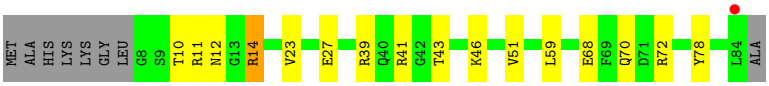
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



• Molecule 22: 50S ribosomal protein L27

Chain 10:

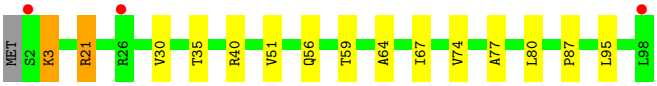


• Molecule 22: 50S ribosomal protein L27

Chain 20:

• Molecule 23: 50S ribosomal protein L28

Chain 11:

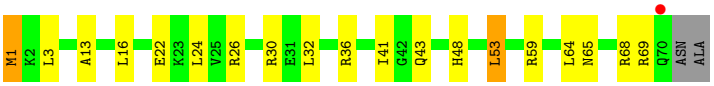


• Molecule 23: 50S ribosomal protein L28

Chain 21:

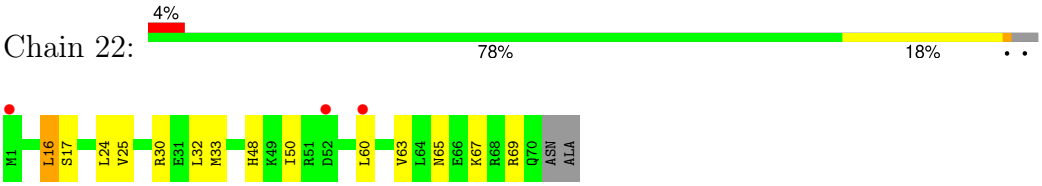
• Molecule 24: 50S ribosomal protein L29

Chain 12:



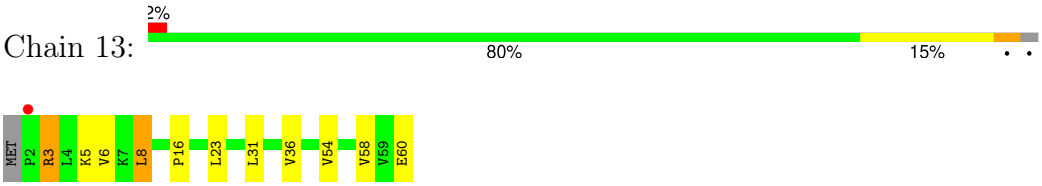
• Molecule 24: 50S ribosomal protein L29

Chain 22:



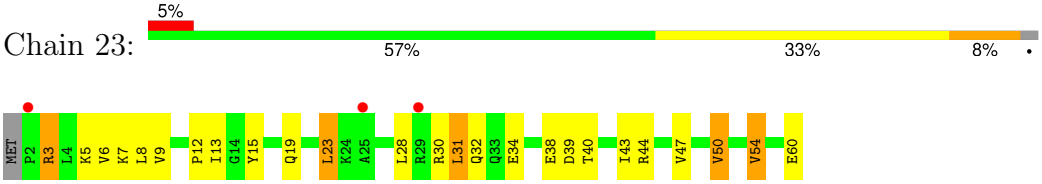
• Molecule 25: 50S ribosomal protein L30

Chain 13:



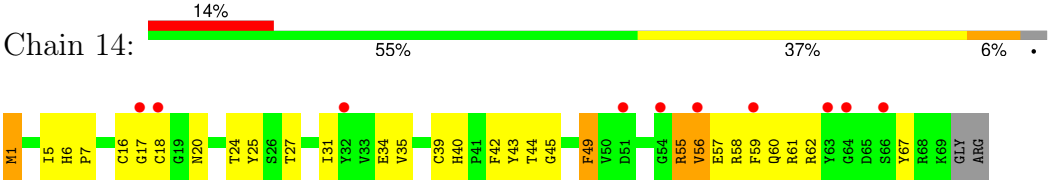
• Molecule 25: 50S ribosomal protein L30

Chain 23:



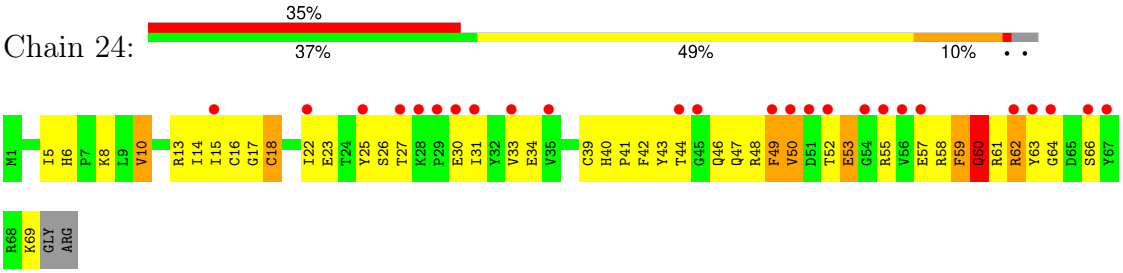
• Molecule 26: 50S ribosomal protein L31

Chain 14:



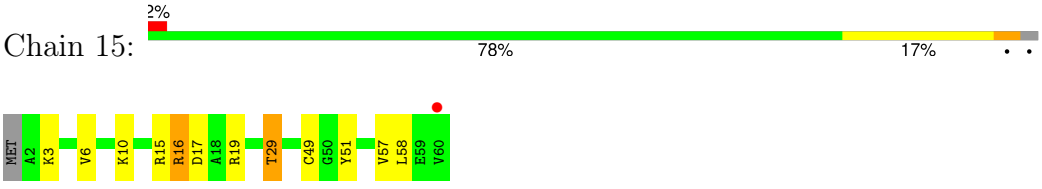
• Molecule 26: 50S ribosomal protein L31

Chain 24:



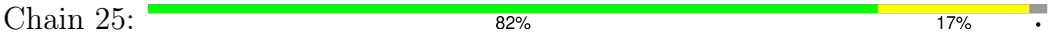
• Molecule 27: 50S ribosomal protein L32

Chain 15:



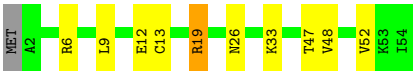
• Molecule 27: 50S ribosomal protein L32

Chain 25:



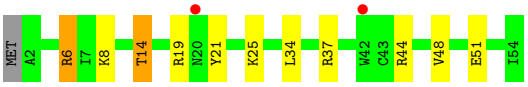
• Molecule 28: 50S ribosomal protein L33

Chain 16:



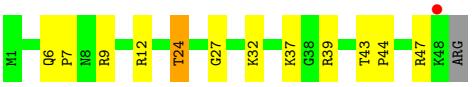
• Molecule 28: 50S ribosomal protein L33

Chain 26:



• Molecule 29: 50S ribosomal protein L34

Chain 17:



• Molecule 29: 50S ribosomal protein L34

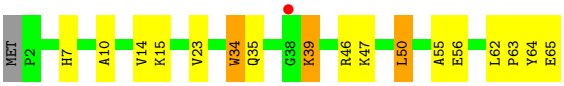
Chain 27:

• Molecule 30: 50S ribosomal protein L35

Chain 18:

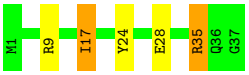
• Molecule 30: 50S ribosomal protein L35

Chain 28:



• Molecule 31: 50S ribosomal protein L36

Chain 19:

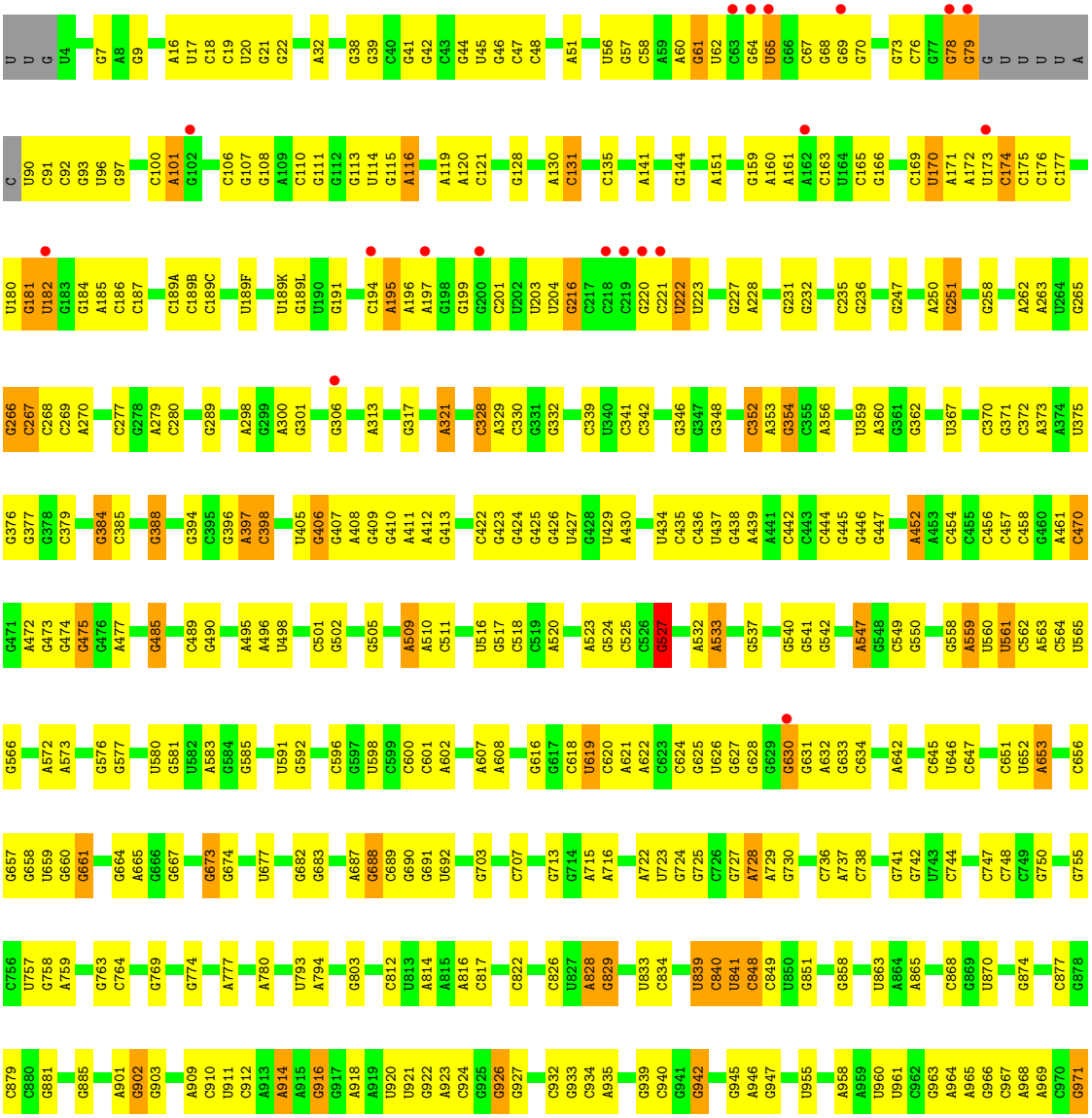


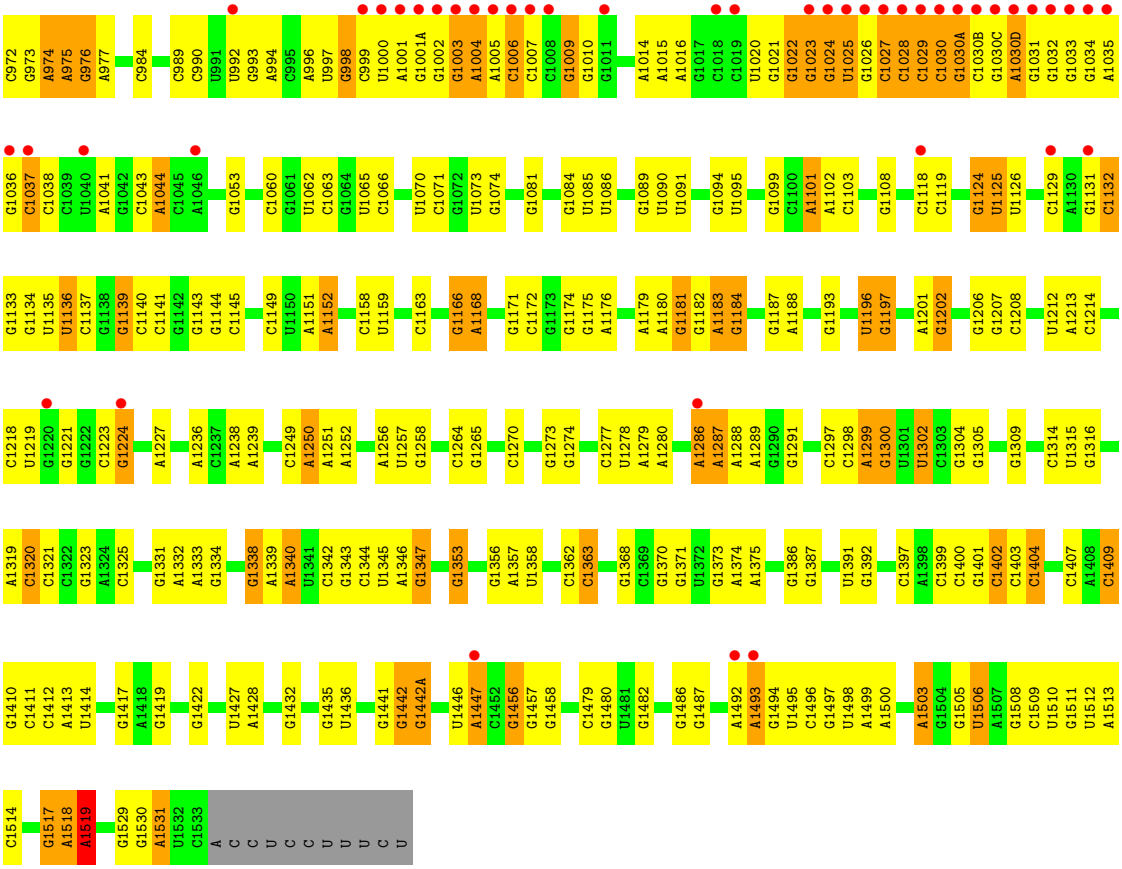
• Molecule 31: 50S ribosomal protein L36

Chain 29:

• Molecule 32: 16S Ribosomal RNA

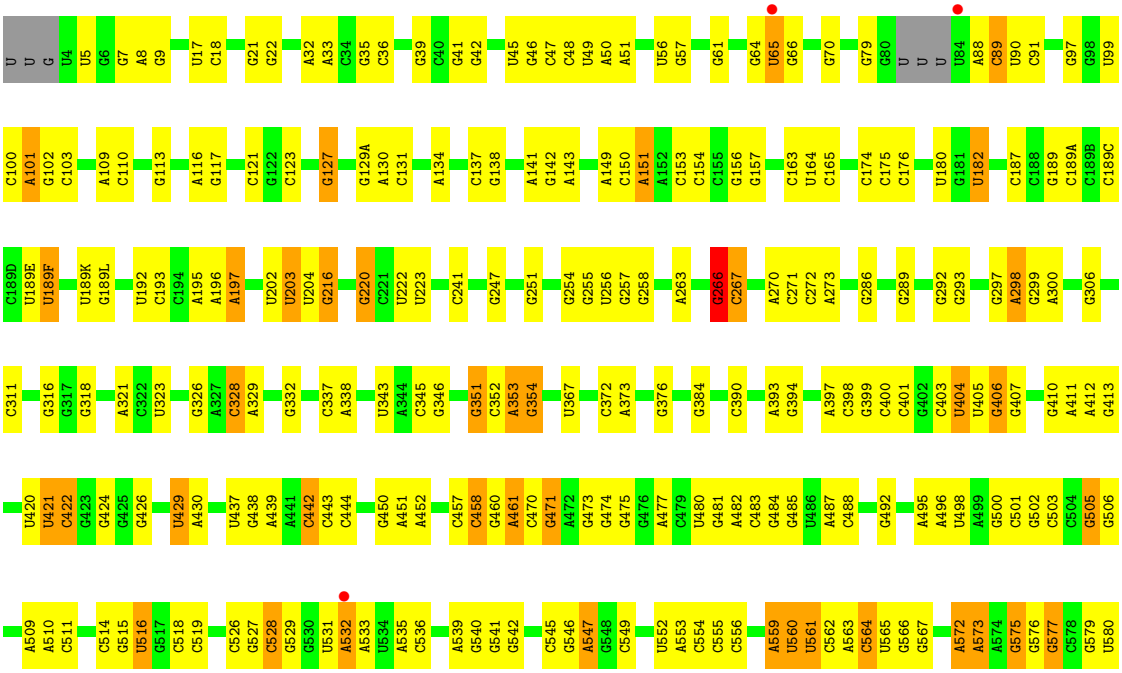
Chain 1a:

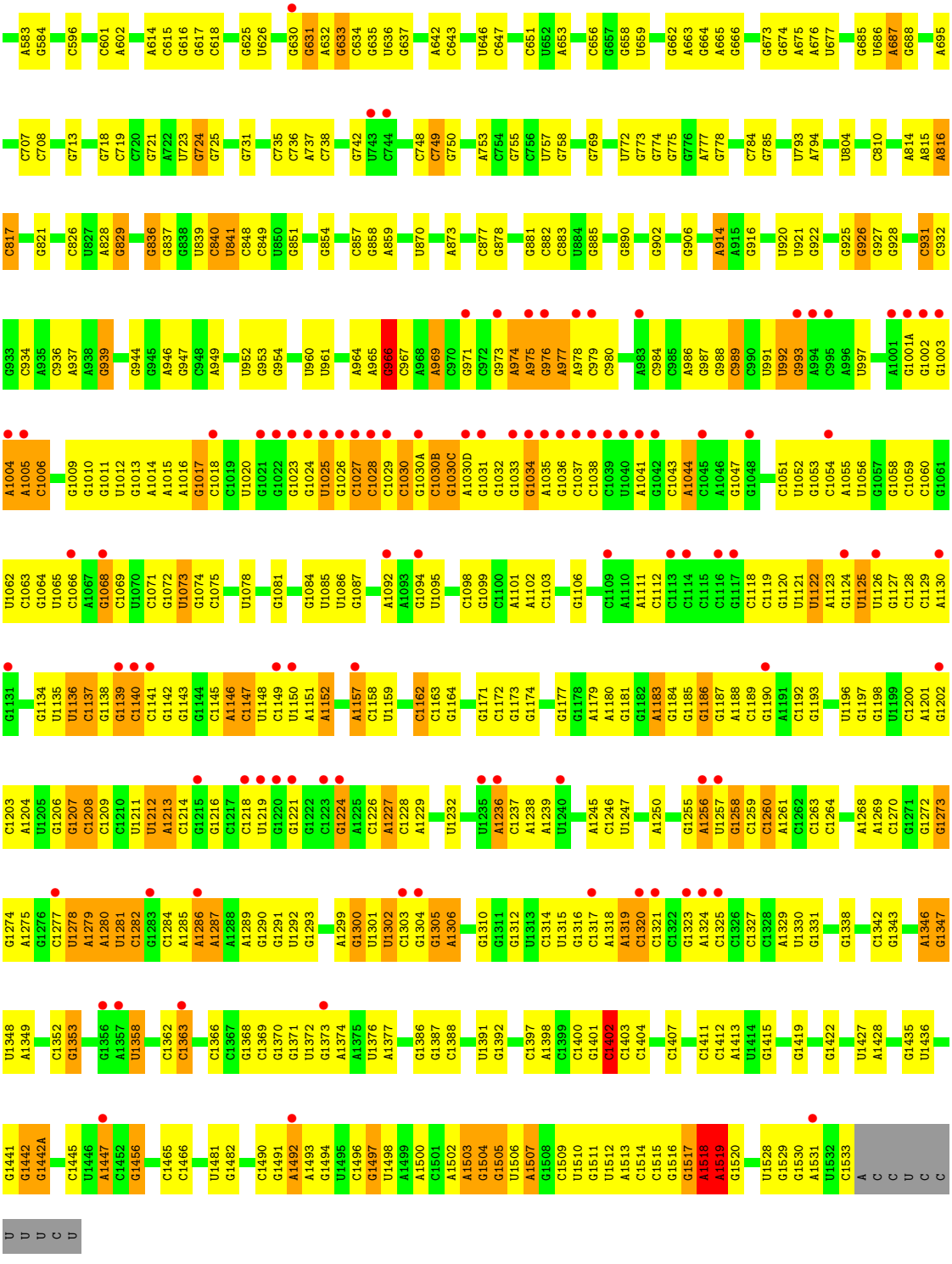




• Molecule 32: 16S Ribosomal RNA

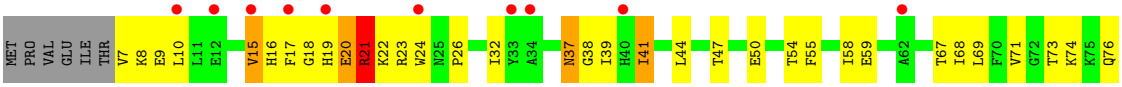
Chain 2a:

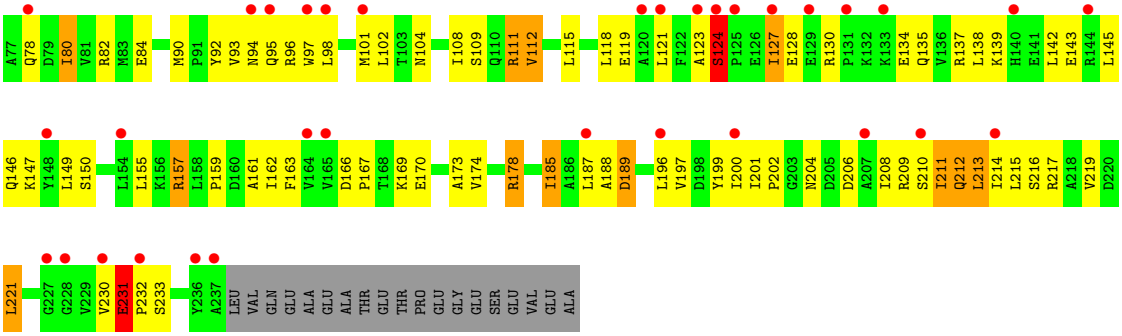




• Molecule 33: 30S ribosomal protein S2

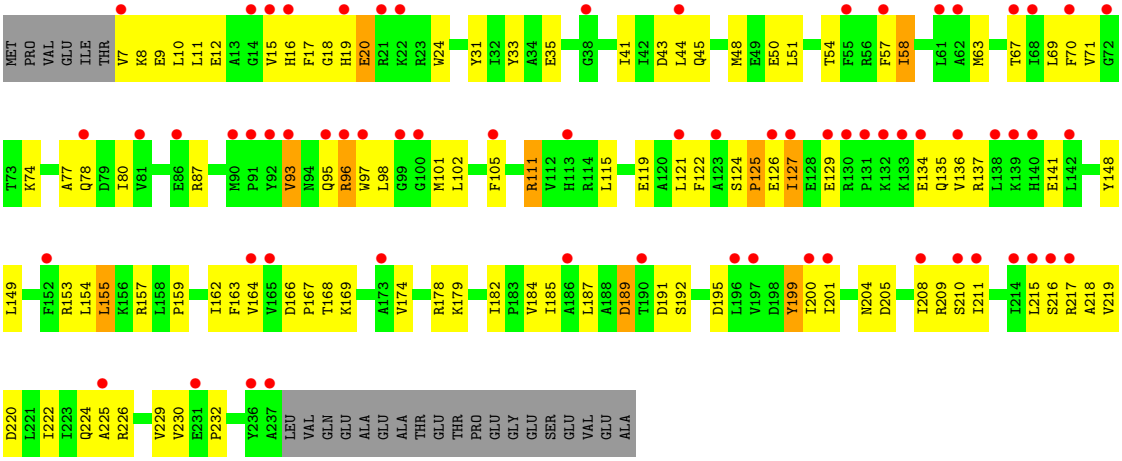
Chain 1b:





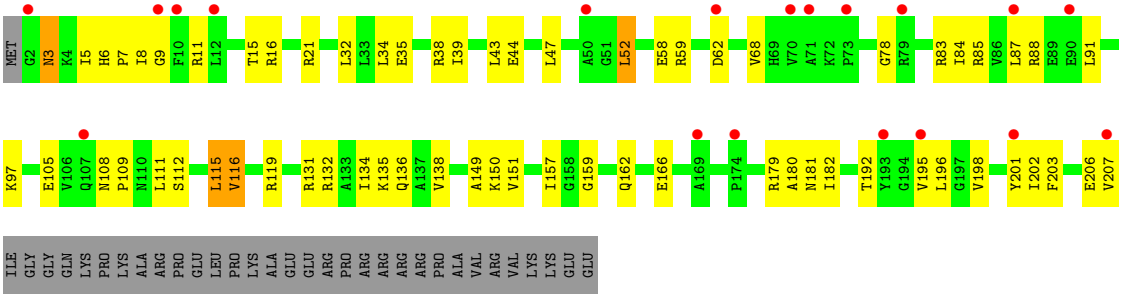
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



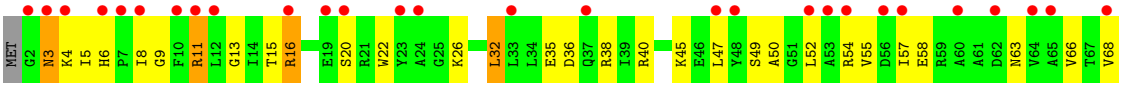
• Molecule 34: 30S ribosomal protein S3

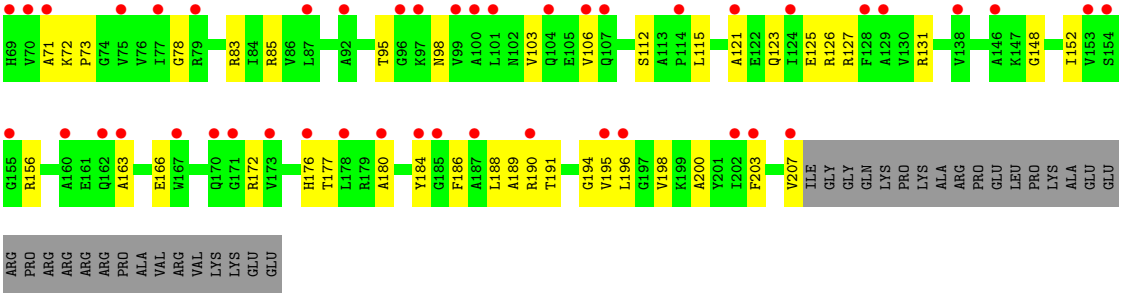
Chain 1c:



• Molecule 34: 30S ribosomal protein S3

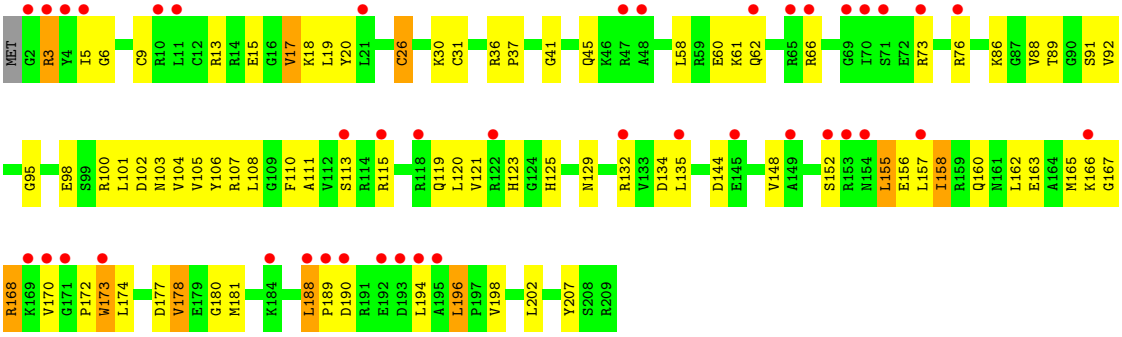
Chain 2c:





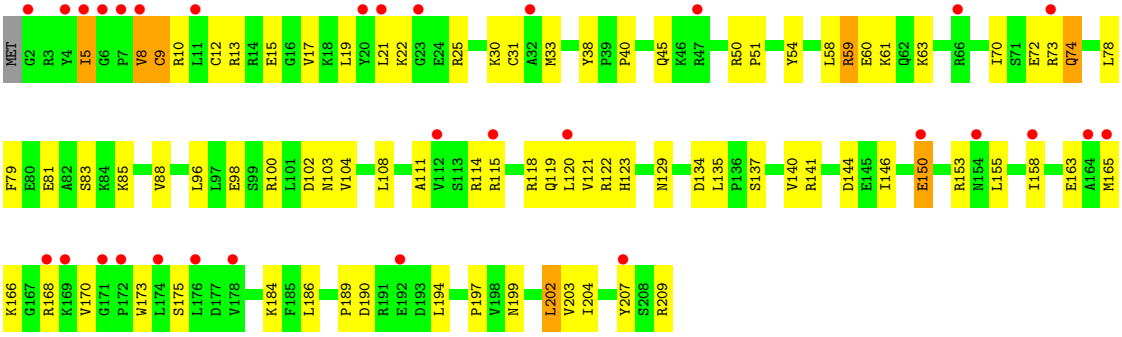
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



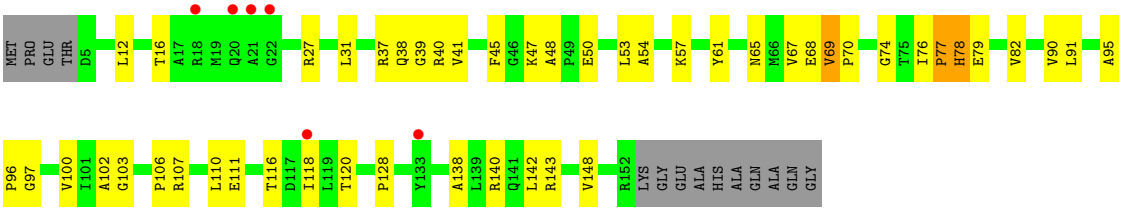
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



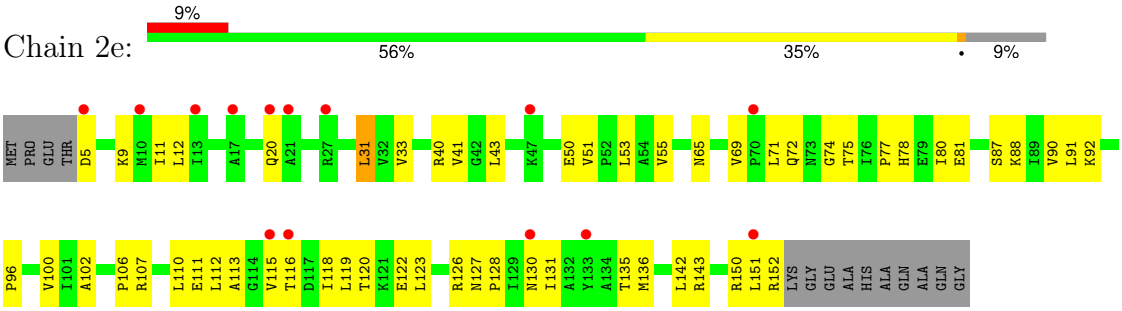
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



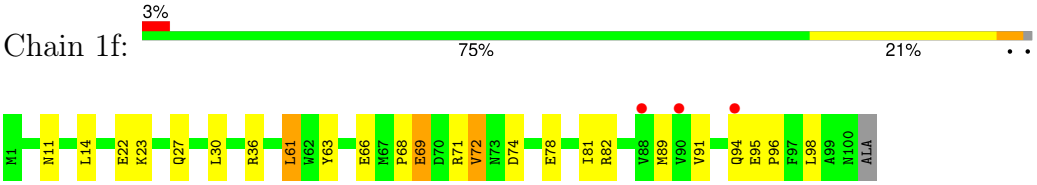
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



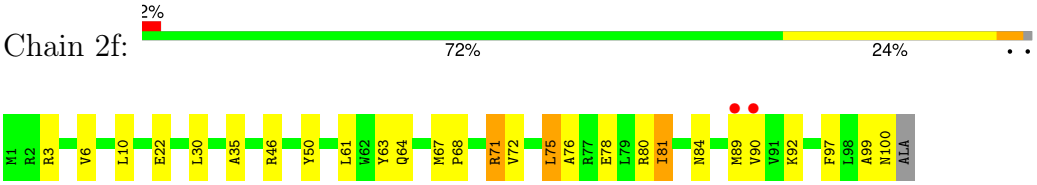
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



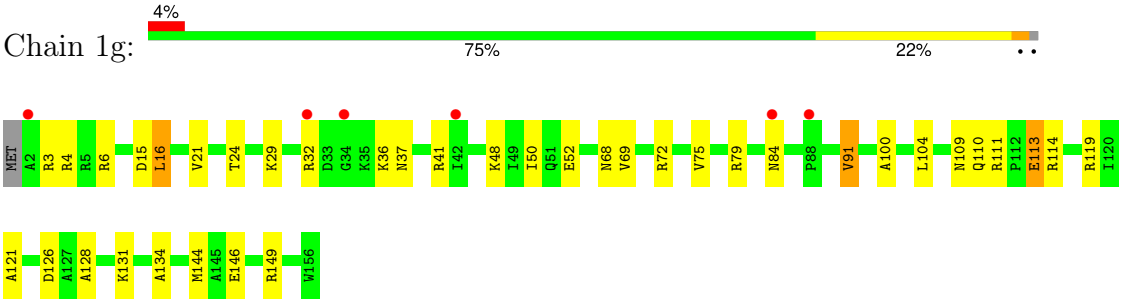
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



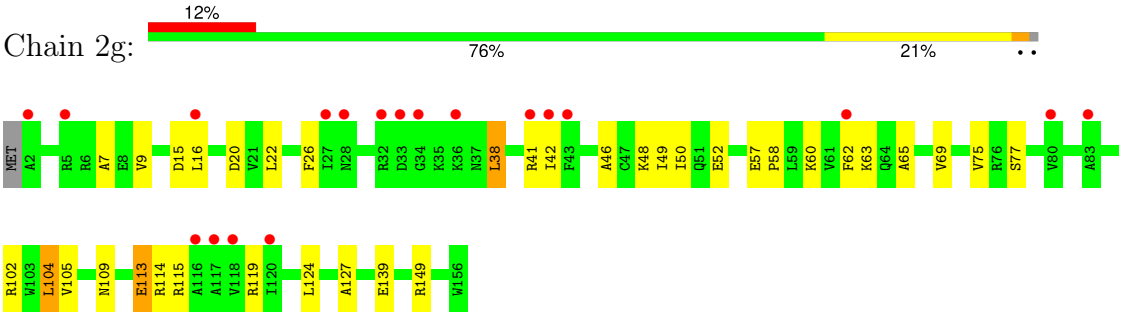
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



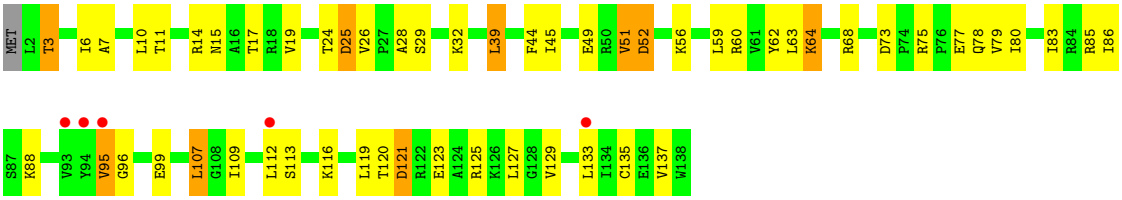
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



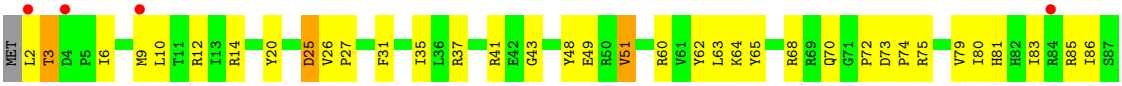
• Molecule 39: 30S ribosomal protein S8

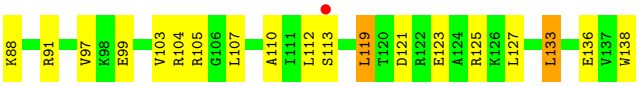
Chain 1h:



• Molecule 39: 30S ribosomal protein S8

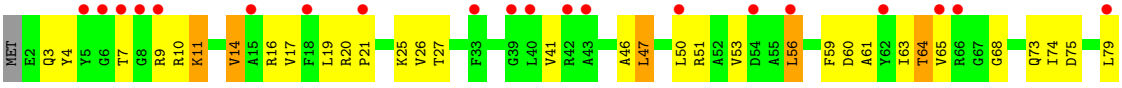
Chain 2h:

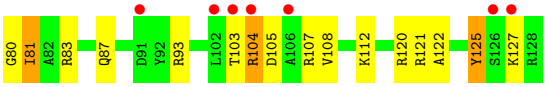




• Molecule 40: 30S ribosomal protein S9

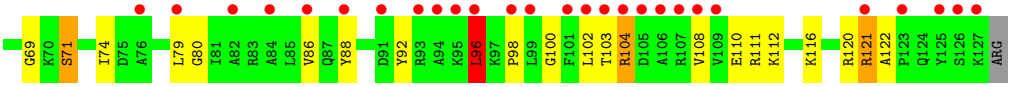
Chain 1i:





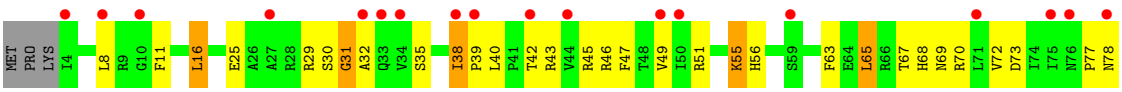
• Molecule 40: 30S ribosomal protein S9

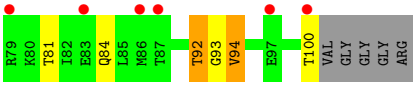
Chain 2i:



• Molecule 41: 30S ribosomal protein S10

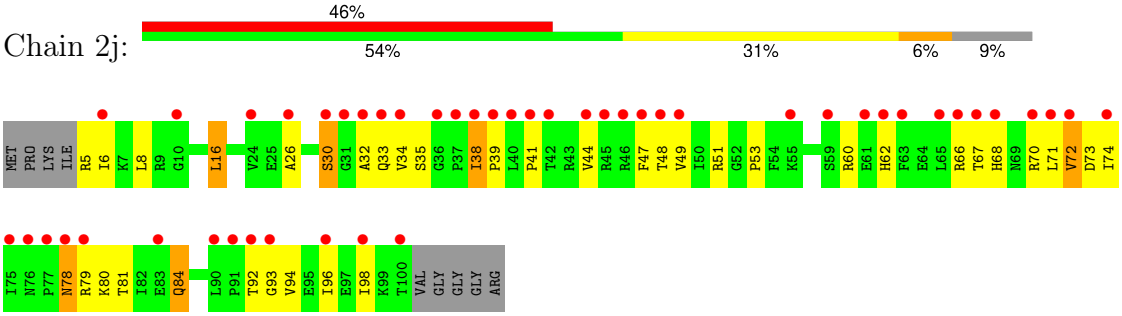
Chain 1j:





