



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 11:44 am BST

PDB ID : 6CFJ
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with histidyl-CAM and bound to mRNA and A-, P-, and E-site tRNAs at 2.8Å resolution
Authors : Tereshchenkov, A.G.; Dobosz-Bartoszek, M.; Osterman, I.A.; Marks, J.; Sergeeva, V.A.; Kasatsky, P.; Komarova, E.S.; Stavrianidi, A.N.; Rodin, I.A.; Konevega, A.L.; Sergiev, P.V.; Sumbatyan, N.V.; Mankin, A.S.; Bogdanov, A.A.; Polikanov, Y.S.
Deposited on : 2018-02-15
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

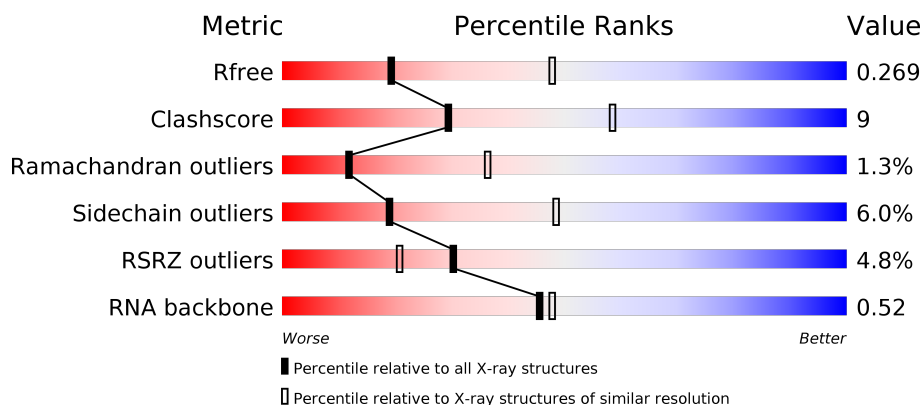
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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











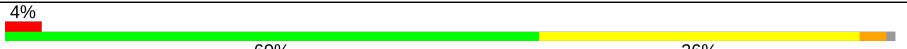

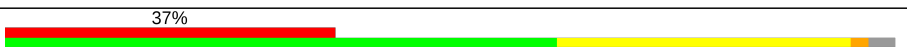





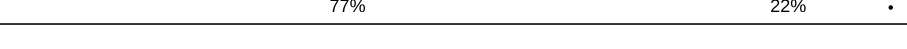


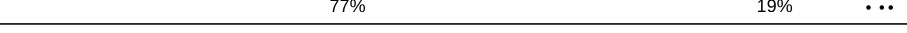





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div></div> <div>60% 32% 6% .</div> </div>
1	2A	2915	<div> <div></div> <div>52% 36% 8% .</div> </div>
2	1B	121	<div> <div></div> <div>64% 30% 5% .</div> </div>



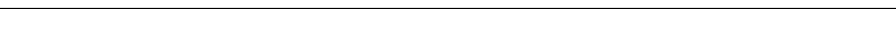
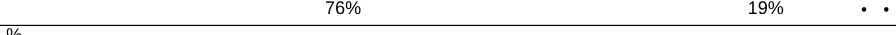


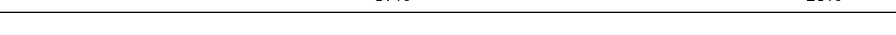



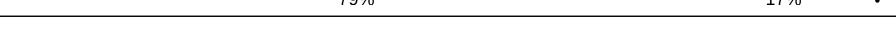


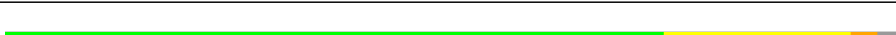




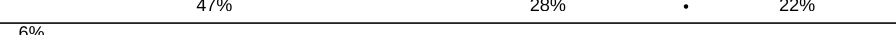


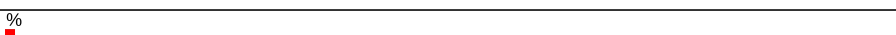



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Mol	Chain	Length	Quality of chain
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	

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

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Mol	Chain	Length	Quality of chain
27	25	60	
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	

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Mol	Chain	Length	Quality of chain
40	1i	128	<div> <div>23%</div> <div>96%</div> <div>..</div> </div>
40	2i	128	<div> <div>54%</div> <div>96%</div> <div>..</div> </div>
41	1j	105	<div> <div>24%</div> <div>87%</div> <div>6% 8%</div> </div>
41	2j	105	<div> <div>35%</div> <div>83%</div> <div>9% 9%</div> </div>
42	1k	129	<div> <div>%</div> <div>84%</div> <div>• 12%</div> </div>
42	2k	129	<div> <div>5%</div> <div>82%</div> <div>6% 12%</div> </div>
43	1l	132	<div> <div></div> <div>84%</div> <div>8% 8%</div> </div>
43	2l	132	<div> <div>6%</div> <div>89%</div> <div>• 8%</div> </div>
44	1m	126	<div> <div>7%</div> <div>93%</div> <div>5% •</div> </div>
44	2m	126	<div> <div>13%</div> <div>93%</div> <div>• •</div> </div>
45	1n	61	<div> <div>16%</div> <div>89%</div> <div>10% •</div> </div>
45	2n	61	<div> <div>67%</div> <div>90%</div> <div>8% •</div> </div>
46	1o	89	<div> <div>2%</div> <div>96%</div> <div>• •</div> </div>
46	2o	89	<div> <div>%</div> <div>96%</div> <div>• • •</div> </div>
47	1p	88	<div> <div>6%</div> <div>89%</div> <div>5% 7%</div> </div>
47	2p	88	<div> <div>%</div> <div>90%</div> <div>• 7%</div> </div>
48	1q	105	<div> <div>3%</div> <div>90%</div> <div>• 6%</div> </div>
48	2q	105	<div> <div>19%</div> <div>90%</div> <div>5% 6%</div> </div>
49	1r	88	<div> <div>5%</div> <div>73%</div> <div>5% 23%</div> </div>
49	2r	88	<div> <div>2%</div> <div>75%</div> <div>• 23%</div> </div>
50	1s	93	<div> <div>%</div> <div>86%</div> <div>• 11%</div> </div>
50	2s	93	<div> <div>17%</div> <div>84%</div> <div>5% 11%</div> </div>
51	1t	106	<div> <div>13%</div> <div>83%</div> <div>8% 9%</div> </div>
51	2t	106	<div> <div>17%</div> <div>80%</div> <div>10% 9%</div> </div>
52	1u	27	<div> <div>15%</div> <div>81%</div> <div>• 15%</div> </div>

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Mol	Chain	Length	Quality of chain
52	2u	27	
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
56	MG	1A	3201	-	-	-	X
56	MG	1A	3226	-	-	-	X
56	MG	1B	211	-	-	-	X
56	MG	2W	202	-	-	-	X
56	MG	2v	3002	-	-	-	X

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 299109 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	1273	G	UNK	conflict	GB 37223181
2A	1227	G	UNK	conflict	GB 37223181

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			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
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
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			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			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1x	8	4SU	G	conflict	GB 205271127
2x	8	4SU	G	conflict	GB 205271127

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	10	Total	Mg	0	0
			10	10		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	17	5	Total 5	Mg 5	0	0
56	2d	2	Total 2	Mg 2	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1N	5	Total 5	Mg 5	0	0
56	20	3	Total 3	Mg 3	0	0
56	18	3	Total 3	Mg 3	0	0
56	2W	3	Total 3	Mg 3	0	0
56	1Y	2	Total 2	Mg 2	0	0
56	13	2	Total 2	Mg 2	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1P	3	Total 3	Mg 3	0	0
56	2B	21	Total 21	Mg 21	0	0
56	2l	4	Total 4	Mg 4	0	0
56	1q	1	Total 1	Mg 1	0	0
56	2a	233	Total 233	Mg 233	0	0
56	1E	13	Total 13	Mg 13	0	0
56	1b	2	Total 2	Mg 2	0	0
56	25	3	Total 3	Mg 3	0	0
56	2F	4	Total 4	Mg 4	0	0
56	16	3	Total 3	Mg 3	0	0
56	28	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2e	1	Total 1	Mg 1	0	0
56	1W	5	Total 5	Mg 5	0	0
56	1A	1063	Total 1063	Mg 1063	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1n	2	Total 2	Mg 2	0	0
56	2P	1	Total 1	Mg 1	0	0
56	1X	6	Total 6	Mg 6	0	0
56	12	2	Total 2	Mg 2	0	0
56	1y	4	Total 4	Mg 4	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1p	1	Total 1	Mg 1	0	0
56	2T	3	Total 3	Mg 3	0	0
56	1D	14	Total 14	Mg 14	0	0
56	23	1	Total 1	Mg 1	0	0
56	1e	1	Total 1	Mg 1	0	0
56	2G	1	Total 1	Mg 1	0	0
56	1I	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	1V	3	Total 3	Mg 3	0	0
56	2X	2	Total 2	Mg 2	0	0
56	1w	11	Total 11	Mg 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1a	215	Total 215	Mg 215	0	0
56	2Q	3	Total 3	Mg 3	0	0
56	15	6	Total 6	Mg 6	0	0
56	1x	15	Total 15	Mg 15	0	0
56	2j	2	Total 2	Mg 2	0	0
56	1R	5	Total 5	Mg 5	0	0
56	1s	1	Total 1	Mg 1	0	0
56	1m	1	Total 1	Mg 1	0	0
56	2U	6	Total 6	Mg 6	0	0
56	1G	5	Total 5	Mg 5	0	0
56	2O	2	Total 2	Mg 2	0	0
56	11	5	Total 5	Mg 5	0	0
56	2r	2	Total 2	Mg 2	0	0
56	21	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2w	9	Total 9	Mg 9	0	0
56	1v	1	Total 1	Mg 1	0	0
56	2x	5	Total 5	Mg 5	0	0
56	2R	4	Total 4	Mg 4	0	0
56	1Z	4	Total 4	Mg 4	0	0
56	2D	7	Total 7	Mg 7	0	0

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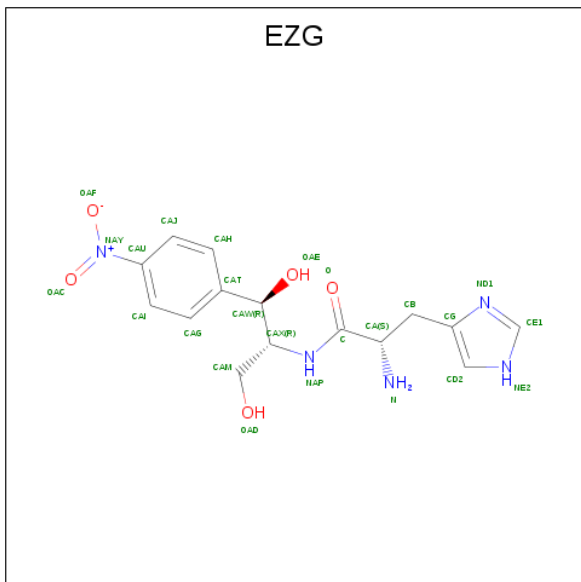
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2q	4	Total Mg 4 4	0	0
56	1U	6	Total Mg 6 6	0	0
56	1O	7	Total Mg 7 7	0	0
56	1r	1	Total Mg 1 1	0	0
56	19	1	Total Mg 1 1	0	0
56	1l	3	Total Mg 3 3	0	0
56	2V	2	Total Mg 2 2	0	0
56	1F	9	Total Mg 9 9	0	0
56	10	5	Total Mg 5 5	0	0
56	2t	1	Total Mg 1 1	0	0
56	1Q	5	Total Mg 5 5	0	0
56	2A	754	Total Mg 754 754	0	0
56	2Z	1	Total Mg 1 1	0	0
56	1B	38	Total Mg 38 38	0	0
56	2y	7	Total Mg 7 7	0	0
56	27	2	Total Mg 2 2	0	0
56	2v	5	Total Mg 5 5	0	0

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	2	Total K 2 2	0	0
57	2A	2	Total K 2 2	0	0

- Molecule 58 is N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]-L-histidinamide (three-letter code: EZG) (formula: C₁₅H₁₉N₅O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1A	1	Total	C	N	O	0	0
			25	15	5	5		
58	2A	1	Total	C	N	O	0	0
			25	15	5	5		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

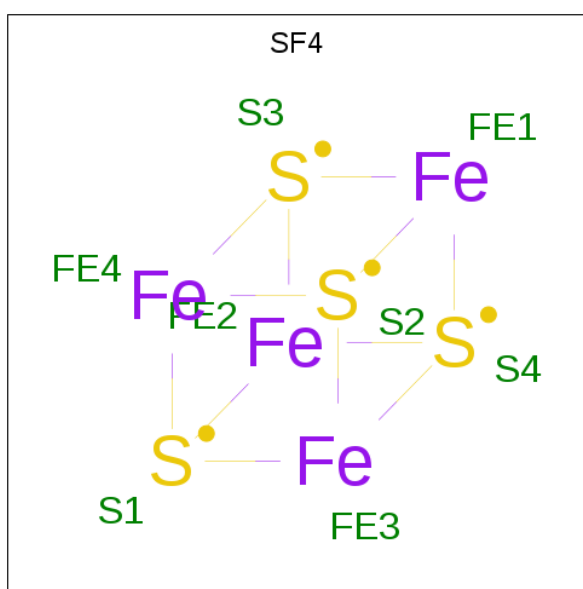
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	24	1	Total 1	Zn 1	0	0
59	2n	1	Total 1	Zn 1	0	0
59	2Y	1	Total 1	Zn 1	0	0
59	16	1	Total 1	Zn 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1d	1	Total 8	Fe 4	S 4	0	0
60	2d	1	Total 8	Fe 4	S 4	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1433	Total 1433	O 1433	0	0
61	1B	65	Total 65	O 65	0	0
61	1D	24	Total 24	O 24	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1E	30	Total 30	O 30	0	0
61	1F	10	Total 10	O 10	0	0
61	1G	8	Total 8	O 8	0	0
61	1H	1	Total 1	O 1	0	0
61	1I	2	Total 2	O 2	0	0
61	1N	6	Total 6	O 6	0	0
61	1O	8	Total 8	O 8	0	0
61	1P	18	Total 18	O 18	0	0
61	1Q	12	Total 12	O 12	0	0
61	1R	12	Total 12	O 12	0	0
61	1S	4	Total 4	O 4	0	0
61	1T	7	Total 7	O 7	0	0
61	1U	9	Total 9	O 9	0	0
61	1V	8	Total 8	O 8	0	0
61	1W	8	Total 8	O 8	0	0
61	1X	8	Total 8	O 8	0	0
61	1Y	2	Total 2	O 2	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	10	Total 10	O 10	0	0
61	11	7	Total 7	O 7	0	0
61	12	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	4	Total 4	O 4	0	0
61	15	5	Total 5	O 5	0	0
61	16	2	Total 2	O 2	0	0
61	17	9	Total 9	O 9	0	0
61	18	7	Total 7	O 7	0	0
61	1a	315	Total 315	O 315	0	0
61	1b	1	Total 1	O 1	0	0
61	1e	1	Total 1	O 1	0	0
61	1f	1	Total 1	O 1	0	0
61	1g	1	Total 1	O 1	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	6	Total 6	O 6	0	0
61	1m	1	Total 1	O 1	0	0
61	1n	1	Total 1	O 1	0	0
61	1q	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	6	Total 6	O 6	0	0
61	1w	20	Total 20	O 20	0	0
61	1x	14	Total 14	O 14	0	0
61	1y	2	Total 2	O 2	0	0
61	2A	885	Total 885	O 885	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2B	26	Total 26	O 26	0	0
61	2D	18	Total 18	O 18	0	0
61	2E	14	Total 14	O 14	0	0
61	2F	18	Total 18	O 18	0	0
61	2I	4	Total 4	O 4	0	0
61	2N	1	Total 1	O 1	0	0
61	2P	12	Total 12	O 12	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	6	Total 6	O 6	0	0
61	2U	3	Total 3	O 3	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	3	Total 3	O 3	0	0
61	2X	1	Total 1	O 1	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	2	Total 2	O 2	0	0
61	20	4	Total 4	O 4	0	0
61	21	8	Total 8	O 8	0	0
61	22	1	Total 1	O 1	0	0
61	23	1	Total 1	O 1	0	0
61	25	4	Total 4	O 4	0	0

