



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 04:42 AM UTC

PDB ID : 8EV7 / pdb_00008ev7
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with kanamycin, mRNA, and A-, P-, and E-site tRNAs
Authors : Seely, S.M.; Gagnon, M.G.
Deposited on : 2022-10-19
Resolution : 2.89 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

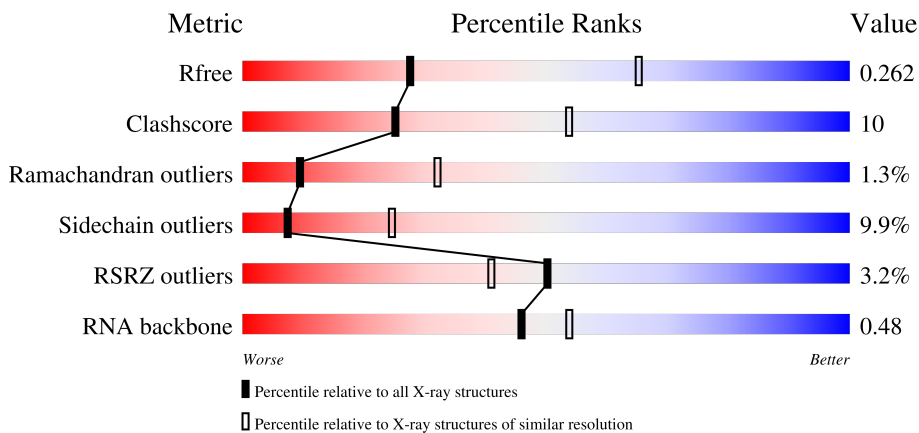
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1A	2915	
1	2A	2915	
2	1B	121	
2	2B	121	

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Mol	Chain	Length	Quality of chain
3	1D	276	2% 74% 23% .
3	2D	276	3% 72% 24% .
4	1E	206	73% 21% 5% .
4	2E	206	% 69% 24% 6% .
5	1F	210	65% 27% 5% .
5	2F	210	2% 59% 32% 5% .
6	1G	182	2% 69% 25% 5% .
6	2G	182	9% 62% 31% 5% ..
7	1H	180	2% 69% 26% . .
7	2H	180	7% 57% 34% 5% .
8	1I	148	2% 70% 22% 7% .
8	2I	148	7% 66% 30% . .
9	1N	140	76% 21% .
9	2N	140	3% 61% 34% 5%
10	1O	122	2% 73% 25% .
10	2O	122	% 66% 30% .
11	1P	150	2% 65% 27% 7% .
11	2P	150	2% 64% 31% . . .
12	1Q	141	% 70% 24% 6%
12	2Q	141	8% 58% 36% 6%
13	1R	118	69% 26% .
13	2R	118	% 69% 27% .
14	1S	112	76% 20% . .
14	2S	112	9% 55% 36% 7% .
15	1T	146	2% 60% 29% . . 10%




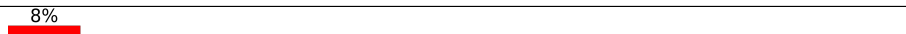
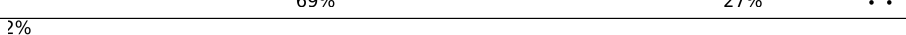
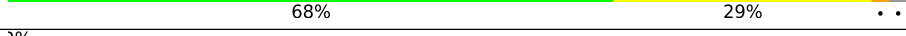



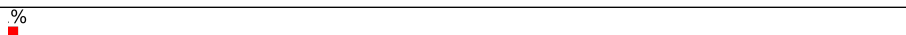
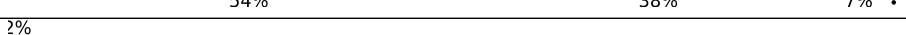
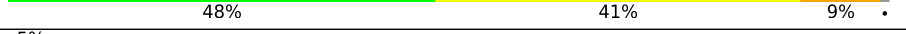
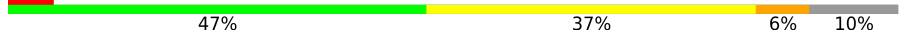


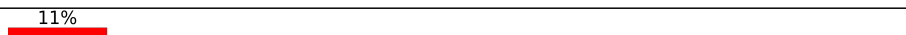






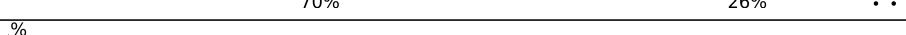


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Mol	Chain	Length	Quality of chain
15	2T	146	2% 54% 33% 10%
16	1U	118	80% 17% ..
16	2U	118	% 69% 26% ..
17	1V	101	75% 24% .
17	2V	101	2% 72% 21% 6% .
18	1W	113	2% 68% 26% 5% .
18	2W	113	% 75% 21% ..
19	1X	96	% 72% 25% ...
19	2X	96	5% 77% 21% ..
20	1Y	110	% 65% 27% 5% .
20	2Y	110	12% 69% 23% 5% .
21	1Z	206	2% 46% 25% . 25%
21	2Z	206	6% 44% 29% . 22%
22	10	85	8% 79% 16% ..
22	20	85	14% 61% 34% ..
23	11	98	% 77% 20% ..
23	21	98	4% 64% 34% ..
24	12	72	3% 62% 33% ..
24	22	72	75% 19% ..
25	13	60	3% 70% 22% 7% .
25	23	60	3% 58% 33% 7% .
26	14	71	10% 55% 35% 6% ..
26	24	71	14% 45% 38% 14% .
27	15	60	2% 75% 22% ..
27	25	60	2% 75% 20% ..

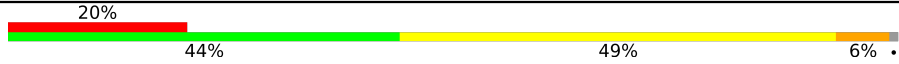
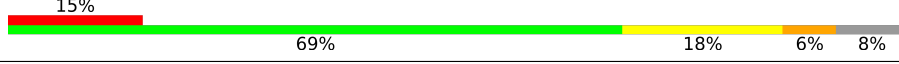



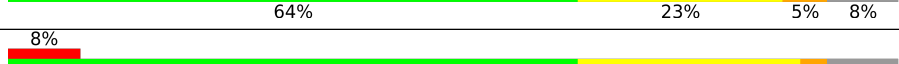
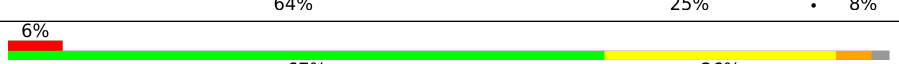

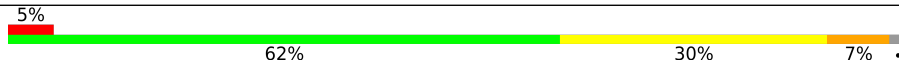


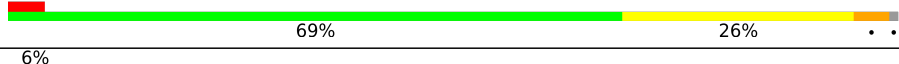
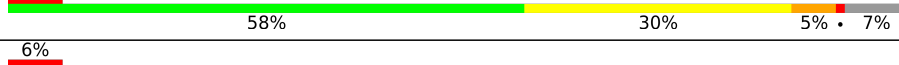

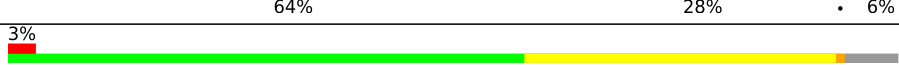
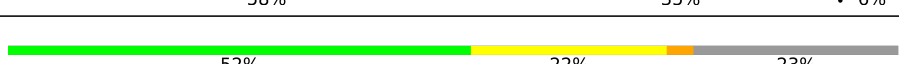









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Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
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	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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	PSU	2y	55	-	-	X	-
56	MG	1A	3532	-	-	-	X
56	MG	1a	1709	-	-	-	X
56	MG	1v	101	-	-	-	X

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 297628 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	1S	110	873	550	174	149	0	0	0
14	2S	110	870	549	173	148	0	0	0

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

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

- 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
			771	495	140	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
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	932	Total	Mg	0	0
			932	932		
56	1B	29	Total	Mg	0	0
			29	29		
56	1D	4	Total	Mg	0	0
			4	4		
56	1E	4	Total	Mg	0	0
			4	4		
56	1F	3	Total	Mg	0	0
			3	3		
56	1G	2	Total	Mg	0	0
			2	2		
56	1N	2	Total	Mg	0	0
			2	2		
56	1O	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1P	2	Total 2	Mg 2	0	0
56	1Q	3	Total 3	Mg 3	0	0
56	1R	1	Total 1	Mg 1	0	0
56	1T	1	Total 1	Mg 1	0	0
56	1U	2	Total 2	Mg 2	0	0
56	1V	2	Total 2	Mg 2	0	0
56	1W	2	Total 2	Mg 2	0	0
56	1X	1	Total 1	Mg 1	0	0
56	1Y	1	Total 1	Mg 1	0	0
56	10	1	Total 1	Mg 1	0	0
56	11	1	Total 1	Mg 1	0	0
56	12	1	Total 1	Mg 1	0	0
56	13	4	Total 4	Mg 4	0	0
56	14	1	Total 1	Mg 1	0	0
56	15	3	Total 3	Mg 3	0	0
56	16	1	Total 1	Mg 1	0	0
56	17	1	Total 1	Mg 1	0	0
56	18	4	Total 4	Mg 4	0	0
56	19	3	Total 3	Mg 3	0	0
56	1a	354	Total 354	Mg 354	0	0
56	1d	2	Total 2	Mg 2	0	0

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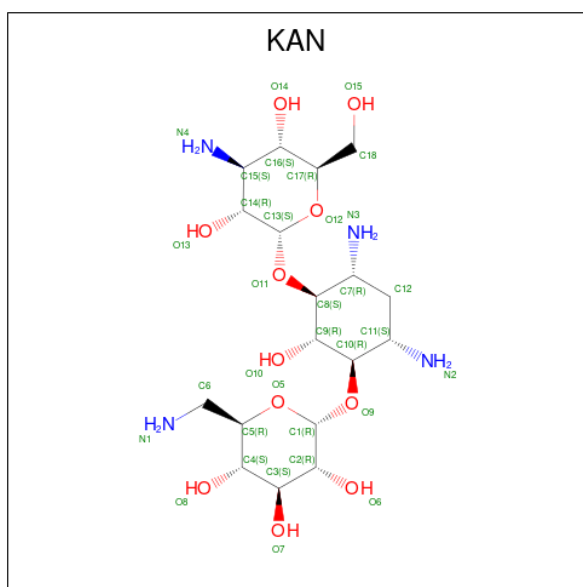
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1e	1	Total 1	Mg 1	0	0
56	1i	1	Total 1	Mg 1	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1l	3	Total 3	Mg 3	0	0
56	1m	2	Total 2	Mg 2	0	0
56	1o	3	Total 3	Mg 3	0	0
56	1q	2	Total 2	Mg 2	0	0
56	1r	1	Total 1	Mg 1	0	0
56	1v	3	Total 3	Mg 3	0	0
56	1w	5	Total 5	Mg 5	0	0
56	1x	24	Total 24	Mg 24	0	0
56	1y	1	Total 1	Mg 1	0	0
56	2A	567	Total 567	Mg 567	0	0
56	2B	13	Total 13	Mg 13	0	0
56	2D	3	Total 3	Mg 3	0	0
56	2E	2	Total 2	Mg 2	0	0
56	2F	4	Total 4	Mg 4	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2Q	2	Total 2	Mg 2	0	0
56	2T	2	Total 2	Mg 2	0	0
56	2W	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	20	2	Total 2	Mg 2	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	1	Total 1	Mg 1	0	0
56	26	1	Total 1	Mg 1	0	0
56	28	2	Total 2	Mg 2	0	0
56	2a	227	Total 227	Mg 227	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2q	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	2	Total 2	Mg 2	0	0
56	2w	1	Total 1	Mg 1	0	0
56	2x	7	Total 7	Mg 7	0	0

- Molecule 57 is KANAMYCIN A (CCD ID: KAN) (formula: $C_{18}H_{36}N_4O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
57	1A	1	Total	C	N	O	0	0
			33	18	4	11		
57	1A	1	Total	C	N	O	0	0
			33	18	4	11		
57	1A	1	Total	C	N	O	0	0
			33	18	4	11		
57	1a	1	Total	C	N	O	0	0
			33	18	4	11		
57	2A	1	Total	C	N	O	0	0
			33	18	4	11		
57	2A	1	Total	C	N	O	0	0
			33	18	4	11		
57	2a	1	Total	C	N	O	0	0
			33	18	4	11		

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

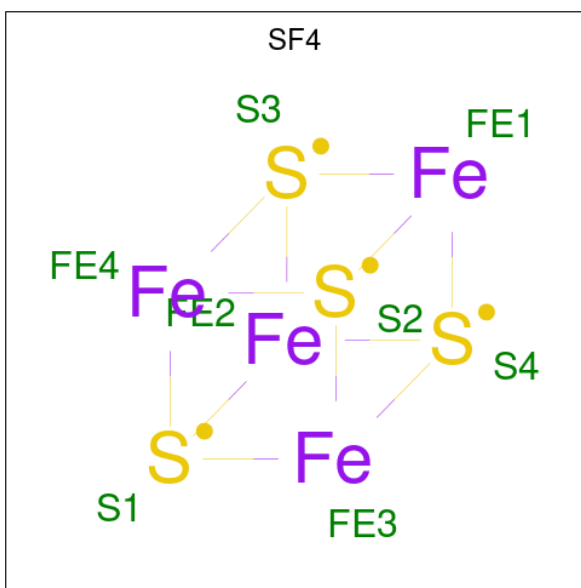
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		

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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	938	Total O 938 938	0	0
60	1B	25	Total O 25 25	0	0
60	1D	9	Total O 9 9	0	0
60	1E	7	Total O 7 7	0	0
60	1F	9	Total O 9 9	0	0
60	1G	1	Total O 1 1	0	0
60	1H	1	Total O 1 1	0	0
60	1N	2	Total O 2 2	0	0
60	1O	4	Total O 4 4	0	0
60	1P	12	Total O 12 12	0	0
60	1Q	4	Total O 4 4	0	0
60	1R	5	Total O 5 5	0	0
60	1S	2	Total O 2 2	0	0
60	1T	8	Total O 8 8	0	0
60	1U	5	Total O 5 5	0	0
60	1V	4	Total O 4 4	0	0
60	1W	5	Total O 5 5	0	0
60	1X	4	Total O 4 4	0	0
60	1Y	5	Total O 5 5	0	0
60	1Z	1	Total O 1 1	0	0
60	10	4	Total O 4 4	0	0
60	11	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	12	2	Total O 2 2	0	0
60	13	1	Total O 1 1	0	0
60	14	1	Total O 1 1	0	0
60	15	1	Total O 1 1	0	0
60	16	3	Total O 3 3	0	0
60	17	3	Total O 3 3	0	0
60	18	2	Total O 2 2	0	0
60	19	1	Total O 1 1	0	0
60	1a	371	Total O 371 371	0	0
60	1d	4	Total O 4 4	0	0
60	1e	4	Total O 4 4	0	0
60	1f	2	Total O 2 2	0	0
60	1h	1	Total O 1 1	0	0
60	1i	2	Total O 2 2	0	0
60	1j	1	Total O 1 1	0	0
60	1k	1	Total O 1 1	0	0
60	1l	3	Total O 3 3	0	0
60	1m	2	Total O 2 2	0	0
60	1n	1	Total O 1 1	0	0
60	1o	3	Total O 3 3	0	0
60	1p	1	Total O 1 1	0	0

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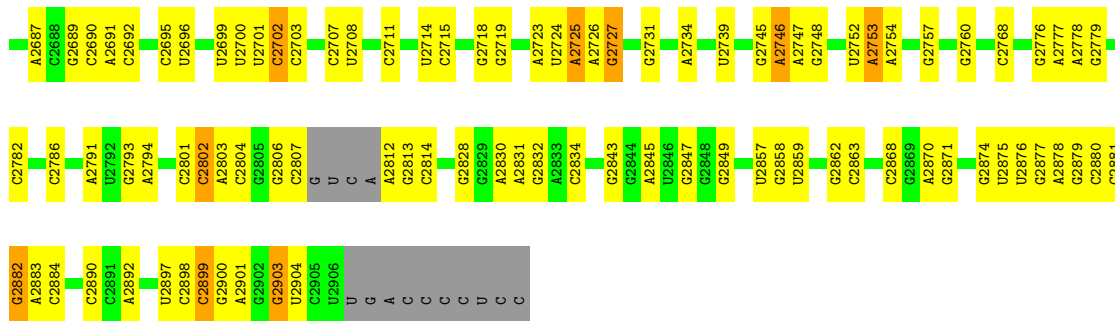
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1s	1	Total O 1 1	0	0
60	1t	1	Total O 1 1	0	0
60	1v	3	Total O 3 3	0	0
60	1w	2	Total O 2 2	0	0
60	1x	16	Total O 16 16	0	0
60	2A	401	Total O 401 401	0	0
60	2B	18	Total O 18 18	0	0
60	2D	6	Total O 6 6	0	0
60	2E	3	Total O 3 3	0	0
60	2F	3	Total O 3 3	0	0
60	2O	1	Total O 1 1	0	0
60	2P	5	Total O 5 5	0	0
60	2R	2	Total O 2 2	0	0
60	2U	2	Total O 2 2	0	0
60	2W	1	Total O 1 1	0	0
60	2X	2	Total O 2 2	0	0
60	2Y	1	Total O 1 1	0	0
60	20	3	Total O 3 3	0	0
60	21	4	Total O 4 4	0	0
60	25	1	Total O 1 1	0	0
60	26	1	Total O 1 1	0	0

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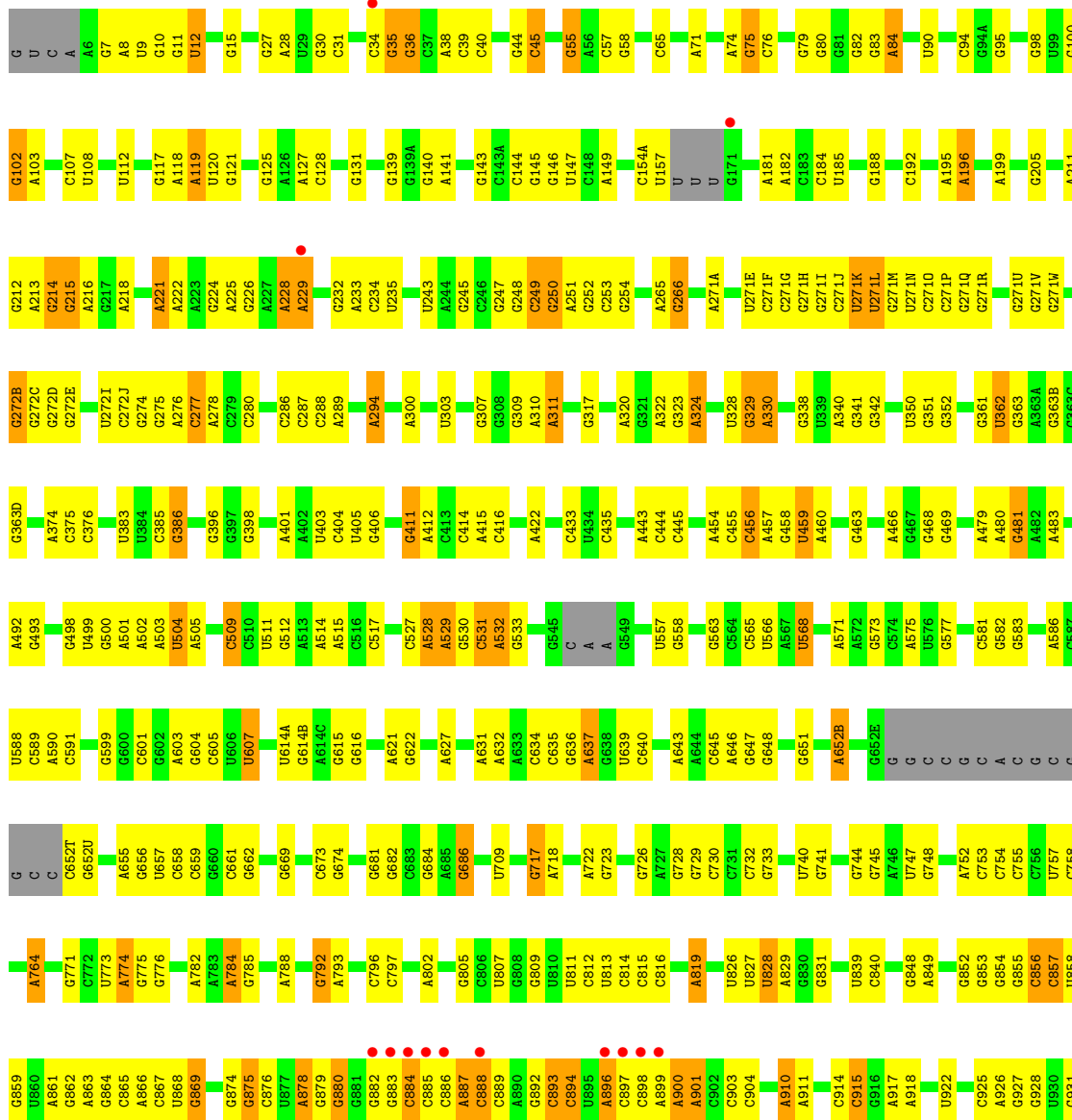
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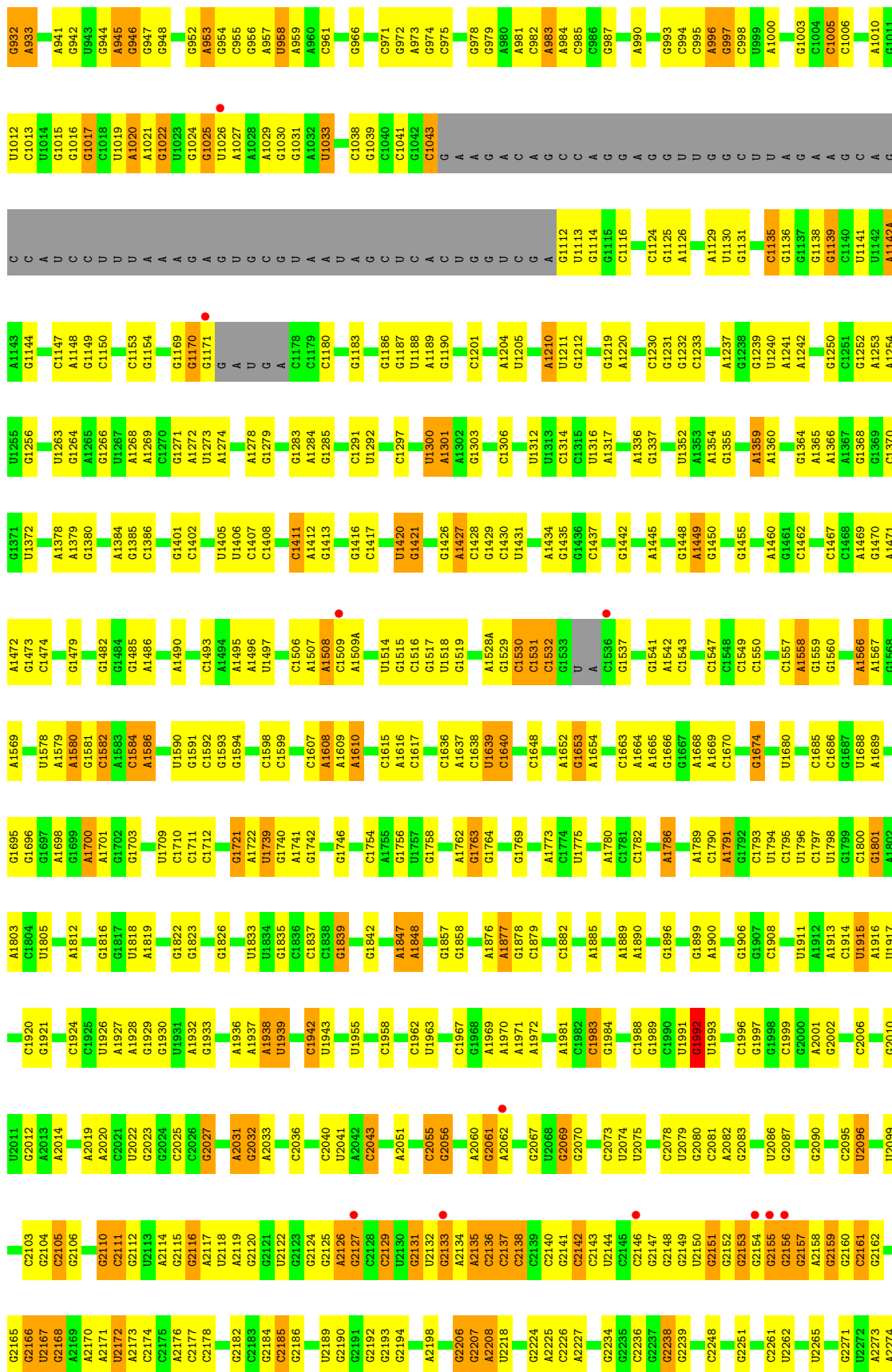
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	27	1	Total O 1 1	0	0
60	28	3	Total O 3 3	0	0
60	29	1	Total O 1 1	0	0
60	2a	160	Total O 160 160	0	0
60	2e	2	Total O 2 2	0	0
60	2i	1	Total O 1 1	0	0
60	2l	2	Total O 2 2	0	0
60	2m	2	Total O 2 2	0	0
60	2o	1	Total O 1 1	0	0
60	2t	3	Total O 3 3	0	0
60	2w	1	Total O 1 1	0	0
60	2x	2	Total O 2 2	0	0

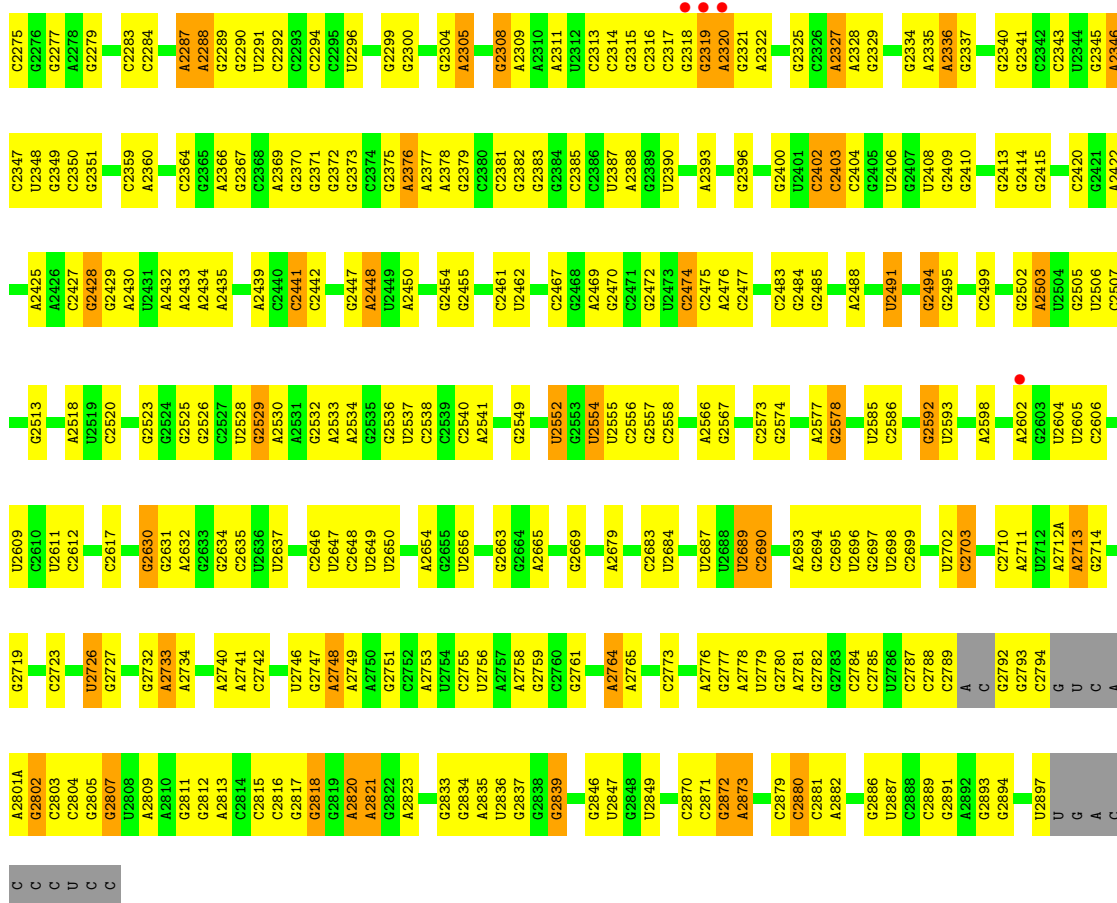
C1138	C1139	C1140	C1141	C1142	C1143	U1147	C1148	C1149	C1150	C1151	C1152	C1153	U1154	C1155	C1156	C1157	C1158	C1159	C1160	C1161	C1162	C1163	G1168	G1171	C1172	C1173	C1174	C1175	C1176	C1177	C1180	C1181	C1182	C1183	U1186	U1187	C1188	C1189	G1197	C1198	C1199	C1200	A1201	A1202	G1210	U1211	C1212	C1216	U1217	C1218																																																																																																																																																		
A1219	U1220	G1221	A1222	C1223	C1224	G1228	C1231	C1232	C1233	C1236	C1246	A1255	C1263	A1265	C1270	G1275	G1282	A1283	A1288	A1293	G1296	C1297	G1298	A1299	G1302	G1310	A1311	C1312	U1313	U1314	A1315	C1316	G1317	A1318	U1319	A1320	A1321	A1324	G1327	U1338	C1339	U1340	C1341	U1346	A1347	G1355	C1356	C1361	U1362	A1363	C1366	C1367	A1368	C1379	G1383	A1384	C1391	U1398	A1400	G1401	G1404	A1405	A1406	G1410	A1411	A1412	A1413	U1418	A1419	A1425	G1426	A1430	G1431	A1438	U1439	A1440	A1441	U1442	C1445	G1446	G1447	U1451	U1452	C1453	G1459	G1460																																																																																																														
U1461	G1462	C1463	C1464	U1465	C1467	C1468	A1469	C1470	C1471	G1472	A1473	C1474	C1476	A1491	G1495	A1496	G1497	U1501	G1502	G1513	C1514	C1515	A1516	G1529	C1538	C1539	C1552	A1554	A1555	A1556	U1560	C1561	U1562	U1566	C1567	G1572	G1573	A1574	A1575	G1579	G	U	A	C	G1584	A1589	C1593	C1604	A1605	G1606	A1613	A1614	G1615	A1616	U1625	A1626	A1627	G1628	C1631	A1632	A1633	C1634	C1635	G1639	G1640	C1653	A1654	A1655	A1656	A1662	C1663	A1679	G1682	U1686	C1687	A1688	G1689	C1695	A1702	A1715	A1716	C1717	G1721	U1727	C1730	A1731	C1732																																																																																																													
C1733	G1734	U1735	U1740	G1743	A1747	U1748	G1749	G1750	C1757	G1764	A1767	C1775	G1781	C1785	A1786	G1787	U1788	G1789	A1790	G1794	G1795	A1804	G1807	U1808	U1809	U1810	A1811	C1812	C1813	A1814	A1815	A1816	A1817	C1821	A1822	U1825	C1826	U1827	U1828	U1829	U1830	C1831	A1832	A1833	A1834	U1835	U1836	U1837	U1838	U1839	U1840	A1841	C1842	A1843	C1844	C1845	C1846	C1847	A1848	C1849	C1850	C1851	C1852	U1853	A1854	G1855	C1856	C1857	C1858	C1859	C1860	C1861	C1862	A1863	A1864	U1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	C1900	C1901	C1902	C1903	C1904	C1905	A1911	A1912	G1921	A1922	G1925	G1928	U1933	A1934	A1935	C1936	U1937	U1938	U1939	A1940	A1941	C1942	G1943	G1951	U1952	U1953	A1954	G1955	C1956	C1959	C1960	C1961																																																						
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• Molecule 1: 23S Ribosomal RNA



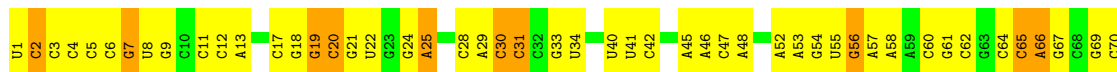
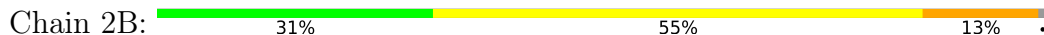




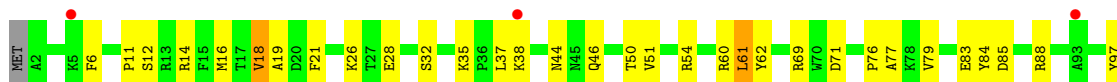
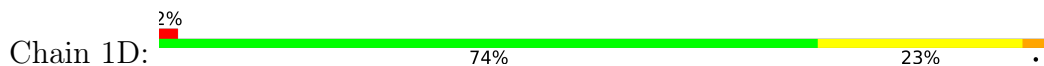
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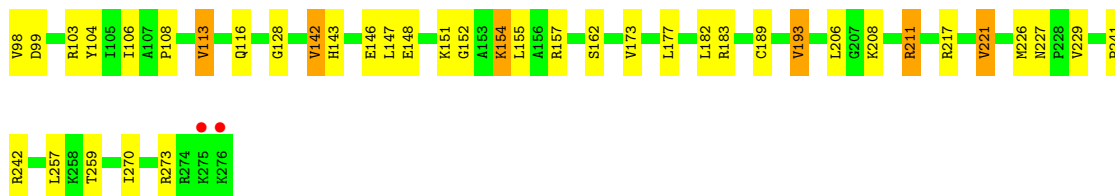


• Molecule 2: 5S Ribosomal RNA

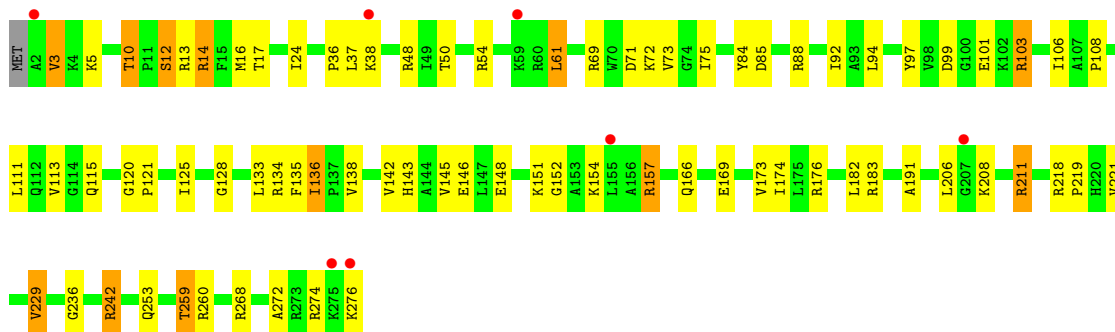
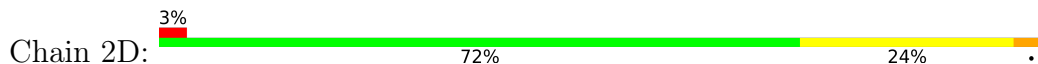


• Molecule 3: 50S ribosomal protein L2

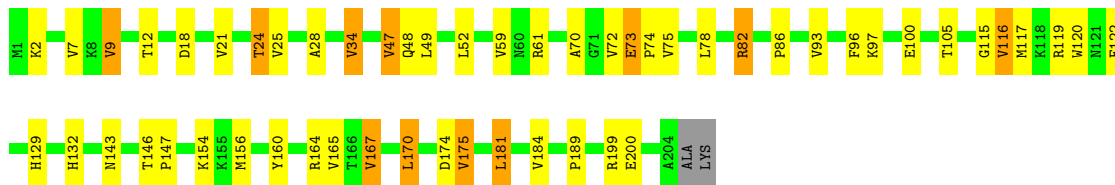




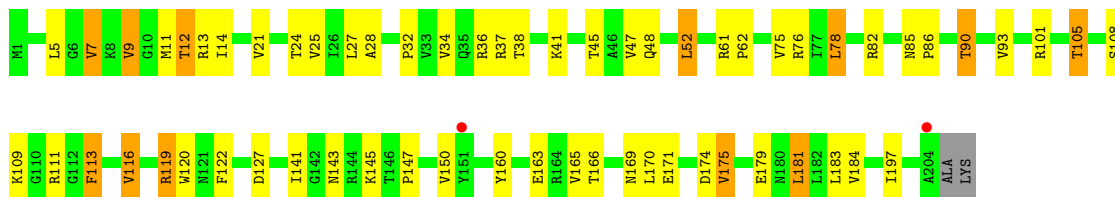
- Molecule 3: 50S ribosomal protein L2



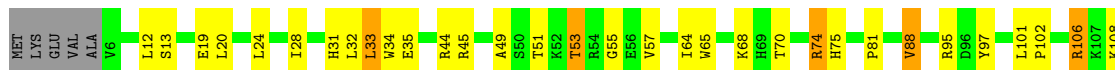
- Molecule 4: 50S ribosomal protein L3

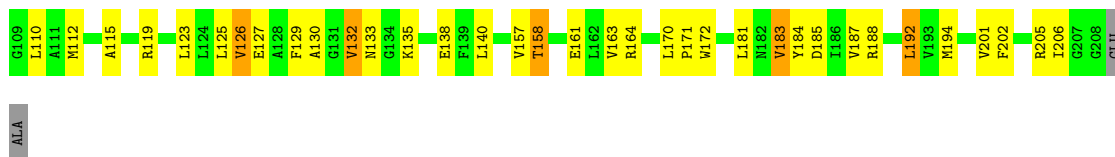


- Molecule 4: 50S ribosomal protein L3

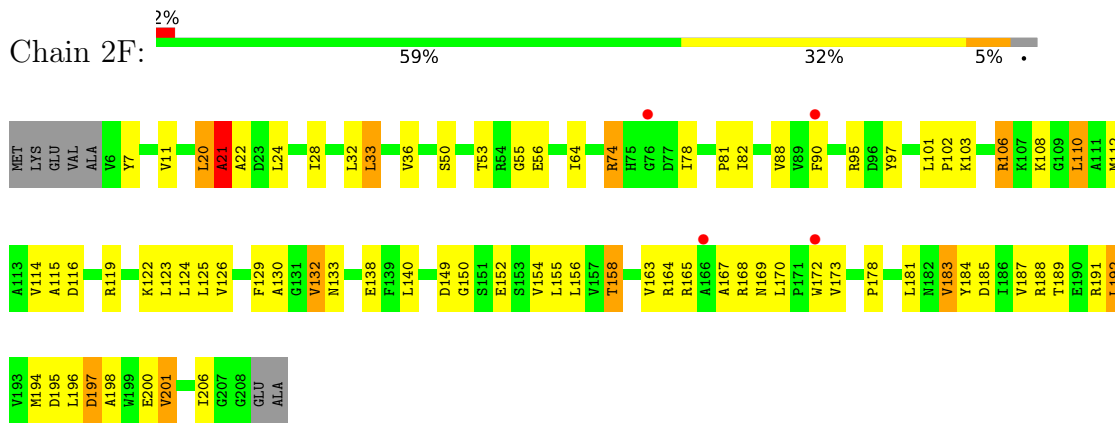


- Molecule 5: 50S ribosomal protein L4

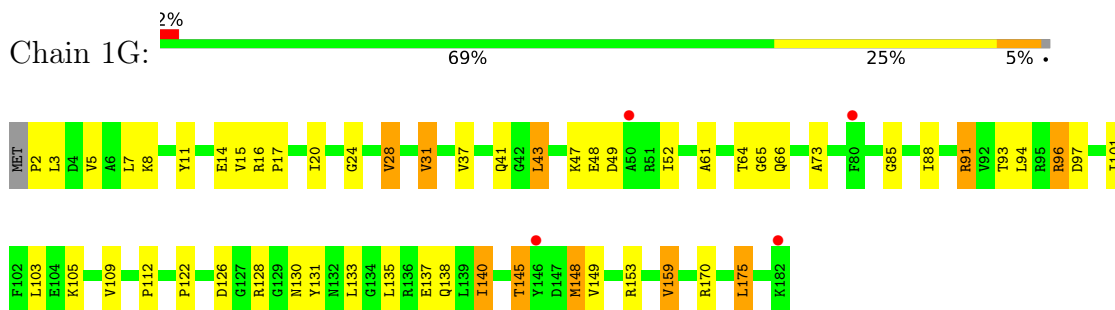




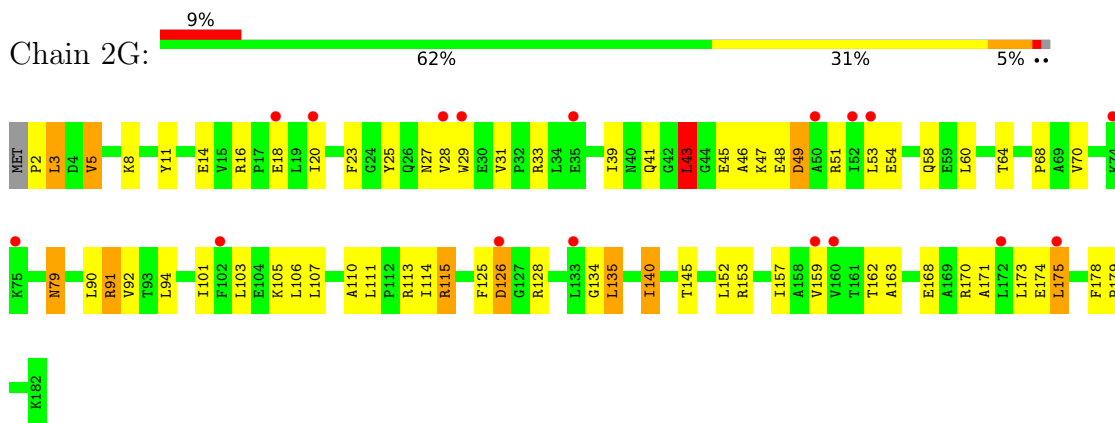
• Molecule 5: 50S ribosomal protein L4



• Molecule 6: 50S ribosomal protein L5

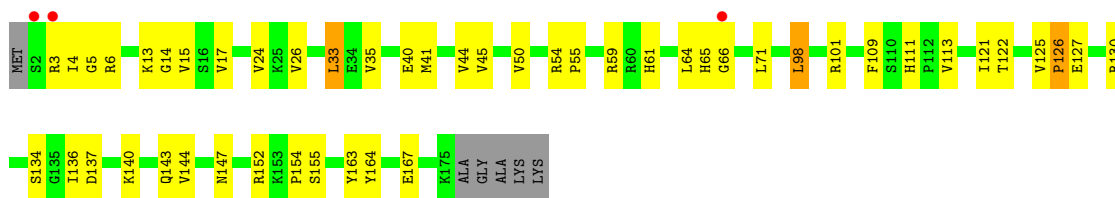


• Molecule 6: 50S ribosomal protein L5

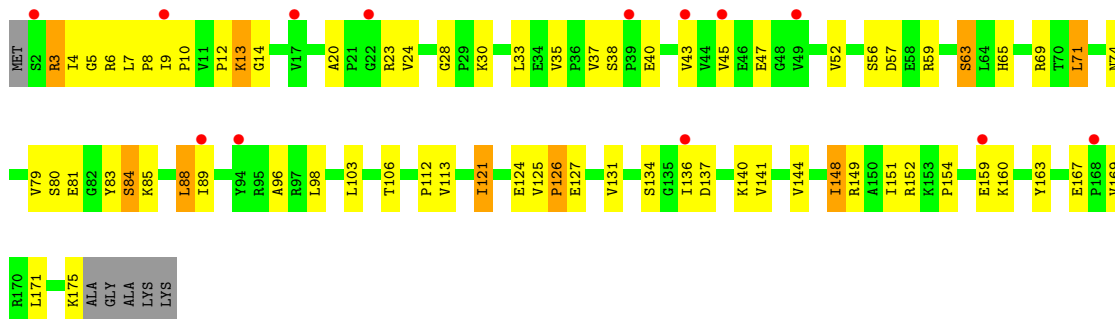


• Molecule 7: 50S ribosomal protein L6

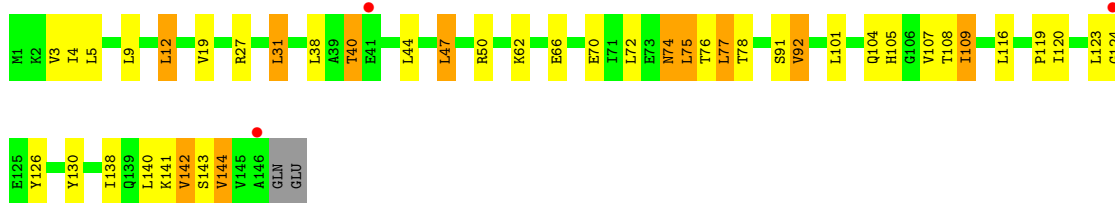




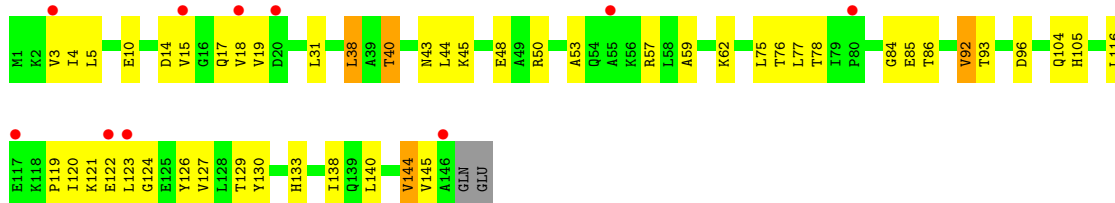
- Molecule 7: 50S ribosomal protein L6



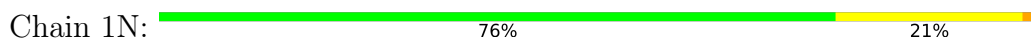
- Molecule 8: 50S ribosomal protein L9

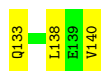


- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13

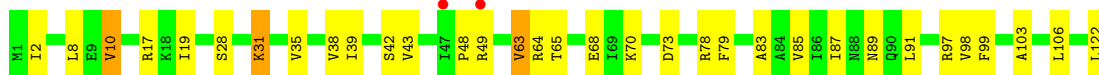
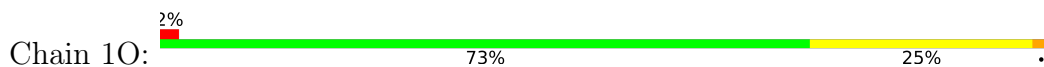