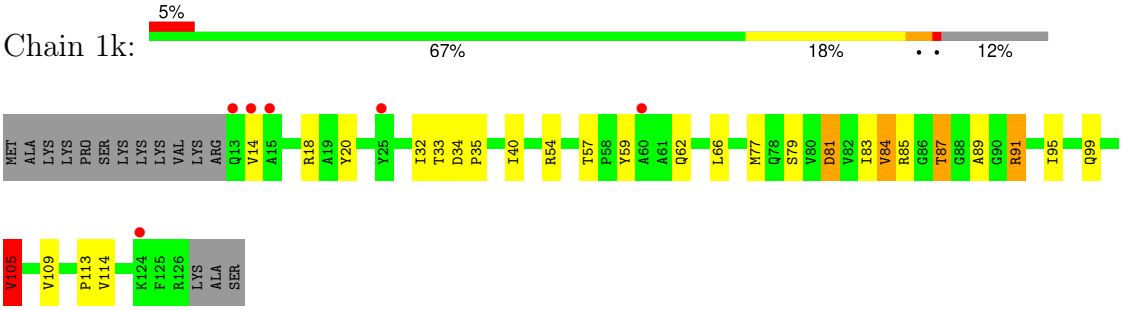
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



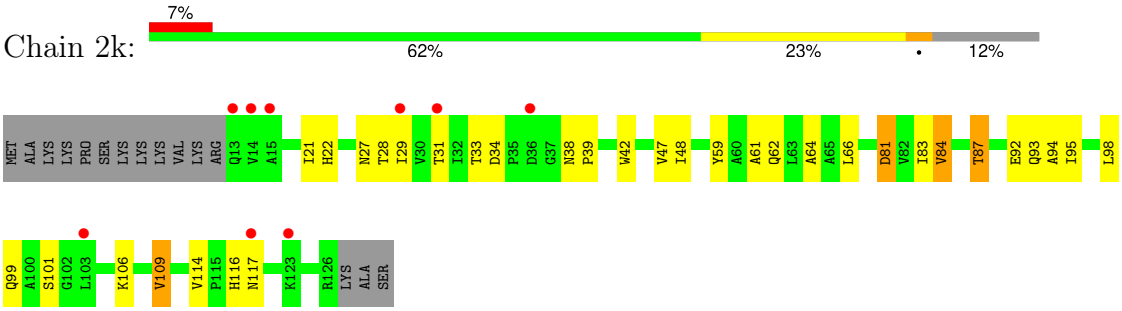
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



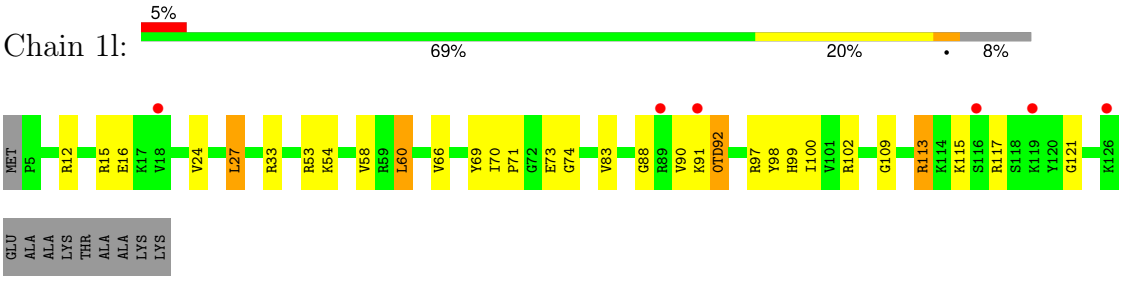
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



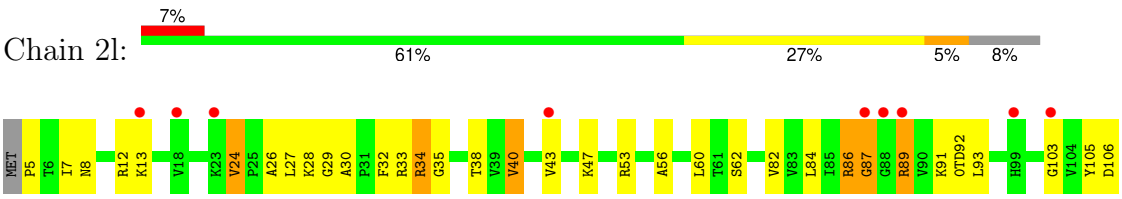
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



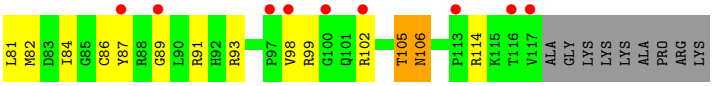
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



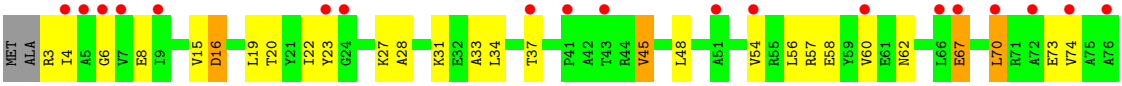
• Molecule 44: 30S ribosomal protein S13

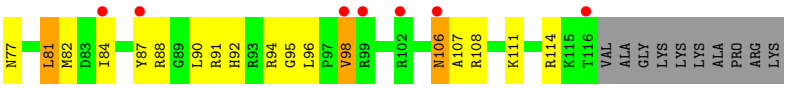
Chain 1m:



• Molecule 44: 30S ribosomal protein S13

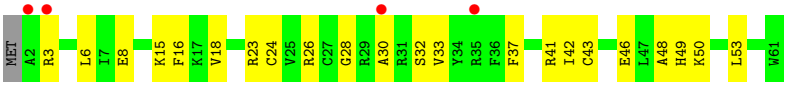
Chain 2m:





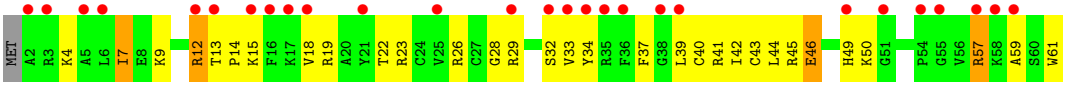
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



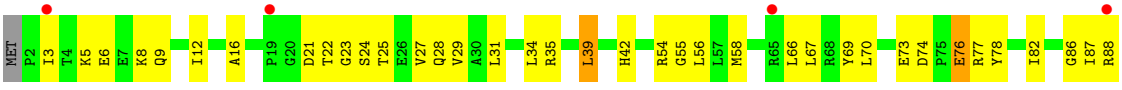
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



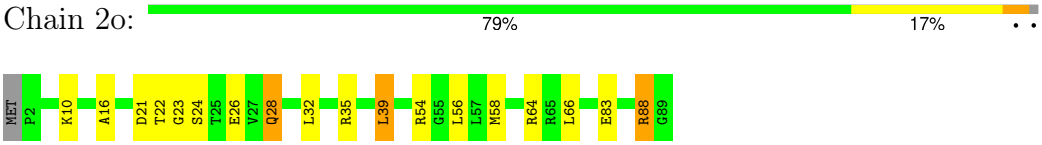
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



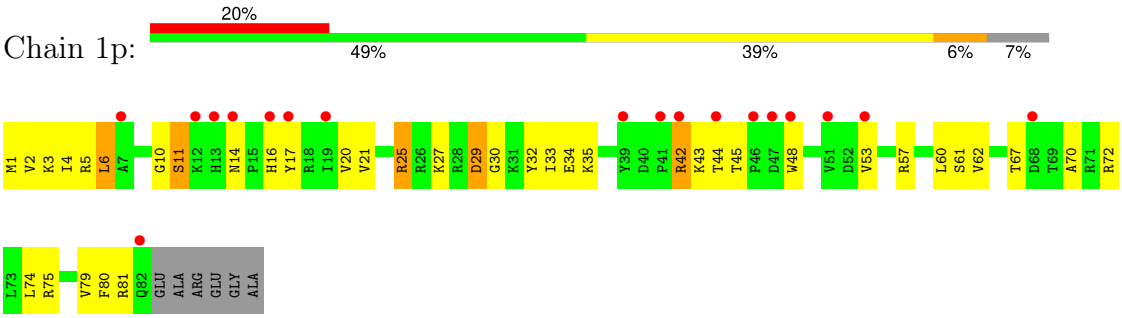
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



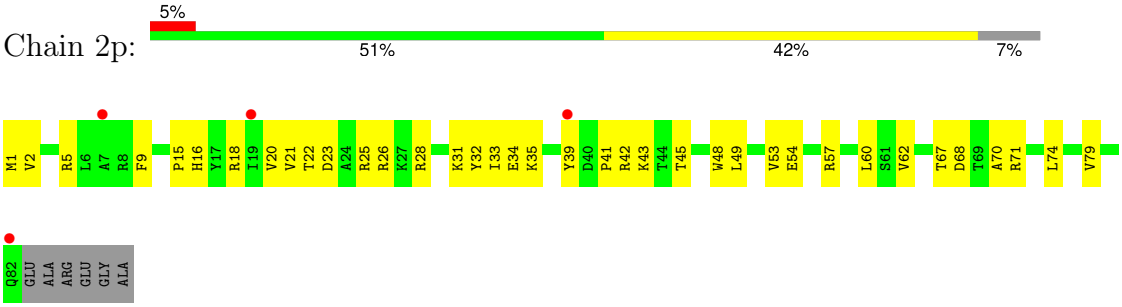
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



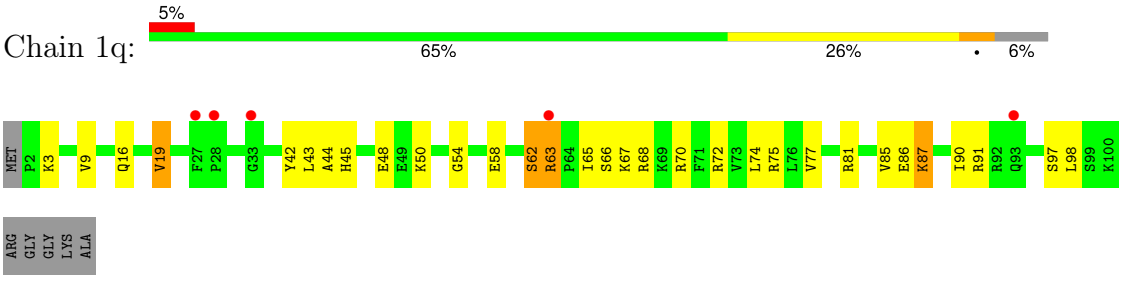
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



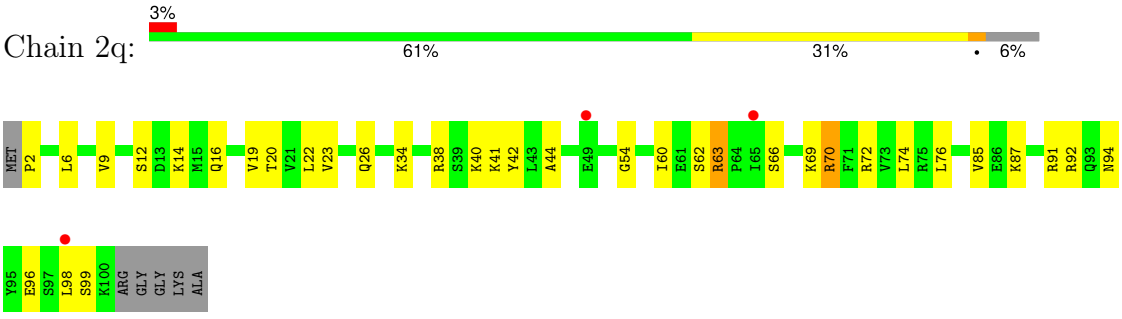
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



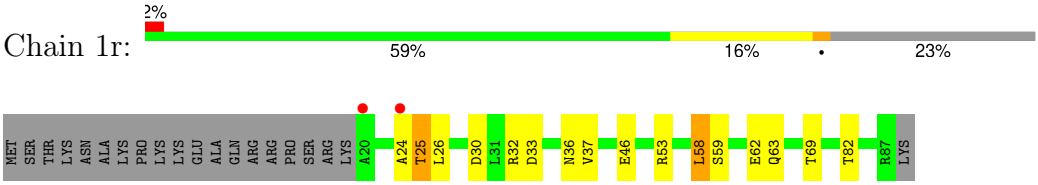
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



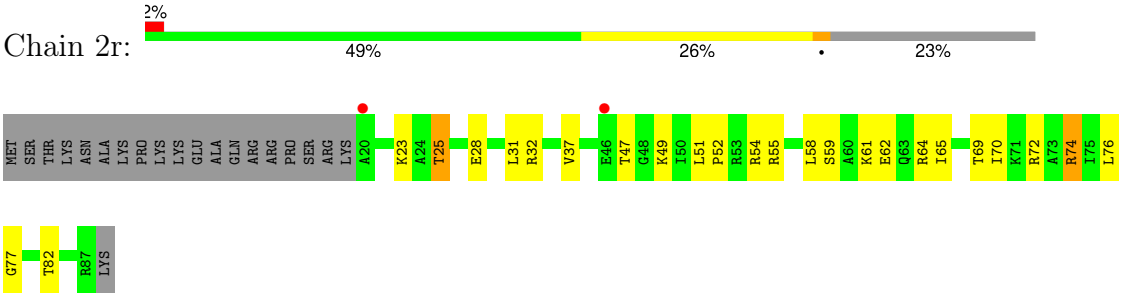
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



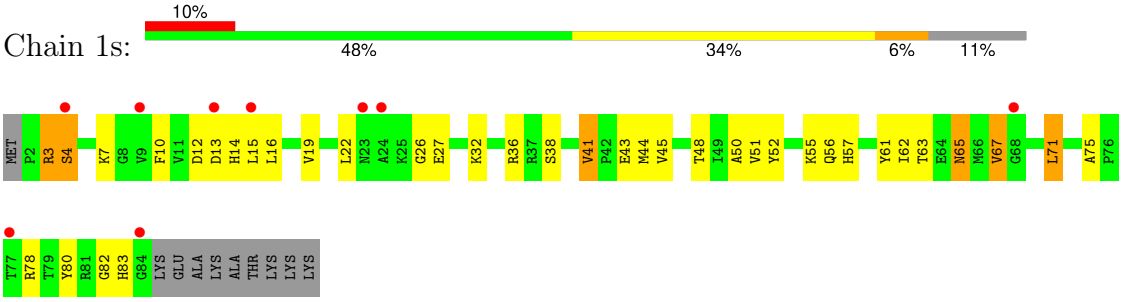
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



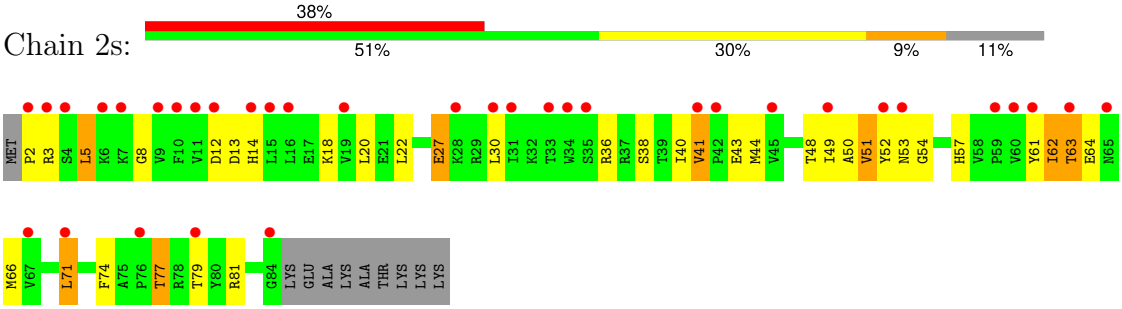
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



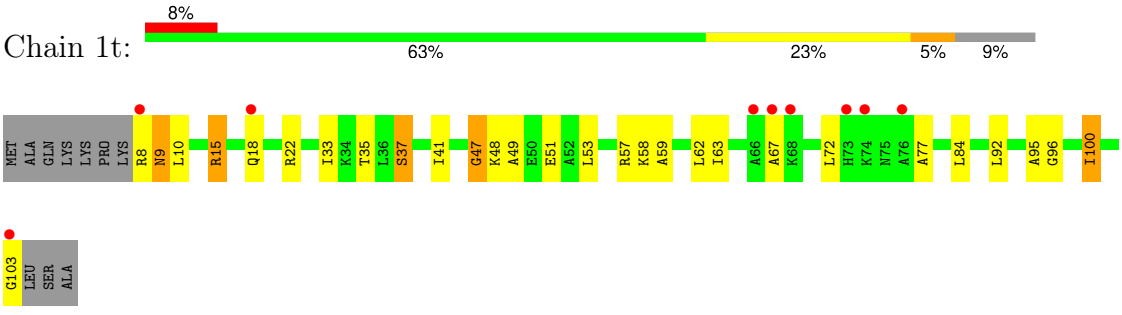
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



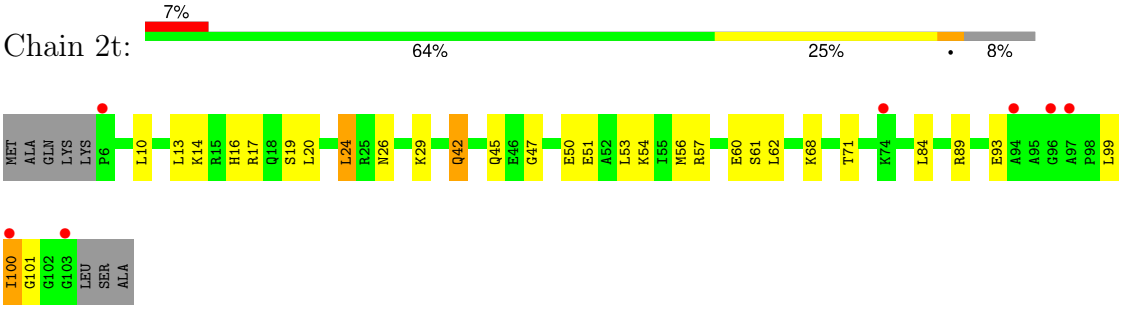
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



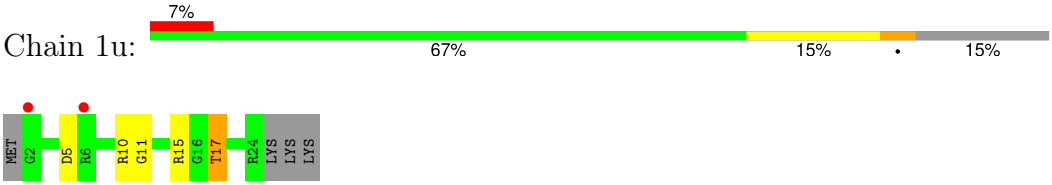
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



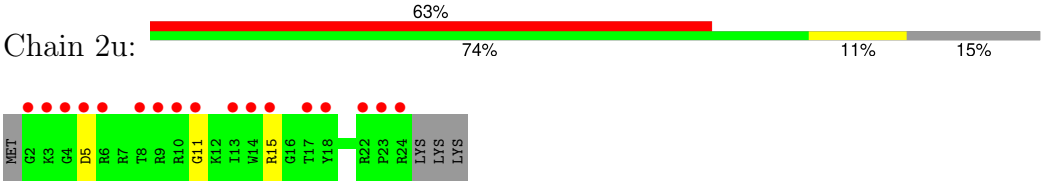
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



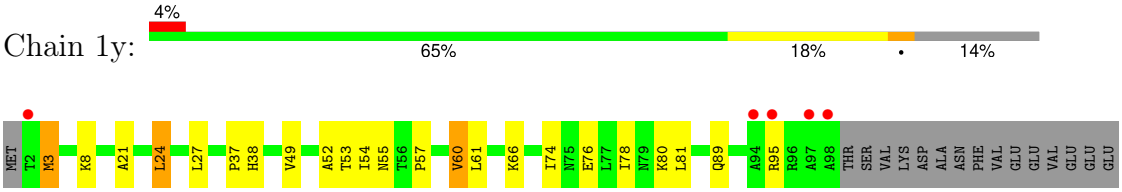
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



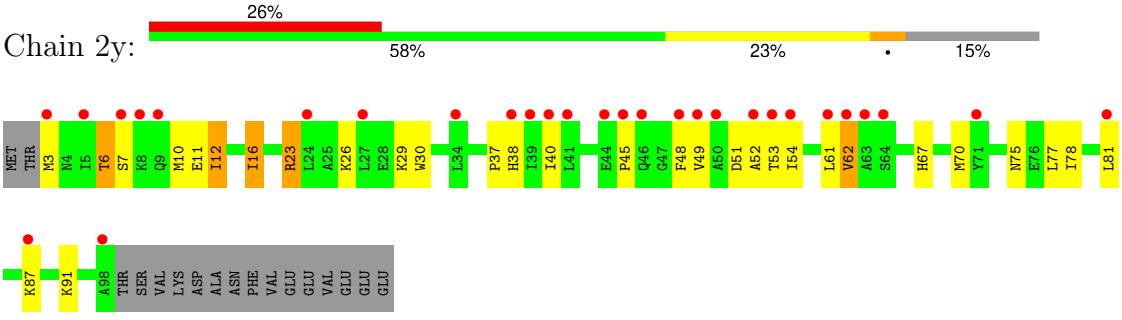
• Molecule 53: Ribosome-associated inhibitor A

Chain 1y:



• Molecule 53: Ribosome-associated inhibitor A

Chain 2y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.42Å 450.57Å 623.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	365.11 – 2.85 365.11 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (365.11-2.85) 99.9 (365.11-2.85)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.212 , 0.265 0.211 , 0.262	Depositor DCC
R_{free} test set	68254 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 178.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	297568	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A1CQ7, 0TD, PSU, 5MU, MG, 2MA, ZN, OMG, OMC, G7M, OMU, 2MG, MPD, 4OC, UR3, SF4, MA6, 5MC, M2G

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	0.28	0/69031	0.44	0/107754
1	2A	0.23	0/68903	0.41	1/107552 (0.0%)
2	1B	0.22	0/2876	0.39	0/4486
2	2B	0.21	0/2878	0.37	0/4490
3	1D	0.28	0/2181	0.51	0/2940
3	2D	0.23	0/2186	0.47	0/2944
4	1E	0.40	1/1592 (0.1%)	0.53	0/2149
4	2E	0.22	0/1592	0.47	0/2149
5	1F	0.27	0/1619	0.47	0/2193
5	2F	0.21	0/1615	0.49	0/2188
6	1G	0.22	0/1451	0.43	0/1961
6	2G	0.21	0/1449	0.44	0/1957
7	1H	0.23	0/1356	0.44	0/1834
7	2H	0.19	0/1350	0.39	0/1826
8	1I	0.20	0/1109	0.44	0/1512
8	2I	0.20	0/1091	0.43	1/1490 (0.1%)
9	1N	0.25	0/1148	0.47	0/1547
9	2N	0.20	0/1144	0.41	0/1543
10	1O	0.29	0/943	0.50	0/1269
10	2O	0.22	0/943	0.45	0/1269
11	1P	0.27	0/1152	0.51	0/1533
11	2P	0.22	0/1152	0.49	0/1533
12	1Q	0.26	0/1143	0.46	0/1527
12	2Q	0.20	0/1143	0.40	0/1527
13	1R	0.28	0/982	0.50	0/1312
13	2R	0.23	0/982	0.48	0/1312
14	1S	0.21	0/887	0.49	0/1180
14	2S	0.21	0/880	0.44	0/1172
15	1T	0.28	0/1105	0.51	0/1477
15	2T	0.23	0/1097	0.44	0/1468
16	1U	0.29	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.22	0/977	0.43	0/1301
17	1V	0.25	0/786	0.46	0/1053
17	2V	0.22	0/782	0.45	0/1049
18	1W	0.26	0/897	0.47	0/1205
18	2W	0.22	0/897	0.42	0/1205
19	1X	0.28	0/764	0.52	0/1025
19	2X	0.22	0/764	0.49	0/1025
20	1Y	0.26	0/823	0.52	0/1099
20	2Y	0.22	0/823	0.46	0/1100
21	1Z	0.23	0/1620	0.45	0/2200
21	2Z	0.23	0/1590	0.45	0/2162
22	10	0.26	0/616	0.52	0/821
22	20	0.21	0/616	0.47	0/821
23	11	0.27	0/761	0.45	0/1013
23	21	0.26	0/766	0.44	0/1018
24	12	0.24	0/590	0.46	0/781
24	22	0.19	0/594	0.38	0/785
25	13	0.27	0/474	0.45	0/635
25	23	0.19	0/469	0.40	0/630
26	14	0.27	0/559	0.61	0/754
26	24	0.30	0/549	0.68	2/741 (0.3%)
27	15	0.28	0/473	0.50	0/639
27	25	0.24	0/469	0.44	0/635
28	16	0.24	0/460	0.45	0/613
28	26	0.23	0/456	0.44	0/608
29	17	0.30	0/426	0.50	0/561
29	27	0.24	0/426	0.49	0/561
30	18	0.29	0/525	0.43	0/691
30	28	0.20	0/525	0.41	0/691
31	19	0.30	0/310	0.48	0/407
31	29	0.22	0/310	0.46	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.20	1/35890 (0.0%)	0.38	2/56012 (0.0%)
33	1b	0.24	0/1876	0.49	0/2533
33	2b	0.26	0/1860	0.49	0/2518
34	1c	0.20	0/1582	0.43	0/2137
34	2c	0.23	0/1566	0.44	0/2119
35	1d	0.24	0/1695	0.48	0/2274
35	2d	0.20	0/1698	0.44	0/2277
36	1e	0.21	0/1149	0.47	0/1548
36	2e	0.20	0/1149	0.43	0/1548
37	1f	0.20	0/827	0.42	0/1120
37	2f	0.20	0/829	0.44	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.19	0/1254	0.40	0/1683
38	2g	0.21	0/1248	0.40	0/1676
39	1h	0.19	0/1118	0.42	0/1506
39	2h	0.19	0/1108	0.43	0/1494
40	1i	0.22	0/1005	0.47	0/1351
40	2i	0.23	0/985	0.48	0/1329
41	1j	0.19	0/732	0.40	0/993
41	2j	0.26	0/723	0.50	0/984
42	1k	0.20	0/849	0.43	0/1150
42	2k	0.20	0/848	0.47	0/1149
43	1l	0.20	0/937	0.43	0/1260
43	2l	0.22	0/937	0.53	1/1260 (0.1%)
44	1m	0.19	0/924	0.46	0/1242
44	2m	0.22	0/905	0.48	0/1217
45	1n	0.20	0/501	0.42	0/664
45	2n	0.21	0/501	0.44	0/664
46	1o	0.19	0/739	0.42	0/985
46	2o	0.19	0/739	0.42	0/985
47	1p	0.21	0/697	0.46	0/939
47	2p	0.21	0/693	0.44	0/935
48	1q	0.22	0/836	0.46	0/1117
48	2q	0.22	0/836	0.44	0/1117
49	1r	0.19	0/560	0.40	0/746
49	2r	0.22	0/560	0.44	0/746
50	1s	0.20	0/663	0.48	0/895
50	2s	0.20	0/660	0.41	0/893
51	1t	0.22	0/734	0.48	0/969
51	2t	0.20	0/736	0.41	0/976
52	1u	0.21	0/203	0.43	0/266
52	2u	0.25	0/203	0.50	0/266
53	1y	0.22	0/776	0.36	0/1048
53	2y	0.19	0/761	0.35	0/1030
All	All	0.24	2/309941 (0.0%)	0.42	7/463239 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
26	24	0	1
33	1b	0	1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1E	143	ASN	CA-C	-11.58	1.47	1.53
32	2a	527	G7M	O3'-P	5.01	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	87	GLY	N-CA-C	6.52	121.13	112.65
26	24	59	PHE	CA-C-N	5.88	132.29	121.70
26	24	59	PHE	C-N-CA	5.88	132.29	121.70
32	2a	266	G	C2'-C3'-O3'	5.88	118.31	109.50
1	2A	1992	G	C2'-C3'-O3'	5.85	118.28	109.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	231	GLU	Peptide
26	24	18	CYS	Peptide
33	2b	199	TYR	Peptide
43	2l	86	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61869	0	31205	587	0
1	2A	61758	0	31153	681	0
2	1B	2572	0	1305	19	0
2	2B	2573	0	1306	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1D	2131	0	2207	61	0
3	2D	2136	0	2218	32	0
4	1E	1559	0	1618	35	0
4	2E	1559	0	1618	52	0
5	1F	1584	0	1625	37	0
5	2F	1580	0	1619	48	0
6	1G	1426	0	1445	39	0
6	2G	1424	0	1441	64	0
7	1H	1330	0	1407	28	0
7	2H	1324	0	1402	34	0
8	1I	1094	0	1127	25	0
8	2I	1076	0	1094	19	0
9	1N	1121	0	1195	21	0
9	2N	1117	0	1184	19	0
10	1O	933	0	996	28	0
10	2O	933	0	996	17	0
11	1P	1135	0	1212	31	0
11	2P	1135	0	1212	26	0
12	1Q	1122	0	1179	21	0
12	2Q	1122	0	1179	27	0
13	1R	968	0	1033	29	0
13	2R	968	0	1033	26	0
14	1S	877	0	938	21	0
14	2S	870	0	923	16	0
15	1T	1091	0	1151	22	0
15	2T	1083	0	1136	25	0
16	1U	959	0	1019	9	0
16	2U	959	0	1019	23	0
17	1V	775	0	841	14	0
17	2V	771	0	830	19	0
18	1W	886	0	940	11	0
18	2W	886	0	940	13	0
19	1X	750	0	814	18	0
19	2X	750	0	814	18	0
20	1Y	810	0	892	14	0
20	2Y	810	0	887	16	0
21	1Z	1587	0	1598	35	0
21	2Z	1557	0	1564	55	0
22	10	608	0	622	12	0
22	20	608	0	622	10	0
23	11	754	0	823	9	0
23	21	759	0	837	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	12	588	0	643	14	0
24	22	592	0	654	8	0
25	13	469	0	518	5	0
25	23	464	0	514	15	0
26	14	546	0	522	21	0
26	24	536	0	514	29	0
27	15	459	0	476	11	0
27	25	455	0	465	6	0
28	16	453	0	473	4	0
28	26	449	0	469	7	0
29	17	418	0	467	11	0
29	27	418	0	467	2	0
30	18	517	0	582	15	0
30	28	517	0	582	11	0
31	19	307	0	335	3	0
31	29	307	0	335	14	0
32	1a	32246	0	16294	459	0
32	2a	32331	0	16338	501	0
33	1b	1842	0	1862	62	0
33	2b	1825	0	1828	73	0
34	1c	1558	0	1557	40	0
34	2c	1542	0	1517	44	0
35	1d	1665	0	1687	64	0
35	2d	1668	0	1703	68	0
36	1e	1133	0	1191	31	0
36	2e	1133	0	1191	34	0
37	1f	814	0	808	10	0
37	2f	816	0	808	23	0
38	1g	1235	0	1249	26	0
38	2g	1229	0	1238	19	0
39	1h	1098	0	1143	42	0
39	2h	1088	0	1126	38	0
40	1i	986	0	990	34	0
40	2i	966	0	953	32	0
41	1j	719	0	672	22	0
41	2j	710	0	661	28	0
42	1k	834	0	838	16	0
42	2k	833	0	836	19	0
43	1l	932	0	981	18	0
43	2l	932	0	981	28	0
44	1m	914	0	954	31	0
44	2m	895	0	920	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	1n	492	0	529	12	0
45	2n	492	0	529	24	0
46	1o	728	0	760	21	0
46	2o	728	0	760	9	0
47	1p	681	0	697	30	0
47	2p	677	0	686	25	0
48	1q	823	0	891	22	0
48	2q	823	0	891	24	0
49	1r	555	0	618	9	0
49	2r	555	0	618	17	0
50	1s	648	0	658	28	0
50	2s	645	0	635	27	0
51	1t	732	0	809	17	0
51	2t	733	0	795	19	0
52	1u	199	0	208	3	0
52	2u	199	0	208	2	0
53	1y	764	0	786	15	0
53	2y	749	0	757	19	0
54	10	7	0	0	0	0
54	11	5	0	0	0	0
54	13	4	0	0	0	0
54	14	1	0	0	0	0
54	15	8	0	0	0	0
54	17	5	0	0	0	0
54	18	3	0	0	0	0
54	19	3	0	0	0	0
54	1A	1010	0	0	0	0
54	1B	31	0	0	0	0
54	1D	18	0	0	0	0
54	1E	9	0	0	0	0
54	1F	17	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	4	0	0	0	0
54	1O	1	0	0	0	0
54	1P	7	0	0	0	0
54	1Q	5	0	0	0	0
54	1R	9	0	0	0	0
54	1T	4	0	0	0	0
54	1U	6	0	0	0	0
54	1V	7	0	0	0	0
54	1W	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1Y	1	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	277	0	0	0	0
54	1b	1	0	0	0	0
54	1d	5	0	0	0	0
54	1e	2	0	0	0	0
54	1f	2	0	0	0	0
54	1g	3	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0
54	1k	1	0	0	0	0
54	1l	3	0	0	0	0
54	1m	1	0	0	0	0
54	1n	2	0	0	0	0
54	1o	2	0	0	0	0
54	1t	2	0	0	0	0
54	1y	3	0	0	0	0
54	20	2	0	0	0	0
54	21	3	0	0	0	0
54	23	1	0	0	0	0
54	25	1	0	0	0	0
54	26	2	0	0	0	0
54	28	1	0	0	0	0
54	29	1	0	0	0	0
54	2A	740	0	0	0	0
54	2B	20	0	0	0	0
54	2D	6	0	0	0	0
54	2E	7	0	0	0	0
54	2F	4	0	0	0	0
54	2G	3	0	0	0	0
54	2I	1	0	0	0	0
54	2O	1	0	0	0	0
54	2P	3	0	0	0	0
54	2Q	4	0	0	0	0
54	2R	2	0	0	0	0
54	2T	4	0	0	0	0
54	2U	1	0	0	0	0
54	2V	3	0	0	0	0
54	2W	3	0	0	0	0
54	2X	1	0	0	0	0
54	2Y	1	0	0	0	0
54	2a	187	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2e	1	0	0	0	0
54	2f	1	0	0	0	0
54	2h	1	0	0	0	0
54	2j	1	0	0	0	0
54	2k	2	0	0	0	0
54	2l	1	0	0	0	0
54	2n	1	0	0	0	0
54	2p	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	38	0	0	0	0
55	2A	38	0	0	0	0
56	18	8	0	14	2	0
56	1A	8	0	14	1	0
56	1T	8	0	14	1	0
56	1a	8	0	11	3	0
56	2A	16	0	28	1	0
56	2B	8	0	14	0	0
57	1B	12	0	12	3	0
57	1F	12	0	12	3	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	0	0
59	2d	8	0	0	3	0
60	10	27	0	0	2	0
60	11	23	0	0	0	0
60	12	18	0	0	3	0
60	13	25	0	0	0	0
60	14	2	0	0	0	0
60	15	25	0	0	2	0
60	16	21	0	0	0	0
60	17	14	0	0	0	0
60	18	32	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	19	10	0	0	0	0
60	1A	3924	0	0	130	0
60	1B	103	0	0	8	0
60	1D	114	0	0	7	0
60	1E	82	0	0	2	0
60	1F	72	0	0	3	0
60	1G	16	0	0	0	0
60	1H	19	0	0	0	0
60	1I	8	0	0	0	0
60	1N	54	0	0	2	0
60	1O	26	0	0	1	0
60	1P	63	0	0	3	0
60	1Q	39	0	0	1	0
60	1R	32	0	0	2	0
60	1S	8	0	0	0	0
60	1T	39	0	0	1	0
60	1U	47	0	0	4	0
60	1V	37	0	0	1	0
60	1W	27	0	0	1	0
60	1X	21	0	0	0	0
60	1Y	19	0	0	0	0
60	1Z	14	0	0	2	0
60	1a	576	0	0	41	0
60	1b	1	0	0	0	0
60	1d	11	0	0	1	0
60	1e	10	0	0	0	0
60	1f	1	0	0	0	0
60	1j	2	0	0	0	0
60	1l	5	0	0	0	0
60	1m	2	0	0	0	0
60	1o	4	0	0	0	0
60	1p	4	0	0	0	0
60	1t	2	0	0	0	0
60	1y	4	0	0	1	0
60	20	6	0	0	0	0
60	21	17	0	0	1	0
60	22	1	0	0	0	0
60	23	3	0	0	1	0
60	24	2	0	0	1	0
60	25	8	0	0	0	0
60	26	6	0	0	1	0
60	27	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	28	14	0	0	1	0
60	29	1	0	0	0	0
60	2A	2074	0	0	112	0
60	2B	44	0	0	2	0
60	2D	55	0	0	1	0
60	2E	37	0	0	5	0
60	2F	26	0	0	2	0
60	2G	7	0	0	1	0
60	2H	3	0	0	0	0
60	2I	3	0	0	1	0
60	2N	7	0	0	1	0
60	2O	19	0	0	0	0
60	2P	23	0	0	1	0
60	2Q	19	0	0	0	0
60	2R	19	0	0	3	0
60	2S	4	0	0	0	0
60	2T	9	0	0	0	0
60	2U	13	0	0	2	0
60	2V	7	0	0	0	0
60	2W	18	0	0	1	0
60	2X	7	0	0	0	0
60	2Y	3	0	0	0	0
60	2Z	14	0	0	2	0
60	2a	438	0	0	26	0
60	2d	4	0	0	0	0
60	2e	1	0	0	0	0
60	2f	1	0	0	0	0
60	2j	2	0	0	1	0
60	2l	6	0	0	0	0
60	2m	1	0	0	0	0
60	2n	1	0	0	0	0
60	2o	3	0	0	0	0
60	2p	2	0	0	0	0
60	2q	1	0	0	0	0
60	2r	4	0	0	0	0
60	2t	2	0	0	0	0
60	2y	4	0	0	0	0
All	All	297568	0	194515	4119	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 4119 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.40	1.18
32:2a:1003:G:H2'	32:2a:1004:A:H4'	1.41	1.01
1:1A:1082:U:O4	1:1A:1086:A:N1	1.95	0.99
15:1T:55:ASN:H	15:1T:59:THR:HG22	1.30	0.94
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.47	0.93