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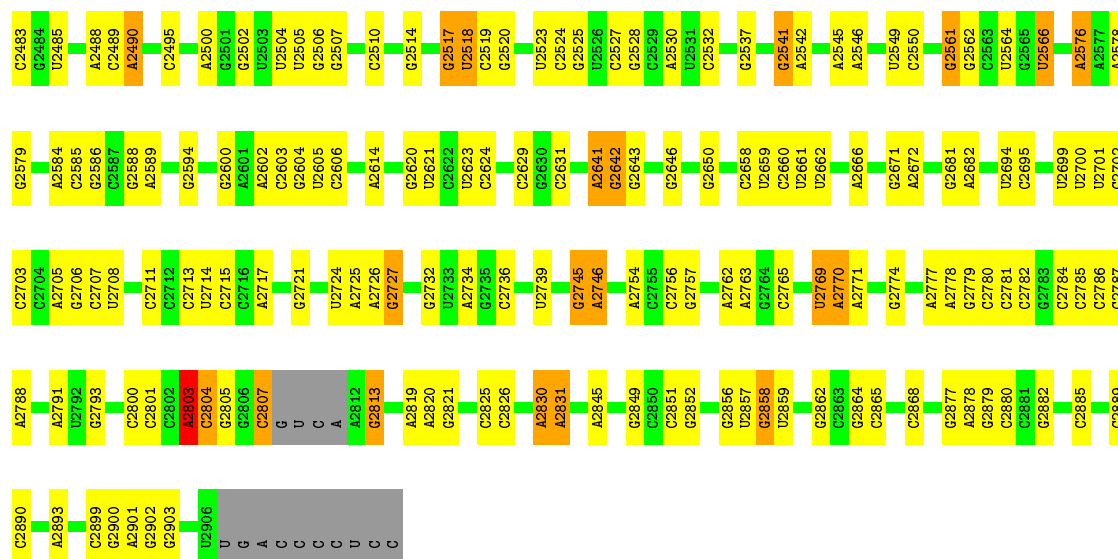
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61	26	1	Total 1	O 1	0	0
61	27	4	Total 4	O 4	0	0
61	28	4	Total 4	O 4	0	0
61	29	1	Total 1	O 1	0	0
61	2a	258	Total 258	O 258	0	0
61	2c	1	Total 1	O 1	0	0
61	2d	3	Total 3	O 3	0	0
61	2e	1	Total 1	O 1	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2l	6	Total 6	O 6	0	0
61	2o	1	Total 1	O 1	0	0
61	2p	2	Total 2	O 2	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	5	Total 5	O 5	0	0
61	2u	1	Total 1	O 1	0	0
61	2v	2	Total 2	O 2	0	0
61	2w	2	Total 2	O 2	0	0
61	2x	6	Total 6	O 6	0	0

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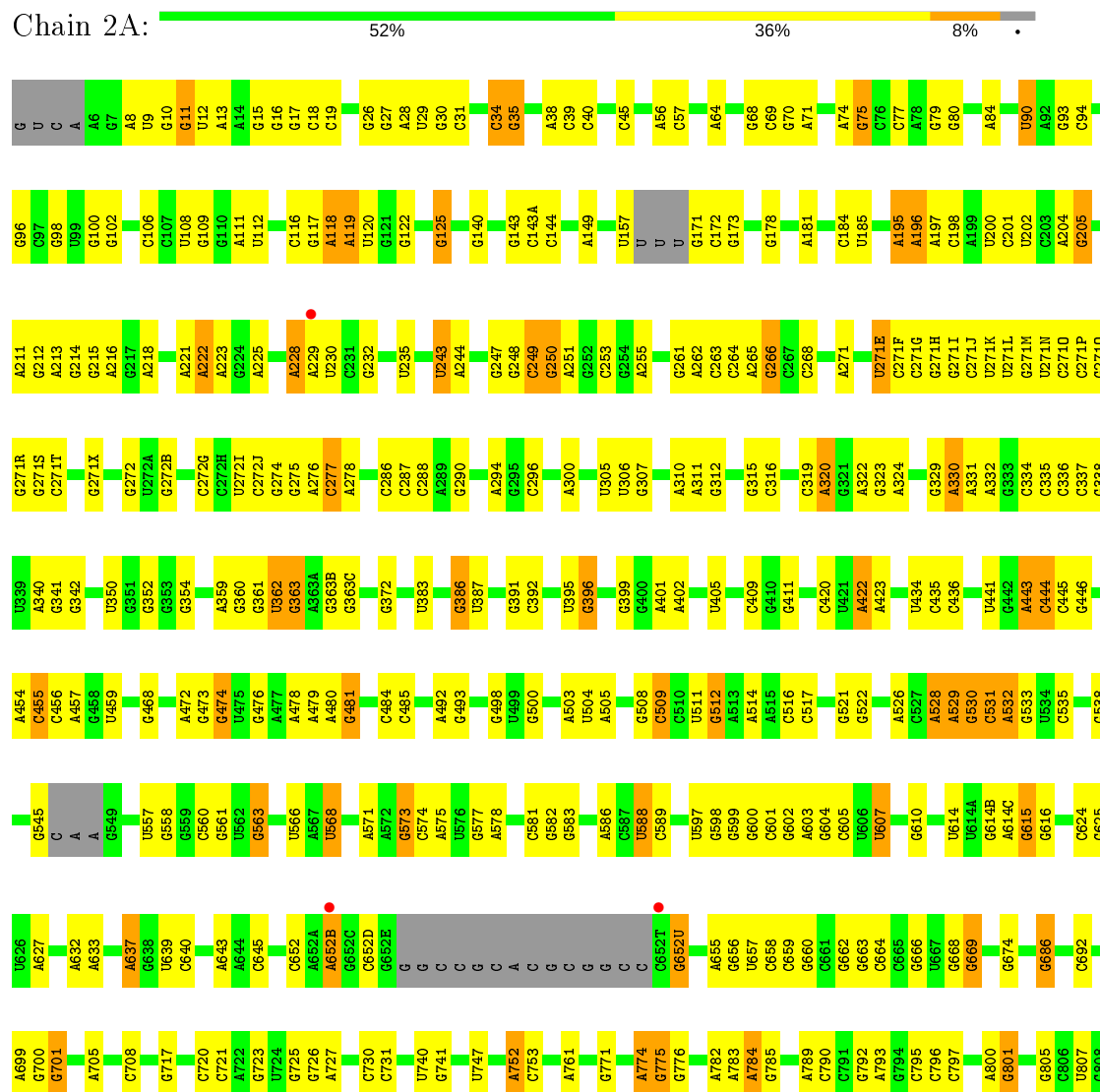
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2y	18	Total	O	0	0
			18	18		