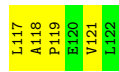
• Molecule 9: 50S ribosomal protein L13



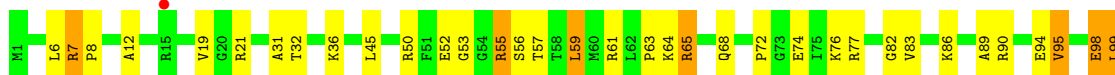
• Molecule 10: 50S ribosomal protein L14



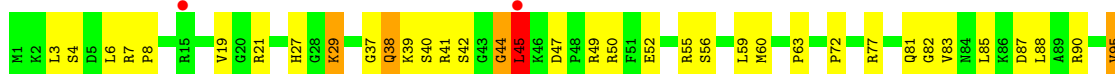
• Molecule 10: 50S ribosomal protein L14



• Molecule 11: 50S ribosomal protein L15

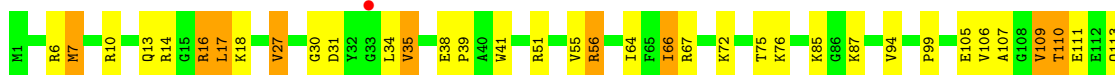


• Molecule 11: 50S ribosomal protein L15

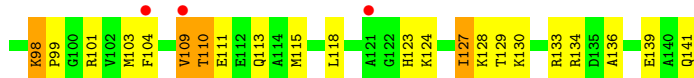
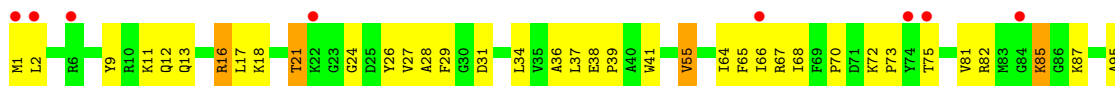




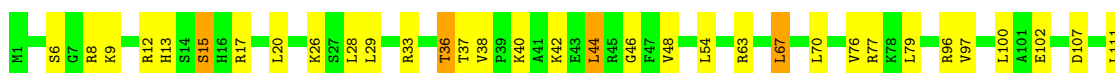
- Molecule 12: 50S ribosomal protein L16



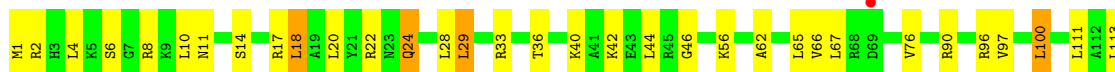
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17

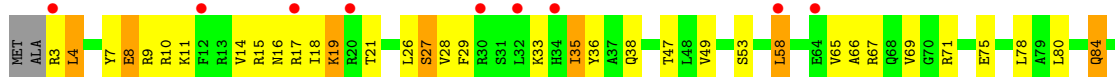


- Molecule 14: 50S ribosomal protein L18

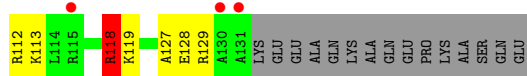




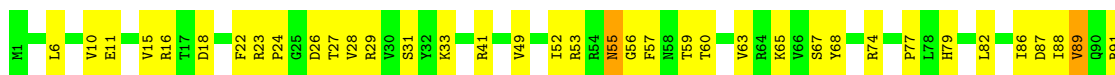
- Molecule 14: 50S ribosomal protein L18



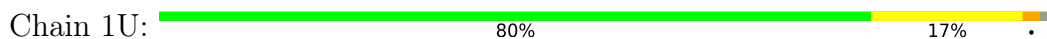
- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



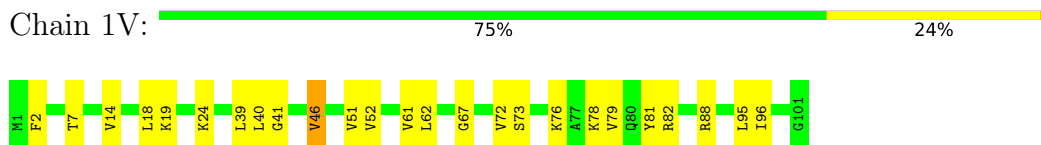
- Molecule 16: 50S ribosomal protein L20



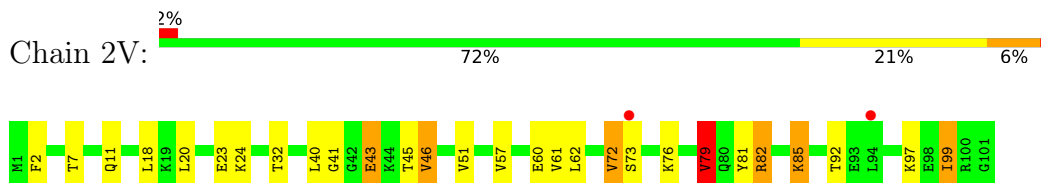
- Molecule 16: 50S ribosomal protein L20



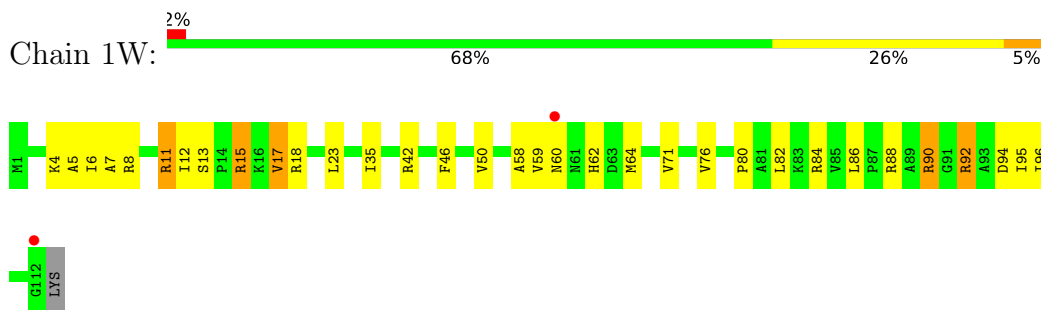
- Molecule 17: 50S ribosomal protein L21



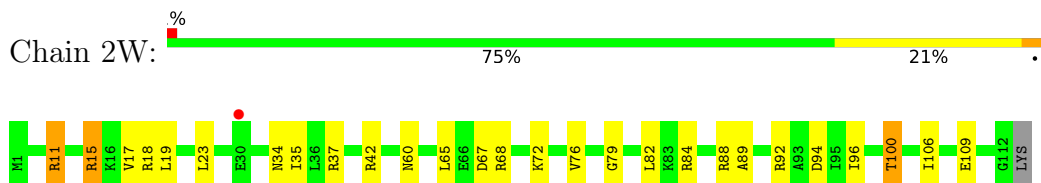
- Molecule 17: 50S ribosomal protein L21



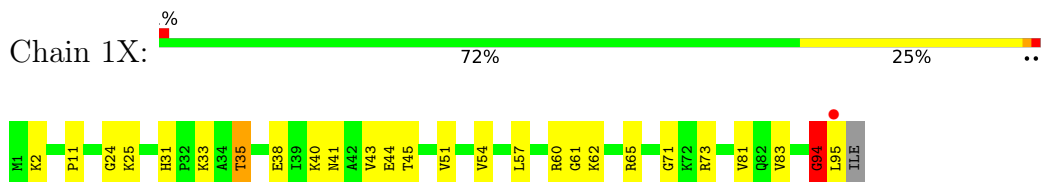
- Molecule 18: 50S ribosomal protein L22



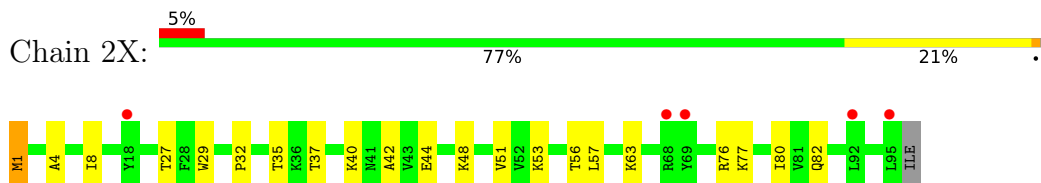
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



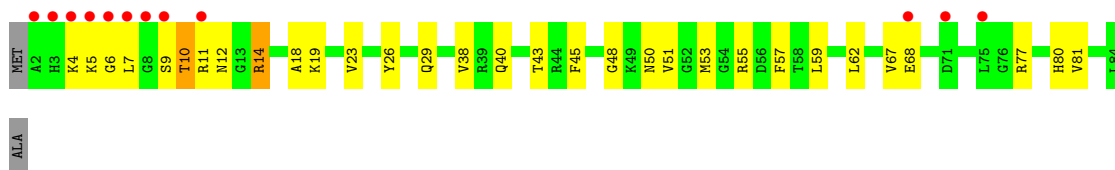
- Molecule 19: 50S ribosomal protein L23



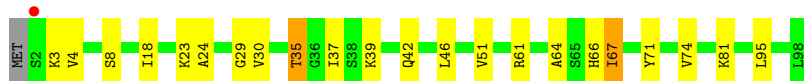
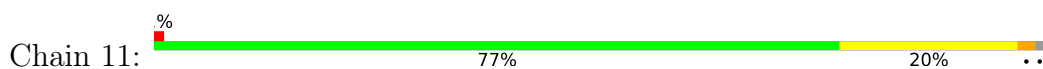
- Molecule 20: 50S ribosomal protein L24



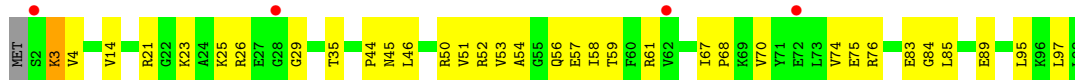
- Molecule 22: 50S ribosomal protein L27



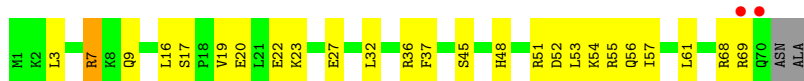
- Molecule 23: 50S ribosomal protein L28



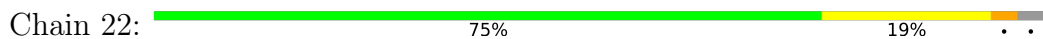
- Molecule 23: 50S ribosomal protein L28



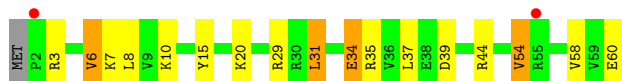
- Molecule 24: 50S ribosomal protein L29



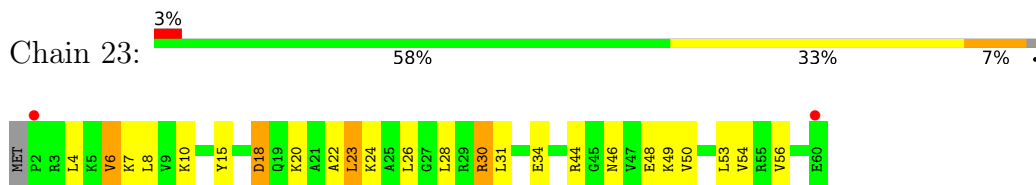
- Molecule 24: 50S ribosomal protein L29



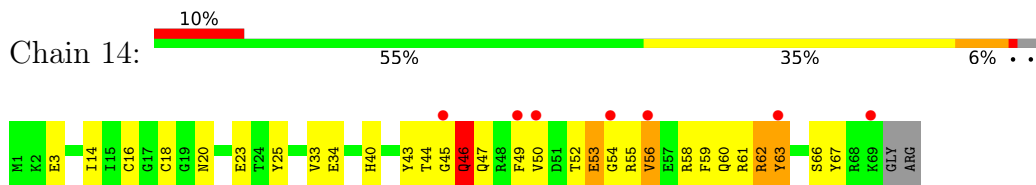
- Molecule 25: 50S ribosomal protein L30



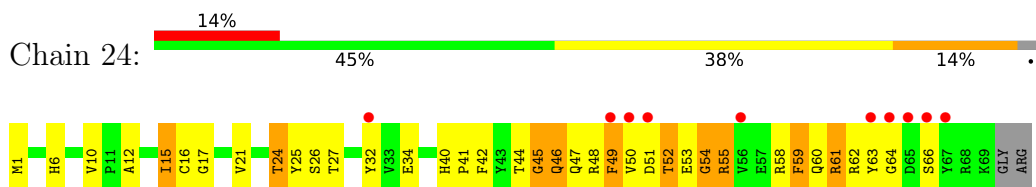
- Molecule 25: 50S ribosomal protein L30



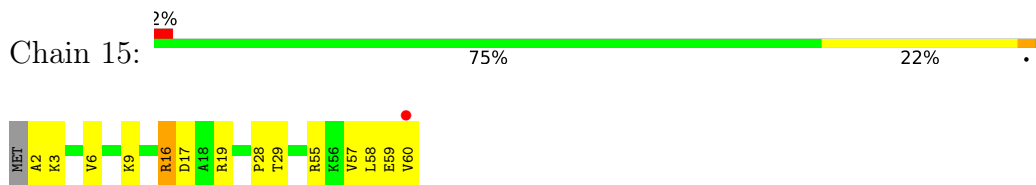
- Molecule 26: 50S ribosomal protein L31



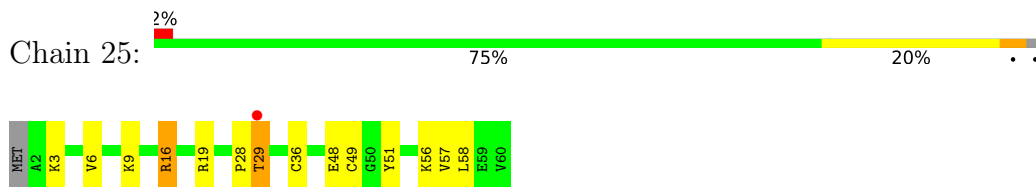
- Molecule 26: 50S ribosomal protein L31



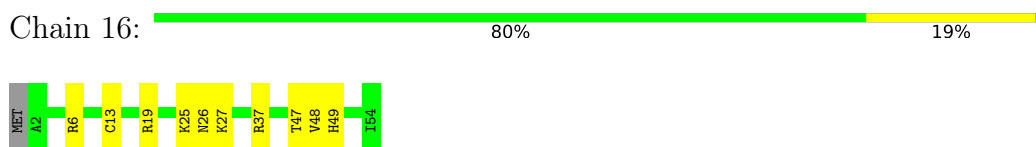
- Molecule 27: 50S ribosomal protein L32



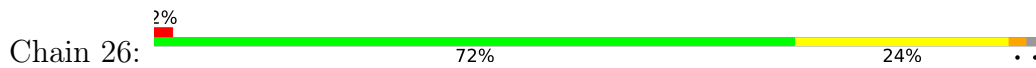
- Molecule 27: 50S ribosomal protein L32

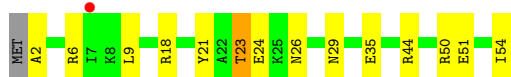


- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33





- Molecule 29: 50S ribosomal protein L34



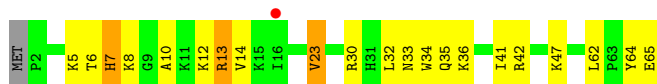
- Molecule 29: 50S ribosomal protein L34



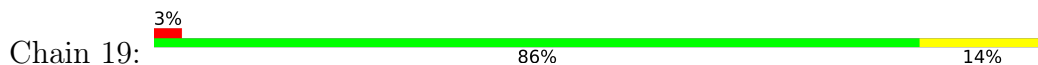
- Molecule 30: 50S ribosomal protein L35



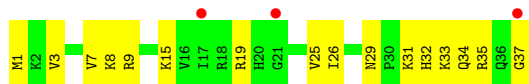
- Molecule 30: 50S ribosomal protein L35



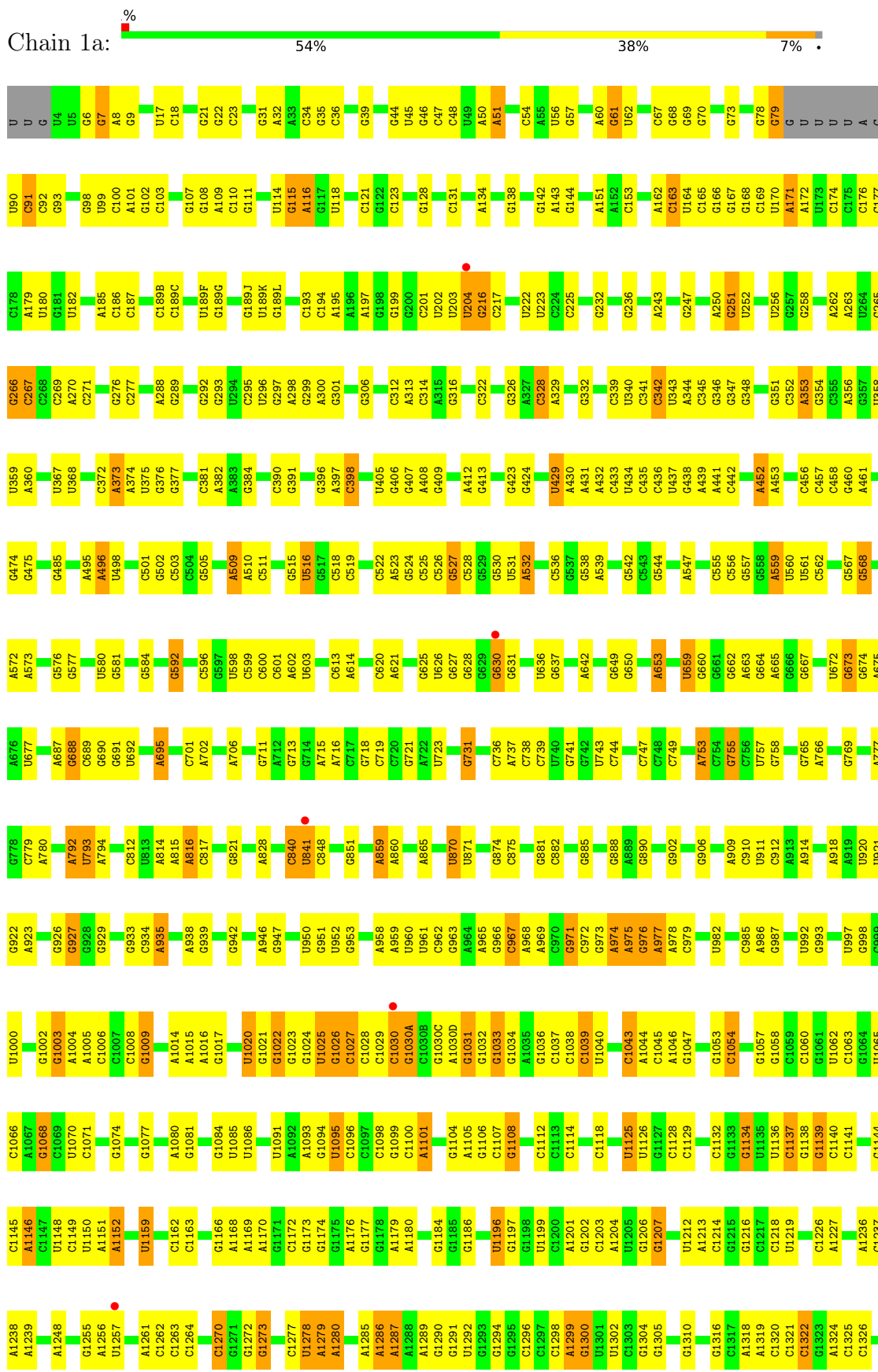
- Molecule 31: 50S ribosomal protein L36

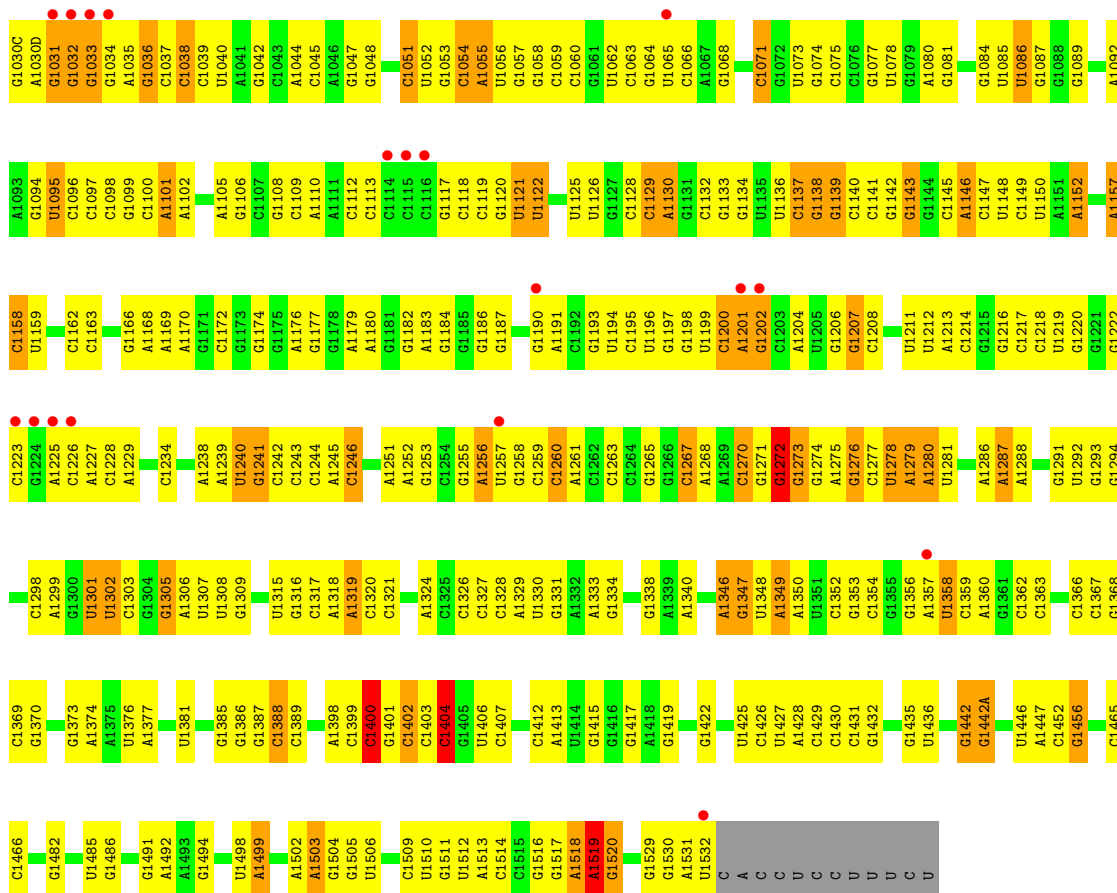


- Molecule 31: 50S ribosomal protein L36

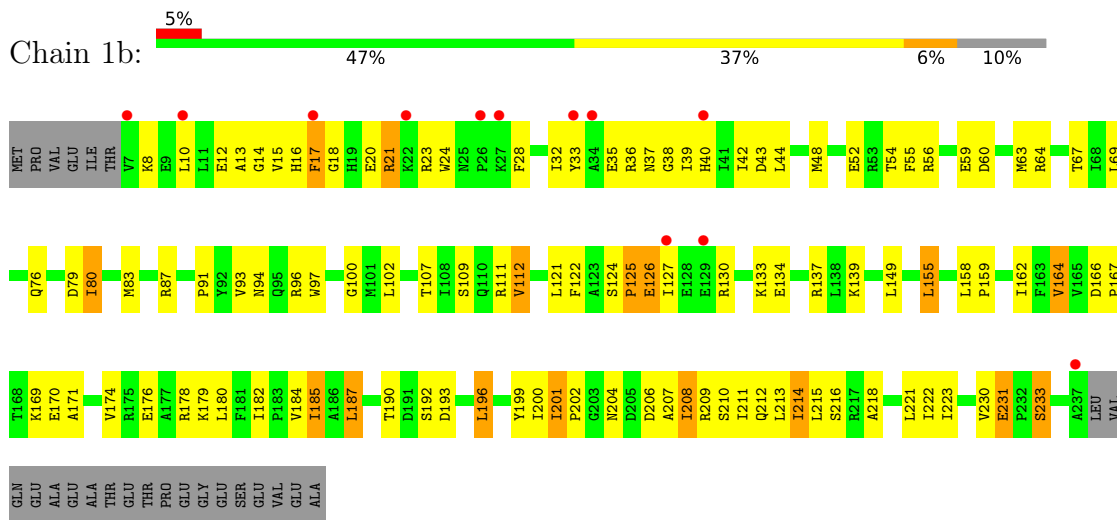


- Molecule 32: 16S Ribosomal RNA

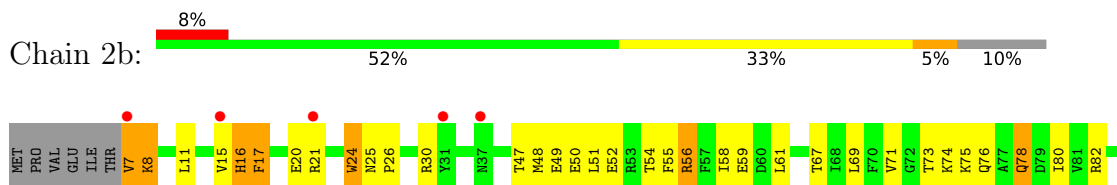


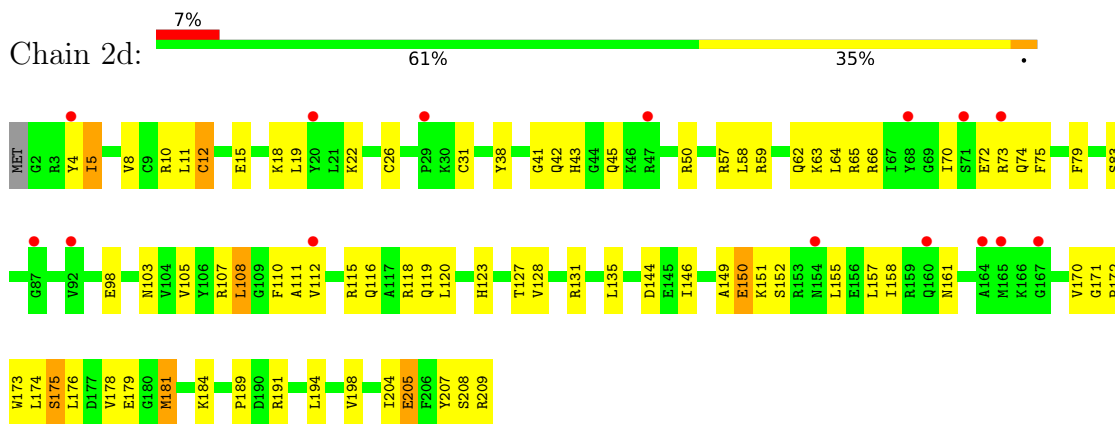


• Molecule 33: 30S ribosomal protein S2

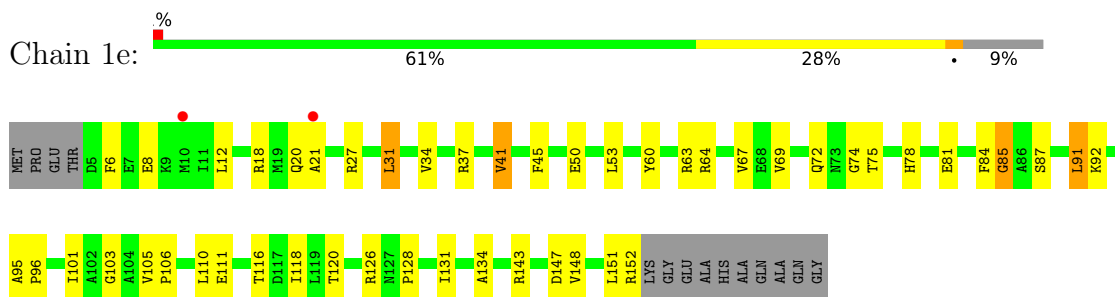


• Molecule 33: 30S ribosomal protein S2

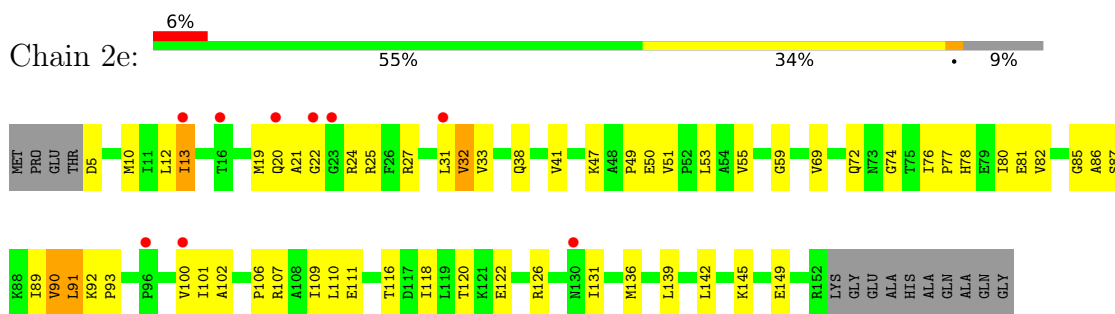




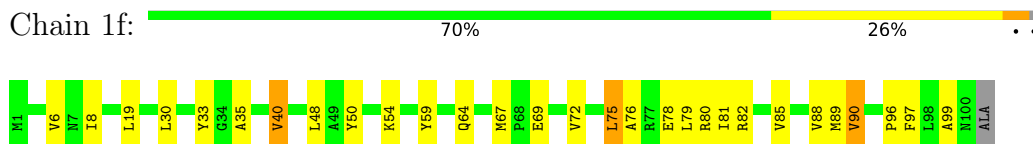
- Molecule 36: 30S ribosomal protein S5



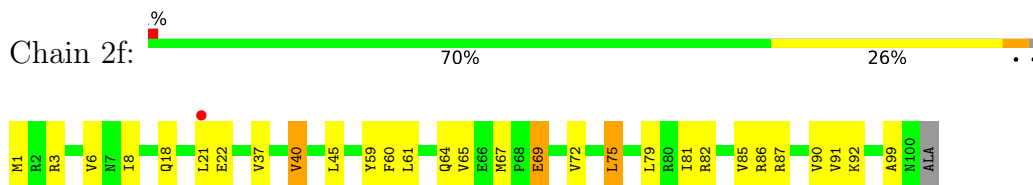
- Molecule 36: 30S ribosomal protein S5



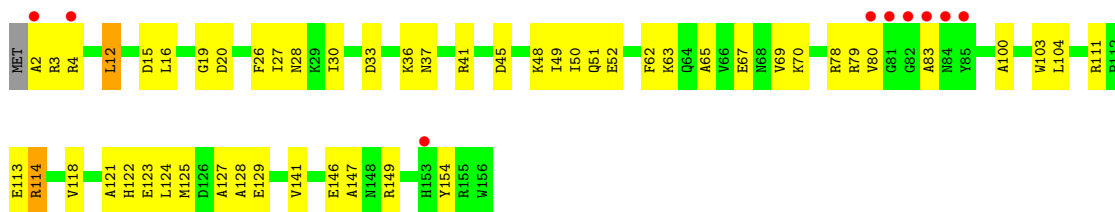
- Molecule 37: 30S ribosomal protein S6



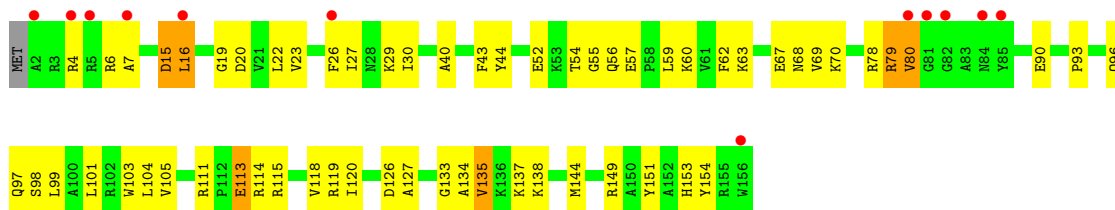
- Molecule 37: 30S ribosomal protein S6



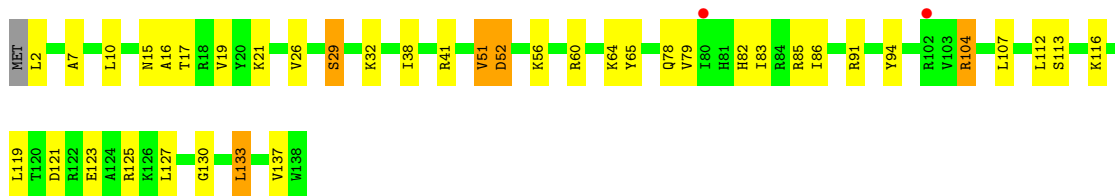
- Molecule 38: 30S ribosomal protein S7



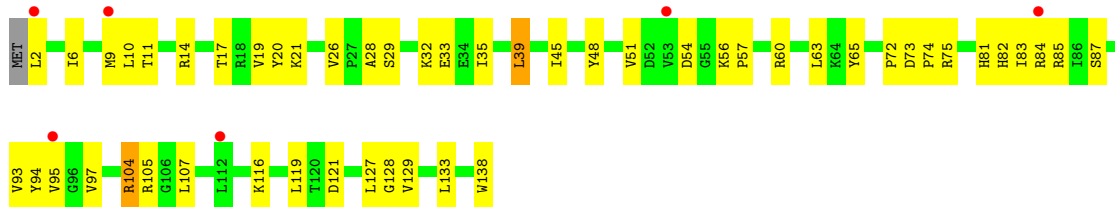
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8



- Molecule 39: 30S ribosomal protein S8

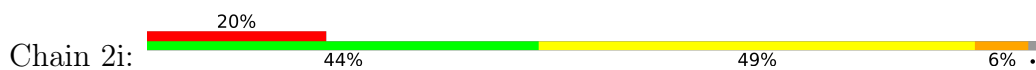


- Molecule 40: 30S ribosomal protein S9

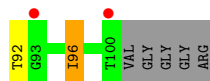
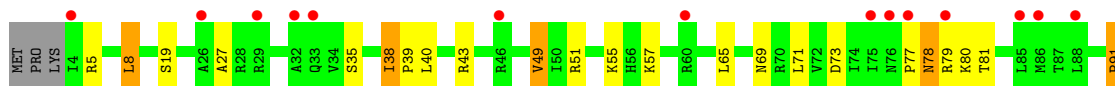




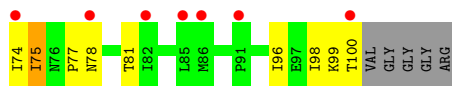
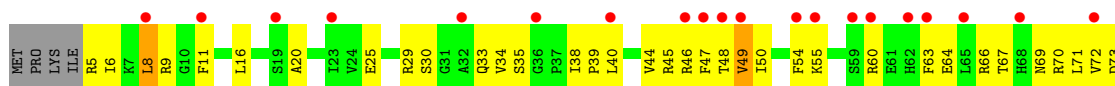
- Molecule 40: 30S ribosomal protein S9



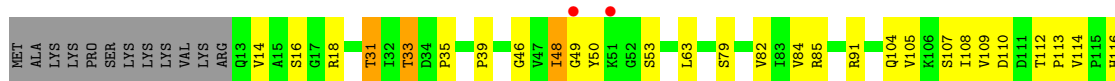
- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10

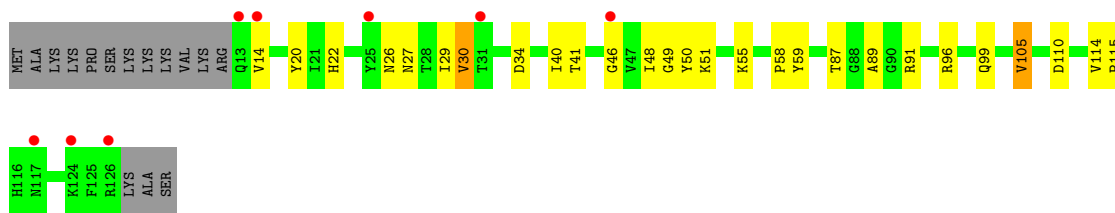


- Molecule 42: 30S ribosomal protein S11

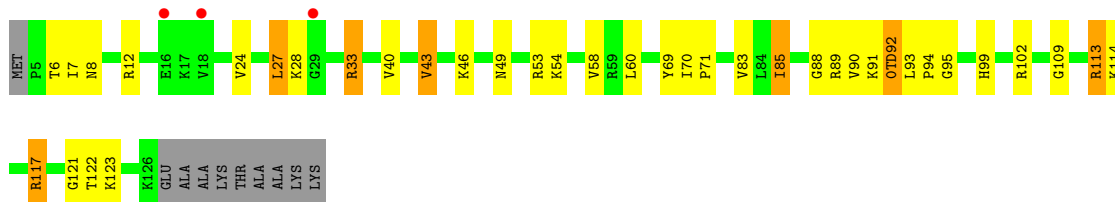


- Molecule 42: 30S ribosomal protein S11

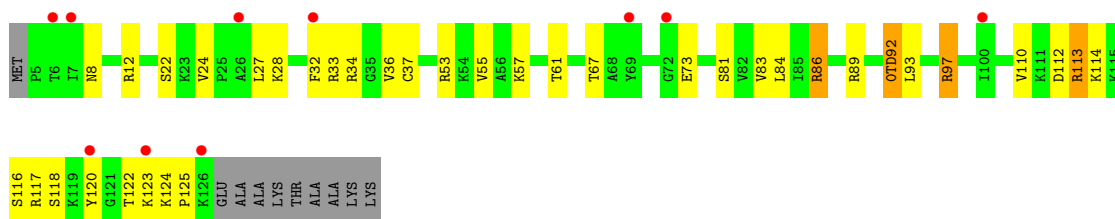




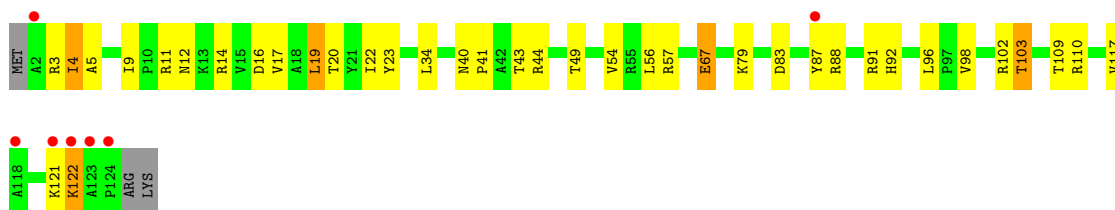
- Molecule 43: 30S ribosomal protein S12



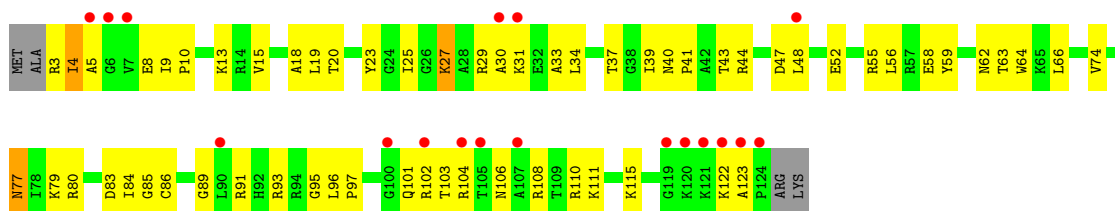
- Molecule 43: 30S ribosomal protein S12



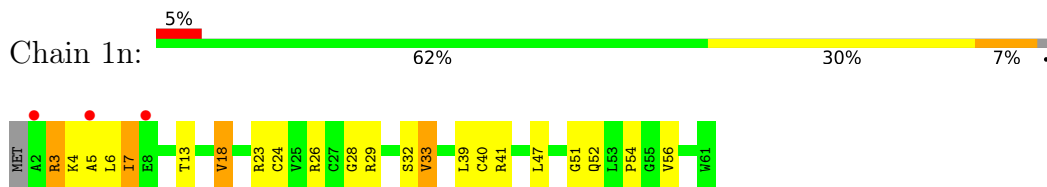
- Molecule 44: 30S ribosomal protein S13



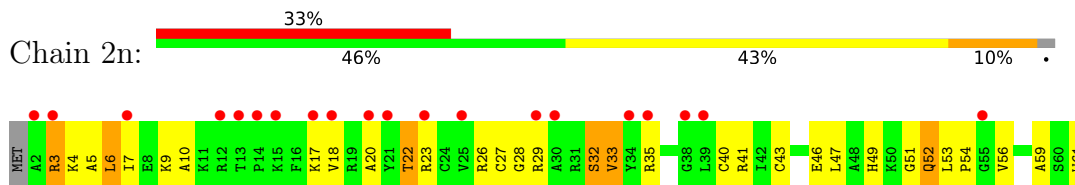
- Molecule 44: 30S ribosomal protein S13



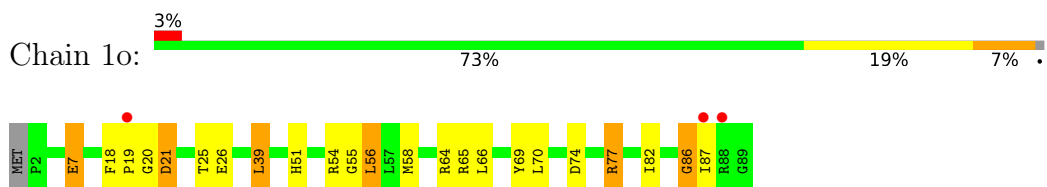
- Molecule 45: 30S ribosomal protein S14 type Z



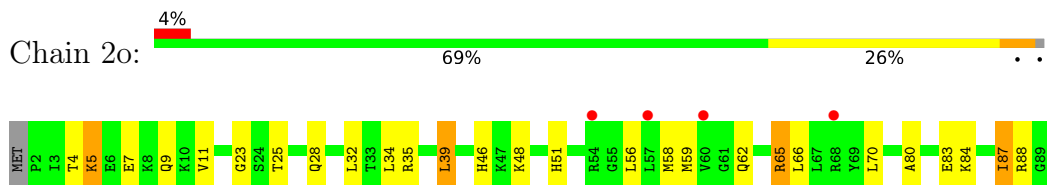
- Molecule 45: 30S ribosomal protein S14 type Z



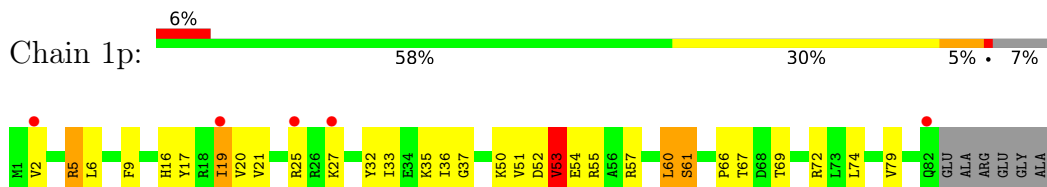
- Molecule 46: 30S ribosomal protein S15



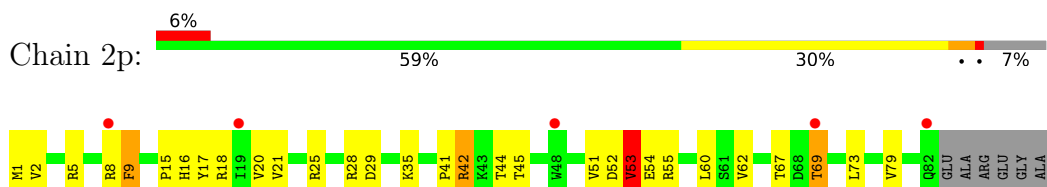
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