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	260 (95%)	13 (5%)	0	100 100
3	2D	273/276 (99%)	256 (94%)	17 (6%)	0	100 100
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24 42
4	2E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	24 42
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24 42
5	2F	201/210 (96%)	186 (92%)	14 (7%)	1 (0%)	24 42
6	1G	179/182 (98%)	159 (89%)	18 (10%)	2 (1%)	11 24
6	2G	179/182 (98%)	159 (89%)	18 (10%)	2 (1%)	11 24
7	1H	172/180 (96%)	158 (92%)	13 (8%)	1 (1%)	21 38
7	2H	171/180 (95%)	148 (86%)	21 (12%)	2 (1%)	10 22
8	1I	145/148 (98%)	129 (89%)	15 (10%)	1 (1%)	18 35
8	2I	144/148 (97%)	124 (86%)	18 (12%)	2 (1%)	9 19
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100 100
9	2N	138/140 (99%)	132 (96%)	3 (2%)	3 (2%)	5 12
10	1O	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16 31
10	2O	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18 35
11	2P	147/150 (98%)	137 (93%)	8 (5%)	2 (1%)	9 19
12	1Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	18 35
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	18 35
13	1R	116/118 (98%)	108 (93%)	8 (7%)	0	100 100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100 100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100 100
14	2S	108/112 (96%)	100 (93%)	5 (5%)	3 (3%)	4 9
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100 100
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100 100
16	1U	114/118 (97%)	111 (97%)	3 (3%)	0	100 100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100 100
17	1V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12 25
17	2V	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	6 13
18	1W	110/113 (97%)	110 (100%)	0	0	100 100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100 100
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11 24
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100 100
20	2Y	105/110 (96%)	96 (91%)	9 (9%)	0	100 100
21	1Z	201/206 (98%)	187 (93%)	14 (7%)	0	100 100
21	2Z	199/206 (97%)	174 (87%)	25 (13%)	0	100 100
22	10	75/85 (88%)	73 (97%)	2 (3%)	0	100 100
22	20	75/85 (88%)	72 (96%)	3 (4%)	0	100 100
23	11	95/98 (97%)	94 (99%)	0	1 (1%)	11 24
23	21	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11 24
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
24	22	68/72 (94%)	63 (93%)	5 (7%)	0	100 100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
25	23	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	6 15
26	14	67/71 (94%)	49 (73%)	14 (21%)	4 (6%)	1 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
26	24	67/71 (94%)	48 (72%)	13 (19%)	6 (9%)	0 0
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
27	25	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	6 15
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
29	17	46/49 (94%)	46 (100%)	0	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	62 (100%)	0	0	100 100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100 100
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	32 (91%)	3 (9%)	0	100 100
33	1b	229/256 (90%)	192 (84%)	27 (12%)	10 (4%)	2 3
33	2b	229/256 (90%)	192 (84%)	32 (14%)	5 (2%)	5 12
34	1c	204/239 (85%)	189 (93%)	15 (7%)	0	100 100
34	2c	204/239 (85%)	177 (87%)	25 (12%)	2 (1%)	12 25
35	1d	206/209 (99%)	186 (90%)	18 (9%)	2 (1%)	12 25
35	2d	206/209 (99%)	189 (92%)	17 (8%)	0	100 100
36	1e	146/162 (90%)	129 (88%)	16 (11%)	1 (1%)	18 35
36	2e	146/162 (90%)	140 (96%)	6 (4%)	0	100 100
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100 100
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100 100
38	1g	153/156 (98%)	146 (95%)	7 (5%)	0	100 100
38	2g	153/156 (98%)	141 (92%)	11 (7%)	1 (1%)	18 35
39	1h	135/138 (98%)	130 (96%)	5 (4%)	0	100 100
39	2h	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	18 35
40	1i	125/128 (98%)	113 (90%)	10 (8%)	2 (2%)	7 17
40	2i	124/128 (97%)	106 (86%)	15 (12%)	3 (2%)	4 10
41	1j	95/105 (90%)	74 (78%)	16 (17%)	5 (5%)	1 2
41	2j	94/105 (90%)	80 (85%)	11 (12%)	3 (3%)	3 7
42	1k	112/129 (87%)	99 (88%)	12 (11%)	1 (1%)	14 28
42	2k	112/129 (87%)	102 (91%)	10 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
43	1l	119/132 (90%)	106 (89%)	11 (9%)	2 (2%)	7 16
43	2l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	16 31
44	1m	114/126 (90%)	105 (92%)	7 (6%)	2 (2%)	6 15
44	2m	112/126 (89%)	97 (87%)	13 (12%)	2 (2%)	6 15
45	1n	58/61 (95%)	53 (91%)	5 (9%)	0	100 100
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7 16
46	1o	86/89 (97%)	84 (98%)	1 (1%)	1 (1%)	10 22
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100 100
47	1p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	9 21
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100 100
48	1q	97/105 (92%)	86 (89%)	11 (11%)	0	100 100
48	2q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	12 25
49	1r	66/88 (75%)	61 (92%)	4 (6%)	1 (2%)	8 18
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100 100
50	1s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	10 22
50	2s	81/93 (87%)	66 (82%)	15 (18%)	0	100 100
51	1t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	3 7
51	2t	96/106 (91%)	88 (92%)	7 (7%)	1 (1%)	12 25
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	17 (81%)	4 (19%)	0	100 100
53	1y	95/113 (84%)	92 (97%)	3 (3%)	0	100 100
53	2y	94/113 (83%)	86 (92%)	7 (7%)	1 (1%)	11 24
All	All	11629/12354 (94%)	10696 (92%)	834 (7%)	99 (1%)	14 28

5 of 99 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	47	LYS
7	1H	92	ILE
26	14	49	PHE
33	1b	8	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	214/218 (98%)	191 (89%)	23 (11%)	6 13
3	2D	215/218 (99%)	190 (88%)	25 (12%)	5 10
4	1E	164/166 (99%)	145 (88%)	19 (12%)	5 10
4	2E	164/166 (99%)	141 (86%)	23 (14%)	3 6
5	1F	160/166 (96%)	136 (85%)	24 (15%)	3 5
5	2F	159/166 (96%)	135 (85%)	24 (15%)	3 5
6	1G	144/156 (92%)	130 (90%)	14 (10%)	8 17
6	2G	142/156 (91%)	122 (86%)	20 (14%)	3 6
7	1H	144/148 (97%)	126 (88%)	18 (12%)	4 8
7	2H	143/148 (97%)	119 (83%)	24 (17%)	2 3
8	1I	111/124 (90%)	97 (87%)	14 (13%)	4 8
8	2I	108/124 (87%)	93 (86%)	15 (14%)	3 6
9	1N	119/119 (100%)	104 (87%)	15 (13%)	4 8
9	2N	118/119 (99%)	95 (80%)	23 (20%)	1 2
10	1O	100/100 (100%)	91 (91%)	9 (9%)	9 19
10	2O	100/100 (100%)	93 (93%)	7 (7%)	14 29
11	1P	115/116 (99%)	103 (90%)	12 (10%)	7 14
11	2P	115/116 (99%)	108 (94%)	7 (6%)	17 35
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11 23
12	2Q	111/111 (100%)	96 (86%)	15 (14%)	4 7
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6 12
13	2R	101/101 (100%)	84 (83%)	17 (17%)	2 3
14	1S	87/88 (99%)	77 (88%)	10 (12%)	5 10
14	2S	85/88 (97%)	76 (89%)	9 (11%)	6 13
15	1T	115/127 (91%)	108 (94%)	7 (6%)	17 35
15	2T	113/127 (89%)	101 (89%)	12 (11%)	6 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	1U	93/94 (99%)	80 (86%)	13 (14%)	3 6
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20 42
17	1V	81/82 (99%)	73 (90%)	8 (10%)	7 16
17	2V	80/82 (98%)	71 (89%)	9 (11%)	5 11
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11 25
18	2W	90/92 (98%)	79 (88%)	11 (12%)	5 9
19	1X	77/78 (99%)	72 (94%)	5 (6%)	15 32
19	2X	77/78 (99%)	71 (92%)	6 (8%)	11 25
20	1Y	86/91 (94%)	77 (90%)	9 (10%)	6 13
20	2Y	86/91 (94%)	79 (92%)	7 (8%)	11 23
21	1Z	169/179 (94%)	152 (90%)	17 (10%)	7 15
21	2Z	165/179 (92%)	147 (89%)	18 (11%)	6 12
22	10	61/67 (91%)	58 (95%)	3 (5%)	22 45
22	20	61/67 (91%)	59 (97%)	2 (3%)	33 58
23	11	79/83 (95%)	75 (95%)	4 (5%)	21 43
23	21	81/83 (98%)	73 (90%)	8 (10%)	7 16
24	12	65/67 (97%)	61 (94%)	4 (6%)	16 34
24	22	66/67 (98%)	61 (92%)	5 (8%)	12 26
25	13	51/52 (98%)	45 (88%)	6 (12%)	5 10
25	23	50/52 (96%)	44 (88%)	6 (12%)	5 9
26	14	58/63 (92%)	52 (90%)	6 (10%)	7 14
26	24	54/63 (86%)	47 (87%)	7 (13%)	4 7
27	15	51/52 (98%)	47 (92%)	4 (8%)	11 25
27	25	50/52 (96%)	47 (94%)	3 (6%)	17 36
28	16	51/52 (98%)	47 (92%)	4 (8%)	11 25
28	26	50/52 (96%)	46 (92%)	4 (8%)	11 24
29	17	41/42 (98%)	39 (95%)	2 (5%)	22 45
29	27	41/42 (98%)	36 (88%)	5 (12%)	5 9
30	18	54/55 (98%)	51 (94%)	3 (6%)	19 40
30	28	54/55 (98%)	48 (89%)	6 (11%)	6 12
31	19	34/34 (100%)	31 (91%)	3 (9%)	9 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	29	34/34 (100%)	31 (91%)	3 (9%)	9 20
33	1b	191/220 (87%)	159 (83%)	32 (17%)	2 3
33	2b	187/220 (85%)	165 (88%)	22 (12%)	5 10
34	1c	144/188 (77%)	132 (92%)	12 (8%)	10 22
34	2c	140/188 (74%)	124 (89%)	16 (11%)	5 11
35	1d	171/181 (94%)	150 (88%)	21 (12%)	4 8
35	2d	172/181 (95%)	156 (91%)	16 (9%)	8 18
36	1e	114/123 (93%)	107 (94%)	7 (6%)	17 35
36	2e	114/123 (93%)	102 (90%)	12 (10%)	6 13
37	1f	85/90 (94%)	76 (89%)	9 (11%)	6 13
37	2f	85/90 (94%)	80 (94%)	5 (6%)	18 37
38	1g	120/127 (94%)	109 (91%)	11 (9%)	8 19
38	2g	119/127 (94%)	111 (93%)	8 (7%)	15 31
39	1h	116/119 (98%)	101 (87%)	15 (13%)	4 7
39	2h	114/119 (96%)	101 (89%)	13 (11%)	5 11
40	1i	91/99 (92%)	78 (86%)	13 (14%)	3 6
40	2i	88/99 (89%)	74 (84%)	14 (16%)	2 4
41	1j	68/92 (74%)	58 (85%)	10 (15%)	3 5
41	2j	68/92 (74%)	56 (82%)	12 (18%)	2 3
42	1k	83/99 (84%)	74 (89%)	9 (11%)	6 12
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8 17
43	1l	96/108 (89%)	90 (94%)	6 (6%)	16 34
43	2l	96/108 (89%)	87 (91%)	9 (9%)	8 18
44	1m	90/101 (89%)	79 (88%)	11 (12%)	5 9
44	2m	87/101 (86%)	75 (86%)	12 (14%)	3 7
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5 9
45	2n	49/50 (98%)	41 (84%)	8 (16%)	2 4
46	1o	78/80 (98%)	69 (88%)	9 (12%)	5 10
46	2o	78/80 (98%)	69 (88%)	9 (12%)	5 10
47	1p	69/74 (93%)	58 (84%)	11 (16%)	2 4
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
48	1q	94/97 (97%)	85 (90%)	9 (10%)	8 17
48	2q	94/97 (97%)	84 (89%)	10 (11%)	6 13
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10 22
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7 15
50	1s	68/80 (85%)	60 (88%)	8 (12%)	5 10
50	2s	67/80 (84%)	53 (79%)	14 (21%)	1 1
51	1t	71/82 (87%)	64 (90%)	7 (10%)	7 16
51	2t	70/82 (85%)	62 (89%)	8 (11%)	5 11
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6 12
52	2u	18/22 (82%)	18 (100%)	0	100 100
53	1y	82/98 (84%)	78 (95%)	4 (5%)	22 45
53	2y	79/98 (81%)	68 (86%)	11 (14%)	3 6
All	All	9524/10260 (93%)	8477 (89%)	1047 (11%)	6 12

5 of 1047 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	2i	71	SER
43	2l	34	ARG
40	2i	65	VAL
53	2y	23	ARG
39	1h	121	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
40	2i	3	GLN
44	2m	12	ASN
40	1i	3	GLN
38	1g	110	GLN
46	2o	28	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	437 (15%)	25 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2A	2858/2915 (98%)	499 (17%)	37 (1%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	119/121 (98%)	22 (18%)	0
32	1a	1497/1521 (98%)	251 (16%)	0
32	2a	1501/1521 (98%)	276 (18%)	0
All	All	8959/9114 (98%)	1497 (16%)	62 (0%)

5 of 1497 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	71	A

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	266	G
1	2A	2406	U
1	2A	856	C
1	2A	2321	G
1	2A	2602	A

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

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	5MU	2A	1939	1,54	19,22,23	1.50	6 (31%)	27,32,35	2.12	6 (22%)
32	4OC	2a	1402	32	20,23,24	0.75	0	25,32,35	1.08	2 (8%)
32	MA6	2a	1519	32	23,26,27	0.39	0	33,38,41	2.08	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MC	2A	1962	1,54	19,22,23	1.57	3 (15%)	26,32,35	1.08	2 (7%)
1	5MU	1A	1915	1	19,22,23	1.42	5 (26%)	27,32,35	2.38	8 (29%)
1	PSU	1A	1911	1	18,21,22	1.35	2 (11%)	21,30,33	2.08	5 (23%)
32	PSU	2a	516	54,32	18,21,22	1.34	3 (16%)	21,30,33	2.09	5 (23%)
1	5MC	1A	1962	1,54	19,22,23	1.57	3 (15%)	26,32,35	1.15	4 (15%)
43	0TD	1l	92	43	8,9,10	4.52	1 (12%)	6,11,13	4.26	2 (33%)
32	5MC	2a	1407	32	19,22,23	1.70	3 (15%)	26,32,35	1.20	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.70	2 (10%)	26,32,35	1.15	4 (15%)
1	OMU	2A	2552	1,54	19,22,23	1.18	3 (15%)	25,31,34	1.90	5 (20%)
32	MA6	1a	1519	32	23,26,27	0.45	0	33,38,41	1.98	9 (27%)
1	OMG	2A	2251	1,54	23,26,27	1.19	3 (13%)	32,38,41	2.01	6 (18%)
32	2MG	2a	1207	32	23,26,27	1.25	3 (13%)	33,38,41	2.10	7 (21%)
32	2MG	1a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.38	9 (27%)
1	2MA	1A	2503	1,54	22,25,26	1.49	5 (22%)	32,37,40	2.31	6 (18%)
1	5MC	1A	1942	1	19,22,23	1.57	3 (15%)	26,32,35	1.14	3 (11%)
32	5MC	2a	1404	32	19,22,23	1.67	3 (15%)	26,32,35	1.12	2 (7%)
32	G7M	2a	527	54,32	23,26,27	1.51	4 (17%)	34,39,42	1.71	5 (14%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	0.95	1 (4%)
32	5MC	2a	967	32	19,22,23	1.84	3 (15%)	26,32,35	1.07	2 (7%)
32	UR3	2a	1498	32	19,22,23	0.97	1 (5%)	26,32,35	1.66	3 (11%)
32	UR3	1a	1498	32	19,22,23	0.93	1 (5%)	26,32,35	1.75	3 (11%)
1	2MA	2A	2503	1,54	22,25,26	1.47	4 (18%)	32,37,40	2.33	8 (25%)
32	M2G	2a	966	54,32	24,27,28	1.28	3 (12%)	33,40,43	1.82	6 (18%)
32	5MC	1a	1400	32	19,22,23	1.66	3 (15%)	26,32,35	1.07	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.36	2 (11%)	21,30,33	1.88	3 (14%)
1	OMC	2A	1920	1	19,22,23	0.78	0	25,31,34	0.95	1 (4%)
32	PSU	1a	516	54,32	18,21,22	1.38	2 (11%)	21,30,33	1.88	5 (23%)
32	M2G	1a	966	32	24,27,28	1.29	3 (12%)	33,40,43	1.81	5 (15%)
1	PSU	1A	2605	1	18,21,22	1.37	4 (22%)	21,30,33	1.80	4 (19%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.00	4 (19%)
1	5MC	2A	1942	1	19,22,23	1.60	3 (15%)	26,32,35	1.14	2 (7%)
1	5MU	1A	1939	1,54	19,22,23	1.41	5 (26%)	27,32,35	2.18	6 (22%)
1	5MU	2A	1915	1	19,22,23	1.47	4 (21%)	27,32,35	2.24	9 (33%)
32	5MC	2a	1400	32	19,22,23	1.58	3 (15%)	26,32,35	1.24	3 (11%)
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	1.98	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.04	3 (14%)
32	G7M	1a	527	54,32	23,26,27	1.59	3 (13%)	34,39,42	1.75	5 (14%)
43	0TD	2l	92	43	8,9,10	4.44	1 (12%)	6,11,13	3.01	3 (50%)
32	5MC	1a	967	32	19,22,23	1.57	3 (15%)	26,32,35	1.05	2 (7%)
1	OMG	1A	2251	1,54	23,26,27	1.24	3 (13%)	32,38,41	2.06	6 (18%)
1	OMU	1A	2552	1,54	19,22,23	1.27	3 (15%)	25,31,34	1.71	5 (20%)
1	OMC	1A	1920	1	19,22,23	0.79	0	25,31,34	0.88	0
32	5MC	1a	1404	32	19,22,23	1.70	3 (15%)	26,32,35	1.13	2 (7%)
32	MA6	2a	1518	32	23,26,27	0.39	0	33,38,41	2.01	9 (27%)
32	MA6	1a	1518	32	23,26,27	0.43	0	33,38,41	2.02	9 (27%)

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	5MU	2A	1939	1,54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	5MC	2A	1962	1,54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	54,32	-	1/7/25/26	0/2/2/2
1	5MC	1A	1962	1,54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,54	-	0/9/27/28	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
1	OMG	2A	2251	1,54	-	0/9/27/28	0/3/3/3
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	2MG	1a	1207	32	-	2/9/27/28	0/3/3/3
1	2MA	1A	2503	1,54	-	2/7/25/26	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	54,32	-	2/7/25/26	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,54	-	0/7/25/26	0/3/3/3
32	M2G	2a	966	54,32	-	1/11/29/30	0/3/3/3
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
32	PSU	1a	516	54,32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	54,32	-	3/7/25/26	0/3/3/3
43	0TD	2l	92	43	-	1/7/12/14	-
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,54	-	0/9/27/28	0/3/3/3
1	OMU	1A	2552	1,54	-	0/9/27/28	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	1a	1404	32	-	2/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/11/29/30	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3

The worst 5 of 118 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.30	1.69	1.82
43	2l	92	0TD	CB-SB	-12.18	1.70	1.82
32	2a	967	5MC	C5-C4	6.80	1.49	1.44
32	1a	1407	5MC	C5-C4	6.35	1.48	1.44
32	2a	1407	5MC	C5-C4	6.18	1.48	1.44

The worst 5 of 215 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	9.97	120.28	102.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2503	2MA	C5-C4-N3	-8.76	117.95	127.18
1	2A	2503	2MA	C5-C4-N3	-8.19	118.55	127.18
32	1a	1207	2MG	C2-N3-C4	7.45	121.31	112.00
32	1a	1498	UR3	C4-N3-C2	-6.94	119.00	124.58

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
1	2A	1915	5MU	O4'-C1'-N1-C2

There are no ring outliers.

22 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1939	5MU	2	0
32	2a	1402	4OC	2	0
32	2a	1519	MA6	2	0
1	1A	1915	5MU	1	0
32	2a	516	PSU	1	0
43	1l	92	0TD	2	0
1	2A	2552	OMU	1	0
32	1a	1519	MA6	1	0
1	2A	2251	OMG	2	0
32	2a	1207	2MG	3	0
1	1A	1942	5MC	1	0
32	1a	1402	4OC	1	0
1	2A	2503	2MA	1	0
32	2a	966	M2G	1	0
1	1A	1939	5MU	2	0
1	2A	1915	5MU	2	0
1	2A	1911	PSU	1	0
32	1a	527	G7M	1	0
1	1A	2251	OMG	1	0
1	1A	1920	OMC	1	0
32	2a	1518	MA6	3	0
32	1a	1518	MA6	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2519 ligands modelled in this entry, 2506 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	$\#\|Z\|>2$
56	MPD	2A	3743	-	7,7,7	0.31	0	9,10,10	0.25	0
56	MPD	1A	4012	-	7,7,7	0.37	0	9,10,10	0.23	0
56	MPD	1T	205	-	7,7,7	0.34	0	9,10,10	0.32	0
57	ARG	1B	232	-	10,11,11	0.74	1 (10%)	9,13,13	0.95	1 (11%)
55	A1CQ7	1A	4011	-	40,42,42	3.04	10 (25%)	54,65,65	2.42	21 (38%)
56	MPD	1a	3278	32	7,7,7	0.34	0	9,10,10	0.48	0
56	MPD	2B	221	-	7,7,7	0.32	0	9,10,10	0.32	0
55	A1CQ7	2A	3741	-	40,42,42	3.06	13 (32%)	54,65,65	2.40	19 (35%)
56	MPD	2A	3742	-	7,7,7	0.28	0	9,10,10	0.35	0
56	MPD	18	104	-	7,7,7	0.33	0	9,10,10	0.30	0
59	SF4	1d	306	35	0,12,12	-	-	-		
57	ARG	1F	318	-	10,11,11	0.72	1 (10%)	9,13,13	1.02	1 (11%)
59	SF4	2d	501	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	MPD	2A	3743	-	-	2/5/5/5	-
56	MPD	1A	4012	-	-	2/5/5/5	-
56	MPD	1T	205	-	-	0/5/5/5	-
57	ARG	1B	232	-	-	4/11/11/11	-
55	A1CQ7	1A	4011	-	-	0/15/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	MPD	1a	3278	32	-	3/5/5/5	-
56	MPD	2B	221	-	-	1/5/5/5	-
55	A1CQ7	2A	3741	-	-	1/15/77/77	0/5/5/5
56	MPD	2A	3742	-	-	2/5/5/5	-
56	MPD	18	104	-	-	2/5/5/5	-
59	SF4	1d	306	35	-	-	0/6/5/5
57	ARG	1F	318	-	-	3/11/11/11	-
59	SF4	2d	501	35	-	-	0/6/5/5

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2A	3741	A1CQ7	CBG-CBE	-10.72	1.31	1.47
55	1A	4011	A1CQ7	CBG-CBE	-10.47	1.32	1.47
55	1A	4011	A1CQ7	CAA-CAQ	-9.08	1.39	1.53
55	2A	3741	A1CQ7	CAA-CAQ	-8.70	1.40	1.53
55	1A	4011	A1CQ7	CAT-CAQ	-8.66	1.37	1.51

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1A	4011	A1CQ7	CAK-CAC-CAB	-8.76	106.88	116.28
55	2A	3741	A1CQ7	CAK-CAC-CAB	-7.87	107.83	116.28
55	1A	4011	A1CQ7	CAZ-CAB-CAC	-5.23	103.47	108.81
55	2A	3741	A1CQ7	CAE-CAF-CAG	-4.90	106.06	112.38
55	2A	3741	A1CQ7	CAZ-CAB-CAC	-4.61	104.10	108.81

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	2A	3741	A1CQ7	CAK-CAJ-CAN-CBA
56	1a	3278	MPD	C2-C3-C4-O4
56	1a	3278	MPD	C2-C3-C4-C5
56	2A	3742	MPD	C2-C3-C4-O4
56	2A	3742	MPD	C2-C3-C4-C5

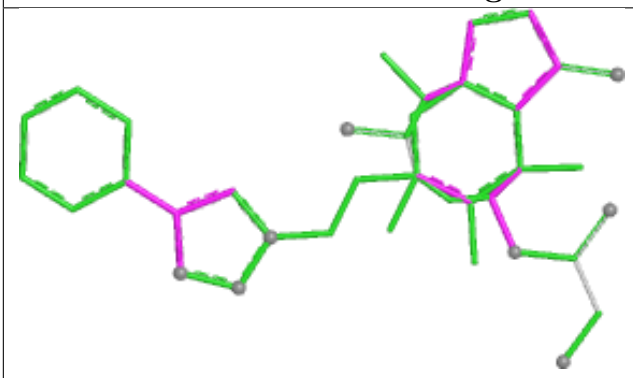
There are no ring outliers.

8 monomers are involved in 17 short contacts:

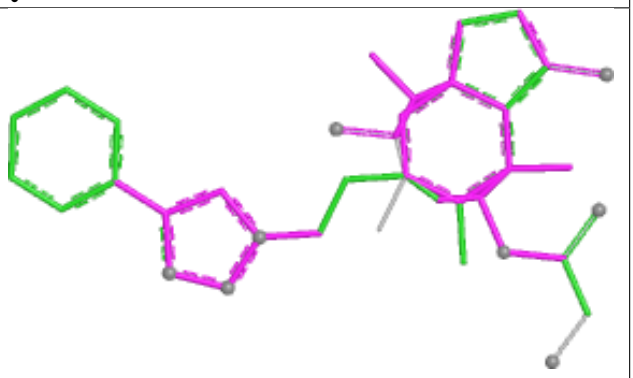
Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	1A	4012	MPD	1	0
56	1T	205	MPD	1	0
57	1B	232	ARG	3	0
56	1a	3278	MPD	3	0
56	2A	3742	MPD	1	0
56	18	104	MPD	2	0
57	1F	318	ARG	3	0
59	2d	501	SF4	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

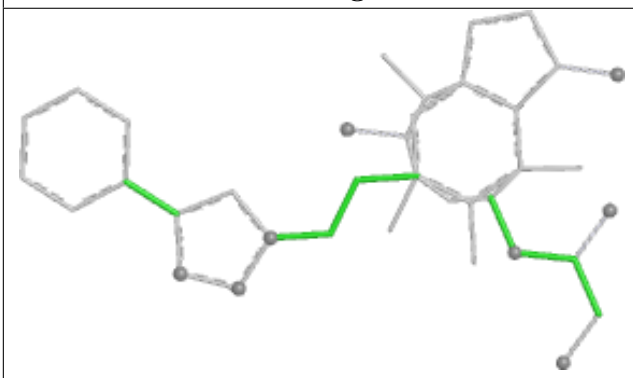
Ligand A1CQ7 1A 4011



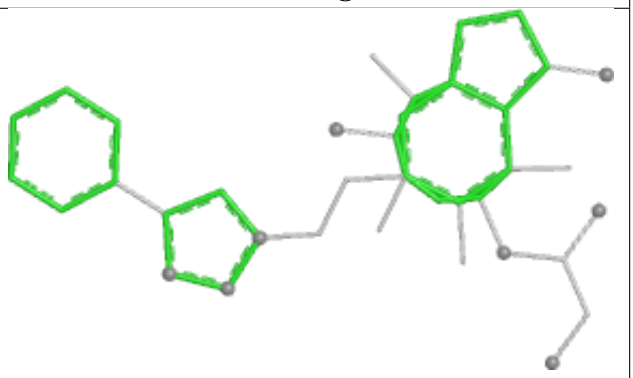
Bond lengths



Bond angles

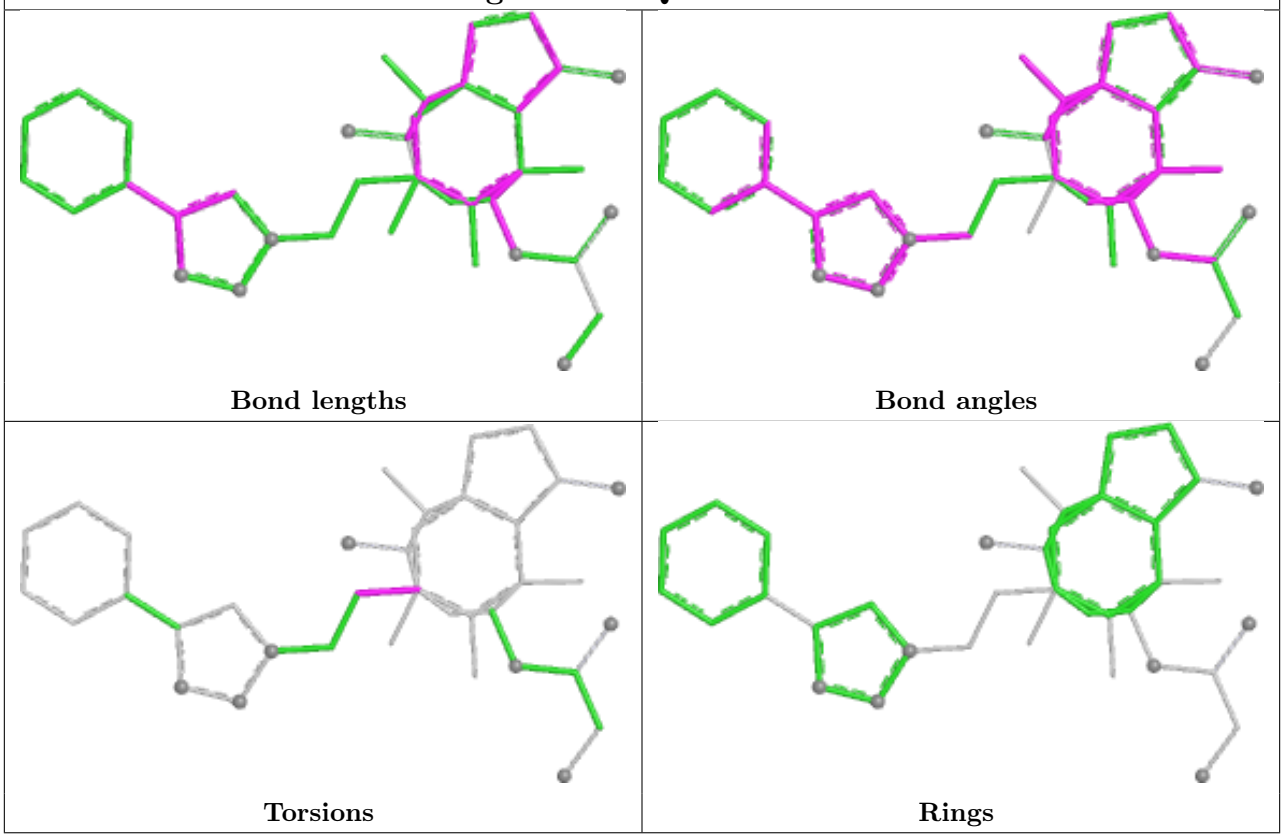


Torsions



Rings

Ligand A1CQ7 2A 3741



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, 95^{th} 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%)	-0.40	139 (4%) 35 27	10, 26, 87, 103	0
1	2A	2856/2915 (97%)	0.07	173 (6%) 27 20	23, 45, 90, 103	0
2	1B	120/121 (99%)	-0.15	1 (0%) 82 78	22, 42, 58, 75	0
2	2B	120/121 (99%)	0.98	4 (3%) 49 40	46, 72, 81, 84	0
3	1D	275/276 (99%)	-0.26	1 (0%) 88 87	11, 26, 41, 64	0
3	2D	275/276 (99%)	-0.03	3 (1%) 78 73	22, 38, 54, 73	0
4	1E	204/206 (99%)	-0.29	1 (0%) 87 85	9, 29, 49, 66	0
4	2E	204/206 (99%)	0.18	3 (1%) 72 65	21, 45, 62, 71	0
5	1F	203/210 (96%)	-0.25	2 (0%) 79 74	9, 30, 57, 76	0
5	2F	203/210 (96%)	0.39	4 (1%) 65 57	24, 53, 69, 81	0
6	1G	181/182 (99%)	0.64	11 (6%) 27 20	38, 55, 72, 83	0
6	2G	181/182 (99%)	1.64	53 (29%) 1 1	66, 76, 84, 88	0
7	1H	174/180 (96%)	0.15	5 (2%) 53 45	27, 42, 56, 64	0
7	2H	173/180 (96%)	1.09	12 (6%) 23 17	59, 72, 78, 84	0
8	1I	147/148 (99%)	0.66	5 (3%) 48 38	31, 61, 73, 79	0
8	2I	146/148 (98%)	0.77	8 (5%) 30 23	42, 65, 75, 83	0
9	1N	140/140 (100%)	-0.21	1 (0%) 84 80	15, 28, 50, 64	0
9	2N	140/140 (100%)	0.42	4 (2%) 53 45	33, 51, 65, 72	0
10	1O	122/122 (100%)	-0.25	1 (0%) 82 78	17, 28, 46, 52	0
10	2O	122/122 (100%)	0.01	1 (0%) 82 78	32, 43, 56, 68	0
11	1P	149/150 (99%)	-0.25	0 100 100	11, 34, 53, 65	0
11	2P	149/150 (99%)	0.41	5 (3%) 48 38	25, 55, 70, 81	0
12	1Q	141/141 (100%)	-0.29	0 100 100	15, 29, 44, 58	0
12	2Q	141/141 (100%)	0.41	4 (2%) 55 46	34, 51, 63, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.31	0 100 100	15, 25, 40, 54	0
13	2R	118/118 (100%)	-0.10	0 100 100	27, 39, 50, 58	0
14	1S	110/112 (98%)	0.14	1 (0%) 81 76	28, 41, 55, 58	0
14	2S	110/112 (98%)	1.52	26 (23%) 2 2	53, 67, 75, 77	0
15	1T	131/146 (89%)	-0.06	3 (2%) 61 52	23, 33, 60, 69	0
15	2T	131/146 (89%)	0.30	4 (3%) 51 43	38, 47, 67, 79	0
16	1U	116/118 (98%)	-0.46	0 100 100	13, 21, 38, 54	0
16	2U	116/118 (98%)	0.36	0 100 100	30, 47, 64, 70	0
17	1V	101/101 (100%)	-0.23	0 100 100	13, 31, 47, 57	0
17	2V	101/101 (100%)	0.70	2 (1%) 65 57	28, 58, 68, 75	0
18	1W	112/113 (99%)	-0.36	0 100 100	13, 21, 44, 75	0
18	2W	112/113 (99%)	-0.06	1 (0%) 81 76	27, 37, 56, 77	0
19	1X	95/96 (98%)	-0.24	1 (1%) 78 73	17, 27, 49, 59	0
19	2X	95/96 (98%)	0.48	3 (3%) 50 41	34, 48, 63, 68	0
20	1Y	107/110 (97%)	0.11	2 (1%) 66 59	26, 38, 57, 64	0
20	2Y	107/110 (97%)	0.92	7 (6%) 25 18	42, 60, 70, 77	0
21	1Z	203/206 (98%)	0.41	3 (1%) 72 65	31, 47, 65, 75	0
21	2Z	201/206 (97%)	1.15	22 (10%) 10 8	51, 66, 77, 86	0
22	10	77/85 (90%)	-0.06	1 (1%) 75 68	19, 27, 42, 54	0
22	20	77/85 (90%)	0.72	4 (5%) 33 25	41, 51, 61, 66	0
23	11	97/98 (98%)	0.07	3 (3%) 51 43	19, 34, 60, 67	0
23	21	97/98 (98%)	0.38	2 (2%) 63 55	28, 43, 64, 69	0
24	12	70/72 (97%)	-0.10	1 (1%) 73 67	24, 36, 51, 79	0
24	22	70/72 (97%)	0.69	3 (4%) 40 31	47, 60, 67, 71	0
25	13	59/60 (98%)	0.00	1 (1%) 69 63	19, 27, 51, 62	0
25	23	59/60 (98%)	0.44	3 (5%) 33 26	37, 51, 64, 72	0
26	14	69/71 (97%)	1.18	10 (14%) 6 4	51, 69, 85, 89	0
26	24	69/71 (97%)	1.80	25 (36%) 1 1	70, 81, 89, 92	0
27	15	59/60 (98%)	-0.28	1 (1%) 69 63	11, 25, 50, 60	0
27	25	59/60 (98%)	0.08	0 100 100	25, 42, 59, 69	0
28	16	53/54 (98%)	-0.15	0 100 100	23, 32, 43, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.48	2 (3%) 44 35	43, 49, 57, 65	0
29	17	48/49 (97%)	-0.41	1 (2%) 63 55	11, 16, 49, 55	0
29	27	48/49 (97%)	0.08	3 (6%) 26 19	20, 30, 56, 65	0
30	18	64/65 (98%)	-0.33	0 100 100	17, 22, 31, 42	0
30	28	64/65 (98%)	0.27	1 (1%) 70 64	34, 42, 51, 60	0
31	19	37/37 (100%)	-0.31	0 100 100	19, 30, 45, 54	0
31	29	37/37 (100%)	0.82	0 100 100	46, 55, 64, 68	0
32	1a	1488/1521 (97%)	0.54	64 (4%) 40 31	25, 63, 87, 103	0
32	2a	1492/1521 (98%)	0.69	99 (6%) 24 18	33, 67, 89, 102	0
33	1b	231/256 (90%)	1.25	43 (18%) 3 3	58, 71, 81, 87	0
33	2b	231/256 (90%)	1.59	67 (29%) 1 1	62, 76, 84, 89	0
34	1c	206/239 (86%)	1.15	19 (9%) 14 11	58, 68, 77, 81	0
34	2c	206/239 (86%)	1.78	73 (35%) 1 1	63, 77, 82, 91	0
35	1d	208/209 (99%)	1.39	42 (20%) 3 3	48, 65, 74, 82	0
35	2d	208/209 (99%)	1.10	31 (14%) 5 4	52, 63, 71, 76	0
36	1e	148/162 (91%)	0.65	6 (4%) 41 32	38, 56, 66, 78	0
36	2e	148/162 (91%)	1.05	14 (9%) 14 11	53, 64, 73, 80	0
37	1f	100/101 (99%)	0.73	3 (3%) 52 44	47, 59, 68, 72	0
37	2f	100/101 (99%)	0.69	2 (2%) 65 57	46, 60, 70, 73	0
38	1g	155/156 (99%)	0.72	6 (3%) 43 34	55, 64, 72, 78	0
38	2g	155/156 (99%)	1.12	19 (12%) 8 6	61, 71, 77, 83	0
39	1h	137/138 (99%)	0.70	5 (3%) 46 36	47, 59, 67, 73	0
39	2h	137/138 (99%)	0.75	5 (3%) 46 36	52, 62, 69, 79	0
40	1i	127/128 (99%)	1.44	27 (21%) 2 2	53, 71, 79, 83	0
40	2i	126/128 (98%)	1.96	57 (45%) 0 0	68, 78, 85, 86	0
41	1j	97/105 (92%)	1.54	24 (24%) 2 1	56, 73, 80, 84	0
41	2j	96/105 (91%)	2.08	48 (50%) 0 0	69, 78, 85, 87	0
42	1k	114/129 (88%)	0.70	6 (5%) 32 24	34, 54, 68, 73	0
42	2k	114/129 (88%)	0.97	9 (7%) 18 14	51, 63, 71, 78	0
43	1l	121/132 (91%)	0.37	6 (4%) 34 27	40, 50, 61, 70	0
43	2l	121/132 (91%)	0.87	9 (7%) 20 14	46, 57, 65, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	116/126 (92%)	1.12	13 (11%) 10 8	56, 68, 74, 80	0
44	2m	114/126 (90%)	1.40	26 (22%) 2 2	66, 77, 83, 87	0
45	1n	60/61 (98%)	1.01	4 (6%) 24 17	56, 66, 72, 76	0
45	2n	60/61 (98%)	2.06	27 (45%) 0 0	68, 77, 82, 84	0
46	1o	88/89 (98%)	0.79	4 (4%) 38 29	42, 58, 67, 76	0
46	2o	88/89 (98%)	0.66	0 100 100	47, 61, 70, 73	0
47	1p	82/88 (93%)	1.35	18 (21%) 2 2	51, 64, 74, 81	0
47	2p	82/88 (93%)	0.88	4 (4%) 35 27	50, 61, 72, 77	0
48	1q	99/105 (94%)	0.90	5 (5%) 33 26	41, 58, 67, 71	0
48	2q	99/105 (94%)	0.72	3 (3%) 52 44	47, 60, 69, 72	0
49	1r	68/88 (77%)	0.85	2 (2%) 53 45	48, 57, 68, 73	0
49	2r	68/88 (77%)	0.60	2 (2%) 53 45	52, 61, 69, 72	0
50	1s	83/93 (89%)	1.18	9 (10%) 11 8	61, 70, 79, 79	0
50	2s	83/93 (89%)	1.82	35 (42%) 0 0	67, 81, 87, 90	0
51	1t	96/106 (90%)	0.94	9 (9%) 14 11	49, 64, 72, 75	0
51	2t	98/106 (92%)	0.83	7 (7%) 22 16	48, 60, 72, 74	0
52	1u	23/27 (85%)	1.38	2 (8%) 16 12	59, 67, 71, 72	0
52	2u	23/27 (85%)	2.37	17 (73%) 0 0	68, 75, 79, 81	0
53	1y	97/113 (85%)	0.70	5 (5%) 33 25	46, 59, 68, 77	0
53	2y	96/113 (84%)	1.73	29 (30%) 1 1	62, 74, 82, 88	0
All	All	20766/21468 (96%)	0.40	1482 (7%) 22 16	9, 54, 82, 103	0