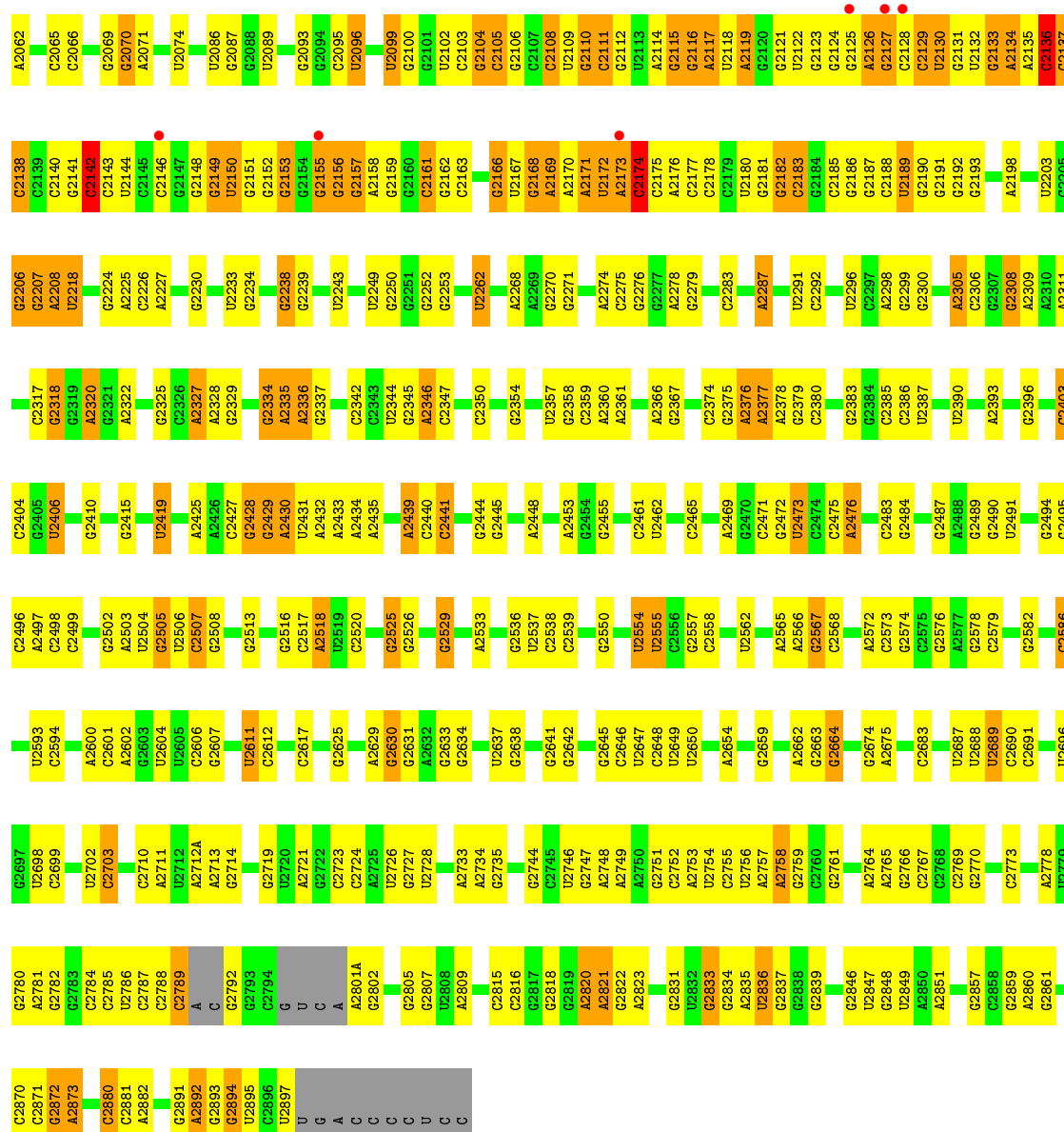




• Molecule 1: 23S Ribosomal RNA

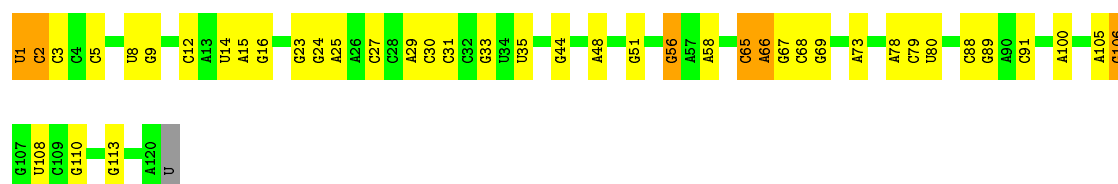


A1966	C1830	A1722	C1617	C1530	G1442	G1347	A1247	G1169	A	C1038	G956	C884	G809
C1967	G1831	U1739	G1622	C1531	A1445	U1352	G1248	G1170	G	G1039	A957	C885	U810
A1970	G1835	G1740	G1626	C1532	G1446	U1353	U1249	G1171	C	C1040	U958	C886	U811
A1971	C1836	G1746	G1627	G1533	G1448	A1354	G1250	G	U	C1041	A959	A887	C812
A1972	C1837	C1751	G1628	A	A1449	A1355	G1251	U	C	G1042	A960	C888	C816
C1973	G1838	C1751	U1629	C1536	G1450	A1359	A1252	A	A	G1043	A961	C889	C816
C1983	G1839	C1754	G1629	G1537	C1450A	A1360	A1253	U	C	G	A962	A890	C816
C1983	C1839	C1754	G1629	G1538	C1451	A1360	A1254	A	U	G	G966	A892	A819
A1847	C1840	A1755	C1636	G1539	G1455	C1363	G1256	C1178	U	A	G966	A893	A820
A1848	C1841	A1756	A1637	G1540	G1456	G1364	G1257	C1179	U	A	G974	C894	A821
C1992	C1842	U1757	C1638	A1542	A1460	A1365	G1258	C1180	U	A	C975	C895	A824
U1993	G1857	G1758	U1639	C1543	G1461	A1366	A1259	A1181	C	C	A980	C896	A824
C1996	C1866	A1762	C1640	C1546	C1462	A1367	A1260	A1182	G	A	A981	C897	A824
G1997	A1876	G1763	G1647	C1547	C1463	C1370	G1261	G1183	A	G	A982	C898	U826
G1998	G1877	G1764	C1648	C1548	G1464	U1371	G1262	G1184	U	C	A983	A899	U827
C2001	G1878	G1769	G1651	C1549	C1465	U1372	A1265	G1185	A	A	C986	A901	U828
G2002	C1879	A1773	G1652	C1557	G1466	A1379	G1266	G1186	G	G	G987	C902	A829
G2010	C1882	A1773	A1654	A1558	G1467	G1380	U1267	G1187	A	A	A990	C903	U833
U2011	A1889	A1773	G1654	G1559	G1468	U1379	A1268	G1188	G	G	C991	U905	G836
G2012	A1890	A1780	C1658	A1566	G1469	A1384	C1270	C1119	U	U	C992	U907	U839
A2013	C1889	A1783	G1663	G1567	G1470	G1385	G1271	U1199	G	G	G993	C908	C840
A2014	A1900	A1784	A1664	G1568	A1471	C1386	A1272	G1200	U	U	C994	A909	C840
A2019	A1901	A1785	A1665	A1569	G1472	U1394	U1273	C1201	G	G	C995	A910	G848
G2020	G1906	A1786	A1669	A1572	G1473	U1395	A1274	G1202	C	C	A996	A911	A849
U2022	G1907	C1790	G1674	A1578	G1474	C1405	A1284	U1204	U	U	U999	C912	C850
G2023	A1912	A1791	C1675	U1579	A1486	U1406	G1285	U1205	A	A	A1000	C915	U851
G2024	A1913	U1794	A1676	A1580	G1487	A1405	A1286	G1206	U	U	A1001	G916	G852
C2025	C1914	C1795	C1677	G1581	G1488	U1406	A1287	G1207	G	G	A1002	G917	G853
C2026	A1915	U1796	U1680	A1582	U1489	A1412	U1292	A1210	A	A	G1003	A918	G854
A2031	A1916	C1797	G1681	C1584	A1490	G1413	C1293	G1212	C	C	C1007	G919	C856
C2032	C1920	U1798	G1682	A1586	C1493	G1414	G1298	A1213	A	G	A1010	G921	U858
A2033	G1921	C1800	C1683	A1587	A1494	G1415	G1299	G1217	C	C	A1011	G922	G859
U2034	C1922	G1801	A1684	C1588	A1495	G1416	G1300	C1218	U	U	U1012	G923	U860
G2035	A1927	G1802	A1689	C1589	A1496	G1417	A1301	G1219	C	C	C1013	G927	A861
C2036	C1928	A1803	C1690	G1593	U1497	U1419	A1302	A1220	A	A	G1016	G928	A863
G2037	G1929	C1804	U1692	G1594	A1507	G1421	G1309	C1221	C	C	U1017	G932	A866
C2038	C1930	U1805	C1694	G1595	A1508	G1422	G1310	G1221A	U	U	U1019	A933	U868
C2040	A1936	C1811	G1695	A1596	A1509A	G1423	G1311	A1226	U	U	A1020	G938	A869
U2041	A1937	G1812	G1696	A1597	A1509B	G1424	U1312	G1227	A	A	G1021	A941	G874
A2042	U1938	G1813	G1697	C1599	G1510	G1425	G1313	G1228	U	U	U1022	G947	C876
C2043	C1939	G1814	A1698	A1603	G1511	A1427	G1314	G1229	C	C	G1023	U877	U877
C2044	U1946	G1815	G1699	A1604	G1512	G1428	C1315	G1230	G	G	A1024	A1029	A878
A2051	C1947	A1816	A1700	C1607	U1517	G1429	G1325	G1236	A	A	G1025	G950	G879
G2052	U1955	G1817	A1701	A1608	U1523	U1430	G1326	A1237	G	G	U1026	G951	G880
C2055	C1958	U1818	G1703	A1609	G1524	U1431	A1336	G1238	U	U	A1027	G952	G881
G2056	U1963	G1824	C1711	A1610	G1525	A1434	G1337	G1239	C	C	A1028	G953	G882
A2059	C1964	G1825	C1712	G1613	G1526	G1435	U1341	A1241	U	U	G1030	G954	G883
A2060	G1965	G1826	G1721	A1614	G1527	G1436	C1345	A1242	A	A	G1031	G955	G883
G2061				A1615	A1528A	C1437	G1346	G1244	U	U	U1033	A952	



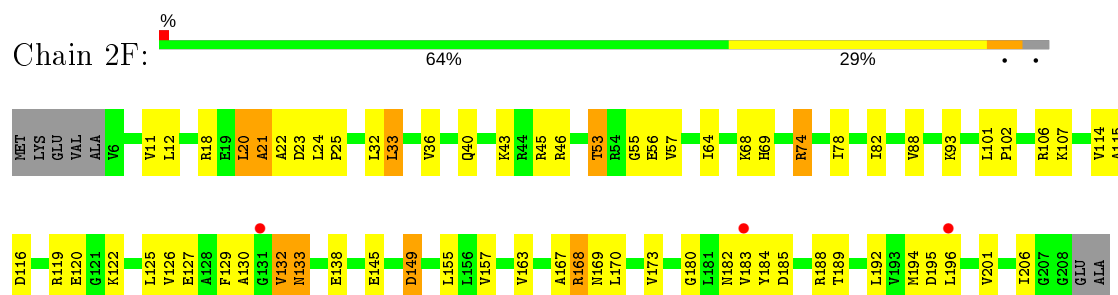
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 64% 30% 5%

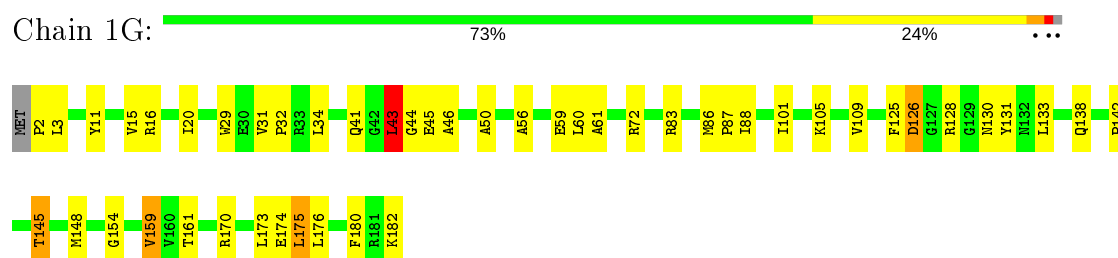




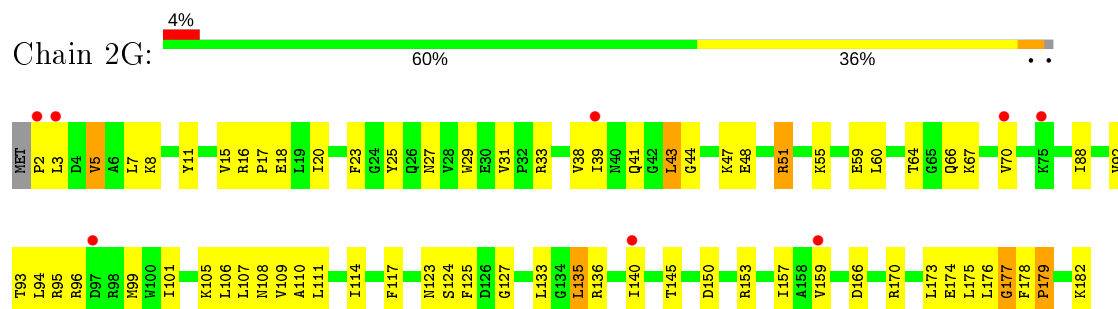
- Molecule 5: 50S ribosomal protein L4



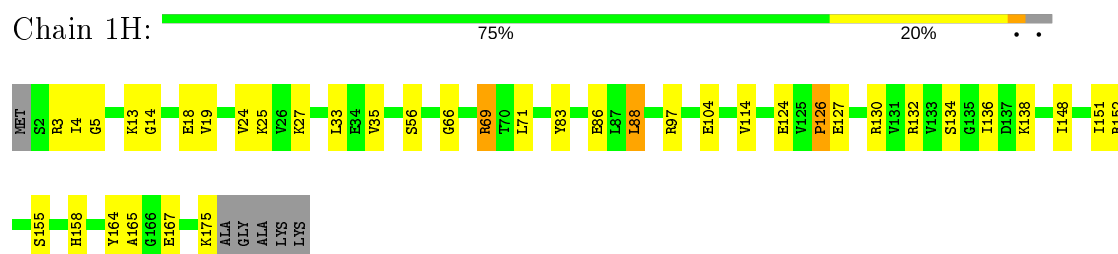
- Molecule 6: 50S ribosomal protein L5



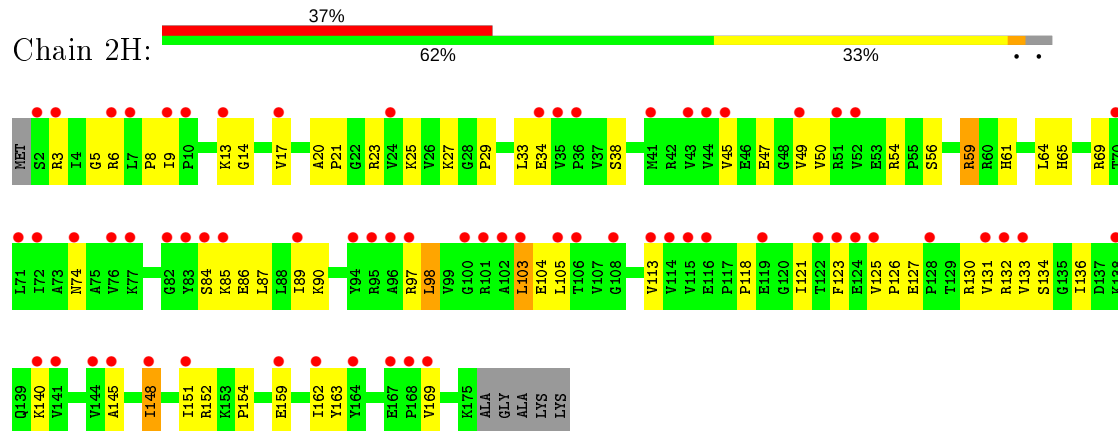
- Molecule 6: 50S ribosomal protein L5



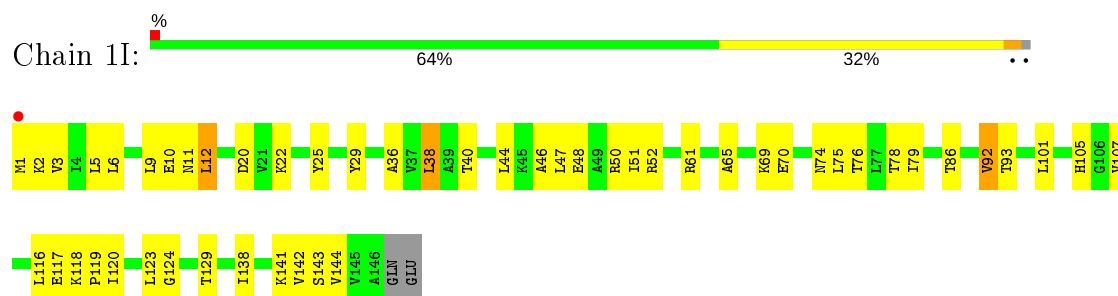
- Molecule 7: 50S ribosomal protein L6



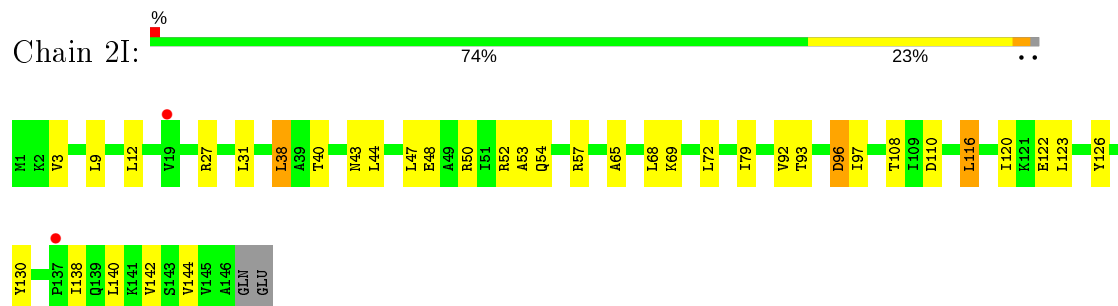
- Molecule 7: 50S ribosomal protein L6



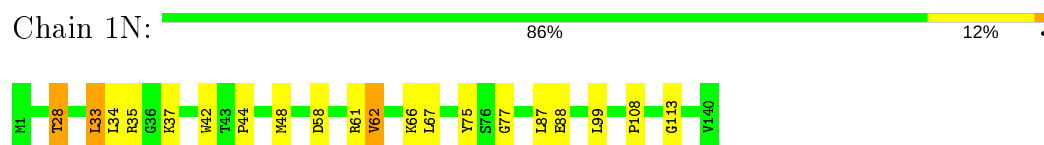
- Molecule 8: 50S ribosomal protein L9



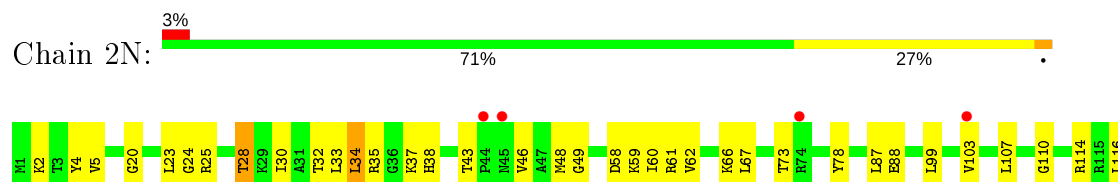
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13

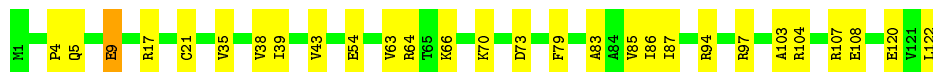
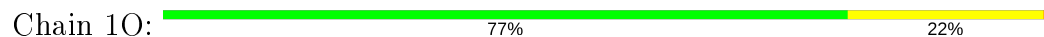


- Molecule 9: 50S ribosomal protein L13

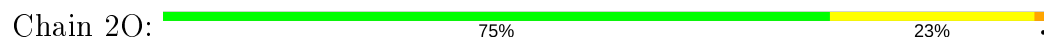




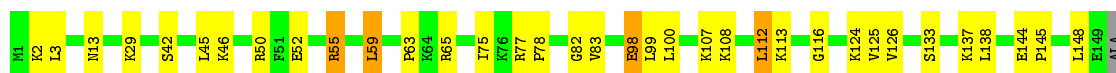
- Molecule 10: 50S ribosomal protein L14