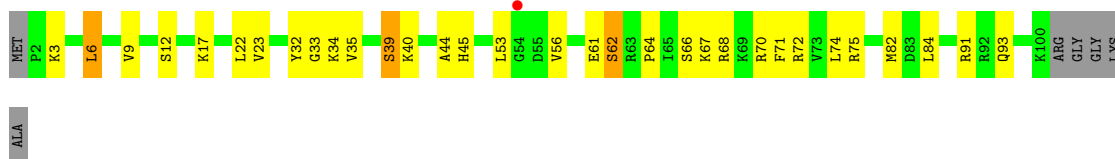


- Molecule 47: 30S ribosomal protein S16

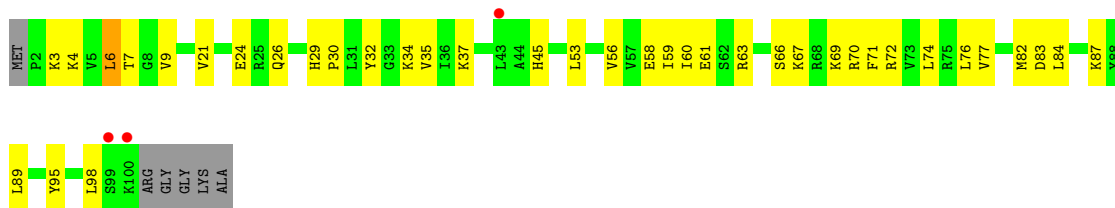


- Molecule 48: 30S ribosomal protein S17

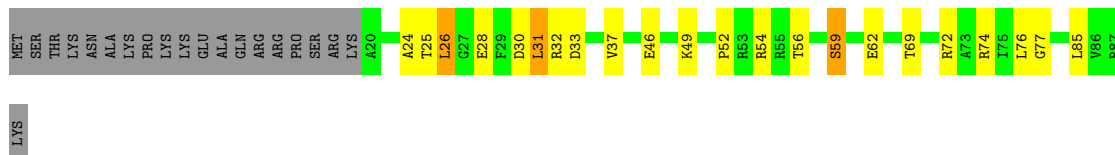




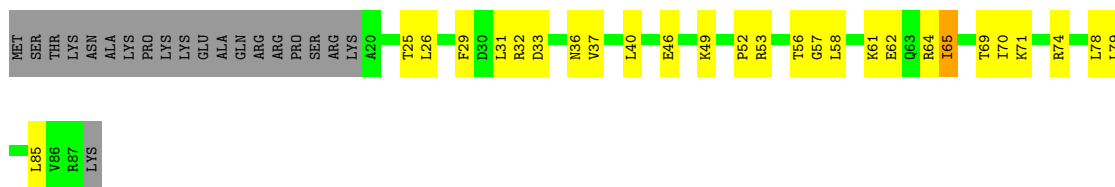
• Molecule 48: 30S ribosomal protein S17



• Molecule 49: 30S ribosomal protein S18



• Molecule 49: 30S ribosomal protein S18



• Molecule 50: 30S ribosomal protein S19

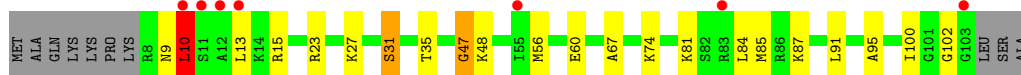


• Molecule 50: 30S ribosomal protein S19

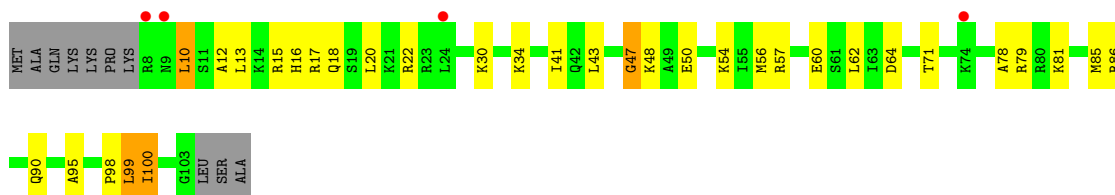




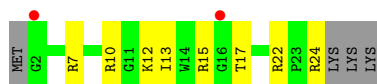
• Molecule 51: 30S ribosomal protein S20



• Molecule 51: 30S ribosomal protein S20



• Molecule 52: 30S ribosomal protein Thx



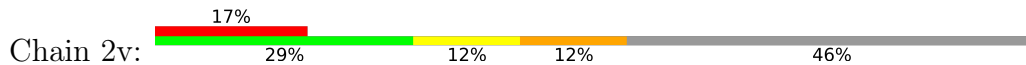
• Molecule 52: 30S ribosomal protein Thx



• Molecule 53: mRNA



• Molecule 53: mRNA





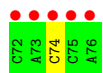
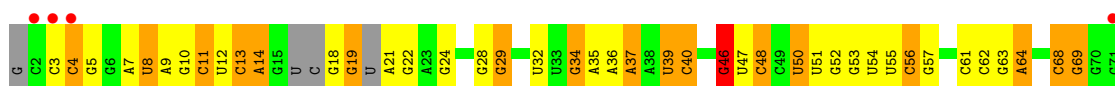
• Molecule 54: A-site and E-site tRNAs



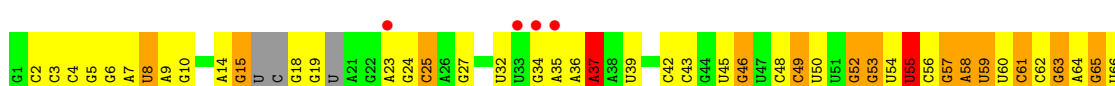
• Molecule 54: A-site and E-site tRNAs



• Molecule 54: A-site and E-site tRNAs

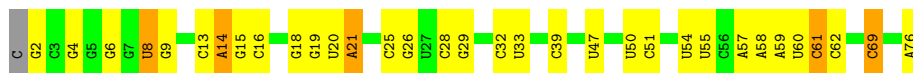


• Molecule 54: A-site and E-site tRNAs



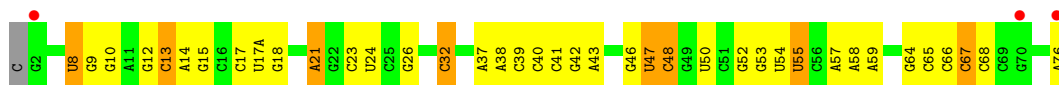
• Molecule 55: P-site tRNA





- Molecule 55: P-site tRNA

Chain 2x: 4% 48% 40% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.36Å 447.53Å 617.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.88 – 2.89 152.88 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.5 (152.88-2.89) 98.5 (152.88-2.89)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.216 , 0.263 0.217 , 0.262	Depositor DCC
R_{free} test set	63210 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtrriage
Anisotropy	0.207	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	297628	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 4SU, OMG, MIA, MG, M2G, SF4, 2MG, KAN, UR3, PSU, ZN, 5MC, 2MU, MA6, 4OC, 7MG, 2MA, 0TD

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	0/69009	0.44	2/107712 (0.0%)
1	2A	0.21	0/67293	0.40	1/105034 (0.0%)
2	1B	0.22	0/2882	0.40	0/4494
2	2B	0.20	0/2879	0.38	0/4487
3	1D	0.28	0/2186	0.52	0/2944
3	2D	0.25	0/2186	0.51	0/2944
4	1E	0.27	0/1592	0.50	0/2149
4	2E	0.30	1/1592 (0.1%)	0.44	0/2149
5	1F	0.27	0/1619	0.50	0/2193
5	2F	0.22	0/1615	0.49	2/2188 (0.1%)
6	1G	0.23	0/1448	0.51	1/1957 (0.1%)
6	2G	0.26	0/1453	0.51	2/1963 (0.1%)
7	1H	0.24	0/1356	0.42	0/1834
7	2H	0.22	0/1356	0.41	0/1834
8	1I	0.19	0/1112	0.39	0/1514
8	2I	0.20	0/1079	0.42	0/1475
9	1N	0.25	0/1144	0.46	0/1543
9	2N	0.19	0/1144	0.41	0/1543
10	1O	0.26	0/943	0.48	0/1269
10	2O	0.22	0/943	0.48	0/1269
11	1P	0.26	0/1152	0.50	0/1533
11	2P	0.24	0/1152	0.52	2/1533 (0.1%)
12	1Q	0.28	0/1143	0.49	0/1527
12	2Q	0.21	0/1143	0.44	0/1527
13	1R	0.27	0/982	0.48	0/1312
13	2R	0.22	0/982	0.49	0/1312
14	1S	0.21	0/883	0.45	0/1176
14	2S	0.21	0/880	0.46	0/1172
15	1T	0.24	0/1105	0.51	0/1477
15	2T	0.23	0/1097	0.44	0/1468
16	1U	0.29	0/977	0.48	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.40	0/1301
17	1V	0.25	0/782	0.48	0/1049
17	2V	0.19	0/782	0.44	0/1049
18	1W	0.28	0/897	0.47	0/1205
18	2W	0.20	0/897	0.40	0/1205
19	1X	0.30	0/764	0.54	2/1025 (0.2%)
19	2X	0.19	0/764	0.45	0/1025
20	1Y	0.23	0/819	0.46	0/1095
20	2Y	0.19	0/819	0.44	0/1095
21	1Z	0.23	0/1267	0.52	0/1717
21	2Z	0.23	0/1299	0.44	1/1763 (0.1%)
22	10	0.28	0/662	0.54	0/881
22	20	0.23	0/662	0.45	0/881
23	11	0.32	1/762 (0.1%)	0.47	0/1014
23	21	0.23	0/762	0.43	0/1014
24	12	0.31	0/590	0.50	1/781 (0.1%)
24	22	0.20	0/590	0.40	0/781
25	13	0.28	0/474	0.48	0/635
25	23	0.19	0/469	0.41	0/630
26	14	0.25	0/565	0.61	0/761
26	24	0.28	0/545	0.65	1/737 (0.1%)
27	15	0.27	0/469	0.47	0/635
27	25	0.24	0/469	0.45	0/635
28	16	0.26	0/460	0.49	0/613
28	26	0.21	0/456	0.45	0/608
29	17	0.29	0/426	0.47	0/561
29	27	0.26	0/426	0.57	0/561
30	18	0.26	0/525	0.49	0/691
30	28	0.22	0/525	0.39	0/691
31	19	0.28	0/310	0.51	0/407
31	29	0.20	0/310	0.47	0/407
32	1a	0.21	0/35795	0.40	5/55864 (0.0%)
32	2a	0.20	0/35886	0.38	1/56005 (0.0%)
33	1b	0.22	0/1881	0.50	0/2542
33	2b	0.23	0/1860	0.52	2/2518 (0.1%)
34	1c	0.20	0/1572	0.41	0/2126
34	2c	0.22	0/1566	0.45	0/2119
35	1d	0.21	0/1685	0.45	0/2262
35	2d	0.19	0/1704	0.47	0/2284
36	1e	0.22	0/1145	0.47	0/1543
36	2e	0.22	0/1149	0.49	0/1548
37	1f	0.22	0/823	0.41	0/1115
37	2f	0.19	0/829	0.38	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.20	0/1250	0.42	1/1679 (0.1%)
38	2g	0.19	0/1254	0.38	0/1683
39	1h	0.21	0/1108	0.43	0/1494
39	2h	0.19	0/1108	0.42	0/1494
40	1i	0.21	0/1002	0.50	0/1346
40	2i	0.23	0/997	0.52	0/1343
41	1j	0.21	0/722	0.45	0/982
41	2j	0.34	0/727	0.50	0/988
42	1k	0.21	0/844	0.42	0/1145
42	2k	0.23	0/848	0.46	0/1149
43	1l	0.22	0/937	0.46	0/1260
43	2l	0.21	0/937	0.49	1/1260 (0.1%)
44	1m	0.22	0/969	0.48	0/1302
44	2m	0.20	0/961	0.46	0/1291
45	1n	0.21	0/501	0.44	0/664
45	2n	0.25	0/501	0.47	0/664
46	1o	0.19	0/739	0.40	0/985
46	2o	0.18	0/739	0.39	0/985
47	1p	0.20	0/697	0.50	0/939
47	2p	0.19	0/693	0.45	0/935
48	1q	0.20	0/836	0.43	0/1117
48	2q	0.19	0/836	0.38	0/1117
49	1r	0.19	0/560	0.41	0/746
49	2r	0.20	0/560	0.41	0/746
50	1s	0.20	0/667	0.50	0/900
50	2s	0.25	0/661	0.58	0/893
51	1t	0.23	0/730	0.51	0/965
51	2t	0.24	0/729	0.49	0/965
52	1u	0.24	0/203	0.55	0/266
52	2u	0.27	0/203	0.56	0/266
53	1v	0.18	0/310	0.31	0/480
53	2v	0.25	0/310	0.39	0/480
54	1w	0.27	1/1606 (0.1%)	0.45	0/2497
54	1y	0.29	1/1606 (0.1%)	0.44	0/2497
54	2w	0.27	1/1556 (0.1%)	0.41	0/2418
54	2y	0.31	0/1583	0.48	0/2459
55	1x	0.26	0/1725	0.41	0/2689
55	2x	0.26	1/1725 (0.1%)	0.41	0/2689
All	All	0.23	6/316686 (0.0%)	0.43	25/474113 (0.0%)

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

sidechain that are expected to be planar.

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2E	109	LYS	C-N	-8.64	1.29	1.33
54	1y	8	4SU	O3'-P	5.29	1.61	1.56
54	1w	8	4SU	O3'-P	5.17	1.61	1.56
54	2w	8	4SU	O3'-P	5.05	1.61	1.56
55	2x	8	4SU	O3'-P	5.04	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	359	U	OP1-P-OP2	-14.11	77.28	119.60
32	1a	359	U	O5'-P-OP1	-11.14	74.58	108.00
32	1a	358	U	OP2-P-O3'	-10.54	76.39	108.00
32	1a	358	U	OP1-P-O3'	8.76	134.28	108.00
32	1a	359	U	O5'-P-OP2	7.88	131.63	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	8	LYS	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	61852	0	31194	621	0
1	2A	60322	0	30423	738	0
2	1B	2577	0	1305	20	0
2	2B	2575	0	1303	62	0
3	1D	2136	0	2218	49	0
3	2D	2136	0	2218	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1E	1559	0	1618	35	0
4	2E	1559	0	1618	43	0
5	1F	1584	0	1625	45	0
5	2F	1580	0	1619	55	0
6	1G	1423	0	1436	36	0
6	2G	1428	0	1438	48	0
7	1H	1330	0	1407	25	0
7	2H	1330	0	1407	41	0
8	1I	1097	0	1140	28	0
8	2I	1064	0	1082	30	0
9	1N	1117	0	1184	19	0
9	2N	1117	0	1184	29	0
10	1O	933	0	996	26	0
10	2O	933	0	996	25	0
11	1P	1135	0	1212	44	0
11	2P	1135	0	1212	43	0
12	1Q	1122	0	1179	33	0
12	2Q	1122	0	1179	41	0
13	1R	968	0	1033	21	0
13	2R	968	0	1033	26	0
14	1S	873	0	927	17	0
14	2S	870	0	923	34	0
15	1T	1091	0	1151	29	0
15	2T	1083	0	1136	37	0
16	1U	959	0	1019	14	0
16	2U	959	0	1019	24	0
17	1V	771	0	830	11	0
17	2V	771	0	830	15	0
18	1W	886	0	940	24	0
18	2W	886	0	940	14	0
19	1X	750	0	814	21	0
19	2X	750	0	814	13	0
20	1Y	806	0	881	22	0
20	2Y	806	0	881	18	0
21	1Z	1240	0	1240	35	0
21	2Z	1271	0	1273	49	0
22	10	653	0	674	13	0
22	20	653	0	674	20	0
23	11	755	0	826	15	0
23	21	755	0	826	23	0
24	12	588	0	643	15	0
24	22	588	0	643	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	13	469	0	518	9	0
25	23	464	0	514	16	0
26	14	552	0	533	18	0
26	24	532	0	503	32	0
27	15	455	0	465	9	0
27	25	455	0	465	9	0
28	16	453	0	473	6	0
28	26	449	0	469	9	0
29	17	418	0	467	16	0
29	27	418	0	467	12	0
30	18	517	0	582	17	0
30	28	517	0	582	20	0
31	19	307	0	335	2	0
31	29	307	0	335	12	0
32	1a	32246	0	16296	447	0
32	2a	32327	0	16336	557	0
33	1b	1846	0	1867	68	0
33	2b	1825	0	1828	71	0
34	1c	1548	0	1535	31	0
34	2c	1542	0	1517	55	0
35	1d	1655	0	1672	47	0
35	2d	1674	0	1714	54	0
36	1e	1129	0	1185	35	0
36	2e	1133	0	1191	40	0
37	1f	810	0	804	18	0
37	2f	816	0	808	17	0
38	1g	1231	0	1238	35	0
38	2g	1235	0	1249	50	0
39	1h	1088	0	1126	31	0
39	2h	1088	0	1126	36	0
40	1i	983	0	986	27	0
40	2i	978	0	966	61	0
41	1j	709	0	650	20	0
41	2j	714	0	672	34	0
42	1k	829	0	825	15	0
42	2k	833	0	836	18	0
43	1l	932	0	981	26	0
43	2l	932	0	981	23	0
44	1m	958	0	1002	22	0
44	2m	950	0	988	55	0
45	1n	492	0	529	20	0
45	2n	492	0	529	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	1o	728	0	760	15	0
46	2o	728	0	760	20	0
47	1p	681	0	697	24	0
47	2p	677	0	686	22	0
48	1q	823	0	891	24	0
48	2q	823	0	891	25	0
49	1r	555	0	618	13	0
49	2r	555	0	618	17	0
50	1s	652	0	662	16	0
50	2s	646	0	644	30	0
51	1t	728	0	798	13	0
51	2t	727	0	796	18	0
52	1u	199	0	208	8	0
52	2u	199	0	208	9	0
53	1v	277	0	140	3	0
53	2v	277	0	140	7	0
54	1w	1592	0	819	32	0
54	1y	1585	0	804	38	0
54	2w	1544	0	788	31	0
54	2y	1565	0	795	46	0
55	1x	1625	0	829	20	0
55	2x	1625	0	829	23	0
56	10	1	0	0	0	0
56	11	1	0	0	0	0
56	12	1	0	0	0	0
56	13	4	0	0	0	0
56	14	1	0	0	0	0
56	15	3	0	0	0	0
56	16	1	0	0	0	0
56	17	1	0	0	0	0
56	18	4	0	0	0	0
56	19	3	0	0	0	0
56	1A	932	0	0	0	0
56	1B	29	0	0	0	0
56	1D	4	0	0	0	0
56	1E	4	0	0	0	0
56	1F	3	0	0	0	0
56	1G	2	0	0	0	0
56	1N	2	0	0	0	0
56	1O	2	0	0	0	0
56	1P	2	0	0	0	0
56	1Q	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1R	1	0	0	0	0
56	1T	1	0	0	0	0
56	1U	2	0	0	0	0
56	1V	2	0	0	0	0
56	1W	2	0	0	0	0
56	1X	1	0	0	0	0
56	1Y	1	0	0	0	0
56	1a	354	0	0	0	0
56	1d	2	0	0	0	0
56	1e	1	0	0	0	0
56	1i	1	0	0	0	0
56	1k	1	0	0	0	0
56	1l	3	0	0	0	0
56	1m	2	0	0	0	0
56	1o	3	0	0	0	0
56	1q	2	0	0	0	0
56	1r	1	0	0	0	0
56	1v	3	0	0	0	0
56	1w	5	0	0	0	0
56	1x	24	0	0	0	0
56	1y	1	0	0	0	0
56	20	2	0	0	0	0
56	21	1	0	0	0	0
56	23	1	0	0	0	0
56	26	1	0	0	0	0
56	28	2	0	0	0	0
56	2A	567	0	0	0	0
56	2B	13	0	0	0	0
56	2D	3	0	0	0	0
56	2E	2	0	0	0	0
56	2F	4	0	0	0	0
56	2G	1	0	0	0	0
56	2Q	2	0	0	0	0
56	2T	2	0	0	0	0
56	2W	1	0	0	0	0
56	2a	227	0	0	0	0
56	2e	1	0	0	0	0
56	2g	1	0	0	0	0
56	2q	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	2	0	0	0	0
56	2w	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2x	7	0	0	0	0
57	1A	99	0	108	6	0
57	1a	33	0	36	3	0
57	2A	66	0	72	4	0
57	2a	33	0	36	2	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	1	0
59	2d	8	0	0	1	0
60	10	4	0	0	0	0
60	11	4	0	0	1	0
60	12	2	0	0	0	0
60	13	1	0	0	0	0
60	14	1	0	0	1	0
60	15	1	0	0	0	0
60	16	3	0	0	1	0
60	17	3	0	0	0	0
60	18	2	0	0	0	0
60	19	1	0	0	0	0
60	1A	938	0	0	27	0
60	1B	25	0	0	0	0
60	1D	9	0	0	1	0
60	1E	7	0	0	1	0
60	1F	9	0	0	0	0
60	1G	1	0	0	0	0
60	1H	1	0	0	0	0
60	1N	2	0	0	0	0
60	1O	4	0	0	0	0
60	1P	12	0	0	4	0
60	1Q	4	0	0	1	0
60	1R	5	0	0	2	0
60	1S	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1T	8	0	0	3	0
60	1U	5	0	0	0	0
60	1V	4	0	0	0	0
60	1W	5	0	0	1	0
60	1X	4	0	0	1	0
60	1Y	5	0	0	0	0
60	1Z	1	0	0	0	0
60	1a	371	0	0	12	0
60	1d	4	0	0	0	0
60	1e	4	0	0	0	0
60	1f	2	0	0	0	0
60	1h	1	0	0	1	0
60	1i	2	0	0	0	0
60	1j	1	0	0	0	0
60	1k	1	0	0	0	0
60	1l	3	0	0	0	0
60	1m	2	0	0	0	0
60	1n	1	0	0	0	0
60	1o	3	0	0	1	0
60	1p	1	0	0	0	0
60	1s	1	0	0	0	0
60	1t	1	0	0	0	0
60	1v	3	0	0	0	0
60	1w	2	0	0	0	0
60	1x	16	0	0	2	0
60	20	3	0	0	0	0
60	21	4	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	27	1	0	0	0	0
60	28	3	0	0	0	0
60	29	1	0	0	0	0
60	2A	401	0	0	20	0
60	2B	18	0	0	2	0
60	2D	6	0	0	0	0
60	2E	3	0	0	1	0
60	2F	3	0	0	0	0
60	2O	1	0	0	0	0
60	2P	5	0	0	0	0
60	2R	2	0	0	0	0
60	2U	2	0	0	0	0
60	2W	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2X	2	0	0	1	0
60	2Y	1	0	0	0	0
60	2a	160	0	0	11	0
60	2e	2	0	0	0	0
60	2i	1	0	0	0	0
60	2l	2	0	0	0	0
60	2m	2	0	0	0	0
60	2o	1	0	0	0	0
60	2t	3	0	0	0	0
60	2w	1	0	0	0	0
60	2x	2	0	0	0	0
All	All	297628	0	196941	4569	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 10.

The worst 5 of 4569 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:1128:U:H3	1:1A:1132:A:N6	1.28	1.31
32:2a:1399:C:H4'	32:2a:1400:5MC:H5'	1.35	1.07
32:1a:998:G:H1	32:1a:1043:C:N4	1.52	1.06
1:1A:1128:U:O4	1:1A:1132:A:N1	1.88	1.06
1:2A:2138:C:N4	1:2A:2153:G:H1	1.55	1.03

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%)	255 (93%)	18 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2D	273/276 (99%)	252 (92%)	19 (7%)	2 (1%)	18	48
4	1E	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	12	39
4	2E	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	12	39
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	54
5	2F	201/210 (96%)	185 (92%)	13 (6%)	3 (2%)	8	28
6	1G	179/182 (98%)	163 (91%)	14 (8%)	2 (1%)	11	36
6	2G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	21	51
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21	51
7	2H	172/180 (96%)	150 (87%)	19 (11%)	3 (2%)	7	26
8	1I	144/148 (97%)	130 (90%)	14 (10%)	0	100	100
8	2I	144/148 (97%)	121 (84%)	20 (14%)	3 (2%)	5	21
9	1N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
9	2N	138/140 (99%)	128 (93%)	8 (6%)	2 (1%)	9	30
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	7	26
11	1P	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
11	2P	147/150 (98%)	130 (88%)	13 (9%)	4 (3%)	4	16
12	1Q	139/141 (99%)	132 (95%)	5 (4%)	2 (1%)	9	30
12	2Q	139/141 (99%)	127 (91%)	11 (8%)	1 (1%)	18	48
13	1R	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	14	41
13	2R	116/118 (98%)	103 (89%)	12 (10%)	1 (1%)	14	41
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	6	23
15	1T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	16	44
15	2T	129/146 (88%)	120 (93%)	6 (5%)	3 (2%)	5	19
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
17	1V	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	39
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11	36
19	2X	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	1Y	105/110 (96%)	94 (90%)	8 (8%)	3 (3%)	3	15
20	2Y	105/110 (96%)	92 (88%)	11 (10%)	2 (2%)	6	23
21	1Z	148/206 (72%)	128 (86%)	19 (13%)	1 (1%)	18	48
21	2Z	156/206 (76%)	127 (81%)	26 (17%)	3 (2%)	6	23
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	75 (93%)	5 (6%)	1 (1%)	10	34
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	92 (97%)	1 (1%)	2 (2%)	5	21
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	2
26	24	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1	2
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	45 (98%)	0	1 (2%)	5	20
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	7	27
31	19	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	198 (86%)	23 (10%)	8 (4%)	3	12
33	2b	229/256 (90%)	200 (87%)	20 (9%)	9 (4%)	2	10
34	1c	204/239 (85%)	181 (89%)	20 (10%)	3 (2%)	8	28
34	2c	204/239 (85%)	172 (84%)	27 (13%)	5 (2%)	4	17
35	1d	206/209 (99%)	192 (93%)	11 (5%)	3 (2%)	8	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	182 (88%)	20 (10%)	4 (2%)	6	23
36	1e	146/162 (90%)	133 (91%)	10 (7%)	3 (2%)	5	21
36	2e	146/162 (90%)	131 (90%)	11 (8%)	4 (3%)	4	16
37	1f	98/101 (97%)	92 (94%)	5 (5%)	1 (1%)	12	39
37	2f	98/101 (97%)	91 (93%)	6 (6%)	1 (1%)	12	39
38	1g	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	9	32
38	2g	153/156 (98%)	137 (90%)	13 (8%)	3 (2%)	6	22
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	124 (92%)	11 (8%)	0	100	100
40	1i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16	44
40	2i	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	16	44
41	1j	95/105 (90%)	76 (80%)	15 (16%)	4 (4%)	2	9
41	2j	94/105 (90%)	79 (84%)	10 (11%)	5 (5%)	1	5
42	1k	112/129 (87%)	102 (91%)	7 (6%)	3 (3%)	4	16
42	2k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	6	25
43	1l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
43	2l	119/132 (90%)	107 (90%)	12 (10%)	0	100	100
44	1m	121/126 (96%)	110 (91%)	10 (8%)	1 (1%)	16	44
44	2m	120/126 (95%)	106 (88%)	13 (11%)	1 (1%)	16	44
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	7	26
46	1o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	5	19
46	2o	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
47	1p	80/88 (91%)	67 (84%)	12 (15%)	1 (1%)	9	32
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	9	32
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	12	39
48	2q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/88 (75%)	61 (92%)	4 (6%)	1 (2%)	8	28
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	81/93 (87%)	69 (85%)	9 (11%)	3 (4%)	2	11
50	2s	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	4	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	1	5
51	2t	94/106 (89%)	83 (88%)	6 (6%)	5 (5%)	1	5
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11370/12128 (94%)	10373 (91%)	846 (7%)	151 (1%)	9	32

5 of 151 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	49	ASP
15	1T	118	ARG
26	14	62	ARG
33	1b	10	LEU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	193 (90%)	22 (10%)	7	23
3	2D	215/218 (99%)	186 (86%)	29 (14%)	4	12
4	1E	164/166 (99%)	146 (89%)	18 (11%)	6	20
4	2E	164/166 (99%)	147 (90%)	17 (10%)	7	23
5	1F	160/166 (96%)	140 (88%)	20 (12%)	4	15
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8	26
6	1G	143/156 (92%)	130 (91%)	13 (9%)	9	28
6	2G	143/156 (92%)	121 (85%)	22 (15%)	2	9
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9	28
7	2H	144/148 (97%)	129 (90%)	15 (10%)	7	23
8	1I	113/124 (91%)	96 (85%)	17 (15%)	3	10
8	2I	105/124 (85%)	92 (88%)	13 (12%)	4	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	1N	118/119 (99%)	106 (90%)	12 (10%)	7	23
9	2N	118/119 (99%)	103 (87%)	15 (13%)	4	14
10	1O	100/100 (100%)	92 (92%)	8 (8%)	11	34
10	2O	100/100 (100%)	92 (92%)	8 (8%)	11	34
11	1P	115/116 (99%)	100 (87%)	15 (13%)	4	13
11	2P	115/116 (99%)	105 (91%)	10 (9%)	9	30
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	9	28
12	2Q	111/111 (100%)	96 (86%)	15 (14%)	4	12
13	1R	101/101 (100%)	87 (86%)	14 (14%)	3	11
13	2R	101/101 (100%)	92 (91%)	9 (9%)	9	28
14	1S	86/88 (98%)	74 (86%)	12 (14%)	3	11
14	2S	85/88 (97%)	71 (84%)	14 (16%)	2	8
15	1T	115/127 (91%)	108 (94%)	7 (6%)	17	46
15	2T	113/127 (89%)	108 (96%)	5 (4%)	25	59
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15	44
16	2U	93/94 (99%)	87 (94%)	6 (6%)	15	44
17	1V	80/82 (98%)	68 (85%)	12 (15%)	3	10
17	2V	80/82 (98%)	67 (84%)	13 (16%)	2	8
18	1W	90/92 (98%)	80 (89%)	10 (11%)	6	20
18	2W	90/92 (98%)	81 (90%)	9 (10%)	7	24
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40	73
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	63
20	1Y	85/91 (93%)	71 (84%)	14 (16%)	2	8
20	2Y	85/91 (93%)	77 (91%)	8 (9%)	8	26
21	1Z	135/179 (75%)	116 (86%)	19 (14%)	3	11
21	2Z	137/179 (76%)	119 (87%)	18 (13%)	4	13
22	10	65/67 (97%)	60 (92%)	5 (8%)	12	35
22	20	65/67 (97%)	60 (92%)	5 (8%)	12	35
23	11	80/83 (96%)	77 (96%)	3 (4%)	29	64
23	21	80/83 (96%)	75 (94%)	5 (6%)	16	45
24	12	65/67 (97%)	61 (94%)	4 (6%)	16	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	27
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	12
25	23	50/52 (96%)	45 (90%)	5 (10%)	7	24
26	14	59/63 (94%)	47 (80%)	12 (20%)	1	4
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	10
27	15	50/52 (96%)	45 (90%)	5 (10%)	7	24
27	25	50/52 (96%)	45 (90%)	5 (10%)	7	24
28	16	51/52 (98%)	49 (96%)	2 (4%)	28	63
28	26	50/52 (96%)	46 (92%)	4 (8%)	11	34
29	17	41/42 (98%)	37 (90%)	4 (10%)	7	25
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	25
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	50
30	28	54/55 (98%)	48 (89%)	6 (11%)	6	20
31	19	34/34 (100%)	32 (94%)	2 (6%)	18	48
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	48
33	1b	192/220 (87%)	166 (86%)	26 (14%)	4	12
33	2b	187/220 (85%)	166 (89%)	21 (11%)	6	19
34	1c	142/188 (76%)	127 (89%)	15 (11%)	6	22
34	2c	140/188 (74%)	129 (92%)	11 (8%)	11	34
35	1d	169/181 (93%)	153 (90%)	16 (10%)	8	26
35	2d	173/181 (96%)	157 (91%)	16 (9%)	8	27
36	1e	113/123 (92%)	108 (96%)	5 (4%)	25	59
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	26
37	1f	84/90 (93%)	78 (93%)	6 (7%)	13	40
37	2f	85/90 (94%)	78 (92%)	7 (8%)	10	32
38	1g	119/127 (94%)	114 (96%)	5 (4%)	26	60
38	2g	120/127 (94%)	109 (91%)	11 (9%)	8	27
39	1h	114/119 (96%)	105 (92%)	9 (8%)	11	34
39	2h	114/119 (96%)	107 (94%)	7 (6%)	17	46
40	1i	90/99 (91%)	78 (87%)	12 (13%)	4	12
40	2i	89/99 (90%)	77 (86%)	12 (14%)	4	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	1j	66/92 (72%)	62 (94%)	4 (6%)	17	46
41	2j	69/92 (75%)	64 (93%)	5 (7%)	13	39
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6	20
42	2k	83/99 (84%)	78 (94%)	5 (6%)	17	47
43	1l	96/108 (89%)	84 (88%)	12 (12%)	4	15
43	2l	96/108 (89%)	86 (90%)	10 (10%)	7	23
44	1m	93/101 (92%)	84 (90%)	9 (10%)	8	25
44	2m	92/101 (91%)	86 (94%)	6 (6%)	15	44
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	16
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5	16
46	1o	78/80 (98%)	70 (90%)	8 (10%)	7	23
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16	44
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	18
47	2p	68/74 (92%)	57 (84%)	11 (16%)	2	8
48	1q	94/97 (97%)	89 (95%)	5 (5%)	20	52
48	2q	94/97 (97%)	88 (94%)	6 (6%)	16	44
49	1r	59/77 (77%)	52 (88%)	7 (12%)	5	16
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10	31
50	1s	69/80 (86%)	64 (93%)	5 (7%)	13	39
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4	12
51	1t	70/82 (85%)	66 (94%)	4 (6%)	18	49
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18	49
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	50
All	All	9303/10064 (92%)	8378 (90%)	925 (10%)	7	24

5 of 925 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2D	10	THR
46	2o	58	MET
9	2N	5	VAL
44	2m	106	ASN
35	2d	170	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
46	1o	46	HIS
40	2i	3	GLN
4	2E	169	ASN
38	2g	148	ASN
46	2o	62	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	459 (16%)	29 (1%)
1	2A	2791/2915 (95%)	494 (17%)	23 (0%)
2	1B	120/121 (99%)	9 (7%)	1 (0%)
2	2B	118/121 (97%)	33 (27%)	0
32	1a	1497/1521 (98%)	237 (15%)	0
32	2a	1501/1521 (98%)	290 (19%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	4 (33%)	0
54	1w	72/76 (94%)	21 (29%)	0
54	1y	72/76 (94%)	24 (33%)	0
54	2w	69/76 (90%)	24 (34%)	0
54	2y	70/76 (92%)	24 (34%)	0
55	1x	75/77 (97%)	9 (12%)	0
55	2x	75/77 (97%)	14 (18%)	0
All	All	9348/9620 (97%)	1643 (17%)	53 (0%)

5 of 1643 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	15	G
1	1A	34	C
1	1A	45	C

5 of 53 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2701	U
1	2A	271(M)	G
1	2A	1992	G

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Mol	Chain	Res	Type
2	1B	1	U
1	2A	228	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	PSU	1A	2617	1	18,21,22	1.40	4 (22%)	21,30,33	1.95	4 (19%)
32	5MC	1a	1400	32	19,22,23	1.76	3 (15%)	26,32,35	1.20	3 (11%)
54	PSU	2w	39	54	18,21,22	1.43	2 (11%)	21,30,33	1.73	4 (19%)
55	5MC	1x	32	55	19,22,23	1.71	3 (15%)	26,32,35	1.12	3 (11%)
32	MA6	2a	1518	32	23,26,27	1.58	4 (17%)	33,38,41	2.28	10 (30%)
1	5MC	1A	1984	1	19,22,23	1.54	3 (15%)	26,32,35	1.22	3 (11%)
1	5MC	2A	1942	1	19,22,23	1.66	3 (15%)	26,32,35	1.08	2 (7%)
54	PSU	1y	55	54	18,21,22	1.34	2 (11%)	21,30,33	2.11	5 (23%)
32	4OC	1a	1402	32,56	20,23,24	0.75	0	25,32,35	0.92	1 (4%)
1	5MU	1A	1961	1,56	19,22,23	1.36	4 (21%)	27,32,35	2.20	6 (22%)
32	5MC	1a	1404	32,56	19,22,23	1.78	3 (15%)	26,32,35	1.10	3 (11%)
32	2MG	1a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.25	9 (27%)
1	4OC	2A	1920	1	19,22,24	0.78	0	25,31,35	0.85	0
1	2MA	2A	2503	1,56	22,25,26	1.37	5 (22%)	32,37,40	2.38	9 (28%)
32	5MC	2a	1407	32	19,22,23	1.50	2 (10%)	26,32,35	1.27	3 (11%)
32	5MC	1a	967	32	19,22,23	1.72	3 (15%)	26,32,35	1.16	3 (11%)
1	PSU	2A	1917	1,56	18,21,22	1.41	2 (11%)	21,30,33	2.09	4 (19%)
55	5MU	1x	54	55	19,22,23	1.43	6 (31%)	27,32,35	1.93	7 (25%)
32	M2G	1a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.89	6 (18%)
54	PSU	2y	39	54	18,21,22	1.37	2 (11%)	21,30,33	1.91	3 (14%)
32	7MG	1a	527	32	23,26,27	1.44	4 (17%)	27,39,42	2.57	5 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1A	1933	1	18,21,22	1.40	2 (11%)	21,30,33	2.15	3 (14%)
1	5MU	1A	1937	1	19,22,23	1.38	6 (31%)	27,32,35	2.23	6 (22%)
54	PSU	1w	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.04	3 (14%)
54	5MU	2y	54	54	19,22,23	1.51	4 (21%)	27,32,35	2.13	9 (33%)
32	UR3	2a	1498	32	19,22,23	1.06	1 (5%)	26,32,35	1.79	3 (11%)
54	5MU	1y	54	54	19,22,23	1.57	6 (31%)	27,32,35	1.99	6 (22%)
54	5MU	1w	54	54	19,22,23	1.48	5 (26%)	27,32,35	1.85	6 (22%)
54	PSU	2y	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.94	4 (19%)
54	PSU	1y	32	54	18,21,22	1.41	3 (16%)	21,30,33	1.87	4 (19%)
54	4SU	1w	8	54	18,21,22	1.71	4 (22%)	25,30,33	2.11	4 (16%)
54	PSU	1w	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.97	3 (14%)
55	5MU	2x	54	55	19,22,23	1.42	5 (26%)	27,32,35	2.31	6 (22%)
54	7MG	1y	46	54	23,26,27	1.34	4 (17%)	27,39,42	2.59	6 (22%)
54	PSU	2w	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.14	4 (19%)
54	PSU	1y	39	54	18,21,22	1.42	2 (11%)	21,30,33	1.85	4 (19%)
54	7MG	1w	46	54	23,26,27	1.43	4 (17%)	27,39,42	2.50	5 (18%)
55	4SU	1x	8	55	18,21,22	2.12	4 (22%)	25,30,33	1.43	5 (20%)
32	4OC	2a	1402	32,56	20,23,24	0.78	0	25,32,35	1.18	2 (8%)
54	PSU	1w	39	54	18,21,22	1.36	2 (11%)	21,30,33	1.96	3 (14%)
1	OMG	2A	2251	1,55	23,26,27	1.25	3 (13%)	32,38,41	2.06	6 (18%)
43	0TD	1l	92	43	8,9,10	4.60	1 (12%)	6,11,13	3.70	3 (50%)
54	PSU	2y	55	54	18,21,22	1.31	3 (16%)	21,30,33	1.90	5 (23%)
1	5MU	2A	1915	1	19,22,23	1.52	5 (26%)	27,32,35	2.14	8 (29%)
1	PSU	1A	1939	1	18,21,22	1.45	4 (22%)	21,30,33	2.07	3 (14%)
32	PSU	1a	516	32,56	18,21,22	1.33	2 (11%)	21,30,33	2.02	5 (23%)
1	4OC	1A	1942	1,56	19,22,24	0.80	0	25,31,35	0.88	0
43	0TD	2l	92	43	8,9,10	4.48	1 (12%)	6,11,13	1.74	2 (33%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	21,30,33	1.99	4 (19%)
32	MA6	2a	1519	32	23,26,27	1.59	4 (17%)	33,38,41	2.24	11 (33%)
32	MA6	1a	1519	32	23,26,27	1.55	4 (17%)	33,38,41	2.30	12 (36%)
32	5MC	1a	1407	32	19,22,23	1.41	3 (15%)	26,32,35	1.20	2 (7%)
1	5MC	2A	1962	1,56	19,22,23	1.50	3 (15%)	26,32,35	1.20	2 (7%)
54	MIA	1y	37	54	21,24,32	1.61	3 (14%)	30,35,47	2.01	10 (33%)
1	5MU	2A	1939	1	19,22,23	1.43	5 (26%)	27,32,35	2.37	6 (22%)
55	5MC	2x	32	55	19,22,23	1.78	2 (10%)	26,32,35	1.16	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	4SU	2y	8	54	18,21,22	1.88	5 (27%)	25,30,33	2.27	5 (20%)
32	UR3	1a	1498	32	19,22,23	1.09	1 (5%)	26,32,35	1.83	3 (11%)
54	MIA	2w	37	54	24,27,32	2.11	5 (20%)	32,39,47	2.37	11 (34%)
54	MIA	1w	37	54	28,31,32	2.42	7 (25%)	38,44,47	2.75	14 (36%)
54	7MG	2w	46	54	23,26,27	1.34	5 (21%)	27,39,42	2.66	7 (25%)
55	4SU	2x	8	55,56	18,21,22	1.98	4 (22%)	25,30,33	1.43	4 (16%)
1	OMG	1A	2263	1,55,56	23,26,27	1.24	3 (13%)	32,38,41	2.05	5 (15%)
54	7MG	2y	46	54	23,26,27	1.47	4 (17%)	27,39,42	2.79	6 (22%)
54	MIA	2y	37	54,32	21,24,32	1.60	4 (19%)	30,35,47	2.10	9 (30%)
1	5MC	1A	1964	1	19,22,23	1.44	3 (15%)	26,32,35	1.16	3 (11%)
54	4SU	1y	8	54	18,21,22	1.71	3 (16%)	25,30,33	1.91	6 (24%)
32	M2G	2a	966	32	24,27,28	1.32	3 (12%)	33,40,43	1.85	6 (18%)
1	2MU	2A	2552	1,56	19,22,24	1.23	2 (10%)	25,31,36	1.92	5 (20%)
32	7MG	2a	527	32	23,26,27	1.36	3 (13%)	27,39,42	2.62	6 (22%)
32	5MC	2a	1404	32	19,22,23	1.82	3 (15%)	26,32,35	1.20	3 (11%)
32	2MG	2a	1207	32	23,26,27	1.24	2 (8%)	33,38,41	2.18	7 (21%)
1	PSU	2A	2605	1	18,21,22	1.34	3 (16%)	21,30,33	2.12	4 (19%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	1.93	5 (23%)
1	2MA	1A	2515	1,56	22,25,26	1.46	4 (18%)	32,37,40	2.42	8 (25%)
32	MA6	1a	1518	32	23,26,27	1.49	5 (21%)	33,38,41	2.28	13 (39%)
54	PSU	2w	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.94	3 (14%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.95	3 (14%)
55	PSU	1x	55	55	18,21,22	1.29	2 (11%)	21,30,33	2.01	4 (19%)
54	4SU	2w	8	54	18,21,22	1.74	4 (22%)	25,30,33	2.37	5 (20%)
32	5MC	2a	967	32	19,22,23	1.75	3 (15%)	26,32,35	1.19	3 (11%)
1	2MU	1A	2564	1,56	19,22,24	1.21	2 (10%)	25,31,36	2.16	6 (24%)
54	5MU	2w	54	54	19,22,23	1.34	4 (21%)	27,32,35	1.82	6 (22%)
32	5MC	2a	1400	32	19,22,23	1.58	3 (15%)	26,32,35	1.07	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/11/29/30	0/3/3/3
1	5MC	1A	1984	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
32	4OC	1a	1402	32,56	-	1/9/29/30	0/2/2/2
1	5MU	1A	1961	1,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32,56	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
1	2MA	2A	2503	1,56	-	1/7/25/26	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
1	PSU	2A	1917	1,56	-	2/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32	-	3/7/37/38	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	2/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	3/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	1/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	2/7/37/38	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	3/7/37/38	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	0TD	1l	92	43	-	2/7/12/14	-
54	PSU	2y	55	54	-	2/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1,56	-	1/9/27/30	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/11/29/30	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	1/7/25/34	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
54	7MG	2w	46	54	-	4/7/37/38	0/3/3/3
55	4SU	2x	8	55,56	-	1/7/25/26	0/2/2/2
1	OMG	1A	2263	1,55,56	-	1/9/27/28	0/3/3/3
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
54	MIA	2y	37	54,32	-	3/7/25/34	0/3/3/3
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	2MU	2A	2552	1,56	-	1/9/27/28	0/2/2/2
32	7MG	2a	527	32	-	3/7/37/38	0/3/3/3
32	5MC	2a	1404	32	-	1/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	1/9/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	1,56	-	1/7/25/26	0/3/3/3
32	MA6	1a	1518	32	-	1/11/29/30	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	2/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	967	32	-	2/7/25/26	0/2/2/2
1	2MU	1A	2564	1,56	-	0/9/27/28	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2

The worst 5 of 259 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.58	1.69	1.82
43	2l	92	0TD	CB-SB	-12.36	1.69	1.82
54	1w	37	MIA	C2-S10	-7.87	1.69	1.75
54	2w	37	MIA	C2-S10	-7.10	1.69	1.75
32	2a	1404	5MC	C5-C4	6.80	1.49	1.44

The worst 5 of 423 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	46	7MG	N9-C4-N3	10.02	140.14	125.46
54	1w	37	MIA	C12-C13-C14	-9.24	110.43	127.01
54	1y	46	7MG	N9-C4-N3	9.05	138.72	125.46
54	2w	46	7MG	N9-C4-N3	8.97	138.60	125.46
32	2a	527	7MG	N9-C4-N3	8.81	138.38	125.46

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	2263	OMG	C1'-C2'-O2'-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
54	1w	37	MIA	C12-C13-C14-C16
54	1y	46	7MG	C4'-C5'-O5'-P

There are no ring outliers.