The worst 5 of 1482 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1076	C	9.0
1	1A	2174	C	8.9
1	1A	1064	C	8.4
1	2A	2162	G	8.0
1	2A	2173	A	7.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	2MG	2a	1207	24/25	0.78	0.15	75,82,89,96	0
1	5MU	2A	1915	21/22	0.83	0.12	66,77,84,95	0
32	5MC	2a	967	21/22	0.84	0.15	64,70,78,89	0
32	M2G	2a	966	25/26	0.85	0.15	58,66,74,85	0
1	5MU	1A	1915	21/22	0.88	0.12	63,73,82,86	0
32	2MG	1a	1207	24/25	0.89	0.12	65,69,74,80	0
1	PSU	2A	1917	20/21	0.89	0.09	68,73,88,94	0
32	G7M	2a	527	24/25	0.89	0.12	55,62,66,67	0
1	PSU	2A	1911	20/21	0.90	0.10	58,63,77,79	0
32	PSU	2a	516	20/21	0.90	0.11	65,72,77,82	0
1	PSU	1A	1917	20/21	0.90	0.11	53,62,79,79	0
1	PSU	1A	1911	20/21	0.91	0.11	44,57,61,62	0
32	4OC	2a	1402	22/23	0.91	0.13	50,62,64,66	0
32	5MC	2a	1400	21/22	0.92	0.11	56,64,70,73	0
43	0TD	1l	92	10/11	0.92	0.12	46,51,55,57	0
43	0TD	2l	92	10/11	0.92	0.11	52,55,61,69	0
32	PSU	1a	516	20/21	0.93	0.11	54,57,62,63	0
1	OMC	2A	1920	21/22	0.93	0.10	49,61,64,68	0
32	M2G	1a	966	25/26	0.94	0.10	48,55,60,64	0
32	5MC	2a	1407	21/22	0.94	0.10	45,53,57,58	0
32	MA6	2a	1518	24/25	0.94	0.11	47,57,60,63	0
32	5MC	1a	967	21/22	0.94	0.10	49,57,70,70	0
32	MA6	1a	1519	24/25	0.95	0.10	31,38,42,47	0
32	G7M	1a	527	24/25	0.95	0.09	35,46,51,56	0
32	UR3	2a	1498	21/22	0.95	0.10	48,54,60,64	0
32	5MC	1a	1400	21/22	0.95	0.10	33,48,53,57	0
32	5MC	1a	1407	21/22	0.95	0.09	34,44,46,48	0
1	OMC	1A	1920	21/22	0.96	0.09	38,45,54,55	0
32	5MC	2a	1404	21/22	0.96	0.08	41,52,57,57	0
32	UR3	1a	1498	21/22	0.96	0.10	35,40,47,53	0
1	5MC	2A	1942	21/22	0.96	0.10	33,42,46,48	0
1	2MA	2A	2503	23/24	0.96	0.10	19,27,31,34	0
32	MA6	2a	1519	24/25	0.96	0.11	44,54,59,60	0
32	4OC	1a	1402	22/23	0.96	0.09	39,44,48,56	0
32	MA6	1a	1518	24/25	0.97	0.09	33,37,41,48	0
32	5MC	1a	1404	21/22	0.97	0.08	31,35,40,42	0
1	5MC	1A	1962	21/22	0.97	0.08	23,27,30,34	0
1	5MU	2A	1939	21/22	0.97	0.09	28,32,35,35	0
1	5MC	1A	1942	21/22	0.97	0.08	19,26,30,32	0
1	5MC	2A	1962	21/22	0.97	0.07	27,34,44,57	0
1	OMG	2A	2251	24/25	0.97	0.07	24,31,33,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	1A	2605	20/21	0.98	0.06	13,18,26,27	0
1	5MU	1A	1939	21/22	0.98	0.07	14,18,21,22	0
1	2MA	1A	2503	23/24	0.98	0.07	7,11,12,15	0
1	OMU	2A	2552	21/22	0.98	0.06	23,31,35,36	0
1	PSU	2A	2605	20/21	0.98	0.07	26,30,34,35	0
1	OMU	1A	2552	21/22	0.98	0.07	16,19,25,28	0
1	OMG	1A	2251	24/25	0.99	0.06	12,15,17,17	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(Å^2)	Q<0.9
54	MG	1a	3200	1/1	0.48	0.18	67,67,67,67	0
54	MG	1a	3152	1/1	0.52	0.20	68,68,68,68	0
54	MG	1A	3750	1/1	0.53	0.22	61,61,61,61	0
54	MG	1A	3881	1/1	0.59	0.20	50,50,50,50	0
54	MG	2A	3505	1/1	0.60	0.25	62,62,62,62	0
54	MG	2j	201	1/1	0.60	0.12	80,80,80,80	0
54	MG	1t	202	1/1	0.64	0.14	56,56,56,56	0
54	MG	1A	3287	1/1	0.64	0.15	75,75,75,75	0
54	MG	2A	3523	1/1	0.64	0.16	71,71,71,71	0
54	MG	1A	3634	1/1	0.64	0.15	61,61,61,61	0
54	MG	2A	3715	1/1	0.65	0.13	70,70,70,70	0
56	MPD	2B	221	8/8	0.65	0.33	56,65,69,70	0
54	MG	2A	3721	1/1	0.66	0.28	70,70,70,70	0
54	MG	2a	3140	1/1	0.66	0.30	79,79,79,79	0
54	MG	1A	3027	1/1	0.66	0.27	58,58,58,58	0
54	MG	1a	3077	1/1	0.66	0.20	67,67,67,67	0
54	MG	2A	3734	1/1	0.68	0.21	69,69,69,69	0
54	MG	1a	3168	1/1	0.68	0.19	80,80,80,80	0
54	MG	1a	3164	1/1	0.69	0.17	61,61,61,61	0
54	MG	2A	3171	1/1	0.69	0.19	59,59,59,59	0
54	MG	1A	3859	1/1	0.70	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3055	1/1	0.70	0.32	64,64,64,64	0
54	MG	2a	3063	1/1	0.70	0.18	69,69,69,69	0
54	MG	1a	3006	1/1	0.71	0.14	58,58,58,58	0
54	MG	2G	202	1/1	0.71	0.14	69,69,69,69	0
54	MG	1B	226	1/1	0.71	0.13	46,46,46,46	0
54	MG	1a	3236	1/1	0.71	0.15	67,67,67,67	0
54	MG	2a	3145	1/1	0.71	0.15	79,79,79,79	0
54	MG	1a	3244	1/1	0.71	0.16	71,71,71,71	0
54	MG	1a	3066	1/1	0.71	0.25	68,68,68,68	0
54	MG	2A	3488	1/1	0.72	0.19	58,58,58,58	0
54	MG	1A	3087	1/1	0.72	0.12	59,59,59,59	0
54	MG	1F	316	1/1	0.72	0.24	40,40,40,40	0
54	MG	1a	3274	1/1	0.73	0.35	70,70,70,70	0
54	MG	2B	207	1/1	0.73	0.18	71,71,71,71	0
54	MG	1f	201	1/1	0.73	0.17	57,57,57,57	0
54	MG	2a	3007	1/1	0.73	0.12	57,57,57,57	0
54	MG	1a	3157	1/1	0.73	0.12	64,64,64,64	0
54	MG	2A	3611	1/1	0.73	0.21	66,66,66,66	0
54	MG	1A	3564	1/1	0.73	0.22	61,61,61,61	0
54	MG	2A	3418	1/1	0.73	0.17	51,51,51,51	0
54	MG	2k	201	1/1	0.73	0.22	69,69,69,69	0
54	MG	2A	3726	1/1	0.73	0.25	69,69,69,69	0
54	MG	2B	219	1/1	0.74	0.18	76,76,76,76	0
54	MG	1a	3033	1/1	0.74	0.13	45,45,45,45	0
54	MG	2Q	202	1/1	0.74	0.26	49,49,49,49	0
54	MG	2T	202	1/1	0.74	0.14	55,55,55,55	0
54	MG	2A	3100	1/1	0.74	0.18	61,61,61,61	0
54	MG	2A	3714	1/1	0.74	0.15	54,54,54,54	0
54	MG	2A	3108	1/1	0.74	0.19	63,63,63,63	0
54	MG	14	101	1/1	0.74	0.13	72,72,72,72	0
54	MG	1a	3254	1/1	0.74	0.26	65,65,65,65	0
54	MG	1a	3198	1/1	0.74	0.15	71,71,71,71	0
54	MG	2n	101	1/1	0.74	0.17	61,61,61,61	0
54	MG	1a	3158	1/1	0.74	0.25	58,58,58,58	0
54	MG	1A	3905	1/1	0.75	0.14	25,25,25,25	0
54	MG	2a	3113	1/1	0.75	0.24	63,63,63,63	0
54	MG	1a	3020	1/1	0.75	0.13	59,59,59,59	0
54	MG	1a	3114	1/1	0.75	0.14	73,73,73,73	0
54	MG	1a	3255	1/1	0.75	0.20	50,50,50,50	0
54	MG	2A	3260	1/1	0.75	0.19	59,59,59,59	0
54	MG	1Z	301	1/1	0.75	0.16	54,54,54,54	0
54	MG	2t	201	1/1	0.75	0.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3186	1/1	0.75	0.11	50,50,50,50	0
54	MG	1B	224	1/1	0.76	0.13	46,46,46,46	0
54	MG	1a	3084	1/1	0.76	0.20	60,60,60,60	0
54	MG	2a	3162	1/1	0.76	0.15	51,51,51,51	0
54	MG	2A	3195	1/1	0.76	0.22	61,61,61,61	0
54	MG	1a	3195	1/1	0.76	0.17	52,52,52,52	0
54	MG	2a	3020	1/1	0.76	0.23	58,58,58,58	0
54	MG	2A	3697	1/1	0.76	0.47	50,50,50,50	0
54	MG	1a	3268	1/1	0.76	0.14	58,58,58,58	0
54	MG	1A	3976	1/1	0.77	0.19	54,54,54,54	0
54	MG	1B	209	1/1	0.77	0.21	57,57,57,57	0
54	MG	2a	3058	1/1	0.77	0.16	65,65,65,65	0
54	MG	1a	3039	1/1	0.77	0.24	67,67,67,67	0
54	MG	2a	3077	1/1	0.77	0.20	59,59,59,59	0
54	MG	2a	3106	1/1	0.77	0.15	69,69,69,69	0
54	MG	2A	3719	1/1	0.77	0.27	65,65,65,65	0
54	MG	2a	3125	1/1	0.77	0.16	73,73,73,73	0
54	MG	1A	3849	1/1	0.77	0.17	60,60,60,60	0
54	MG	1h	202	1/1	0.77	0.18	52,52,52,52	0
54	MG	2A	3493	1/1	0.77	0.21	29,29,29,29	0
54	MG	2a	3164	1/1	0.77	0.44	93,93,93,93	0
54	MG	1A	3407	1/1	0.77	0.17	50,50,50,50	0
54	MG	1a	3163	1/1	0.77	0.18	61,61,61,61	0
54	MG	1a	3008	1/1	0.77	0.22	59,59,59,59	0
54	MG	2A	3652	1/1	0.77	0.25	58,58,58,58	0
54	MG	2A	3666	1/1	0.77	0.15	53,53,53,53	0
54	MG	2A	3438	1/1	0.78	0.18	61,61,61,61	0
54	MG	2A	3448	1/1	0.78	0.17	63,63,63,63	0
54	MG	1A	3630	1/1	0.78	0.42	23,23,23,23	0
54	MG	21	103	1/1	0.78	0.34	62,62,62,62	0
54	MG	1a	3111	1/1	0.78	0.16	61,61,61,61	0
54	MG	1A	3771	1/1	0.78	0.13	20,20,20,20	0
54	MG	1a	3141	1/1	0.78	0.16	56,56,56,56	0
54	MG	2a	3061	1/1	0.78	0.22	67,67,67,67	0
54	MG	1A	3938	1/1	0.78	0.14	50,50,50,50	0
54	MG	1A	3861	1/1	0.78	0.22	74,74,74,74	0
56	MPD	2A	3742	8/8	0.78	0.27	31,44,48,53	0
54	MG	1N	203	1/1	0.78	0.14	63,63,63,63	0
54	MG	1A	3598	1/1	0.79	0.15	36,36,36,36	0
54	MG	1A	3283	1/1	0.79	0.53	37,37,37,37	0
54	MG	2A	3706	1/1	0.79	0.36	38,38,38,38	0
54	MG	1A	3153	1/1	0.79	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3101	1/1	0.79	0.15	65,65,65,65	0
54	MG	1A	3689	1/1	0.79	0.14	54,54,54,54	0
54	MG	2A	3401	1/1	0.79	0.25	54,54,54,54	0
54	MG	1A	3148	1/1	0.79	0.26	49,49,49,49	0
54	MG	1a	3269	1/1	0.79	0.14	61,61,61,61	0
54	MG	1A	3219	1/1	0.79	0.13	53,53,53,53	0
54	MG	1d	303	1/1	0.79	0.36	74,74,74,74	0
54	MG	2A	3491	1/1	0.79	0.33	63,63,63,63	0
54	MG	1a	3169	1/1	0.79	0.16	71,71,71,71	0
54	MG	1A	3981	1/1	0.79	0.13	58,58,58,58	0
54	MG	2A	3509	1/1	0.79	0.14	66,66,66,66	0
54	MG	1A	3990	1/1	0.79	0.15	62,62,62,62	0
54	MG	1y	202	1/1	0.79	0.16	63,63,63,63	0
54	MG	1A	3584	1/1	0.79	0.13	54,54,54,54	0
54	MG	1A	3683	1/1	0.80	0.17	52,52,52,52	0
54	MG	2A	3512	1/1	0.80	0.19	48,48,48,48	0
54	MG	1A	3980	1/1	0.80	0.21	39,39,39,39	0
54	MG	2a	3155	1/1	0.80	0.13	57,57,57,57	0
54	MG	2a	3024	1/1	0.80	0.19	55,55,55,55	0
54	MG	2A	3564	1/1	0.80	0.21	73,73,73,73	0
54	MG	1f	202	1/1	0.80	0.14	49,49,49,49	0
54	MG	2A	3482	1/1	0.80	0.20	69,69,69,69	0
54	MG	2A	3288	1/1	0.80	0.11	43,43,43,43	0
54	MG	2A	3289	1/1	0.80	0.13	50,50,50,50	0
54	MG	2A	3354	1/1	0.80	0.12	54,54,54,54	0
54	MG	11	104	1/1	0.80	0.14	44,44,44,44	0
54	MG	1A	3608	1/1	0.81	0.20	65,65,65,65	0
54	MG	2a	3002	1/1	0.81	0.17	56,56,56,56	0
54	MG	2A	3507	1/1	0.81	0.16	63,63,63,63	0
54	MG	2A	3148	1/1	0.81	0.25	58,58,58,58	0
54	MG	1a	3249	1/1	0.81	0.11	51,51,51,51	0
54	MG	2a	3050	1/1	0.81	0.24	49,49,49,49	0
54	MG	2a	3055	1/1	0.81	0.21	61,61,61,61	0
54	MG	2A	3181	1/1	0.81	0.17	60,60,60,60	0
54	MG	1B	207	1/1	0.81	0.13	36,36,36,36	0
54	MG	2A	3204	1/1	0.81	0.19	59,59,59,59	0
54	MG	2A	3645	1/1	0.81	0.10	33,33,33,33	0
54	MG	1A	3930	1/1	0.81	0.11	37,37,37,37	0
54	MG	1a	3263	1/1	0.81	0.16	81,81,81,81	0
54	MG	1A	3852	1/1	0.81	0.12	56,56,56,56	0
54	MG	2A	3345	1/1	0.81	0.20	57,57,57,57	0
54	MG	1a	3086	1/1	0.81	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3661	1/1	0.81	0.12	55,55,55,55	0
54	MG	1a	3170	1/1	0.81	0.12	59,59,59,59	0
54	MG	1D	316	1/1	0.81	0.13	58,58,58,58	0
54	MG	1a	3120	1/1	0.81	0.10	49,49,49,49	0
54	MG	2A	3457	1/1	0.81	0.20	63,63,63,63	0
54	MG	1A	3758	1/1	0.81	0.15	43,43,43,43	0
54	MG	2A	3487	1/1	0.81	0.13	63,63,63,63	0
54	MG	1a	3232	1/1	0.81	0.12	63,63,63,63	0
54	MG	1A	3548	1/1	0.81	0.22	49,49,49,49	0
54	MG	1a	3239	1/1	0.81	0.21	66,66,66,66	0
54	MG	2A	3262	1/1	0.82	0.21	58,58,58,58	0
54	MG	1a	3230	1/1	0.82	0.10	60,60,60,60	0
54	MG	2A	3634	1/1	0.82	0.22	61,61,61,61	0
54	MG	1A	3571	1/1	0.82	0.13	36,36,36,36	0
54	MG	1A	3635	1/1	0.82	0.13	45,45,45,45	0
54	MG	1A	3428	1/1	0.82	0.18	33,33,33,33	0
54	MG	1A	3545	1/1	0.82	0.10	23,23,23,23	0
54	MG	1A	3964	1/1	0.82	0.15	35,35,35,35	0
54	MG	2A	3022	1/1	0.82	0.14	47,47,47,47	0
54	MG	2A	3039	1/1	0.82	0.27	53,53,53,53	0
54	MG	2a	3108	1/1	0.82	0.21	69,69,69,69	0
54	MG	2A	3451	1/1	0.82	0.15	52,52,52,52	0
54	MG	1a	3180	1/1	0.82	0.13	70,70,70,70	0
54	MG	1a	3073	1/1	0.82	0.12	46,46,46,46	0
54	MG	1A	3065	1/1	0.82	0.12	56,56,56,56	0
54	MG	2A	3150	1/1	0.82	0.14	42,42,42,42	0
54	MG	1a	3267	1/1	0.82	0.14	73,73,73,73	0
54	MG	1A	3286	1/1	0.82	0.16	53,53,53,53	0
54	MG	2P	202	1/1	0.82	0.10	47,47,47,47	0
54	MG	1a	3221	1/1	0.82	0.14	60,60,60,60	0
54	MG	2A	3198	1/1	0.82	0.12	49,49,49,49	0
54	MG	1a	3229	1/1	0.82	0.14	40,40,40,40	0
56	MPD	1T	205	8/8	0.82	0.30	57,61,72,72	0
54	MG	2A	3258	1/1	0.82	0.24	45,45,45,45	0
54	MG	1b	301	1/1	0.82	0.13	72,72,72,72	0
54	MG	2A	3386	1/1	0.83	0.14	53,53,53,53	0
54	MG	2a	3035	1/1	0.83	0.11	69,69,69,69	0
54	MG	2a	3045	1/1	0.83	0.33	72,72,72,72	0
54	MG	1a	3095	1/1	0.83	0.17	63,63,63,63	0
54	MG	2A	3413	1/1	0.83	0.13	53,53,53,53	0
54	MG	2A	3678	1/1	0.83	0.13	58,58,58,58	0
54	MG	1a	3109	1/1	0.83	0.16	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3011	1/1	0.83	0.15	51,51,51,51	0
54	MG	1A	3415	1/1	0.83	0.14	53,53,53,53	0
54	MG	1A	3616	1/1	0.83	0.16	30,30,30,30	0
54	MG	1A	3672	1/1	0.83	0.14	43,43,43,43	0
54	MG	1A	3626	1/1	0.83	0.12	33,33,33,33	0
54	MG	1a	3062	1/1	0.83	0.21	59,59,59,59	0
54	MG	2a	3119	1/1	0.83	0.10	47,47,47,47	0
54	MG	2A	3729	1/1	0.83	0.14	62,62,62,62	0
54	MG	2a	3137	1/1	0.83	0.10	38,38,38,38	0
54	MG	1A	3196	1/1	0.83	0.15	47,47,47,47	0
54	MG	2A	3738	1/1	0.83	0.11	47,47,47,47	0
54	MG	2A	3215	1/1	0.83	0.19	52,52,52,52	0
54	MG	1A	3690	1/1	0.83	0.26	43,43,43,43	0
54	MG	1A	3702	1/1	0.83	0.36	59,59,59,59	0
54	MG	1a	3078	1/1	0.83	0.21	73,73,73,73	0
54	MG	2A	3274	1/1	0.83	0.11	40,40,40,40	0
54	MG	2A	3015	1/1	0.83	0.14	44,44,44,44	0
54	MG	1A	3744	1/1	0.83	0.20	40,40,40,40	0
54	MG	1A	3527	1/1	0.83	0.14	35,35,35,35	0
56	MPD	1a	3278	8/8	0.83	0.17	44,56,68,69	0
54	MG	2A	3091	1/1	0.83	0.21	52,52,52,52	0
54	MG	2A	3364	1/1	0.83	0.12	49,49,49,49	0
54	MG	1a	3136	1/1	0.84	0.17	62,62,62,62	0
54	MG	2A	3532	1/1	0.84	0.14	59,59,59,59	0
54	MG	1a	3171	1/1	0.84	0.20	53,53,53,53	0
54	MG	1a	3137	1/1	0.84	0.12	52,52,52,52	0
54	MG	1a	3190	1/1	0.84	0.16	58,58,58,58	0
54	MG	1A	3633	1/1	0.84	0.31	21,21,21,21	0
54	MG	2A	3077	1/1	0.84	0.18	39,39,39,39	0
54	MG	2A	3078	1/1	0.84	0.13	74,74,74,74	0
54	MG	2A	3382	1/1	0.84	0.12	60,60,60,60	0
54	MG	2a	3068	1/1	0.84	0.20	65,65,65,65	0
54	MG	2A	3080	1/1	0.84	0.12	57,57,57,57	0
54	MG	2a	3078	1/1	0.84	0.23	44,44,44,44	0
54	MG	2A	3397	1/1	0.84	0.13	44,44,44,44	0
54	MG	1a	3261	1/1	0.84	0.08	40,40,40,40	0
54	MG	1A	3837	1/1	0.84	0.18	34,34,34,34	0
54	MG	10	105	1/1	0.84	0.11	43,43,43,43	0
54	MG	2A	3133	1/1	0.84	0.20	48,48,48,48	0
54	MG	1a	3215	1/1	0.84	0.11	66,66,66,66	0
54	MG	1a	3217	1/1	0.84	0.20	59,59,59,59	0
54	MG	1a	3272	1/1	0.84	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3473	1/1	0.84	0.20	61,61,61,61	0
54	MG	1A	3586	1/1	0.84	0.14	21,21,21,21	0
54	MG	2B	215	1/1	0.84	0.13	61,61,61,61	0
54	MG	2A	3182	1/1	0.84	0.10	46,46,46,46	0
54	MG	1a	3222	1/1	0.84	0.31	67,67,67,67	0
54	MG	2I	201	1/1	0.84	0.10	55,55,55,55	0
54	MG	1A	3295	1/1	0.84	0.10	36,36,36,36	0
54	MG	1A	3480	1/1	0.84	0.11	12,12,12,12	0
54	MG	1F	309	1/1	0.84	0.20	39,39,39,39	0
54	MG	2A	3228	1/1	0.84	0.10	47,47,47,47	0
54	MG	1g	202	1/1	0.84	0.07	50,50,50,50	0
54	MG	1A	3993	1/1	0.84	0.14	40,40,40,40	0
54	MG	2A	3475	1/1	0.85	0.17	55,55,55,55	0
54	MG	1G	202	1/1	0.85	0.13	48,48,48,48	0
54	MG	1A	3944	1/1	0.85	0.12	17,17,17,17	0
54	MG	1A	3959	1/1	0.85	0.14	65,65,65,65	0
54	MG	2A	3207	1/1	0.85	0.14	47,47,47,47	0
54	MG	1A	3783	1/1	0.85	0.13	47,47,47,47	0
54	MG	1a	3112	1/1	0.85	0.12	48,48,48,48	0
54	MG	2A	3235	1/1	0.85	0.14	56,56,56,56	0
54	MG	11	102	1/1	0.85	0.11	48,48,48,48	0
54	MG	2a	3010	1/1	0.85	0.14	56,56,56,56	0
54	MG	1i	3101	1/1	0.85	0.19	65,65,65,65	0
54	MG	1A	3289	1/1	0.85	0.16	74,74,74,74	0
54	MG	2A	3530	1/1	0.85	0.44	46,46,46,46	0
54	MG	1A	3841	1/1	0.85	0.15	28,28,28,28	0
54	MG	2a	3046	1/1	0.85	0.14	66,66,66,66	0
54	MG	1A	3462	1/1	0.85	0.13	45,45,45,45	0
54	MG	2A	3587	1/1	0.85	0.11	38,38,38,38	0
54	MG	2A	3594	1/1	0.85	0.14	24,24,24,24	0
54	MG	1A	3986	1/1	0.85	0.24	37,37,37,37	0
54	MG	2A	3624	1/1	0.85	0.10	55,55,55,55	0
54	MG	2A	3293	1/1	0.85	0.10	57,57,57,57	0
54	MG	1a	3144	1/1	0.85	0.14	60,60,60,60	0
54	MG	1A	3987	1/1	0.85	0.11	31,31,31,31	0
54	MG	1A	3202	1/1	0.85	0.14	49,49,49,49	0
54	MG	2A	3672	1/1	0.85	0.17	71,71,71,71	0
54	MG	1A	3694	1/1	0.85	0.20	47,47,47,47	0
54	MG	2A	3683	1/1	0.85	0.14	26,26,26,26	0
54	MG	2a	3118	1/1	0.85	0.14	47,47,47,47	0
54	MG	2A	3692	1/1	0.85	0.11	45,45,45,45	0
54	MG	2A	3085	1/1	0.85	0.33	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3704	1/1	0.85	0.11	52,52,52,52	0
54	MG	1A	3511	1/1	0.85	0.09	39,39,39,39	0
54	MG	2A	3398	1/1	0.85	0.27	62,62,62,62	0
54	MG	2a	3146	1/1	0.85	0.14	79,79,79,79	0
54	MG	2A	3399	1/1	0.85	0.19	59,59,59,59	0
54	MG	1A	3864	1/1	0.85	0.13	64,64,64,64	0
54	MG	1A	3867	1/1	0.85	0.28	30,30,30,30	0
54	MG	2a	3167	1/1	0.85	0.10	75,75,75,75	0
54	MG	2a	3181	1/1	0.85	0.12	83,83,83,83	0
54	MG	1A	3303	1/1	0.85	0.14	61,61,61,61	0
54	MG	1B	230	1/1	0.85	0.08	47,47,47,47	0
54	MG	1A	3659	1/1	0.85	0.16	54,54,54,54	0
54	MG	1A	3180	1/1	0.85	0.34	33,33,33,33	0
54	MG	2B	203	1/1	0.85	0.24	72,72,72,72	0
54	MG	2B	204	1/1	0.85	0.10	61,61,61,61	0
54	MG	1a	3183	1/1	0.85	0.09	72,72,72,72	0
54	MG	1A	3277	1/1	0.85	0.14	44,44,44,44	0
54	MG	2A	3111	1/1	0.86	0.19	58,58,58,58	0
54	MG	2A	3115	1/1	0.86	0.15	60,60,60,60	0
54	MG	10	106	1/1	0.86	0.14	52,52,52,52	0
54	MG	1A	3729	1/1	0.86	0.27	38,38,38,38	0
54	MG	2G	203	1/1	0.86	0.10	70,70,70,70	0
54	MG	1a	3139	1/1	0.86	0.23	73,73,73,73	0
54	MG	1A	3984	1/1	0.86	0.32	42,42,42,42	0
54	MG	2P	203	1/1	0.86	0.12	57,57,57,57	0
54	MG	1A	3254	1/1	0.86	0.14	56,56,56,56	0
54	MG	2A	3500	1/1	0.86	0.20	54,54,54,54	0
54	MG	2A	3501	1/1	0.86	0.15	65,65,65,65	0
54	MG	1a	3145	1/1	0.86	0.09	63,63,63,63	0
54	MG	1A	3507	1/1	0.86	0.11	9,9,9,9	0
54	MG	1A	3260	1/1	0.86	0.08	51,51,51,51	0
54	MG	1A	3760	1/1	0.86	0.16	54,54,54,54	0
54	MG	1A	3878	1/1	0.86	0.14	30,30,30,30	0
54	MG	2a	3034	1/1	0.86	0.11	65,65,65,65	0
54	MG	2A	3213	1/1	0.86	0.10	62,62,62,62	0
54	MG	1A	3762	1/1	0.86	0.13	19,19,19,19	0
54	MG	2A	3552	1/1	0.86	0.14	45,45,45,45	0
54	MG	2A	3559	1/1	0.86	0.09	31,31,31,31	0
54	MG	2a	3054	1/1	0.86	0.09	52,52,52,52	0
54	MG	1a	3167	1/1	0.86	0.09	70,70,70,70	0
54	MG	1B	213	1/1	0.86	0.13	61,61,61,61	0
54	MG	2A	3241	1/1	0.86	0.65	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3062	1/1	0.86	0.10	73,73,73,73	0
54	MG	2A	3608	1/1	0.86	0.10	66,66,66,66	0
54	MG	1B	215	1/1	0.86	0.31	57,57,57,57	0
54	MG	2a	3074	1/1	0.86	0.10	52,52,52,52	0
54	MG	2A	3613	1/1	0.86	0.16	55,55,55,55	0
54	MG	1d	302	1/1	0.86	0.11	59,59,59,59	0
54	MG	1B	217	1/1	0.86	0.10	47,47,47,47	0
54	MG	1A	3177	1/1	0.86	0.12	47,47,47,47	0
54	MG	1a	3174	1/1	0.86	0.19	65,65,65,65	0
54	MG	1A	3913	1/1	0.86	0.13	25,25,25,25	0
54	MG	1A	3914	1/1	0.86	0.12	29,29,29,29	0
54	MG	2A	3333	1/1	0.86	0.14	58,58,58,58	0
54	MG	1A	3778	1/1	0.86	0.10	44,44,44,44	0
54	MG	2a	3129	1/1	0.86	0.10	62,62,62,62	0
54	MG	1a	3082	1/1	0.86	0.13	49,49,49,49	0
54	MG	1E	308	1/1	0.86	0.12	24,24,24,24	0
54	MG	2A	3698	1/1	0.86	0.12	70,70,70,70	0
54	MG	1A	3593	1/1	0.86	0.11	39,39,39,39	0
54	MG	1a	3202	1/1	0.86	0.23	88,88,88,88	0
54	MG	2A	3026	1/1	0.86	0.10	41,41,41,41	0
54	MG	1A	3788	1/1	0.86	0.20	50,50,50,50	0
54	MG	2A	3717	1/1	0.86	0.12	31,31,31,31	0
54	MG	2A	3051	1/1	0.86	0.15	49,49,49,49	0
54	MG	1A	3798	1/1	0.86	0.18	78,78,78,78	0
54	MG	1A	3692	1/1	0.86	0.16	36,36,36,36	0
54	MG	2A	3727	1/1	0.86	0.20	54,54,54,54	0
54	MG	1P	204	1/1	0.86	0.21	21,21,21,21	0
54	MG	1A	3378	1/1	0.86	0.11	32,32,32,32	0
54	MG	1a	3116	1/1	0.86	0.35	54,54,54,54	0
54	MG	1a	3231	1/1	0.86	0.15	67,67,67,67	0
54	MG	1A	3469	1/1	0.86	0.09	10,10,10,10	0
54	MG	1a	3070	1/1	0.87	0.16	36,36,36,36	0
54	MG	2A	3142	1/1	0.87	0.16	45,45,45,45	0
54	MG	2A	3467	1/1	0.87	0.19	47,47,47,47	0
54	MG	2B	209	1/1	0.87	0.18	49,49,49,49	0
54	MG	1A	3931	1/1	0.87	0.24	66,66,66,66	0
54	MG	1A	3441	1/1	0.87	0.18	51,51,51,51	0
54	MG	2A	3169	1/1	0.87	0.10	58,58,58,58	0
54	MG	2A	3483	1/1	0.87	0.12	46,46,46,46	0
54	MG	1d	301	1/1	0.87	0.12	62,62,62,62	0
54	MG	1a	3204	1/1	0.87	0.16	50,50,50,50	0
54	MG	1a	3214	1/1	0.87	0.19	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3187	1/1	0.87	0.18	59,59,59,59	0
54	MG	1A	3184	1/1	0.87	0.14	43,43,43,43	0
54	MG	1A	3684	1/1	0.87	0.08	66,66,66,66	0
54	MG	1A	3862	1/1	0.87	0.09	28,28,28,28	0
54	MG	1A	3785	1/1	0.87	0.15	68,68,68,68	0
54	MG	1a	3225	1/1	0.87	0.10	64,64,64,64	0
54	MG	2A	3214	1/1	0.87	0.10	46,46,46,46	0
54	MG	2a	3021	1/1	0.87	0.08	42,42,42,42	0
54	MG	2A	3513	1/1	0.87	0.14	48,48,48,48	0
54	MG	1l	202	1/1	0.87	0.12	49,49,49,49	0
54	MG	1o	102	1/1	0.87	0.10	36,36,36,36	0
54	MG	2a	3042	1/1	0.87	0.14	59,59,59,59	0
54	MG	1t	201	1/1	0.87	0.12	55,55,55,55	0
54	MG	2A	3543	1/1	0.87	0.10	60,60,60,60	0
54	MG	2a	3047	1/1	0.87	0.12	51,51,51,51	0
54	MG	2A	3548	1/1	0.87	0.13	34,34,34,34	0
54	MG	1A	3331	1/1	0.87	0.21	60,60,60,60	0
54	MG	1a	3166	1/1	0.87	0.33	61,61,61,61	0
54	MG	1A	3362	1/1	0.87	0.10	26,26,26,26	0
54	MG	1A	3823	1/1	0.87	0.16	41,41,41,41	0
54	MG	2A	3265	1/1	0.87	0.15	61,61,61,61	0
54	MG	2A	3602	1/1	0.87	0.14	30,30,30,30	0
54	MG	1A	3367	1/1	0.87	0.16	35,35,35,35	0
54	MG	2A	3032	1/1	0.87	0.17	54,54,54,54	0
54	MG	1A	3907	1/1	0.87	0.11	26,26,26,26	0
54	MG	2A	3615	1/1	0.87	0.19	59,59,59,59	0
54	MG	2a	3083	1/1	0.87	0.13	51,51,51,51	0
54	MG	2A	3290	1/1	0.87	0.12	41,41,41,41	0
54	MG	1A	3838	1/1	0.87	0.10	38,38,38,38	0
54	MG	2A	3322	1/1	0.87	0.13	54,54,54,54	0
54	MG	2A	3074	1/1	0.87	0.14	43,43,43,43	0
54	MG	2A	3076	1/1	0.87	0.47	44,44,44,44	0
54	MG	2A	3347	1/1	0.87	0.12	65,65,65,65	0
54	MG	1a	3173	1/1	0.87	0.10	62,62,62,62	0
54	MG	2a	3128	1/1	0.87	0.15	60,60,60,60	0
54	MG	1A	3432	1/1	0.87	0.20	56,56,56,56	0
54	MG	2a	3132	1/1	0.87	0.17	69,69,69,69	0
54	MG	2A	3371	1/1	0.87	0.16	38,38,38,38	0
54	MG	1a	3126	1/1	0.87	0.09	61,61,61,61	0
54	MG	1a	3257	1/1	0.87	0.13	57,57,57,57	0
54	MG	2A	3703	1/1	0.87	0.16	51,51,51,51	0
54	MG	2a	3152	1/1	0.87	0.12	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3061	1/1	0.87	0.14	66,66,66,66	0
54	MG	2a	3158	1/1	0.87	0.13	63,63,63,63	0
54	MG	2A	3092	1/1	0.87	0.24	52,52,52,52	0
54	MG	1A	3765	1/1	0.87	0.12	24,24,24,24	0
54	MG	2A	3102	1/1	0.87	0.21	48,48,48,48	0
54	MG	2A	3403	1/1	0.87	0.20	29,29,29,29	0
54	MG	2A	3408	1/1	0.87	0.15	57,57,57,57	0
54	MG	2A	3105	1/1	0.87	0.09	37,37,37,37	0
54	MG	1a	3192	1/1	0.87	0.14	50,50,50,50	0
54	MG	2A	3420	1/1	0.87	0.09	55,55,55,55	0
54	MG	1a	3193	1/1	0.87	0.13	52,52,52,52	0
54	MG	2A	3447	1/1	0.87	0.17	55,55,55,55	0
54	MG	1P	207	1/1	0.87	0.07	53,53,53,53	0
54	MG	2A	3739	1/1	0.87	0.11	48,48,48,48	0
54	MG	1a	3049	1/1	0.88	0.12	50,50,50,50	0
54	MG	1A	3894	1/1	0.88	0.13	47,47,47,47	0
54	MG	1A	3411	1/1	0.88	0.15	10,10,10,10	0
54	MG	1n	101	1/1	0.88	0.14	58,58,58,58	0
54	MG	1a	3175	1/1	0.88	0.13	55,55,55,55	0
54	MG	1A	3789	1/1	0.88	0.14	50,50,50,50	0
54	MG	2A	3708	1/1	0.88	0.13	38,38,38,38	0
54	MG	1a	3064	1/1	0.88	0.12	36,36,36,36	0
54	MG	1a	3185	1/1	0.88	0.22	57,57,57,57	0
54	MG	2A	3355	1/1	0.88	0.18	54,54,54,54	0
54	MG	1y	203	1/1	0.88	0.13	61,61,61,61	0
54	MG	2A	3366	1/1	0.88	0.10	24,24,24,24	0
54	MG	2A	3725	1/1	0.88	0.21	49,49,49,49	0
54	MG	2A	3368	1/1	0.88	0.14	46,46,46,46	0
54	MG	1A	3588	1/1	0.88	0.16	48,48,48,48	0
54	MG	2A	3020	1/1	0.88	0.19	52,52,52,52	0
54	MG	2A	3730	1/1	0.88	0.14	40,40,40,40	0
54	MG	1A	3812	1/1	0.88	0.30	32,32,32,32	0
54	MG	2A	3393	1/1	0.88	0.13	44,44,44,44	0
54	MG	2A	3396	1/1	0.88	0.18	60,60,60,60	0
54	MG	1B	227	1/1	0.88	0.12	50,50,50,50	0
54	MG	1A	3816	1/1	0.88	0.12	51,51,51,51	0
54	MG	2B	206	1/1	0.88	0.18	44,44,44,44	0
54	MG	1B	231	1/1	0.88	0.09	47,47,47,47	0
54	MG	2A	3044	1/1	0.88	0.13	42,42,42,42	0
54	MG	1A	3710	1/1	0.88	0.42	34,34,34,34	0
54	MG	2A	3404	1/1	0.88	0.15	40,40,40,40	0
54	MG	2A	3405	1/1	0.88	0.20	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3826	1/1	0.88	0.12	38,38,38,38	0
54	MG	1a	3203	1/1	0.88	0.11	49,49,49,49	0
54	MG	1A	3540	1/1	0.88	0.17	39,39,39,39	0
54	MG	1a	3088	1/1	0.88	0.28	56,56,56,56	0
54	MG	2A	3429	1/1	0.88	0.07	37,37,37,37	0
54	MG	1A	3953	1/1	0.88	0.11	59,59,59,59	0
54	MG	2A	3440	1/1	0.88	0.10	57,57,57,57	0
54	MG	1a	3096	1/1	0.88	0.15	46,46,46,46	0
54	MG	2a	3003	1/1	0.88	0.14	60,60,60,60	0
54	MG	1a	3218	1/1	0.88	0.12	59,59,59,59	0
54	MG	1a	3097	1/1	0.88	0.21	44,44,44,44	0
54	MG	2a	3013	1/1	0.88	0.14	54,54,54,54	0
54	MG	2a	3018	1/1	0.88	0.19	66,66,66,66	0
54	MG	2A	3093	1/1	0.88	0.11	55,55,55,55	0
54	MG	2A	3458	1/1	0.88	0.14	39,39,39,39	0
54	MG	2A	3464	1/1	0.88	0.13	51,51,51,51	0
54	MG	1a	3106	1/1	0.88	0.14	74,74,74,74	0
54	MG	2A	3470	1/1	0.88	0.11	49,49,49,49	0