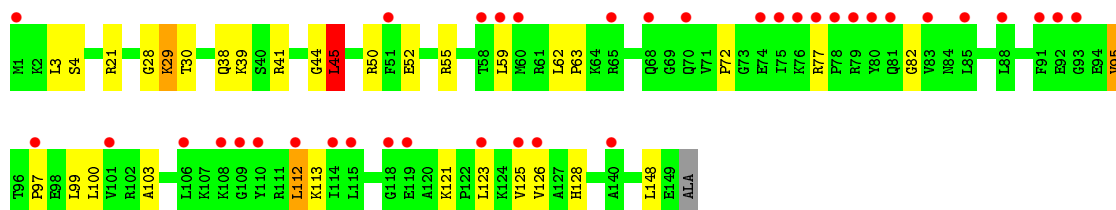
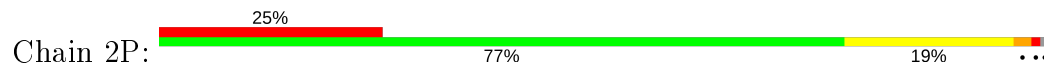
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15

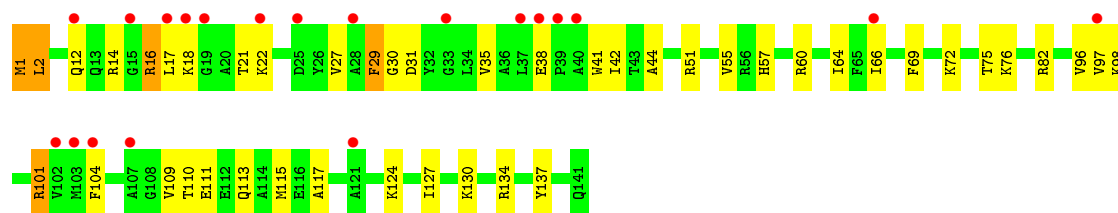


- Molecule 12: 50S ribosomal protein L16



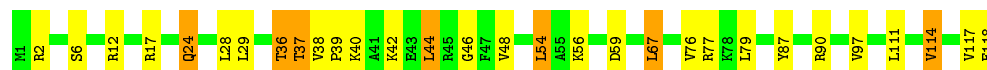
- Molecule 12: 50S ribosomal protein L16





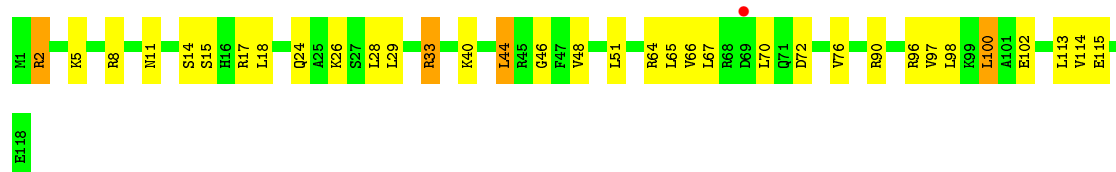
- Molecule 13: 50S ribosomal protein L17

Chain 1R: 75% 19% 6%



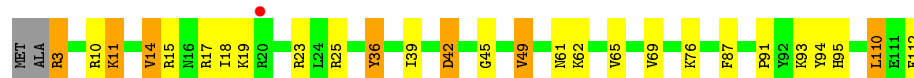
- Molecule 13: 50S ribosomal protein L17

Chain 2R: 71% 25% 4%



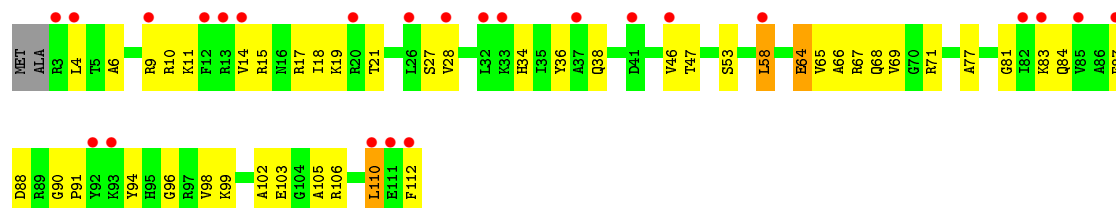
- Molecule 14: 50S ribosomal protein L18

Chain 1S: 74% 18% 6%



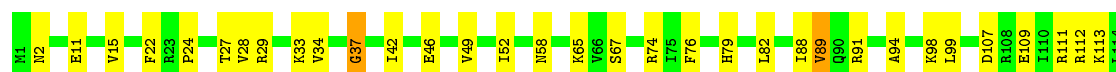
- Molecule 14: 50S ribosomal protein L18

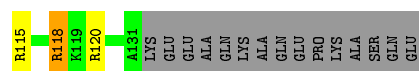
Chain 2S: 58% 38% 4%



- Molecule 15: 50S ribosomal protein L19

Chain 1T: 65% 23% 10%





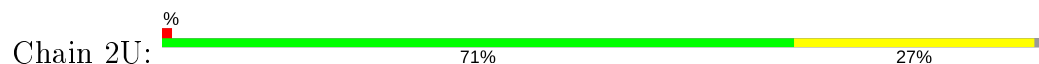
- Molecule 15: 50S ribosomal protein L19



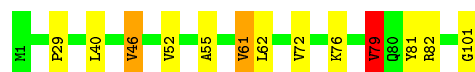
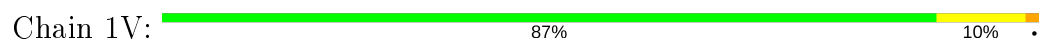
- Molecule 16: 50S ribosomal protein L20



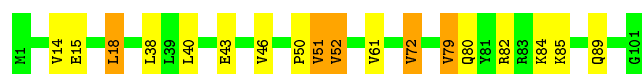
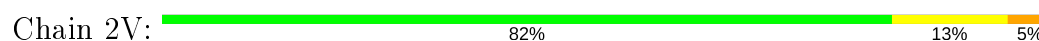
- Molecule 16: 50S ribosomal protein L20



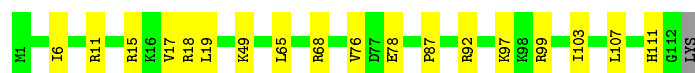
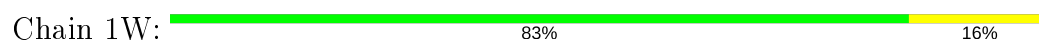
- Molecule 17: 50S ribosomal protein L21



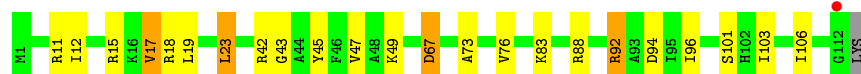
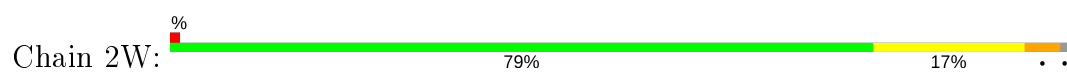
- Molecule 17: 50S ribosomal protein L21



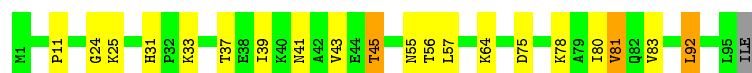
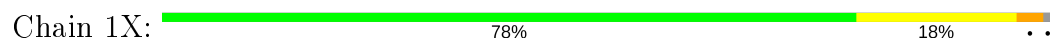
- Molecule 18: 50S ribosomal protein L22



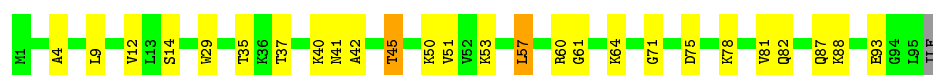
- Molecule 18: 50S ribosomal protein L22



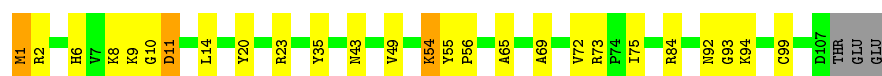
- Molecule 19: 50S ribosomal protein L23



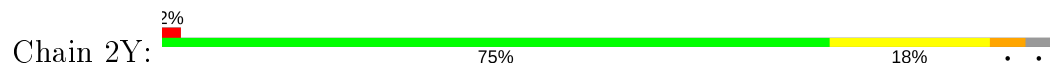
- Molecule 19: 50S ribosomal protein L23



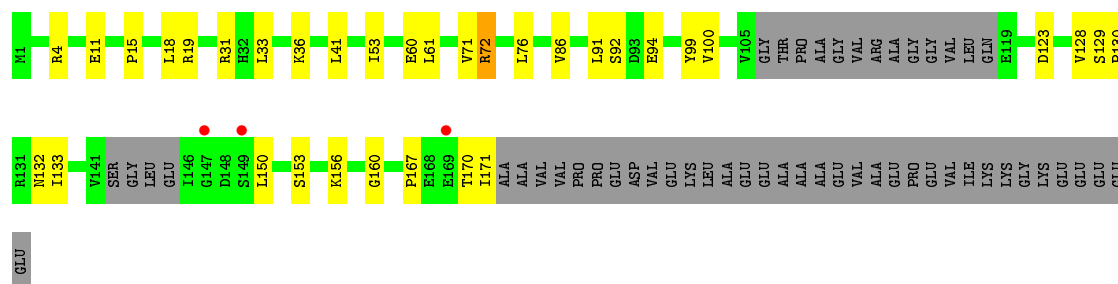
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

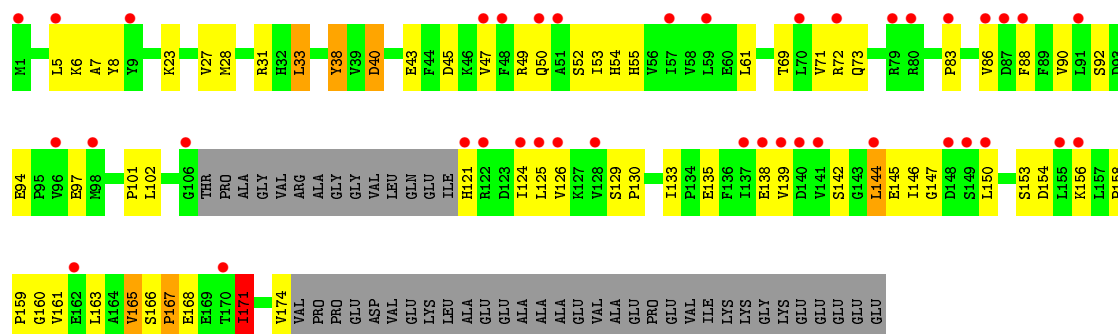


- Molecule 21: 50S ribosomal protein L25

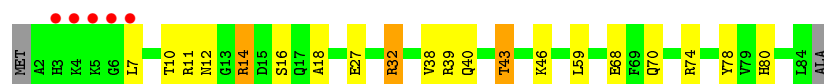
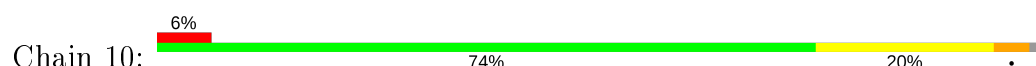


- Molecule 21: 50S ribosomal protein L25





- Molecule 22: 50S ribosomal protein L27



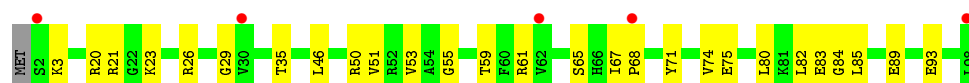
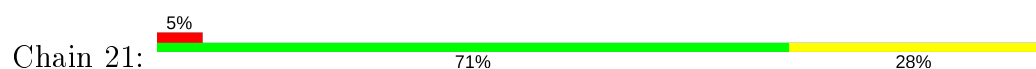
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



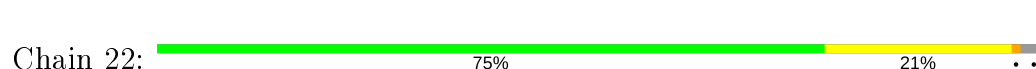
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

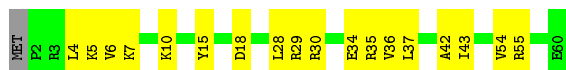


- Molecule 24: 50S ribosomal protein L29

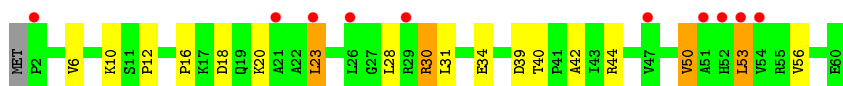




- Molecule 25: 50S ribosomal protein L30



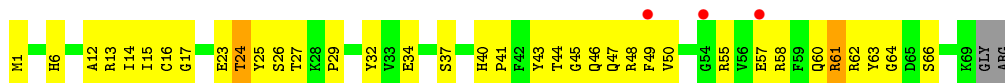
- Molecule 25: 50S ribosomal protein L30



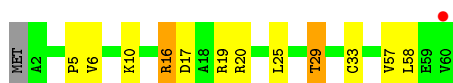
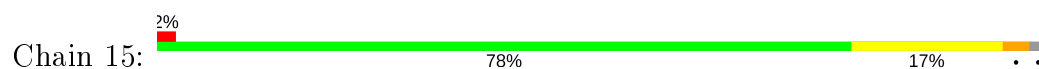
- Molecule 26: 50S ribosomal protein L31



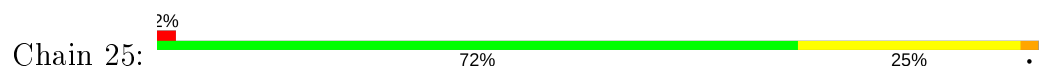
- Molecule 26: 50S ribosomal protein L31



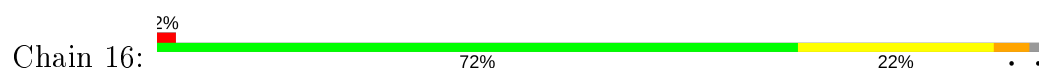
- Molecule 27: 50S ribosomal protein L32



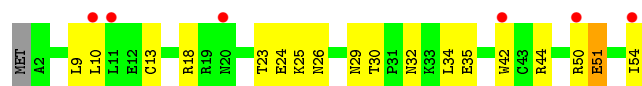
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



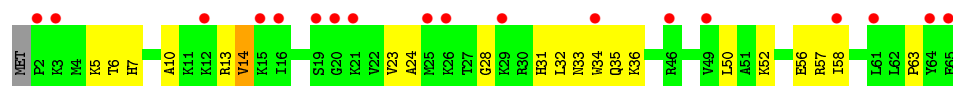
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