44 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2w	39	PSU	3	0
32	2a	1518	MA6	3	0
1	2A	1942	5MC	1	0
54	1y	55	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1961	5MU	1	0
32	1a	1404	5MC	1	0
32	1a	1207	2MG	1	0
1	2A	1920	4OC	1	0
1	2A	2503	2MA	1	0
32	1a	967	5MC	1	0
54	1y	39	PSU	1	0
54	1w	46	7MG	1	0
55	1x	8	4SU	2	0
32	2a	1402	4OC	2	0
43	1l	92	0TD	3	0
54	2y	55	PSU	8	0
1	2A	1915	5MU	1	0
32	1a	516	PSU	1	0
1	1A	1942	4OC	2	0
43	2l	92	0TD	2	0
55	2x	55	PSU	1	0
32	2a	1519	MA6	2	0
32	1a	1519	MA6	1	0
54	1y	37	MIA	1	0
1	2A	1939	5MU	1	0
55	2x	32	5MC	1	0
54	2y	8	4SU	1	0
32	1a	1498	UR3	1	0
54	2w	37	MIA	1	0
54	1w	37	MIA	1	0
54	2w	46	7MG	1	0
55	2x	8	4SU	1	0
54	2y	46	7MG	1	0
54	2y	37	MIA	1	0
54	1y	8	4SU	3	0
32	2a	966	M2G	1	0
1	2A	2552	2MU	2	0
32	2a	1404	5MC	1	0
32	2a	1207	2MG	2	0
32	1a	1518	MA6	1	0
54	2w	8	4SU	2	0
32	2a	967	5MC	2	0
1	1A	2564	2MU	1	0
32	2a	1400	5MC	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2280 ligands modelled in this entry, 2271 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	KAN	2a	1828	-	34,35,35	1.63	6 (17%)	47,52,52	1.50	8 (17%)
59	SF4	2d	501	35	0,12,12	-	-	-	-	-
57	KAN	2A	3569	56	34,35,35	1.57	6 (17%)	47,52,52	1.98	15 (31%)
57	KAN	1a	1955	-	34,35,35	1.62	6 (17%)	47,52,52	1.10	5 (10%)
57	KAN	2A	3568	56	34,35,35	1.52	5 (14%)	47,52,52	1.68	6 (12%)
57	KAN	1A	3935	56	34,35,35	1.66	6 (17%)	47,52,52	1.76	12 (25%)
57	KAN	1A	3934	-	34,35,35	1.48	5 (14%)	47,52,52	1.63	11 (23%)
57	KAN	1A	3933	-	34,35,35	1.69	6 (17%)	47,52,52	1.29	5 (10%)
59	SF4	1d	303	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
57	KAN	2a	1828	-	-	1/12/72/72	0/3/3/3
59	SF4	2d	501	35	-	-	0/6/5/5
57	KAN	2A	3569	56	-	2/12/72/72	0/3/3/3
57	KAN	1a	1955	-	-	3/12/72/72	0/3/3/3
57	KAN	2A	3568	56	-	4/12/72/72	0/3/3/3
57	KAN	1A	3935	56	-	2/12/72/72	0/3/3/3
57	KAN	1A	3934	-	-	4/12/72/72	0/3/3/3
57	KAN	1A	3933	-	-	4/12/72/72	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	1d	303	35	-	-	0/6/5/5

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1A	3933	KAN	C14-C15	-5.68	1.46	1.53
57	2a	1828	KAN	C14-C15	-5.67	1.46	1.53
57	1A	3935	KAN	C14-C15	-5.25	1.46	1.53
57	1a	1955	KAN	C14-C15	-5.24	1.47	1.53
57	2A	3568	KAN	C14-C15	-5.12	1.47	1.53

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2A	3568	KAN	C17-C16-C15	5.82	117.11	110.67
57	2A	3568	KAN	O12-C17-C16	5.04	118.78	109.70
57	2A	3568	KAN	C13-O11-C8	-4.78	106.66	117.98
57	2a	1828	KAN	O12-C17-C16	4.68	118.14	109.70
57	2a	1828	KAN	C17-C16-C15	4.57	115.72	110.67

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	2A	3568	KAN	C11-C10-O9-C1
57	1A	3934	KAN	C9-C8-O11-C13
57	1A	3935	KAN	O12-C17-C18-O15
57	1A	3935	KAN	C16-C17-C18-O15
57	1A	3933	KAN	O12-C17-C18-O15

There are no ring outliers.

8 monomers are involved in 17 short contacts:

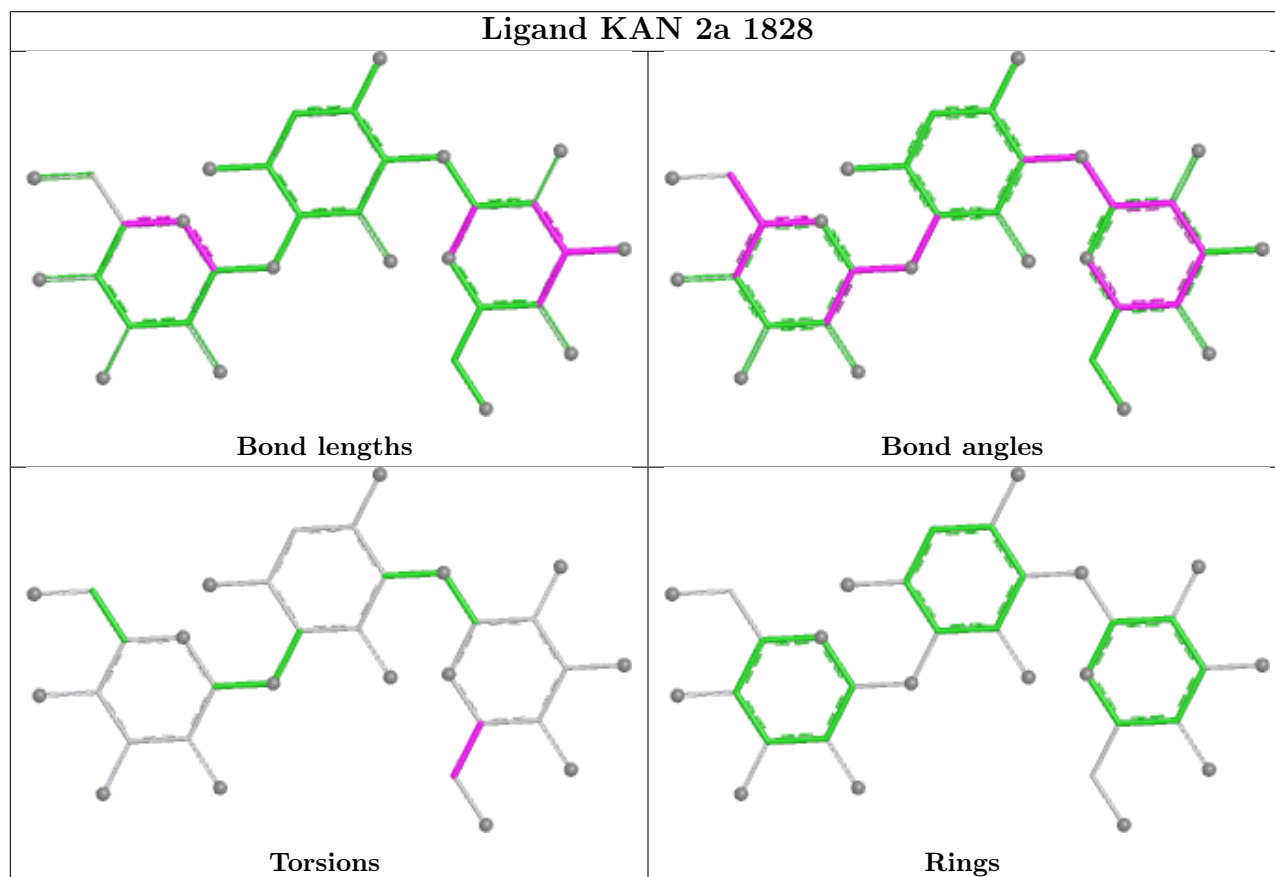
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	2a	1828	KAN	2	0
59	2d	501	SF4	1	0
57	2A	3569	KAN	2	0
57	1a	1955	KAN	3	0
57	2A	3568	KAN	2	0
57	1A	3935	KAN	2	0
57	1A	3934	KAN	4	0

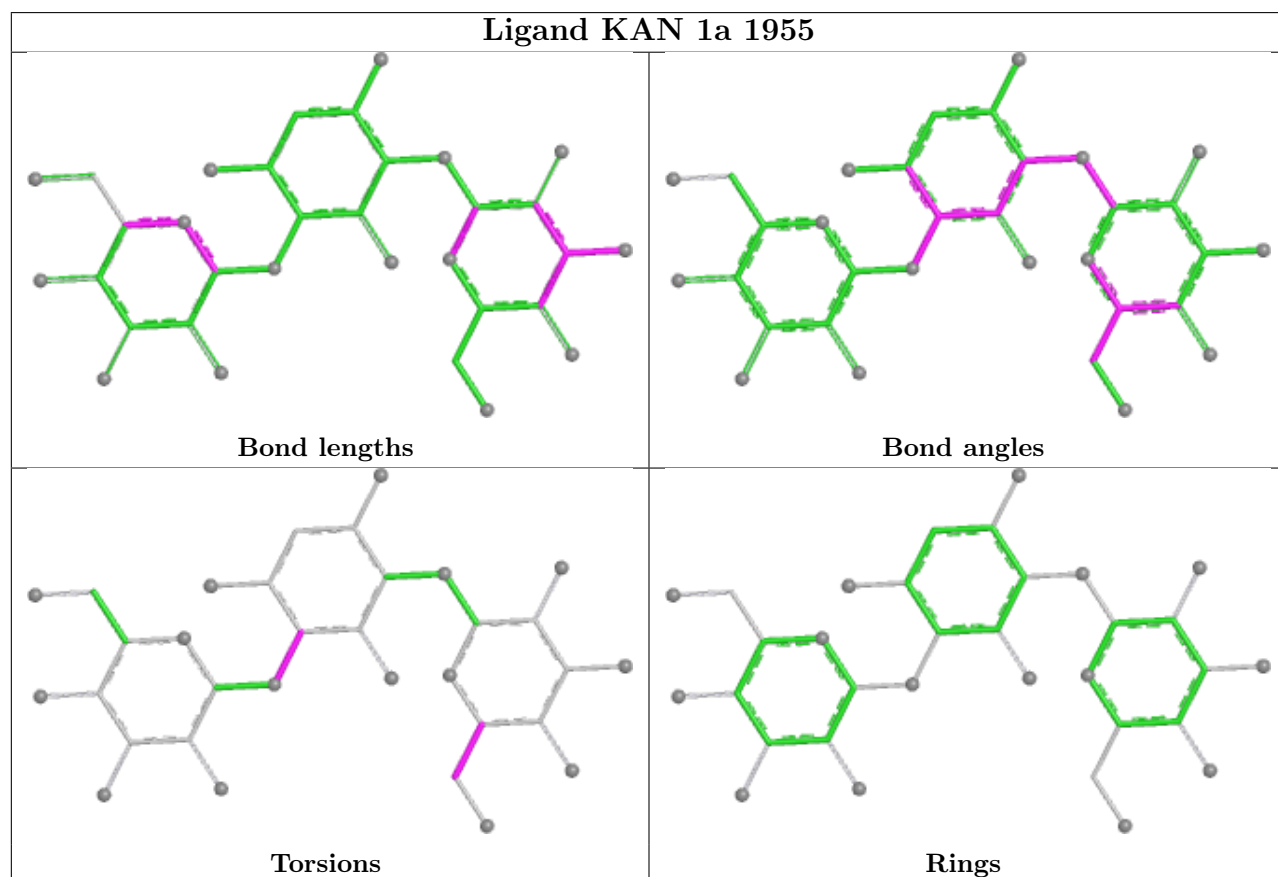
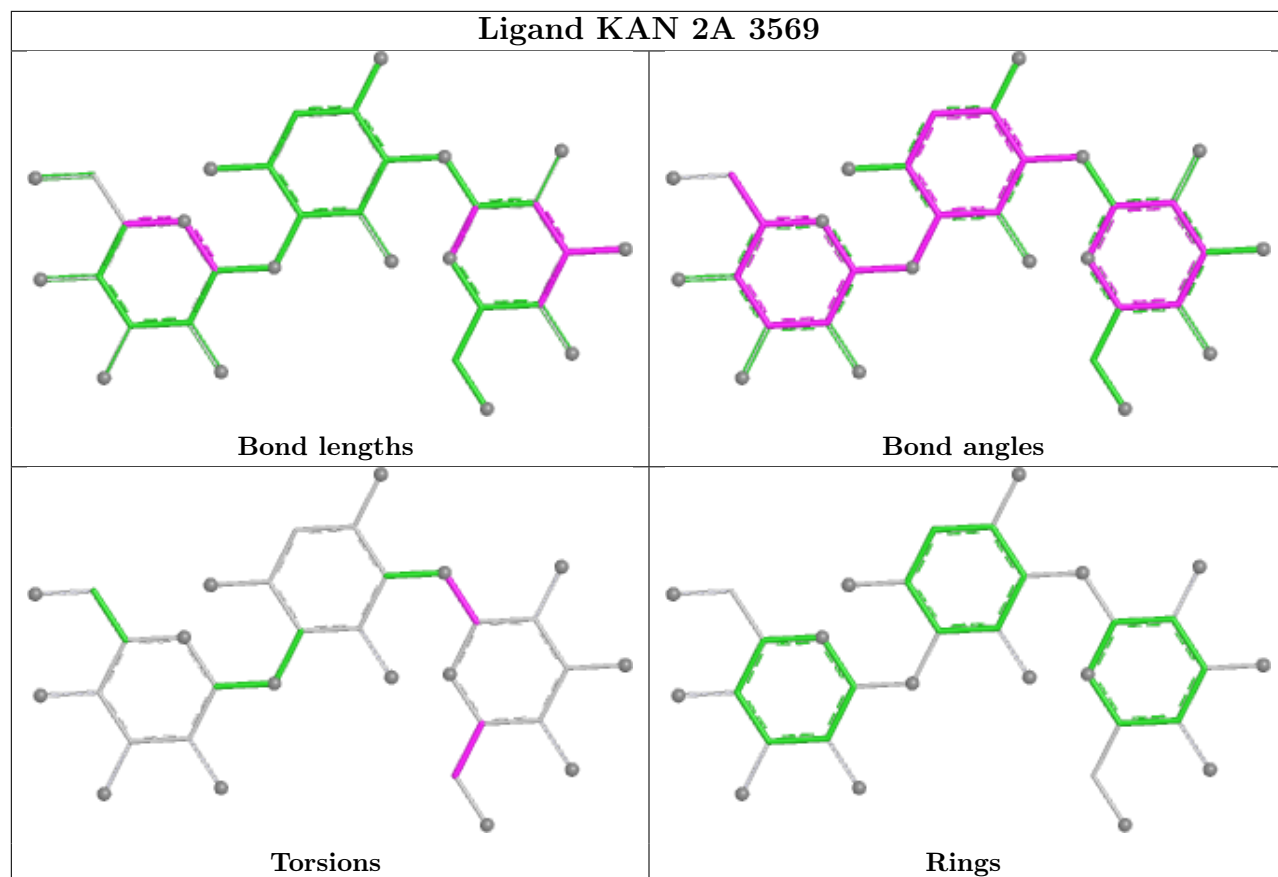
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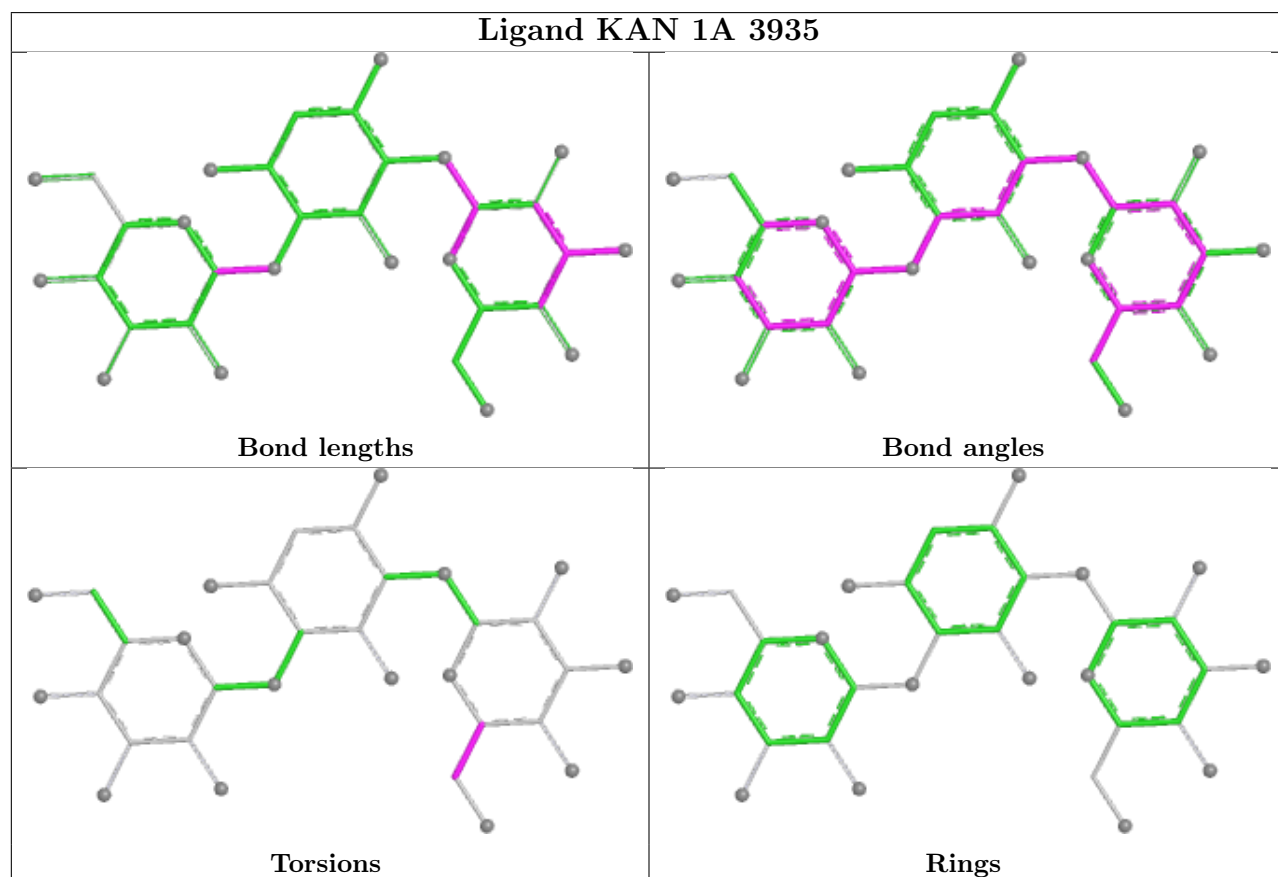
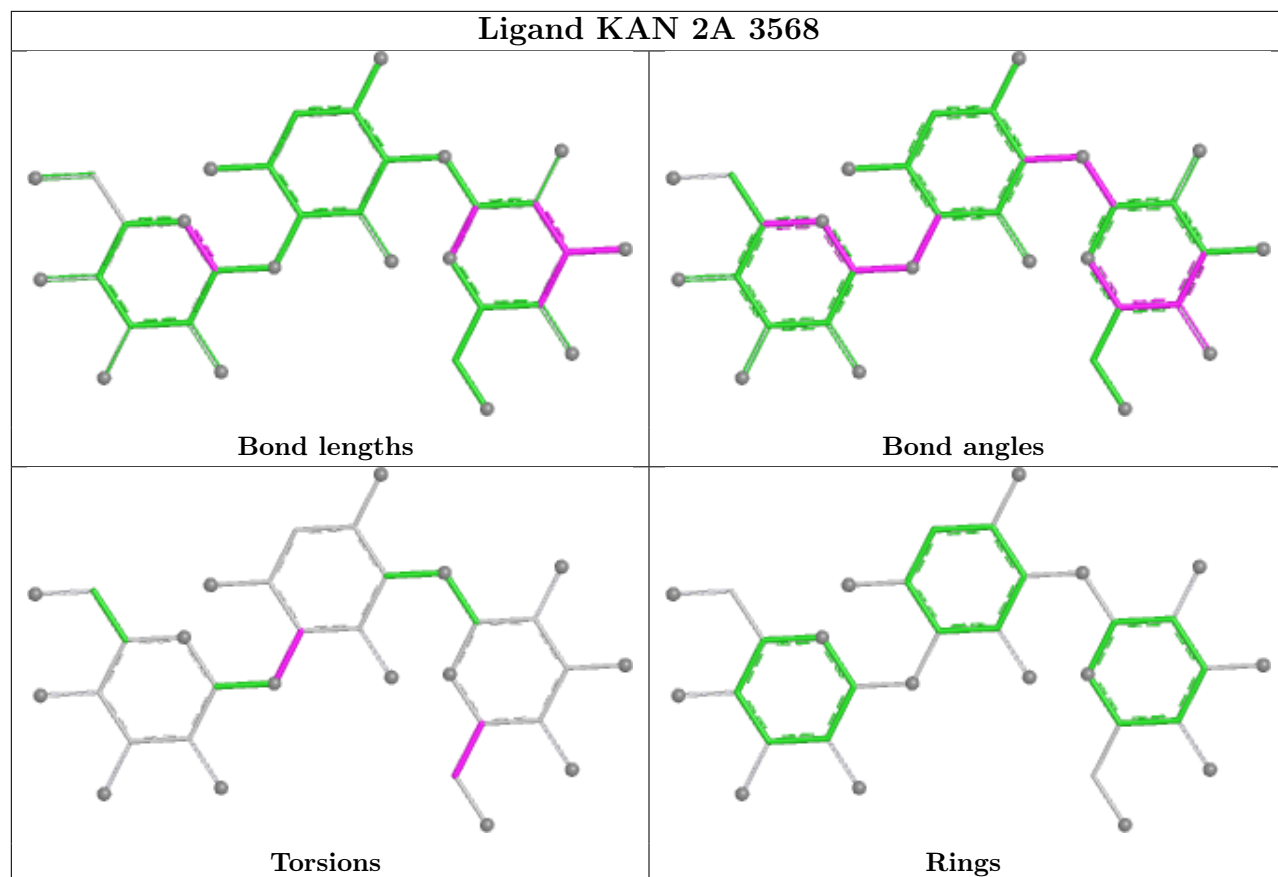
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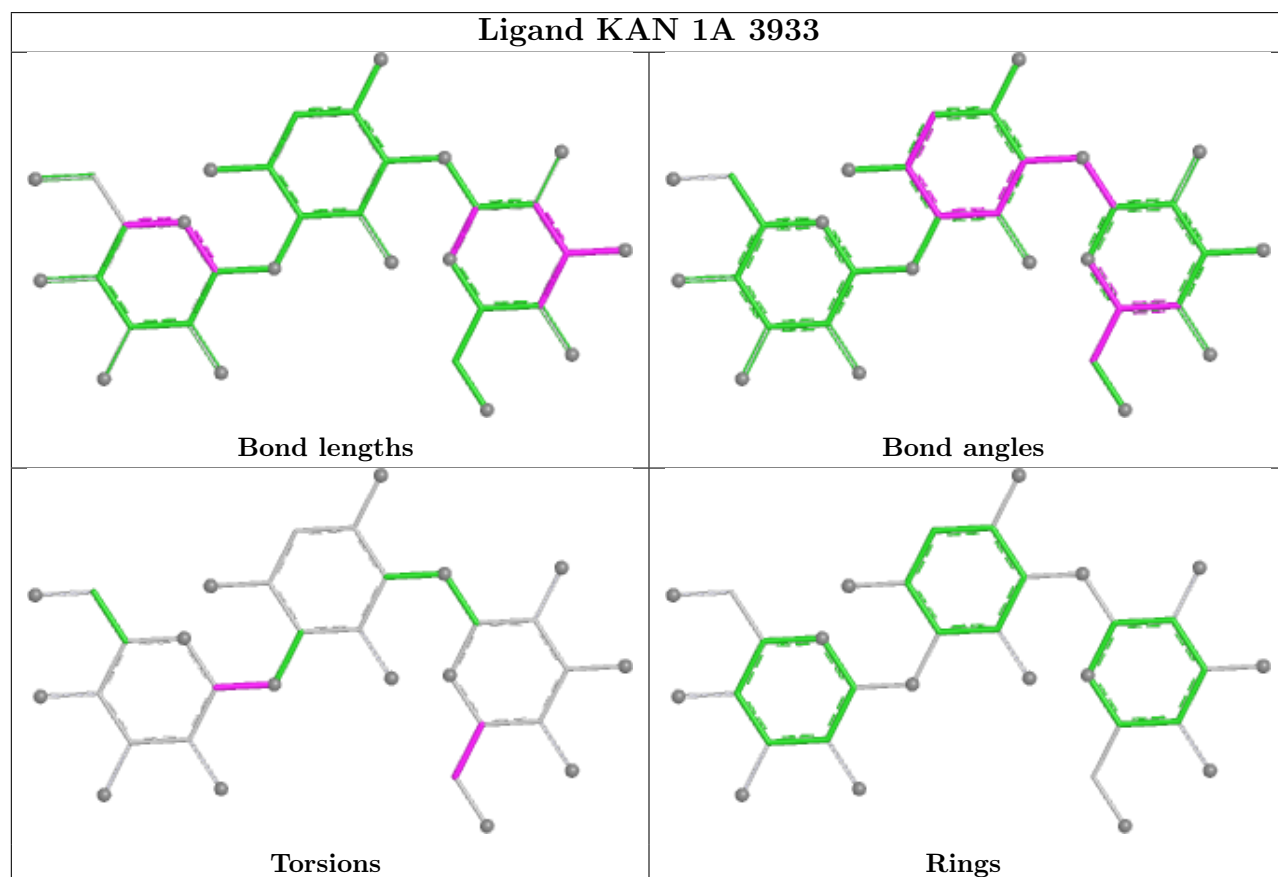
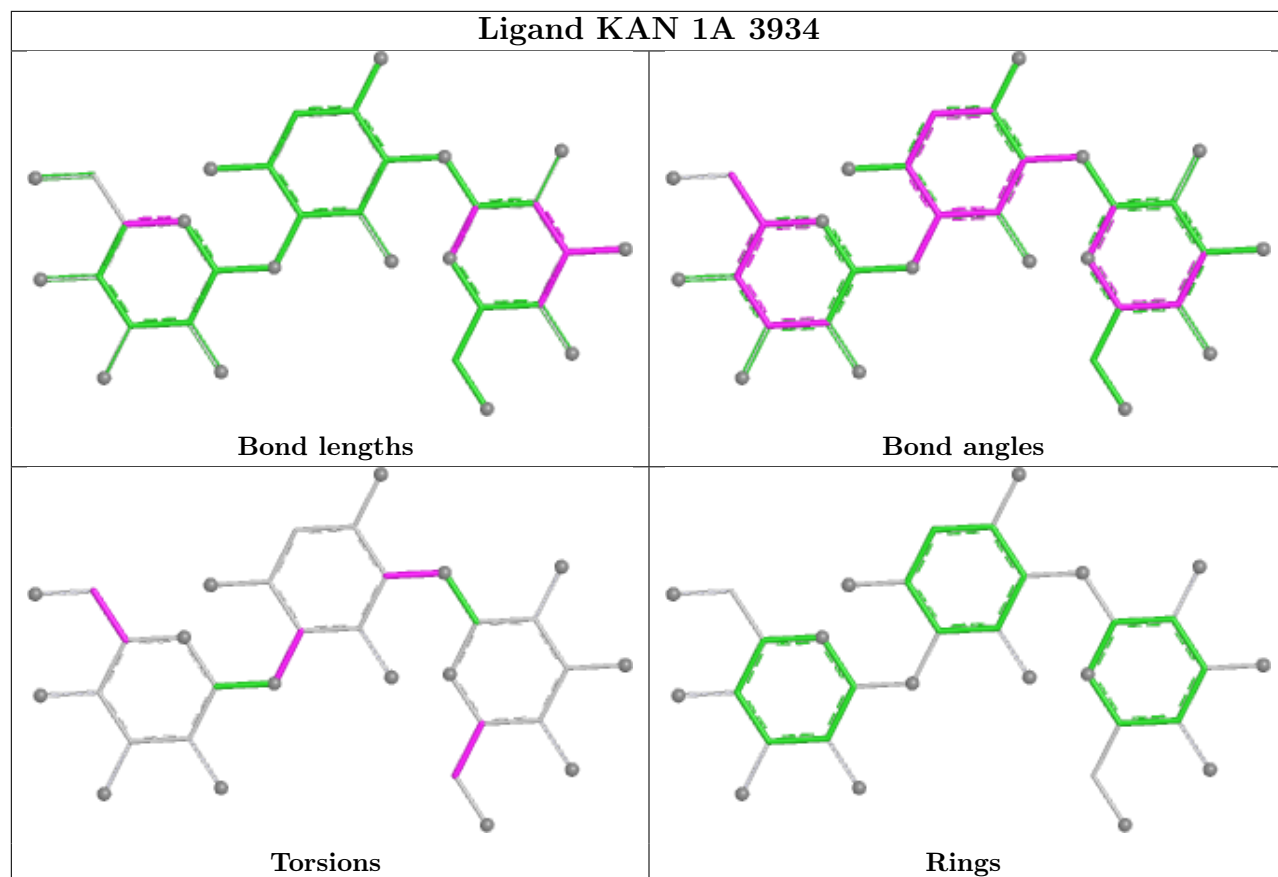
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1d	303	SF4	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.56	21 (0%) 84 79	23, 43, 106, 122	0
1	2A	2789/2915 (95%)	-0.22	28 (1%) 79 73	38, 65, 105, 122	0
2	1B	120/121 (99%)	-0.53	0 100 100	37, 56, 75, 100	0
2	2B	120/121 (99%)	0.26	0 100 100	69, 87, 98, 111	0
3	1D	275/276 (99%)	-0.02	5 (1%) 67 59	25, 44, 60, 83	0
3	2D	275/276 (99%)	0.22	7 (2%) 58 48	36, 56, 69, 83	0
4	1E	204/206 (99%)	-0.18	0 100 100	27, 46, 67, 86	0
4	2E	204/206 (99%)	0.15	2 (0%) 79 73	39, 68, 80, 91	0
5	1F	203/210 (96%)	-0.12	0 100 100	24, 49, 75, 96	0
5	2F	203/210 (96%)	0.33	4 (1%) 65 56	43, 75, 91, 103	0
6	1G	181/182 (99%)	0.38	4 (2%) 62 53	46, 64, 81, 96	0
6	2G	181/182 (99%)	0.89	17 (9%) 14 12	74, 88, 97, 104	0
7	1H	174/180 (96%)	0.09	3 (1%) 69 61	45, 62, 75, 81	0
7	2H	174/180 (96%)	0.87	13 (7%) 20 16	77, 91, 102, 106	0
8	1I	146/148 (98%)	0.33	3 (2%) 63 54	51, 82, 93, 97	0
8	2I	146/148 (98%)	0.83	10 (6%) 23 18	65, 86, 96, 101	0
9	1N	140/140 (100%)	-0.06	0 100 100	34, 46, 69, 79	0
9	2N	140/140 (100%)	0.49	4 (2%) 53 45	55, 73, 88, 93	0
10	1O	122/122 (100%)	0.09	2 (1%) 70 62	33, 46, 64, 70	0
10	2O	122/122 (100%)	0.26	1 (0%) 82 77	52, 64, 78, 86	0
11	1P	149/150 (99%)	0.06	3 (2%) 65 56	23, 51, 76, 86	0
11	2P	149/150 (99%)	0.30	3 (2%) 65 56	46, 76, 92, 100	0
12	1Q	141/141 (100%)	-0.13	1 (0%) 84 79	34, 47, 60, 86	0
12	2Q	141/141 (100%)	0.80	11 (7%) 19 16	58, 76, 88, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.26	0 100 100	29, 40, 53, 64	0
13	2R	118/118 (100%)	0.02	1 (0%) 82 77	47, 59, 70, 77	0
14	1S	110/112 (98%)	-0.01	0 100 100	42, 56, 68, 76	0
14	2S	110/112 (98%)	0.95	10 (9%) 15 12	70, 81, 90, 94	0
15	1T	131/146 (89%)	0.11	3 (2%) 61 52	39, 50, 76, 95	0
15	2T	131/146 (89%)	0.51	3 (2%) 61 52	56, 68, 88, 96	0
16	1U	116/118 (98%)	-0.29	0 100 100	27, 37, 54, 71	0
16	2U	116/118 (98%)	0.30	1 (0%) 81 75	49, 70, 82, 89	0
17	1V	101/101 (100%)	-0.32	0 100 100	28, 46, 62, 79	0
17	2V	101/101 (100%)	0.49	2 (1%) 65 56	50, 79, 90, 93	0
18	1W	112/113 (99%)	-0.18	2 (1%) 67 59	26, 38, 59, 92	0
18	2W	112/113 (99%)	0.19	1 (0%) 81 75	45, 56, 75, 96	0
19	1X	95/96 (98%)	-0.16	1 (1%) 78 71	30, 44, 66, 87	0
19	2X	95/96 (98%)	0.47	5 (5%) 32 25	48, 67, 81, 90	0
20	1Y	107/110 (97%)	0.03	1 (0%) 81 75	47, 57, 80, 89	0
20	2Y	107/110 (97%)	1.02	13 (12%) 8 7	69, 81, 94, 95	0
21	1Z	154/206 (74%)	0.28	5 (3%) 50 41	50, 67, 93, 100	0
21	2Z	160/206 (77%)	0.71	12 (7%) 20 16	77, 92, 105, 111	0
22	10	83/85 (97%)	0.26	7 (8%) 17 14	33, 44, 72, 89	0
22	20	83/85 (97%)	1.09	12 (14%) 6 4	52, 72, 86, 95	0
23	11	97/98 (98%)	0.22	1 (1%) 79 73	28, 45, 76, 80	0
23	21	97/98 (98%)	0.68	4 (4%) 41 33	46, 62, 84, 97	0
24	12	70/72 (97%)	-0.10	2 (2%) 53 45	42, 54, 65, 94	0
24	22	70/72 (97%)	0.48	0 100 100	61, 78, 87, 89	0
25	13	59/60 (98%)	-0.13	2 (3%) 48 39	30, 42, 66, 84	0
25	23	59/60 (98%)	0.64	2 (3%) 48 39	65, 74, 90, 102	0
26	14	69/71 (97%)	0.64	7 (10%) 12 10	57, 81, 99, 107	0
26	24	69/71 (97%)	1.04	10 (14%) 6 4	87, 95, 106, 110	0
27	15	59/60 (98%)	-0.15	1 (1%) 69 61	26, 39, 57, 70	0
27	25	59/60 (98%)	0.25	1 (1%) 69 61	46, 60, 75, 79	0
28	16	53/54 (98%)	-0.33	0 100 100	34, 46, 61, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.41	1 (1%) 66 58	57, 65, 77, 82	0
29	17	48/49 (97%)	-0.05	1 (2%) 63 54	30, 34, 65, 72	0
29	27	48/49 (97%)	0.22	4 (8%) 17 14	37, 46, 70, 82	0
30	18	64/65 (98%)	-0.06	1 (1%) 70 62	31, 39, 48, 65	0
30	28	64/65 (98%)	0.65	1 (1%) 70 62	48, 63, 70, 76	0
31	19	37/37 (100%)	-0.01	1 (2%) 56 47	39, 46, 66, 70	0
31	29	37/37 (100%)	0.83	3 (8%) 18 15	67, 78, 90, 92	0
32	1a	1488/1521 (97%)	-0.18	9 (0%) 85 81	42, 71, 104, 121	0
32	2a	1491/1521 (98%)	0.17	27 (1%) 67 59	55, 85, 106, 122	0
33	1b	231/256 (90%)	0.59	12 (5%) 33 26	72, 89, 104, 110	0
33	2b	231/256 (90%)	0.89	20 (8%) 16 13	84, 97, 104, 110	0
34	1c	206/239 (86%)	0.26	5 (2%) 59 50	60, 76, 89, 94	0
34	2c	206/239 (86%)	1.14	27 (13%) 7 6	84, 94, 100, 107	0
35	1d	208/209 (99%)	0.70	10 (4%) 35 28	58, 74, 88, 98	0
35	2d	208/209 (99%)	0.93	15 (7%) 21 17	67, 80, 93, 101	0
36	1e	148/162 (91%)	0.21	2 (1%) 73 65	58, 69, 81, 94	0
36	2e	148/162 (91%)	0.82	9 (6%) 27 21	78, 86, 94, 102	0
37	1f	100/101 (99%)	0.07	0 100 100	57, 72, 83, 86	0
37	2f	100/101 (99%)	0.17	1 (1%) 79 73	64, 77, 86, 96	0
38	1g	155/156 (99%)	0.48	9 (5%) 29 22	63, 75, 91, 102	0
38	2g	155/156 (99%)	0.58	12 (7%) 19 16	76, 87, 98, 113	0
39	1h	137/138 (99%)	0.47	2 (1%) 72 64	62, 74, 82, 89	0
39	2h	137/138 (99%)	0.87	6 (4%) 39 30	74, 86, 93, 97	0
40	1i	127/128 (99%)	0.87	8 (6%) 26 20	59, 81, 91, 94	0
40	2i	127/128 (99%)	1.40	26 (20%) 2 2	79, 94, 101, 105	0
41	1j	97/105 (92%)	1.13	16 (16%) 4 3	58, 83, 96, 101	0
41	2j	96/105 (91%)	1.59	27 (28%) 1 1	84, 95, 104, 110	0
42	1k	114/129 (88%)	0.37	2 (1%) 67 59	52, 72, 83, 87	0
42	2k	114/129 (88%)	0.76	8 (7%) 22 18	63, 81, 90, 93	0
43	1l	121/132 (91%)	0.16	3 (2%) 58 48	47, 56, 73, 82	0
43	2l	121/132 (91%)	0.75	10 (8%) 17 14	60, 73, 84, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.58	7 (5%) 29 23	60, 72, 85, 98	0
44	2m	122/126 (96%)	1.21	18 (14%) 5 4	78, 92, 98, 105	0
45	1n	60/61 (98%)	0.51	3 (5%) 34 27	61, 70, 77, 82	0
45	2n	60/61 (98%)	1.94	20 (33%) 1 1	83, 92, 98, 99	0
46	1o	88/89 (98%)	0.47	3 (3%) 48 39	57, 69, 83, 91	0
46	2o	88/89 (98%)	0.54	4 (4%) 38 30	64, 81, 89, 95	0
47	1p	82/88 (93%)	0.96	5 (6%) 27 21	62, 74, 85, 96	0
47	2p	82/88 (93%)	0.81	5 (6%) 27 21	64, 76, 86, 92	0
48	1q	99/105 (94%)	0.54	1 (1%) 79 73	57, 73, 84, 89	0
48	2q	99/105 (94%)	0.60	3 (3%) 52 43	68, 80, 89, 95	0
49	1r	68/88 (77%)	0.01	0 100 100	61, 72, 85, 88	0
49	2r	68/88 (77%)	0.31	0 100 100	64, 81, 90, 96	0
50	1s	83/93 (89%)	0.38	2 (2%) 59 50	62, 75, 84, 94	0
50	2s	83/93 (89%)	1.21	15 (18%) 3 3	87, 94, 102, 107	0
51	1t	96/106 (90%)	0.82	7 (7%) 21 17	64, 77, 88, 96	0
51	2t	96/106 (90%)	0.61	4 (4%) 40 32	65, 77, 91, 94	0
52	1u	23/27 (85%)	0.70	2 (8%) 16 13	64, 72, 77, 80	0
52	2u	23/27 (85%)	2.14	14 (60%) 0 0	80, 89, 93, 94	0
53	1v	13/24 (54%)	0.49	1 (7%) 19 16	50, 62, 88, 105	0
53	2v	13/24 (54%)	1.68	4 (30%) 1 1	75, 95, 115, 118	0
54	1w	67/76 (88%)	0.42	3 (4%) 38 30	60, 98, 112, 115	0
54	1y	67/76 (88%)	0.57	2 (2%) 52 43	44, 104, 112, 121	0
54	2w	65/76 (85%)	0.77	9 (13%) 6 5	85, 108, 116, 120	0
54	2y	66/76 (86%)	1.02	4 (6%) 27 21	62, 113, 118, 119	0
55	1x	72/77 (93%)	-0.04	0 100 100	45, 72, 93, 99	0
55	2x	72/77 (93%)	0.27	3 (4%) 40 32	61, 86, 100, 106	0
All	All	20875/21748 (95%)	0.15	668 (3%) 50 41	23, 70, 100, 122	0

The worst 5 of 668 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	9.6
44	1m	124	PRO	8.6

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Mol	Chain	Res	Type	RSRZ
23	21	2	SER	8.1
44	2m	122	LYS	7.5
44	2m	124	PRO	6.8