54	MG	1A	3642	1/1	0.88	0.11	66,66,66,66	0
54	MG	1A	3645	1/1	0.88	0.23	45,45,45,45	0
54	MG	1O	201	1/1	0.88	0.11	44,44,44,44	0
54	MG	1A	3116	1/1	0.88	0.15	30,30,30,30	0
54	MG	1A	3602	1/1	0.88	0.28	28,28,28,28	0
54	MG	2A	3117	1/1	0.88	0.25	57,57,57,57	0
54	MG	1R	208	1/1	0.88	0.09	19,19,19,19	0
54	MG	2a	3057	1/1	0.88	0.17	61,61,61,61	0
54	MG	2A	3140	1/1	0.88	0.11	46,46,46,46	0
54	MG	2a	3059	1/1	0.88	0.12	54,54,54,54	0
54	MG	2A	3497	1/1	0.88	0.17	51,51,51,51	0
54	MG	1a	3238	1/1	0.88	0.14	60,60,60,60	0
54	MG	1A	3605	1/1	0.88	0.20	40,40,40,40	0
54	MG	2a	3066	1/1	0.88	0.10	49,49,49,49	0
54	MG	1A	3860	1/1	0.88	0.15	33,33,33,33	0
54	MG	2A	3506	1/1	0.88	0.14	50,50,50,50	0
54	MG	1A	3205	1/1	0.88	0.13	32,32,32,32	0
54	MG	1a	3250	1/1	0.88	0.14	59,59,59,59	0
54	MG	1A	3503	1/1	0.88	0.13	38,38,38,38	0
54	MG	1A	3775	1/1	0.88	0.17	21,21,21,21	0
54	MG	2A	3185	1/1	0.88	0.23	41,41,41,41	0
54	MG	1a	3142	1/1	0.88	0.12	57,57,57,57	0
54	MG	13	102	1/1	0.88	0.09	24,24,24,24	0
54	MG	2a	3117	1/1	0.88	0.09	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3318	1/1	0.88	0.11	46,46,46,46	0
54	MG	2A	3547	1/1	0.88	0.11	33,33,33,33	0
54	MG	1a	3146	1/1	0.88	0.13	64,64,64,64	0
54	MG	18	102	1/1	0.88	0.41	28,28,28,28	0
54	MG	1a	3001	1/1	0.88	0.19	59,59,59,59	0
54	MG	1A	4005	1/1	0.88	0.54	44,44,44,44	0
54	MG	2A	3567	1/1	0.88	0.14	34,34,34,34	0
54	MG	1a	3159	1/1	0.88	0.14	56,56,56,56	0
54	MG	2a	3143	1/1	0.88	0.11	56,56,56,56	0
54	MG	2A	3590	1/1	0.88	0.12	29,29,29,29	0
54	MG	2A	3216	1/1	0.88	0.12	54,54,54,54	0
54	MG	2a	3150	1/1	0.88	0.12	42,42,42,42	0
54	MG	1A	4008	1/1	0.88	0.13	49,49,49,49	0
54	MG	2A	3232	1/1	0.88	0.19	45,45,45,45	0
54	MG	2A	3610	1/1	0.88	0.14	50,50,50,50	0
54	MG	1B	205	1/1	0.88	0.15	48,48,48,48	0
54	MG	1a	3012	1/1	0.88	0.18	65,65,65,65	0
54	MG	2A	3249	1/1	0.88	0.11	39,39,39,39	0
54	MG	1B	206	1/1	0.88	0.17	47,47,47,47	0
54	MG	2A	3259	1/1	0.88	0.28	58,58,58,58	0
54	MG	1d	304	1/1	0.88	0.10	82,82,82,82	0
54	MG	1A	3255	1/1	0.88	0.14	53,53,53,53	0
54	MG	2A	3663	1/1	0.88	0.09	52,52,52,52	0
54	MG	1A	3631	1/1	0.88	0.11	42,42,42,42	0
54	MG	1a	3040	1/1	0.88	0.12	49,49,49,49	0
54	MG	2A	3279	1/1	0.88	0.15	52,52,52,52	0
56	MPD	2A	3743	8/8	0.88	0.23	57,60,63,66	0
54	MG	1g	203	1/1	0.88	0.21	67,67,67,67	0
57	ARG	1F	318	12/12	0.88	0.13	39,51,70,70	0
54	MG	2B	202	1/1	0.89	0.19	58,58,58,58	0
54	MG	1a	3075	1/1	0.89	0.17	47,47,47,47	0
54	MG	2A	3206	1/1	0.89	0.10	50,50,50,50	0
54	MG	1a	3076	1/1	0.89	0.18	64,64,64,64	0
54	MG	1a	3188	1/1	0.89	0.09	53,53,53,53	0
54	MG	1A	3560	1/1	0.89	0.12	39,39,39,39	0
54	MG	1A	3802	1/1	0.89	0.10	56,56,56,56	0
54	MG	2B	217	1/1	0.89	0.08	69,69,69,69	0
54	MG	2A	3480	1/1	0.89	0.17	52,52,52,52	0
54	MG	1A	3946	1/1	0.89	0.13	32,32,32,32	0
54	MG	2A	3219	1/1	0.89	0.08	43,43,43,43	0
54	MG	1A	3627	1/1	0.89	0.12	24,24,24,24	0
54	MG	2P	201	1/1	0.89	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3230	1/1	0.89	0.17	42,42,42,42	0
54	MG	1A	3140	1/1	0.89	0.10	40,40,40,40	0
54	MG	1A	3055	1/1	0.89	0.13	46,46,46,46	0
54	MG	2A	3237	1/1	0.89	0.29	36,36,36,36	0
54	MG	1a	3091	1/1	0.89	0.12	53,53,53,53	0
54	MG	26	102	1/1	0.89	0.17	50,50,50,50	0
54	MG	1A	3966	1/1	0.89	0.13	38,38,38,38	0
54	MG	2A	3001	1/1	0.89	0.15	46,46,46,46	0
54	MG	1A	3969	1/1	0.89	0.10	49,49,49,49	0
54	MG	1U	206	1/1	0.89	0.26	29,29,29,29	0
54	MG	1Y	201	1/1	0.89	0.15	72,72,72,72	0
54	MG	1A	3706	1/1	0.89	0.16	24,24,24,24	0
54	MG	2A	3270	1/1	0.89	0.15	18,18,18,18	0
54	MG	2A	3514	1/1	0.89	0.10	43,43,43,43	0
54	MG	1A	3828	1/1	0.89	0.09	25,25,25,25	0
54	MG	2A	3037	1/1	0.89	0.09	38,38,38,38	0
54	MG	1A	3305	1/1	0.89	0.12	61,61,61,61	0
54	MG	2a	3039	1/1	0.89	0.17	57,57,57,57	0
54	MG	1A	3037	1/1	0.89	0.12	44,44,44,44	0
54	MG	2A	3545	1/1	0.89	0.12	26,26,26,26	0
54	MG	1A	3743	1/1	0.89	0.11	19,19,19,19	0
54	MG	2A	3063	1/1	0.89	0.15	42,42,42,42	0
54	MG	2A	3302	1/1	0.89	0.17	43,43,43,43	0
54	MG	2a	3053	1/1	0.89	0.11	53,53,53,53	0
54	MG	2A	3309	1/1	0.89	0.12	40,40,40,40	0
54	MG	2A	3318	1/1	0.89	0.09	34,34,34,34	0
54	MG	1A	3587	1/1	0.89	0.14	41,41,41,41	0
54	MG	2A	3569	1/1	0.89	0.10	28,28,28,28	0
54	MG	2A	3585	1/1	0.89	0.11	45,45,45,45	0
54	MG	2A	3323	1/1	0.89	0.10	44,44,44,44	0
54	MG	1A	3638	1/1	0.89	0.15	41,41,41,41	0
54	MG	1a	3132	1/1	0.89	0.16	41,41,41,41	0
54	MG	2a	3065	1/1	0.89	0.08	54,54,54,54	0
54	MG	1A	3992	1/1	0.89	0.21	49,49,49,49	0
54	MG	1a	3234	1/1	0.89	0.12	67,67,67,67	0
54	MG	2a	3072	1/1	0.89	0.15	45,45,45,45	0
54	MG	1A	3754	1/1	0.89	0.13	41,41,41,41	0
54	MG	1A	3225	1/1	0.89	0.20	32,32,32,32	0
54	MG	1a	3007	1/1	0.89	0.13	59,59,59,59	0
54	MG	1A	3431	1/1	0.89	0.13	51,51,51,51	0
54	MG	2a	3098	1/1	0.89	0.17	51,51,51,51	0
54	MG	2a	3100	1/1	0.89	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3651	1/1	0.89	0.09	13,13,13,13	0
54	MG	2a	3102	1/1	0.89	0.09	60,60,60,60	0
54	MG	1A	3535	1/1	0.89	0.10	20,20,20,20	0
54	MG	1A	3770	1/1	0.89	0.10	32,32,32,32	0
54	MG	1a	3022	1/1	0.89	0.10	47,47,47,47	0
54	MG	2a	3114	1/1	0.89	0.23	53,53,53,53	0
54	MG	2a	3115	1/1	0.89	0.18	71,71,71,71	0
54	MG	1a	3030	1/1	0.89	0.20	50,50,50,50	0
54	MG	1a	3031	1/1	0.89	0.14	45,45,45,45	0
54	MG	1A	3355	1/1	0.89	0.10	31,31,31,31	0
54	MG	2a	3120	1/1	0.89	0.12	68,68,68,68	0
54	MG	2A	3673	1/1	0.89	0.13	31,31,31,31	0
54	MG	2A	3127	1/1	0.89	0.16	51,51,51,51	0
54	MG	1a	3034	1/1	0.89	0.19	47,47,47,47	0
54	MG	1a	3038	1/1	0.89	0.17	64,64,64,64	0
54	MG	1A	3167	1/1	0.89	0.15	40,40,40,40	0
54	MG	1A	3677	1/1	0.89	0.19	58,58,58,58	0
54	MG	2A	3149	1/1	0.89	0.13	71,71,71,71	0
54	MG	2A	3412	1/1	0.89	0.10	44,44,44,44	0
54	MG	2A	3705	1/1	0.89	0.10	42,42,42,42	0
54	MG	1A	3904	1/1	0.89	0.09	11,11,11,11	0
54	MG	2a	3151	1/1	0.89	0.09	84,84,84,84	0
54	MG	1A	3780	1/1	0.89	0.16	53,53,53,53	0
54	MG	2a	3153	1/1	0.89	0.12	61,61,61,61	0
54	MG	1A	3679	1/1	0.89	0.12	25,25,25,25	0
54	MG	2A	3424	1/1	0.89	0.11	51,51,51,51	0
54	MG	2A	3174	1/1	0.89	0.22	68,68,68,68	0
54	MG	2A	3431	1/1	0.89	0.24	57,57,57,57	0
54	MG	2A	3435	1/1	0.89	0.09	46,46,46,46	0
54	MG	2a	3177	1/1	0.89	0.12	58,58,58,58	0
54	MG	2A	3436	1/1	0.89	0.25	43,43,43,43	0
54	MG	2h	201	1/1	0.89	0.20	60,60,60,60	0
54	MG	1A	3784	1/1	0.89	0.10	34,34,34,34	0
54	MG	1A	3169	1/1	0.89	0.12	39,39,39,39	0
54	MG	2l	201	1/1	0.89	0.09	53,53,53,53	0
54	MG	2A	3728	1/1	0.89	0.22	49,49,49,49	0
54	MG	2A	3444	1/1	0.89	0.09	64,64,64,64	0
54	MG	1A	3613	1/1	0.89	0.11	11,11,11,11	0
54	MG	2A	3733	1/1	0.89	0.29	50,50,50,50	0
54	MG	1d	305	1/1	0.89	0.07	42,42,42,42	0
54	MG	1A	3556	1/1	0.89	0.09	54,54,54,54	0
54	MG	1A	3932	1/1	0.89	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3740	1/1	0.89	0.10	60,60,60,60	0
54	MG	1A	3299	1/1	0.90	0.15	44,44,44,44	0
54	MG	1A	3413	1/1	0.90	0.08	51,51,51,51	0
54	MG	1A	3131	1/1	0.90	0.21	32,32,32,32	0
54	MG	1a	3041	1/1	0.90	0.12	52,52,52,52	0
54	MG	2A	3190	1/1	0.90	0.12	48,48,48,48	0
54	MG	2A	3193	1/1	0.90	0.10	49,49,49,49	0
54	MG	1A	3547	1/1	0.90	0.27	36,36,36,36	0
54	MG	1e	201	1/1	0.90	0.11	51,51,51,51	0
54	MG	2A	3460	1/1	0.90	0.10	49,49,49,49	0
54	MG	2A	3202	1/1	0.90	0.20	41,41,41,41	0
54	MG	2B	218	1/1	0.90	0.08	50,50,50,50	0
54	MG	1a	3052	1/1	0.90	0.13	48,48,48,48	0
54	MG	2F	302	1/1	0.90	0.10	32,32,32,32	0
54	MG	1B	216	1/1	0.90	0.08	47,47,47,47	0
54	MG	2A	3471	1/1	0.90	0.10	42,42,42,42	0
54	MG	1A	3875	1/1	0.90	0.10	9,9,9,9	0
54	MG	1A	3757	1/1	0.90	0.12	44,44,44,44	0
54	MG	2A	3477	1/1	0.90	0.07	45,45,45,45	0
54	MG	1A	3213	1/1	0.90	0.40	26,26,26,26	0
54	MG	1A	3555	1/1	0.90	0.18	45,45,45,45	0
54	MG	1a	3069	1/1	0.90	0.21	38,38,38,38	0
54	MG	2W	203	1/1	0.90	0.11	54,54,54,54	0
54	MG	21	102	1/1	0.90	0.14	49,49,49,49	0
54	MG	2A	3484	1/1	0.90	0.14	42,42,42,42	0
54	MG	1A	3896	1/1	0.90	0.09	29,29,29,29	0
54	MG	1A	3637	1/1	0.90	0.25	27,27,27,27	0
54	MG	2A	3229	1/1	0.90	0.13	44,44,44,44	0
54	MG	1A	3195	1/1	0.90	0.09	47,47,47,47	0
54	MG	2A	3494	1/1	0.90	0.09	43,43,43,43	0
54	MG	2a	3011	1/1	0.90	0.10	53,53,53,53	0
54	MG	1A	3281	1/1	0.90	0.28	44,44,44,44	0
54	MG	2A	3499	1/1	0.90	0.31	49,49,49,49	0
54	MG	1A	3439	1/1	0.90	0.11	33,33,33,33	0
54	MG	1A	3567	1/1	0.90	0.12	40,40,40,40	0
54	MG	1a	3194	1/1	0.90	0.10	54,54,54,54	0
54	MG	2a	3027	1/1	0.90	0.14	50,50,50,50	0
54	MG	2A	3014	1/1	0.90	0.17	54,54,54,54	0
54	MG	2A	3252	1/1	0.90	0.16	56,56,56,56	0
54	MG	2a	3037	1/1	0.90	0.13	50,50,50,50	0
54	MG	1a	3080	1/1	0.90	0.11	53,53,53,53	0
54	MG	1a	3081	1/1	0.90	0.13	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3021	1/1	0.90	0.11	54,54,54,54	0
54	MG	1A	3918	1/1	0.90	0.06	44,44,44,44	0
54	MG	2A	3517	1/1	0.90	0.09	28,28,28,28	0
54	MG	1a	3083	1/1	0.90	0.11	51,51,51,51	0
54	MG	1A	3654	1/1	0.90	0.15	44,44,44,44	0
54	MG	2A	3033	1/1	0.90	0.15	67,67,67,67	0
54	MG	2A	3539	1/1	0.90	0.12	67,67,67,67	0
54	MG	2A	3275	1/1	0.90	0.19	41,41,41,41	0
54	MG	2A	3034	1/1	0.90	0.14	41,41,41,41	0
54	MG	1A	3658	1/1	0.90	0.24	19,19,19,19	0
54	MG	1A	3332	1/1	0.90	0.16	21,21,21,21	0
54	MG	1A	3935	1/1	0.90	0.11	40,40,40,40	0
54	MG	2A	3292	1/1	0.90	0.08	20,20,20,20	0
54	MG	1A	3581	1/1	0.90	0.10	23,23,23,23	0
54	MG	2A	3294	1/1	0.90	0.16	45,45,45,45	0
54	MG	2A	3295	1/1	0.90	0.20	52,52,52,52	0
54	MG	1A	3940	1/1	0.90	0.19	71,71,71,71	0
54	MG	2A	3306	1/1	0.90	0.10	36,36,36,36	0
54	MG	2a	3076	1/1	0.90	0.13	58,58,58,58	0
54	MG	2A	3072	1/1	0.90	0.14	65,65,65,65	0
54	MG	1A	3669	1/1	0.90	0.10	48,48,48,48	0
54	MG	2A	3596	1/1	0.90	0.13	31,31,31,31	0
54	MG	1A	3458	1/1	0.90	0.07	24,24,24,24	0
54	MG	1A	3353	1/1	0.90	0.09	52,52,52,52	0
54	MG	2A	3330	1/1	0.90	0.16	55,55,55,55	0
54	MG	1a	3227	1/1	0.90	0.10	59,59,59,59	0
54	MG	1A	3156	1/1	0.90	0.15	38,38,38,38	0
54	MG	1A	3682	1/1	0.90	0.10	59,59,59,59	0
54	MG	2A	3622	1/1	0.90	0.12	41,41,41,41	0
54	MG	1A	3361	1/1	0.90	0.09	28,28,28,28	0
54	MG	2A	3631	1/1	0.90	0.10	81,81,81,81	0
54	MG	1A	3486	1/1	0.90	0.09	20,20,20,20	0
54	MG	2A	3636	1/1	0.90	0.08	38,38,38,38	0
54	MG	1A	3818	1/1	0.90	0.22	28,28,28,28	0
54	MG	2A	3649	1/1	0.90	0.10	18,18,18,18	0
54	MG	1A	3820	1/1	0.90	0.10	20,20,20,20	0
54	MG	2A	3653	1/1	0.90	0.09	68,68,68,68	0
54	MG	2A	3658	1/1	0.90	0.10	59,59,59,59	0
54	MG	1A	3232	1/1	0.90	0.30	31,31,31,31	0
54	MG	2A	3369	1/1	0.90	0.15	50,50,50,50	0
54	MG	1a	3133	1/1	0.90	0.08	47,47,47,47	0
54	MG	2a	3142	1/1	0.90	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3372	1/1	0.90	0.12	29,29,29,29	0
54	MG	1a	3135	1/1	0.90	0.18	57,57,57,57	0
54	MG	1A	3599	1/1	0.90	0.36	25,25,25,25	0
54	MG	1A	3241	1/1	0.90	0.13	66,66,66,66	0
54	MG	2A	3116	1/1	0.90	0.14	44,44,44,44	0
54	MG	1A	3243	1/1	0.90	0.12	33,33,33,33	0
54	MG	1A	3516	1/1	0.90	0.12	46,46,46,46	0
54	MG	2A	3130	1/1	0.90	0.16	43,43,43,43	0
54	MG	1A	3518	1/1	0.90	0.15	50,50,50,50	0
54	MG	2A	3402	1/1	0.90	0.18	46,46,46,46	0
54	MG	1A	3846	1/1	0.90	0.11	45,45,45,45	0
54	MG	1A	3709	1/1	0.90	0.20	77,77,77,77	0
54	MG	2a	3171	1/1	0.90	0.14	65,65,65,65	0
54	MG	2a	3175	1/1	0.90	0.15	67,67,67,67	0
54	MG	2A	3143	1/1	0.90	0.11	68,68,68,68	0
54	MG	1a	3028	1/1	0.90	0.16	51,51,51,51	0
54	MG	2a	3187	1/1	0.90	0.10	61,61,61,61	0
54	MG	1A	3526	1/1	0.90	0.15	21,21,21,21	0
54	MG	1a	3156	1/1	0.90	0.08	40,40,40,40	0
54	MG	2A	3722	1/1	0.90	0.16	46,46,46,46	0
54	MG	2A	3151	1/1	0.90	0.13	49,49,49,49	0
54	MG	2A	3419	1/1	0.90	0.31	33,33,33,33	0
54	MG	2A	3161	1/1	0.90	0.12	40,40,40,40	0
54	MG	1B	202	1/1	0.90	0.13	52,52,52,52	0
54	MG	2A	3428	1/1	0.90	0.14	51,51,51,51	0
54	MG	2A	3170	1/1	0.90	0.11	51,51,51,51	0
54	MG	1A	3718	1/1	0.90	0.08	19,19,19,19	0
54	MG	1A	3173	1/1	0.90	0.07	31,31,31,31	0
54	MG	2A	3179	1/1	0.90	0.10	44,44,44,44	0
54	MG	1a	3079	1/1	0.91	0.11	40,40,40,40	0
54	MG	2A	3002	1/1	0.91	0.09	47,47,47,47	0
54	MG	2B	208	1/1	0.91	0.19	59,59,59,59	0
54	MG	1A	3585	1/1	0.91	0.09	43,43,43,43	0
54	MG	2B	210	1/1	0.91	0.11	39,39,39,39	0
54	MG	2A	3233	1/1	0.91	0.13	38,38,38,38	0
54	MG	1A	3508	1/1	0.91	0.10	29,29,29,29	0
54	MG	1A	3655	1/1	0.91	0.11	13,13,13,13	0
54	MG	10	102	1/1	0.91	0.38	36,36,36,36	0
54	MG	2E	303	1/1	0.91	0.10	22,22,22,22	0
54	MG	2E	304	1/1	0.91	0.11	46,46,46,46	0
54	MG	2A	3247	1/1	0.91	0.28	52,52,52,52	0
54	MG	1A	3420	1/1	0.91	0.09	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3513	1/1	0.91	0.08	42,42,42,42	0
54	MG	2A	3254	1/1	0.91	0.26	45,45,45,45	0
54	MG	2A	3029	1/1	0.91	0.09	41,41,41,41	0
54	MG	1a	3199	1/1	0.91	0.08	60,60,60,60	0
54	MG	1a	3087	1/1	0.91	0.18	52,52,52,52	0
54	MG	1A	3272	1/1	0.91	0.13	44,44,44,44	0
54	MG	1a	3090	1/1	0.91	0.19	61,61,61,61	0
54	MG	2T	203	1/1	0.91	0.12	49,49,49,49	0
54	MG	1A	3296	1/1	0.91	0.08	30,30,30,30	0
54	MG	21	101	1/1	0.91	0.19	56,56,56,56	0
54	MG	2A	3043	1/1	0.91	0.16	55,55,55,55	0
54	MG	1a	3206	1/1	0.91	0.20	64,64,64,64	0
54	MG	2A	3276	1/1	0.91	0.15	52,52,52,52	0
54	MG	2A	3047	1/1	0.91	0.18	36,36,36,36	0
54	MG	1a	3208	1/1	0.91	0.13	83,83,83,83	0
54	MG	1a	3092	1/1	0.91	0.12	35,35,35,35	0
54	MG	2a	3009	1/1	0.91	0.10	61,61,61,61	0
54	MG	2A	3516	1/1	0.91	0.18	45,45,45,45	0
54	MG	1a	3093	1/1	0.91	0.08	48,48,48,48	0
54	MG	2A	3291	1/1	0.91	0.08	35,35,35,35	0
54	MG	2a	3015	1/1	0.91	0.15	48,48,48,48	0
54	MG	2a	3017	1/1	0.91	0.09	37,37,37,37	0
54	MG	1A	3521	1/1	0.91	0.12	40,40,40,40	0
54	MG	1A	3865	1/1	0.91	0.10	22,22,22,22	0
54	MG	1A	3242	1/1	0.91	0.11	44,44,44,44	0
54	MG	2A	3540	1/1	0.91	0.09	56,56,56,56	0
54	MG	1a	3098	1/1	0.91	0.23	50,50,50,50	0
54	MG	2a	3028	1/1	0.91	0.18	70,70,70,70	0
54	MG	2A	3544	1/1	0.91	0.13	31,31,31,31	0
54	MG	1A	3151	1/1	0.91	0.08	35,35,35,35	0
54	MG	2A	3305	1/1	0.91	0.09	23,23,23,23	0
54	MG	1a	3004	1/1	0.91	0.20	63,63,63,63	0
54	MG	1A	3876	1/1	0.91	0.09	66,66,66,66	0
54	MG	2A	3558	1/1	0.91	0.12	53,53,53,53	0
54	MG	1A	3053	1/1	0.91	0.22	28,28,28,28	0
54	MG	1B	201	1/1	0.91	0.13	40,40,40,40	0
54	MG	1a	3009	1/1	0.91	0.09	51,51,51,51	0
54	MG	1A	3450	1/1	0.91	0.10	32,32,32,32	0
54	MG	2A	3579	1/1	0.91	0.10	59,59,59,59	0
54	MG	2A	3581	1/1	0.91	0.09	30,30,30,30	0
54	MG	2A	3583	1/1	0.91	0.18	57,57,57,57	0
54	MG	1a	3121	1/1	0.91	0.14	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3341	1/1	0.91	0.16	66,66,66,66	0
54	MG	2A	3588	1/1	0.91	0.18	51,51,51,51	0
54	MG	1a	3125	1/1	0.91	0.07	51,51,51,51	0
54	MG	2A	3110	1/1	0.91	0.07	36,36,36,36	0
54	MG	1B	204	1/1	0.91	0.07	37,37,37,37	0
54	MG	1A	3369	1/1	0.91	0.12	32,32,32,32	0
54	MG	2a	3067	1/1	0.91	0.14	54,54,54,54	0
54	MG	2A	3356	1/1	0.91	0.09	38,38,38,38	0
54	MG	1A	3619	1/1	0.91	0.10	10,10,10,10	0
54	MG	1A	3459	1/1	0.91	0.07	36,36,36,36	0
54	MG	1A	3316	1/1	0.91	0.07	21,21,21,21	0
54	MG	2A	3128	1/1	0.91	0.14	35,35,35,35	0
54	MG	1A	3793	1/1	0.91	0.27	41,41,41,41	0
54	MG	1A	3383	1/1	0.91	0.08	23,23,23,23	0
54	MG	2a	3089	1/1	0.91	0.07	65,65,65,65	0
54	MG	2a	3096	1/1	0.91	0.15	53,53,53,53	0
54	MG	2A	3376	1/1	0.91	0.09	32,32,32,32	0
54	MG	1A	3699	1/1	0.91	0.15	45,45,45,45	0
54	MG	1A	3472	1/1	0.91	0.11	24,24,24,24	0
54	MG	1A	3923	1/1	0.91	0.16	52,52,52,52	0
54	MG	2A	3146	1/1	0.91	0.20	39,39,39,39	0
54	MG	2a	3107	1/1	0.91	0.13	55,55,55,55	0
54	MG	1A	3474	1/1	0.91	0.08	14,14,14,14	0
54	MG	1A	3191	1/1	0.91	0.22	41,41,41,41	0
54	MG	1a	3044	1/1	0.91	0.15	65,65,65,65	0
54	MG	1A	3154	1/1	0.91	0.21	43,43,43,43	0
54	MG	1a	3276	1/1	0.91	0.13	63,63,63,63	0
54	MG	2A	3166	1/1	0.91	0.22	53,53,53,53	0
54	MG	2A	3168	1/1	0.91	0.36	31,31,31,31	0
54	MG	2A	3676	1/1	0.91	0.15	47,47,47,47	0
54	MG	1A	3488	1/1	0.91	0.08	24,24,24,24	0
54	MG	1D	310	1/1	0.91	0.21	28,28,28,28	0
54	MG	2A	3684	1/1	0.91	0.11	55,55,55,55	0
54	MG	2a	3131	1/1	0.91	0.07	71,71,71,71	0
54	MG	2A	3685	1/1	0.91	0.10	49,49,49,49	0
54	MG	2A	3687	1/1	0.91	0.22	50,50,50,50	0
54	MG	1a	3057	1/1	0.91	0.27	56,56,56,56	0
54	MG	2A	3694	1/1	0.91	0.13	46,46,46,46	0
54	MG	2A	3172	1/1	0.91	0.14	59,59,59,59	0
54	MG	2A	3414	1/1	0.91	0.14	61,61,61,61	0
54	MG	2A	3701	1/1	0.91	0.16	43,43,43,43	0
54	MG	1a	3160	1/1	0.91	0.21	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3161	1/1	0.91	0.18	56,56,56,56	0
54	MG	1a	3058	1/1	0.91	0.12	60,60,60,60	0
54	MG	1A	3824	1/1	0.91	0.08	33,33,33,33	0
54	MG	1e	202	1/1	0.91	0.15	57,57,57,57	0
54	MG	2a	3157	1/1	0.91	0.16	57,57,57,57	0
54	MG	1E	304	1/1	0.91	0.10	11,11,11,11	0
54	MG	1a	3063	1/1	0.91	0.13	55,55,55,55	0
54	MG	2A	3432	1/1	0.91	0.08	45,45,45,45	0
54	MG	2A	3192	1/1	0.91	0.19	52,52,52,52	0
54	MG	1g	201	1/1	0.91	0.20	61,61,61,61	0
54	MG	2a	3172	1/1	0.91	0.08	61,61,61,61	0
54	MG	2a	3174	1/1	0.91	0.10	51,51,51,51	0
54	MG	1A	3728	1/1	0.91	0.09	31,31,31,31	0
54	MG	1a	3065	1/1	0.91	0.22	56,56,56,56	0
54	MG	2a	3178	1/1	0.91	0.24	64,64,64,64	0
54	MG	2A	3200	1/1	0.91	0.19	52,52,52,52	0
54	MG	2A	3445	1/1	0.91	0.09	37,37,37,37	0
54	MG	2e	201	1/1	0.91	0.30	57,57,57,57	0
54	MG	1A	3572	1/1	0.91	0.12	16,16,16,16	0
54	MG	1A	3945	1/1	0.91	0.07	34,34,34,34	0
54	MG	1l	201	1/1	0.91	0.34	55,55,55,55	0
54	MG	2A	3456	1/1	0.91	0.10	53,53,53,53	0
54	MG	1A	3264	1/1	0.91	0.10	37,37,37,37	0
54	MG	1A	3949	1/1	0.91	0.12	59,59,59,59	0
54	MG	1A	3951	1/1	0.91	0.14	48,48,48,48	0
54	MG	1A	3333	1/1	0.91	0.10	32,32,32,32	0
54	MG	2B	201	1/1	0.91	0.11	62,62,62,62	0
54	MG	1a	3182	1/1	0.91	0.10	53,53,53,53	0
54	MG	1A	3840	1/1	0.91	0.22	43,43,43,43	0
54	MG	1A	3650	1/1	0.91	0.09	21,21,21,21	0
58	ZN	24	501	1/1	0.91	0.13	142,142,142,142	0
54	MG	2A	3224	1/1	0.92	0.09	52,52,52,52	0
54	MG	1A	3929	1/1	0.92	0.17	28,28,28,28	0
54	MG	1A	3546	1/1	0.92	0.08	39,39,39,39	0
54	MG	1a	3181	1/1	0.92	0.13	59,59,59,59	0
54	MG	2A	3231	1/1	0.92	0.08	49,49,49,49	0
54	MG	2D	306	1/1	0.92	0.10	47,47,47,47	0
54	MG	1A	3324	1/1	0.92	0.15	32,32,32,32	0
54	MG	1D	311	1/1	0.92	0.14	36,36,36,36	0
54	MG	2A	3019	1/1	0.92	0.08	36,36,36,36	0
54	MG	2G	201	1/1	0.92	0.18	66,66,66,66	0
54	MG	1D	313	1/1	0.92	0.09	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3477	1/1	0.92	0.09	23,23,23,23	0
54	MG	2A	3244	1/1	0.92	0.28	38,38,38,38	0
54	MG	2O	201	1/1	0.92	0.14	36,36,36,36	0
54	MG	1D	318	1/1	0.92	0.10	34,34,34,34	0
54	MG	2A	3248	1/1	0.92	0.08	37,37,37,37	0
54	MG	1A	3551	1/1	0.92	0.13	36,36,36,36	0
54	MG	2A	3251	1/1	0.92	0.14	37,37,37,37	0
54	MG	1A	3014	1/1	0.92	0.08	41,41,41,41	0
54	MG	1A	3419	1/1	0.92	0.11	24,24,24,24	0
54	MG	2T	204	1/1	0.92	0.07	36,36,36,36	0
54	MG	2A	3257	1/1	0.92	0.12	42,42,42,42	0
54	MG	20	102	1/1	0.92	0.11	53,53,53,53	0
54	MG	1A	3712	1/1	0.92	0.09	22,22,22,22	0
54	MG	1A	3285	1/1	0.92	0.34	40,40,40,40	0
54	MG	1A	3727	1/1	0.92	0.31	31,31,31,31	0
54	MG	1A	3948	1/1	0.92	0.11	48,48,48,48	0
54	MG	28	101	1/1	0.92	0.08	38,38,38,38	0
54	MG	2A	3040	1/1	0.92	0.09	36,36,36,36	0
54	MG	2A	3042	1/1	0.92	0.13	37,37,37,37	0
54	MG	2A	3521	1/1	0.92	0.08	46,46,46,46	0
54	MG	1A	3829	1/1	0.92	0.10	36,36,36,36	0
54	MG	1A	3950	1/1	0.92	0.09	59,59,59,59	0
54	MG	1A	3494	1/1	0.92	0.09	24,24,24,24	0
54	MG	2A	3048	1/1	0.92	0.15	40,40,40,40	0
54	MG	2A	3286	1/1	0.92	0.09	37,37,37,37	0
54	MG	2A	3287	1/1	0.92	0.13	51,51,51,51	0
54	MG	1A	3187	1/1	0.92	0.09	45,45,45,45	0
54	MG	2A	3056	1/1	0.92	0.07	37,37,37,37	0
54	MG	2A	3060	1/1	0.92	0.20	47,47,47,47	0
54	MG	1a	3089	1/1	0.92	0.13	42,42,42,42	0
54	MG	2A	3066	1/1	0.92	0.12	41,41,41,41	0
54	MG	1a	3210	1/1	0.92	0.10	51,51,51,51	0
54	MG	2a	3033	1/1	0.92	0.13	55,55,55,55	0
54	MG	1V	205	1/1	0.92	0.11	45,45,45,45	0
54	MG	1A	3957	1/1	0.92	0.10	37,37,37,37	0
54	MG	2A	3299	1/1	0.92	0.08	54,54,54,54	0
54	MG	1A	3737	1/1	0.92	0.08	44,44,44,44	0
54	MG	1A	3960	1/1	0.92	0.26	25,25,25,25	0
54	MG	1A	3963	1/1	0.92	0.22	61,61,61,61	0
54	MG	1A	3569	1/1	0.92	0.08	46,46,46,46	0
54	MG	1A	3965	1/1	0.92	0.13	58,58,58,58	0
54	MG	2a	3048	1/1	0.92	0.07	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3321	1/1	0.92	0.09	31,31,31,31	0
54	MG	2a	3051	1/1	0.92	0.16	59,59,59,59	0
54	MG	1A	3506	1/1	0.92	0.09	10,10,10,10	0
54	MG	2A	3589	1/1	0.92	0.12	64,64,64,64	0
54	MG	1A	3746	1/1	0.92	0.08	39,39,39,39	0
54	MG	13	103	1/1	0.92	0.12	52,52,52,52	0
54	MG	1A	3429	1/1	0.92	0.12	47,47,47,47	0
54	MG	2A	3597	1/1	0.92	0.10	45,45,45,45	0
54	MG	2A	3598	1/1	0.92	0.10	58,58,58,58	0
54	MG	2A	3601	1/1	0.92	0.12	31,31,31,31	0
54	MG	2A	3104	1/1	0.92	0.07	38,38,38,38	0
54	MG	2A	3343	1/1	0.92	0.11	47,47,47,47	0
54	MG	1A	3978	1/1	0.92	0.10	39,39,39,39	0
54	MG	2A	3107	1/1	0.92	0.12	45,45,45,45	0
54	MG	1A	3979	1/1	0.92	0.08	57,57,57,57	0
54	MG	1a	3003	1/1	0.92	0.13	61,61,61,61	0
54	MG	2a	3073	1/1	0.92	0.09	46,46,46,46	0
54	MG	2A	3619	1/1	0.92	0.15	44,44,44,44	0
54	MG	2A	3621	1/1	0.92	0.11	50,50,50,50	0
54	MG	1A	3216	1/1	0.92	0.10	46,46,46,46	0
54	MG	2A	3362	1/1	0.92	0.08	57,57,57,57	0
54	MG	2a	3079	1/1	0.92	0.09	52,52,52,52	0
54	MG	2A	3114	1/1	0.92	0.49	37,37,37,37	0
54	MG	1A	3258	1/1	0.92	0.15	37,37,37,37	0
54	MG	2A	3367	1/1	0.92	0.11	26,26,26,26	0
54	MG	2A	3637	1/1	0.92	0.13	52,52,52,52	0
54	MG	2a	3099	1/1	0.92	0.09	52,52,52,52	0
54	MG	1a	3240	1/1	0.92	0.11	54,54,54,54	0
54	MG	1a	3243	1/1	0.92	0.08	63,63,63,63	0
54	MG	1a	3123	1/1	0.92	0.08	46,46,46,46	0
54	MG	1A	3188	1/1	0.92	0.21	47,47,47,47	0
54	MG	1A	3514	1/1	0.92	0.07	17,17,17,17	0
54	MG	2A	3378	1/1	0.92	0.12	48,48,48,48	0
54	MG	2A	3664	1/1	0.92	0.10	39,39,39,39	0
54	MG	1a	3129	1/1	0.92	0.08	52,52,52,52	0
54	MG	1A	3863	1/1	0.92	0.07	26,26,26,26	0
54	MG	1A	3988	1/1	0.92	0.16	32,32,32,32	0
54	MG	1a	3134	1/1	0.92	0.10	49,49,49,49	0
54	MG	1A	3022	1/1	0.92	0.12	34,34,34,34	0
54	MG	2A	3682	1/1	0.92	0.11	32,32,32,32	0
54	MG	2a	3121	1/1	0.92	0.07	51,51,51,51	0
54	MG	1a	3018	1/1	0.92	0.17	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3019	1/1	0.92	0.10	46,46,46,46	0
54	MG	1A	3109	1/1	0.92	0.32	19,19,19,19	0
54	MG	2A	3686	1/1	0.92	0.12	47,47,47,47	0
54	MG	1A	3302	1/1	0.92	0.07	32,32,32,32	0
54	MG	1A	4000	1/1	0.92	0.15	35,35,35,35	0
54	MG	1a	3275	1/1	0.92	0.09	55,55,55,55	0
54	MG	2A	3167	1/1	0.92	0.09	53,53,53,53	0
54	MG	1A	3594	1/1	0.92	0.07	29,29,29,29	0
54	MG	2A	3700	1/1	0.92	0.09	67,67,67,67	0
54	MG	1A	4007	1/1	0.92	0.10	42,42,42,42	0
54	MG	1A	3772	1/1	0.92	0.17	23,23,23,23	0
54	MG	1a	3147	1/1	0.92	0.10	43,43,43,43	0
54	MG	1A	3671	1/1	0.92	0.09	59,59,59,59	0
54	MG	2A	3173	1/1	0.92	0.09	39,39,39,39	0
54	MG	2a	3154	1/1	0.92	0.08	57,57,57,57	0
54	MG	1a	3153	1/1	0.92	0.10	46,46,46,46	0
54	MG	2A	3710	1/1	0.92	0.09	45,45,45,45	0
54	MG	2A	3423	1/1	0.92	0.11	42,42,42,42	0
54	MG	2A	3177	1/1	0.92	0.14	37,37,37,37	0
54	MG	1a	3155	1/1	0.92	0.16	62,62,62,62	0
54	MG	1A	3275	1/1	0.92	0.11	52,52,52,52	0
54	MG	2A	3720	1/1	0.92	0.13	52,52,52,52	0
54	MG	1A	3165	1/1	0.92	0.11	44,44,44,44	0
54	MG	1A	3529	1/1	0.92	0.14	45,45,45,45	0
54	MG	1A	3902	1/1	0.92	0.10	20,20,20,20	0
54	MG	1A	3467	1/1	0.92	0.10	36,36,36,36	0
54	MG	1A	3607	1/1	0.92	0.09	32,32,32,32	0
54	MG	2a	3180	1/1	0.92	0.09	61,61,61,61	0
54	MG	1A	3279	1/1	0.92	0.61	38,38,38,38	0
54	MG	2a	3183	1/1	0.92	0.10	47,47,47,47	0