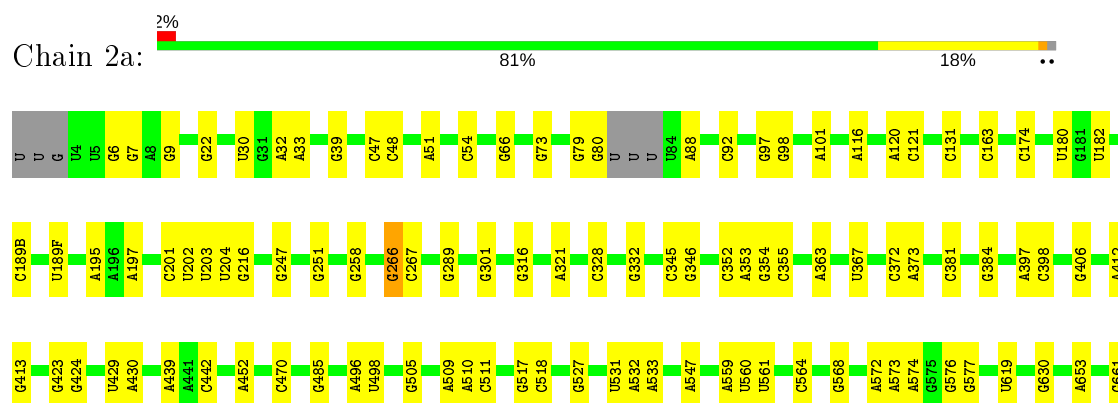
- Molecule 30: 50S ribosomal protein L35

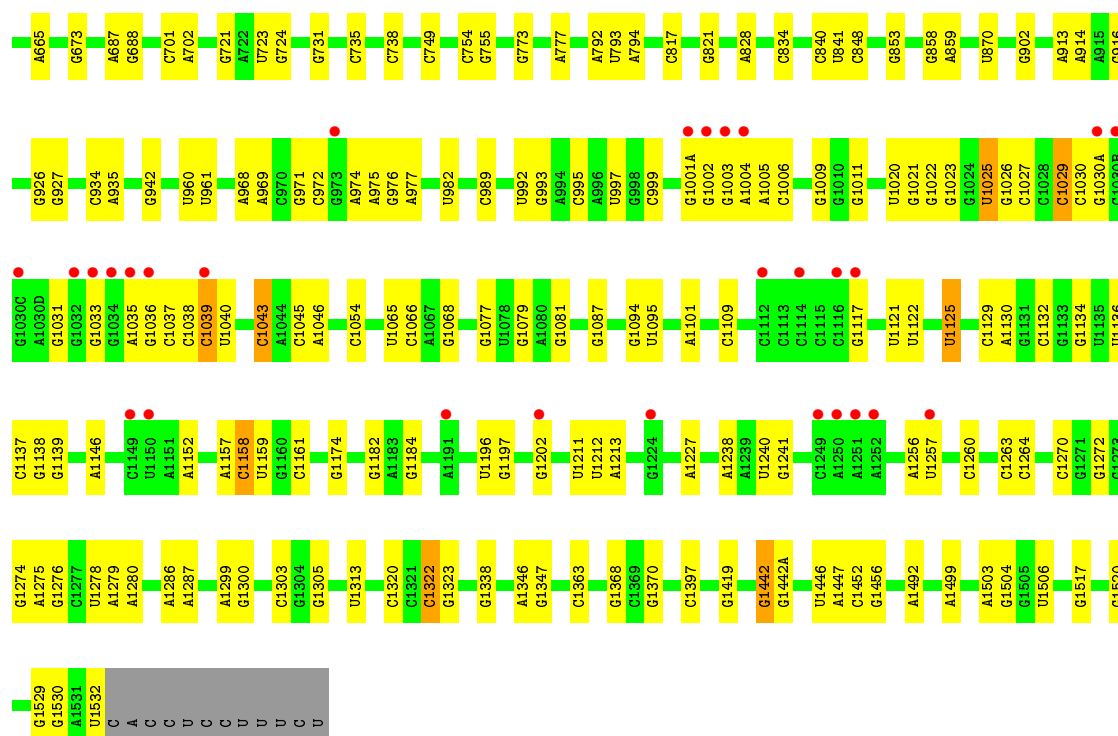


- Molecule 31: 50S ribosomal protein L36

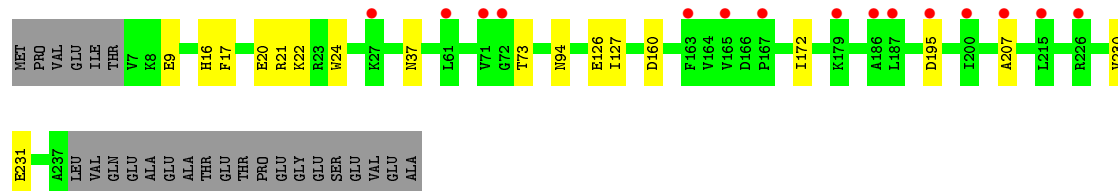
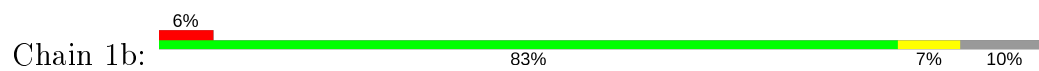


- Molecule 31: 50S ribosomal protein L36

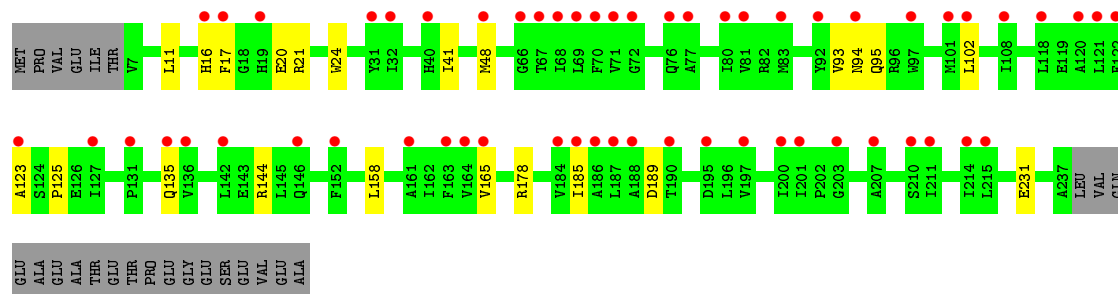
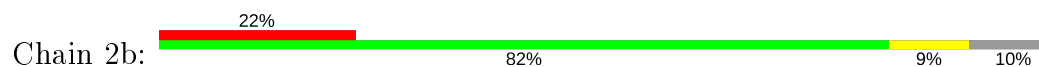




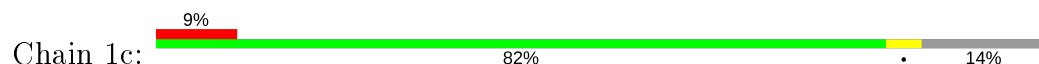
• Molecule 33: 30S ribosomal protein S2

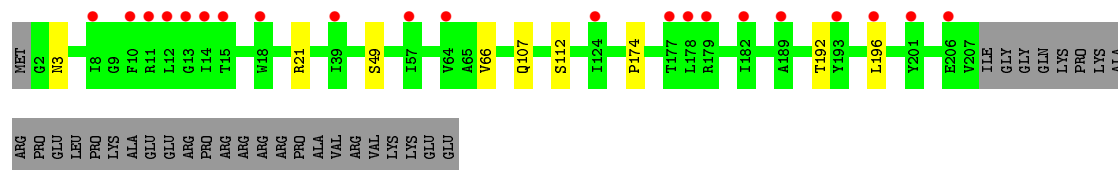


• Molecule 33: 30S ribosomal protein S2

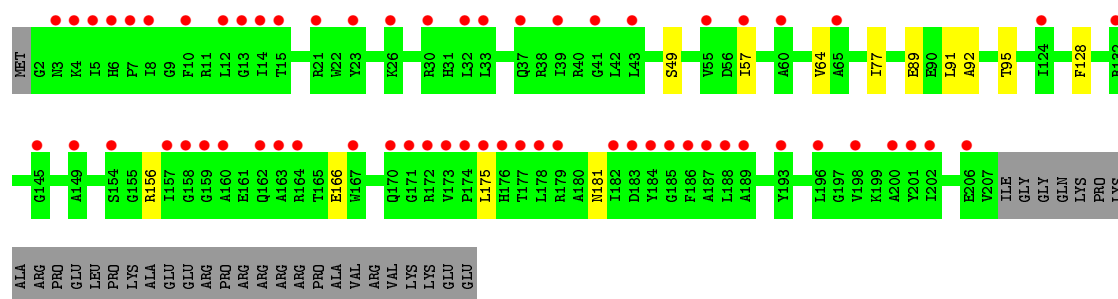
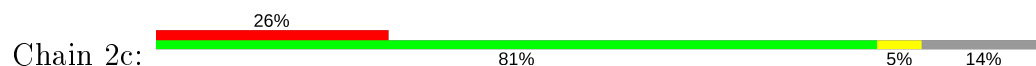


• Molecule 34: 30S ribosomal protein S3

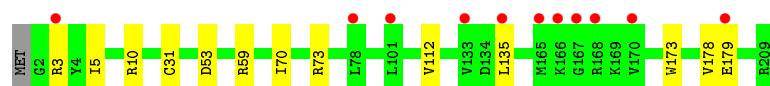




- Molecule 34: 30S ribosomal protein S3



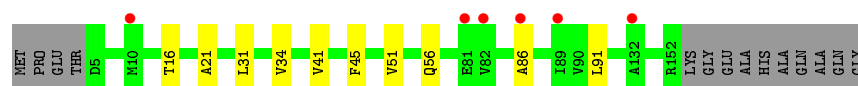
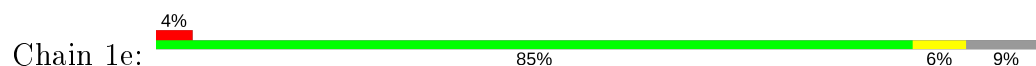
- Molecule 35: 30S ribosomal protein S4



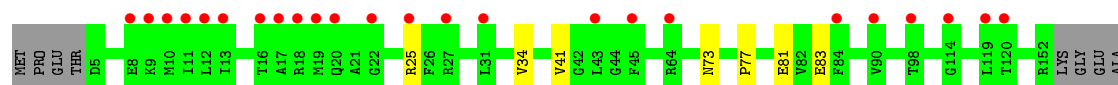
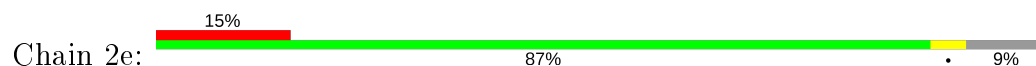
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



HIS
ALA
GLN
ALA
GLN
GLY

• Molecule 37: 30S ribosomal protein S6

Chain 1f:  96% ..

H1
V72
N73
S93
H100
ALA

• Molecule 37: 30S ribosomal protein S6

Chain 2f:  96% ..

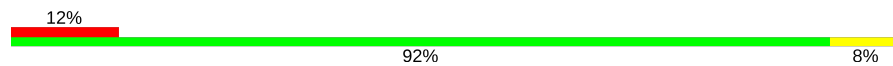
H1
L10
R28
Y59
L75
H100
ALA

• Molecule 38: 30S ribosomal protein S7

Chain 1g:  10% 94% 5% .

MET
A2
R3
R4
R5
R6
L12
L16
T24
S77
R78
R79
Y80
G81
Q82
A83
R84
Y85
Q86
E90
R94
H153
Y154
R155
W156

• Molecule 38: 30S ribosomal protein S7

Chain 2g:  12% 92% 8% .

MET
A2
R3
R4
V9
D15
L16
T24
L27
R32
L42
G55
R78
R79
V80
G81
G82
A83
R84
Y85
Q86
R95
S98
L104
E113
R114
R115
Y154
R155
W156

• Molecule 39: 30S ribosomal protein S8

Chain 1h:  3% 94% ..

MET
L2
D25
S29
E49
I83
R84
R85
Y86
L112
L119
L133
W138

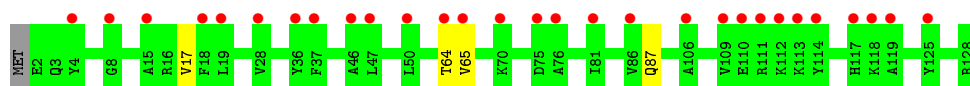
• Molecule 39: 30S ribosomal protein S8

Chain 2h:  10% 93% 5% ..

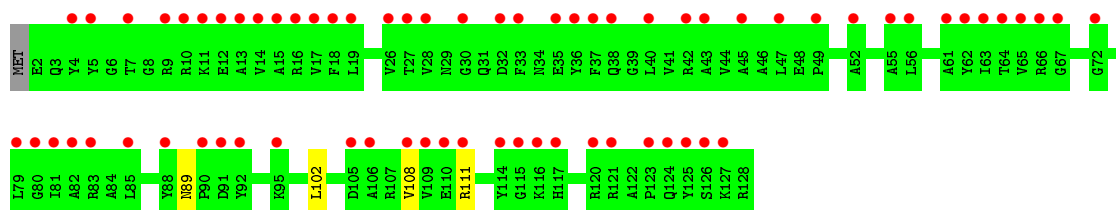
MET
L2
T3
N9
L10
T11
R12
N15
A16
T17
R18
V19
Y20
K21
D25
R68
D73
L80
I83
R84
S87
R91
Y111
L112
L133
W138

• Molecule 40: 30S ribosomal protein S9

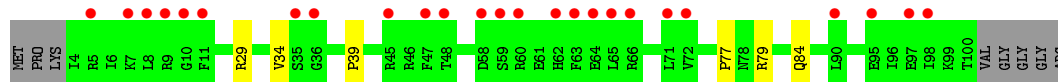
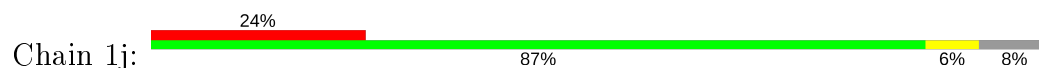
Chain 1i:  23% 96% ..