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, 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	7MG	2y	46	24/25	0.53	0.14	108,115,122,143	0
54	5MU	2y	54	21/22	0.53	0.14	100,108,120,137	0
54	7MG	2w	46	24/25	0.54	0.12	104,113,124,141	0
54	7MG	1y	46	24/25	0.55	0.14	101,112,119,130	0
54	MIA	2y	37	22/30	0.55	0.16	92,104,116,129	0
54	4SU	2y	8	20/21	0.61	0.14	111,115,121,124	0
54	7MG	1w	46	24/25	0.62	0.13	88,103,119,135	0
54	PSU	2y	32	20/21	0.64	0.18	99,110,119,121	0
54	5MU	1y	54	21/22	0.65	0.15	97,103,113,129	0
54	PSU	2y	55	20/21	0.66	0.11	102,113,127,129	0
54	PSU	1y	55	20/21	0.70	0.14	101,108,115,126	0
54	4SU	2w	8	20/21	0.71	0.10	109,114,122,137	0
54	4SU	1y	8	20/21	0.71	0.10	101,107,113,113	0
54	MIA	1y	37	22/30	0.78	0.12	81,90,97,99	0
55	PSU	2x	55	20/21	0.78	0.12	80,89,100,105	0
54	4SU	1w	8	20/21	0.79	0.10	91,99,107,109	0
54	PSU	2y	39	20/21	0.81	0.12	91,101,110,111	0
54	PSU	1y	32	20/21	0.81	0.11	84,92,101,101	0
55	4SU	2x	8	20/21	0.82	0.11	77,88,93,93	0
32	2MG	2a	1207	24/25	0.83	0.13	86,91,99,102	0
55	5MU	2x	54	21/22	0.84	0.12	88,93,99,109	0
54	5MU	2w	54	21/22	0.84	0.09	79,91,95,99	0
54	PSU	1w	55	20/21	0.84	0.09	70,90,98,99	0
54	PSU	2w	32	20/21	0.85	0.13	87,95,100,102	0
54	PSU	2w	55	20/21	0.85	0.09	92,97,106,108	0
54	PSU	1w	32	20/21	0.88	0.12	68,78,82,83	0
1	5MU	2A	1915	21/22	0.88	0.10	76,83,88,89	0
54	PSU	1y	39	20/21	0.88	0.09	85,91,104,106	0
32	PSU	2a	516	20/21	0.89	0.10	76,83,89,89	0
1	PSU	2A	1917	20/21	0.90	0.08	72,78,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	5MU	1x	54	21/22	0.90	0.08	64,75,79,84	0
55	PSU	1x	55	20/21	0.90	0.08	66,70,78,83	0
32	7MG	2a	527	24/25	0.91	0.11	66,72,78,82	0
54	MIA	2w	37	25/30	0.91	0.11	79,89,94,97	0
55	5MC	2x	32	21/22	0.91	0.13	75,83,87,88	0
1	5MU	1A	1937	21/22	0.92	0.10	56,63,70,74	0
32	M2G	2a	966	25/26	0.92	0.15	68,79,87,92	0
32	5MC	2a	967	21/22	0.92	0.13	78,81,86,94	0
54	PSU	2w	39	20/21	0.92	0.11	82,94,99,99	0
55	4SU	1x	8	20/21	0.92	0.11	60,68,78,79	0
32	5MC	2a	1400	21/22	0.92	0.17	72,81,85,92	0
54	5MU	1w	54	21/22	0.93	0.08	62,76,84,85	0
32	5MC	2a	1407	21/22	0.93	0.10	60,65,71,82	0
1	5MC	2A	1942	21/22	0.94	0.09	56,70,78,85	0
32	UR3	2a	1498	21/22	0.94	0.10	60,64,69,78	0
43	0TD	2l	92	10/11	0.94	0.10	64,69,74,81	0
1	5MC	2A	1962	21/22	0.94	0.11	50,57,68,78	0
32	7MG	1a	527	24/25	0.94	0.09	47,53,57,59	0
1	4OC	2A	1920	21/23	0.94	0.08	67,72,75,78	0
32	4OC	2a	1402	22/23	0.94	0.10	64,71,75,78	0
1	PSU	2A	1911	20/21	0.95	0.07	66,72,75,75	0
32	5MC	2a	1404	21/22	0.95	0.09	54,63,68,70	0
43	0TD	1l	92	10/11	0.95	0.07	48,51,54,65	0
32	PSU	1a	516	20/21	0.95	0.08	54,64,71,71	0
32	MA6	2a	1519	24/25	0.95	0.12	57,69,76,82	0
1	OMG	2A	2251	24/25	0.95	0.10	45,51,56,60	0
1	2MA	2A	2503	23/24	0.95	0.13	34,44,50,54	0
1	PSU	2A	2605	20/21	0.95	0.09	34,47,51,52	0
1	PSU	1A	1933	20/21	0.96	0.08	44,51,56,58	0
54	MIA	1w	37	29/30	0.96	0.11	51,58,69,70	0
54	PSU	1w	39	20/21	0.96	0.09	53,72,76,78	0
1	PSU	1A	1939	20/21	0.96	0.08	40,57,64,66	0
32	2MG	1a	1207	24/25	0.96	0.06	54,70,73,76	0
32	5MC	1a	1400	21/22	0.96	0.10	43,54,62,67	0
1	5MU	1A	1961	21/22	0.96	0.08	36,39,43,51	0
55	5MC	1x	32	21/22	0.96	0.10	52,57,62,65	0
1	5MC	1A	1964	21/22	0.96	0.08	46,50,55,56	0
32	MA6	2a	1518	24/25	0.96	0.10	54,70,74,77	0
1	2MA	1A	2515	23/24	0.97	0.07	21,27,32,34	0
1	2MU	1A	2564	21/23	0.97	0.07	31,36,40,44	0
32	5MC	1a	1404	21/22	0.97	0.09	42,46,51,51	0
1	2MU	2A	2552	21/23	0.97	0.06	40,45,56,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	5MC	1a	1407	21/22	0.97	0.07	40,46,50,53	0
32	UR3	1a	1498	21/22	0.97	0.08	34,45,49,55	0
32	MA6	1a	1519	24/25	0.97	0.10	43,48,53,58	0
1	4OC	1A	1942	21/23	0.97	0.09	41,49,55,56	0
1	OMG	1A	2263	24/25	0.97	0.08	24,30,34,38	0
32	M2G	1a	966	25/26	0.97	0.10	56,61,69,70	0
1	5MU	2A	1939	21/22	0.97	0.07	47,51,55,58	0
32	5MC	1a	967	21/22	0.97	0.11	57,63,68,70	0
32	4OC	1a	1402	22/23	0.98	0.07	46,53,58,68	0
32	MA6	1a	1518	24/25	0.98	0.08	40,48,52,58	0
1	5MC	1A	1984	21/22	0.98	0.06	31,45,47,49	0
1	PSU	1A	2617	20/21	0.98	0.07	24,35,39,40	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(\AA^2)	Q<0.9
56	MG	1A	3915	1/1	0.24	0.19	86,86,86,86	0
56	MG	2A	3456	1/1	0.33	0.29	97,97,97,97	0
56	MG	1x	123	1/1	0.36	0.16	85,85,85,85	0
56	MG	2A	3515	1/1	0.37	0.27	86,86,86,86	0
56	MG	2a	1642	1/1	0.40	0.36	84,84,84,84	0
56	MG	1a	1883	1/1	0.41	0.24	89,89,89,89	0
56	MG	1A	3920	1/1	0.42	0.16	95,95,95,95	0
56	MG	2a	1725	1/1	0.42	0.25	96,96,96,96	0
56	MG	1A	3838	1/1	0.43	0.29	84,84,84,84	0
56	MG	2l	101	1/1	0.43	0.22	82,82,82,82	0
56	MG	2v	102	1/1	0.43	0.36	89,89,89,89	0
56	MG	2A	3498	1/1	0.45	0.19	90,90,90,90	0
56	MG	1a	1832	1/1	0.45	0.18	78,78,78,78	0
56	MG	1A	3751	1/1	0.46	0.31	72,72,72,72	0
56	MG	1a	1853	1/1	0.47	0.21	81,81,81,81	0
56	MG	1A	3730	1/1	0.47	0.16	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3464	1/1	0.47	0.27	82,82,82,82	0
56	MG	2a	1803	1/1	0.48	0.29	82,82,82,82	0
56	MG	2a	1817	1/1	0.50	0.20	75,75,75,75	0
56	MG	2A	3329	1/1	0.51	0.17	86,86,86,86	0
56	MG	1A	3865	1/1	0.52	0.14	79,79,79,79	0
56	MG	2A	3110	1/1	0.54	0.11	85,85,85,85	0
56	MG	1a	1918	1/1	0.54	0.19	86,86,86,86	0
56	MG	1a	1936	1/1	0.54	0.16	71,71,71,71	0
56	MG	1Q	203	1/1	0.54	0.18	63,63,63,63	0
56	MG	1A	3770	1/1	0.55	0.18	74,74,74,74	0
56	MG	2a	1685	1/1	0.56	0.30	81,81,81,81	0
56	MG	2a	1779	1/1	0.57	0.24	81,81,81,81	0
56	MG	1A	3175	1/1	0.57	0.16	83,83,83,83	0
56	MG	1a	1739	1/1	0.58	0.21	75,75,75,75	0
56	MG	1A	3892	1/1	0.58	0.15	69,69,69,69	0
56	MG	1A	3766	1/1	0.58	0.18	98,98,98,98	0
56	MG	2a	1802	1/1	0.59	0.21	81,81,81,81	0
56	MG	1A	3803	1/1	0.59	0.23	55,55,55,55	0
56	MG	1B	220	1/1	0.59	0.32	81,81,81,81	0
56	MG	1a	1872	1/1	0.59	0.19	71,71,71,71	0
56	MG	1w	104	1/1	0.61	0.17	93,93,93,93	0
56	MG	2A	3197	1/1	0.61	0.34	66,66,66,66	0
56	MG	1A	3488	1/1	0.62	0.22	94,94,94,94	0
56	MG	2a	1798	1/1	0.62	0.17	89,89,89,89	0
56	MG	2a	1797	1/1	0.63	0.18	99,99,99,99	0
56	MG	2A	3061	1/1	0.63	0.28	79,79,79,79	0
56	MG	1A	3919	1/1	0.63	0.17	85,85,85,85	0
56	MG	1A	3627	1/1	0.63	0.21	56,56,56,56	0
56	MG	1a	1738	1/1	0.63	0.13	95,95,95,95	0
56	MG	2a	1827	1/1	0.63	0.16	74,74,74,74	0
56	MG	2A	3517	1/1	0.63	0.15	91,91,91,91	0
56	MG	2a	1700	1/1	0.64	0.23	77,77,77,77	0
56	MG	1a	1717	1/1	0.64	0.22	77,77,77,77	0
56	MG	2A	3333	1/1	0.64	0.20	79,79,79,79	0
56	MG	2A	3530	1/1	0.64	0.14	74,74,74,74	0
56	MG	1a	1746	1/1	0.64	0.15	85,85,85,85	0
56	MG	2a	1607	1/1	0.64	0.16	83,83,83,83	0
56	MG	1d	302	1/1	0.64	0.24	81,81,81,81	0
56	MG	2a	1663	1/1	0.64	0.28	85,85,85,85	0
56	MG	1a	1674	1/1	0.64	0.18	78,78,78,78	0
56	MG	2a	1699	1/1	0.64	0.11	81,81,81,81	0
56	MG	1A	3140	1/1	0.65	0.17	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3855	1/1	0.65	0.16	69,69,69,69	0
56	MG	2a	1621	1/1	0.66	0.15	99,99,99,99	0
56	MG	2A	3513	1/1	0.66	0.21	82,82,82,82	0
56	MG	1A	3706	1/1	0.66	0.20	55,55,55,55	0
56	MG	2a	1800	1/1	0.66	0.16	86,86,86,86	0
56	MG	2a	1664	1/1	0.66	0.13	89,89,89,89	0
56	MG	2A	3075	1/1	0.66	0.37	81,81,81,81	0
56	MG	1A	3772	1/1	0.66	0.22	76,76,76,76	0
56	MG	2A	3144	1/1	0.66	0.16	91,91,91,91	0
56	MG	1a	1879	1/1	0.66	0.13	87,87,87,87	0
56	MG	1a	1831	1/1	0.67	0.15	102,102,102,102	0
56	MG	1a	1615	1/1	0.67	0.14	83,83,83,83	0
56	MG	1a	1691	1/1	0.67	0.17	75,75,75,75	0
56	MG	2a	1723	1/1	0.67	0.18	84,84,84,84	0
56	MG	2A	3524	1/1	0.67	0.29	79,79,79,79	0
56	MG	2A	3510	1/1	0.67	0.17	87,87,87,87	0
56	MG	2T	202	1/1	0.67	0.20	82,82,82,82	0
56	MG	2A	3346	1/1	0.68	0.25	69,69,69,69	0
56	MG	2A	3447	1/1	0.68	0.18	86,86,86,86	0
56	MG	2a	1764	1/1	0.68	0.22	75,75,75,75	0
56	MG	1a	1896	1/1	0.68	0.15	73,73,73,73	0
56	MG	2A	3065	1/1	0.68	0.20	79,79,79,79	0
56	MG	2a	1649	1/1	0.68	0.17	81,81,81,81	0
56	MG	2A	3548	1/1	0.69	0.22	58,58,58,58	0
56	MG	1o	103	1/1	0.69	0.17	75,75,75,75	0
56	MG	2a	1721	1/1	0.69	0.35	82,82,82,82	0
56	MG	1a	1609	1/1	0.69	0.33	81,81,81,81	0
56	MG	2A	3451	1/1	0.69	0.19	84,84,84,84	0
56	MG	1x	112	1/1	0.69	0.13	72,72,72,72	0
56	MG	2a	1778	1/1	0.69	0.10	87,87,87,87	0
56	MG	2a	1698	1/1	0.69	0.32	86,86,86,86	0
56	MG	1A	3866	1/1	0.70	0.25	69,69,69,69	0
56	MG	2a	1672	1/1	0.70	0.16	94,94,94,94	0
56	MG	2a	1811	1/1	0.70	0.12	79,79,79,79	0
56	MG	1A	3784	1/1	0.70	0.18	76,76,76,76	0
56	MG	2A	3361	1/1	0.70	0.32	67,67,67,67	0
56	MG	2A	3459	1/1	0.70	0.16	56,56,56,56	0
56	MG	2A	3500	1/1	0.71	0.09	80,80,80,80	0
56	MG	2a	1614	1/1	0.71	0.31	84,84,84,84	0
56	MG	2A	3063	1/1	0.71	0.26	69,69,69,69	0
56	MG	1A	3648	1/1	0.71	0.13	77,77,77,77	0
56	MG	2a	1644	1/1	0.71	0.17	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3442	1/1	0.71	0.15	78,78,78,78	0
56	MG	2a	1787	1/1	0.71	0.18	84,84,84,84	0
56	MG	2a	1654	1/1	0.71	0.25	76,76,76,76	0
56	MG	1A	3085	1/1	0.71	0.24	73,73,73,73	0
56	MG	1A	3727	1/1	0.71	0.16	65,65,65,65	0
56	MG	1a	1912	1/1	0.71	0.20	71,71,71,71	0
56	MG	2A	3541	1/1	0.71	0.11	85,85,85,85	0
56	MG	2a	1686	1/1	0.71	0.18	80,80,80,80	0
56	MG	1a	1862	1/1	0.71	0.13	78,78,78,78	0
56	MG	2a	1821	1/1	0.71	0.34	67,67,67,67	0
56	MG	2A	3020	1/1	0.71	0.26	72,72,72,72	0
56	MG	1A	3185	1/1	0.71	0.25	73,73,73,73	0
56	MG	2a	1623	1/1	0.72	0.23	70,70,70,70	0
56	MG	1A	3868	1/1	0.72	0.10	83,83,83,83	0
56	MG	1a	1882	1/1	0.72	0.14	86,86,86,86	0
56	MG	1A	3658	1/1	0.72	0.21	66,66,66,66	0
56	MG	2a	1782	1/1	0.72	0.36	65,65,65,65	0
56	MG	1a	1894	1/1	0.72	0.14	67,67,67,67	0
56	MG	1A	3900	1/1	0.72	0.17	75,75,75,75	0
56	MG	1A	3647	1/1	0.72	0.15	91,91,91,91	0
56	MG	1A	3253	1/1	0.72	0.17	73,73,73,73	0
56	MG	2A	3545	1/1	0.72	0.20	72,72,72,72	0
56	MG	1a	1859	1/1	0.72	0.12	79,79,79,79	0
56	MG	1A	3794	1/1	0.72	0.17	59,59,59,59	0
56	MG	2A	3140	1/1	0.72	0.18	71,71,71,71	0
56	MG	1A	3800	1/1	0.72	0.11	68,68,68,68	0
56	MG	1v	101	1/1	0.72	0.41	73,73,73,73	0
56	MG	2A	3503	1/1	0.72	0.12	89,89,89,89	0
56	MG	2a	1658	1/1	0.73	0.22	77,77,77,77	0
56	MG	2A	3496	1/1	0.73	0.23	91,91,91,91	0
56	MG	2A	3340	1/1	0.73	0.13	69,69,69,69	0
56	MG	2A	3086	1/1	0.73	0.21	67,67,67,67	0
56	MG	1A	3449	1/1	0.73	0.14	51,51,51,51	0
56	MG	2A	3435	1/1	0.73	0.15	74,74,74,74	0
56	MG	1a	1890	1/1	0.73	0.12	83,83,83,83	0
56	MG	1A	3151	1/1	0.73	0.14	68,68,68,68	0
56	MG	1a	1693	1/1	0.73	0.17	63,63,63,63	0
56	MG	2a	1717	1/1	0.73	0.21	77,77,77,77	0
56	MG	2A	3308	1/1	0.73	0.24	58,58,58,58	0
56	MG	2A	3526	1/1	0.73	0.14	76,76,76,76	0
56	MG	2a	1822	1/1	0.73	0.21	71,71,71,71	0
56	MG	1A	3752	1/1	0.73	0.16	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1616	1/1	0.73	0.13	61,61,61,61	0
56	MG	2A	3441	1/1	0.74	0.18	85,85,85,85	0
56	MG	1A	3887	1/1	0.74	0.13	61,61,61,61	0
56	MG	1A	3761	1/1	0.74	0.13	79,79,79,79	0
56	MG	1a	1723	1/1	0.74	0.17	80,80,80,80	0
56	MG	1A	3929	1/1	0.74	0.34	69,69,69,69	0
56	MG	1x	102	1/1	0.74	0.14	80,80,80,80	0
56	MG	2A	3341	1/1	0.74	0.24	81,81,81,81	0
56	MG	1a	1666	1/1	0.74	0.18	90,90,90,90	0
56	MG	2a	1722	1/1	0.74	0.20	79,79,79,79	0
56	MG	2A	3353	1/1	0.74	0.22	81,81,81,81	0
56	MG	2a	1819	1/1	0.74	0.34	57,57,57,57	0
56	MG	1A	3631	1/1	0.74	0.16	77,77,77,77	0
56	MG	2a	1732	1/1	0.74	0.23	90,90,90,90	0
56	MG	2G	201	1/1	0.74	0.20	75,75,75,75	0
56	MG	1A	3856	1/1	0.74	0.21	70,70,70,70	0
56	MG	2x	103	1/1	0.74	0.11	83,83,83,83	0
56	MG	2x	107	1/1	0.74	0.17	80,80,80,80	0
56	MG	1A	3922	1/1	0.75	0.14	67,67,67,67	0
56	MG	2A	3291	1/1	0.75	0.23	82,82,82,82	0
56	MG	2A	3458	1/1	0.75	0.23	73,73,73,73	0
56	MG	2a	1730	1/1	0.75	0.17	83,83,83,83	0
56	MG	1A	3313	1/1	0.75	0.21	75,75,75,75	0
56	MG	2a	1734	1/1	0.75	0.14	59,59,59,59	0
56	MG	1A	3208	1/1	0.75	0.22	84,84,84,84	0
56	MG	2a	1775	1/1	0.75	0.22	73,73,73,73	0
56	MG	2A	3471	1/1	0.75	0.20	78,78,78,78	0
56	MG	2A	3484	1/1	0.75	0.25	67,67,67,67	0
56	MG	2A	3055	1/1	0.75	0.28	69,69,69,69	0
56	MG	1a	1953	1/1	0.75	0.10	83,83,83,83	0
56	MG	1F	303	1/1	0.75	0.24	75,75,75,75	0
56	MG	2A	3342	1/1	0.75	0.13	77,77,77,77	0
56	MG	1l	203	1/1	0.75	0.23	71,71,71,71	0
56	MG	2A	3350	1/1	0.75	0.10	66,66,66,66	0
56	MG	1o	101	1/1	0.75	0.14	80,80,80,80	0
56	MG	2a	1667	1/1	0.75	0.20	81,81,81,81	0
56	MG	1A	3166	1/1	0.75	0.33	58,58,58,58	0
56	MG	2A	3370	1/1	0.75	0.26	60,60,60,60	0
56	MG	2A	3387	1/1	0.75	0.18	73,73,73,73	0
56	MG	1A	3726	1/1	0.75	0.23	63,63,63,63	0
56	MG	1a	1855	1/1	0.75	0.13	63,63,63,63	0
56	MG	2A	3543	1/1	0.75	0.13	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3757	1/1	0.75	0.23	65,65,65,65	0
56	MG	2A	3151	1/1	0.75	0.26	65,65,65,65	0
56	MG	1A	3230	1/1	0.76	0.16	76,76,76,76	0
56	MG	1A	3654	1/1	0.76	0.13	76,76,76,76	0
56	MG	1A	3417	1/1	0.76	0.20	51,51,51,51	0
56	MG	2a	1695	1/1	0.76	0.23	80,80,80,80	0
56	MG	1a	1814	1/1	0.76	0.17	76,76,76,76	0
56	MG	1A	3024	1/1	0.76	0.23	74,74,74,74	0
56	MG	2A	3059	1/1	0.76	0.25	75,75,75,75	0
56	MG	1A	3880	1/1	0.76	0.19	66,66,66,66	0
56	MG	1a	1709	1/1	0.76	0.44	68,68,68,68	0
56	MG	1a	1610	1/1	0.76	0.17	71,71,71,71	0
56	MG	1A	3484	1/1	0.76	0.18	51,51,51,51	0
56	MG	2a	1724	1/1	0.76	0.21	77,77,77,77	0
56	MG	1a	1931	1/1	0.77	0.12	92,92,92,92	0
56	MG	2A	3047	1/1	0.77	0.24	46,46,46,46	0
56	MG	1a	1724	1/1	0.77	0.29	75,75,75,75	0
56	MG	1a	1942	1/1	0.77	0.18	79,79,79,79	0
56	MG	1B	206	1/1	0.77	0.10	61,61,61,61	0
56	MG	1A	3409	1/1	0.77	0.17	69,69,69,69	0
56	MG	2a	1620	1/1	0.77	0.11	92,92,92,92	0
56	MG	1A	3218	1/1	0.77	0.15	75,75,75,75	0
56	MG	2A	3067	1/1	0.77	0.27	80,80,80,80	0
56	MG	1a	1757	1/1	0.77	0.12	69,69,69,69	0
56	MG	2A	3505	1/1	0.77	0.12	82,82,82,82	0
56	MG	2A	3509	1/1	0.77	0.20	57,57,57,57	0
56	MG	1a	1774	1/1	0.77	0.12	76,76,76,76	0
56	MG	2A	3511	1/1	0.77	0.21	87,87,87,87	0
56	MG	2A	3364	1/1	0.77	0.29	62,62,62,62	0
56	MG	1A	3668	1/1	0.77	0.26	69,69,69,69	0
56	MG	2A	3130	1/1	0.77	0.15	73,73,73,73	0
56	MG	1v	102	1/1	0.77	0.23	67,67,67,67	0
56	MG	2a	1804	1/1	0.77	0.26	78,78,78,78	0
56	MG	2a	1676	1/1	0.77	0.09	84,84,84,84	0
56	MG	2a	1815	1/1	0.77	0.22	71,71,71,71	0
56	MG	14	502	1/1	0.77	0.09	79,79,79,79	0
56	MG	2A	3529	1/1	0.77	0.12	82,82,82,82	0
56	MG	1A	3438	1/1	0.77	0.12	78,78,78,78	0
56	MG	2A	3538	1/1	0.77	0.18	66,66,66,66	0
56	MG	2A	3163	1/1	0.77	0.10	76,76,76,76	0
56	MG	1A	3782	1/1	0.77	0.23	76,76,76,76	0
56	MG	1A	3532	1/1	0.77	0.43	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3547	1/1	0.77	0.11	81,81,81,81	0
56	MG	2a	1763	1/1	0.78	0.28	55,55,55,55	0
56	MG	1A	3755	1/1	0.78	0.15	54,54,54,54	0
56	MG	2A	3540	1/1	0.78	0.10	84,84,84,84	0
56	MG	1a	1781	1/1	0.78	0.08	75,75,75,75	0
56	MG	2A	3542	1/1	0.78	0.13	83,83,83,83	0
56	MG	2a	1781	1/1	0.78	0.21	73,73,73,73	0
56	MG	2A	3495	1/1	0.78	0.10	74,74,74,74	0
56	MG	1q	202	1/1	0.78	0.10	76,76,76,76	0
56	MG	2A	3307	1/1	0.78	0.20	75,75,75,75	0
56	MG	2A	3407	1/1	0.78	0.27	59,59,59,59	0
56	MG	2A	3413	1/1	0.78	0.18	47,47,47,47	0
56	MG	2a	1801	1/1	0.78	0.11	75,75,75,75	0
56	MG	2A	3433	1/1	0.78	0.25	51,51,51,51	0
56	MG	1a	1922	1/1	0.78	0.10	82,82,82,82	0
56	MG	1a	1923	1/1	0.78	0.13	81,81,81,81	0
56	MG	2a	1707	1/1	0.78	0.14	72,72,72,72	0
56	MG	1a	1924	1/1	0.78	0.14	83,83,83,83	0
56	MG	1A	3642	1/1	0.78	0.12	63,63,63,63	0
56	MG	1A	3630	1/1	0.78	0.20	78,78,78,78	0
56	MG	13	104	1/1	0.78	0.20	70,70,70,70	0
56	MG	2a	1631	1/1	0.78	0.20	100,100,100,100	0
56	MG	1A	3817	1/1	0.78	0.18	49,49,49,49	0
56	MG	1B	204	1/1	0.78	0.13	63,63,63,63	0
56	MG	2A	3461	1/1	0.78	0.11	58,58,58,58	0
56	MG	1A	3537	1/1	0.78	0.19	57,57,57,57	0
56	MG	1A	3029	1/1	0.79	0.26	63,63,63,63	0
56	MG	1A	3331	1/1	0.79	0.12	55,55,55,55	0
56	MG	1A	3377	1/1	0.79	0.13	63,63,63,63	0
56	MG	2A	3563	1/1	0.79	0.18	78,78,78,78	0
56	MG	1a	1925	1/1	0.79	0.11	64,64,64,64	0
56	MG	1a	1891	1/1	0.79	0.16	78,78,78,78	0
56	MG	2A	3169	1/1	0.79	0.15	67,67,67,67	0
56	MG	1a	1934	1/1	0.79	0.16	57,57,57,57	0
56	MG	2A	3255	1/1	0.79	0.09	76,76,76,76	0
56	MG	2a	1616	1/1	0.79	0.19	81,81,81,81	0
56	MG	1A	3293	1/1	0.79	0.19	38,38,38,38	0
56	MG	1a	1868	1/1	0.79	0.15	68,68,68,68	0
56	MG	1x	111	1/1	0.79	0.09	70,70,70,70	0
56	MG	2a	1627	1/1	0.79	0.28	78,78,78,78	0
56	MG	2A	3489	1/1	0.79	0.11	72,72,72,72	0
56	MG	2A	3493	1/1	0.79	0.19	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1B	229	1/1	0.79	0.11	68,68,68,68	0
56	MG	2A	3417	1/1	0.79	0.19	68,68,68,68	0
56	MG	2a	1729	1/1	0.79	0.26	84,84,84,84	0
56	MG	2a	1652	1/1	0.79	0.21	76,76,76,76	0
56	MG	2a	1731	1/1	0.79	0.21	72,72,72,72	0
56	MG	2a	1823	1/1	0.79	0.10	88,88,88,88	0
56	MG	2a	1825	1/1	0.79	0.13	58,58,58,58	0
56	MG	2A	3332	1/1	0.79	0.34	80,80,80,80	0
56	MG	1a	1847	1/1	0.79	0.13	74,74,74,74	0
56	MG	2x	102	1/1	0.79	0.15	73,73,73,73	0
56	MG	2a	1739	1/1	0.79	0.14	79,79,79,79	0
56	MG	2a	1751	1/1	0.79	0.25	62,62,62,62	0
56	MG	2B	206	1/1	0.80	0.24	73,73,73,73	0
56	MG	1A	3138	1/1	0.80	0.29	65,65,65,65	0
56	MG	1B	218	1/1	0.80	0.17	76,76,76,76	0
56	MG	1A	3873	1/1	0.80	0.09	52,52,52,52	0
56	MG	2A	3229	1/1	0.80	0.20	72,72,72,72	0
56	MG	1A	3398	1/1	0.80	0.21	78,78,78,78	0
56	MG	2a	1737	1/1	0.80	0.14	72,72,72,72	0
56	MG	1w	103	1/1	0.80	0.13	81,81,81,81	0
56	MG	1A	3057	1/1	0.80	0.19	91,91,91,91	0
56	MG	1A	3635	1/1	0.80	0.12	69,69,69,69	0
56	MG	1A	3716	1/1	0.80	0.12	63,63,63,63	0
56	MG	1A	3904	1/1	0.80	0.21	41,41,41,41	0
56	MG	2a	1777	1/1	0.80	0.13	85,85,85,85	0
56	MG	1A	3909	1/1	0.80	0.13	75,75,75,75	0
56	MG	1A	3914	1/1	0.80	0.10	64,64,64,64	0
56	MG	2A	3043	1/1	0.80	0.13	53,53,53,53	0
56	MG	1a	1819	1/1	0.80	0.23	70,70,70,70	0
56	MG	1A	3494	1/1	0.80	0.15	69,69,69,69	0
56	MG	1A	3852	1/1	0.80	0.18	61,61,61,61	0
56	MG	1a	1929	1/1	0.80	0.11	87,87,87,87	0
56	MG	1A	3168	1/1	0.80	0.24	81,81,81,81	0
56	MG	1A	3771	1/1	0.80	0.10	64,64,64,64	0
56	MG	2A	3367	1/1	0.80	0.31	69,69,69,69	0
56	MG	2A	3369	1/1	0.80	0.25	68,68,68,68	0
56	MG	1a	1684	1/1	0.80	0.21	81,81,81,81	0
56	MG	2a	1805	1/1	0.80	0.09	95,95,95,95	0
56	MG	1A	3149	1/1	0.80	0.10	70,70,70,70	0
56	MG	1A	3932	1/1	0.80	0.22	65,65,65,65	0
56	MG	1a	1700	1/1	0.80	0.11	73,73,73,73	0
56	MG	2A	3127	1/1	0.80	0.15	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1l	202	1/1	0.80	0.31	70,70,70,70	0
56	MG	2A	3134	1/1	0.80	0.26	69,69,69,69	0
56	MG	1A	3749	1/1	0.80	0.14	66,66,66,66	0
56	MG	2a	1712	1/1	0.80	0.11	74,74,74,74	0
56	MG	1a	1876	1/1	0.80	0.23	83,83,83,83	0
56	MG	2A	3546	1/1	0.80	0.22	70,70,70,70	0
56	MG	2w	101	1/1	0.80	0.14	83,83,83,83	0
56	MG	2A	3150	1/1	0.80	0.31	65,65,65,65	0
56	MG	1o	102	1/1	0.80	0.15	76,76,76,76	0
56	MG	2A	3154	1/1	0.80	0.26	46,46,46,46	0
56	MG	2B	211	1/1	0.81	0.14	90,90,90,90	0
56	MG	2F	304	1/1	0.81	0.13	75,75,75,75	0
56	MG	2A	3294	1/1	0.81	0.36	64,64,64,64	0
56	MG	1A	3507	1/1	0.81	0.18	49,49,49,49	0
56	MG	1A	3194	1/1	0.81	0.08	58,58,58,58	0
56	MG	2A	3474	1/1	0.81	0.39	67,67,67,67	0
56	MG	2A	3314	1/1	0.81	0.27	67,67,67,67	0
56	MG	2A	3328	1/1	0.81	0.24	69,69,69,69	0
56	MG	2a	1746	1/1	0.81	0.26	77,77,77,77	0
56	MG	2a	1617	1/1	0.81	0.07	101,101,101,101	0
56	MG	1a	1726	1/1	0.81	0.08	75,75,75,75	0
56	MG	1A	3199	1/1	0.81	0.29	68,68,68,68	0
56	MG	1A	3105	1/1	0.81	0.28	41,41,41,41	0
56	MG	1a	1741	1/1	0.81	0.11	73,73,73,73	0
56	MG	1A	3741	1/1	0.81	0.14	49,49,49,49	0
56	MG	1a	1754	1/1	0.81	0.22	62,62,62,62	0
56	MG	1a	1877	1/1	0.81	0.17	70,70,70,70	0
56	MG	2a	1648	1/1	0.81	0.23	76,76,76,76	0
56	MG	1a	1680	1/1	0.81	0.38	83,83,83,83	0
56	MG	1A	3129	1/1	0.81	0.09	83,83,83,83	0
56	MG	1a	1775	1/1	0.81	0.16	62,62,62,62	0
56	MG	1a	1780	1/1	0.81	0.16	67,67,67,67	0
56	MG	1A	3882	1/1	0.81	0.10	72,72,72,72	0
56	MG	1a	1785	1/1	0.81	0.12	64,64,64,64	0
56	MG	1a	1787	1/1	0.81	0.16	83,83,83,83	0
56	MG	1a	1898	1/1	0.81	0.18	78,78,78,78	0
56	MG	2A	3527	1/1	0.81	0.23	73,73,73,73	0
56	MG	1a	1908	1/1	0.81	0.16	72,72,72,72	0
56	MG	1a	1800	1/1	0.81	0.32	80,80,80,80	0
56	MG	2a	1694	1/1	0.81	0.17	77,77,77,77	0
56	MG	1A	3146	1/1	0.81	0.11	69,69,69,69	0
56	MG	2A	3418	1/1	0.81	0.08	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3186	1/1	0.81	0.16	68,68,68,68	0
56	MG	2A	3190	1/1	0.81	0.26	61,61,61,61	0
56	MG	1x	115	1/1	0.81	0.17	79,79,79,79	0
56	MG	2A	3223	1/1	0.81	0.27	38,38,38,38	0
56	MG	19	101	1/1	0.81	0.18	70,70,70,70	0
56	MG	1A	3898	1/1	0.81	0.14	41,41,41,41	0
56	MG	2A	3287	1/1	0.81	0.26	60,60,60,60	0
56	MG	2A	3290	1/1	0.81	0.18	55,55,55,55	0
56	MG	2A	3030	1/1	0.81	0.22	56,56,56,56	0
56	MG	1a	1902	1/1	0.82	0.08	85,85,85,85	0
56	MG	2A	3445	1/1	0.82	0.12	84,84,84,84	0
56	MG	1A	3312	1/1	0.82	0.30	65,65,65,65	0
56	MG	2A	3281	1/1	0.82	0.28	40,40,40,40	0
56	MG	2A	3561	1/1	0.82	0.22	64,64,64,64	0
56	MG	1A	3137	1/1	0.82	0.22	70,70,70,70	0
56	MG	1a	1686	1/1	0.82	0.17	64,64,64,64	0
56	MG	1A	3215	1/1	0.82	0.10	67,67,67,67	0
56	MG	1A	3759	1/1	0.82	0.28	73,73,73,73	0
56	MG	1A	3217	1/1	0.82	0.41	63,63,63,63	0
56	MG	2Q	202	1/1	0.82	0.31	75,75,75,75	0
56	MG	1A	3187	1/1	0.82	0.16	81,81,81,81	0
56	MG	2A	3473	1/1	0.82	0.29	66,66,66,66	0
56	MG	2a	1606	1/1	0.82	0.26	87,87,87,87	0
56	MG	2A	3311	1/1	0.82	0.26	60,60,60,60	0
56	MG	2a	1749	1/1	0.82	0.18	62,62,62,62	0
56	MG	2A	3481	1/1	0.82	0.24	71,71,71,71	0
56	MG	2a	1756	1/1	0.82	0.26	68,68,68,68	0
56	MG	2a	1760	1/1	0.82	0.36	61,61,61,61	0
56	MG	2a	1762	1/1	0.82	0.43	62,62,62,62	0
56	MG	2a	1615	1/1	0.82	0.23	81,81,81,81	0
56	MG	1a	1711	1/1	0.82	0.18	75,75,75,75	0
56	MG	2a	1771	1/1	0.82	0.28	82,82,82,82	0
56	MG	1A	3768	1/1	0.82	0.17	71,71,71,71	0
56	MG	2a	1619	1/1	0.82	0.23	80,80,80,80	0
56	MG	2A	3490	1/1	0.82	0.10	68,68,68,68	0
56	MG	2A	3491	1/1	0.82	0.13	68,68,68,68	0
56	MG	2A	3062	1/1	0.82	0.23	59,59,59,59	0
56	MG	1A	3769	1/1	0.82	0.11	66,66,66,66	0
56	MG	1A	3876	1/1	0.82	0.12	59,59,59,59	0
56	MG	2a	1790	1/1	0.82	0.12	92,92,92,92	0
56	MG	2a	1795	1/1	0.82	0.11	85,85,85,85	0
56	MG	2a	1635	1/1	0.82	0.25	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1637	1/1	0.82	0.22	64,64,64,64	0
56	MG	2A	3066	1/1	0.82	0.29	59,59,59,59	0
56	MG	1A	3403	1/1	0.82	0.13	56,56,56,56	0
56	MG	1A	3604	1/1	0.82	0.18	71,71,71,71	0
56	MG	1A	3176	1/1	0.82	0.35	77,77,77,77	0
56	MG	1e	201	1/1	0.82	0.11	77,77,77,77	0
56	MG	1A	3775	1/1	0.82	0.15	59,59,59,59	0
56	MG	1A	3161	1/1	0.82	0.19	67,67,67,67	0
56	MG	1A	3202	1/1	0.82	0.22	74,74,74,74	0
56	MG	1A	3298	1/1	0.82	0.16	58,58,58,58	0
56	MG	1A	3798	1/1	0.82	0.22	64,64,64,64	0
56	MG	1a	1888	1/1	0.82	0.13	75,75,75,75	0
56	MG	1A	3744	1/1	0.82	0.15	72,72,72,72	0
56	MG	1a	1778	1/1	0.82	0.21	53,53,53,53	0
56	MG	2A	3411	1/1	0.82	0.23	69,69,69,69	0
56	MG	1v	103	1/1	0.82	0.24	79,79,79,79	0
56	MG	1a	1892	1/1	0.82	0.15	68,68,68,68	0
56	MG	1A	3641	1/1	0.82	0.14	66,66,66,66	0
56	MG	1A	3461	1/1	0.82	0.12	58,58,58,58	0
56	MG	2A	3208	1/1	0.82	0.29	42,42,42,42	0
56	MG	1a	1782	1/1	0.82	0.20	81,81,81,81	0
56	MG	1a	1764	1/1	0.83	0.22	69,69,69,69	0
56	MG	2a	1679	1/1	0.83	0.20	73,73,73,73	0
56	MG	2a	1776	1/1	0.83	0.12	80,80,80,80	0
56	MG	1A	3881	1/1	0.83	0.22	62,62,62,62	0
56	MG	1A	3452	1/1	0.83	0.09	52,52,52,52	0
56	MG	1A	3796	1/1	0.83	0.11	73,73,73,73	0
56	MG	1A	3130	1/1	0.83	0.18	54,54,54,54	0
56	MG	2a	1608	1/1	0.83	0.31	61,61,61,61	0
56	MG	2A	3522	1/1	0.83	0.11	81,81,81,81	0
56	MG	1A	3860	1/1	0.83	0.09	88,88,88,88	0
56	MG	1a	1613	1/1	0.83	0.15	74,74,74,74	0
56	MG	2A	3258	1/1	0.83	0.38	43,43,43,43	0
56	MG	1B	205	1/1	0.83	0.10	50,50,50,50	0
56	MG	2A	3082	1/1	0.83	0.22	63,63,63,63	0
56	MG	2A	3536	1/1	0.83	0.38	57,57,57,57	0
56	MG	1A	3113	1/1	0.83	0.17	69,69,69,69	0
56	MG	2A	3381	1/1	0.83	0.11	59,59,59,59	0
56	MG	2A	3382	1/1	0.83	0.10	84,84,84,84	0
56	MG	1a	1619	1/1	0.83	0.30	71,71,71,71	0
56	MG	2a	1809	1/1	0.83	0.10	74,74,74,74	0
56	MG	1a	1805	1/1	0.83	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1659	1/1	0.83	0.23	40,40,40,40	0
56	MG	1A	3802	1/1	0.83	0.11	65,65,65,65	0
56	MG	2a	1646	1/1	0.83	0.37	58,58,58,58	0
56	MG	2A	3494	1/1	0.83	0.08	79,79,79,79	0
56	MG	1a	1947	1/1	0.83	0.16	81,81,81,81	0
56	MG	1A	3002	1/1	0.83	0.13	66,66,66,66	0
56	MG	1A	3591	1/1	0.83	0.23	53,53,53,53	0
56	MG	2a	1655	1/1	0.83	0.22	72,72,72,72	0
56	MG	1A	3640	1/1	0.83	0.14	68,68,68,68	0
56	MG	2B	209	1/1	0.83	0.10	76,76,76,76	0
56	MG	2A	3439	1/1	0.83	0.18	75,75,75,75	0
56	MG	1A	3846	1/1	0.83	0.09	42,42,42,42	0
56	MG	1a	1900	1/1	0.83	0.19	72,72,72,72	0
56	MG	1A	3453	1/1	0.84	0.30	56,56,56,56	0
56	MG	1a	1790	1/1	0.84	0.15	69,69,69,69	0
56	MG	1A	3296	1/1	0.84	0.26	73,73,73,73	0
56	MG	2a	1713	1/1	0.84	0.14	72,72,72,72	0
56	MG	2a	1715	1/1	0.84	0.23	69,69,69,69	0
56	MG	1A	3418	1/1	0.84	0.13	55,55,55,55	0
56	MG	2A	3549	1/1	0.84	0.12	53,53,53,53	0
56	MG	2A	3552	1/1	0.84	0.15	70,70,70,70	0
56	MG	2A	3254	1/1	0.84	0.36	63,63,63,63	0
56	MG	1x	116	1/1	0.84	0.10	78,78,78,78	0
56	MG	2B	203	1/1	0.84	0.18	75,75,75,75	0
56	MG	2a	1727	1/1	0.84	0.09	97,97,97,97	0
56	MG	1A	3645	1/1	0.84	0.18	60,60,60,60	0
56	MG	2A	3261	1/1	0.84	0.30	71,71,71,71	0
56	MG	2A	3454	1/1	0.84	0.28	81,81,81,81	0
56	MG	2F	301	1/1	0.84	0.20	63,63,63,63	0
56	MG	2A	3270	1/1	0.84	0.25	64,64,64,64	0
56	MG	1A	3611	1/1	0.84	0.12	57,57,57,57	0
56	MG	1a	1823	1/1	0.84	0.16	69,69,69,69	0
56	MG	2A	3032	1/1	0.84	0.10	68,68,68,68	0
56	MG	1A	3806	1/1	0.84	0.14	58,58,58,58	0
56	MG	2a	1605	1/1	0.84	0.40	73,73,73,73	0
56	MG	2A	3469	1/1	0.84	0.14	71,71,71,71	0
56	MG	1A	3809	1/1	0.84	0.18	86,86,86,86	0
56	MG	2A	3303	1/1	0.84	0.31	56,56,56,56	0
56	MG	2a	1611	1/1	0.84	0.28	80,80,80,80	0
56	MG	1a	1844	1/1	0.84	0.14	53,53,53,53	0
56	MG	1A	3422	1/1	0.84	0.20	61,61,61,61	0
56	MG	1A	3254	1/1	0.84	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1607	1/1	0.84	0.24	63,63,63,63	0
56	MG	2A	3327	1/1	0.84	0.21	86,86,86,86	0
56	MG	1A	3655	1/1	0.84	0.16	73,73,73,73	0
56	MG	1A	3850	1/1	0.84	0.21	59,59,59,59	0
56	MG	1a	1944	1/1	0.84	0.09	70,70,70,70	0
56	MG	1a	1611	1/1	0.84	0.14	64,64,64,64	0
56	MG	2a	1786	1/1	0.84	0.20	72,72,72,72	0
56	MG	1a	1745	1/1	0.84	0.26	71,71,71,71	0
56	MG	1a	1954	1/1	0.84	0.10	70,70,70,70	0
56	MG	2a	1793	1/1	0.84	0.16	73,73,73,73	0
56	MG	2a	1794	1/1	0.84	0.15	88,88,88,88	0
56	MG	1A	3851	1/1	0.84	0.16	61,61,61,61	0
56	MG	2A	3098	1/1	0.84	0.19	74,74,74,74	0
56	MG	1A	3142	1/1	0.84	0.13	60,60,60,60	0
56	MG	2a	1799	1/1	0.84	0.09	68,68,68,68	0
56	MG	1A	3665	1/1	0.84	0.11	59,59,59,59	0
56	MG	2A	3354	1/1	0.84	0.13	84,84,84,84	0
56	MG	2A	3128	1/1	0.84	0.25	73,73,73,73	0
56	MG	1A	3666	1/1	0.84	0.14	80,80,80,80	0
56	MG	2A	3132	1/1	0.84	0.12	84,84,84,84	0
56	MG	1a	1621	1/1	0.84	0.20	39,39,39,39	0
56	MG	2a	1808	1/1	0.84	0.14	77,77,77,77	0
56	MG	2A	3136	1/1	0.84	0.23	55,55,55,55	0
56	MG	1a	1886	1/1	0.84	0.11	81,81,81,81	0
56	MG	1A	3858	1/1	0.84	0.15	71,71,71,71	0