54	MG	1h	201	1/1	0.92	0.06	37,37,37,37	0
54	MG	2A	3196	1/1	0.92	0.08	50,50,50,50	0
54	MG	1a	3053	1/1	0.92	0.08	54,54,54,54	0
54	MG	1A	3609	1/1	0.92	0.17	25,25,25,25	0
54	MG	1A	3790	1/1	0.92	0.10	76,76,76,76	0
54	MG	2A	3452	1/1	0.92	0.14	49,49,49,49	0
54	MG	1A	3916	1/1	0.92	0.16	46,46,46,46	0
54	MG	1l	203	1/1	0.92	0.08	47,47,47,47	0
54	MG	1a	3060	1/1	0.92	0.12	59,59,59,59	0
54	MG	1n	102	1/1	0.92	0.24	61,61,61,61	0
54	MG	1B	219	1/1	0.92	0.09	28,28,28,28	0
54	MG	1A	3544	1/1	0.92	0.15	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3919	1/1	0.92	0.10	50,50,50,50	0
54	MG	1A	3059	1/1	0.92	0.13	41,41,41,41	0
54	MG	2A	3222	1/1	0.92	0.32	48,48,48,48	0
54	MG	1A	3570	1/1	0.93	0.13	9,9,9,9	0
54	MG	1a	3027	1/1	0.93	0.12	53,53,53,53	0
54	MG	1A	3365	1/1	0.93	0.07	34,34,34,34	0
54	MG	2B	205	1/1	0.93	0.23	54,54,54,54	0
54	MG	1A	3248	1/1	0.93	0.11	37,37,37,37	0
54	MG	1A	3576	1/1	0.93	0.13	33,33,33,33	0
54	MG	2A	3463	1/1	0.93	0.10	53,53,53,53	0
54	MG	1A	3200	1/1	0.93	0.10	30,30,30,30	0
54	MG	2A	3217	1/1	0.93	0.16	53,53,53,53	0
54	MG	2B	213	1/1	0.93	0.12	53,53,53,53	0
54	MG	2B	214	1/1	0.93	0.07	52,52,52,52	0
54	MG	1A	3374	1/1	0.93	0.07	25,25,25,25	0
54	MG	1A	3691	1/1	0.93	0.32	23,23,23,23	0
54	MG	1A	3842	1/1	0.93	0.13	26,26,26,26	0
54	MG	2A	3474	1/1	0.93	0.08	38,38,38,38	0
54	MG	2D	301	1/1	0.93	0.43	27,27,27,27	0
54	MG	2A	3226	1/1	0.93	0.12	40,40,40,40	0
54	MG	2A	3476	1/1	0.93	0.15	45,45,45,45	0
54	MG	1A	4003	1/1	0.93	0.06	27,27,27,27	0
54	MG	2E	306	1/1	0.93	0.17	44,44,44,44	0
54	MG	1A	3125	1/1	0.93	0.17	34,34,34,34	0
54	MG	1A	3256	1/1	0.93	0.11	36,36,36,36	0
54	MG	1A	3388	1/1	0.93	0.08	8,8,8,8	0
54	MG	1A	3701	1/1	0.93	0.09	24,24,24,24	0
54	MG	2A	3485	1/1	0.93	0.09	56,56,56,56	0
54	MG	2A	3018	1/1	0.93	0.23	36,36,36,36	0
54	MG	1A	3400	1/1	0.93	0.10	28,28,28,28	0
54	MG	1A	3703	1/1	0.93	0.24	46,46,46,46	0
54	MG	2A	3239	1/1	0.93	0.09	37,37,37,37	0
54	MG	1a	3178	1/1	0.93	0.12	65,65,65,65	0
54	MG	2A	3496	1/1	0.93	0.10	20,20,20,20	0
54	MG	1A	3402	1/1	0.93	0.10	40,40,40,40	0
54	MG	2A	3246	1/1	0.93	0.12	45,45,45,45	0
54	MG	2A	3024	1/1	0.93	0.14	43,43,43,43	0
54	MG	1A	3707	1/1	0.93	0.23	19,19,19,19	0
54	MG	2A	3503	1/1	0.93	0.10	59,59,59,59	0
54	MG	2A	3504	1/1	0.93	0.07	46,46,46,46	0
54	MG	2A	3027	1/1	0.93	0.10	37,37,37,37	0
54	MG	1A	3130	1/1	0.93	0.05	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3030	1/1	0.93	0.09	39,39,39,39	0
54	MG	29	101	1/1	0.93	0.20	52,52,52,52	0
54	MG	1A	3509	1/1	0.93	0.06	34,34,34,34	0
54	MG	2A	3255	1/1	0.93	0.12	49,49,49,49	0
54	MG	1a	3184	1/1	0.93	0.09	64,64,64,64	0
54	MG	1A	3209	1/1	0.93	0.44	24,24,24,24	0
54	MG	1a	3187	1/1	0.93	0.09	53,53,53,53	0
54	MG	1A	3304	1/1	0.93	0.13	50,50,50,50	0
54	MG	1A	3720	1/1	0.93	0.09	41,41,41,41	0
54	MG	1A	3185	1/1	0.93	0.14	34,34,34,34	0
54	MG	2A	3525	1/1	0.93	0.12	68,68,68,68	0
54	MG	1A	3606	1/1	0.93	0.21	21,21,21,21	0
54	MG	1a	3068	1/1	0.93	0.08	32,32,32,32	0
54	MG	1A	3889	1/1	0.93	0.08	49,49,49,49	0
54	MG	2a	3022	1/1	0.93	0.17	42,42,42,42	0
54	MG	1a	3197	1/1	0.93	0.11	59,59,59,59	0
54	MG	1A	3267	1/1	0.93	0.07	42,42,42,42	0
54	MG	2A	3280	1/1	0.93	0.10	37,37,37,37	0
54	MG	2a	3029	1/1	0.93	0.08	50,50,50,50	0
54	MG	2A	3283	1/1	0.93	0.07	20,20,20,20	0
54	MG	2A	3546	1/1	0.93	0.12	54,54,54,54	0
54	MG	1A	3730	1/1	0.93	0.06	21,21,21,21	0
54	MG	2A	3057	1/1	0.93	0.12	44,44,44,44	0
54	MG	1A	3897	1/1	0.93	0.29	28,28,28,28	0
54	MG	2a	3040	1/1	0.93	0.10	68,68,68,68	0
54	MG	2A	3556	1/1	0.93	0.10	42,42,42,42	0
54	MG	1A	3517	1/1	0.93	0.08	14,14,14,14	0
54	MG	1A	3214	1/1	0.93	0.19	52,52,52,52	0
54	MG	2A	3560	1/1	0.93	0.14	52,52,52,52	0
54	MG	2A	3067	1/1	0.93	0.25	39,39,39,39	0
54	MG	1A	3425	1/1	0.93	0.09	39,39,39,39	0
54	MG	1A	3426	1/1	0.93	0.10	11,11,11,11	0
54	MG	2A	3576	1/1	0.93	0.08	57,57,57,57	0
54	MG	1A	3910	1/1	0.93	0.45	23,23,23,23	0
54	MG	1D	317	1/1	0.93	0.12	59,59,59,59	0
54	MG	1a	3212	1/1	0.93	0.11	82,82,82,82	0
54	MG	1A	3320	1/1	0.93	0.10	17,17,17,17	0
54	MG	2A	3304	1/1	0.93	0.07	42,42,42,42	0
54	MG	2A	3084	1/1	0.93	0.07	43,43,43,43	0
54	MG	1A	3752	1/1	0.93	0.08	31,31,31,31	0
54	MG	2A	3307	1/1	0.93	0.07	33,33,33,33	0
54	MG	2a	3064	1/1	0.93	0.11	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3593	1/1	0.93	0.09	20,20,20,20	0
54	MG	2A	3088	1/1	0.93	0.20	44,44,44,44	0
54	MG	2A	3315	1/1	0.93	0.08	22,22,22,22	0
54	MG	1A	3623	1/1	0.93	0.09	17,17,17,17	0
54	MG	1F	304	1/1	0.93	0.24	22,22,22,22	0
54	MG	1A	3322	1/1	0.93	0.09	18,18,18,18	0
54	MG	2A	3094	1/1	0.93	0.09	34,34,34,34	0
54	MG	2a	3075	1/1	0.93	0.12	49,49,49,49	0
54	MG	2A	3606	1/1	0.93	0.10	49,49,49,49	0
54	MG	2A	3329	1/1	0.93	0.12	21,21,21,21	0
54	MG	2A	3097	1/1	0.93	0.29	35,35,35,35	0
54	MG	1A	3531	1/1	0.93	0.07	43,43,43,43	0
54	MG	2A	3337	1/1	0.93	0.09	49,49,49,49	0
54	MG	1A	3533	1/1	0.93	0.07	17,17,17,17	0
54	MG	2a	3094	1/1	0.93	0.09	50,50,50,50	0
54	MG	1A	3007	1/1	0.93	0.07	27,27,27,27	0
54	MG	1a	3228	1/1	0.93	0.09	42,42,42,42	0
54	MG	1A	3536	1/1	0.93	0.07	25,25,25,25	0
54	MG	1A	3766	1/1	0.93	0.10	33,33,33,33	0
54	MG	1A	3768	1/1	0.93	0.11	12,12,12,12	0
54	MG	1A	3537	1/1	0.93	0.06	19,19,19,19	0
54	MG	1U	203	1/1	0.93	0.12	33,33,33,33	0
54	MG	1U	205	1/1	0.93	0.24	33,33,33,33	0
54	MG	2A	3638	1/1	0.93	0.15	50,50,50,50	0
54	MG	2a	3112	1/1	0.93	0.06	58,58,58,58	0
54	MG	1a	3237	1/1	0.93	0.10	68,68,68,68	0
54	MG	1A	3328	1/1	0.93	0.18	7,7,7,7	0
54	MG	1a	3101	1/1	0.93	0.14	38,38,38,38	0
54	MG	1A	3541	1/1	0.93	0.12	32,32,32,32	0
54	MG	2A	3370	1/1	0.93	0.09	33,33,33,33	0
54	MG	1a	3242	1/1	0.93	0.07	42,42,42,42	0
54	MG	1W	201	1/1	0.93	0.13	30,30,30,30	0
54	MG	2A	3374	1/1	0.93	0.09	39,39,39,39	0
54	MG	2A	3670	1/1	0.93	0.15	64,64,64,64	0
54	MG	2A	3671	1/1	0.93	0.13	63,63,63,63	0
54	MG	1A	3437	1/1	0.93	0.07	35,35,35,35	0
54	MG	1a	3245	1/1	0.93	0.09	64,64,64,64	0
54	MG	1A	3104	1/1	0.93	0.22	16,16,16,16	0
54	MG	1A	3644	1/1	0.93	0.11	49,49,49,49	0
54	MG	2A	3390	1/1	0.93	0.08	48,48,48,48	0
54	MG	1a	3253	1/1	0.93	0.09	43,43,43,43	0
54	MG	2A	3394	1/1	0.93	0.07	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3115	1/1	0.93	0.12	60,60,60,60	0
54	MG	1A	3220	1/1	0.93	0.13	40,40,40,40	0
54	MG	2a	3148	1/1	0.93	0.09	63,63,63,63	0
54	MG	1A	3443	1/1	0.93	0.09	29,29,29,29	0
54	MG	2A	3157	1/1	0.93	0.12	35,35,35,35	0
54	MG	1A	3010	1/1	0.93	0.08	35,35,35,35	0
54	MG	1A	3653	1/1	0.93	0.07	14,14,14,14	0
54	MG	1A	3550	1/1	0.93	0.07	27,27,27,27	0
54	MG	2A	3699	1/1	0.93	0.17	48,48,48,48	0
54	MG	1A	3351	1/1	0.93	0.06	16,16,16,16	0
54	MG	1a	3127	1/1	0.93	0.07	67,67,67,67	0
54	MG	2a	3161	1/1	0.93	0.08	49,49,49,49	0
54	MG	2A	3406	1/1	0.93	0.08	69,69,69,69	0
54	MG	1A	3110	1/1	0.93	0.08	36,36,36,36	0
54	MG	2a	3165	1/1	0.93	0.07	56,56,56,56	0
54	MG	1a	3131	1/1	0.93	0.18	61,61,61,61	0
54	MG	15	101	1/1	0.93	0.20	34,34,34,34	0
54	MG	15	108	1/1	0.93	0.09	57,57,57,57	0
54	MG	1A	3354	1/1	0.93	0.13	45,45,45,45	0
54	MG	2A	3175	1/1	0.93	0.13	37,37,37,37	0
54	MG	1A	3799	1/1	0.93	0.15	46,46,46,46	0
54	MG	2A	3422	1/1	0.93	0.15	60,60,60,60	0
54	MG	2A	3718	1/1	0.93	0.10	50,50,50,50	0
54	MG	1A	3466	1/1	0.93	0.09	43,43,43,43	0
54	MG	1A	3804	1/1	0.93	0.14	15,15,15,15	0
54	MG	1A	3806	1/1	0.93	0.09	26,26,26,26	0
54	MG	1A	3663	1/1	0.93	0.14	31,31,31,31	0
54	MG	2A	3723	1/1	0.93	0.11	58,58,58,58	0
54	MG	1A	3971	1/1	0.93	0.13	44,44,44,44	0
54	MG	1A	3664	1/1	0.93	0.10	26,26,26,26	0
54	MG	2A	3434	1/1	0.93	0.08	46,46,46,46	0
54	MG	1A	3561	1/1	0.93	0.23	30,30,30,30	0
54	MG	2p	101	1/1	0.93	0.09	34,34,34,34	0
54	MG	1A	3192	1/1	0.93	0.11	49,49,49,49	0
56	MPD	1A	4012	8/8	0.93	0.19	38,44,54,56	0
54	MG	1a	3013	1/1	0.93	0.07	14,14,14,14	0
54	MG	1a	3150	1/1	0.93	0.09	64,64,64,64	0
54	MG	1a	3016	1/1	0.93	0.11	57,57,57,57	0
54	MG	1A	3075	1/1	0.93	0.10	39,39,39,39	0
54	MG	2A	3201	1/1	0.93	0.08	50,50,50,50	0
54	MG	1A	3179	1/1	0.93	0.10	48,48,48,48	0
54	MG	1A	3982	1/1	0.93	0.06	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3808	1/1	0.94	0.08	34,34,34,34	0
54	MG	1a	3271	1/1	0.94	0.09	66,66,66,66	0
54	MG	10	103	1/1	0.94	0.07	28,28,28,28	0
54	MG	1A	3338	1/1	0.94	0.09	35,35,35,35	0
54	MG	1A	3345	1/1	0.94	0.10	47,47,47,47	0
54	MG	11	101	1/1	0.94	0.44	36,36,36,36	0
54	MG	2A	3732	1/1	0.94	0.17	58,58,58,58	0
54	MG	1A	3532	1/1	0.94	0.09	41,41,41,41	0
54	MG	1A	3440	1/1	0.94	0.17	44,44,44,44	0
54	MG	2A	3736	1/1	0.94	0.23	37,37,37,37	0
54	MG	1A	3534	1/1	0.94	0.07	22,22,22,22	0
54	MG	1A	3348	1/1	0.94	0.07	18,18,18,18	0
54	MG	1A	3229	1/1	0.94	0.30	26,26,26,26	0
54	MG	2A	3446	1/1	0.94	0.09	46,46,46,46	0
54	MG	1A	3975	1/1	0.94	0.07	70,70,70,70	0
54	MG	15	105	1/1	0.94	0.33	20,20,20,20	0
54	MG	1A	3610	1/1	0.94	0.10	24,24,24,24	0
54	MG	17	103	1/1	0.94	0.24	25,25,25,25	0
54	MG	1a	3140	1/1	0.94	0.07	34,34,34,34	0
54	MG	17	105	1/1	0.94	0.09	39,39,39,39	0
54	MG	1A	3704	1/1	0.94	0.21	31,31,31,31	0
54	MG	2A	3203	1/1	0.94	0.09	50,50,50,50	0
54	MG	1A	3612	1/1	0.94	0.10	35,35,35,35	0
54	MG	2B	212	1/1	0.94	0.11	56,56,56,56	0
54	MG	1A	3128	1/1	0.94	0.06	39,39,39,39	0
54	MG	2A	3465	1/1	0.94	0.16	23,23,23,23	0
54	MG	1A	3456	1/1	0.94	0.09	44,44,44,44	0
54	MG	2A	3208	1/1	0.94	0.09	48,48,48,48	0
54	MG	2A	3209	1/1	0.94	0.19	37,37,37,37	0
54	MG	2A	3472	1/1	0.94	0.07	28,28,28,28	0
54	MG	2B	220	1/1	0.94	0.09	66,66,66,66	0
54	MG	1A	3079	1/1	0.94	0.12	34,34,34,34	0
54	MG	2D	304	1/1	0.94	0.18	40,40,40,40	0
54	MG	1A	3711	1/1	0.94	0.14	25,25,25,25	0
54	MG	1a	3151	1/1	0.94	0.12	60,60,60,60	0
54	MG	1A	3171	1/1	0.94	0.06	29,29,29,29	0
54	MG	1A	3288	1/1	0.94	0.06	37,37,37,37	0
54	MG	2E	307	1/1	0.94	0.10	49,49,49,49	0
54	MG	1a	3154	1/1	0.94	0.08	55,55,55,55	0
54	MG	2A	3221	1/1	0.94	0.22	36,36,36,36	0
54	MG	1a	3010	1/1	0.94	0.07	41,41,41,41	0
54	MG	1A	3719	1/1	0.94	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3225	1/1	0.94	0.19	43,43,43,43	0
54	MG	1A	3197	1/1	0.94	0.09	27,27,27,27	0
54	MG	1A	3290	1/1	0.94	0.11	43,43,43,43	0
54	MG	1a	3014	1/1	0.94	0.09	61,61,61,61	0
54	MG	1A	3293	1/1	0.94	0.11	36,36,36,36	0
54	MG	1A	3999	1/1	0.94	0.18	34,34,34,34	0
54	MG	2A	3004	1/1	0.94	0.10	40,40,40,40	0
54	MG	1A	3632	1/1	0.94	0.20	14,14,14,14	0
54	MG	2A	3498	1/1	0.94	0.27	33,33,33,33	0
54	MG	2V	201	1/1	0.94	0.08	56,56,56,56	0
54	MG	1A	3019	1/1	0.94	0.33	21,21,21,21	0
54	MG	1A	3733	1/1	0.94	0.06	25,25,25,25	0
54	MG	2A	3238	1/1	0.94	0.13	30,30,30,30	0
54	MG	2A	3502	1/1	0.94	0.19	41,41,41,41	0
54	MG	1a	3023	1/1	0.94	0.17	56,56,56,56	0
54	MG	25	101	1/1	0.94	0.11	48,48,48,48	0
54	MG	26	101	1/1	0.94	0.10	51,51,51,51	0
54	MG	1A	4006	1/1	0.94	0.10	54,54,54,54	0
54	MG	1A	3136	1/1	0.94	0.06	21,21,21,21	0
54	MG	1A	3738	1/1	0.94	0.16	41,41,41,41	0
54	MG	1A	4010	1/1	0.94	0.15	56,56,56,56	0
54	MG	2A	3508	1/1	0.94	0.08	53,53,53,53	0
54	MG	1A	3739	1/1	0.94	0.13	43,43,43,43	0
54	MG	2A	3511	1/1	0.94	0.06	43,43,43,43	0
54	MG	1A	3554	1/1	0.94	0.06	25,25,25,25	0
54	MG	1a	3036	1/1	0.94	0.08	52,52,52,52	0
54	MG	1a	3176	1/1	0.94	0.08	65,65,65,65	0
54	MG	1A	3877	1/1	0.94	0.09	23,23,23,23	0
54	MG	2a	3016	1/1	0.94	0.06	47,47,47,47	0
54	MG	1a	3179	1/1	0.94	0.08	54,54,54,54	0
54	MG	2A	3520	1/1	0.94	0.14	16,16,16,16	0
54	MG	1A	3203	1/1	0.94	0.51	34,34,34,34	0
54	MG	1A	3103	1/1	0.94	0.15	38,38,38,38	0
54	MG	2A	3524	1/1	0.94	0.10	57,57,57,57	0
54	MG	2a	3023	1/1	0.94	0.15	49,49,49,49	0
54	MG	1A	3749	1/1	0.94	0.06	28,28,28,28	0
54	MG	2A	3526	1/1	0.94	0.07	52,52,52,52	0
54	MG	1A	3639	1/1	0.94	0.08	29,29,29,29	0
54	MG	1A	3895	1/1	0.94	0.11	48,48,48,48	0
54	MG	2A	3533	1/1	0.94	0.09	52,52,52,52	0
54	MG	1A	3385	1/1	0.94	0.09	14,14,14,14	0
54	MG	2A	3267	1/1	0.94	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3036	1/1	0.94	0.12	52,52,52,52	0
54	MG	1A	3031	1/1	0.94	0.09	14,14,14,14	0
54	MG	2A	3272	1/1	0.94	0.17	34,34,34,34	0
54	MG	2A	3046	1/1	0.94	0.15	42,42,42,42	0
54	MG	1a	3054	1/1	0.94	0.07	58,58,58,58	0
54	MG	1a	3189	1/1	0.94	0.13	37,37,37,37	0
54	MG	2A	3050	1/1	0.94	0.23	63,63,63,63	0
54	MG	1A	3259	1/1	0.94	0.23	26,26,26,26	0
54	MG	2A	3052	1/1	0.94	0.10	28,28,28,28	0
54	MG	1a	3056	1/1	0.94	0.11	59,59,59,59	0
54	MG	1A	3565	1/1	0.94	0.18	26,26,26,26	0
54	MG	1B	221	1/1	0.94	0.07	55,55,55,55	0
54	MG	1A	3033	1/1	0.94	0.08	27,27,27,27	0
54	MG	1B	225	1/1	0.94	0.12	53,53,53,53	0
54	MG	2a	3056	1/1	0.94	0.09	33,33,33,33	0
54	MG	1A	3652	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3572	1/1	0.94	0.07	42,42,42,42	0
54	MG	1A	3306	1/1	0.94	0.45	30,30,30,30	0
54	MG	2a	3060	1/1	0.94	0.12	50,50,50,50	0
54	MG	2A	3073	1/1	0.94	0.12	49,49,49,49	0
54	MG	1A	3313	1/1	0.94	0.20	27,27,27,27	0
54	MG	1A	3025	1/1	0.94	0.23	35,35,35,35	0
54	MG	1D	301	1/1	0.94	0.08	30,30,30,30	0
54	MG	1A	3266	1/1	0.94	0.11	51,51,51,51	0
54	MG	2A	3079	1/1	0.94	0.07	23,23,23,23	0
54	MG	1a	3205	1/1	0.94	0.12	51,51,51,51	0
54	MG	1A	3575	1/1	0.94	0.26	30,30,30,30	0
54	MG	2a	3070	1/1	0.94	0.16	45,45,45,45	0
54	MG	1A	3418	1/1	0.94	0.10	34,34,34,34	0
54	MG	1A	3071	1/1	0.94	0.30	22,22,22,22	0
54	MG	2A	3595	1/1	0.94	0.07	55,55,55,55	0
54	MG	2A	3314	1/1	0.94	0.05	24,24,24,24	0
54	MG	2A	3090	1/1	0.94	0.12	38,38,38,38	0
54	MG	1a	3074	1/1	0.94	0.09	29,29,29,29	0
54	MG	1A	3927	1/1	0.94	0.10	36,36,36,36	0
54	MG	1A	3928	1/1	0.94	0.10	58,58,58,58	0
54	MG	2a	3082	1/1	0.94	0.12	43,43,43,43	0
54	MG	2A	3605	1/1	0.94	0.08	56,56,56,56	0
54	MG	2a	3087	1/1	0.94	0.10	53,53,53,53	0
54	MG	1A	3268	1/1	0.94	0.20	37,37,37,37	0
54	MG	2A	3327	1/1	0.94	0.06	40,40,40,40	0
54	MG	2A	3609	1/1	0.94	0.11	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1E	305	1/1	0.94	0.13	32,32,32,32	0
54	MG	1a	3220	1/1	0.94	0.10	56,56,56,56	0
54	MG	2A	3612	1/1	0.94	0.14	50,50,50,50	0
54	MG	2A	3332	1/1	0.94	0.07	27,27,27,27	0
54	MG	1A	3667	1/1	0.94	0.09	51,51,51,51	0
54	MG	2A	3617	1/1	0.94	0.10	54,54,54,54	0
54	MG	2A	3103	1/1	0.94	0.08	26,26,26,26	0
54	MG	1A	3668	1/1	0.94	0.08	56,56,56,56	0
54	MG	2A	3342	1/1	0.94	0.14	38,38,38,38	0
54	MG	1a	3224	1/1	0.94	0.11	37,37,37,37	0
54	MG	2A	3106	1/1	0.94	0.12	41,41,41,41	0
54	MG	2A	3632	1/1	0.94	0.17	49,49,49,49	0
54	MG	1A	3041	1/1	0.94	0.13	43,43,43,43	0
54	MG	2A	3635	1/1	0.94	0.09	40,40,40,40	0
54	MG	1F	310	1/1	0.94	0.07	33,33,33,33	0
54	MG	1F	314	1/1	0.94	0.09	34,34,34,34	0
54	MG	1F	315	1/1	0.94	0.13	50,50,50,50	0
54	MG	2A	3359	1/1	0.94	0.12	49,49,49,49	0
54	MG	2a	3126	1/1	0.94	0.07	52,52,52,52	0
54	MG	1a	3085	1/1	0.94	0.11	44,44,44,44	0
54	MG	1A	3670	1/1	0.94	0.08	42,42,42,42	0
54	MG	1G	201	1/1	0.94	0.08	65,65,65,65	0
54	MG	2A	3654	1/1	0.94	0.07	70,70,70,70	0
54	MG	2A	3655	1/1	0.94	0.10	54,54,54,54	0
54	MG	1A	3787	1/1	0.94	0.07	80,80,80,80	0
54	MG	2A	3123	1/1	0.94	0.12	37,37,37,37	0
54	MG	2A	3125	1/1	0.94	0.12	56,56,56,56	0
54	MG	2a	3144	1/1	0.94	0.12	53,53,53,53	0
54	MG	1G	203	1/1	0.94	0.12	56,56,56,56	0
54	MG	2A	3668	1/1	0.94	0.12	48,48,48,48	0
54	MG	1A	3161	1/1	0.94	0.33	21,21,21,21	0
54	MG	2a	3149	1/1	0.94	0.10	36,36,36,36	0
54	MG	1A	3942	1/1	0.94	0.08	21,21,21,21	0
54	MG	2A	3373	1/1	0.94	0.12	24,24,24,24	0
54	MG	2A	3132	1/1	0.94	0.13	47,47,47,47	0
54	MG	2A	3375	1/1	0.94	0.09	46,46,46,46	0
54	MG	1A	3126	1/1	0.94	0.12	30,30,30,30	0
54	MG	2A	3680	1/1	0.94	0.10	46,46,46,46	0
54	MG	2A	3139	1/1	0.94	0.11	28,28,28,28	0
54	MG	1P	205	1/1	0.94	0.10	66,66,66,66	0
54	MG	1P	206	1/1	0.94	0.13	28,28,28,28	0
54	MG	1A	3227	1/1	0.94	0.33	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3590	1/1	0.94	0.11	26,26,26,26	0
54	MG	2A	3147	1/1	0.94	0.09	47,47,47,47	0
54	MG	1T	201	1/1	0.94	0.08	23,23,23,23	0
54	MG	2a	3170	1/1	0.94	0.11	78,78,78,78	0
54	MG	2A	3693	1/1	0.94	0.12	45,45,45,45	0
54	MG	1T	202	1/1	0.94	0.08	51,51,51,51	0
54	MG	2A	3696	1/1	0.94	0.12	44,44,44,44	0
54	MG	1T	203	1/1	0.94	0.06	33,33,33,33	0
54	MG	1a	3252	1/1	0.94	0.09	65,65,65,65	0
54	MG	2A	3153	1/1	0.94	0.19	40,40,40,40	0
54	MG	2A	3155	1/1	0.94	0.07	29,29,29,29	0
54	MG	2A	3156	1/1	0.94	0.07	38,38,38,38	0
54	MG	1a	3107	1/1	0.94	0.09	37,37,37,37	0
54	MG	2A	3158	1/1	0.94	0.19	39,39,39,39	0
54	MG	2A	3160	1/1	0.94	0.07	36,36,36,36	0
54	MG	2A	3407	1/1	0.94	0.09	39,39,39,39	0
54	MG	2A	3707	1/1	0.94	0.07	28,28,28,28	0
54	MG	1A	3525	1/1	0.94	0.09	49,49,49,49	0
54	MG	2A	3709	1/1	0.94	0.18	38,38,38,38	0
54	MG	2A	3410	1/1	0.94	0.08	25,25,25,25	0
54	MG	2A	3713	1/1	0.94	0.07	44,44,44,44	0
54	MG	2A	3163	1/1	0.94	0.05	64,64,64,64	0
54	MG	2A	3164	1/1	0.94	0.16	56,56,56,56	0
54	MG	1A	3228	1/1	0.94	0.27	27,27,27,27	0
54	MG	1a	3256	1/1	0.94	0.10	44,44,44,44	0
54	MG	1A	3596	1/1	0.94	0.17	36,36,36,36	0
54	MG	1A	3685	1/1	0.94	0.09	19,19,19,19	0
54	MG	1A	3337	1/1	0.94	0.10	29,29,29,29	0
54	MG	1A	3955	1/1	0.94	0.09	32,32,32,32	0
54	MG	1A	3807	1/1	0.94	0.06	27,27,27,27	0
54	MG	2A	3081	1/1	0.95	0.17	44,44,44,44	0
54	MG	2A	3363	1/1	0.95	0.07	42,42,42,42	0
54	MG	2A	3082	1/1	0.95	0.21	38,38,38,38	0
54	MG	2A	3083	1/1	0.95	0.07	50,50,50,50	0
54	MG	1A	3776	1/1	0.95	0.12	34,34,34,34	0
54	MG	1A	3194	1/1	0.95	0.10	40,40,40,40	0
54	MG	19	101	1/1	0.95	0.06	37,37,37,37	0
54	MG	2A	3089	1/1	0.95	0.10	29,29,29,29	0
54	MG	2A	3702	1/1	0.95	0.09	52,52,52,52	0
54	MG	1A	3149	1/1	0.95	0.07	23,23,23,23	0
54	MG	1A	3962	1/1	0.95	0.07	28,28,28,28	0
54	MG	1A	3781	1/1	0.95	0.16	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3005	1/1	0.95	0.16	49,49,49,49	0
54	MG	1A	3097	1/1	0.95	0.13	47,47,47,47	0
54	MG	1A	3098	1/1	0.95	0.11	52,52,52,52	0
54	MG	2A	3099	1/1	0.95	0.07	33,33,33,33	0
54	MG	2A	3379	1/1	0.95	0.17	49,49,49,49	0
54	MG	2A	3712	1/1	0.95	0.08	33,33,33,33	0
54	MG	2A	3380	1/1	0.95	0.07	30,30,30,30	0
54	MG	1A	3005	1/1	0.95	0.04	8,8,8,8	0
54	MG	1a	3186	1/1	0.95	0.09	64,64,64,64	0
54	MG	2A	3716	1/1	0.95	0.10	33,33,33,33	0
54	MG	2A	3387	1/1	0.95	0.09	23,23,23,23	0
54	MG	1A	3435	1/1	0.95	0.10	24,24,24,24	0
54	MG	1A	3549	1/1	0.95	0.07	31,31,31,31	0
54	MG	1A	3972	1/1	0.95	0.07	29,29,29,29	0
54	MG	1A	3973	1/1	0.95	0.09	48,48,48,48	0
54	MG	1A	3974	1/1	0.95	0.06	38,38,38,38	0
54	MG	1A	3326	1/1	0.95	0.07	9,9,9,9	0
54	MG	1A	3023	1/1	0.95	0.14	17,17,17,17	0
54	MG	1A	3977	1/1	0.95	0.07	18,18,18,18	0
54	MG	1a	3196	1/1	0.95	0.08	63,63,63,63	0
54	MG	1A	3108	1/1	0.95	0.23	30,30,30,30	0
54	MG	1A	3795	1/1	0.95	0.07	27,27,27,27	0
54	MG	1A	3011	1/1	0.95	0.08	28,28,28,28	0
54	MG	2A	3731	1/1	0.95	0.07	51,51,51,51	0
54	MG	2A	3122	1/1	0.95	0.15	45,45,45,45	0
54	MG	1A	3660	1/1	0.95	0.07	35,35,35,35	0
54	MG	1a	3024	1/1	0.95	0.11	48,48,48,48	0
54	MG	1A	3801	1/1	0.95	0.33	35,35,35,35	0
54	MG	1A	3208	1/1	0.95	0.08	25,25,25,25	0
54	MG	2A	3129	1/1	0.95	0.06	29,29,29,29	0
54	MG	1a	3029	1/1	0.95	0.09	37,37,37,37	0
54	MG	2A	3416	1/1	0.95	0.11	21,21,21,21	0
54	MG	1A	3557	1/1	0.95	0.07	34,34,34,34	0
54	MG	1a	3207	1/1	0.95	0.11	45,45,45,45	0
54	MG	2A	3134	1/1	0.95	0.11	52,52,52,52	0
54	MG	1A	3558	1/1	0.95	0.08	40,40,40,40	0
54	MG	1a	3209	1/1	0.95	0.06	50,50,50,50	0
54	MG	1a	3032	1/1	0.95	0.10	27,27,27,27	0
54	MG	2A	3427	1/1	0.95	0.08	45,45,45,45	0
54	MG	1A	3665	1/1	0.95	0.13	47,47,47,47	0
54	MG	1a	3213	1/1	0.95	0.08	63,63,63,63	0
54	MG	1A	3666	1/1	0.95	0.16	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3035	1/1	0.95	0.07	37,37,37,37	0
54	MG	1A	3991	1/1	0.95	0.06	46,46,46,46	0
54	MG	1a	3037	1/1	0.95	0.16	50,50,50,50	0
54	MG	2B	216	1/1	0.95	0.06	43,43,43,43	0
54	MG	1A	3271	1/1	0.95	0.09	36,36,36,36	0
54	MG	1A	3454	1/1	0.95	0.08	8,8,8,8	0
54	MG	2A	3439	1/1	0.95	0.10	23,23,23,23	0
54	MG	2A	3154	1/1	0.95	0.06	49,49,49,49	0
54	MG	2A	3442	1/1	0.95	0.09	33,33,33,33	0
54	MG	2D	302	1/1	0.95	0.09	41,41,41,41	0
54	MG	2D	303	1/1	0.95	0.21	43,43,43,43	0
54	MG	1A	3996	1/1	0.95	0.08	50,50,50,50	0
54	MG	2D	305	1/1	0.95	0.08	26,26,26,26	0
54	MG	1A	3026	1/1	0.95	0.34	21,21,21,21	0
54	MG	1a	3042	1/1	0.95	0.14	39,39,39,39	0
54	MG	1a	3043	1/1	0.95	0.12	47,47,47,47	0
54	MG	1A	3341	1/1	0.95	0.07	33,33,33,33	0
54	MG	2A	3449	1/1	0.95	0.08	49,49,49,49	0
54	MG	2A	3450	1/1	0.95	0.08	35,35,35,35	0
54	MG	1A	4002	1/1	0.95	0.06	34,34,34,34	0
54	MG	1A	3343	1/1	0.95	0.07	17,17,17,17	0
54	MG	2A	3455	1/1	0.95	0.06	40,40,40,40	0
54	MG	1A	3568	1/1	0.95	0.06	54,54,54,54	0
54	MG	2A	3165	1/1	0.95	0.10	41,41,41,41	0
54	MG	1A	3273	1/1	0.95	0.18	35,35,35,35	0
54	MG	1a	3233	1/1	0.95	0.08	48,48,48,48	0
54	MG	2A	3461	1/1	0.95	0.08	40,40,40,40	0
54	MG	2Q	201	1/1	0.95	0.13	39,39,39,39	0
54	MG	1A	3463	1/1	0.95	0.07	44,44,44,44	0
54	MG	2R	201	1/1	0.95	0.10	42,42,42,42	0
54	MG	1a	3235	1/1	0.95	0.16	58,58,58,58	0
54	MG	1A	3210	1/1	0.95	0.39	29,29,29,29	0
54	MG	2A	3466	1/1	0.95	0.08	34,34,34,34	0
54	MG	1A	3830	1/1	0.95	0.10	37,37,37,37	0
54	MG	2V	202	1/1	0.95	0.21	38,38,38,38	0
54	MG	2V	203	1/1	0.95	0.06	37,37,37,37	0
54	MG	2A	3469	1/1	0.95	0.06	42,42,42,42	0
54	MG	1A	3835	1/1	0.95	0.06	32,32,32,32	0
54	MG	1a	3059	1/1	0.95	0.10	60,60,60,60	0
54	MG	1A	3060	1/1	0.95	0.18	43,43,43,43	0
54	MG	1A	3574	1/1	0.95	0.07	29,29,29,29	0
54	MG	1A	3278	1/1	0.95	0.07	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3124	1/1	0.95	0.08	22,22,22,22	0
54	MG	1A	3577	1/1	0.95	0.09	53,53,53,53	0
54	MG	1B	208	1/1	0.95	0.07	39,39,39,39	0
54	MG	2A	3479	1/1	0.95	0.12	40,40,40,40	0
54	MG	2A	3184	1/1	0.95	0.13	56,56,56,56	0
54	MG	2A	3481	1/1	0.95	0.16	50,50,50,50	0
54	MG	2a	3005	1/1	0.95	0.15	50,50,50,50	0
54	MG	2a	3006	1/1	0.95	0.16	65,65,65,65	0
54	MG	1A	3843	1/1	0.95	0.11	34,34,34,34	0
54	MG	2a	3008	1/1	0.95	0.12	39,39,39,39	0
54	MG	1A	3280	1/1	0.95	0.12	32,32,32,32	0
54	MG	2A	3189	1/1	0.95	0.10	39,39,39,39	0
54	MG	1A	3847	1/1	0.95	0.10	31,31,31,31	0
54	MG	1A	3475	1/1	0.95	0.11	14,14,14,14	0
54	MG	2a	3014	1/1	0.95	0.16	46,46,46,46	0
54	MG	1a	3071	1/1	0.95	0.07	53,53,53,53	0
54	MG	2A	3489	1/1	0.95	0.08	61,61,61,61	0
54	MG	1a	3072	1/1	0.95	0.15	37,37,37,37	0
54	MG	1A	3850	1/1	0.95	0.15	24,24,24,24	0
54	MG	2a	3019	1/1	0.95	0.06	56,56,56,56	0
54	MG	1a	3260	1/1	0.95	0.09	25,25,25,25	0
54	MG	2A	3495	1/1	0.95	0.10	35,35,35,35	0
54	MG	2A	3199	1/1	0.95	0.07	47,47,47,47	0
54	MG	1B	218	1/1	0.95	0.06	31,31,31,31	0
54	MG	1A	3359	1/1	0.95	0.07	7,7,7,7	0
54	MG	1a	3264	1/1	0.95	0.13	52,52,52,52	0
54	MG	1A	3856	1/1	0.95	0.09	23,23,23,23	0
54	MG	1A	3172	1/1	0.95	0.19	35,35,35,35	0
54	MG	2a	3032	1/1	0.95	0.09	32,32,32,32	0
54	MG	1A	3700	1/1	0.95	0.08	41,41,41,41	0
54	MG	1A	3482	1/1	0.95	0.09	13,13,13,13	0
54	MG	1A	3218	1/1	0.95	0.27	24,24,24,24	0
54	MG	1B	228	1/1	0.95	0.08	45,45,45,45	0
54	MG	2A	3212	1/1	0.95	0.12	49,49,49,49	0
54	MG	1A	3002	1/1	0.95	0.10	43,43,43,43	0
54	MG	1A	3592	1/1	0.95	0.09	47,47,47,47	0
54	MG	1a	3277	1/1	0.95	0.07	43,43,43,43	0
54	MG	2A	3510	1/1	0.95	0.12	53,53,53,53	0
54	MG	1A	3066	1/1	0.95	0.07	34,34,34,34	0
54	MG	1D	304	1/1	0.95	0.17	26,26,26,26	0
54	MG	2A	3218	1/1	0.95	0.07	44,44,44,44	0