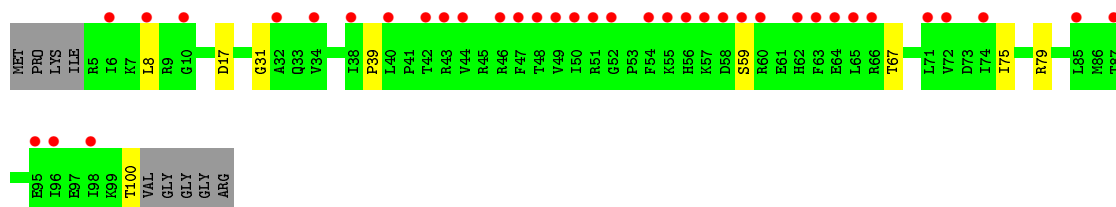
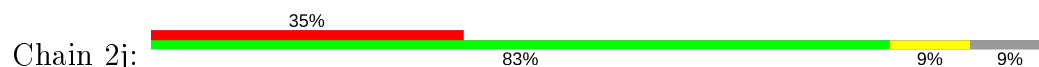
- Molecule 40: 30S ribosomal protein S9



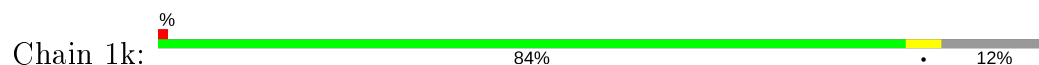
- Molecule 41: 30S ribosomal protein S10



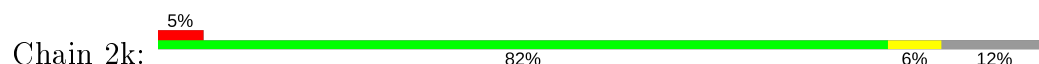
- Molecule 41: 30S ribosomal protein S10




- Molecule 42: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S11




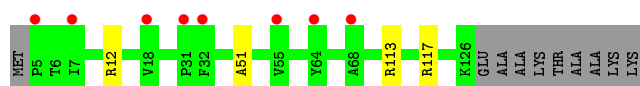
- Molecule 43: 30S ribosomal protein S12

Chain 1l:  84% 8% 8%



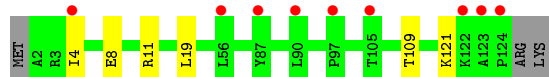
- Molecule 43: 30S ribosomal protein S12

Chain 2l:  6% 89% 8%



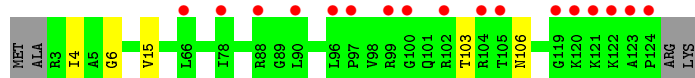
- Molecule 44: 30S ribosomal protein S13

Chain 1m:  7% 93% 5%




- Molecule 44: 30S ribosomal protein S13

Chain 2m:  13% 93% 5%




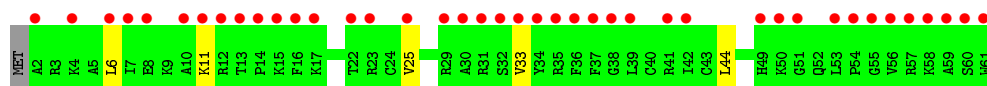
- Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:  16% 89% 10%



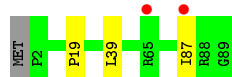
- Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:  67% 90% 8%

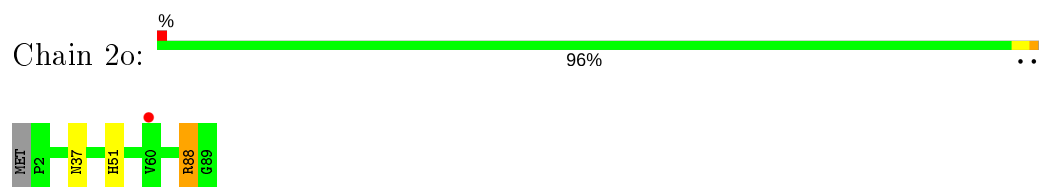


- Molecule 46: 30S ribosomal protein S15

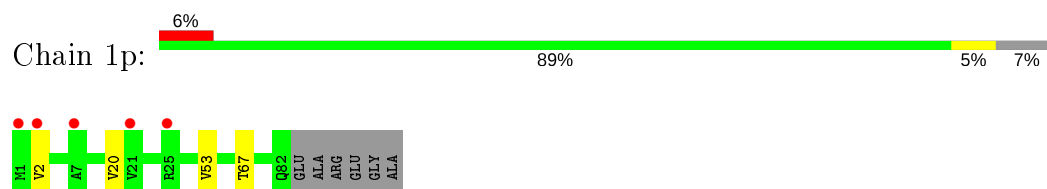
Chain 1o:  2% 96%



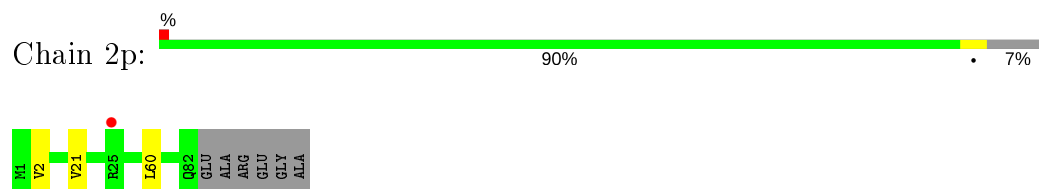
- Molecule 46: 30S ribosomal protein S15



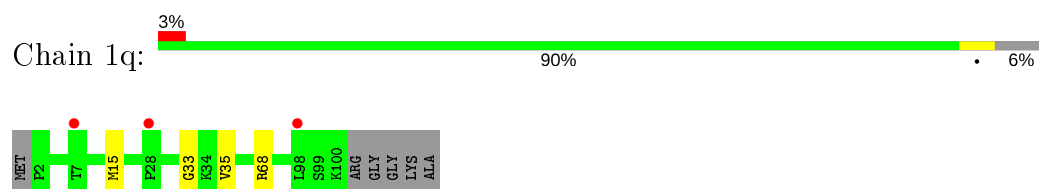
- Molecule 47: 30S ribosomal protein S16



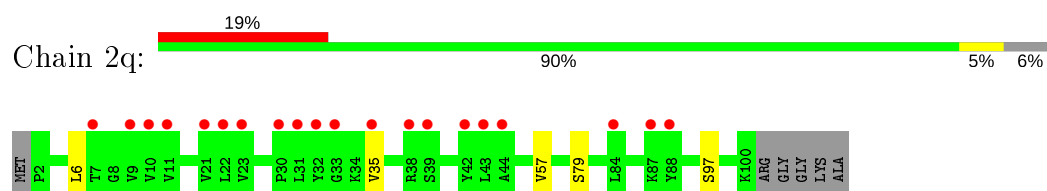
- Molecule 47: 30S ribosomal protein S16



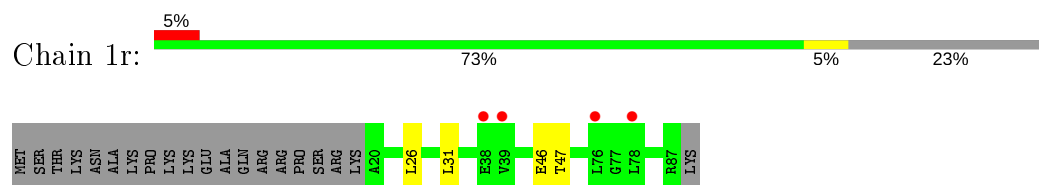
- Molecule 48: 30S ribosomal protein S17



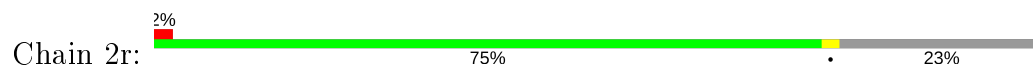
- Molecule 48: 30S ribosomal protein S17

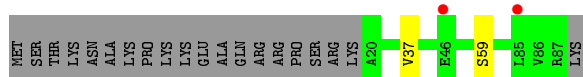


- Molecule 49: 30S ribosomal protein S18

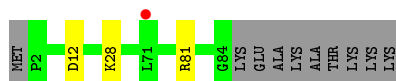
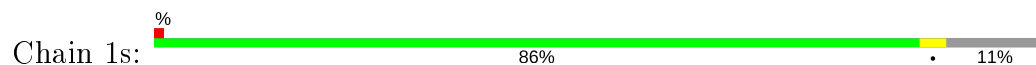


- Molecule 49: 30S ribosomal protein S18

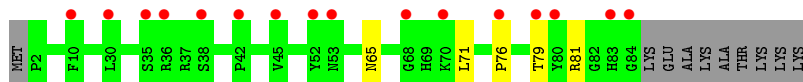
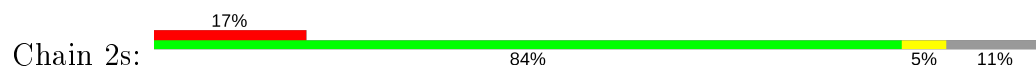




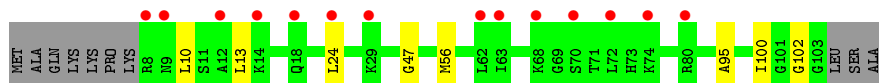
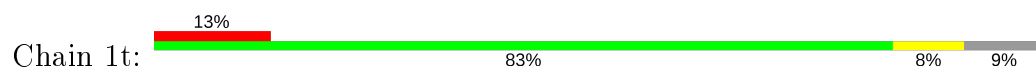
- Molecule 50: 30S ribosomal protein S19



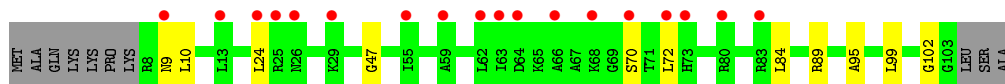
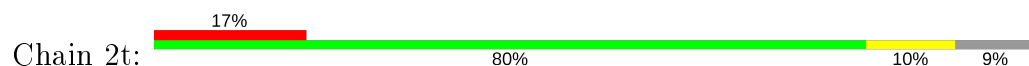
- Molecule 50: 30S ribosomal protein S19



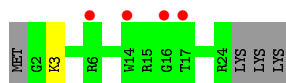
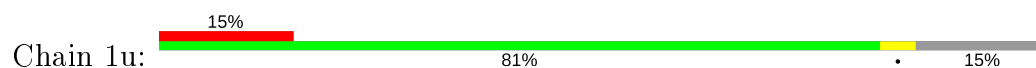
- Molecule 51: 30S ribosomal protein S20



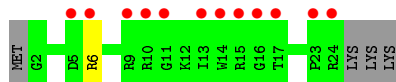
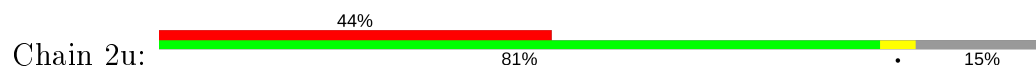
- Molecule 51: 30S ribosomal protein S20



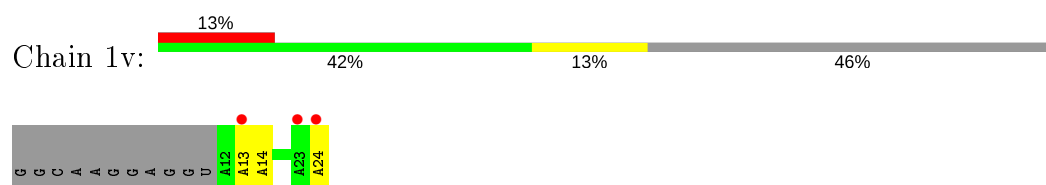
- Molecule 52: 30S ribosomal protein Thx



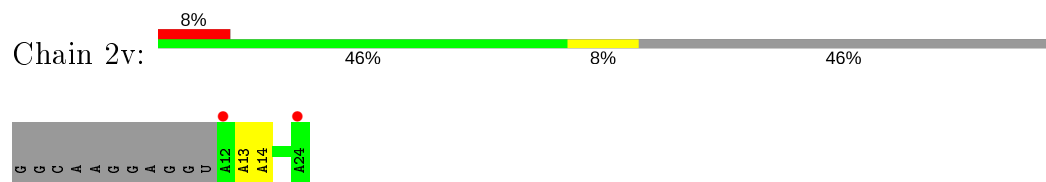
- Molecule 52: 30S ribosomal protein Thx