56	MG	1a	1662	1/1	0.84	0.43	76,76,76,76	0
56	MG	2a	1669	1/1	0.84	0.09	91,91,91,91	0
56	MG	2A	3399	1/1	0.84	0.15	41,41,41,41	0
56	MG	1A	3785	1/1	0.84	0.17	73,73,73,73	0
56	MG	2A	3532	1/1	0.84	0.32	64,64,64,64	0
56	MG	2a	1824	1/1	0.84	0.19	73,73,73,73	0
56	MG	1A	3792	1/1	0.84	0.26	78,78,78,78	0
56	MG	1A	3793	1/1	0.84	0.21	65,65,65,65	0
56	MG	2g	201	1/1	0.84	0.15	88,88,88,88	0
56	MG	2a	1691	1/1	0.84	0.11	90,90,90,90	0
56	MG	1A	3412	1/1	0.84	0.10	49,49,49,49	0
56	MG	2x	101	1/1	0.84	0.33	58,58,58,58	0
56	MG	1a	1897	1/1	0.84	0.07	83,83,83,83	0
56	MG	2A	3426	1/1	0.84	0.17	56,56,56,56	0
56	MG	2A	3429	1/1	0.84	0.19	74,74,74,74	0
56	MG	2W	201	1/1	0.85	0.21	76,76,76,76	0
56	MG	20	102	1/1	0.85	0.40	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1863	1/1	0.85	0.08	80,80,80,80	0
56	MG	28	102	1/1	0.85	0.13	69,69,69,69	0
56	MG	2A	3102	1/1	0.85	0.50	66,66,66,66	0
56	MG	1A	3428	1/1	0.85	0.19	69,69,69,69	0
56	MG	2A	3492	1/1	0.85	0.19	69,69,69,69	0
56	MG	1A	3508	1/1	0.85	0.17	63,63,63,63	0
56	MG	2a	1609	1/1	0.85	0.25	79,79,79,79	0
56	MG	2a	1738	1/1	0.85	0.41	75,75,75,75	0
56	MG	2a	1610	1/1	0.85	0.15	83,83,83,83	0
56	MG	1A	3048	1/1	0.85	0.27	46,46,46,46	0
56	MG	2A	3129	1/1	0.85	0.23	73,73,73,73	0
56	MG	1A	3121	1/1	0.85	0.19	49,49,49,49	0
56	MG	1a	1747	1/1	0.85	0.18	63,63,63,63	0
56	MG	1A	3329	1/1	0.85	0.10	47,47,47,47	0
56	MG	1A	3928	1/1	0.85	0.10	62,62,62,62	0
56	MG	2A	3504	1/1	0.85	0.16	74,74,74,74	0
56	MG	1a	1763	1/1	0.85	0.14	73,73,73,73	0
56	MG	2a	1769	1/1	0.85	0.20	70,70,70,70	0
56	MG	1A	3646	1/1	0.85	0.08	64,64,64,64	0
56	MG	2a	1774	1/1	0.85	0.16	79,79,79,79	0
56	MG	1a	1626	1/1	0.85	0.12	75,75,75,75	0
56	MG	1a	1651	1/1	0.85	0.28	56,56,56,56	0
56	MG	1A	3869	1/1	0.85	0.12	65,65,65,65	0
56	MG	1a	1779	1/1	0.85	0.10	68,68,68,68	0
56	MG	2a	1640	1/1	0.85	0.28	64,64,64,64	0
56	MG	1A	3592	1/1	0.85	0.20	48,48,48,48	0
56	MG	2A	3183	1/1	0.85	0.25	61,61,61,61	0
56	MG	1A	3213	1/1	0.85	0.24	57,57,57,57	0
56	MG	2A	3196	1/1	0.85	0.27	57,57,57,57	0
56	MG	1A	3824	1/1	0.85	0.17	62,62,62,62	0
56	MG	1a	1899	1/1	0.85	0.18	77,77,77,77	0
56	MG	2A	3211	1/1	0.85	0.29	42,42,42,42	0
56	MG	1a	1679	1/1	0.85	0.24	70,70,70,70	0
56	MG	1a	1786	1/1	0.85	0.13	75,75,75,75	0
56	MG	2A	3237	1/1	0.85	0.13	55,55,55,55	0
56	MG	2A	3539	1/1	0.85	0.13	86,86,86,86	0
56	MG	2a	1666	1/1	0.85	0.27	75,75,75,75	0
56	MG	2A	3239	1/1	0.85	0.24	40,40,40,40	0
56	MG	2A	3007	1/1	0.85	0.16	72,72,72,72	0
56	MG	1B	209	1/1	0.85	0.10	67,67,67,67	0
56	MG	2a	1673	1/1	0.85	0.07	88,88,88,88	0
56	MG	2A	3023	1/1	0.85	0.10	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3833	1/1	0.85	0.12	67,67,67,67	0
56	MG	1A	3649	1/1	0.85	0.11	65,65,65,65	0
56	MG	2A	3448	1/1	0.85	0.17	71,71,71,71	0
56	MG	2a	1814	1/1	0.85	0.10	73,73,73,73	0
56	MG	2a	1688	1/1	0.85	0.35	72,72,72,72	0
56	MG	1B	228	1/1	0.85	0.10	80,80,80,80	0
56	MG	2a	1693	1/1	0.85	0.11	85,85,85,85	0
56	MG	1A	3883	1/1	0.85	0.24	43,43,43,43	0
56	MG	1A	3842	1/1	0.85	0.23	63,63,63,63	0
56	MG	1A	3358	1/1	0.85	0.15	62,62,62,62	0
56	MG	1A	3617	1/1	0.85	0.13	50,50,50,50	0
56	MG	1a	1714	1/1	0.85	0.10	80,80,80,80	0
56	MG	1A	3080	1/1	0.85	0.12	57,57,57,57	0
56	MG	15	103	1/1	0.85	0.14	77,77,77,77	0
56	MG	1a	1938	1/1	0.85	0.14	84,84,84,84	0
56	MG	1A	3419	1/1	0.85	0.14	55,55,55,55	0
56	MG	1A	3908	1/1	0.85	0.13	61,61,61,61	0
56	MG	2A	3475	1/1	0.85	0.14	62,62,62,62	0
56	MG	1a	1730	1/1	0.85	0.11	76,76,76,76	0
56	MG	2x	104	1/1	0.85	0.10	68,68,68,68	0
56	MG	2x	106	1/1	0.85	0.22	54,54,54,54	0
56	MG	1A	3378	1/1	0.85	0.16	56,56,56,56	0
56	MG	2A	3312	1/1	0.86	0.08	75,75,75,75	0
56	MG	1A	3180	1/1	0.86	0.11	56,56,56,56	0
56	MG	1A	3333	1/1	0.86	0.37	45,45,45,45	0
56	MG	2a	1684	1/1	0.86	0.17	74,74,74,74	0
56	MG	2A	3514	1/1	0.86	0.21	70,70,70,70	0
56	MG	1A	3522	1/1	0.86	0.22	30,30,30,30	0
56	MG	1A	3336	1/1	0.86	0.10	54,54,54,54	0
56	MG	2A	3330	1/1	0.86	0.15	62,62,62,62	0
56	MG	2A	3331	1/1	0.86	0.27	56,56,56,56	0
56	MG	1a	1771	1/1	0.86	0.15	63,63,63,63	0
56	MG	1A	3344	1/1	0.86	0.33	36,36,36,36	0
56	MG	1a	1620	1/1	0.86	0.15	72,72,72,72	0
56	MG	1A	3557	1/1	0.86	0.25	59,59,59,59	0
56	MG	1A	3141	1/1	0.86	0.14	75,75,75,75	0
56	MG	2a	1701	1/1	0.86	0.14	61,61,61,61	0
56	MG	2a	1702	1/1	0.86	0.13	84,84,84,84	0
56	MG	2a	1705	1/1	0.86	0.18	79,79,79,79	0
56	MG	2A	3533	1/1	0.86	0.12	64,64,64,64	0
56	MG	1a	1633	1/1	0.86	0.14	55,55,55,55	0
56	MG	1a	1641	1/1	0.86	0.21	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3657	1/1	0.86	0.16	69,69,69,69	0
56	MG	1a	1653	1/1	0.86	0.25	60,60,60,60	0
56	MG	1A	3083	1/1	0.86	0.20	71,71,71,71	0
56	MG	2A	3363	1/1	0.86	0.12	65,65,65,65	0
56	MG	1A	3926	1/1	0.86	0.12	83,83,83,83	0
56	MG	1A	3300	1/1	0.86	0.22	43,43,43,43	0
56	MG	1a	1796	1/1	0.86	0.07	74,74,74,74	0
56	MG	2A	3115	1/1	0.86	0.29	67,67,67,67	0
56	MG	2A	3374	1/1	0.86	0.10	60,60,60,60	0
56	MG	2A	3378	1/1	0.86	0.49	57,57,57,57	0
56	MG	1a	1935	1/1	0.86	0.16	70,70,70,70	0
56	MG	1A	3607	1/1	0.86	0.27	46,46,46,46	0
56	MG	1A	3388	1/1	0.86	0.27	74,74,74,74	0
56	MG	2A	3565	1/1	0.86	0.08	64,64,64,64	0
56	MG	2A	3391	1/1	0.86	0.11	78,78,78,78	0
56	MG	2B	205	1/1	0.86	0.06	91,91,91,91	0
56	MG	2a	1744	1/1	0.86	0.29	68,68,68,68	0
56	MG	1A	3669	1/1	0.86	0.11	62,62,62,62	0
56	MG	2a	1747	1/1	0.86	0.40	72,72,72,72	0
56	MG	2B	207	1/1	0.86	0.16	65,65,65,65	0
56	MG	1A	3864	1/1	0.86	0.15	68,68,68,68	0
56	MG	2A	3408	1/1	0.86	0.20	58,58,58,58	0
56	MG	2D	302	1/1	0.86	0.13	68,68,68,68	0
56	MG	1A	3671	1/1	0.86	0.11	70,70,70,70	0
56	MG	1a	1826	1/1	0.86	0.11	74,74,74,74	0
56	MG	1A	3700	1/1	0.86	0.19	72,72,72,72	0
56	MG	2a	1767	1/1	0.86	0.28	59,59,59,59	0
56	MG	1a	1692	1/1	0.86	0.09	86,86,86,86	0
56	MG	1A	3154	1/1	0.86	0.05	67,67,67,67	0
56	MG	1a	1694	1/1	0.86	0.25	46,46,46,46	0
56	MG	1a	1852	1/1	0.86	0.20	72,72,72,72	0
56	MG	1A	3620	1/1	0.86	0.19	63,63,63,63	0
56	MG	2A	3164	1/1	0.86	0.27	42,42,42,42	0
56	MG	2a	1602	1/1	0.86	0.22	74,74,74,74	0
56	MG	1a	1854	1/1	0.86	0.18	83,83,83,83	0
56	MG	2A	3170	1/1	0.86	0.23	40,40,40,40	0
56	MG	1B	225	1/1	0.86	0.12	80,80,80,80	0
56	MG	1A	3722	1/1	0.86	0.20	54,54,54,54	0
56	MG	1a	1712	1/1	0.86	0.15	69,69,69,69	0
56	MG	1A	3454	1/1	0.86	0.09	59,59,59,59	0
56	MG	2A	3198	1/1	0.86	0.39	50,50,50,50	0
56	MG	2a	1612	1/1	0.86	0.15	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3455	1/1	0.86	0.27	56,56,56,56	0
56	MG	1A	3039	1/1	0.86	0.13	50,50,50,50	0
56	MG	1O	3102	1/1	0.86	0.10	60,60,60,60	0
56	MG	1A	3480	1/1	0.86	0.14	74,74,74,74	0
56	MG	11	101	1/1	0.86	0.18	69,69,69,69	0
56	MG	1x	104	1/1	0.86	0.33	76,76,76,76	0
56	MG	1A	3324	1/1	0.86	0.20	49,49,49,49	0
56	MG	1a	1880	1/1	0.86	0.11	81,81,81,81	0
56	MG	2a	1624	1/1	0.86	0.15	61,61,61,61	0
56	MG	2a	1625	1/1	0.86	0.32	51,51,51,51	0
56	MG	2a	1807	1/1	0.86	0.19	79,79,79,79	0
56	MG	1x	114	1/1	0.86	0.14	86,86,86,86	0
56	MG	1A	3486	1/1	0.86	0.09	50,50,50,50	0
56	MG	1A	3410	1/1	0.86	0.09	72,72,72,72	0
56	MG	2a	1812	1/1	0.86	0.15	96,96,96,96	0
56	MG	2A	3264	1/1	0.86	0.30	37,37,37,37	0
56	MG	2A	3268	1/1	0.86	0.16	77,77,77,77	0
56	MG	2a	1816	1/1	0.86	0.07	89,89,89,89	0
56	MG	1x	119	1/1	0.86	0.08	78,78,78,78	0
56	MG	1x	120	1/1	0.86	0.14	80,80,80,80	0
56	MG	2A	3284	1/1	0.86	0.26	60,60,60,60	0
56	MG	1A	3888	1/1	0.86	0.07	68,68,68,68	0
56	MG	2A	3002	1/1	0.86	0.25	55,55,55,55	0
56	MG	1a	1742	1/1	0.86	0.12	69,69,69,69	0
56	MG	2A	3008	1/1	0.86	0.09	57,57,57,57	0
56	MG	2A	3296	1/1	0.86	0.36	52,52,52,52	0
56	MG	2A	3011	1/1	0.86	0.26	55,55,55,55	0
56	MG	2A	3304	1/1	0.86	0.17	56,56,56,56	0
56	MG	2A	3501	1/1	0.86	0.10	74,74,74,74	0
56	MG	2a	1665	1/1	0.86	0.28	61,61,61,61	0
56	MG	2A	3305	1/1	0.86	0.17	60,60,60,60	0
56	MG	1A	3891	1/1	0.86	0.19	69,69,69,69	0
56	MG	1A	3271	1/1	0.86	0.31	33,33,33,33	0
56	MG	2a	1670	1/1	0.86	0.10	74,74,74,74	0
56	MG	1A	3810	1/1	0.86	0.16	65,65,65,65	0
56	MG	1a	1856	1/1	0.87	0.21	56,56,56,56	0
56	MG	1A	3427	1/1	0.87	0.17	43,43,43,43	0
56	MG	1A	3008	1/1	0.87	0.09	61,61,61,61	0
56	MG	1A	3188	1/1	0.87	0.16	52,52,52,52	0
56	MG	2A	3179	1/1	0.87	0.23	51,51,51,51	0
56	MG	2A	3550	1/1	0.87	0.21	64,64,64,64	0
56	MG	2a	1708	1/1	0.87	0.12	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3409	1/1	0.87	0.21	68,68,68,68	0
56	MG	2A	3557	1/1	0.87	0.14	62,62,62,62	0
56	MG	1a	1867	1/1	0.87	0.17	72,72,72,72	0
56	MG	1A	3558	1/1	0.87	0.29	58,58,58,58	0
56	MG	2A	3564	1/1	0.87	0.15	65,65,65,65	0
56	MG	2A	3414	1/1	0.87	0.10	55,55,55,55	0
56	MG	2A	3416	1/1	0.87	0.19	57,57,57,57	0
56	MG	1a	1869	1/1	0.87	0.09	64,64,64,64	0
56	MG	1a	1736	1/1	0.87	0.19	79,79,79,79	0
56	MG	1a	1737	1/1	0.87	0.07	89,89,89,89	0
56	MG	1A	3559	1/1	0.87	0.25	54,54,54,54	0
56	MG	1A	3827	1/1	0.87	0.22	39,39,39,39	0
56	MG	2A	3434	1/1	0.87	0.17	79,79,79,79	0
56	MG	2A	3214	1/1	0.87	0.32	41,41,41,41	0
56	MG	2A	3222	1/1	0.87	0.27	49,49,49,49	0
56	MG	1A	3578	1/1	0.87	0.36	38,38,38,38	0
56	MG	1A	3394	1/1	0.87	0.11	69,69,69,69	0
56	MG	2A	3443	1/1	0.87	0.12	70,70,70,70	0
56	MG	1A	3395	1/1	0.87	0.17	70,70,70,70	0
56	MG	1a	1618	1/1	0.87	0.06	75,75,75,75	0
56	MG	1A	3844	1/1	0.87	0.15	79,79,79,79	0
56	MG	23	101	1/1	0.87	0.16	73,73,73,73	0
56	MG	1a	1889	1/1	0.87	0.08	75,75,75,75	0
56	MG	2a	1754	1/1	0.87	0.36	63,63,63,63	0
56	MG	2a	1755	1/1	0.87	0.40	63,63,63,63	0
56	MG	1A	3327	1/1	0.87	0.30	62,62,62,62	0
56	MG	1a	1755	1/1	0.87	0.09	68,68,68,68	0
56	MG	2a	1761	1/1	0.87	0.16	69,69,69,69	0
56	MG	1A	3660	1/1	0.87	0.10	69,69,69,69	0
56	MG	1A	3400	1/1	0.87	0.21	66,66,66,66	0
56	MG	1A	3923	1/1	0.87	0.25	44,44,44,44	0
56	MG	2A	3025	1/1	0.87	0.26	54,54,54,54	0
56	MG	2A	3282	1/1	0.87	0.27	46,46,46,46	0
56	MG	2A	3026	1/1	0.87	0.13	39,39,39,39	0
56	MG	1A	3183	1/1	0.87	0.13	75,75,75,75	0
56	MG	2A	3288	1/1	0.87	0.23	74,74,74,74	0
56	MG	1a	1644	1/1	0.87	0.21	63,63,63,63	0
56	MG	2A	3034	1/1	0.87	0.26	55,55,55,55	0
56	MG	2A	3480	1/1	0.87	0.44	70,70,70,70	0
56	MG	2A	3037	1/1	0.87	0.14	59,59,59,59	0
56	MG	2A	3041	1/1	0.87	0.20	39,39,39,39	0
56	MG	2A	3300	1/1	0.87	0.20	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3464	1/1	0.87	0.09	83,83,83,83	0
56	MG	2A	3046	1/1	0.87	0.16	76,76,76,76	0
56	MG	1A	3280	1/1	0.87	0.30	51,51,51,51	0
56	MG	1A	3780	1/1	0.87	0.09	70,70,70,70	0
56	MG	1A	3093	1/1	0.87	0.26	21,21,21,21	0
56	MG	2a	1633	1/1	0.87	0.21	55,55,55,55	0
56	MG	1a	1663	1/1	0.87	0.23	65,65,65,65	0
56	MG	1A	3694	1/1	0.87	0.15	39,39,39,39	0
56	MG	1a	1672	1/1	0.87	0.13	60,60,60,60	0
56	MG	1A	3061	1/1	0.87	0.11	72,72,72,72	0
56	MG	1A	3790	1/1	0.87	0.15	66,66,66,66	0
56	MG	1a	1789	1/1	0.87	0.11	77,77,77,77	0
56	MG	2A	3071	1/1	0.87	0.18	72,72,72,72	0
56	MG	1A	3414	1/1	0.87	0.18	54,54,54,54	0
56	MG	2A	3506	1/1	0.87	0.09	90,90,90,90	0
56	MG	1a	1683	1/1	0.87	0.17	75,75,75,75	0
56	MG	1a	1799	1/1	0.87	0.20	76,76,76,76	0
56	MG	2a	1656	1/1	0.87	0.09	85,85,85,85	0
56	MG	1A	3203	1/1	0.87	0.16	70,70,70,70	0
56	MG	1A	3636	1/1	0.87	0.14	62,62,62,62	0
56	MG	2a	1813	1/1	0.87	0.09	90,90,90,90	0
56	MG	1A	3874	1/1	0.87	0.16	65,65,65,65	0
56	MG	1a	1939	1/1	0.87	0.24	68,68,68,68	0
56	MG	1A	3638	1/1	0.87	0.16	73,73,73,73	0
56	MG	1A	3878	1/1	0.87	0.10	57,57,57,57	0
56	MG	1N	201	1/1	0.87	0.21	66,66,66,66	0
56	MG	2A	3525	1/1	0.87	0.16	81,81,81,81	0
56	MG	1a	1698	1/1	0.87	0.29	75,75,75,75	0
56	MG	1A	3347	1/1	0.87	0.23	31,31,31,31	0
56	MG	1A	3233	1/1	0.87	0.18	48,48,48,48	0
56	MG	1W	202	1/1	0.87	0.13	47,47,47,47	0
56	MG	1a	1850	1/1	0.87	0.09	73,73,73,73	0
56	MG	1A	3251	1/1	0.87	0.20	49,49,49,49	0
56	MG	2A	3372	1/1	0.87	0.18	60,60,60,60	0
56	MG	2a	1687	1/1	0.87	0.14	71,71,71,71	0
56	MG	1A	3644	1/1	0.87	0.18	57,57,57,57	0
56	MG	1a	1715	1/1	0.87	0.29	58,58,58,58	0
56	MG	2A	3379	1/1	0.87	0.10	59,59,59,59	0
56	MG	1A	3804	1/1	0.87	0.27	77,77,77,77	0
56	MG	2A	3161	1/1	0.87	0.33	61,61,61,61	0
56	MG	2A	3383	1/1	0.87	0.12	43,43,43,43	0
56	MG	2A	3553	1/1	0.88	0.12	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3554	1/1	0.88	0.09	74,74,74,74	0
56	MG	2A	3421	1/1	0.88	0.26	59,59,59,59	0
56	MG	1B	215	1/1	0.88	0.16	53,53,53,53	0
56	MG	2A	3428	1/1	0.88	0.12	78,78,78,78	0
56	MG	2a	1711	1/1	0.88	0.06	81,81,81,81	0
56	MG	1A	3193	1/1	0.88	0.08	55,55,55,55	0
56	MG	1A	3637	1/1	0.88	0.15	61,61,61,61	0
56	MG	2A	3265	1/1	0.88	0.29	42,42,42,42	0
56	MG	2A	3266	1/1	0.88	0.18	39,39,39,39	0
56	MG	1A	3875	1/1	0.88	0.08	72,72,72,72	0
56	MG	1a	1675	1/1	0.88	0.25	68,68,68,68	0
56	MG	1A	3016	1/1	0.88	0.09	61,61,61,61	0
56	MG	1A	3174	1/1	0.88	0.09	63,63,63,63	0
56	MG	2A	3057	1/1	0.88	0.20	52,52,52,52	0
56	MG	1a	1681	1/1	0.88	0.43	64,64,64,64	0
56	MG	2F	302	1/1	0.88	0.15	69,69,69,69	0
56	MG	1a	1793	1/1	0.88	0.11	74,74,74,74	0
56	MG	2A	3449	1/1	0.88	0.29	61,61,61,61	0
56	MG	1D	303	1/1	0.88	0.06	65,65,65,65	0
56	MG	2A	3453	1/1	0.88	0.21	74,74,74,74	0
56	MG	1E	304	1/1	0.88	0.12	70,70,70,70	0
56	MG	1F	301	1/1	0.88	0.25	52,52,52,52	0
56	MG	1A	3144	1/1	0.88	0.27	72,72,72,72	0
56	MG	2a	1741	1/1	0.88	0.31	50,50,50,50	0
56	MG	2A	3298	1/1	0.88	0.21	50,50,50,50	0
56	MG	26	101	1/1	0.88	0.15	61,61,61,61	0
56	MG	1A	3421	1/1	0.88	0.12	61,61,61,61	0
56	MG	1A	3364	1/1	0.88	0.16	49,49,49,49	0
56	MG	2a	1603	1/1	0.88	0.12	67,67,67,67	0
56	MG	2a	1752	1/1	0.88	0.23	57,57,57,57	0
56	MG	2a	1753	1/1	0.88	0.33	46,46,46,46	0
56	MG	2a	1604	1/1	0.88	0.21	43,43,43,43	0
56	MG	2A	3462	1/1	0.88	0.23	48,48,48,48	0
56	MG	1a	1940	1/1	0.88	0.15	47,47,47,47	0
56	MG	2a	1758	1/1	0.88	0.24	61,61,61,61	0
56	MG	2A	3466	1/1	0.88	0.25	61,61,61,61	0
56	MG	1Q	202	1/1	0.88	0.15	62,62,62,62	0
56	MG	2A	3083	1/1	0.88	0.28	69,69,69,69	0
56	MG	1a	1696	1/1	0.88	0.24	46,46,46,46	0
56	MG	2A	3089	1/1	0.88	0.31	61,61,61,61	0
56	MG	1A	3032	1/1	0.88	0.18	69,69,69,69	0
56	MG	2A	3099	1/1	0.88	0.19	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3315	1/1	0.88	0.25	57,57,57,57	0
56	MG	2A	3483	1/1	0.88	0.15	75,75,75,75	0
56	MG	2A	3317	1/1	0.88	0.26	38,38,38,38	0
56	MG	1V	201	1/1	0.88	0.12	43,43,43,43	0
56	MG	1a	1834	1/1	0.88	0.08	64,64,64,64	0
56	MG	1A	3204	1/1	0.88	0.15	61,61,61,61	0
56	MG	1Y	201	1/1	0.88	0.08	64,64,64,64	0
56	MG	1A	3821	1/1	0.88	0.14	30,30,30,30	0
56	MG	1A	3433	1/1	0.88	0.12	41,41,41,41	0
56	MG	2a	1785	1/1	0.88	0.12	60,60,60,60	0
56	MG	1A	3826	1/1	0.88	0.20	82,82,82,82	0
56	MG	1a	1716	1/1	0.88	0.23	70,70,70,70	0
56	MG	1A	3434	1/1	0.88	0.10	78,78,78,78	0
56	MG	1a	1720	1/1	0.88	0.08	80,80,80,80	0
56	MG	2A	3344	1/1	0.88	0.18	47,47,47,47	0
56	MG	1A	3585	1/1	0.88	0.32	28,28,28,28	0
56	MG	1A	3590	1/1	0.88	0.34	55,55,55,55	0
56	MG	1A	3386	1/1	0.88	0.15	54,54,54,54	0
56	MG	1A	3177	1/1	0.88	0.17	65,65,65,65	0
56	MG	2A	3360	1/1	0.88	0.13	77,77,77,77	0
56	MG	1a	1735	1/1	0.88	0.20	80,80,80,80	0
56	MG	2A	3157	1/1	0.88	0.08	74,74,74,74	0
56	MG	2A	3159	1/1	0.88	0.23	69,69,69,69	0
56	MG	1A	3845	1/1	0.88	0.29	65,65,65,65	0
56	MG	2A	3368	1/1	0.88	0.14	80,80,80,80	0
56	MG	1A	3595	1/1	0.88	0.27	51,51,51,51	0
56	MG	2a	1661	1/1	0.88	0.14	79,79,79,79	0
56	MG	1A	3917	1/1	0.88	0.13	67,67,67,67	0
56	MG	2A	3371	1/1	0.88	0.13	62,62,62,62	0
56	MG	1A	3136	1/1	0.88	0.21	56,56,56,56	0
56	MG	1A	3068	1/1	0.88	0.20	62,62,62,62	0
56	MG	1A	3610	1/1	0.88	0.10	54,54,54,54	0
56	MG	1a	1743	1/1	0.88	0.15	66,66,66,66	0
56	MG	1A	3069	1/1	0.88	0.28	62,62,62,62	0
56	MG	1A	3614	1/1	0.88	0.15	73,73,73,73	0
56	MG	1x	121	1/1	0.88	0.08	57,57,57,57	0
56	MG	2a	1674	1/1	0.88	0.17	90,90,90,90	0
56	MG	1a	1625	1/1	0.88	0.12	72,72,72,72	0
56	MG	2A	3390	1/1	0.88	0.35	72,72,72,72	0
56	MG	1A	3053	1/1	0.88	0.15	40,40,40,40	0
56	MG	2A	3398	1/1	0.88	0.12	76,76,76,76	0
56	MG	1a	1627	1/1	0.88	0.12	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3212	1/1	0.88	0.36	43,43,43,43	0
56	MG	1A	3401	1/1	0.88	0.10	61,61,61,61	0
56	MG	1A	3165	1/1	0.88	0.23	52,52,52,52	0
56	MG	1A	3704	1/1	0.88	0.11	49,49,49,49	0
56	MG	1A	3081	1/1	0.88	0.17	51,51,51,51	0
56	MG	1A	3192	1/1	0.88	0.12	41,41,41,41	0
56	MG	1A	3252	1/1	0.88	0.10	67,67,67,67	0
56	MG	1a	1660	1/1	0.88	0.18	47,47,47,47	0
56	MG	1B	210	1/1	0.88	0.24	35,35,35,35	0
57	KAN	2A	3568	33/33	0.88	0.09	51,58,63,65	0
57	KAN	2A	3569	33/33	0.88	0.13	56,65,71,73	0
56	MG	2a	1660	1/1	0.89	0.11	57,57,57,57	0
56	MG	1a	1860	1/1	0.89	0.15	73,73,73,73	0
56	MG	1A	3216	1/1	0.89	0.31	49,49,49,49	0
56	MG	1x	124	1/1	0.89	0.17	65,65,65,65	0
56	MG	1y	101	1/1	0.89	0.20	66,66,66,66	0
56	MG	1a	1719	1/1	0.89	0.09	95,95,95,95	0
56	MG	1A	3691	1/1	0.89	0.19	37,37,37,37	0
56	MG	1A	3615	1/1	0.89	0.14	50,50,50,50	0
56	MG	1A	3357	1/1	0.89	0.38	31,31,31,31	0
56	MG	2A	3289	1/1	0.89	0.06	80,80,80,80	0
56	MG	1A	3885	1/1	0.89	0.21	53,53,53,53	0
56	MG	1a	1874	1/1	0.89	0.11	71,71,71,71	0
56	MG	2a	1675	1/1	0.89	0.08	94,94,94,94	0
56	MG	1a	1727	1/1	0.89	0.14	65,65,65,65	0
56	MG	2a	1677	1/1	0.89	0.10	67,67,67,67	0
56	MG	19	102	1/1	0.89	0.12	55,55,55,55	0
56	MG	2A	3027	1/1	0.89	0.20	58,58,58,58	0
56	MG	2A	3299	1/1	0.89	0.26	64,64,64,64	0
56	MG	2A	3029	1/1	0.89	0.18	67,67,67,67	0
56	MG	2A	3301	1/1	0.89	0.18	65,65,65,65	0
56	MG	1a	1734	1/1	0.89	0.21	76,76,76,76	0
56	MG	1a	1602	1/1	0.89	0.23	67,67,67,67	0
56	MG	1A	3886	1/1	0.89	0.16	39,39,39,39	0
56	MG	1A	3012	1/1	0.89	0.15	51,51,51,51	0
56	MG	1A	3501	1/1	0.89	0.07	51,51,51,51	0
56	MG	1a	1887	1/1	0.89	0.10	75,75,75,75	0
56	MG	2A	3516	1/1	0.89	0.06	78,78,78,78	0
56	MG	1A	3710	1/1	0.89	0.09	43,43,43,43	0
56	MG	2A	3519	1/1	0.89	0.26	56,56,56,56	0
56	MG	2A	3520	1/1	0.89	0.22	59,59,59,59	0
56	MG	2a	1703	1/1	0.89	0.19	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3313	1/1	0.89	0.20	28,28,28,28	0
56	MG	1A	3711	1/1	0.89	0.07	46,46,46,46	0
56	MG	2A	3054	1/1	0.89	0.20	57,57,57,57	0
56	MG	1A	3172	1/1	0.89	0.07	79,79,79,79	0
56	MG	2A	3325	1/1	0.89	0.20	62,62,62,62	0
56	MG	1A	3368	1/1	0.89	0.30	24,24,24,24	0
56	MG	2A	3058	1/1	0.89	0.41	55,55,55,55	0
56	MG	2A	3531	1/1	0.89	0.13	57,57,57,57	0
56	MG	1A	3518	1/1	0.89	0.18	45,45,45,45	0
56	MG	1a	1893	1/1	0.89	0.07	79,79,79,79	0
56	MG	1A	3519	1/1	0.89	0.30	46,46,46,46	0
56	MG	1a	1895	1/1	0.89	0.36	51,51,51,51	0
56	MG	2A	3064	1/1	0.89	0.20	59,59,59,59	0
56	MG	2a	1726	1/1	0.89	0.33	65,65,65,65	0
56	MG	2A	3334	1/1	0.89	0.24	62,62,62,62	0
56	MG	1A	3229	1/1	0.89	0.11	63,63,63,63	0
56	MG	1a	1752	1/1	0.89	0.14	56,56,56,56	0
56	MG	1a	1753	1/1	0.89	0.14	58,58,58,58	0
56	MG	1A	3525	1/1	0.89	0.28	34,34,34,34	0
56	MG	1A	3200	1/1	0.89	0.12	66,66,66,66	0
56	MG	2a	1736	1/1	0.89	0.15	64,64,64,64	0
56	MG	1A	3747	1/1	0.89	0.23	66,66,66,66	0
56	MG	1a	1906	1/1	0.89	0.11	54,54,54,54	0
56	MG	1A	3302	1/1	0.89	0.37	61,61,61,61	0
56	MG	2A	3355	1/1	0.89	0.22	76,76,76,76	0
56	MG	1A	3750	1/1	0.89	0.11	67,67,67,67	0
56	MG	1a	1913	1/1	0.89	0.18	66,66,66,66	0
56	MG	1A	3834	1/1	0.89	0.14	68,68,68,68	0
56	MG	2A	3555	1/1	0.89	0.16	58,58,58,58	0
56	MG	1A	3835	1/1	0.89	0.11	59,59,59,59	0
56	MG	2A	3558	1/1	0.89	0.24	46,46,46,46	0
56	MG	2A	3105	1/1	0.89	0.30	56,56,56,56	0
56	MG	2A	3109	1/1	0.89	0.21	57,57,57,57	0
56	MG	1A	3837	1/1	0.89	0.18	51,51,51,51	0
56	MG	1A	3387	1/1	0.89	0.20	74,74,74,74	0
56	MG	2A	3567	1/1	0.89	0.09	67,67,67,67	0
56	MG	2A	3122	1/1	0.89	0.13	33,33,33,33	0
56	MG	2A	3124	1/1	0.89	0.20	45,45,45,45	0
56	MG	1A	3840	1/1	0.89	0.16	71,71,71,71	0
56	MG	1a	1927	1/1	0.89	0.14	70,70,70,70	0
56	MG	1a	1928	1/1	0.89	0.11	70,70,70,70	0
56	MG	2a	1765	1/1	0.89	0.37	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	3841	1/1	0.89	0.14	73,73,73,73	0
56	MG	1A	3309	1/1	0.89	0.28	42,42,42,42	0
56	MG	2A	3133	1/1	0.89	0.18	72,72,72,72	0
56	MG	2a	1773	1/1	0.89	0.13	91,91,91,91	0
56	MG	1A	3173	1/1	0.89	0.07	70,70,70,70	0
56	MG	1A	3577	1/1	0.89	0.28	51,51,51,51	0
56	MG	1B	208	1/1	0.89	0.09	61,61,61,61	0
56	MG	2Q	201	1/1	0.89	0.10	71,71,71,71	0
56	MG	1A	3241	1/1	0.89	0.26	36,36,36,36	0
56	MG	2T	201	1/1	0.89	0.19	55,55,55,55	0
56	MG	1A	3004	1/1	0.89	0.16	68,68,68,68	0
56	MG	1a	1676	1/1	0.89	0.17	73,73,73,73	0
56	MG	2a	1784	1/1	0.89	0.21	66,66,66,66	0
56	MG	1B	214	1/1	0.89	0.23	49,49,49,49	0
56	MG	1a	1795	1/1	0.89	0.10	55,55,55,55	0
56	MG	1A	3764	1/1	0.89	0.14	64,64,64,64	0
56	MG	1a	1949	1/1	0.89	0.13	78,78,78,78	0
56	MG	2a	1792	1/1	0.89	0.24	59,59,59,59	0
56	MG	1A	3117	1/1	0.89	0.30	41,41,41,41	0
56	MG	1A	3023	1/1	0.89	0.10	55,55,55,55	0
56	MG	2A	3165	1/1	0.89	0.39	77,77,77,77	0
56	MG	2A	3167	1/1	0.89	0.24	64,64,64,64	0
56	MG	1B	221	1/1	0.89	0.28	58,58,58,58	0
56	MG	1a	1807	1/1	0.89	0.22	76,76,76,76	0
56	MG	2A	3171	1/1	0.89	0.36	51,51,51,51	0
56	MG	1A	3036	1/1	0.89	0.23	32,32,32,32	0
56	MG	1A	3656	1/1	0.89	0.09	71,71,71,71	0
56	MG	2A	3187	1/1	0.89	0.27	39,39,39,39	0
56	MG	1m	202	1/1	0.89	0.09	58,58,58,58	0
56	MG	2A	3192	1/1	0.89	0.32	36,36,36,36	0
56	MG	2A	3440	1/1	0.89	0.16	57,57,57,57	0
56	MG	1A	3859	1/1	0.89	0.09	69,69,69,69	0
56	MG	1a	1825	1/1	0.89	0.21	76,76,76,76	0
56	MG	1A	3263	1/1	0.89	0.19	31,31,31,31	0
56	MG	2A	3199	1/1	0.89	0.30	38,38,38,38	0
56	MG	1a	1827	1/1	0.89	0.20	68,68,68,68	0
56	MG	1A	3598	1/1	0.89	0.21	60,60,60,60	0
56	MG	1A	3774	1/1	0.89	0.06	83,83,83,83	0
56	MG	2A	3213	1/1	0.89	0.33	48,48,48,48	0
56	MG	1A	3601	1/1	0.89	0.15	43,43,43,43	0
56	MG	2A	3218	1/1	0.89	0.35	56,56,56,56	0
56	MG	1a	1841	1/1	0.89	0.11	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1843	1/1	0.89	0.15	63,63,63,63	0
56	MG	2A	3224	1/1	0.89	0.19	45,45,45,45	0
56	MG	2a	1636	1/1	0.89	0.19	69,69,69,69	0
56	MG	1A	3662	1/1	0.89	0.12	60,60,60,60	0
56	MG	1a	1702	1/1	0.89	0.26	58,58,58,58	0
56	MG	1a	1707	1/1	0.89	0.32	41,41,41,41	0
56	MG	2A	3243	1/1	0.89	0.44	53,53,53,53	0
56	MG	2A	3245	1/1	0.89	0.31	63,63,63,63	0
56	MG	1A	3476	1/1	0.89	0.14	63,63,63,63	0
56	MG	1A	3478	1/1	0.89	0.11	60,60,60,60	0
56	MG	2a	1650	1/1	0.89	0.34	73,73,73,73	0
56	MG	1A	3269	1/1	0.89	0.22	33,33,33,33	0
56	MG	1A	3789	1/1	0.89	0.06	78,78,78,78	0
56	MG	2A	3262	1/1	0.89	0.17	65,65,65,65	0
56	MG	1A	3179	1/1	0.89	0.11	70,70,70,70	0
56	MG	1A	3791	1/1	0.89	0.22	54,54,54,54	0
56	MG	1a	1909	1/1	0.90	0.09	62,62,62,62	0
56	MG	1a	1671	1/1	0.90	0.18	69,69,69,69	0
56	MG	1A	3524	1/1	0.90	0.38	44,44,44,44	0
56	MG	1A	3171	1/1	0.90	0.06	61,61,61,61	0
56	MG	1B	223	1/1	0.90	0.08	63,63,63,63	0
56	MG	2A	3310	1/1	0.90	0.31	56,56,56,56	0
56	MG	1A	3529	1/1	0.90	0.24	33,33,33,33	0
56	MG	1A	3713	1/1	0.90	0.12	61,61,61,61	0
56	MG	2A	3085	1/1	0.90	0.17	67,67,67,67	0
56	MG	2a	1683	1/1	0.90	0.14	83,83,83,83	0
56	MG	1A	3530	1/1	0.90	0.34	43,43,43,43	0
56	MG	1a	1926	1/1	0.90	0.08	77,77,77,77	0
56	MG	1A	3717	1/1	0.90	0.14	62,62,62,62	0
56	MG	2A	3323	1/1	0.90	0.22	40,40,40,40	0
56	MG	1A	3396	1/1	0.90	0.15	61,61,61,61	0
56	MG	1A	3447	1/1	0.90	0.16	53,53,53,53	0
56	MG	1a	1685	1/1	0.90	0.12	79,79,79,79	0
56	MG	2A	3106	1/1	0.90	0.26	52,52,52,52	0
56	MG	1a	1933	1/1	0.90	0.11	74,74,74,74	0
56	MG	1A	3539	1/1	0.90	0.18	33,33,33,33	0
56	MG	1a	1688	1/1	0.90	0.20	72,72,72,72	0
56	MG	2A	3528	1/1	0.90	0.15	64,64,64,64	0
56	MG	1a	1811	1/1	0.90	0.19	63,63,63,63	0
56	MG	1a	1937	1/1	0.90	0.24	52,52,52,52	0
56	MG	2A	3125	1/1	0.90	0.23	69,69,69,69	0
56	MG	1A	3153	1/1	0.90	0.10	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1816	1/1	0.90	0.10	81,81,81,81	0
56	MG	2A	3535	1/1	0.90	0.12	65,65,65,65	0
56	MG	1a	1818	1/1	0.90	0.13	64,64,64,64	0
56	MG	1A	3884	1/1	0.90	0.20	59,59,59,59	0
56	MG	1a	1821	1/1	0.90	0.08	88,88,88,88	0
56	MG	2a	1714	1/1	0.90	0.09	58,58,58,58	0
56	MG	1A	3232	1/1	0.90	0.19	58,58,58,58	0
56	MG	1A	3087	1/1	0.90	0.29	40,40,40,40	0
56	MG	1A	3564	1/1	0.90	0.22	43,43,43,43	0
56	MG	1A	3567	1/1	0.90	0.17	37,37,37,37	0
56	MG	2A	3142	1/1	0.90	0.21	73,73,73,73	0
56	MG	2A	3362	1/1	0.90	0.13	58,58,58,58	0
56	MG	1X	101	1/1	0.90	0.19	56,56,56,56	0
56	MG	2A	3149	1/1	0.90	0.08	75,75,75,75	0
56	MG	1A	3402	1/1	0.90	0.12	63,63,63,63	0
56	MG	1a	1706	1/1	0.90	0.25	52,52,52,52	0
56	MG	2A	3153	1/1	0.90	0.11	69,69,69,69	0
56	MG	1a	1839	1/1	0.90	0.10	75,75,75,75	0
56	MG	1A	3458	1/1	0.90	0.50	54,54,54,54	0
56	MG	1a	1842	1/1	0.90	0.20	55,55,55,55	0
56	MG	2a	1735	1/1	0.90	0.09	71,71,71,71	0
56	MG	1A	3354	1/1	0.90	0.32	25,25,25,25	0
56	MG	1A	3653	1/1	0.90	0.07	84,84,84,84	0
56	MG	2A	3560	1/1	0.90	0.14	82,82,82,82	0
56	MG	1A	3405	1/1	0.90	0.09	60,60,60,60	0
56	MG	2A	3562	1/1	0.90	0.13	73,73,73,73	0
56	MG	1A	3758	1/1	0.90	0.10	58,58,58,58	0
56	MG	1a	1851	1/1	0.90	0.10	64,64,64,64	0
56	MG	2A	3168	1/1	0.90	0.09	71,71,71,71	0
56	MG	2A	3386	1/1	0.90	0.13	66,66,66,66	0
56	MG	1A	3264	1/1	0.90	0.25	32,32,32,32	0
56	MG	2A	3388	1/1	0.90	0.14	53,53,53,53	0
56	MG	19	103	1/1	0.90	0.18	63,63,63,63	0
56	MG	1A	3912	1/1	0.90	0.13	61,61,61,61	0
56	MG	2A	3392	1/1	0.90	0.16	57,57,57,57	0
56	MG	1w	105	1/1	0.90	0.31	55,55,55,55	0
56	MG	2A	3181	1/1	0.90	0.29	50,50,50,50	0
56	MG	2a	1759	1/1	0.90	0.11	63,63,63,63	0
56	MG	2D	303	1/1	0.90	0.13	67,67,67,67	0
56	MG	1a	1604	1/1	0.90	0.20	62,62,62,62	0
56	MG	1A	3913	1/1	0.90	0.07	65,65,65,65	0
56	MG	2A	3189	1/1	0.90	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1a	1857	1/1	0.90	0.19	71,71,71,71	0
56	MG	1a	1608	1/1	0.90	0.12	65,65,65,65	0
56	MG	2A	3194	1/1	0.90	0.35	47,47,47,47	0
56	MG	1A	3310	1/1	0.90	0.15	53,53,53,53	0
56	MG	1A	3763	1/1	0.90	0.20	53,53,53,53	0
56	MG	1A	3267	1/1	0.90	0.32	40,40,40,40	0
56	MG	2A	3419	1/1	0.90	0.14	62,62,62,62	0
56	MG	1x	118	1/1	0.90	0.10	71,71,71,71	0
56	MG	2A	3205	1/1	0.90	0.33	49,49,49,49	0
56	MG	1a	1865	1/1	0.90	0.10	59,59,59,59	0
56	MG	28	101	1/1	0.90	0.16	47,47,47,47	0
56	MG	1A	3235	1/1	0.90	0.09	55,55,55,55	0
56	MG	1A	3659	1/1	0.90	0.12	65,65,65,65	0
56	MG	1A	3485	1/1	0.90	0.12	64,64,64,64	0
56	MG	2a	1783	1/1	0.90	0.26	60,60,60,60	0
56	MG	1a	1871	1/1	0.90	0.17	53,53,53,53	0
56	MG	1a	1617	1/1	0.90	0.11	84,84,84,84	0
56	MG	2A	3219	1/1	0.90	0.36	35,35,35,35	0
56	MG	1a	1873	1/1	0.90	0.17	62,62,62,62	0
56	MG	2a	1788	1/1	0.90	0.26	62,62,62,62	0
56	MG	1A	3415	1/1	0.90	0.24	48,48,48,48	0
56	MG	1A	3371	1/1	0.90	0.15	60,60,60,60	0
56	MG	2A	3010	1/1	0.90	0.27	49,49,49,49	0
56	MG	2A	3236	1/1	0.90	0.34	33,33,33,33	0
56	MG	1A	3927	1/1	0.90	0.22	86,86,86,86	0
56	MG	2A	3015	1/1	0.90	0.10	51,51,51,51	0
56	MG	2A	3019	1/1	0.90	0.15	58,58,58,58	0
56	MG	1A	3375	1/1	0.90	0.27	25,25,25,25	0
56	MG	2A	3253	1/1	0.90	0.21	50,50,50,50	0
56	MG	2a	1618	1/1	0.90	0.07	129,129,129,129	0
56	MG	1a	1622	1/1	0.90	0.24	56,56,56,56	0
56	MG	2A	3024	1/1	0.90	0.22	48,48,48,48	0
56	MG	1A	3019	1/1	0.90	0.11	63,63,63,63	0
56	MG	1A	3325	1/1	0.90	0.20	41,41,41,41	0
56	MG	2a	1806	1/1	0.90	0.12	90,90,90,90	0