54	MG	2a	3049	1/1	0.95	0.17	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1D	305	1/1	0.95	0.07	24,24,24,24	0
54	MG	2A	3220	1/1	0.95	0.07	54,54,54,54	0
54	MG	2a	3052	1/1	0.95	0.08	50,50,50,50	0
54	MG	1A	3501	1/1	0.95	0.10	58,58,58,58	0
54	MG	1A	3871	1/1	0.95	0.07	22,22,22,22	0
54	MG	1A	3873	1/1	0.95	0.10	52,52,52,52	0
54	MG	1A	3708	1/1	0.95	0.10	33,33,33,33	0
54	MG	1A	3368	1/1	0.95	0.07	17,17,17,17	0
54	MG	1A	3597	1/1	0.95	0.06	39,39,39,39	0
54	MG	1A	3224	1/1	0.95	0.09	39,39,39,39	0
54	MG	2A	3529	1/1	0.95	0.09	59,59,59,59	0
54	MG	1a	3094	1/1	0.95	0.08	49,49,49,49	0
54	MG	1A	3880	1/1	0.95	0.13	36,36,36,36	0
54	MG	1A	3069	1/1	0.95	0.35	31,31,31,31	0
54	MG	2A	3536	1/1	0.95	0.08	19,19,19,19	0
54	MG	1A	3714	1/1	0.95	0.06	35,35,35,35	0
54	MG	1A	3018	1/1	0.95	0.36	26,26,26,26	0
54	MG	1A	3382	1/1	0.95	0.07	13,13,13,13	0
54	MG	1F	311	1/1	0.95	0.12	14,14,14,14	0
54	MG	2a	3069	1/1	0.95	0.12	27,27,27,27	0
54	MG	1A	3510	1/1	0.95	0.07	14,14,14,14	0
54	MG	1A	3721	1/1	0.95	0.08	25,25,25,25	0
54	MG	2A	3242	1/1	0.95	0.11	34,34,34,34	0
54	MG	1m	201	1/1	0.95	0.07	63,63,63,63	0
54	MG	2A	3551	1/1	0.95	0.11	38,38,38,38	0
54	MG	2A	3245	1/1	0.95	0.12	34,34,34,34	0
54	MG	1A	3723	1/1	0.95	0.09	32,32,32,32	0
54	MG	1F	317	1/1	0.95	0.07	40,40,40,40	0
54	MG	1a	3113	1/1	0.95	0.09	47,47,47,47	0
54	MG	1A	3183	1/1	0.95	0.46	26,26,26,26	0
54	MG	2A	3250	1/1	0.95	0.22	40,40,40,40	0
54	MG	1A	3512	1/1	0.95	0.14	43,43,43,43	0
54	MG	1A	3008	1/1	0.95	0.10	28,28,28,28	0
54	MG	2a	3090	1/1	0.95	0.08	52,52,52,52	0
54	MG	1G	204	1/1	0.95	0.10	38,38,38,38	0
54	MG	2A	3575	1/1	0.95	0.13	62,62,62,62	0
54	MG	2a	3097	1/1	0.95	0.12	69,69,69,69	0
54	MG	1H	201	1/1	0.95	0.10	52,52,52,52	0
54	MG	2A	3256	1/1	0.95	0.17	40,40,40,40	0
54	MG	2A	3580	1/1	0.95	0.07	27,27,27,27	0
54	MG	1N	201	1/1	0.95	0.09	33,33,33,33	0
54	MG	2A	3003	1/1	0.95	0.09	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3103	1/1	0.95	0.08	68,68,68,68	0
54	MG	1N	202	1/1	0.95	0.21	34,34,34,34	0
54	MG	2A	3005	1/1	0.95	0.09	42,42,42,42	0
54	MG	2A	3261	1/1	0.95	0.10	63,63,63,63	0
54	MG	2a	3111	1/1	0.95	0.10	44,44,44,44	0
54	MG	2A	3010	1/1	0.95	0.13	44,44,44,44	0
54	MG	2A	3263	1/1	0.95	0.10	46,46,46,46	0
54	MG	1A	3231	1/1	0.95	0.20	48,48,48,48	0
54	MG	1A	3731	1/1	0.95	0.15	38,38,38,38	0
54	MG	2A	3017	1/1	0.95	0.31	33,33,33,33	0
54	MG	1A	3611	1/1	0.95	0.08	43,43,43,43	0
54	MG	1a	3130	1/1	0.95	0.09	41,41,41,41	0
54	MG	1A	3734	1/1	0.95	0.07	31,31,31,31	0
54	MG	1A	3395	1/1	0.95	0.11	14,14,14,14	0
54	MG	2a	3122	1/1	0.95	0.14	43,43,43,43	0
54	MG	2a	3123	1/1	0.95	0.07	60,60,60,60	0
54	MG	1A	3397	1/1	0.95	0.07	12,12,12,12	0
54	MG	2A	3604	1/1	0.95	0.07	53,53,53,53	0
54	MG	1Q	204	1/1	0.95	0.11	40,40,40,40	0
54	MG	1R	201	1/1	0.95	0.18	19,19,19,19	0
54	MG	1R	206	1/1	0.95	0.12	27,27,27,27	0
54	MG	1A	3922	1/1	0.95	0.12	32,32,32,32	0
54	MG	2a	3133	1/1	0.95	0.10	46,46,46,46	0
54	MG	2a	3134	1/1	0.95	0.07	75,75,75,75	0
54	MG	1R	209	1/1	0.95	0.06	35,35,35,35	0
54	MG	2A	3031	1/1	0.95	0.25	46,46,46,46	0
54	MG	1A	3398	1/1	0.95	0.07	20,20,20,20	0
54	MG	1A	3924	1/1	0.95	0.11	44,44,44,44	0
54	MG	1A	3925	1/1	0.95	0.10	31,31,31,31	0
54	MG	1A	3132	1/1	0.95	0.07	20,20,20,20	0
54	MG	1U	204	1/1	0.95	0.34	25,25,25,25	0
54	MG	1A	3620	1/1	0.95	0.14	43,43,43,43	0
54	MG	2A	3041	1/1	0.95	0.09	44,44,44,44	0
54	MG	1A	3621	1/1	0.95	0.06	30,30,30,30	0
54	MG	2A	3625	1/1	0.95	0.10	47,47,47,47	0
54	MG	1A	3748	1/1	0.95	0.07	28,28,28,28	0
54	MG	1A	3236	1/1	0.95	0.22	33,33,33,33	0
54	MG	1A	3624	1/1	0.95	0.17	21,21,21,21	0
54	MG	1A	3934	1/1	0.95	0.05	16,16,16,16	0
54	MG	10	101	1/1	0.95	0.06	27,27,27,27	0
54	MG	2A	3310	1/1	0.95	0.09	47,47,47,47	0
54	MG	2A	3049	1/1	0.95	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3640	1/1	0.95	0.10	29,29,29,29	0
54	MG	2A	3641	1/1	0.95	0.07	42,42,42,42	0
54	MG	1A	3625	1/1	0.95	0.13	61,61,61,61	0
54	MG	2A	3646	1/1	0.95	0.08	24,24,24,24	0
54	MG	2A	3647	1/1	0.95	0.08	39,39,39,39	0
54	MG	1A	3034	1/1	0.95	0.16	41,41,41,41	0
54	MG	1A	3080	1/1	0.95	0.39	26,26,26,26	0
54	MG	1A	3412	1/1	0.95	0.08	5,5,5,5	0
54	MG	1A	3141	1/1	0.95	0.06	27,27,27,27	0
54	MG	2a	3176	1/1	0.95	0.07	52,52,52,52	0
54	MG	2A	3058	1/1	0.95	0.07	43,43,43,43	0
54	MG	1A	3246	1/1	0.95	0.27	55,55,55,55	0
54	MG	1A	3142	1/1	0.95	0.14	26,26,26,26	0
54	MG	2A	3331	1/1	0.95	0.07	38,38,38,38	0
54	MG	2A	3665	1/1	0.95	0.08	42,42,42,42	0
54	MG	2a	3186	1/1	0.95	0.07	48,48,48,48	0
54	MG	2A	3064	1/1	0.95	0.17	20,20,20,20	0
54	MG	11	105	1/1	0.95	0.08	25,25,25,25	0
54	MG	2A	3334	1/1	0.95	0.06	25,25,25,25	0
54	MG	2A	3335	1/1	0.95	0.10	51,51,51,51	0
54	MG	1A	3308	1/1	0.95	0.10	29,29,29,29	0
54	MG	2A	3340	1/1	0.95	0.09	32,32,32,32	0
54	MG	1A	3020	1/1	0.95	0.33	31,31,31,31	0
54	MG	13	104	1/1	0.95	0.18	38,38,38,38	0
54	MG	1A	3422	1/1	0.95	0.04	14,14,14,14	0
55	A1CQ7	2A	3741	38/38	0.95	0.11	25,32,37,39	0
54	MG	2A	3075	1/1	0.95	0.24	33,33,33,33	0
54	MG	1A	3423	1/1	0.95	0.08	12,12,12,12	0
54	MG	1A	3952	1/1	0.95	0.07	49,49,49,49	0
54	MG	15	106	1/1	0.95	0.07	40,40,40,40	0
54	MG	1A	3314	1/1	0.95	0.23	26,26,26,26	0
54	MG	2A	3357	1/1	0.95	0.07	24,24,24,24	0
57	ARG	1B	232	12/12	0.95	0.10	23,36,42,46	0
54	MG	2A	3690	1/1	0.95	0.07	40,40,40,40	0
54	MG	1A	3641	1/1	0.95	0.06	44,44,44,44	0
54	MG	1A	3094	1/1	0.96	0.09	25,25,25,25	0
54	MG	2A	3131	1/1	0.96	0.09	45,45,45,45	0
54	MG	1A	3004	1/1	0.96	0.12	34,34,34,34	0
54	MG	1A	3844	1/1	0.96	0.08	37,37,37,37	0
54	MG	1A	3176	1/1	0.96	0.18	15,15,15,15	0
54	MG	2A	3137	1/1	0.96	0.09	46,46,46,46	0
54	MG	2A	3138	1/1	0.96	0.18	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3485	1/1	0.96	0.11	54,54,54,54	0
54	MG	1B	203	1/1	0.96	0.05	34,34,34,34	0
54	MG	2A	3141	1/1	0.96	0.06	35,35,35,35	0
54	MG	1A	3848	1/1	0.96	0.09	11,11,11,11	0
54	MG	2A	3724	1/1	0.96	0.08	40,40,40,40	0
54	MG	1A	3591	1/1	0.96	0.06	37,37,37,37	0
54	MG	2A	3145	1/1	0.96	0.15	42,42,42,42	0
54	MG	2A	3417	1/1	0.96	0.09	47,47,47,47	0
54	MG	1a	3223	1/1	0.96	0.06	69,69,69,69	0
54	MG	1A	3363	1/1	0.96	0.06	22,22,22,22	0
54	MG	1A	3047	1/1	0.96	0.15	29,29,29,29	0
54	MG	1A	3855	1/1	0.96	0.06	27,27,27,27	0
54	MG	1A	3489	1/1	0.96	0.09	36,36,36,36	0
54	MG	1B	210	1/1	0.96	0.08	40,40,40,40	0
54	MG	2A	3426	1/1	0.96	0.05	38,38,38,38	0
54	MG	2A	3152	1/1	0.96	0.14	37,37,37,37	0
54	MG	1a	3046	1/1	0.96	0.16	35,35,35,35	0
54	MG	1a	3048	1/1	0.96	0.11	46,46,46,46	0
54	MG	2A	3430	1/1	0.96	0.09	51,51,51,51	0
54	MG	1A	3858	1/1	0.96	0.05	29,29,29,29	0
54	MG	1a	3051	1/1	0.96	0.14	38,38,38,38	0
54	MG	1A	3595	1/1	0.96	0.06	19,19,19,19	0
54	MG	1A	3493	1/1	0.96	0.05	25,25,25,25	0
54	MG	1A	3135	1/1	0.96	0.34	37,37,37,37	0
54	MG	2A	3437	1/1	0.96	0.07	59,59,59,59	0
54	MG	1A	3222	1/1	0.96	0.06	29,29,29,29	0
54	MG	1A	3502	1/1	0.96	0.10	41,41,41,41	0
54	MG	1B	220	1/1	0.96	0.09	54,54,54,54	0
54	MG	2A	3441	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	3600	1/1	0.96	0.05	52,52,52,52	0
54	MG	1A	3715	1/1	0.96	0.07	21,21,21,21	0
54	MG	1A	3717	1/1	0.96	0.06	71,71,71,71	0
54	MG	1A	3869	1/1	0.96	0.16	35,35,35,35	0
54	MG	1A	3601	1/1	0.96	0.11	44,44,44,44	0
54	MG	1A	3100	1/1	0.96	0.09	24,24,24,24	0
54	MG	1B	229	1/1	0.96	0.05	47,47,47,47	0
54	MG	1A	3604	1/1	0.96	0.22	25,25,25,25	0
54	MG	1A	3370	1/1	0.96	0.05	41,41,41,41	0
54	MG	1a	3067	1/1	0.96	0.13	45,45,45,45	0
54	MG	2A	3454	1/1	0.96	0.07	17,17,17,17	0
54	MG	1A	3722	1/1	0.96	0.08	47,47,47,47	0
54	MG	1D	303	1/1	0.96	0.10	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3178	1/1	0.96	0.05	30,30,30,30	0
54	MG	1A	3029	1/1	0.96	0.08	28,28,28,28	0
54	MG	2A	3180	1/1	0.96	0.09	45,45,45,45	0
54	MG	1a	3259	1/1	0.96	0.12	45,45,45,45	0
54	MG	1A	3724	1/1	0.96	0.20	32,32,32,32	0
54	MG	1A	3725	1/1	0.96	0.24	46,46,46,46	0
54	MG	2F	301	1/1	0.96	0.23	30,30,30,30	0
54	MG	1A	3882	1/1	0.96	0.09	36,36,36,36	0
54	MG	2F	303	1/1	0.96	0.07	39,39,39,39	0
54	MG	1D	312	1/1	0.96	0.24	25,25,25,25	0
54	MG	1a	3265	1/1	0.96	0.07	44,44,44,44	0
54	MG	1a	3266	1/1	0.96	0.08	73,73,73,73	0
54	MG	1A	3884	1/1	0.96	0.26	16,16,16,16	0
54	MG	1D	314	1/1	0.96	0.19	26,26,26,26	0
54	MG	1A	3226	1/1	0.96	0.11	25,25,25,25	0
54	MG	1a	3270	1/1	0.96	0.09	49,49,49,49	0
54	MG	1A	3893	1/1	0.96	0.10	65,65,65,65	0
54	MG	1A	3038	1/1	0.96	0.13	41,41,41,41	0
54	MG	1a	3273	1/1	0.96	0.07	44,44,44,44	0
54	MG	1E	302	1/1	0.96	0.41	27,27,27,27	0
54	MG	2T	201	1/1	0.96	0.14	40,40,40,40	0
54	MG	1A	3105	1/1	0.96	0.44	20,20,20,20	0
54	MG	1A	3144	1/1	0.96	0.10	17,17,17,17	0
54	MG	1E	307	1/1	0.96	0.05	25,25,25,25	0
54	MG	2U	201	1/1	0.96	0.07	67,67,67,67	0
54	MG	1A	3230	1/1	0.96	0.30	23,23,23,23	0
54	MG	1E	309	1/1	0.96	0.07	32,32,32,32	0
54	MG	1F	303	1/1	0.96	0.15	26,26,26,26	0
54	MG	1A	3899	1/1	0.96	0.09	9,9,9,9	0
54	MG	2X	101	1/1	0.96	0.10	45,45,45,45	0
54	MG	1F	307	1/1	0.96	0.14	14,14,14,14	0
54	MG	1F	308	1/1	0.96	0.14	18,18,18,18	0
54	MG	1A	3900	1/1	0.96	0.08	23,23,23,23	0
54	MG	1A	3732	1/1	0.96	0.04	15,15,15,15	0
54	MG	1A	3393	1/1	0.96	0.13	9,9,9,9	0
54	MG	1F	313	1/1	0.96	0.31	29,29,29,29	0
54	MG	1A	3147	1/1	0.96	0.17	21,21,21,21	0
54	MG	1A	3736	1/1	0.96	0.07	30,30,30,30	0
54	MG	1A	3297	1/1	0.96	0.09	23,23,23,23	0
54	MG	1A	3107	1/1	0.96	0.17	21,21,21,21	0
54	MG	1A	3399	1/1	0.96	0.08	22,22,22,22	0
54	MG	2a	3004	1/1	0.96	0.08	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3099	1/1	0.96	0.05	26,26,26,26	0
54	MG	1k	201	1/1	0.96	0.16	35,35,35,35	0
54	MG	1a	3100	1/1	0.96	0.07	37,37,37,37	0
54	MG	2A	3227	1/1	0.96	0.19	35,35,35,35	0
54	MG	1A	3915	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3740	1/1	0.96	0.08	29,29,29,29	0
54	MG	1A	3917	1/1	0.96	0.19	44,44,44,44	0
54	MG	2a	3012	1/1	0.96	0.05	48,48,48,48	0
54	MG	1A	3300	1/1	0.96	0.23	30,30,30,30	0
54	MG	1a	3110	1/1	0.96	0.06	37,37,37,37	0
54	MG	1o	101	1/1	0.96	0.12	44,44,44,44	0
54	MG	2A	3234	1/1	0.96	0.10	41,41,41,41	0
54	MG	1A	3523	1/1	0.96	0.07	24,24,24,24	0
54	MG	2A	3236	1/1	0.96	0.09	48,48,48,48	0
54	MG	1A	3921	1/1	0.96	0.22	48,48,48,48	0
54	MG	1A	3524	1/1	0.96	0.09	51,51,51,51	0
54	MG	1y	201	1/1	0.96	0.07	68,68,68,68	0
54	MG	1A	3235	1/1	0.96	0.39	21,21,21,21	0
54	MG	1A	3404	1/1	0.96	0.06	28,28,28,28	0
54	MG	1A	3189	1/1	0.96	0.25	24,24,24,24	0
54	MG	2A	3522	1/1	0.96	0.09	46,46,46,46	0
54	MG	1a	3118	1/1	0.96	0.09	52,52,52,52	0
54	MG	1A	3628	1/1	0.96	0.08	42,42,42,42	0
54	MG	1A	3240	1/1	0.96	0.29	24,24,24,24	0
54	MG	1a	3122	1/1	0.96	0.08	53,53,53,53	0
54	MG	2A	3528	1/1	0.96	0.07	60,60,60,60	0
54	MG	1Q	202	1/1	0.96	0.05	23,23,23,23	0
54	MG	1a	3124	1/1	0.96	0.06	42,42,42,42	0
54	MG	1A	3756	1/1	0.96	0.06	28,28,28,28	0
54	MG	2A	3016	1/1	0.96	0.24	43,43,43,43	0
54	MG	2A	3253	1/1	0.96	0.06	26,26,26,26	0
54	MG	1Q	205	1/1	0.96	0.07	22,22,22,22	0
54	MG	2a	3043	1/1	0.96	0.18	56,56,56,56	0
54	MG	2a	3044	1/1	0.96	0.04	44,44,44,44	0
54	MG	1A	3081	1/1	0.96	0.21	22,22,22,22	0
54	MG	2A	3542	1/1	0.96	0.08	65,65,65,65	0
54	MG	1a	3128	1/1	0.96	0.18	35,35,35,35	0
54	MG	1A	3150	1/1	0.96	0.26	22,22,22,22	0
54	MG	1A	3193	1/1	0.96	0.07	38,38,38,38	0
54	MG	1A	3082	1/1	0.96	0.10	34,34,34,34	0
54	MG	1A	3152	1/1	0.96	0.07	21,21,21,21	0
54	MG	1A	3936	1/1	0.96	0.18	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3249	1/1	0.96	0.15	21,21,21,21	0
54	MG	1T	204	1/1	0.96	0.05	48,48,48,48	0
54	MG	2A	3264	1/1	0.96	0.09	45,45,45,45	0
54	MG	2A	3557	1/1	0.96	0.06	33,33,33,33	0
54	MG	1U	201	1/1	0.96	0.09	21,21,21,21	0
54	MG	2A	3266	1/1	0.96	0.09	23,23,23,23	0
54	MG	1A	3421	1/1	0.96	0.07	13,13,13,13	0
54	MG	2A	3269	1/1	0.96	0.06	41,41,41,41	0
54	MG	1A	3941	1/1	0.96	0.15	23,23,23,23	0
54	MG	1A	3317	1/1	0.96	0.08	21,21,21,21	0
54	MG	2A	3570	1/1	0.96	0.06	48,48,48,48	0
54	MG	1A	3083	1/1	0.96	0.07	36,36,36,36	0
54	MG	1V	203	1/1	0.96	0.15	31,31,31,31	0
54	MG	2A	3038	1/1	0.96	0.09	21,21,21,21	0
54	MG	2A	3578	1/1	0.96	0.06	20,20,20,20	0
54	MG	1A	3542	1/1	0.96	0.06	46,46,46,46	0
54	MG	1V	206	1/1	0.96	0.13	38,38,38,38	0
54	MG	1V	207	1/1	0.96	0.04	42,42,42,42	0
54	MG	1A	3773	1/1	0.96	0.06	22,22,22,22	0
54	MG	1a	3148	1/1	0.96	0.13	45,45,45,45	0
54	MG	1a	3149	1/1	0.96	0.09	56,56,56,56	0
54	MG	1W	202	1/1	0.96	0.06	31,31,31,31	0
54	MG	1W	203	1/1	0.96	0.13	23,23,23,23	0
54	MG	1A	3643	1/1	0.96	0.06	26,26,26,26	0
54	MG	1A	3319	1/1	0.96	0.16	57,57,57,57	0
54	MG	1A	3111	1/1	0.96	0.24	25,25,25,25	0
54	MG	1A	3647	1/1	0.96	0.14	40,40,40,40	0
54	MG	1A	3198	1/1	0.96	0.07	44,44,44,44	0
54	MG	2a	3084	1/1	0.96	0.06	61,61,61,61	0
54	MG	2A	3298	1/1	0.96	0.06	35,35,35,35	0
54	MG	2a	3088	1/1	0.96	0.10	30,30,30,30	0
54	MG	2A	3054	1/1	0.96	0.10	39,39,39,39	0
54	MG	2A	3301	1/1	0.96	0.11	39,39,39,39	0
54	MG	2a	3091	1/1	0.96	0.12	44,44,44,44	0
54	MG	2a	3092	1/1	0.96	0.06	34,34,34,34	0
54	MG	2a	3093	1/1	0.96	0.08	40,40,40,40	0
54	MG	10	104	1/1	0.96	0.06	42,42,42,42	0
54	MG	2a	3095	1/1	0.96	0.07	33,33,33,33	0
54	MG	1A	3323	1/1	0.96	0.07	13,13,13,13	0
54	MG	1A	3257	1/1	0.96	0.15	24,24,24,24	0
54	MG	1A	3113	1/1	0.96	0.11	33,33,33,33	0
54	MG	2A	3061	1/1	0.96	0.22	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3308	1/1	0.96	0.07	31,31,31,31	0
54	MG	1A	3433	1/1	0.96	0.05	11,11,11,11	0
54	MG	1A	3434	1/1	0.96	0.12	46,46,46,46	0
54	MG	2A	3311	1/1	0.96	0.07	23,23,23,23	0
54	MG	2a	3104	1/1	0.96	0.09	57,57,57,57	0
54	MG	2a	3105	1/1	0.96	0.08	41,41,41,41	0
54	MG	2A	3065	1/1	0.96	0.08	43,43,43,43	0
54	MG	1A	3961	1/1	0.96	0.04	18,18,18,18	0
54	MG	2A	3316	1/1	0.96	0.08	47,47,47,47	0
54	MG	2a	3110	1/1	0.96	0.09	62,62,62,62	0
54	MG	1A	3201	1/1	0.96	0.11	33,33,33,33	0
54	MG	2A	3319	1/1	0.96	0.05	32,32,32,32	0
54	MG	2A	3069	1/1	0.96	0.13	38,38,38,38	0
54	MG	2A	3623	1/1	0.96	0.07	44,44,44,44	0
54	MG	2A	3070	1/1	0.96	0.08	36,36,36,36	0
54	MG	1A	3086	1/1	0.96	0.52	35,35,35,35	0
54	MG	2A	3326	1/1	0.96	0.08	40,40,40,40	0
54	MG	1A	3791	1/1	0.96	0.06	30,30,30,30	0
54	MG	2A	3633	1/1	0.96	0.07	42,42,42,42	0
54	MG	1A	3261	1/1	0.96	0.14	29,29,29,29	0
54	MG	1A	3262	1/1	0.96	0.08	25,25,25,25	0
54	MG	15	103	1/1	0.96	0.20	20,20,20,20	0
54	MG	15	104	1/1	0.96	0.27	18,18,18,18	0
54	MG	1A	3796	1/1	0.96	0.23	35,35,35,35	0
54	MG	1A	3970	1/1	0.96	0.05	35,35,35,35	0
54	MG	15	107	1/1	0.96	0.09	36,36,36,36	0
54	MG	2A	3642	1/1	0.96	0.08	41,41,41,41	0
54	MG	2A	3643	1/1	0.96	0.08	78,78,78,78	0
54	MG	2A	3644	1/1	0.96	0.06	39,39,39,39	0
54	MG	2A	3336	1/1	0.96	0.07	18,18,18,18	0
54	MG	1a	3177	1/1	0.96	0.11	71,71,71,71	0
54	MG	2a	3139	1/1	0.96	0.07	57,57,57,57	0
54	MG	2A	3339	1/1	0.96	0.07	31,31,31,31	0
54	MG	1A	3335	1/1	0.96	0.07	19,19,19,19	0
54	MG	17	101	1/1	0.96	0.06	28,28,28,28	0
54	MG	1A	3336	1/1	0.96	0.05	35,35,35,35	0
54	MG	1A	3449	1/1	0.96	0.06	31,31,31,31	0
54	MG	2A	3087	1/1	0.96	0.13	48,48,48,48	0
54	MG	1A	3162	1/1	0.96	0.12	30,30,30,30	0
54	MG	2A	3661	1/1	0.96	0.08	30,30,30,30	0
54	MG	2A	3662	1/1	0.96	0.07	26,26,26,26	0
54	MG	2A	3350	1/1	0.96	0.06	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3351	1/1	0.96	0.12	34,34,34,34	0
54	MG	1A	3803	1/1	0.96	0.07	26,26,26,26	0
54	MG	1A	3164	1/1	0.96	0.10	38,38,38,38	0
54	MG	1a	3002	1/1	0.96	0.11	28,28,28,28	0
54	MG	2A	3669	1/1	0.96	0.07	38,38,38,38	0
54	MG	1A	3206	1/1	0.96	0.28	27,27,27,27	0
54	MG	2a	3160	1/1	0.96	0.07	63,63,63,63	0
54	MG	1A	3207	1/1	0.96	0.20	23,23,23,23	0
54	MG	2A	3361	1/1	0.96	0.07	47,47,47,47	0
54	MG	1A	3344	1/1	0.96	0.06	27,27,27,27	0
54	MG	2A	3675	1/1	0.96	0.09	49,49,49,49	0
54	MG	2a	3166	1/1	0.96	0.09	40,40,40,40	0
54	MG	2A	3095	1/1	0.96	0.07	17,17,17,17	0
54	MG	2a	3168	1/1	0.96	0.07	40,40,40,40	0
54	MG	2A	3677	1/1	0.96	0.14	50,50,50,50	0
54	MG	2A	3096	1/1	0.96	0.09	42,42,42,42	0
54	MG	2A	3679	1/1	0.96	0.06	38,38,38,38	0
54	MG	2a	3173	1/1	0.96	0.10	47,47,47,47	0
54	MG	2A	3365	1/1	0.96	0.07	42,42,42,42	0
54	MG	1A	3809	1/1	0.96	0.09	45,45,45,45	0
54	MG	1A	3460	1/1	0.96	0.06	42,42,42,42	0
54	MG	1A	3815	1/1	0.96	0.35	19,19,19,19	0
54	MG	2A	3101	1/1	0.96	0.14	48,48,48,48	0
54	MG	1A	3057	1/1	0.96	0.09	44,44,44,44	0
54	MG	1A	3985	1/1	0.96	0.07	21,21,21,21	0
54	MG	2a	3182	1/1	0.96	0.06	55,55,55,55	0
54	MG	1A	3675	1/1	0.96	0.08	54,54,54,54	0
54	MG	2a	3185	1/1	0.96	0.05	36,36,36,36	0
54	MG	1A	3089	1/1	0.96	0.10	38,38,38,38	0
54	MG	1A	3573	1/1	0.96	0.09	29,29,29,29	0
54	MG	1A	3989	1/1	0.96	0.07	71,71,71,71	0
54	MG	2A	3695	1/1	0.96	0.11	55,55,55,55	0
54	MG	1A	3091	1/1	0.96	0.06	33,33,33,33	0
54	MG	1A	3352	1/1	0.96	0.09	40,40,40,40	0
54	MG	2k	202	1/1	0.96	0.07	44,44,44,44	0
54	MG	1A	3468	1/1	0.96	0.07	32,32,32,32	0
54	MG	1A	3211	1/1	0.96	0.13	34,34,34,34	0
54	MG	2A	3381	1/1	0.96	0.07	28,28,28,28	0
54	MG	1A	3687	1/1	0.96	0.09	29,29,29,29	0
55	A1CQ7	1A	4011	38/38	0.96	0.10	12,17,27,29	0
54	MG	2A	3383	1/1	0.96	0.07	30,30,30,30	0
54	MG	1A	3998	1/1	0.96	0.06	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3832	1/1	0.96	0.07	34,34,34,34	0
54	MG	2A	3119	1/1	0.96	0.15	39,39,39,39	0
54	MG	1A	3580	1/1	0.96	0.08	37,37,37,37	0
54	MG	1A	3276	1/1	0.96	0.13	45,45,45,45	0
54	MG	1A	3583	1/1	0.96	0.15	45,45,45,45	0
54	MG	1A	3092	1/1	0.96	0.33	31,31,31,31	0
54	MG	1a	3211	1/1	0.96	0.07	51,51,51,51	0
54	MG	1A	3357	1/1	0.96	0.06	33,33,33,33	0
58	ZN	2n	102	1/1	0.96	0.07	97,97,97,97	0
54	MG	1A	3473	1/1	0.97	0.06	14,14,14,14	0
54	MG	2A	3023	1/1	0.97	0.20	36,36,36,36	0
54	MG	2B	211	1/1	0.97	0.13	43,43,43,43	0
54	MG	13	101	1/1	0.97	0.15	23,23,23,23	0
54	MG	1A	3294	1/1	0.97	0.22	19,19,19,19	0
54	MG	1A	3827	1/1	0.97	0.05	30,30,30,30	0
54	MG	2A	3028	1/1	0.97	0.12	19,19,19,19	0
54	MG	1A	3582	1/1	0.97	0.06	30,30,30,30	0
54	MG	1A	3695	1/1	0.97	0.21	22,22,22,22	0
54	MG	1A	3697	1/1	0.97	0.18	18,18,18,18	0
54	MG	15	102	1/1	0.97	0.22	22,22,22,22	0
54	MG	1A	3698	1/1	0.97	0.07	36,36,36,36	0
54	MG	1A	3834	1/1	0.97	0.24	31,31,31,31	0
54	MG	2A	3486	1/1	0.97	0.05	29,29,29,29	0
54	MG	2A	3035	1/1	0.97	0.06	40,40,40,40	0
54	MG	2A	3036	1/1	0.97	0.08	35,35,35,35	0
54	MG	1A	3234	1/1	0.97	0.74	30,30,30,30	0
54	MG	2A	3490	1/1	0.97	0.04	32,32,32,32	0
54	MG	2E	301	1/1	0.97	0.11	31,31,31,31	0
54	MG	1A	3476	1/1	0.97	0.06	23,23,23,23	0
54	MG	2A	3492	1/1	0.97	0.08	46,46,46,46	0
54	MG	1A	3017	1/1	0.97	0.24	17,17,17,17	0
54	MG	1A	3839	1/1	0.97	0.14	32,32,32,32	0
54	MG	1A	3478	1/1	0.97	0.06	14,14,14,14	0
54	MG	17	102	1/1	0.97	0.14	19,19,19,19	0
54	MG	1A	3479	1/1	0.97	0.06	17,17,17,17	0
54	MG	2F	304	1/1	0.97	0.27	41,41,41,41	0
54	MG	1A	3373	1/1	0.97	0.08	39,39,39,39	0
54	MG	1A	3705	1/1	0.97	0.08	22,22,22,22	0
54	MG	1A	3481	1/1	0.97	0.07	44,44,44,44	0
54	MG	19	103	1/1	0.97	0.07	47,47,47,47	0
54	MG	1A	3845	1/1	0.97	0.03	27,27,27,27	0
54	MG	1a	3172	1/1	0.97	0.07	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3067	1/1	0.97	0.03	13,13,13,13	0
54	MG	1A	3483	1/1	0.97	0.07	10,10,10,10	0
54	MG	2A	3053	1/1	0.97	0.04	20,20,20,20	0
54	MG	1A	3484	1/1	0.97	0.05	23,23,23,23	0
54	MG	2Q	204	1/1	0.97	0.09	46,46,46,46	0
54	MG	2A	3055	1/1	0.97	0.06	30,30,30,30	0
54	MG	2R	202	1/1	0.97	0.07	30,30,30,30	0
54	MG	1A	4009	1/1	0.97	0.06	42,42,42,42	0
54	MG	1A	3376	1/1	0.97	0.07	38,38,38,38	0
54	MG	1A	3298	1/1	0.97	0.11	30,30,30,30	0
54	MG	1A	3380	1/1	0.97	0.05	12,12,12,12	0
54	MG	1A	3713	1/1	0.97	0.06	12,12,12,12	0
54	MG	2A	3062	1/1	0.97	0.17	26,26,26,26	0
54	MG	2A	3515	1/1	0.97	0.06	32,32,32,32	0
54	MG	1A	3238	1/1	0.97	0.20	21,21,21,21	0
54	MG	2W	201	1/1	0.97	0.37	39,39,39,39	0
54	MG	2W	202	1/1	0.97	0.08	40,40,40,40	0
54	MG	1A	3857	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3143	1/1	0.97	0.04	23,23,23,23	0
54	MG	20	101	1/1	0.97	0.14	32,32,32,32	0
54	MG	1A	3301	1/1	0.97	0.12	18,18,18,18	0
54	MG	1A	3498	1/1	0.97	0.05	22,22,22,22	0
54	MG	2A	3277	1/1	0.97	0.08	28,28,28,28	0
54	MG	1A	3499	1/1	0.97	0.07	33,33,33,33	0
54	MG	1a	3017	1/1	0.97	0.06	58,58,58,58	0
54	MG	2A	3281	1/1	0.97	0.08	40,40,40,40	0
54	MG	2A	3527	1/1	0.97	0.06	49,49,49,49	0
54	MG	2A	3071	1/1	0.97	0.05	39,39,39,39	0
54	MG	2A	3284	1/1	0.97	0.06	31,31,31,31	0
54	MG	2a	3001	1/1	0.97	0.07	38,38,38,38	0
54	MG	2A	3285	1/1	0.97	0.07	19,19,19,19	0
54	MG	1A	3500	1/1	0.97	0.06	10,10,10,10	0
54	MG	1A	3386	1/1	0.97	0.05	13,13,13,13	0
54	MG	2A	3534	1/1	0.97	0.05	34,34,34,34	0
54	MG	1B	214	1/1	0.97	0.13	36,36,36,36	0
54	MG	1a	3191	1/1	0.97	0.08	60,60,60,60	0
54	MG	1A	3068	1/1	0.97	0.06	22,22,22,22	0
54	MG	2A	3541	1/1	0.97	0.07	54,54,54,54	0
54	MG	1A	3389	1/1	0.97	0.06	17,17,17,17	0
54	MG	1A	3028	1/1	0.97	0.18	14,14,14,14	0
54	MG	1a	3025	1/1	0.97	0.05	45,45,45,45	0
54	MG	1a	3026	1/1	0.97	0.05	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3070	1/1	0.97	0.34	29,29,29,29	0
54	MG	2A	3296	1/1	0.97	0.11	27,27,27,27	0
54	MG	2A	3297	1/1	0.97	0.10	43,43,43,43	0
54	MG	2A	3550	1/1	0.97	0.06	23,23,23,23	0
54	MG	1A	3106	1/1	0.97	0.26	32,32,32,32	0
54	MG	1A	3012	1/1	0.97	0.07	27,27,27,27	0
54	MG	2A	3553	1/1	0.97	0.05	32,32,32,32	0
54	MG	2A	3554	1/1	0.97	0.04	44,44,44,44	0
54	MG	1A	3307	1/1	0.97	0.07	40,40,40,40	0
54	MG	1B	222	1/1	0.97	0.04	31,31,31,31	0
54	MG	2A	3303	1/1	0.97	0.06	27,27,27,27	0
54	MG	2a	3025	1/1	0.97	0.09	48,48,48,48	0
54	MG	2a	3026	1/1	0.97	0.06	47,47,47,47	0
54	MG	2A	3086	1/1	0.97	0.13	39,39,39,39	0
54	MG	1B	223	1/1	0.97	0.05	32,32,32,32	0
54	MG	2A	3561	1/1	0.97	0.17	25,25,25,25	0
54	MG	2a	3030	1/1	0.97	0.19	54,54,54,54	0
54	MG	2a	3031	1/1	0.97	0.09	38,38,38,38	0
54	MG	2A	3562	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3072	1/1	0.97	0.04	25,25,25,25	0
54	MG	2A	3566	1/1	0.97	0.06	55,55,55,55	0
54	MG	1A	3311	1/1	0.97	0.20	23,23,23,23	0
54	MG	2A	3568	1/1	0.97	0.05	31,31,31,31	0
54	MG	1A	3312	1/1	0.97	0.39	29,29,29,29	0
54	MG	2a	3038	1/1	0.97	0.11	40,40,40,40	0
54	MG	1A	3879	1/1	0.97	0.05	52,52,52,52	0
54	MG	1A	3617	1/1	0.97	0.07	39,39,39,39	0
54	MG	2A	3573	1/1	0.97	0.06	54,54,54,54	0
54	MG	1A	3405	1/1	0.97	0.15	35,35,35,35	0
54	MG	1A	3735	1/1	0.97	0.06	27,27,27,27	0
54	MG	1A	3042	1/1	0.97	0.05	25,25,25,25	0
54	MG	1A	3410	1/1	0.97	0.04	16,16,16,16	0
54	MG	1D	302	1/1	0.97	0.11	42,42,42,42	0
54	MG	2A	3098	1/1	0.97	0.07	39,39,39,39	0
54	MG	2A	3582	1/1	0.97	0.04	32,32,32,32	0
54	MG	2A	3320	1/1	0.97	0.05	22,22,22,22	0
54	MG	1A	3076	1/1	0.97	0.43	35,35,35,35	0
54	MG	1A	3078	1/1	0.97	0.15	22,22,22,22	0
54	MG	1a	3216	1/1	0.97	0.10	56,56,56,56	0
54	MG	1A	3112	1/1	0.97	0.23	20,20,20,20	0
54	MG	1a	3047	1/1	0.97	0.06	46,46,46,46	0
54	MG	2A	3592	1/1	0.97	0.06	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3219	1/1	0.97	0.10	57,57,57,57	0
54	MG	1D	306	1/1	0.97	0.14	26,26,26,26	0
54	MG	1D	308	1/1	0.97	0.06	28,28,28,28	0
54	MG	1a	3050	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3741	1/1	0.97	0.09	18,18,18,18	0
54	MG	2A	3109	1/1	0.97	0.12	26,26,26,26	0
54	MG	2A	3599	1/1	0.97	0.08	43,43,43,43	0
54	MG	1A	3204	1/1	0.97	0.25	33,33,33,33	0
54	MG	1A	3898	1/1	0.97	0.11	12,12,12,12	0