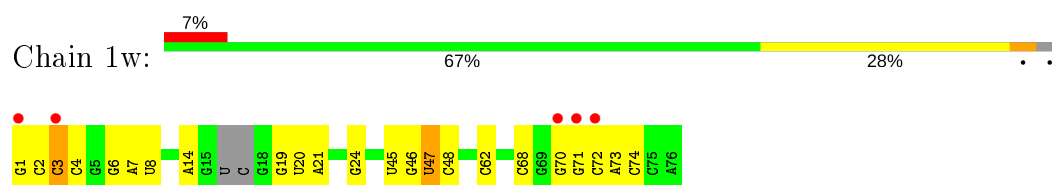
- Molecule 53: mRNA



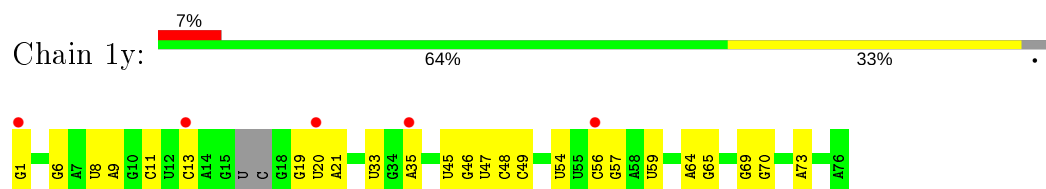
- Molecule 53: mRNA



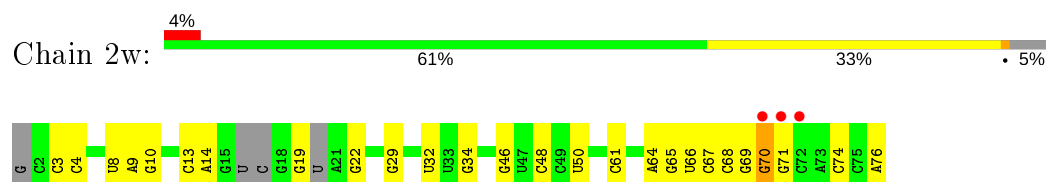
- Molecule 54: A-site and E-site tRNAs



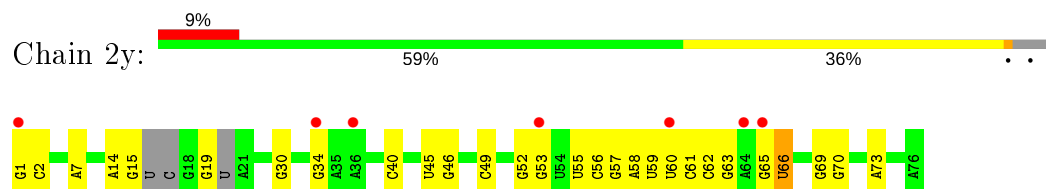
- Molecule 54: A-site and E-site tRNAs



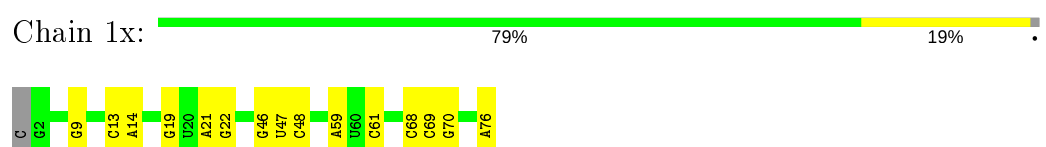
- Molecule 54: A-site and E-site tRNAs




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

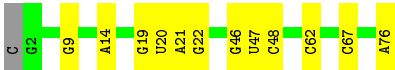


- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA

Chain 2x:  83% 16% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.78Å 449.83Å 622.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.54 – 2.80 181.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.0 (152.54-2.80) 94.0 (181.84-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.214 , 0.269 0.214 , 0.269	Depositor DCC
R_{free} test set	67418 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	299109	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.50	0/69009	0.96	49/107712 (0.0%)
1	2A	0.39	0/67293	0.89	43/105034 (0.0%)
2	1B	0.45	1/2882 (0.0%)	0.88	0/4494
2	2B	0.40	1/2879 (0.0%)	0.92	2/4487 (0.0%)
3	1D	0.35	0/2186	0.55	0/2944
3	2D	0.34	0/2186	0.55	0/2944
4	1E	0.35	0/1592	0.56	0/2149
4	2E	0.30	0/1592	0.51	0/2149
5	1F	0.33	0/1619	0.53	0/2193
5	2F	0.31	0/1615	0.50	0/2188
6	1G	0.30	0/1448	0.49	0/1957
6	2G	0.29	0/1453	0.48	1/1963 (0.1%)
7	1H	0.33	0/1356	0.51	0/1834
7	2H	0.31	0/1356	0.49	1/1834 (0.1%)
8	1I	0.29	0/1112	0.48	0/1514
8	2I	0.28	0/1079	0.47	0/1475
9	1N	0.34	0/1144	0.50	0/1543
9	2N	0.28	0/1144	0.47	0/1543
10	1O	0.36	0/943	0.55	0/1269
10	2O	0.31	0/943	0.52	0/1269
11	1P	0.35	0/1152	0.55	0/1533
11	2P	0.31	0/1152	0.53	0/1533
12	1Q	0.33	0/1143	0.51	0/1527
12	2Q	0.29	0/1143	0.49	0/1527
13	1R	0.32	0/982	0.53	0/1312
13	2R	0.28	0/982	0.49	0/1312
14	1S	0.31	0/883	0.52	0/1176
14	2S	0.29	0/880	0.49	0/1172
15	1T	0.32	0/1105	0.51	0/1477
15	2T	0.28	0/1097	0.47	0/1468
16	1U	0.36	0/977	0.51	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.29	0/977	0.43	0/1301
17	1V	0.34	0/782	0.56	0/1049
17	2V	0.29	0/782	0.53	0/1049
18	1W	0.34	0/897	0.54	0/1205
18	2W	0.30	0/897	0.51	0/1205
19	1X	0.35	0/764	0.56	0/1025
19	2X	0.30	0/764	0.54	1/1025 (0.1%)
20	1Y	0.34	0/819	0.54	0/1095
20	2Y	0.32	0/819	0.51	0/1095
21	1Z	0.32	0/1267	0.52	0/1717
21	2Z	0.30	0/1299	0.51	0/1763
22	10	0.35	0/662	0.55	0/881
22	20	0.32	0/662	0.49	0/881
23	11	0.34	0/762	0.52	0/1014
23	21	0.31	0/762	0.54	0/1014
24	12	0.33	0/590	0.46	0/781
24	22	0.27	0/590	0.43	0/781
25	13	0.33	0/474	0.50	0/635
25	23	0.28	0/469	0.46	0/630
26	14	0.35	0/565	0.59	0/761
26	24	0.30	0/545	0.50	0/737
27	15	0.36	0/469	0.54	0/635
27	25	0.32	0/469	0.50	0/635
28	16	0.35	0/460	0.53	0/613
28	26	0.31	0/456	0.51	0/608
29	17	0.34	0/426	0.55	0/561
29	27	0.32	0/426	0.54	0/561
30	18	0.34	0/525	0.56	0/691
30	28	0.31	0/525	0.49	0/691
31	19	0.34	0/310	0.53	0/407
31	29	0.30	0/310	0.51	0/407
32	1a	0.36	0/35795	0.88	25/55864 (0.0%)
32	2a	0.36	2/35886 (0.0%)	0.90	38/56005 (0.1%)
33	1b	0.29	0/1881	0.47	0/2542
33	2b	0.30	0/1860	0.50	0/2518
34	1c	0.29	0/1572	0.47	0/2126
34	2c	0.29	0/1566	0.47	0/2119
35	1d	0.29	0/1685	0.46	0/2262
35	2d	0.29	0/1704	0.47	0/2284
36	1e	0.30	0/1145	0.49	0/1543
36	2e	0.29	0/1149	0.52	0/1548
37	1f	0.29	0/823	0.48	0/1115
37	2f	0.30	0/829	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.30	0/1250	0.46	0/1679
38	2g	0.28	0/1254	0.43	0/1683
39	1h	0.29	0/1108	0.47	0/1494
39	2h	0.28	0/1108	0.47	0/1494
40	1i	0.29	0/1002	0.47	0/1346
40	2i	0.29	0/997	0.49	0/1343
41	1j	0.27	0/722	0.47	0/982
41	2j	0.29	0/727	0.50	0/988
42	1k	0.27	0/844	0.47	0/1145
42	2k	0.27	0/848	0.47	0/1149
43	1l	0.31	0/937	0.52	0/1260
43	2l	0.30	0/937	0.55	0/1260
44	1m	0.28	0/969	0.46	0/1302
44	2m	0.28	0/961	0.49	0/1291
45	1n	0.31	0/501	0.47	0/664
45	2n	0.33	0/501	0.50	0/664
46	1o	0.27	0/739	0.42	0/985
46	2o	0.28	0/739	0.46	0/985
47	1p	0.28	0/697	0.50	0/939
47	2p	0.27	0/693	0.47	0/935
48	1q	0.28	0/836	0.48	0/1117
48	2q	0.29	0/836	0.47	0/1117
49	1r	0.30	0/560	0.46	0/746
49	2r	0.28	0/560	0.46	0/746
50	1s	0.29	0/667	0.52	0/900
50	2s	0.30	0/661	0.56	0/893
51	1t	0.28	0/730	0.48	0/965
51	2t	0.27	0/729	0.42	0/965
52	1u	0.28	0/203	0.50	0/266
52	2u	0.30	0/203	0.50	0/266
53	1v	0.38	0/310	0.88	0/480
53	2v	0.49	0/310	0.94	0/480
54	1w	0.51	1/1606 (0.1%)	1.05	5/2497 (0.2%)
54	1y	0.53	1/1606 (0.1%)	1.14	7/2497 (0.3%)
54	2w	0.47	0/1556	1.17	4/2418 (0.2%)
54	2y	0.54	1/1583 (0.1%)	1.09	2/2459 (0.1%)
55	1x	0.48	0/1725	1.09	12/2689 (0.4%)
55	2x	0.45	0/1725	1.09	10/2689 (0.4%)
All	All	0.40	7/316686 (0.0%)	0.83	200/474113 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	1	G	OP3-P	-10.33	1.48	1.61
54	1y	1	G	OP3-P	-10.31	1.48	1.61
54	2y	1	G	OP3-P	-10.09	1.49	1.61
2	1B	1	U	OP3-P	-10.05	1.49	1.61
2	2B	1	U	OP3-P	-10.04	1.49	1.61

The worst 5 of 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C5-C6-O6	19.26	140.16	128.60
32	2a	1263	C	N1-C2-O2	17.07	129.14	118.90
32	2a	1272	G	N1-C2-N2	-15.02	102.68	116.20
32	2a	1272	G	N3-C2-N2	14.88	130.32	119.90
32	2a	1272	G	N1-C6-O6	-12.36	112.48	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31192	701	0
1	2A	60322	0	30423	818	0
2	1B	2577	0	1305	26	0
2	2B	2575	0	1303	44	0
3	1D	2136	0	2218	48	0
3	2D	2136	0	2218	50	0
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	39	0
5	1F	1584	0	1625	37	0
5	2F	1580	0	1619	45	0
6	1G	1423	0	1436	29	0
6	2G	1428	0	1438	45	0
7	1H	1330	0	1407	24	0
7	2H	1330	0	1407	44	0
8	1I	1097	0	1140	32	0
8	2I	1064	0	1082	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	1N	1117	0	1184	14	0
9	2N	1117	0	1184	23	0
10	1O	933	0	996	20	0
10	2O	933	0	996	23	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	37	0
12	1Q	1122	0	1179	27	0
12	2Q	1122	0	1179	32	0
13	1R	968	0	1033	20	0
13	2R	968	0	1033	22	0
14	1S	873	0	927	23	0
14	2S	870	0	923	37	0
15	1T	1091	0	1151	22	0
15	2T	1083	0	1136	27	0
16	1U	959	0	1019	18	0
16	2U	959	0	1019	26	0
17	1V	771	0	830	6	0
17	2V	771	0	830	10	0
18	1W	886	0	940	15	0
18	2W	886	0	940	14	0
19	1X	750	0	814	15	0
19	2X	750	0	814	18	0
20	1Y	806	0	881	15	0
20	2Y	806	0	881	15	0
21	1Z	1240	0	1240	16	0
21	2Z	1271	0	1273	39	0
22	10	653	0	674	19	0
22	20	653	0	674	19	0
23	11	755	0	826	15	0
23	21	755	0	826	23	0
24	12	588	0	643	9	0
24	22	588	0	643	13	0
25	13	469	0	518	13	0
25	23	464	0	514	12	0
26	14	552	0	533	13	0
26	24	532	0	503	23	0
27	15	455	0	465	9	0
27	25	455	0	465	14	0
28	16	453	0	473	9	0
28	26	449	0	469	9	0
29	17	418	0	467	9	0
29	27	418	0	467	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	18	517	0	582	18	0
30	28	517	0	582	19	0
31	19	307	0	335	7	0
31	29	307	0	335	8	0
32	1a	32246	0	16295	0	0
32	2a	32327	0	16339	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1672	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1184	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0
38	1g	1231	0	1238	0	0
38	2g	1235	0	1249	0	0
39	1h	1088	0	1126	0	0
39	2h	1088	0	1126	0	0
40	1i	983	0	986	0	0
40	2i	978	0	966	0	0
41	1j	709	0	650	0	0
41	2j	714	0	672	0	0
42	1k	829	0	825	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	958	0	1002	0	0
44	2m	950	0	988	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	652	0	662	0	0
50	2s	646	0	644	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	1t	728	0	798	0	0
51	2t	727	0	796	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1v	277	0	140	0	0
53	2v	277	0	140	0	0
54	1w	1592	0	819	0	0
54	1y	1585	0	804	0	0
54	2w	1544	0	788	0	0
54	2y	1565	0	795	0	0
55	1x	1625	0	827	0	0
55	2x	1625	0	828	0	0
56	10	5	0	0	0	0
56	11	5	0	0	0	0
56	12	2	0	0	0	0
56	13	2	0	0	0	0
56	15	6	0	0	0	0
56	16	3	0	0	0	0
56	17	5	0	0	0	0
56	18	3	0	0	0	0
56	19	1	0	0	0	0
56	1A	1063	0	0	0	0
56	1B	38	0	0	0	0
56	1D	14	0	0	0	0
56	1E	13	0	0	0	0
56	1F	9	0	0	0	0
56	1G	5	0	0	0	0
56	1I	1	0	0	0	0
56	1N	5	0	0	0	0
56	1O	7	0	0	0	0
56	1P	3	0	0	0	0
56	1Q	5	0	0	0	0
56	1R	5	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	6	0	0	0	0
56	1V	3	0	0	0	0
56	1W	5	0	0	0	0
56	1X	6	0	0	0	0
56	1Y	2	0	0	0	0
56	1Z	4	0	0	0	0
56	1a	215	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1b	2	0	0	0	0
56	1e	1	0	0	0	0
56	1f	1	0	0	0	0
56	1l	3	0	0	0	0
56	1m	1	0	0	0	0
56	1n	2	0	0	0	0
56	1p	1	0	0	0	0
56	1q	1	0	0	0	0
56	1r	1	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	11	0	0	0	0
56	1x	15	0	0	0	0
56	1y	4	0	0	0	0
56	20	3	0	0	0	0
56	21	1	0	0	0	0
56	23	1	0	0	0	0
56	25	3	0	0	0	0
56	27	2	0	0	0	0
56	28	2	0	0	0	0
56	2A	754	0	0	0	0
56	2B	21	0	0	0	0
56	2D	7	0	0	0	0
56	2E	10	0	0	0	0
56	2F	4	0	0	0	0
56	2G	1	0	0	0	0
56	2O	2	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	3	0	0	0	0
56	2R	4	0	0	0	0
56	2T	3	0	0	0	0
56	2U	6	0	0	0	0
56	2V	2	0	0	0	0
56	2W	3	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	233	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2g	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2j	2	0	0	0	0
56	2l	4	0	0	0	0
56	2q	4	0	0	0	0
56	2r	2	0	0	0	0
56	2t	1	0	0	0	0
56	2v	5	0	0	0	0
56	2w	9	0	0	0	0
56	2x	5	0	0	0	0
56	2y	7	0	0	0	0
57	1A	2	0	0	0	0
57	2A	2	0	0	0	0
58	1A	25	0	0	2	0
58	2A	25	0	0	1	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0
61	10	10	0	0	0	0
61	11	7	0	0	0	0
61	12	2	0	0	0	0
61	13	4	0	0	0	0
61	15	5	0	0	1	0
61	16	2	0	0	0	0
61	17	9	0	0	1	0
61	18	7	0	0	1	0
61	1A	1433	0	0	74	0
61	1B	65	0	0	2	0
61	1D	24	0	0	0	0
61	1E	30	0	0	4	0
61	1F	10	0	0	4	0
61	1G	8	0	0	2	0
61	1H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1I	2	0	0	0	0
61	1N	6	0	0	1	0
61	1O	8	0	0	0	0
61	1P	18	0	0	1	0
61	1Q	12	0	0	0	0
61	1R	12	0	0	0	0
61	1S	4	0	0	0	0
61	1T	7	0	0	0	0
61	1U	9	0	0	0	0
61	1V	8	0	0	0	0
61	1W	8	0	0	0	0
61	1X	8	0	0	1	0
61	1Y	2	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	315	0	0	0	0
61	1b	1	0	0	0	0
61	1e	1	0	0	0	0
61	1f	1	0	0	0	0
61	1g	1	0	0	0	0
61	1j	1	0	0	0	0
61	1l	6	0	0	0	0
61	1m	1	0	0	0	0
61	1n	1	0	0	0	0
61	1q	3	0	0	0	0
61	1u	1	0	0	0	0
61	1v	6	0	0	0	0
61	1w	20	0	0	0	0
61	1x	14	0	0	0	0
61	1y	2	0	0	0	0
61	20	4	0	0	0	0
61	21	8	0	0	0	0
61	22	1	0	0	0	0
61	23	1	0	0	0	0
61	25	4	0	0	0	0
61	26	1	0	0	0	0
61	27	4	0	0	0	0
61	28	4	0	0	0	0
61	29	1	0	0	0	0
61	2A	885	0	0	53	0
61	2B	26	0	0	0	0
61	2D	18	0	0	4	0
61	2E	14	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2F	18	0	0	0	0
61	2I	4	0	0	0	0
61	2N	1	0	0	0	0
61	2P	12	0	0	1	0
61	2Q	2	0	0	0	0
61	2R	2	0	0	0	0
61	2T	6	0	0	0	0
61	2U	3	0	0	0	0
61	2V	1	0	0	0	0
61	2W	3	0	0	0	0
61	2X	1	0	0	0	0
61	2Y	1	0	0	1	0
61	2Z	2	0	0	0	0
61	2a	258	0	0	0	0
61	2c	1	0	0	0	0
61	2d	3	0	0	0	0
61	2e	1	0	0	0	0
61	2g	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	4	0	0	0	0
61	2l	6	0	0	0	0
61	2o	1	0	0	0	0
61	2p	2	0	0	0	0
61	2q	1	0	0	0	0
61	2r	1	0	0	0	0
61	2t	5	0	0	0	0
61	2u	1	0	0	0	0
61	2v	2	0	0	0	0
61	2w	2	0	0	0	0
61	2x	6	0	0	0	0
61	2y	18	0	0	0	0
All	All	299109	0	196685	2479	0