56	MG	1a	1885	1/1	0.90	0.07	71,71,71,71	0
56	MG	1B	203	1/1	0.90	0.13	74,74,74,74	0
56	MG	1A	3778	1/1	0.90	0.13	64,64,64,64	0
56	MG	2a	1629	1/1	0.90	0.20	55,55,55,55	0
56	MG	1a	1748	1/1	0.90	0.10	59,59,59,59	0
56	MG	2A	3468	1/1	0.90	0.14	73,73,73,73	0
56	MG	1a	1749	1/1	0.90	0.14	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1a	1634	1/1	0.90	0.18	61,61,61,61	0
56	MG	2A	3279	1/1	0.90	0.29	31,31,31,31	0
56	MG	2A	3038	1/1	0.90	0.12	57,57,57,57	0
56	MG	1A	3326	1/1	0.90	0.22	42,42,42,42	0
56	MG	2a	1820	1/1	0.90	0.28	58,58,58,58	0
56	MG	1A	3680	1/1	0.90	0.17	58,58,58,58	0
56	MG	1a	1645	1/1	0.90	0.14	71,71,71,71	0
56	MG	1a	1646	1/1	0.90	0.17	67,67,67,67	0
56	MG	1A	3682	1/1	0.90	0.09	41,41,41,41	0
56	MG	2A	3485	1/1	0.90	0.19	58,58,58,58	0
56	MG	1A	3861	1/1	0.90	0.07	81,81,81,81	0
56	MG	2e	201	1/1	0.90	0.09	74,74,74,74	0
56	MG	1a	1658	1/1	0.90	0.35	46,46,46,46	0
56	MG	2A	3292	1/1	0.90	0.33	50,50,50,50	0
56	MG	1A	3242	1/1	0.90	0.13	62,62,62,62	0
56	MG	2A	3295	1/1	0.90	0.30	57,57,57,57	0
56	MG	1B	213	1/1	0.90	0.21	40,40,40,40	0
56	MG	1A	3282	1/1	0.90	0.28	44,44,44,44	0
56	MG	1A	3625	1/1	0.90	0.10	57,57,57,57	0
56	MG	2A	3497	1/1	0.90	0.18	71,71,71,71	0
56	MG	1A	3224	1/1	0.90	0.27	23,23,23,23	0
56	MG	2A	3499	1/1	0.90	0.19	73,73,73,73	0
56	MG	1a	1670	1/1	0.90	0.12	62,62,62,62	0
56	MG	2A	3206	1/1	0.91	0.31	31,31,31,31	0
56	MG	2A	3207	1/1	0.91	0.27	34,34,34,34	0
56	MG	1A	3436	1/1	0.91	0.07	57,57,57,57	0
56	MG	2A	3210	1/1	0.91	0.31	44,44,44,44	0
56	MG	1A	3025	1/1	0.91	0.11	41,41,41,41	0
56	MG	1x	113	1/1	0.91	0.19	67,67,67,67	0
56	MG	2a	1653	1/1	0.91	0.17	49,49,49,49	0
56	MG	1B	216	1/1	0.91	0.10	67,67,67,67	0
56	MG	1a	1849	1/1	0.91	0.19	61,61,61,61	0
56	MG	2A	3216	1/1	0.91	0.27	38,38,38,38	0
56	MG	1A	3441	1/1	0.91	0.07	26,26,26,26	0
56	MG	2a	1659	1/1	0.91	0.14	69,69,69,69	0
56	MG	1A	3236	1/1	0.91	0.20	48,48,48,48	0
56	MG	2A	3220	1/1	0.91	0.40	59,59,59,59	0
56	MG	2a	1662	1/1	0.91	0.14	73,73,73,73	0
56	MG	1A	3593	1/1	0.91	0.34	55,55,55,55	0
56	MG	1A	3384	1/1	0.91	0.06	72,72,72,72	0
56	MG	1A	3597	1/1	0.91	0.23	45,45,45,45	0
56	MG	2A	3227	1/1	0.91	0.29	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3470	1/1	0.91	0.10	68,68,68,68	0
56	MG	1A	3304	1/1	0.91	0.21	46,46,46,46	0
56	MG	2A	3235	1/1	0.91	0.44	47,47,47,47	0
56	MG	1A	3719	1/1	0.91	0.09	57,57,57,57	0
56	MG	1A	3720	1/1	0.91	0.14	66,66,66,66	0
56	MG	1A	3205	1/1	0.91	0.26	65,65,65,65	0
56	MG	2A	3003	1/1	0.91	0.17	60,60,60,60	0
56	MG	2A	3006	1/1	0.91	0.09	57,57,57,57	0
56	MG	2A	3247	1/1	0.91	0.45	41,41,41,41	0
56	MG	1A	3028	1/1	0.91	0.06	57,57,57,57	0
56	MG	2a	1680	1/1	0.91	0.16	67,67,67,67	0
56	MG	1a	1713	1/1	0.91	0.09	75,75,75,75	0
56	MG	1A	3853	1/1	0.91	0.11	59,59,59,59	0
56	MG	2A	3256	1/1	0.91	0.21	24,24,24,24	0
56	MG	1A	3391	1/1	0.91	0.17	62,62,62,62	0
56	MG	1A	3728	1/1	0.91	0.12	48,48,48,48	0
56	MG	1A	3393	1/1	0.91	0.10	53,53,53,53	0
56	MG	1A	3732	1/1	0.91	0.09	68,68,68,68	0
56	MG	1A	3463	1/1	0.91	0.06	60,60,60,60	0
56	MG	1a	1721	1/1	0.91	0.07	81,81,81,81	0
56	MG	1a	1722	1/1	0.91	0.07	85,85,85,85	0
56	MG	2a	1696	1/1	0.91	0.08	52,52,52,52	0
56	MG	1A	3247	1/1	0.91	0.09	68,68,68,68	0
56	MG	2A	3271	1/1	0.91	0.30	34,34,34,34	0
56	MG	2A	3277	1/1	0.91	0.16	58,58,58,58	0
56	MG	1A	3470	1/1	0.91	0.27	43,43,43,43	0
56	MG	1a	1725	1/1	0.91	0.15	76,76,76,76	0
56	MG	1a	1878	1/1	0.91	0.10	77,77,77,77	0
56	MG	2a	1704	1/1	0.91	0.23	69,69,69,69	0
56	MG	2A	3031	1/1	0.91	0.28	47,47,47,47	0
56	MG	2A	3507	1/1	0.91	0.18	57,57,57,57	0
56	MG	1A	3210	1/1	0.91	0.35	47,47,47,47	0
56	MG	2a	1710	1/1	0.91	0.05	85,85,85,85	0
56	MG	1A	3318	1/1	0.91	0.19	64,64,64,64	0
56	MG	2A	3036	1/1	0.91	0.16	68,68,68,68	0
56	MG	1a	1881	1/1	0.91	0.11	70,70,70,70	0
56	MG	12	101	1/1	0.91	0.15	73,73,73,73	0
56	MG	1A	3622	1/1	0.91	0.27	44,44,44,44	0
56	MG	1a	1884	1/1	0.91	0.16	70,70,70,70	0
56	MG	2a	1718	1/1	0.91	0.11	68,68,68,68	0
56	MG	2A	3044	1/1	0.91	0.23	49,49,49,49	0
56	MG	1A	3397	1/1	0.91	0.07	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	15	101	1/1	0.91	0.24	51,51,51,51	0
56	MG	1A	3872	1/1	0.91	0.22	61,61,61,61	0
56	MG	18	102	1/1	0.91	0.07	55,55,55,55	0
56	MG	1A	3626	1/1	0.91	0.33	47,47,47,47	0
56	MG	1a	1740	1/1	0.91	0.14	67,67,67,67	0
56	MG	1A	3322	1/1	0.91	0.29	58,58,58,58	0
56	MG	1A	3629	1/1	0.91	0.12	73,73,73,73	0
56	MG	1A	3006	1/1	0.91	0.08	59,59,59,59	0
56	MG	1A	3760	1/1	0.91	0.14	52,52,52,52	0
56	MG	2a	1733	1/1	0.91	0.11	74,74,74,74	0
56	MG	1A	3050	1/1	0.91	0.17	43,43,43,43	0
56	MG	1A	3632	1/1	0.91	0.25	71,71,71,71	0
56	MG	1A	3189	1/1	0.91	0.27	51,51,51,51	0
56	MG	1A	3489	1/1	0.91	0.07	45,45,45,45	0
56	MG	2A	3070	1/1	0.91	0.32	61,61,61,61	0
56	MG	1A	3493	1/1	0.91	0.11	52,52,52,52	0
56	MG	1A	3257	1/1	0.91	0.17	57,57,57,57	0
56	MG	2A	3076	1/1	0.91	0.24	47,47,47,47	0
56	MG	2a	1745	1/1	0.91	0.34	44,44,44,44	0
56	MG	1a	1901	1/1	0.91	0.12	76,76,76,76	0
56	MG	1A	3496	1/1	0.91	0.08	47,47,47,47	0
56	MG	1a	1904	1/1	0.91	0.10	70,70,70,70	0
56	MG	1A	3500	1/1	0.91	0.23	61,61,61,61	0
56	MG	2A	3088	1/1	0.91	0.20	49,49,49,49	0
56	MG	1A	3404	1/1	0.91	0.11	58,58,58,58	0
56	MG	2A	3092	1/1	0.91	0.21	55,55,55,55	0
56	MG	1a	1760	1/1	0.91	0.12	59,59,59,59	0
56	MG	1a	1761	1/1	0.91	0.14	69,69,69,69	0
56	MG	1A	3505	1/1	0.91	0.09	46,46,46,46	0
56	MG	1a	1914	1/1	0.91	0.12	74,74,74,74	0
56	MG	1A	3261	1/1	0.91	0.25	25,25,25,25	0
56	MG	2A	3343	1/1	0.91	0.22	67,67,67,67	0
56	MG	2A	3108	1/1	0.91	0.32	58,58,58,58	0
56	MG	1a	1920	1/1	0.91	0.08	66,66,66,66	0
56	MG	2A	3349	1/1	0.91	0.27	48,48,48,48	0
56	MG	1a	1768	1/1	0.91	0.16	75,75,75,75	0
56	MG	1A	3896	1/1	0.91	0.12	65,65,65,65	0
56	MG	2a	1768	1/1	0.91	0.31	71,71,71,71	0
56	MG	2A	3118	1/1	0.91	0.24	42,42,42,42	0
56	MG	1A	3407	1/1	0.91	0.07	85,85,85,85	0
56	MG	1A	3899	1/1	0.91	0.17	53,53,53,53	0
56	MG	1a	1623	1/1	0.91	0.13	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3408	1/1	0.91	0.12	74,74,74,74	0
56	MG	2B	204	1/1	0.91	0.28	60,60,60,60	0
56	MG	1A	3074	1/1	0.91	0.15	50,50,50,50	0
56	MG	1A	3521	1/1	0.91	0.27	31,31,31,31	0
56	MG	1a	1930	1/1	0.91	0.12	72,72,72,72	0
56	MG	2a	1780	1/1	0.91	0.11	56,56,56,56	0
56	MG	2B	208	1/1	0.91	0.07	67,67,67,67	0
56	MG	1A	3079	1/1	0.91	0.11	54,54,54,54	0
56	MG	1a	1783	1/1	0.91	0.31	47,47,47,47	0
56	MG	1A	3158	1/1	0.91	0.20	41,41,41,41	0
56	MG	2A	3135	1/1	0.91	0.24	68,68,68,68	0
56	MG	1A	3225	1/1	0.91	0.29	40,40,40,40	0
56	MG	2A	3373	1/1	0.91	0.16	69,69,69,69	0
56	MG	1A	3007	1/1	0.91	0.06	60,60,60,60	0
56	MG	2a	1789	1/1	0.91	0.11	66,66,66,66	0
56	MG	2A	3376	1/1	0.91	0.11	60,60,60,60	0
56	MG	1A	3353	1/1	0.91	0.21	27,27,27,27	0
56	MG	2A	3143	1/1	0.91	0.10	59,59,59,59	0
56	MG	2A	3380	1/1	0.91	0.28	54,54,54,54	0
56	MG	1A	3163	1/1	0.91	0.14	67,67,67,67	0
56	MG	2a	1796	1/1	0.91	0.16	68,68,68,68	0
56	MG	1a	1792	1/1	0.91	0.19	59,59,59,59	0
56	MG	20	101	1/1	0.91	0.14	52,52,52,52	0
56	MG	1A	3918	1/1	0.91	0.10	55,55,55,55	0
56	MG	1A	3231	1/1	0.91	0.12	51,51,51,51	0
56	MG	1A	3286	1/1	0.91	0.23	23,23,23,23	0
56	MG	1A	3921	1/1	0.91	0.21	43,43,43,43	0
56	MG	1A	3541	1/1	0.91	0.32	43,43,43,43	0
56	MG	1A	3663	1/1	0.91	0.13	54,54,54,54	0
56	MG	1A	3553	1/1	0.91	0.23	34,34,34,34	0
56	MG	2A	3396	1/1	0.91	0.29	63,63,63,63	0
56	MG	1d	301	1/1	0.91	0.24	62,62,62,62	0
56	MG	1A	3556	1/1	0.91	0.11	25,25,25,25	0
56	MG	2A	3403	1/1	0.91	0.16	61,61,61,61	0
56	MG	1a	1667	1/1	0.91	0.10	66,66,66,66	0
56	MG	1A	3363	1/1	0.91	0.16	34,34,34,34	0
56	MG	1A	3423	1/1	0.91	0.09	65,65,65,65	0
56	MG	1A	3931	1/1	0.91	0.13	74,74,74,74	0
56	MG	1A	3670	1/1	0.91	0.16	53,53,53,53	0
56	MG	1B	202	1/1	0.91	0.19	55,55,55,55	0
56	MG	2a	1613	1/1	0.91	0.30	81,81,81,81	0
56	MG	1A	3426	1/1	0.91	0.11	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3679	1/1	0.91	0.11	40,40,40,40	0
56	MG	2A	3182	1/1	0.91	0.32	39,39,39,39	0
56	MG	1A	3054	1/1	0.91	0.19	40,40,40,40	0
56	MG	2A	3185	1/1	0.91	0.32	40,40,40,40	0
56	MG	2A	3423	1/1	0.91	0.15	88,88,88,88	0
56	MG	2A	3424	1/1	0.91	0.17	51,51,51,51	0
56	MG	2A	3186	1/1	0.91	0.34	38,38,38,38	0
56	MG	1A	3143	1/1	0.91	0.10	50,50,50,50	0
56	MG	2A	3188	1/1	0.91	0.32	30,30,30,30	0
56	MG	2v	101	1/1	0.91	0.19	61,61,61,61	0
56	MG	1A	3689	1/1	0.91	0.12	55,55,55,55	0
56	MG	1w	101	1/1	0.91	0.14	72,72,72,72	0
56	MG	1w	102	1/1	0.91	0.12	63,63,63,63	0
56	MG	2A	3437	1/1	0.91	0.16	58,58,58,58	0
56	MG	1A	3234	1/1	0.91	0.24	25,25,25,25	0
56	MG	1A	3299	1/1	0.91	0.29	57,57,57,57	0
56	MG	1a	1840	1/1	0.91	0.14	70,70,70,70	0
56	MG	1B	212	1/1	0.91	0.10	62,62,62,62	0
56	MG	1A	3697	1/1	0.91	0.09	55,55,55,55	0
56	MG	1x	107	1/1	0.91	0.14	71,71,71,71	0
56	MG	1A	3814	1/1	0.92	0.10	73,73,73,73	0
56	MG	1A	3303	1/1	0.92	0.10	42,42,42,42	0
56	MG	1A	3701	1/1	0.92	0.07	42,42,42,42	0
56	MG	2A	3087	1/1	0.92	0.13	76,76,76,76	0
56	MG	1A	3096	1/1	0.92	0.11	59,59,59,59	0
56	MG	1A	3608	1/1	0.92	0.33	57,57,57,57	0
56	MG	1A	3708	1/1	0.92	0.09	33,33,33,33	0
56	MG	1a	1932	1/1	0.92	0.27	72,72,72,72	0
56	MG	2a	1678	1/1	0.92	0.45	72,72,72,72	0
56	MG	1A	3170	1/1	0.92	0.18	73,73,73,73	0
56	MG	2A	3502	1/1	0.92	0.30	70,70,70,70	0
56	MG	1A	3145	1/1	0.92	0.10	52,52,52,52	0
56	MG	1a	1673	1/1	0.92	0.14	68,68,68,68	0
56	MG	1a	1801	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3107	1/1	0.92	0.15	60,60,60,60	0
56	MG	1A	3260	1/1	0.92	0.27	25,25,25,25	0
56	MG	1A	3420	1/1	0.92	0.05	32,32,32,32	0
56	MG	2a	1690	1/1	0.92	0.10	90,90,90,90	0
56	MG	1a	1808	1/1	0.92	0.16	60,60,60,60	0
56	MG	1A	3104	1/1	0.92	0.27	39,39,39,39	0
56	MG	2A	3512	1/1	0.92	0.10	85,85,85,85	0
56	MG	2A	3116	1/1	0.92	0.22	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1813	1/1	0.92	0.07	58,58,58,58	0
56	MG	2a	1697	1/1	0.92	0.09	69,69,69,69	0
56	MG	1A	3314	1/1	0.92	0.32	39,39,39,39	0
56	MG	1A	3621	1/1	0.92	0.07	78,78,78,78	0
56	MG	1A	3133	1/1	0.92	0.25	54,54,54,54	0
56	MG	2A	3126	1/1	0.92	0.18	53,53,53,53	0
56	MG	2A	3324	1/1	0.92	0.46	68,68,68,68	0
56	MG	1a	1682	1/1	0.92	0.17	62,62,62,62	0
56	MG	1A	3723	1/1	0.92	0.12	66,66,66,66	0
56	MG	1A	3321	1/1	0.92	0.20	27,27,27,27	0
56	MG	1A	3510	1/1	0.92	0.11	65,65,65,65	0
56	MG	2A	3131	1/1	0.92	0.28	58,58,58,58	0
56	MG	2a	1709	1/1	0.92	0.10	70,70,70,70	0
56	MG	1A	3514	1/1	0.92	0.22	34,34,34,34	0
56	MG	1k	201	1/1	0.92	0.10	74,74,74,74	0
56	MG	1A	3628	1/1	0.92	0.20	76,76,76,76	0
56	MG	1A	3196	1/1	0.92	0.10	62,62,62,62	0
56	MG	1A	3739	1/1	0.92	0.08	48,48,48,48	0
56	MG	2A	3137	1/1	0.92	0.19	57,57,57,57	0
56	MG	2A	3534	1/1	0.92	0.15	57,57,57,57	0
56	MG	1A	3740	1/1	0.92	0.10	52,52,52,52	0
56	MG	1a	1838	1/1	0.92	0.13	74,74,74,74	0
56	MG	1A	3134	1/1	0.92	0.22	64,64,64,64	0
56	MG	2A	3345	1/1	0.92	0.15	69,69,69,69	0
56	MG	1A	3431	1/1	0.92	0.18	66,66,66,66	0
56	MG	2A	3347	1/1	0.92	0.30	42,42,42,42	0
56	MG	1A	3745	1/1	0.92	0.17	61,61,61,61	0
56	MG	1A	3389	1/1	0.92	0.29	65,65,65,65	0
56	MG	1a	1701	1/1	0.92	0.21	47,47,47,47	0
56	MG	1A	3390	1/1	0.92	0.11	54,54,54,54	0
56	MG	1a	1703	1/1	0.92	0.17	51,51,51,51	0
56	MG	1A	3862	1/1	0.92	0.14	70,70,70,70	0
56	MG	2A	3158	1/1	0.92	0.07	66,66,66,66	0
56	MG	1A	3001	1/1	0.92	0.21	39,39,39,39	0
56	MG	1A	3528	1/1	0.92	0.33	35,35,35,35	0
56	MG	1T	201	1/1	0.92	0.12	55,55,55,55	0
56	MG	1U	201	1/1	0.92	0.23	41,41,41,41	0
56	MG	1A	3106	1/1	0.92	0.21	31,31,31,31	0
56	MG	1x	109	1/1	0.92	0.15	56,56,56,56	0
56	MG	1V	202	1/1	0.92	0.12	47,47,47,47	0
56	MG	2a	1742	1/1	0.92	0.21	51,51,51,51	0
56	MG	1A	3274	1/1	0.92	0.25	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	3446	1/1	0.92	0.25	47,47,47,47	0
56	MG	1A	3870	1/1	0.92	0.12	61,61,61,61	0
56	MG	2A	3172	1/1	0.92	0.30	48,48,48,48	0
56	MG	2a	1748	1/1	0.92	0.13	69,69,69,69	0
56	MG	2A	3173	1/1	0.92	0.25	39,39,39,39	0
56	MG	2A	3174	1/1	0.92	0.27	48,48,48,48	0
56	MG	1a	1718	1/1	0.92	0.10	73,73,73,73	0
56	MG	2B	202	1/1	0.92	0.23	68,68,68,68	0
56	MG	1A	3534	1/1	0.92	0.31	32,32,32,32	0
56	MG	1A	3155	1/1	0.92	0.08	59,59,59,59	0
56	MG	1A	3538	1/1	0.92	0.29	53,53,53,53	0
56	MG	1A	3033	1/1	0.92	0.16	68,68,68,68	0
56	MG	1A	3540	1/1	0.92	0.17	32,32,32,32	0
56	MG	1A	3014	1/1	0.92	0.23	59,59,59,59	0
56	MG	1A	3548	1/1	0.92	0.07	54,54,54,54	0
56	MG	1A	3650	1/1	0.92	0.10	56,56,56,56	0
56	MG	1A	3206	1/1	0.92	0.20	75,75,75,75	0
56	MG	1A	3554	1/1	0.92	0.27	54,54,54,54	0
56	MG	1a	1731	1/1	0.92	0.08	72,72,72,72	0
56	MG	2A	3397	1/1	0.92	0.21	74,74,74,74	0
56	MG	1a	1601	1/1	0.92	0.11	59,59,59,59	0
56	MG	1A	3207	1/1	0.92	0.08	59,59,59,59	0
56	MG	1A	3346	1/1	0.92	0.27	44,44,44,44	0
56	MG	2a	1772	1/1	0.92	0.31	52,52,52,52	0
56	MG	1a	1606	1/1	0.92	0.17	74,74,74,74	0
56	MG	2A	3014	1/1	0.92	0.08	51,51,51,51	0
56	MG	1A	3119	1/1	0.92	0.27	44,44,44,44	0
56	MG	2A	3017	1/1	0.92	0.12	53,53,53,53	0
56	MG	1A	3348	1/1	0.92	0.23	28,28,28,28	0
56	MG	1A	3351	1/1	0.92	0.39	36,36,36,36	0
56	MG	1A	3565	1/1	0.92	0.34	60,60,60,60	0
56	MG	1A	3466	1/1	0.92	0.10	45,45,45,45	0
56	MG	1a	1612	1/1	0.92	0.12	72,72,72,72	0
56	MG	1a	1744	1/1	0.92	0.15	64,64,64,64	0
56	MG	2A	3420	1/1	0.92	0.21	52,52,52,52	0
56	MG	1A	3783	1/1	0.92	0.09	56,56,56,56	0
56	MG	1A	3575	1/1	0.92	0.28	31,31,31,31	0
56	MG	1A	3664	1/1	0.92	0.09	59,59,59,59	0
56	MG	1A	3788	1/1	0.92	0.11	53,53,53,53	0
56	MG	1A	3901	1/1	0.92	0.21	53,53,53,53	0
56	MG	2A	3033	1/1	0.92	0.28	68,68,68,68	0
56	MG	2A	3430	1/1	0.92	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3431	1/1	0.92	0.09	70,70,70,70	0
56	MG	1A	3352	1/1	0.92	0.31	32,32,32,32	0
56	MG	2A	3035	1/1	0.92	0.20	53,53,53,53	0
56	MG	1A	3472	1/1	0.92	0.15	60,60,60,60	0
56	MG	2A	3230	1/1	0.92	0.27	50,50,50,50	0
56	MG	1A	3475	1/1	0.92	0.07	64,64,64,64	0
56	MG	1A	3009	1/1	0.92	0.19	51,51,51,51	0
56	MG	1A	3124	1/1	0.92	0.08	56,56,56,56	0
56	MG	1a	1758	1/1	0.92	0.05	65,65,65,65	0
56	MG	2A	3240	1/1	0.92	0.17	50,50,50,50	0
56	MG	1A	3356	1/1	0.92	0.26	26,26,26,26	0
56	MG	1A	3677	1/1	0.92	0.10	56,56,56,56	0
56	MG	1A	3481	1/1	0.92	0.09	72,72,72,72	0
56	MG	2a	1622	1/1	0.92	0.11	92,92,92,92	0
56	MG	2A	3248	1/1	0.92	0.27	57,57,57,57	0
56	MG	2A	3249	1/1	0.92	0.27	55,55,55,55	0
56	MG	2A	3452	1/1	0.92	0.16	59,59,59,59	0
56	MG	2A	3252	1/1	0.92	0.21	59,59,59,59	0
56	MG	2a	1810	1/1	0.92	0.12	67,67,67,67	0
56	MG	1A	3799	1/1	0.92	0.15	67,67,67,67	0
56	MG	1a	1765	1/1	0.92	0.08	88,88,88,88	0
56	MG	1A	3482	1/1	0.92	0.12	55,55,55,55	0
56	MG	1A	3801	1/1	0.92	0.08	63,63,63,63	0
56	MG	1A	3596	1/1	0.92	0.23	25,25,25,25	0
56	MG	1a	1911	1/1	0.92	0.15	64,64,64,64	0
56	MG	1A	3688	1/1	0.92	0.14	37,37,37,37	0
56	MG	2A	3263	1/1	0.92	0.38	48,48,48,48	0
56	MG	1A	3301	1/1	0.92	0.17	42,42,42,42	0
56	MG	1a	1648	1/1	0.92	0.14	51,51,51,51	0
56	MG	1a	1916	1/1	0.92	0.08	70,70,70,70	0
56	MG	1a	1917	1/1	0.92	0.18	62,62,62,62	0
56	MG	1A	3411	1/1	0.92	0.07	54,54,54,54	0
56	MG	1a	1652	1/1	0.92	0.21	57,57,57,57	0
56	MG	1A	3167	1/1	0.92	0.30	46,46,46,46	0
56	MG	2A	3278	1/1	0.92	0.27	38,38,38,38	0
56	MG	2A	3477	1/1	0.92	0.20	58,58,58,58	0
56	MG	2t	201	1/1	0.92	0.19	55,55,55,55	0
56	MG	2A	3479	1/1	0.92	0.25	46,46,46,46	0
56	MG	2A	3074	1/1	0.92	0.14	51,51,51,51	0
56	MG	1a	1654	1/1	0.92	0.25	41,41,41,41	0
56	MG	1A	3602	1/1	0.92	0.09	48,48,48,48	0
56	MG	2A	3077	1/1	0.92	0.24	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3285	1/1	0.92	0.44	39,39,39,39	0
56	MG	2A	3488	1/1	0.92	0.22	61,61,61,61	0
56	MG	2A	3286	1/1	0.92	0.29	50,50,50,50	0
56	MG	2A	3078	1/1	0.92	0.17	35,35,35,35	0
57	KAN	1A	3933	33/33	0.92	0.10	34,44,58,64	0
57	KAN	1A	3934	33/33	0.92	0.08	39,48,55,63	0
56	MG	2A	3079	1/1	0.92	0.12	74,74,74,74	0
56	MG	1A	3811	1/1	0.92	0.08	81,81,81,81	0
57	KAN	2a	1828	33/33	0.92	0.11	47,61,67,70	0
56	MG	2A	3096	1/1	0.93	0.18	44,44,44,44	0
56	MG	2A	3097	1/1	0.93	0.13	48,48,48,48	0
56	MG	1A	3240	1/1	0.93	0.28	49,49,49,49	0
56	MG	2a	1668	1/1	0.93	0.24	69,69,69,69	0
56	MG	1A	3568	1/1	0.93	0.28	42,42,42,42	0
56	MG	2A	3101	1/1	0.93	0.08	41,41,41,41	0
56	MG	1a	1809	1/1	0.93	0.08	63,63,63,63	0
56	MG	2A	3103	1/1	0.93	0.11	59,59,59,59	0
56	MG	1A	3572	1/1	0.93	0.14	40,40,40,40	0
56	MG	1E	301	1/1	0.93	0.10	37,37,37,37	0
56	MG	1E	302	1/1	0.93	0.24	27,27,27,27	0
56	MG	1a	1941	1/1	0.93	0.10	55,55,55,55	0
56	MG	1a	1815	1/1	0.93	0.23	61,61,61,61	0
56	MG	1a	1687	1/1	0.93	0.10	69,69,69,69	0
56	MG	2A	3113	1/1	0.93	0.10	72,72,72,72	0
56	MG	1A	3573	1/1	0.93	0.13	57,57,57,57	0
56	MG	1A	3413	1/1	0.93	0.41	43,43,43,43	0
56	MG	1a	1950	1/1	0.93	0.20	92,92,92,92	0
56	MG	2A	3120	1/1	0.93	0.25	51,51,51,51	0
56	MG	1F	302	1/1	0.93	0.05	56,56,56,56	0
56	MG	1A	3101	1/1	0.93	0.28	45,45,45,45	0
56	MG	1G	202	1/1	0.93	0.11	47,47,47,47	0
56	MG	2A	3508	1/1	0.93	0.05	68,68,68,68	0
56	MG	1A	3132	1/1	0.93	0.20	33,33,33,33	0
56	MG	1O	3101	1/1	0.93	0.18	64,64,64,64	0
56	MG	1a	1828	1/1	0.93	0.09	66,66,66,66	0
56	MG	1A	3243	1/1	0.93	0.17	51,51,51,51	0
56	MG	1A	3765	1/1	0.93	0.19	60,60,60,60	0
56	MG	1A	3010	1/1	0.93	0.19	66,66,66,66	0
56	MG	1a	1836	1/1	0.93	0.15	72,72,72,72	0
56	MG	1A	3661	1/1	0.93	0.07	70,70,70,70	0
56	MG	1A	3181	1/1	0.93	0.19	60,60,60,60	0
56	MG	1A	3067	1/1	0.93	0.10	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3135	1/1	0.93	0.16	48,48,48,48	0
56	MG	1A	3594	1/1	0.93	0.33	47,47,47,47	0
56	MG	2A	3523	1/1	0.93	0.09	63,63,63,63	0
56	MG	1A	3773	1/1	0.93	0.19	48,48,48,48	0
56	MG	1A	3214	1/1	0.93	0.22	55,55,55,55	0
56	MG	2A	3335	1/1	0.93	0.24	42,42,42,42	0
56	MG	2A	3338	1/1	0.93	0.23	53,53,53,53	0
56	MG	1a	1845	1/1	0.93	0.28	54,54,54,54	0
56	MG	1a	1846	1/1	0.93	0.14	42,42,42,42	0
56	MG	10	101	1/1	0.93	0.30	46,46,46,46	0
56	MG	1a	1848	1/1	0.93	0.26	56,56,56,56	0
56	MG	1A	3667	1/1	0.93	0.11	71,71,71,71	0
56	MG	1A	3777	1/1	0.93	0.12	63,63,63,63	0
56	MG	1A	3082	1/1	0.93	0.24	67,67,67,67	0
56	MG	2a	1719	1/1	0.93	0.22	70,70,70,70	0
56	MG	2a	1720	1/1	0.93	0.22	60,60,60,60	0
56	MG	1A	3424	1/1	0.93	0.17	48,48,48,48	0
56	MG	1A	3380	1/1	0.93	0.10	67,67,67,67	0
56	MG	1A	3599	1/1	0.93	0.09	57,57,57,57	0
56	MG	2A	3352	1/1	0.93	0.11	70,70,70,70	0
56	MG	2A	3160	1/1	0.93	0.07	57,57,57,57	0
56	MG	17	101	1/1	0.93	0.12	54,54,54,54	0
56	MG	1A	3676	1/1	0.93	0.11	57,57,57,57	0
56	MG	2A	3356	1/1	0.93	0.21	54,54,54,54	0
56	MG	2A	3544	1/1	0.93	0.12	69,69,69,69	0
56	MG	2A	3359	1/1	0.93	0.09	54,54,54,54	0
56	MG	1A	3600	1/1	0.93	0.08	52,52,52,52	0
56	MG	1a	1858	1/1	0.93	0.10	68,68,68,68	0
56	MG	1x	117	1/1	0.93	0.13	57,57,57,57	0
56	MG	1A	3258	1/1	0.93	0.22	44,44,44,44	0
56	MG	1A	3385	1/1	0.93	0.20	59,59,59,59	0
56	MG	1a	1861	1/1	0.93	0.12	64,64,64,64	0
56	MG	1A	3603	1/1	0.93	0.15	65,65,65,65	0
56	MG	1x	122	1/1	0.93	0.09	63,63,63,63	0
56	MG	1A	3317	1/1	0.93	0.10	55,55,55,55	0
56	MG	1a	1729	1/1	0.93	0.21	53,53,53,53	0
56	MG	2a	1743	1/1	0.93	0.29	39,39,39,39	0
56	MG	1a	1603	1/1	0.93	0.12	61,61,61,61	0
56	MG	1A	3511	1/1	0.93	0.10	49,49,49,49	0
56	MG	1a	1605	1/1	0.93	0.20	63,63,63,63	0
56	MG	1A	3897	1/1	0.93	0.18	51,51,51,51	0
56	MG	2A	3377	1/1	0.93	0.23	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3184	1/1	0.93	0.16	54,54,54,54	0
56	MG	2a	1750	1/1	0.93	0.19	61,61,61,61	0
56	MG	1A	3512	1/1	0.93	0.14	39,39,39,39	0
56	MG	1A	3693	1/1	0.93	0.09	53,53,53,53	0
56	MG	2A	3009	1/1	0.93	0.13	59,59,59,59	0
56	MG	1A	3795	1/1	0.93	0.09	69,69,69,69	0
56	MG	1A	3110	1/1	0.93	0.11	68,68,68,68	0
56	MG	2A	3012	1/1	0.93	0.21	33,33,33,33	0
56	MG	1A	3797	1/1	0.93	0.14	58,58,58,58	0
56	MG	1A	3905	1/1	0.93	0.09	70,70,70,70	0
56	MG	2A	3016	1/1	0.93	0.21	58,58,58,58	0
56	MG	1A	3907	1/1	0.93	0.07	45,45,45,45	0
56	MG	2B	210	1/1	0.93	0.11	74,74,74,74	0
56	MG	1A	3112	1/1	0.93	0.27	23,23,23,23	0
56	MG	2B	212	1/1	0.93	0.09	64,64,64,64	0
56	MG	2B	213	1/1	0.93	0.11	78,78,78,78	0
56	MG	2A	3394	1/1	0.93	0.08	59,59,59,59	0
56	MG	1A	3139	1/1	0.93	0.13	68,68,68,68	0
56	MG	2E	302	1/1	0.93	0.25	36,36,36,36	0
56	MG	2A	3200	1/1	0.93	0.19	46,46,46,46	0
56	MG	2A	3202	1/1	0.93	0.23	38,38,38,38	0
56	MG	2F	303	1/1	0.93	0.10	65,65,65,65	0
56	MG	1A	3191	1/1	0.93	0.08	57,57,57,57	0
56	MG	2A	3401	1/1	0.93	0.19	59,59,59,59	0
56	MG	2A	3402	1/1	0.93	0.10	56,56,56,56	0
56	MG	1A	3026	1/1	0.93	0.06	32,32,32,32	0
56	MG	1A	3618	1/1	0.93	0.14	58,58,58,58	0
56	MG	1A	3227	1/1	0.93	0.24	54,54,54,54	0
56	MG	1A	3916	1/1	0.93	0.12	63,63,63,63	0
56	MG	1a	1751	1/1	0.93	0.21	62,62,62,62	0
56	MG	1A	3035	1/1	0.93	0.20	39,39,39,39	0
56	MG	1A	3273	1/1	0.93	0.26	21,21,21,21	0
56	MG	1A	3450	1/1	0.93	0.07	47,47,47,47	0
56	MG	2A	3215	1/1	0.93	0.27	35,35,35,35	0
56	MG	1A	3070	1/1	0.93	0.14	44,44,44,44	0
56	MG	1A	3275	1/1	0.93	0.38	39,39,39,39	0
56	MG	1A	3812	1/1	0.93	0.11	68,68,68,68	0
56	MG	1A	3334	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3816	1/1	0.93	0.21	42,42,42,42	0
56	MG	2a	1791	1/1	0.93	0.13	68,68,68,68	0
56	MG	1A	3120	1/1	0.93	0.12	41,41,41,41	0
56	MG	2A	3039	1/1	0.93	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3225	1/1	0.93	0.31	41,41,41,41	0
56	MG	2A	3226	1/1	0.93	0.28	52,52,52,52	0
56	MG	2A	3040	1/1	0.93	0.08	43,43,43,43	0
56	MG	1A	3460	1/1	0.93	0.07	53,53,53,53	0
56	MG	1A	3340	1/1	0.93	0.14	36,36,36,36	0
56	MG	2A	3234	1/1	0.93	0.28	43,43,43,43	0
56	MG	1a	1766	1/1	0.93	0.06	63,63,63,63	0
56	MG	1a	1767	1/1	0.93	0.12	60,60,60,60	0
56	MG	1A	3343	1/1	0.93	0.14	44,44,44,44	0
56	MG	2A	3238	1/1	0.93	0.36	48,48,48,48	0
56	MG	2A	3048	1/1	0.93	0.24	54,54,54,54	0
56	MG	1a	1769	1/1	0.93	0.18	79,79,79,79	0
56	MG	1A	3633	1/1	0.93	0.11	70,70,70,70	0
56	MG	1A	3828	1/1	0.93	0.11	49,49,49,49	0
56	MG	1a	1907	1/1	0.93	0.10	68,68,68,68	0
56	MG	1A	3015	1/1	0.93	0.15	53,53,53,53	0
56	MG	1A	3543	1/1	0.93	0.22	26,26,26,26	0
56	MG	1a	1910	1/1	0.93	0.10	52,52,52,52	0
56	MG	1A	3547	1/1	0.93	0.25	42,42,42,42	0
56	MG	1A	3738	1/1	0.93	0.12	63,63,63,63	0
56	MG	2a	1628	1/1	0.93	0.10	69,69,69,69	0
56	MG	1B	207	1/1	0.93	0.08	52,52,52,52	0
56	MG	1A	3465	1/1	0.93	0.20	48,48,48,48	0
56	MG	1A	3551	1/1	0.93	0.23	28,28,28,28	0
56	MG	2A	3457	1/1	0.93	0.15	44,44,44,44	0
56	MG	1a	1784	1/1	0.93	0.06	67,67,67,67	0
56	MG	1A	3285	1/1	0.93	0.18	26,26,26,26	0
56	MG	2a	1639	1/1	0.93	0.17	71,71,71,71	0
56	MG	1A	3003	1/1	0.93	0.14	55,55,55,55	0
56	MG	1a	1668	1/1	0.93	0.07	62,62,62,62	0
56	MG	2a	1643	1/1	0.93	0.23	59,59,59,59	0
56	MG	1A	3843	1/1	0.93	0.07	69,69,69,69	0
56	MG	2A	3465	1/1	0.93	0.06	76,76,76,76	0
56	MG	1A	3471	1/1	0.93	0.17	66,66,66,66	0
56	MG	1a	1791	1/1	0.93	0.09	69,69,69,69	0
56	MG	1A	3746	1/1	0.93	0.16	54,54,54,54	0
56	MG	1A	3290	1/1	0.93	0.31	40,40,40,40	0
56	MG	2A	3274	1/1	0.93	0.29	32,32,32,32	0
56	MG	2A	3472	1/1	0.93	0.15	84,84,84,84	0
56	MG	1A	3291	1/1	0.93	0.18	31,31,31,31	0
56	MG	2A	3084	1/1	0.93	0.19	43,43,43,43	0
56	MG	2a	1657	1/1	0.93	0.26	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2x	105	1/1	0.93	0.21	61,61,61,61	0
56	MG	1B	219	1/1	0.93	0.22	59,59,59,59	0
56	MG	1A	3125	1/1	0.93	0.11	59,59,59,59	0
56	MG	1A	3099	1/1	0.93	0.22	44,44,44,44	0
56	MG	1A	3150	1/1	0.93	0.04	75,75,75,75	0
56	MG	1a	1804	1/1	0.93	0.08	57,57,57,57	0
56	MG	2A	3091	1/1	0.93	0.24	59,59,59,59	0
56	MG	1A	3753	1/1	0.93	0.07	57,57,57,57	0
56	MG	1A	3011	1/1	0.94	0.24	48,48,48,48	0
56	MG	1A	3294	1/1	0.94	0.26	40,40,40,40	0
56	MG	1a	1762	1/1	0.94	0.08	70,70,70,70	0
56	MG	2a	1681	1/1	0.94	0.13	64,64,64,64	0
56	MG	1A	3376	1/1	0.94	0.12	75,75,75,75	0
56	MG	2A	3177	1/1	0.94	0.18	47,47,47,47	0
56	MG	2A	3178	1/1	0.94	0.33	35,35,35,35	0
56	MG	1A	3209	1/1	0.94	0.32	44,44,44,44	0
56	MG	2A	3518	1/1	0.94	0.08	59,59,59,59	0
56	MG	1A	3849	1/1	0.94	0.06	68,68,68,68	0
56	MG	2a	1689	1/1	0.94	0.09	72,72,72,72	0
56	MG	2A	3348	1/1	0.94	0.27	50,50,50,50	0
56	MG	1a	1656	1/1	0.94	0.21	53,53,53,53	0
56	MG	1a	1657	1/1	0.94	0.29	46,46,46,46	0
56	MG	1A	3328	1/1	0.94	0.21	46,46,46,46	0
56	MG	1A	3379	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3762	1/1	0.94	0.11	57,57,57,57	0
56	MG	1a	1772	1/1	0.94	0.13	58,58,58,58	0
56	MG	1B	217	1/1	0.94	0.26	64,64,64,64	0
56	MG	1A	3467	1/1	0.94	0.16	29,29,29,29	0
56	MG	1a	1776	1/1	0.94	0.08	72,72,72,72	0
56	MG	1A	3297	1/1	0.94	0.10	63,63,63,63	0
56	MG	1A	3533	1/1	0.94	0.19	44,44,44,44	0
56	MG	2A	3195	1/1	0.94	0.24	53,53,53,53	0
56	MG	1A	3605	1/1	0.94	0.13	72,72,72,72	0
56	MG	2A	3366	1/1	0.94	0.07	66,66,66,66	0
56	MG	1a	1669	1/1	0.94	0.05	68,68,68,68	0
56	MG	1A	3058	1/1	0.94	0.11	35,35,35,35	0
56	MG	1a	1903	1/1	0.94	0.08	61,61,61,61	0
56	MG	1A	3675	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	3535	1/1	0.94	0.42	44,44,44,44	0
56	MG	2A	3204	1/1	0.94	0.15	38,38,38,38	0
56	MG	1A	3049	1/1	0.94	0.08	38,38,38,38	0
56	MG	1A	3474	1/1	0.94	0.08	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3375	1/1	0.94	0.13	56,56,56,56	0
56	MG	2a	1716	1/1	0.94	0.09	85,85,85,85	0
56	MG	1A	3612	1/1	0.94	0.11	53,53,53,53	0
56	MG	1a	1788	1/1	0.94	0.09	71,71,71,71	0
56	MG	1A	3195	1/1	0.94	0.21	68,68,68,68	0
56	MG	1a	1677	1/1	0.94	0.09	56,56,56,56	0
56	MG	2A	3052	1/1	0.94	0.17	57,57,57,57	0
56	MG	2A	3551	1/1	0.94	0.15	59,59,59,59	0
56	MG	1a	1678	1/1	0.94	0.20	42,42,42,42	0
56	MG	1A	3684	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3686	1/1	0.94	0.17	15,15,15,15	0
56	MG	1a	1794	1/1	0.94	0.08	40,40,40,40	0
56	MG	2A	3556	1/1	0.94	0.10	56,56,56,56	0
56	MG	2a	1728	1/1	0.94	0.24	60,60,60,60	0
56	MG	2A	3217	1/1	0.94	0.36	38,38,38,38	0
56	MG	1A	3169	1/1	0.94	0.15	48,48,48,48	0
56	MG	2A	3559	1/1	0.94	0.09	66,66,66,66	0
56	MG	1A	3237	1/1	0.94	0.12	56,56,56,56	0
56	MG	1a	1797	1/1	0.94	0.08	72,72,72,72	0
56	MG	2A	3221	1/1	0.94	0.34	35,35,35,35	0
56	MG	2A	3393	1/1	0.94	0.14	52,52,52,52	0
56	MG	1A	3182	1/1	0.94	0.05	53,53,53,53	0
56	MG	1A	3545	1/1	0.94	0.19	31,31,31,31	0
56	MG	1A	3546	1/1	0.94	0.25	33,33,33,33	0
56	MG	1A	3696	1/1	0.94	0.07	49,49,49,49	0
56	MG	2a	1740	1/1	0.94	0.27	58,58,58,58	0
56	MG	1A	3877	1/1	0.94	0.09	70,70,70,70	0
56	MG	1a	1806	1/1	0.94	0.18	62,62,62,62	0
56	MG	1A	3786	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	3879	1/1	0.94	0.12	68,68,68,68	0
56	MG	2A	3405	1/1	0.94	0.34	58,58,58,58	0
56	MG	2A	3231	1/1	0.94	0.27	54,54,54,54	0
56	MG	2A	3232	1/1	0.94	0.17	46,46,46,46	0
56	MG	1A	3787	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3410	1/1	0.94	0.16	50,50,50,50	0
56	MG	1A	3027	1/1	0.94	0.07	28,28,28,28	0
56	MG	2A	3412	1/1	0.94	0.16	54,54,54,54	0
56	MG	1A	3345	1/1	0.94	0.28	36,36,36,36	0
56	MG	1A	3550	1/1	0.94	0.34	29,29,29,29	0
56	MG	1A	3392	1/1	0.94	0.14	49,49,49,49	0
56	MG	2A	3080	1/1	0.94	0.16	45,45,45,45	0