54	MG	2A	3603	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3417	1/1	0.97	0.07	15,15,15,15	0
54	MG	1A	3157	1/1	0.97	0.21	33,33,33,33	0
54	MG	1A	3747	1/1	0.97	0.14	23,23,23,23	0
54	MG	1A	3629	1/1	0.97	0.13	18,18,18,18	0
54	MG	2a	3071	1/1	0.97	0.05	47,47,47,47	0
54	MG	2A	3118	1/1	0.97	0.11	51,51,51,51	0
54	MG	1A	3158	1/1	0.97	0.08	26,26,26,26	0
54	MG	2A	3120	1/1	0.97	0.09	24,24,24,24	0
54	MG	1A	3906	1/1	0.97	0.08	13,13,13,13	0
54	MG	1A	3528	1/1	0.97	0.08	31,31,31,31	0
54	MG	2A	3124	1/1	0.97	0.21	37,37,37,37	0
54	MG	2A	3352	1/1	0.97	0.07	46,46,46,46	0
54	MG	2A	3353	1/1	0.97	0.06	44,44,44,44	0
54	MG	2a	3081	1/1	0.97	0.16	45,45,45,45	0
54	MG	1A	3043	1/1	0.97	0.14	6,6,6,6	0
54	MG	1A	3912	1/1	0.97	0.11	33,33,33,33	0
54	MG	1A	3530	1/1	0.97	0.08	40,40,40,40	0
54	MG	2a	3085	1/1	0.97	0.17	62,62,62,62	0
54	MG	1A	3755	1/1	0.97	0.05	35,35,35,35	0
54	MG	2A	3358	1/1	0.97	0.04	54,54,54,54	0
54	MG	1F	301	1/1	0.97	0.17	18,18,18,18	0
54	MG	1F	302	1/1	0.97	0.15	17,17,17,17	0
54	MG	1A	3115	1/1	0.97	0.19	21,21,21,21	0
54	MG	1A	3263	1/1	0.97	0.15	26,26,26,26	0
54	MG	1A	3044	1/1	0.97	0.11	16,16,16,16	0
54	MG	2A	3135	1/1	0.97	0.12	31,31,31,31	0
54	MG	2A	3136	1/1	0.97	0.08	32,32,32,32	0
54	MG	1A	3424	1/1	0.97	0.15	19,19,19,19	0
54	MG	1A	3265	1/1	0.97	0.18	18,18,18,18	0
54	MG	1a	3247	1/1	0.97	0.06	57,57,57,57	0
54	MG	1A	3330	1/1	0.97	0.06	24,24,24,24	0
54	MG	1A	3427	1/1	0.97	0.07	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1F	312	1/1	0.97	0.10	27,27,27,27	0
54	MG	1A	3767	1/1	0.97	0.06	13,13,13,13	0
54	MG	2A	3144	1/1	0.97	0.13	38,38,38,38	0
54	MG	1A	3117	1/1	0.97	0.27	26,26,26,26	0
54	MG	1A	3769	1/1	0.97	0.07	34,34,34,34	0
54	MG	1A	3118	1/1	0.97	0.06	24,24,24,24	0
54	MG	1A	3212	1/1	0.97	0.28	29,29,29,29	0
54	MG	1A	3646	1/1	0.97	0.06	38,38,38,38	0
54	MG	1A	3269	1/1	0.97	0.21	19,19,19,19	0
54	MG	1A	3119	1/1	0.97	0.14	27,27,27,27	0
54	MG	2A	3659	1/1	0.97	0.05	57,57,57,57	0
54	MG	1a	3262	1/1	0.97	0.05	48,48,48,48	0
54	MG	2A	3385	1/1	0.97	0.07	30,30,30,30	0
54	MG	1A	3170	1/1	0.97	0.28	23,23,23,23	0
54	MG	2a	3116	1/1	0.97	0.09	36,36,36,36	0
54	MG	1A	3215	1/1	0.97	0.29	24,24,24,24	0
54	MG	1A	3779	1/1	0.97	0.09	22,22,22,22	0
54	MG	2A	3391	1/1	0.97	0.07	21,21,21,21	0
54	MG	2A	3392	1/1	0.97	0.08	56,56,56,56	0
54	MG	1A	3274	1/1	0.97	0.25	27,27,27,27	0
54	MG	1A	3120	1/1	0.97	0.11	22,22,22,22	0
54	MG	1N	204	1/1	0.97	0.07	50,50,50,50	0
54	MG	1A	3939	1/1	0.97	0.13	50,50,50,50	0
54	MG	1P	201	1/1	0.97	0.34	25,25,25,25	0
54	MG	2A	3162	1/1	0.97	0.12	40,40,40,40	0
54	MG	2A	3400	1/1	0.97	0.06	39,39,39,39	0
54	MG	1P	203	1/1	0.97	0.29	25,25,25,25	0
54	MG	1A	3782	1/1	0.97	0.13	19,19,19,19	0
54	MG	1A	3217	1/1	0.97	0.14	19,19,19,19	0
54	MG	1A	3656	1/1	0.97	0.04	39,39,39,39	0
54	MG	2a	3135	1/1	0.97	0.07	50,50,50,50	0
54	MG	2a	3136	1/1	0.97	0.06	70,70,70,70	0
54	MG	1A	3943	1/1	0.97	0.15	17,17,17,17	0
54	MG	1Q	201	1/1	0.97	0.13	27,27,27,27	0
54	MG	1A	3657	1/1	0.97	0.20	40,40,40,40	0
54	MG	2a	3141	1/1	0.97	0.07	53,53,53,53	0
54	MG	1A	3786	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3030	1/1	0.97	0.05	20,20,20,20	0
54	MG	2A	3411	1/1	0.97	0.07	40,40,40,40	0
54	MG	2A	3689	1/1	0.97	0.06	51,51,51,51	0
54	MG	1A	3947	1/1	0.97	0.09	33,33,33,33	0
54	MG	2a	3147	1/1	0.97	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1R	202	1/1	0.97	0.12	23,23,23,23	0
54	MG	1a	3102	1/1	0.97	0.07	65,65,65,65	0
54	MG	2A	3415	1/1	0.97	0.10	46,46,46,46	0
54	MG	1R	205	1/1	0.97	0.06	26,26,26,26	0
54	MG	2A	3176	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3552	1/1	0.97	0.15	34,34,34,34	0
54	MG	1a	3108	1/1	0.97	0.04	34,34,34,34	0
54	MG	1R	207	1/1	0.97	0.07	35,35,35,35	0
54	MG	1A	3442	1/1	0.97	0.04	24,24,24,24	0
54	MG	1A	3024	1/1	0.97	0.11	15,15,15,15	0
54	MG	1A	3447	1/1	0.97	0.07	31,31,31,31	0
54	MG	1A	3792	1/1	0.97	0.05	13,13,13,13	0
54	MG	1A	3448	1/1	0.97	0.05	41,41,41,41	0
54	MG	2A	3186	1/1	0.97	0.07	40,40,40,40	0
54	MG	1A	3174	1/1	0.97	0.12	30,30,30,30	0
54	MG	1A	3956	1/1	0.97	0.06	29,29,29,29	0
54	MG	1A	3032	1/1	0.97	0.05	30,30,30,30	0
54	MG	1A	3451	1/1	0.97	0.10	48,48,48,48	0
54	MG	2A	3433	1/1	0.97	0.06	36,36,36,36	0
54	MG	1A	3015	1/1	0.97	0.17	19,19,19,19	0
54	MG	2A	3194	1/1	0.97	0.12	48,48,48,48	0
54	MG	1A	3129	1/1	0.97	0.08	54,54,54,54	0
54	MG	1V	201	1/1	0.97	0.17	16,16,16,16	0
54	MG	2A	3197	1/1	0.97	0.06	40,40,40,40	0
54	MG	1V	202	1/1	0.97	0.12	21,21,21,21	0
54	MG	1A	3566	1/1	0.97	0.05	32,32,32,32	0
54	MG	1V	204	1/1	0.97	0.18	30,30,30,30	0
54	MG	2a	3179	1/1	0.97	0.09	58,58,58,58	0
54	MG	1A	3284	1/1	0.97	0.06	39,39,39,39	0
54	MG	2A	3443	1/1	0.97	0.10	58,58,58,58	0
54	MG	1A	3016	1/1	0.97	0.20	21,21,21,21	0
54	MG	1A	3358	1/1	0.97	0.07	9,9,9,9	0
54	MG	2a	3184	1/1	0.97	0.08	35,35,35,35	0
54	MG	1A	3035	1/1	0.97	0.06	20,20,20,20	0
54	MG	1A	3360	1/1	0.97	0.06	46,46,46,46	0
54	MG	1A	3061	1/1	0.97	0.10	16,16,16,16	0
54	MG	1A	3810	1/1	0.97	0.12	56,56,56,56	0
54	MG	2f	201	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3062	1/1	0.97	0.06	24,24,24,24	0
54	MG	2A	3210	1/1	0.97	0.08	44,44,44,44	0
54	MG	2A	3211	1/1	0.97	0.36	39,39,39,39	0
54	MG	1A	3813	1/1	0.97	0.14	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3063	1/1	0.97	0.05	34,34,34,34	0
54	MG	1A	3139	1/1	0.97	0.16	14,14,14,14	0
54	MG	2A	3007	1/1	0.97	0.08	25,25,25,25	0
54	MG	2A	3008	1/1	0.97	0.09	36,36,36,36	0
54	MG	2A	3737	1/1	0.97	0.12	29,29,29,29	0
54	MG	2A	3009	1/1	0.97	0.15	30,30,30,30	0
54	MG	1A	3471	1/1	0.97	0.05	11,11,11,11	0
54	MG	2A	3013	1/1	0.97	0.10	31,31,31,31	0
56	MPD	18	104	8/8	0.97	0.10	19,20,23,28	0
54	MG	1A	3819	1/1	0.97	0.06	13,13,13,13	0
54	MG	1A	3036	1/1	0.97	0.07	21,21,21,21	0
54	MG	10	107	1/1	0.97	0.07	42,42,42,42	0
54	MG	1a	3143	1/1	0.97	0.06	52,52,52,52	0
54	MG	1A	3821	1/1	0.97	0.10	28,28,28,28	0
54	MG	1A	3822	1/1	0.97	0.06	43,43,43,43	0
58	ZN	14	102	1/1	0.97	0.12	124,124,124,124	0
58	ZN	2Y	202	1/1	0.97	0.04	89,89,89,89	0
54	MG	11	103	1/1	0.97	0.07	28,28,28,28	0
54	MG	1A	3578	1/1	0.97	0.08	44,44,44,44	0
54	MG	1A	3085	1/1	0.98	0.29	27,27,27,27	0
54	MG	1A	3455	1/1	0.98	0.05	25,25,25,25	0
54	MG	1A	3562	1/1	0.98	0.06	8,8,8,8	0
54	MG	1R	203	1/1	0.98	0.11	34,34,34,34	0
54	MG	1R	204	1/1	0.98	0.07	34,34,34,34	0
54	MG	1A	3563	1/1	0.98	0.08	26,26,26,26	0
54	MG	1A	3800	1/1	0.98	0.04	29,29,29,29	0
54	MG	1A	3245	1/1	0.98	0.18	23,23,23,23	0
54	MG	2A	3563	1/1	0.98	0.06	37,37,37,37	0
54	MG	1A	3954	1/1	0.98	0.06	37,37,37,37	0
54	MG	2A	3565	1/1	0.98	0.07	42,42,42,42	0
54	MG	1A	3674	1/1	0.98	0.05	47,47,47,47	0
54	MG	1a	3103	1/1	0.98	0.08	41,41,41,41	0
54	MG	1a	3104	1/1	0.98	0.06	28,28,28,28	0
54	MG	2Y	201	1/1	0.98	0.10	40,40,40,40	0
54	MG	1a	3105	1/1	0.98	0.08	29,29,29,29	0
54	MG	1A	3457	1/1	0.98	0.04	38,38,38,38	0
54	MG	1A	3676	1/1	0.98	0.04	7,7,7,7	0
54	MG	1A	3805	1/1	0.98	0.05	34,34,34,34	0
54	MG	2A	3574	1/1	0.98	0.07	49,49,49,49	0
54	MG	23	101	1/1	0.98	0.07	41,41,41,41	0
54	MG	2A	3159	1/1	0.98	0.08	66,66,66,66	0
54	MG	1A	3364	1/1	0.98	0.05	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3678	1/1	0.98	0.06	35,35,35,35	0
54	MG	1U	202	1/1	0.98	0.44	28,28,28,28	0
54	MG	1A	3050	1/1	0.98	0.20	20,20,20,20	0
54	MG	1A	3680	1/1	0.98	0.07	37,37,37,37	0
54	MG	1A	3366	1/1	0.98	0.05	34,34,34,34	0
54	MG	1A	3811	1/1	0.98	0.08	13,13,13,13	0
54	MG	2A	3584	1/1	0.98	0.04	42,42,42,42	0
54	MG	1A	3247	1/1	0.98	0.31	21,21,21,21	0
54	MG	2A	3586	1/1	0.98	0.04	26,26,26,26	0
54	MG	1a	3117	1/1	0.98	0.04	30,30,30,30	0
54	MG	1A	3968	1/1	0.98	0.05	12,12,12,12	0
54	MG	1A	3166	1/1	0.98	0.09	25,25,25,25	0
54	MG	1A	3814	1/1	0.98	0.18	32,32,32,32	0
54	MG	1A	3133	1/1	0.98	0.23	22,22,22,22	0
54	MG	1A	3250	1/1	0.98	0.20	15,15,15,15	0
54	MG	2A	3377	1/1	0.98	0.05	25,25,25,25	0
54	MG	1A	3817	1/1	0.98	0.05	13,13,13,13	0
54	MG	1A	3688	1/1	0.98	0.12	20,20,20,20	0
54	MG	1A	3371	1/1	0.98	0.05	38,38,38,38	0
54	MG	1A	3372	1/1	0.98	0.04	14,14,14,14	0
54	MG	1A	3252	1/1	0.98	0.07	17,17,17,17	0
54	MG	2A	3600	1/1	0.98	0.07	59,59,59,59	0
54	MG	1A	3253	1/1	0.98	0.06	33,33,33,33	0
54	MG	1A	3693	1/1	0.98	0.06	40,40,40,40	0
54	MG	1A	3375	1/1	0.98	0.07	22,22,22,22	0
54	MG	1A	3825	1/1	0.98	0.06	37,37,37,37	0
54	MG	2A	3388	1/1	0.98	0.05	45,45,45,45	0
54	MG	2A	3389	1/1	0.98	0.08	44,44,44,44	0
54	MG	2A	3607	1/1	0.98	0.07	52,52,52,52	0
54	MG	2A	3183	1/1	0.98	0.06	44,44,44,44	0
54	MG	1A	3168	1/1	0.98	0.04	18,18,18,18	0
54	MG	1A	3983	1/1	0.98	0.07	16,16,16,16	0
54	MG	1A	3696	1/1	0.98	0.09	32,32,32,32	0
54	MG	1A	3579	1/1	0.98	0.08	28,28,28,28	0
54	MG	2A	3395	1/1	0.98	0.04	22,22,22,22	0
54	MG	2A	3614	1/1	0.98	0.04	59,59,59,59	0
54	MG	1A	3377	1/1	0.98	0.08	41,41,41,41	0
54	MG	1A	3052	1/1	0.98	0.20	19,19,19,19	0
54	MG	2A	3618	1/1	0.98	0.04	54,54,54,54	0
54	MG	2A	3191	1/1	0.98	0.09	40,40,40,40	0
54	MG	2A	3006	1/1	0.98	0.07	33,33,33,33	0
54	MG	1A	3831	1/1	0.98	0.04	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3379	1/1	0.98	0.05	15,15,15,15	0
54	MG	2a	3041	1/1	0.98	0.06	52,52,52,52	0
54	MG	1A	3088	1/1	0.98	0.14	28,28,28,28	0
54	MG	1A	3381	1/1	0.98	0.07	7,7,7,7	0
54	MG	2A	3626	1/1	0.98	0.05	52,52,52,52	0
54	MG	2A	3628	1/1	0.98	0.05	25,25,25,25	0
54	MG	2A	3629	1/1	0.98	0.04	54,54,54,54	0
54	MG	2A	3630	1/1	0.98	0.05	34,34,34,34	0
54	MG	1A	3138	1/1	0.98	0.22	20,20,20,20	0
54	MG	1A	3309	1/1	0.98	0.14	27,27,27,27	0
54	MG	1A	3995	1/1	0.98	0.14	6,6,6,6	0
54	MG	1A	3310	1/1	0.98	0.10	12,12,12,12	0
54	MG	1A	3074	1/1	0.98	0.21	27,27,27,27	0
54	MG	2A	3409	1/1	0.98	0.07	43,43,43,43	0
54	MG	1A	3387	1/1	0.98	0.06	6,6,6,6	0
54	MG	1A	3001	1/1	0.98	0.07	24,24,24,24	0
54	MG	2A	3639	1/1	0.98	0.04	25,25,25,25	0
54	MG	1A	4001	1/1	0.98	0.05	44,44,44,44	0
54	MG	2A	3205	1/1	0.98	0.13	46,46,46,46	0
54	MG	1A	3064	1/1	0.98	0.05	21,21,21,21	0
54	MG	1A	3390	1/1	0.98	0.05	23,23,23,23	0
54	MG	1A	4004	1/1	0.98	0.07	20,20,20,20	0
54	MG	1A	3392	1/1	0.98	0.08	7,7,7,7	0
54	MG	1A	3490	1/1	0.98	0.07	42,42,42,42	0
54	MG	1A	3491	1/1	0.98	0.04	13,13,13,13	0
54	MG	1A	3492	1/1	0.98	0.06	58,58,58,58	0
54	MG	2A	3650	1/1	0.98	0.05	58,58,58,58	0
54	MG	2A	3651	1/1	0.98	0.04	52,52,52,52	0
54	MG	2A	3421	1/1	0.98	0.06	36,36,36,36	0
54	MG	17	104	1/1	0.98	0.07	24,24,24,24	0
54	MG	1A	3175	1/1	0.98	0.13	31,31,31,31	0
54	MG	18	101	1/1	0.98	0.29	34,34,34,34	0
54	MG	2A	3656	1/1	0.98	0.05	37,37,37,37	0
54	MG	2A	3425	1/1	0.98	0.05	47,47,47,47	0
54	MG	1a	3162	1/1	0.98	0.10	66,66,66,66	0
54	MG	2A	3660	1/1	0.98	0.04	53,53,53,53	0
54	MG	1A	3394	1/1	0.98	0.05	8,8,8,8	0
54	MG	18	103	1/1	0.98	0.12	39,39,39,39	0
54	MG	1a	3165	1/1	0.98	0.08	46,46,46,46	0
54	MG	1A	3851	1/1	0.98	0.07	28,28,28,28	0
54	MG	2a	3080	1/1	0.98	0.09	48,48,48,48	0
54	MG	19	102	1/1	0.98	0.26	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3495	1/1	0.98	0.09	30,30,30,30	0
54	MG	2A	3223	1/1	0.98	0.17	28,28,28,28	0
54	MG	1A	3853	1/1	0.98	0.11	30,30,30,30	0
54	MG	1A	3315	1/1	0.98	0.05	10,10,10,10	0
54	MG	1A	3114	1/1	0.98	0.12	26,26,26,26	0
54	MG	1A	3603	1/1	0.98	0.13	16,16,16,16	0
54	MG	1A	3093	1/1	0.98	0.22	14,14,14,14	0
54	MG	2A	3674	1/1	0.98	0.05	27,27,27,27	0
54	MG	1A	3178	1/1	0.98	0.16	22,22,22,22	0
54	MG	1A	3077	1/1	0.98	0.48	22,22,22,22	0
54	MG	1A	3401	1/1	0.98	0.04	15,15,15,15	0
54	MG	1A	3726	1/1	0.98	0.04	30,30,30,30	0
54	MG	1A	3146	1/1	0.98	0.06	15,15,15,15	0
54	MG	1A	3403	1/1	0.98	0.05	11,11,11,11	0
54	MG	2A	3681	1/1	0.98	0.05	28,28,28,28	0
54	MG	1A	3181	1/1	0.98	0.14	28,28,28,28	0
54	MG	1A	3866	1/1	0.98	0.07	41,41,41,41	0
54	MG	1A	3182	1/1	0.98	0.23	19,19,19,19	0
54	MG	1a	3015	1/1	0.98	0.12	39,39,39,39	0
54	MG	1A	3095	1/1	0.98	0.13	22,22,22,22	0
54	MG	1A	3870	1/1	0.98	0.05	20,20,20,20	0
54	MG	1A	3408	1/1	0.98	0.04	18,18,18,18	0
54	MG	1A	3614	1/1	0.98	0.05	14,14,14,14	0
54	MG	2A	3691	1/1	0.98	0.07	33,33,33,33	0
54	MG	2A	3059	1/1	0.98	0.09	35,35,35,35	0
54	MG	1A	3409	1/1	0.98	0.04	25,25,25,25	0
54	MG	2a	3109	1/1	0.98	0.08	60,60,60,60	0
54	MG	1a	3021	1/1	0.98	0.04	42,42,42,42	0
54	MG	1A	3270	1/1	0.98	0.23	15,15,15,15	0
54	MG	1A	3618	1/1	0.98	0.11	38,38,38,38	0
54	MG	2A	3459	1/1	0.98	0.05	41,41,41,41	0
54	MG	1A	3327	1/1	0.98	0.06	18,18,18,18	0
54	MG	1A	3515	1/1	0.98	0.06	13,13,13,13	0
54	MG	1A	3221	1/1	0.98	0.07	22,22,22,22	0
54	MG	1A	3622	1/1	0.98	0.04	17,17,17,17	0
54	MG	2A	3068	1/1	0.98	0.10	45,45,45,45	0
54	MG	1A	3329	1/1	0.98	0.04	27,27,27,27	0
54	MG	1A	3883	1/1	0.98	0.20	26,26,26,26	0
54	MG	1A	3003	1/1	0.98	0.07	14,14,14,14	0
54	MG	1A	3885	1/1	0.98	0.04	29,29,29,29	0
54	MG	1A	3887	1/1	0.98	0.05	31,31,31,31	0
54	MG	1a	3201	1/1	0.98	0.06	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3519	1/1	0.98	0.04	25,25,25,25	0
54	MG	2a	3127	1/1	0.98	0.05	50,50,50,50	0
54	MG	1A	3890	1/1	0.98	0.05	36,36,36,36	0
54	MG	2A	3711	1/1	0.98	0.05	36,36,36,36	0
54	MG	2a	3130	1/1	0.98	0.05	71,71,71,71	0
54	MG	1A	3892	1/1	0.98	0.04	21,21,21,21	0
54	MG	1A	3416	1/1	0.98	0.07	13,13,13,13	0
54	MG	1A	3522	1/1	0.98	0.10	35,35,35,35	0
54	MG	1A	3223	1/1	0.98	0.20	30,30,30,30	0
54	MG	1A	3056	1/1	0.98	0.07	35,35,35,35	0
54	MG	1A	3099	1/1	0.98	0.06	15,15,15,15	0
54	MG	1A	3751	1/1	0.98	0.06	27,27,27,27	0
54	MG	1D	315	1/1	0.98	0.08	40,40,40,40	0
54	MG	1A	3334	1/1	0.98	0.05	20,20,20,20	0
54	MG	1A	3753	1/1	0.98	0.07	39,39,39,39	0
54	MG	1a	3045	1/1	0.98	0.20	47,47,47,47	0
54	MG	1A	3121	1/1	0.98	0.04	16,16,16,16	0
54	MG	2A	3278	1/1	0.98	0.12	33,33,33,33	0
54	MG	1E	301	1/1	0.98	0.12	14,14,14,14	0
54	MG	1A	3903	1/1	0.98	0.05	18,18,18,18	0
54	MG	1E	303	1/1	0.98	0.17	18,18,18,18	0
54	MG	2A	3282	1/1	0.98	0.07	21,21,21,21	0
54	MG	1A	3122	1/1	0.98	0.05	14,14,14,14	0
54	MG	1A	3040	1/1	0.98	0.09	28,28,28,28	0
54	MG	1A	3190	1/1	0.98	0.09	24,24,24,24	0
54	MG	1A	3636	1/1	0.98	0.06	26,26,26,26	0
54	MG	1A	3759	1/1	0.98	0.03	14,14,14,14	0
54	MG	1A	3339	1/1	0.98	0.10	45,45,45,45	0
54	MG	2A	3735	1/1	0.98	0.05	33,33,33,33	0
54	MG	1A	3761	1/1	0.98	0.05	35,35,35,35	0
54	MG	1a	3226	1/1	0.98	0.06	57,57,57,57	0
54	MG	2a	3159	1/1	0.98	0.05	59,59,59,59	0
54	MG	1A	3340	1/1	0.98	0.06	13,13,13,13	0
54	MG	1A	3102	1/1	0.98	0.19	23,23,23,23	0
54	MG	1F	306	1/1	0.98	0.04	25,25,25,25	0
54	MG	2a	3163	1/1	0.98	0.09	74,74,74,74	0
54	MG	1A	3640	1/1	0.98	0.08	33,33,33,33	0
54	MG	1A	3155	1/1	0.98	0.15	25,25,25,25	0
54	MG	1A	3282	1/1	0.98	0.25	13,13,13,13	0
54	MG	1A	3430	1/1	0.98	0.06	30,30,30,30	0
54	MG	1A	3058	1/1	0.98	0.05	10,10,10,10	0
54	MG	1A	3346	1/1	0.98	0.07	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3300	1/1	0.98	0.06	34,34,34,34	0
54	MG	1A	3347	1/1	0.98	0.04	8,8,8,8	0
54	MG	1A	3233	1/1	0.98	0.38	18,18,18,18	0
54	MG	1A	3774	1/1	0.98	0.06	28,28,28,28	0
54	MG	2A	3112	1/1	0.98	0.24	31,31,31,31	0
54	MG	1A	3648	1/1	0.98	0.10	33,33,33,33	0
54	MG	1A	3543	1/1	0.98	0.05	35,35,35,35	0
54	MG	1A	3350	1/1	0.98	0.06	18,18,18,18	0
54	MG	2A	3519	1/1	0.98	0.09	20,20,20,20	0
54	MG	1A	3127	1/1	0.98	0.05	26,26,26,26	0
54	MG	1A	3021	1/1	0.98	0.18	26,26,26,26	0
54	MG	1A	3159	1/1	0.98	0.15	17,17,17,17	0
54	MG	1a	3246	1/1	0.98	0.05	33,33,33,33	0
54	MG	2A	3312	1/1	0.98	0.06	29,29,29,29	0
54	MG	2A	3121	1/1	0.98	0.08	40,40,40,40	0
54	MG	1A	3933	1/1	0.98	0.08	45,45,45,45	0
54	MG	1H	202	1/1	0.98	0.03	46,46,46,46	0
54	MG	2A	3317	1/1	0.98	0.08	27,27,27,27	0
54	MG	1A	3237	1/1	0.98	0.21	24,24,24,24	0
54	MG	1a	3251	1/1	0.98	0.11	58,58,58,58	0
54	MG	2A	3126	1/1	0.98	0.06	40,40,40,40	0
54	MG	2E	302	1/1	0.98	0.04	27,27,27,27	0
54	MG	1A	3048	1/1	0.98	0.04	15,15,15,15	0
54	MG	1A	3356	1/1	0.98	0.08	10,10,10,10	0
54	MG	2A	3535	1/1	0.98	0.09	59,59,59,59	0
54	MG	1A	3937	1/1	0.98	0.04	25,25,25,25	0
54	MG	2A	3538	1/1	0.98	0.04	35,35,35,35	0
54	MG	2A	3324	1/1	0.98	0.06	21,21,21,21	0
54	MG	1A	3444	1/1	0.98	0.05	34,34,34,34	0
54	MG	1A	3239	1/1	0.98	0.11	13,13,13,13	0
54	MG	1P	202	1/1	0.98	0.25	18,18,18,18	0
54	MG	1a	3258	1/1	0.98	0.04	52,52,52,52	0
54	MG	1A	3553	1/1	0.98	0.07	29,29,29,29	0
54	MG	1A	3291	1/1	0.98	0.13	13,13,13,13	0
54	MG	1A	3084	1/1	0.98	0.13	24,24,24,24	0
54	MG	1A	3199	1/1	0.98	0.06	34,34,34,34	0
54	MG	1A	3163	1/1	0.98	0.18	22,22,22,22	0
54	MG	1A	3453	1/1	0.98	0.08	26,26,26,26	0
58	ZN	1Y	202	1/1	0.98	0.03	53,53,53,53	0
54	MG	1A	3559	1/1	0.98	0.05	33,33,33,33	0
58	ZN	1n	103	1/1	0.98	0.03	69,69,69,69	0
54	MG	1Q	203	1/1	0.98	0.05	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2Q	203	1/1	0.98	0.06	56,56,56,56	0
58	ZN	25	102	1/1	0.98	0.04	64,64,64,64	0
58	ZN	29	102	1/1	0.98	0.04	60,60,60,60	0
54	MG	1A	3794	1/1	0.98	0.05	38,38,38,38	0
59	SF4	2d	501	8/8	0.98	0.06	51,67,74,74	0
54	MG	2A	3011	1/1	0.99	0.07	21,21,21,21	0
54	MG	2A	3360	1/1	0.99	0.06	32,32,32,32	0
54	MG	2A	3012	1/1	0.99	0.07	36,36,36,36	0
54	MG	1A	3123	1/1	0.99	0.06	24,24,24,24	0
54	MG	2A	3571	1/1	0.99	0.07	21,21,21,21	0
54	MG	1a	3241	1/1	0.99	0.03	34,34,34,34	0
54	MG	2A	3688	1/1	0.99	0.04	45,45,45,45	0
54	MG	1A	3013	1/1	0.99	0.15	17,17,17,17	0
54	MG	1A	3009	1/1	0.99	0.24	23,23,23,23	0
54	MG	2A	3268	1/1	0.99	0.04	17,17,17,17	0
54	MG	2A	3468	1/1	0.99	0.04	32,32,32,32	0
54	MG	2A	3577	1/1	0.99	0.05	34,34,34,34	0
54	MG	1A	3908	1/1	0.99	0.06	8,8,8,8	0
54	MG	1A	3909	1/1	0.99	0.09	31,31,31,31	0
54	MG	2A	3271	1/1	0.99	0.04	47,47,47,47	0
54	MG	1A	3384	1/1	0.99	0.04	26,26,26,26	0
54	MG	2A	3273	1/1	0.99	0.07	22,22,22,22	0
54	MG	1A	3911	1/1	0.99	0.04	35,35,35,35	0
54	MG	1a	3248	1/1	0.99	0.04	44,44,44,44	0
54	MG	1D	307	1/1	0.99	0.04	7,7,7,7	0
54	MG	2A	3188	1/1	0.99	0.04	35,35,35,35	0
54	MG	1A	3414	1/1	0.99	0.05	21,21,21,21	0
54	MG	1D	309	1/1	0.99	0.15	18,18,18,18	0
54	MG	2A	3025	1/1	0.99	0.02	22,22,22,22	0
54	MG	1A	3446	1/1	0.99	0.02	15,15,15,15	0
54	MG	2A	3591	1/1	0.99	0.04	28,28,28,28	0
54	MG	2a	3124	1/1	0.99	0.04	46,46,46,46	0
54	MG	1A	3520	1/1	0.99	0.05	14,14,14,14	0
54	MG	1A	3742	1/1	0.99	0.05	20,20,20,20	0
54	MG	1A	3049	1/1	0.99	0.15	26,26,26,26	0
54	MG	1A	3797	1/1	0.99	0.08	32,32,32,32	0
54	MG	2A	3384	1/1	0.99	0.03	19,19,19,19	0
54	MG	2A	3113	1/1	0.99	0.15	29,29,29,29	0
54	MG	1A	3251	1/1	0.99	0.17	39,39,39,39	0
54	MG	1A	3854	1/1	0.99	0.08	44,44,44,44	0
54	MG	1A	3920	1/1	0.99	0.04	28,28,28,28	0
54	MG	1A	3745	1/1	0.99	0.03	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3649	1/1	0.99	0.06	21,21,21,21	0
54	MG	1A	3292	1/1	0.99	0.10	7,7,7,7	0
54	MG	1A	3160	1/1	0.99	0.07	20,20,20,20	0
54	MG	1A	3039	1/1	0.99	0.03	25,25,25,25	0
54	MG	1A	3926	1/1	0.99	0.11	36,36,36,36	0
54	MG	1E	306	1/1	0.99	0.07	8,8,8,8	0
54	MG	1A	3487	1/1	0.99	0.04	11,11,11,11	0
54	MG	1A	3994	1/1	0.99	0.06	74,74,74,74	0
54	MG	1A	3101	1/1	0.99	0.27	28,28,28,28	0
54	MG	1A	3145	1/1	0.99	0.06	13,13,13,13	0
54	MG	2A	3045	1/1	0.99	0.14	32,32,32,32	0
54	MG	1A	3997	1/1	0.99	0.04	19,19,19,19	0
54	MG	1A	3051	1/1	0.99	0.15	20,20,20,20	0
54	MG	1a	3119	1/1	0.99	0.06	27,27,27,27	0
54	MG	2A	3616	1/1	0.99	0.05	47,47,47,47	0
54	MG	1A	3342	1/1	0.99	0.07	36,36,36,36	0
54	MG	1F	305	1/1	0.99	0.19	23,23,23,23	0
54	MG	1A	3090	1/1	0.99	0.20	24,24,24,24	0
54	MG	2A	3620	1/1	0.99	0.04	51,51,51,51	0
54	MG	1A	3396	1/1	0.99	0.02	7,7,7,7	0
54	MG	2a	3156	1/1	0.99	0.06	58,58,58,58	0
54	MG	1A	3006	1/1	0.99	0.07	17,17,17,17	0
54	MG	1A	3868	1/1	0.99	0.04	17,17,17,17	0
54	MG	1A	3321	1/1	0.99	0.08	45,45,45,45	0
54	MG	1A	3662	1/1	0.99	0.03	29,29,29,29	0
54	MG	2A	3313	1/1	0.99	0.07	23,23,23,23	0
54	MG	1A	3496	1/1	0.99	0.04	40,40,40,40	0
54	MG	1A	3872	1/1	0.99	0.03	13,13,13,13	0
54	MG	2A	3518	1/1	0.99	0.06	24,24,24,24	0
54	MG	1A	3497	1/1	0.99	0.05	27,27,27,27	0
54	MG	1A	3461	1/1	0.99	0.03	31,31,31,31	0
54	MG	1A	3764	1/1	0.99	0.06	21,21,21,21	0
54	MG	1A	3538	1/1	0.99	0.07	32,32,32,32	0
54	MG	2a	3169	1/1	0.99	0.09	52,52,52,52	0
54	MG	1A	3539	1/1	0.99	0.04	24,24,24,24	0
54	MG	1A	3045	1/1	0.99	0.32	17,17,17,17	0
54	MG	1A	3716	1/1	0.99	0.04	21,21,21,21	0
54	MG	1A	3054	1/1	0.99	0.20	23,23,23,23	0
54	MG	1a	3138	1/1	0.99	0.05	33,33,33,33	0
54	MG	2A	3325	1/1	0.99	0.03	26,26,26,26	0
54	MG	1A	3464	1/1	0.99	0.04	16,16,16,16	0
54	MG	1A	3465	1/1	0.99	0.06	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3531	1/1	0.99	0.05	43,43,43,43	0
54	MG	2A	3328	1/1	0.99	0.09	25,25,25,25	0
54	MG	1A	3134	1/1	0.99	0.14	18,18,18,18	0
54	MG	1A	3673	1/1	0.99	0.06	42,42,42,42	0
54	MG	1A	3504	1/1	0.99	0.07	10,10,10,10	0
54	MG	2A	3648	1/1	0.99	0.05	25,25,25,25	0
54	MG	2A	3240	1/1	0.99	0.11	14,14,14,14	0
54	MG	2A	3537	1/1	0.99	0.03	36,36,36,36	0
54	MG	1B	211	1/1	0.99	0.07	37,37,37,37	0
54	MG	1B	212	1/1	0.99	0.03	36,36,36,36	0
54	MG	2A	3243	1/1	0.99	0.07	21,21,21,21	0
54	MG	1A	3505	1/1	0.99	0.03	7,7,7,7	0
54	MG	1A	3349	1/1	0.99	0.07	8,8,8,8	0
54	MG	2E	305	1/1	0.99	0.04	21,21,21,21	0
54	MG	2A	3338	1/1	0.99	0.04	19,19,19,19	0
54	MG	1A	3891	1/1	0.99	0.04	16,16,16,16	0
54	MG	1A	3777	1/1	0.99	0.05	29,29,29,29	0
54	MG	1A	3589	1/1	0.99	0.04	26,26,26,26	0
54	MG	1A	3958	1/1	0.99	0.06	33,33,33,33	0
54	MG	1A	3325	1/1	0.99	0.04	13,13,13,13	0
54	MG	2A	3549	1/1	0.99	0.03	39,39,39,39	0
54	MG	2A	3344	1/1	0.99	0.04	25,25,25,25	0
54	MG	1A	3833	1/1	0.99	0.04	22,22,22,22	0
54	MG	2A	3346	1/1	0.99	0.03	34,34,34,34	0
54	MG	2A	3667	1/1	0.99	0.04	47,47,47,47	0
54	MG	1A	3073	1/1	0.99	0.30	25,25,25,25	0
54	MG	2A	3348	1/1	0.99	0.04	21,21,21,21	0
54	MG	2A	3555	1/1	0.99	0.04	39,39,39,39	0
54	MG	2a	3086	1/1	0.99	0.05	57,57,57,57	0
54	MG	2A	3349	1/1	0.99	0.04	29,29,29,29	0
54	MG	1A	3046	1/1	0.99	0.04	5,5,5,5	0
54	MG	1A	3681	1/1	0.99	0.08	27,27,27,27	0
54	MG	1A	3244	1/1	0.99	0.22	31,31,31,31	0
58	ZN	16	501	1/1	0.99	0.02	29,29,29,29	0
54	MG	1A	3436	1/1	0.99	0.07	35,35,35,35	0
54	MG	2A	3453	1/1	0.99	0.13	56,56,56,56	0
54	MG	1A	3901	1/1	0.99	0.04	45,45,45,45	0
54	MG	1A	3967	1/1	0.99	0.09	9,9,9,9	0
58	ZN	26	103	1/1	0.99	0.02	54,54,54,54	0
54	MG	1A	3137	1/1	0.99	0.17	30,30,30,30	0
54	MG	1A	3096	1/1	0.99	0.10	8,8,8,8	0
59	SF4	1d	306	8/8	0.99	0.04	50,57,65,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3686	1/1	0.99	0.06	31,31,31,31	0
54	MG	1A	3438	1/1	1.00	0.03	10,10,10,10	0
54	MG	2A	3478	1/1	1.00	0.02	28,28,28,28	0
54	MG	2a	3138	1/1	1.00	0.07	38,38,38,38	0
54	MG	1A	3445	1/1	1.00	0.04	8,8,8,8	0
54	MG	1A	3470	1/1	1.00	0.04	25,25,25,25	0
54	MG	1A	3615	1/1	1.00	0.04	17,17,17,17	0
54	MG	1A	3763	1/1	1.00	0.02	21,21,21,21	0
58	ZN	15	109	1/1	1.00	0.02	50,50,50,50	0
54	MG	1A	3836	1/1	1.00	0.02	8,8,8,8	0
58	ZN	19	104	1/1	1.00	0.02	33,33,33,33	0
54	MG	1A	3406	1/1	1.00	0.03	9,9,9,9	0
54	MG	1A	3874	1/1	1.00	0.02	29,29,29,29	0
54	MG	1A	3391	1/1	1.00	0.04	25,25,25,25	0
54	MG	2A	3657	1/1	1.00	0.03	26,26,26,26	0
54	MG	2A	3627	1/1	1.00	0.03	25,25,25,25	0
54	MG	1A	3886	1/1	1.00	0.02	13,13,13,13	0
54	MG	1A	3452	1/1	1.00	0.03	38,38,38,38	0
54	MG	2A	3462	1/1	1.00	0.02	25,25,25,25	0
54	MG	1A	3888	1/1	1.00	0.04	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.