56	MG	1A	3308	1/1	0.94	0.13	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1757	1/1	0.94	0.28	57,57,57,57	0
56	MG	1A	3272	1/1	0.94	0.16	27,27,27,27	0
56	MG	1A	3709	1/1	0.94	0.10	15,15,15,15	0
56	MG	1a	1820	1/1	0.94	0.15	47,47,47,47	0
56	MG	1A	3432	1/1	0.94	0.05	56,56,56,56	0
56	MG	1a	1705	1/1	0.94	0.18	54,54,54,54	0
56	MG	2A	3425	1/1	0.94	0.08	57,57,57,57	0
56	MG	1a	1824	1/1	0.94	0.06	80,80,80,80	0
56	MG	1A	3890	1/1	0.94	0.05	69,69,69,69	0
56	MG	1A	3108	1/1	0.94	0.22	27,27,27,27	0
56	MG	1A	3490	1/1	0.94	0.07	56,56,56,56	0
56	MG	2A	3093	1/1	0.94	0.23	69,69,69,69	0
56	MG	2a	1770	1/1	0.94	0.24	54,54,54,54	0
56	MG	1a	1710	1/1	0.94	0.28	43,43,43,43	0
56	MG	1a	1952	1/1	0.94	0.06	58,58,58,58	0
56	MG	1a	1829	1/1	0.94	0.07	70,70,70,70	0
56	MG	2A	3436	1/1	0.94	0.26	61,61,61,61	0
56	MG	2a	1601	1/1	0.94	0.10	76,76,76,76	0
56	MG	15	102	1/1	0.94	0.19	39,39,39,39	0
56	MG	2A	3438	1/1	0.94	0.16	63,63,63,63	0
56	MG	1A	3893	1/1	0.94	0.07	41,41,41,41	0
56	MG	1a	1833	1/1	0.94	0.11	59,59,59,59	0
56	MG	1A	3715	1/1	0.94	0.10	68,68,68,68	0
56	MG	1a	1835	1/1	0.94	0.12	83,83,83,83	0
56	MG	2A	3269	1/1	0.94	0.18	35,35,35,35	0
56	MG	1A	3492	1/1	0.94	0.11	44,44,44,44	0
56	MG	18	103	1/1	0.94	0.15	58,58,58,58	0
56	MG	2A	3272	1/1	0.94	0.14	58,58,58,58	0
56	MG	1A	3563	1/1	0.94	0.17	39,39,39,39	0
56	MG	1A	3350	1/1	0.94	0.19	30,30,30,30	0
56	MG	1A	3435	1/1	0.94	0.12	54,54,54,54	0
56	MG	1A	3311	1/1	0.94	0.20	42,42,42,42	0
56	MG	1A	3497	1/1	0.94	0.13	59,59,59,59	0
56	MG	1A	3805	1/1	0.94	0.10	74,74,74,74	0
56	MG	2A	3283	1/1	0.94	0.34	50,50,50,50	0
56	MG	2A	3117	1/1	0.94	0.21	32,32,32,32	0
56	MG	1A	3906	1/1	0.94	0.30	53,53,53,53	0
56	MG	1A	3724	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3460	1/1	0.94	0.06	46,46,46,46	0
56	MG	1A	3221	1/1	0.94	0.08	55,55,55,55	0
56	MG	1A	3244	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3503	1/1	0.94	0.25	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3576	1/1	0.94	0.17	22,22,22,22	0
56	MG	1A	3445	1/1	0.94	0.26	51,51,51,51	0
56	MG	2A	3467	1/1	0.94	0.13	60,60,60,60	0
56	MG	1A	3815	1/1	0.94	0.09	45,45,45,45	0
56	MG	1A	3737	1/1	0.94	0.13	61,61,61,61	0
56	MG	1x	105	1/1	0.94	0.27	41,41,41,41	0
56	MG	1a	1732	1/1	0.94	0.21	53,53,53,53	0
56	MG	1x	108	1/1	0.94	0.15	42,42,42,42	0
56	MG	1A	3245	1/1	0.94	0.10	40,40,40,40	0
56	MG	1A	3819	1/1	0.94	0.20	47,47,47,47	0
56	MG	1A	3820	1/1	0.94	0.21	28,28,28,28	0
56	MG	2A	3302	1/1	0.94	0.14	41,41,41,41	0
56	MG	1A	3579	1/1	0.94	0.24	41,41,41,41	0
56	MG	2a	1645	1/1	0.94	0.15	56,56,56,56	0
56	MG	1A	3580	1/1	0.94	0.27	35,35,35,35	0
56	MG	1A	3581	1/1	0.94	0.34	24,24,24,24	0
56	MG	1A	3652	1/1	0.94	0.19	43,43,43,43	0
56	MG	1A	3583	1/1	0.94	0.23	39,39,39,39	0
56	MG	1A	3829	1/1	0.94	0.20	44,44,44,44	0
56	MG	2A	3487	1/1	0.94	0.19	41,41,41,41	0
56	MG	1A	3830	1/1	0.94	0.15	42,42,42,42	0
56	MG	1A	3832	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3156	1/1	0.94	0.07	59,59,59,59	0
56	MG	2A	3152	1/1	0.94	0.10	54,54,54,54	0
56	MG	1A	3018	1/1	0.94	0.22	66,66,66,66	0
56	MG	1a	1632	1/1	0.94	0.11	54,54,54,54	0
56	MG	2A	3319	1/1	0.94	0.09	44,44,44,44	0
56	MG	2A	3322	1/1	0.94	0.33	54,54,54,54	0
56	MG	2q	201	1/1	0.94	0.27	72,72,72,72	0
56	MG	1A	3319	1/1	0.94	0.39	44,44,44,44	0
56	MG	1A	3361	1/1	0.94	0.22	30,30,30,30	0
56	MG	1a	1750	1/1	0.94	0.06	70,70,70,70	0
56	MG	1a	1875	1/1	0.94	0.13	60,60,60,60	0
56	MG	1a	1638	1/1	0.94	0.11	58,58,58,58	0
56	MG	1a	1639	1/1	0.94	0.16	35,35,35,35	0
56	MG	1a	1640	1/1	0.94	0.27	55,55,55,55	0
56	MG	1A	3043	1/1	0.94	0.37	58,58,58,58	0
56	MG	2A	3166	1/1	0.94	0.14	44,44,44,44	0
56	MG	2a	1671	1/1	0.94	0.08	88,88,88,88	0
56	MG	1A	3126	1/1	0.94	0.05	74,74,74,74	0
56	MG	1A	3128	1/1	0.94	0.11	62,62,62,62	0
56	MG	1A	3754	1/1	0.94	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	KAN	1a	1955	33/33	0.94	0.10	44,52,58,59	0
56	MG	2A	3336	1/1	0.94	0.11	68,68,68,68	0
56	MG	2A	3337	1/1	0.94	0.25	61,61,61,61	0
56	MG	2A	3013	1/1	0.94	0.16	60,60,60,60	0
56	MG	1A	3248	1/1	0.95	0.17	66,66,66,66	0
56	MG	1A	3250	1/1	0.95	0.09	59,59,59,59	0
56	MG	2A	3072	1/1	0.95	0.08	64,64,64,64	0
56	MG	1A	3818	1/1	0.95	0.27	52,52,52,52	0
56	MG	1A	3295	1/1	0.95	0.23	39,39,39,39	0
56	MG	1a	1830	1/1	0.95	0.07	70,70,70,70	0
56	MG	1A	3910	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3385	1/1	0.95	0.14	51,51,51,51	0
56	MG	1A	3911	1/1	0.95	0.06	49,49,49,49	0
56	MG	1A	3651	1/1	0.95	0.09	58,58,58,58	0
56	MG	1a	1945	1/1	0.95	0.08	61,61,61,61	0
56	MG	2A	3389	1/1	0.95	0.13	51,51,51,51	0
56	MG	1a	1946	1/1	0.95	0.12	69,69,69,69	0
56	MG	1A	3742	1/1	0.95	0.17	41,41,41,41	0
56	MG	1A	3822	1/1	0.95	0.11	57,57,57,57	0
56	MG	2a	1706	1/1	0.95	0.11	57,57,57,57	0
56	MG	1A	3823	1/1	0.95	0.28	50,50,50,50	0
56	MG	1A	3190	1/1	0.95	0.12	55,55,55,55	0
56	MG	1A	3825	1/1	0.95	0.17	45,45,45,45	0
56	MG	1A	3056	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3443	1/1	0.95	0.15	35,35,35,35	0
56	MG	1A	3097	1/1	0.95	0.32	55,55,55,55	0
56	MG	2A	3400	1/1	0.95	0.16	60,60,60,60	0
56	MG	1A	3582	1/1	0.95	0.25	49,49,49,49	0
56	MG	1i	201	1/1	0.95	0.10	84,84,84,84	0
56	MG	1A	3123	1/1	0.95	0.17	26,26,26,26	0
56	MG	2A	3404	1/1	0.95	0.23	41,41,41,41	0
56	MG	1l	201	1/1	0.95	0.09	58,58,58,58	0
56	MG	2A	3406	1/1	0.95	0.08	57,57,57,57	0
56	MG	1A	3584	1/1	0.95	0.15	28,28,28,28	0
56	MG	1A	3924	1/1	0.95	0.10	52,52,52,52	0
56	MG	1m	201	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3256	1/1	0.95	0.21	43,43,43,43	0
56	MG	1A	3513	1/1	0.95	0.08	32,32,32,32	0
56	MG	1A	3098	1/1	0.95	0.18	48,48,48,48	0
56	MG	2B	201	1/1	0.95	0.07	75,75,75,75	0
56	MG	1A	3515	1/1	0.95	0.16	30,30,30,30	0
56	MG	2A	3257	1/1	0.95	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3930	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3756	1/1	0.95	0.13	67,67,67,67	0
56	MG	1A	3516	1/1	0.95	0.22	31,31,31,31	0
56	MG	1a	1628	1/1	0.95	0.06	55,55,55,55	0
56	MG	2A	3112	1/1	0.95	0.12	42,42,42,42	0
56	MG	1A	3517	1/1	0.95	0.32	41,41,41,41	0
56	MG	2A	3422	1/1	0.95	0.16	57,57,57,57	0
56	MG	2A	3114	1/1	0.95	0.07	60,60,60,60	0
56	MG	1A	3041	1/1	0.95	0.14	25,25,25,25	0
56	MG	1A	3349	1/1	0.95	0.27	26,26,26,26	0
56	MG	1A	3042	1/1	0.95	0.17	42,42,42,42	0
56	MG	2A	3427	1/1	0.95	0.20	67,67,67,67	0
56	MG	1A	3198	1/1	0.95	0.22	52,52,52,52	0
56	MG	1A	3455	1/1	0.95	0.15	41,41,41,41	0
56	MG	2A	3273	1/1	0.95	0.35	54,54,54,54	0
56	MG	2A	3121	1/1	0.95	0.23	33,33,33,33	0
56	MG	2A	3432	1/1	0.95	0.22	44,44,44,44	0
56	MG	1A	3456	1/1	0.95	0.15	44,44,44,44	0
56	MG	2A	3123	1/1	0.95	0.12	33,33,33,33	0
56	MG	1a	1643	1/1	0.95	0.09	51,51,51,51	0
56	MG	1x	106	1/1	0.95	0.12	64,64,64,64	0
56	MG	1A	3526	1/1	0.95	0.24	28,28,28,28	0
56	MG	1A	3306	1/1	0.95	0.25	50,50,50,50	0
56	MG	1a	1866	1/1	0.95	0.14	73,73,73,73	0
56	MG	1A	3147	1/1	0.95	0.09	59,59,59,59	0
56	MG	1a	1647	1/1	0.95	0.12	54,54,54,54	0
56	MG	1A	3127	1/1	0.95	0.14	57,57,57,57	0
56	MG	1a	1870	1/1	0.95	0.07	62,62,62,62	0
56	MG	1a	1649	1/1	0.95	0.19	42,42,42,42	0
56	MG	1A	3854	1/1	0.95	0.11	39,39,39,39	0
56	MG	1A	3531	1/1	0.95	0.26	34,34,34,34	0
56	MG	1A	3355	1/1	0.95	0.10	23,23,23,23	0
56	MG	2A	3293	1/1	0.95	0.41	60,60,60,60	0
56	MG	1A	3022	1/1	0.95	0.14	57,57,57,57	0
56	MG	2A	3138	1/1	0.95	0.09	65,65,65,65	0
56	MG	1A	3063	1/1	0.95	0.12	39,39,39,39	0
56	MG	1A	3051	1/1	0.95	0.08	27,27,27,27	0
56	MG	2a	1766	1/1	0.95	0.19	73,73,73,73	0
56	MG	1A	3536	1/1	0.95	0.25	38,38,38,38	0
56	MG	1A	3613	1/1	0.95	0.13	52,52,52,52	0
56	MG	2A	3147	1/1	0.95	0.19	65,65,65,65	0
56	MG	1A	3863	1/1	0.95	0.08	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3107	1/1	0.95	0.23	30,30,30,30	0
56	MG	1a	1770	1/1	0.95	0.14	60,60,60,60	0
56	MG	1B	226	1/1	0.95	0.10	53,53,53,53	0
56	MG	2A	3463	1/1	0.95	0.07	66,66,66,66	0
56	MG	2A	3306	1/1	0.95	0.13	74,74,74,74	0
56	MG	1A	3779	1/1	0.95	0.16	71,71,71,71	0
56	MG	1a	1773	1/1	0.95	0.13	59,59,59,59	0
56	MG	2A	3309	1/1	0.95	0.36	53,53,53,53	0
56	MG	2A	3156	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3362	1/1	0.95	0.31	36,36,36,36	0
56	MG	1A	3044	1/1	0.95	0.20	34,34,34,34	0
56	MG	1A	3695	1/1	0.95	0.08	55,55,55,55	0
56	MG	1a	1777	1/1	0.95	0.24	71,71,71,71	0
56	MG	1A	3047	1/1	0.95	0.11	32,32,32,32	0
56	MG	2A	3162	1/1	0.95	0.13	59,59,59,59	0
56	MG	2A	3318	1/1	0.95	0.26	39,39,39,39	0
56	MG	2A	3476	1/1	0.95	0.07	69,69,69,69	0
56	MG	2a	1630	1/1	0.95	0.14	57,57,57,57	0
56	MG	1A	3366	1/1	0.95	0.19	59,59,59,59	0
56	MG	2A	3321	1/1	0.95	0.40	54,54,54,54	0
56	MG	2a	1634	1/1	0.95	0.07	59,59,59,59	0
56	MG	1A	3091	1/1	0.95	0.07	64,64,64,64	0
56	MG	1A	3416	1/1	0.95	0.06	64,64,64,64	0
56	MG	2A	3482	1/1	0.95	0.10	60,60,60,60	0
56	MG	1A	3624	1/1	0.95	0.22	40,40,40,40	0
56	MG	1A	3477	1/1	0.95	0.23	44,44,44,44	0
56	MG	2a	1641	1/1	0.95	0.09	62,62,62,62	0
56	MG	2A	3018	1/1	0.95	0.06	32,32,32,32	0
56	MG	1A	3370	1/1	0.95	0.17	33,33,33,33	0
56	MG	1A	3479	1/1	0.95	0.13	38,38,38,38	0
56	MG	2A	3022	1/1	0.95	0.06	36,36,36,36	0
56	MG	1A	3276	1/1	0.95	0.25	52,52,52,52	0
56	MG	2a	1647	1/1	0.95	0.17	54,54,54,54	0
56	MG	1P	201	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3372	1/1	0.95	0.22	36,36,36,36	0
56	MG	1A	3374	1/1	0.95	0.10	57,57,57,57	0
56	MG	2a	1651	1/1	0.95	0.21	46,46,46,46	0
56	MG	1R	201	1/1	0.95	0.14	27,27,27,27	0
56	MG	1A	3320	1/1	0.95	0.31	26,26,26,26	0
56	MG	1A	3277	1/1	0.95	0.25	43,43,43,43	0
56	MG	1U	202	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	3278	1/1	0.95	0.09	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	1A	3718	1/1	0.95	0.11	32,32,32,32	0
56	MG	1W	201	1/1	0.95	0.23	57,57,57,57	0
56	MG	1A	3092	1/1	0.95	0.16	54,54,54,54	0
56	MG	1a	1798	1/1	0.95	0.06	75,75,75,75	0
56	MG	1A	3115	1/1	0.95	0.19	31,31,31,31	0
56	MG	1A	3721	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3562	1/1	0.95	0.38	28,28,28,28	0
56	MG	2A	3191	1/1	0.95	0.13	50,50,50,50	0
56	MG	1a	1915	1/1	0.95	0.12	85,85,85,85	0
56	MG	1A	3211	1/1	0.95	0.23	31,31,31,31	0
56	MG	2A	3042	1/1	0.95	0.25	51,51,51,51	0
56	MG	1a	1697	1/1	0.95	0.16	67,67,67,67	0
56	MG	2a	1826	1/1	0.95	0.14	59,59,59,59	0
56	MG	1A	3116	1/1	0.95	0.13	24,24,24,24	0
56	MG	1a	1699	1/1	0.95	0.07	64,64,64,64	0
56	MG	1a	1921	1/1	0.95	0.09	68,68,68,68	0
56	MG	13	101	1/1	0.95	0.30	26,26,26,26	0
56	MG	2A	3050	1/1	0.95	0.22	53,53,53,53	0
56	MG	2A	3203	1/1	0.95	0.21	48,48,48,48	0
56	MG	13	102	1/1	0.95	0.09	53,53,53,53	0
56	MG	2A	3053	1/1	0.95	0.14	37,37,37,37	0
56	MG	1A	3429	1/1	0.95	0.08	59,59,59,59	0
56	MG	1A	3055	1/1	0.95	0.11	41,41,41,41	0
56	MG	1a	1704	1/1	0.95	0.29	33,33,33,33	0
56	MG	1A	3807	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3095	1/1	0.95	0.29	32,32,32,32	0
56	MG	2a	1682	1/1	0.95	0.07	80,80,80,80	0
56	MG	1A	3571	1/1	0.95	0.26	30,30,30,30	0
56	MG	16	101	1/1	0.95	0.21	52,52,52,52	0
56	MG	1A	3731	1/1	0.95	0.13	56,56,56,56	0
57	KAN	1A	3935	33/33	0.95	0.08	27,36,51,59	0
56	MG	1A	3292	1/1	0.95	0.14	36,36,36,36	0
56	MG	1A	3902	1/1	0.95	0.09	38,38,38,38	0
56	MG	1A	3733	1/1	0.95	0.14	32,32,32,32	0
56	MG	1A	3498	1/1	0.95	0.18	45,45,45,45	0
56	MG	2A	3175	1/1	0.96	0.20	52,52,52,52	0
56	MG	1A	3148	1/1	0.96	0.06	65,65,65,65	0
56	MG	1a	1756	1/1	0.96	0.13	55,55,55,55	0
56	MG	1a	1629	1/1	0.96	0.11	31,31,31,31	0
56	MG	2A	3180	1/1	0.96	0.29	30,30,30,30	0
56	MG	1A	3925	1/1	0.96	0.12	48,48,48,48	0
56	MG	1a	1759	1/1	0.96	0.06	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3451	1/1	0.96	0.10	42,42,42,42	0
56	MG	2A	3351	1/1	0.96	0.18	58,58,58,58	0
56	MG	1A	3238	1/1	0.96	0.29	28,28,28,28	0
56	MG	1a	1635	1/1	0.96	0.07	56,56,56,56	0
56	MG	2A	3521	1/1	0.96	0.23	45,45,45,45	0
56	MG	1a	1636	1/1	0.96	0.14	55,55,55,55	0
56	MG	1a	1637	1/1	0.96	0.13	54,54,54,54	0
56	MG	1A	3279	1/1	0.96	0.21	45,45,45,45	0
56	MG	1A	3005	1/1	0.96	0.12	58,58,58,58	0
56	MG	1A	3623	1/1	0.96	0.26	49,49,49,49	0
56	MG	1A	3330	1/1	0.96	0.23	25,25,25,25	0
56	MG	1a	1642	1/1	0.96	0.08	68,68,68,68	0
56	MG	1A	3725	1/1	0.96	0.08	27,27,27,27	0
56	MG	1B	201	1/1	0.96	0.14	63,63,63,63	0
56	MG	2A	3365	1/1	0.96	0.16	51,51,51,51	0
56	MG	1A	3281	1/1	0.96	0.18	34,34,34,34	0
56	MG	1A	3457	1/1	0.96	0.13	46,46,46,46	0
56	MG	1A	3332	1/1	0.96	0.24	45,45,45,45	0
56	MG	1A	3062	1/1	0.96	0.27	53,53,53,53	0
56	MG	1A	3283	1/1	0.96	0.32	39,39,39,39	0
56	MG	2A	3537	1/1	0.96	0.11	63,63,63,63	0
56	MG	1A	3178	1/1	0.96	0.08	57,57,57,57	0
56	MG	1A	3542	1/1	0.96	0.16	40,40,40,40	0
56	MG	1A	3734	1/1	0.96	0.11	40,40,40,40	0
56	MG	1A	3735	1/1	0.96	0.10	37,37,37,37	0
56	MG	2A	3051	1/1	0.96	0.19	47,47,47,47	0
56	MG	1A	3337	1/1	0.96	0.20	42,42,42,42	0
56	MG	1A	3338	1/1	0.96	0.13	52,52,52,52	0
56	MG	1A	3634	1/1	0.96	0.10	64,64,64,64	0
56	MG	1A	3339	1/1	0.96	0.13	26,26,26,26	0
56	MG	2A	3056	1/1	0.96	0.15	58,58,58,58	0
56	MG	1A	3399	1/1	0.96	0.20	51,51,51,51	0
56	MG	1A	3034	1/1	0.96	0.19	32,32,32,32	0
56	MG	1a	1919	1/1	0.96	0.07	57,57,57,57	0
56	MG	2A	3060	1/1	0.96	0.12	48,48,48,48	0
56	MG	1A	3743	1/1	0.96	0.07	47,47,47,47	0
56	MG	1a	1664	1/1	0.96	0.15	53,53,53,53	0
56	MG	1a	1665	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3549	1/1	0.96	0.17	26,26,26,26	0
56	MG	1A	3341	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3342	1/1	0.96	0.18	51,51,51,51	0
56	MG	1A	3473	1/1	0.96	0.05	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3068	1/1	0.96	0.23	44,44,44,44	0
56	MG	2A	3069	1/1	0.96	0.14	45,45,45,45	0
56	MG	2A	3395	1/1	0.96	0.16	50,50,50,50	0
56	MG	1B	224	1/1	0.96	0.06	39,39,39,39	0
56	MG	1A	3643	1/1	0.96	0.09	54,54,54,54	0
56	MG	2A	3228	1/1	0.96	0.22	28,28,28,28	0
56	MG	1A	3287	1/1	0.96	0.34	49,49,49,49	0
56	MG	2A	3566	1/1	0.96	0.18	43,43,43,43	0
56	MG	2A	3073	1/1	0.96	0.12	44,44,44,44	0
56	MG	1B	227	1/1	0.96	0.11	58,58,58,58	0
56	MG	1A	3555	1/1	0.96	0.12	42,42,42,42	0
56	MG	1A	3289	1/1	0.96	0.18	35,35,35,35	0
56	MG	1D	301	1/1	0.96	0.21	28,28,28,28	0
56	MG	1D	302	1/1	0.96	0.14	57,57,57,57	0
56	MG	1A	3131	1/1	0.96	0.21	52,52,52,52	0
56	MG	1A	3406	1/1	0.96	0.15	49,49,49,49	0
56	MG	1A	3064	1/1	0.96	0.06	36,36,36,36	0
56	MG	1E	303	1/1	0.96	0.29	24,24,24,24	0
56	MG	2A	3242	1/1	0.96	0.41	35,35,35,35	0
56	MG	1A	3857	1/1	0.96	0.06	59,59,59,59	0
56	MG	2A	3244	1/1	0.96	0.46	59,59,59,59	0
56	MG	1A	3560	1/1	0.96	0.24	36,36,36,36	0
56	MG	1A	3246	1/1	0.96	0.10	41,41,41,41	0
56	MG	1a	1812	1/1	0.96	0.12	54,54,54,54	0
56	MG	1a	1943	1/1	0.96	0.06	69,69,69,69	0
56	MG	2A	3250	1/1	0.96	0.13	57,57,57,57	0
56	MG	2A	3251	1/1	0.96	0.29	48,48,48,48	0
56	MG	1A	3065	1/1	0.96	0.16	22,22,22,22	0
56	MG	2A	3090	1/1	0.96	0.06	54,54,54,54	0
56	MG	1G	201	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	3020	1/1	0.96	0.08	47,47,47,47	0
56	MG	1A	3249	1/1	0.96	0.16	42,42,42,42	0
56	MG	2A	3094	1/1	0.96	0.33	61,61,61,61	0
56	MG	1a	1948	1/1	0.96	0.07	69,69,69,69	0
56	MG	2A	3259	1/1	0.96	0.12	42,42,42,42	0
56	MG	2A	3260	1/1	0.96	0.17	43,43,43,43	0
56	MG	1a	1689	1/1	0.96	0.07	48,48,48,48	0
56	MG	1a	1690	1/1	0.96	0.18	53,53,53,53	0
56	MG	1A	3184	1/1	0.96	0.05	61,61,61,61	0
56	MG	2A	3100	1/1	0.96	0.18	37,37,37,37	0
56	MG	1A	3157	1/1	0.96	0.07	62,62,62,62	0
56	MG	1A	3090	1/1	0.96	0.07	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3267	1/1	0.96	0.28	33,33,33,33	0
56	MG	1Q	201	1/1	0.96	0.09	26,26,26,26	0
56	MG	1a	1695	1/1	0.96	0.23	48,48,48,48	0
56	MG	1A	3487	1/1	0.96	0.14	52,52,52,52	0
56	MG	1A	3867	1/1	0.96	0.20	53,53,53,53	0
56	MG	1A	3160	1/1	0.96	0.06	76,76,76,76	0
56	MG	1A	3574	1/1	0.96	0.14	18,18,18,18	0
56	MG	1A	3767	1/1	0.96	0.12	34,34,34,34	0
56	MG	2A	3276	1/1	0.96	0.16	37,37,37,37	0
56	MG	2A	3444	1/1	0.96	0.12	55,55,55,55	0
56	MG	1A	3871	1/1	0.96	0.10	50,50,50,50	0
56	MG	2A	3446	1/1	0.96	0.11	60,60,60,60	0
56	MG	1A	3021	1/1	0.96	0.12	40,40,40,40	0
56	MG	1A	3255	1/1	0.96	0.40	44,44,44,44	0
56	MG	1A	3491	1/1	0.96	0.15	56,56,56,56	0
56	MG	2A	3450	1/1	0.96	0.17	66,66,66,66	0
56	MG	1A	3045	1/1	0.96	0.16	37,37,37,37	0
56	MG	1A	3219	1/1	0.96	0.07	55,55,55,55	0
56	MG	1q	201	1/1	0.96	0.21	66,66,66,66	0
56	MG	2A	3119	1/1	0.96	0.26	45,45,45,45	0
56	MG	1A	3359	1/1	0.96	0.08	32,32,32,32	0
56	MG	1A	3164	1/1	0.96	0.22	38,38,38,38	0
56	MG	1A	3259	1/1	0.96	0.19	27,27,27,27	0
56	MG	1A	3776	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3307	1/1	0.96	0.18	28,28,28,28	0
56	MG	1A	3037	1/1	0.96	0.15	32,32,32,32	0
56	MG	1A	3094	1/1	0.96	0.30	25,25,25,25	0
56	MG	1A	3672	1/1	0.96	0.15	48,48,48,48	0
56	MG	1A	3781	1/1	0.96	0.07	60,60,60,60	0
56	MG	1A	3588	1/1	0.96	0.42	46,46,46,46	0
56	MG	2a	1632	1/1	0.96	0.06	58,58,58,58	0
56	MG	1A	3367	1/1	0.96	0.16	52,52,52,52	0
56	MG	1A	3262	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	3226	1/1	0.96	0.13	61,61,61,61	0
56	MG	18	101	1/1	0.96	0.14	53,53,53,53	0
56	MG	1A	3072	1/1	0.96	0.25	45,45,45,45	0
56	MG	2a	1638	1/1	0.96	0.09	59,59,59,59	0
56	MG	1A	3509	1/1	0.96	0.14	52,52,52,52	0
56	MG	1A	3266	1/1	0.96	0.22	26,26,26,26	0
56	MG	1A	3373	1/1	0.96	0.18	52,52,52,52	0
56	MG	1A	3073	1/1	0.96	0.11	46,46,46,46	0
56	MG	2A	3139	1/1	0.96	0.28	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3268	1/1	0.96	0.20	29,29,29,29	0
56	MG	1a	1728	1/1	0.96	0.06	77,77,77,77	0
56	MG	1A	3013	1/1	0.96	0.20	46,46,46,46	0
56	MG	2A	3478	1/1	0.96	0.16	64,64,64,64	0
56	MG	1A	3437	1/1	0.96	0.20	42,42,42,42	0
56	MG	2a	1818	1/1	0.96	0.06	86,86,86,86	0
56	MG	2A	3145	1/1	0.96	0.07	66,66,66,66	0
56	MG	2A	3146	1/1	0.96	0.27	59,59,59,59	0
56	MG	1A	3075	1/1	0.96	0.07	56,56,56,56	0
56	MG	1A	3439	1/1	0.96	0.05	44,44,44,44	0
56	MG	1a	1733	1/1	0.96	0.06	88,88,88,88	0
56	MG	1a	1864	1/1	0.96	0.07	55,55,55,55	0
56	MG	2A	3486	1/1	0.96	0.12	54,54,54,54	0
56	MG	1A	3440	1/1	0.96	0.09	54,54,54,54	0
56	MG	1A	3077	1/1	0.96	0.10	69,69,69,69	0
56	MG	2A	3320	1/1	0.96	0.13	42,42,42,42	0
56	MG	1A	3520	1/1	0.96	0.24	17,17,17,17	0
56	MG	1A	3606	1/1	0.96	0.18	66,66,66,66	0
56	MG	1A	3702	1/1	0.96	0.06	31,31,31,31	0
56	MG	1A	3703	1/1	0.96	0.10	38,38,38,38	0
56	MG	2A	3005	1/1	0.96	0.32	48,48,48,48	0
56	MG	1A	3442	1/1	0.96	0.12	54,54,54,54	0
56	MG	1A	3705	1/1	0.96	0.09	50,50,50,50	0
56	MG	1a	1614	1/1	0.96	0.05	47,47,47,47	0
56	MG	1A	3100	1/1	0.96	0.21	25,25,25,25	0
56	MG	1A	3707	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3609	1/1	0.96	0.06	57,57,57,57	0
56	MG	1A	3523	1/1	0.96	0.12	43,43,43,43	0
56	MG	1A	3808	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3444	1/1	0.96	0.09	38,38,38,38	0
56	MG	1A	3040	1/1	0.96	0.14	49,49,49,49	0
56	MG	1A	3712	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	3381	1/1	0.96	0.05	59,59,59,59	0
56	MG	1A	3201	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3102	1/1	0.96	0.20	30,30,30,30	0
56	MG	1A	3616	1/1	0.96	0.11	48,48,48,48	0
56	MG	1A	3071	1/1	0.97	0.22	37,37,37,37	0
56	MG	1A	3813	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	3365	1/1	0.97	0.29	20,20,20,20	0
56	MG	2A	3104	1/1	0.97	0.11	45,45,45,45	0
56	MG	1A	3729	1/1	0.97	0.12	41,41,41,41	0
56	MG	1a	1905	1/1	0.97	0.05	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3683	1/1	0.97	0.17	54,54,54,54	0
56	MG	1A	3162	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3222	1/1	0.97	0.26	19,19,19,19	0
56	MG	1A	3060	1/1	0.97	0.06	29,29,29,29	0
56	MG	2A	3111	1/1	0.97	0.15	29,29,29,29	0
56	MG	1A	3504	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3369	1/1	0.97	0.34	43,43,43,43	0
56	MG	2a	1692	1/1	0.97	0.12	67,67,67,67	0
56	MG	1A	3506	1/1	0.97	0.24	43,43,43,43	0
56	MG	1A	3103	1/1	0.97	0.10	62,62,62,62	0
56	MG	2A	3275	1/1	0.97	0.31	33,33,33,33	0
56	MG	2A	3193	1/1	0.97	0.12	51,51,51,51	0
56	MG	1A	3076	1/1	0.97	0.10	45,45,45,45	0
56	MG	1N	202	1/1	0.97	0.07	71,71,71,71	0
56	MG	1x	101	1/1	0.97	0.05	75,75,75,75	0
56	MG	2A	3280	1/1	0.97	0.17	36,36,36,36	0
56	MG	2A	3045	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3265	1/1	0.97	0.26	41,41,41,41	0
56	MG	1x	103	1/1	0.97	0.06	68,68,68,68	0
56	MG	1A	3239	1/1	0.97	0.17	23,23,23,23	0
56	MG	1A	3448	1/1	0.97	0.12	42,42,42,42	0
56	MG	1A	3089	1/1	0.97	0.10	32,32,32,32	0
56	MG	1A	3544	1/1	0.97	0.18	16,16,16,16	0
56	MG	1A	3315	1/1	0.97	0.28	42,42,42,42	0
56	MG	1a	1624	1/1	0.97	0.07	59,59,59,59	0
56	MG	1x	110	1/1	0.97	0.11	68,68,68,68	0
56	MG	1A	3335	1/1	0.97	0.25	27,27,27,27	0
56	MG	1A	3316	1/1	0.97	0.38	51,51,51,51	0
56	MG	1A	3748	1/1	0.97	0.07	47,47,47,47	0
56	MG	1a	1802	1/1	0.97	0.09	52,52,52,52	0
56	MG	1a	1803	1/1	0.97	0.04	59,59,59,59	0
56	MG	1A	3228	1/1	0.97	0.28	33,33,33,33	0
56	MG	2A	3297	1/1	0.97	0.22	41,41,41,41	0
56	MG	1A	3836	1/1	0.97	0.07	27,27,27,27	0
56	MG	2A	3384	1/1	0.97	0.23	42,42,42,42	0
56	MG	1a	1630	1/1	0.97	0.06	49,49,49,49	0
56	MG	1a	1631	1/1	0.97	0.09	64,64,64,64	0
56	MG	1A	3586	1/1	0.97	0.36	54,54,54,54	0
56	MG	1A	3122	1/1	0.97	0.24	40,40,40,40	0
56	MG	1a	1810	1/1	0.97	0.09	63,63,63,63	0
56	MG	2A	3141	1/1	0.97	0.11	40,40,40,40	0
56	MG	1A	3839	1/1	0.97	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3159	1/1	0.97	0.07	54,54,54,54	0
56	MG	1A	3430	1/1	0.97	0.05	51,51,51,51	0
56	MG	2A	3001	1/1	0.97	0.06	88,88,88,88	0
56	MG	1A	3889	1/1	0.97	0.09	61,61,61,61	0
56	MG	1A	3552	1/1	0.97	0.17	34,34,34,34	0
56	MG	2A	3004	1/1	0.97	0.04	42,42,42,42	0
56	MG	1A	3017	1/1	0.97	0.07	64,64,64,64	0
56	MG	1A	3382	1/1	0.97	0.07	56,56,56,56	0
56	MG	1A	3714	1/1	0.97	0.07	34,34,34,34	0
56	MG	13	103	1/1	0.97	0.12	53,53,53,53	0
56	MG	1A	3894	1/1	0.97	0.06	53,53,53,53	0
56	MG	2A	3155	1/1	0.97	0.07	60,60,60,60	0
56	MG	1A	3895	1/1	0.97	0.08	57,57,57,57	0
56	MG	2A	3081	1/1	0.97	0.15	59,59,59,59	0
56	MG	1A	3383	1/1	0.97	0.08	59,59,59,59	0
56	MG	1A	3847	1/1	0.97	0.12	46,46,46,46	0
56	MG	1A	3360	1/1	0.97	0.21	29,29,29,29	0
56	MG	1A	3462	1/1	0.97	0.09	59,59,59,59	0
56	MG	1A	3288	1/1	0.97	0.11	32,32,32,32	0
56	MG	1A	3197	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3527	1/1	0.97	0.29	25,25,25,25	0
56	MG	1A	3903	1/1	0.97	0.16	39,39,39,39	0
56	MG	18	104	1/1	0.97	0.13	52,52,52,52	0
56	MG	2A	3415	1/1	0.97	0.23	43,43,43,43	0
56	MG	1A	3673	1/1	0.97	0.07	43,43,43,43	0
56	MG	2E	301	1/1	0.97	0.13	51,51,51,51	0
56	MG	2A	3021	1/1	0.97	0.16	48,48,48,48	0
56	MG	1A	3561	1/1	0.97	0.31	28,28,28,28	0
56	MG	1A	3495	1/1	0.97	0.04	47,47,47,47	0
56	MG	2A	3095	1/1	0.97	0.16	41,41,41,41	0
56	MG	1A	3639	1/1	0.97	0.08	29,29,29,29	0
56	MG	1A	3678	1/1	0.97	0.18	43,43,43,43	0
56	MG	1a	1661	1/1	0.97	0.41	57,57,57,57	0
56	MG	2A	3339	1/1	0.97	0.21	48,48,48,48	0
56	MG	1A	3305	1/1	0.97	0.27	53,53,53,53	0
56	MG	2A	3176	1/1	0.97	0.18	41,41,41,41	0
56	MG	2A	3028	1/1	0.97	0.18	57,57,57,57	0
58	ZN	24	501	1/1	0.97	0.08	126,126,126,126	0
58	ZN	2n	501	1/1	0.97	0.05	103,103,103,103	0
56	MG	1A	3114	1/1	0.98	0.22	33,33,33,33	0
56	MG	1A	3698	1/1	0.98	0.06	21,21,21,21	0
56	MG	1A	3212	1/1	0.98	0.05	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2D	301	1/1	0.98	0.08	34,34,34,34	0
56	MG	1A	3736	1/1	0.98	0.08	48,48,48,48	0
56	MG	2A	3316	1/1	0.98	0.32	27,27,27,27	0
56	MG	1A	3483	1/1	0.98	0.06	48,48,48,48	0
56	MG	1A	3046	1/1	0.98	0.25	46,46,46,46	0
56	MG	1A	3848	1/1	0.98	0.08	43,43,43,43	0
56	MG	1A	3270	1/1	0.98	0.17	31,31,31,31	0
56	MG	1A	3084	1/1	0.98	0.05	54,54,54,54	0
56	MG	1A	3031	1/1	0.98	0.06	36,36,36,36	0
56	MG	1D	304	1/1	0.98	0.06	57,57,57,57	0
56	MG	1A	3030	1/1	0.98	0.04	27,27,27,27	0
56	MG	1A	3468	1/1	0.98	0.12	40,40,40,40	0
56	MG	2A	3326	1/1	0.98	0.32	30,30,30,30	0
56	MG	1A	3469	1/1	0.98	0.08	37,37,37,37	0
56	MG	1A	3109	1/1	0.98	0.29	47,47,47,47	0
56	MG	1A	3587	1/1	0.98	0.31	40,40,40,40	0
56	MG	1A	3674	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3088	1/1	0.98	0.10	43,43,43,43	0
56	MG	1A	3589	1/1	0.98	0.36	47,47,47,47	0
56	MG	1A	3152	1/1	0.98	0.16	55,55,55,55	0
56	MG	1A	3619	1/1	0.98	0.11	28,28,28,28	0
56	MG	1a	1817	1/1	0.98	0.06	53,53,53,53	0
56	MG	2A	3233	1/1	0.98	0.15	38,38,38,38	0
56	MG	1A	3323	1/1	0.98	0.21	49,49,49,49	0
56	MG	1A	3220	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3681	1/1	0.98	0.06	57,57,57,57	0
56	MG	1A	3111	1/1	0.98	0.35	24,24,24,24	0
56	MG	1P	202	1/1	0.98	0.10	69,69,69,69	0
56	MG	1a	1650	1/1	0.98	0.12	38,38,38,38	0
56	MG	1A	3566	1/1	0.98	0.19	34,34,34,34	0
56	MG	2A	3241	1/1	0.98	0.41	39,39,39,39	0
56	MG	1A	3052	1/1	0.98	0.06	26,26,26,26	0
56	MG	1A	3685	1/1	0.98	0.09	47,47,47,47	0
56	MG	1B	211	1/1	0.98	0.30	42,42,42,42	0
56	MG	1A	3223	1/1	0.98	0.35	30,30,30,30	0
56	MG	2A	3148	1/1	0.98	0.06	51,51,51,51	0
56	MG	1A	3569	1/1	0.98	0.35	34,34,34,34	0
56	MG	1A	3570	1/1	0.98	0.35	25,25,25,25	0
56	MG	1A	3690	1/1	0.98	0.06	33,33,33,33	0
56	MG	1A	3499	1/1	0.98	0.11	38,38,38,38	0
56	MG	1r	101	1/1	0.98	0.05	64,64,64,64	0
56	MG	2A	3201	1/1	0.98	0.23	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3692	1/1	0.98	0.09	29,29,29,29	0
56	MG	2A	3358	1/1	0.98	0.06	60,60,60,60	0
56	MG	1A	3066	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3459	1/1	0.98	0.06	57,57,57,57	0
56	MG	1a	1837	1/1	0.98	0.18	44,44,44,44	0
56	MG	2a	1626	1/1	0.98	0.31	53,53,53,53	0
56	MG	1A	3502	1/1	0.98	0.06	52,52,52,52	0
56	MG	1A	3425	1/1	0.98	0.11	46,46,46,46	0
58	ZN	2Y	501	1/1	0.98	0.04	98,98,98,98	0
56	MG	1a	1708	1/1	0.98	0.25	49,49,49,49	0
56	MG	1B	222	1/1	0.98	0.04	59,59,59,59	0
56	MG	2A	3246	1/1	0.99	0.28	31,31,31,31	0
56	MG	1A	3118	1/1	0.99	0.03	37,37,37,37	0
56	MG	1A	3699	1/1	0.99	0.04	51,51,51,51	0
56	MG	2A	3209	1/1	0.99	0.30	35,35,35,35	0
56	MG	1A	3284	1/1	0.99	0.06	48,48,48,48	0
56	MG	1A	3086	1/1	0.99	0.03	30,30,30,30	0
56	MG	1a	1655	1/1	0.99	0.07	56,56,56,56	0
56	MG	1A	3059	1/1	0.99	0.05	30,30,30,30	0
56	MG	1A	3078	1/1	0.99	0.10	14,14,14,14	0
56	MG	1A	3038	1/1	0.99	0.10	26,26,26,26	0
56	MG	1a	1951	1/1	0.99	0.04	64,64,64,64	0
56	MG	1A	3831	1/1	0.99	0.11	54,54,54,54	0
58	ZN	1Y	202	1/1	0.99	0.02	66,66,66,66	0
58	ZN	14	501	1/1	0.99	0.03	99,99,99,99	0
58	ZN	15	104	1/1	0.99	0.02	49,49,49,49	0
58	ZN	1n	501	1/1	0.99	0.03	64,64,64,64	0
56	MG	2A	3049	1/1	0.99	0.04	79,79,79,79	0
56	MG	2A	3357	1/1	0.99	0.05	51,51,51,51	0
58	ZN	25	501	1/1	0.99	0.05	66,66,66,66	0
58	ZN	26	102	1/1	0.99	0.03	63,63,63,63	0
58	ZN	29	501	1/1	0.99	0.03	88,88,88,88	0
56	MG	1a	1822	1/1	0.99	0.07	55,55,55,55	0
59	SF4	1d	303	8/8	0.99	0.03	60,65,69,72	0
59	SF4	2d	501	8/8	0.99	0.03	60,79,85,85	0
56	MG	1A	3687	1/1	1.00	0.04	33,33,33,33	0
58	ZN	16	102	1/1	1.00	0.04	48,48,48,48	0
58	ZN	19	104	1/1	1.00	0.07	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.