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

The worst 5 of 2479 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:2158:C:N4	1:1A:2177:G:H1	1.36	1.21
1:2A:2136:C:N4	1:2A:2155:G:H1	1.46	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2129:C:N4	1:2A:2159:G:H1	1.49	1.10
1:1A:1128:U:H3	1:1A:1132:A:N6	1.48	1.09
1:1A:2149:G:H1	1:1A:2183:C:N4	1.54	1.05

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	254 (93%)	18 (7%)	1 (0%)	34	66
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	29	61
4	2E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	29	61
5	1F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	29	61
5	2F	201/210 (96%)	184 (92%)	13 (6%)	4 (2%)	7	24
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	25	56
6	2G	179/182 (98%)	156 (87%)	18 (10%)	5 (3%)	5	17
7	1H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	25	56
7	2H	172/180 (96%)	149 (87%)	20 (12%)	3 (2%)	9	29
8	1I	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	22	53
8	2I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	22	53
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	126 (91%)	9 (6%)	3 (2%)	6	22
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	7 (6%)	2 (2%)	9	29
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	2P	147/150 (98%)	134 (91%)	11 (8%)	2 (1%)	11	34
12	1Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	53
12	2Q	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	22	53
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	9	29
14	1S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	17	46
14	2S	108/112 (96%)	100 (93%)	6 (6%)	2 (2%)	8	26
15	1T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	19	49
15	2T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	19	49
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	15	44
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	44
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
20	1Y	105/110 (96%)	96 (91%)	8 (8%)	1 (1%)	15	44
20	2Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	8	26
21	1Z	148/206 (72%)	133 (90%)	14 (10%)	1 (1%)	22	53
21	2Z	156/206 (76%)	132 (85%)	19 (12%)	5 (3%)	4	13
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	13	39
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	63 (93%)	4 (6%)	1 (2%)	10	33
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	8	28
26	14	67/71 (94%)	55 (82%)	8 (12%)	4 (6%)	1	4
26	24	67/71 (94%)	50 (75%)	13 (19%)	4 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	44 (86%)	7 (14%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	6	22
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
33	1b	229/256 (90%)	192 (84%)	27 (12%)	10 (4%)	2	8
33	2b	229/256 (90%)	200 (87%)	20 (9%)	9 (4%)	3	10
34	1c	204/239 (85%)	190 (93%)	11 (5%)	3 (2%)	10	33
34	2c	204/239 (85%)	173 (85%)	25 (12%)	6 (3%)	4	15
35	1d	206/209 (99%)	190 (92%)	13 (6%)	3 (2%)	10	33
35	2d	206/209 (99%)	187 (91%)	15 (7%)	4 (2%)	8	26
36	1e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	11	34
36	2e	146/162 (90%)	131 (90%)	14 (10%)	1 (1%)	22	53
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
38	1g	153/156 (98%)	138 (90%)	12 (8%)	3 (2%)	7	24
38	2g	153/156 (98%)	135 (88%)	15 (10%)	3 (2%)	7	24
39	1h	135/138 (98%)	129 (96%)	4 (3%)	2 (2%)	10	33
39	2h	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	10	33
40	1i	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
40	2i	125/128 (98%)	113 (90%)	12 (10%)	0	100	100
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	9
41	2j	94/105 (90%)	79 (84%)	11 (12%)	4 (4%)	2	8
42	1k	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	17	46
42	2k	112/129 (87%)	103 (92%)	6 (5%)	3 (3%)	5	17
43	1l	119/132 (90%)	110 (92%)	8 (7%)	1 (1%)	19	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	2l	119/132 (90%)	103 (87%)	15 (13%)	1 (1%)	19	49
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100	100
44	2m	120/126 (95%)	102 (85%)	15 (12%)	3 (2%)	5	19
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	39
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	39
47	1p	80/88 (91%)	69 (86%)	10 (12%)	1 (1%)	12	36
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	15	44
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	13	39
50	2s	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	5	19
51	1t	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	2	6
51	2t	94/106 (89%)	83 (88%)	5 (5%)	6 (6%)	1	3
52	1u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	7
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	11370/12128 (94%)	10425 (92%)	802 (7%)	143 (1%)	12	36

5 of 143 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	43	LEU
7	1H	126	PRO
26	14	53	GLU
33	1b	22	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	200 (93%)	15 (7%)	15	40
3	2D	215/218 (99%)	206 (96%)	9 (4%)	30	63
4	1E	164/166 (99%)	152 (93%)	12 (7%)	14	38
4	2E	164/166 (99%)	148 (90%)	16 (10%)	8	24
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7	22
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8	26
6	1G	143/156 (92%)	133 (93%)	10 (7%)	15	40
6	2G	143/156 (92%)	134 (94%)	9 (6%)	18	46
7	1H	144/148 (97%)	138 (96%)	6 (4%)	30	63
7	2H	144/148 (97%)	138 (96%)	6 (4%)	30	63
8	1I	113/124 (91%)	104 (92%)	9 (8%)	12	34
8	2I	105/124 (85%)	99 (94%)	6 (6%)	20	50
9	1N	118/119 (99%)	110 (93%)	8 (7%)	16	42
9	2N	118/119 (99%)	108 (92%)	10 (8%)	10	31
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	75
10	2O	100/100 (100%)	100 (100%)	0	100	100
11	1P	115/116 (99%)	109 (95%)	6 (5%)	23	55
11	2P	115/116 (99%)	111 (96%)	4 (4%)	36	70
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	22	53
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11	33
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6	19
13	2R	101/101 (100%)	92 (91%)	9 (9%)	9	28
14	1S	86/88 (98%)	78 (91%)	8 (9%)	9	26
14	2S	85/88 (97%)	78 (92%)	7 (8%)	11	33
15	1T	115/127 (91%)	112 (97%)	3 (3%)	46	79
15	2T	113/127 (89%)	105 (93%)	8 (7%)	14	39
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	30
16	2U	93/94 (99%)	91 (98%)	2 (2%)	52	83
17	1V	80/82 (98%)	73 (91%)	7 (9%)	10	29
17	2V	80/82 (98%)	71 (89%)	9 (11%)	6	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	1W	90/92 (98%)	87 (97%)	3 (3%)	38	72
18	2W	90/92 (98%)	83 (92%)	7 (8%)	12	35
19	1X	77/78 (99%)	73 (95%)	4 (5%)	23	55
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	66
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	19	49
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	14	39
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	9	28
21	2Z	137/179 (76%)	128 (93%)	9 (7%)	16	44
22	10	65/67 (97%)	62 (95%)	3 (5%)	27	60
22	20	65/67 (97%)	63 (97%)	2 (3%)	40	74
23	11	80/83 (96%)	77 (96%)	3 (4%)	33	67
23	21	80/83 (96%)	80 (100%)	0	100	100
24	12	65/67 (97%)	62 (95%)	3 (5%)	27	60
24	22	65/67 (97%)	64 (98%)	1 (2%)	65	89
25	13	51/52 (98%)	50 (98%)	1 (2%)	55	84
25	23	50/52 (96%)	45 (90%)	5 (10%)	7	22
26	14	59/63 (94%)	55 (93%)	4 (7%)	16	42
26	24	53/63 (84%)	49 (92%)	4 (8%)	13	37
27	15	50/52 (96%)	44 (88%)	6 (12%)	5	15
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	48
28	16	51/52 (98%)	47 (92%)	4 (8%)	12	35
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	22
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	24
29	27	41/42 (98%)	39 (95%)	2 (5%)	25	57
30	18	54/55 (98%)	49 (91%)	5 (9%)	9	26
30	28	54/55 (98%)	49 (91%)	5 (9%)	9	26
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	76
33	1b	192/220 (87%)	184 (96%)	8 (4%)	30	63
33	2b	187/220 (85%)	174 (93%)	13 (7%)	15	40
34	1c	142/188 (76%)	136 (96%)	6 (4%)	30	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	2c	140/188 (74%)	133 (95%)	7 (5%)	24	56
35	1d	169/181 (93%)	159 (94%)	10 (6%)	19	49
35	2d	173/181 (96%)	162 (94%)	11 (6%)	17	45
36	1e	113/123 (92%)	105 (93%)	8 (7%)	14	39
36	2e	114/123 (93%)	108 (95%)	6 (5%)	22	54
37	1f	84/90 (93%)	81 (96%)	3 (4%)	35	69
37	2f	85/90 (94%)	82 (96%)	3 (4%)	36	70
38	1g	119/127 (94%)	114 (96%)	5 (4%)	30	63
38	2g	120/127 (94%)	111 (92%)	9 (8%)	13	37
39	1h	114/119 (96%)	108 (95%)	6 (5%)	22	54
39	2h	114/119 (96%)	107 (94%)	7 (6%)	18	48
40	1i	90/99 (91%)	86 (96%)	4 (4%)	28	61
40	2i	89/99 (90%)	85 (96%)	4 (4%)	27	60
41	1j	66/92 (72%)	64 (97%)	2 (3%)	41	75
41	2j	69/92 (75%)	64 (93%)	5 (7%)	14	38
42	1k	82/99 (83%)	78 (95%)	4 (5%)	25	57
42	2k	83/99 (84%)	78 (94%)	5 (6%)	19	48
43	1l	96/108 (89%)	86 (90%)	10 (10%)	7	21
43	2l	96/108 (89%)	93 (97%)	3 (3%)	40	74
44	1m	93/101 (92%)	87 (94%)	6 (6%)	17	44
44	2m	92/101 (91%)	90 (98%)	2 (2%)	52	83
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	15
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	22
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46	79
46	2o	78/80 (98%)	75 (96%)	3 (4%)	33	67
47	1p	69/74 (93%)	66 (96%)	3 (4%)	29	62
47	2p	68/74 (92%)	65 (96%)	3 (4%)	28	61
48	1q	94/97 (97%)	91 (97%)	3 (3%)	39	73
48	2q	94/97 (97%)	89 (95%)	5 (5%)	22	54
49	1r	59/77 (77%)	55 (93%)	4 (7%)	16	42
49	2r	59/77 (77%)	57 (97%)	2 (3%)	37	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	1s	69/80 (86%)	67 (97%)	2 (3%)	42	76
50	2s	67/80 (84%)	64 (96%)	3 (4%)	27	60
51	1t	70/82 (85%)	67 (96%)	3 (4%)	29	62
51	2t	70/82 (85%)	65 (93%)	5 (7%)	14	39
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	51
All	All	9303/10064 (92%)	8749 (94%)	554 (6%)	19	48

5 of 554 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	1l	117	ARG
5	2F	74	ARG
41	2j	8	LEU
45	1n	6	LEU
3	2D	94	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
44	1m	62	ASN
5	2F	69	HIS
40	2i	3	GLN
45	1n	49	HIS
3	2D	112	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2860/2915 (98%)	472 (16%)	28 (0%)
1	2A	2788/2915 (95%)	502 (18%)	22 (0%)
2	1B	120/121 (99%)	12 (10%)	2 (1%)
2	2B	118/121 (97%)	32 (27%)	0
32	1a	1494/1521 (98%)	243 (16%)	0
32	2a	1498/1521 (98%)	270 (18%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	71/76 (93%)	22 (30%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	1y	71/76 (93%)	21 (29%)	0
54	2w	68/76 (89%)	24 (35%)	0
54	2y	69/76 (90%)	26 (37%)	0
55	1x	75/77 (97%)	12 (16%)	0
55	2x	75/77 (97%)	9 (12%)	0
All	All	9331/9620 (96%)	1650 (17%)	52 (0%)

5 of 1650 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	57	G

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2442	A
2	1B	65	C
1	2A	1913	A
1	1A	2451	A
1	1A	2701	U

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

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
55	5MU	2x	54	55	15,22,23	1.10	1 (6%)	16,32,35	1.64	2 (12%)
1	2MU	2A	2552	1,56	14,22,24	0.91	0	14,31,36	0.94	1 (7%)
55	5MC	2x	32	55	15,22,23	1.28	1 (6%)	19,32,35	1.45	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MA	1A	2515	1,56	17,25,26	1.31	2 (11%)	19,37,40	2.01	2 (10%)
1	5MU	2A	1915	1	15,22,23	1.07	1 (6%)	16,32,35	1.81	2 (12%)
32	5MC	1a	1407	32	15,22,23	1.24	1 (6%)	19,32,35	1.37	2 (10%)
43	0TD	2l	92	43	4,9,10	3.09	1 (25%)	3,11,13	2.37	1 (33%)
32	MA6	1a	1518	32	19,26,27	0.90	1 (5%)	18,38,41	1.72	5 (27%)
55	PSU	2x	55	55	17,21,22	1.51	2 (11%)	20,30,33	3.16	6 (30%)
32	M2G	2a	966	32	20,27,28	1.42	3 (15%)	22,40,43	2.20	7 (31%)
54	5MU	2y	54	54	15,22,23	1.11	1 (6%)	16,32,35	1.72	2 (12%)
54	4SU	2y	8	54	14,21,22	1.27	1 (7%)	15,30,33	1.29	2 (13%)
1	PSU	1A	1933	1	17,21,22	1.67	4 (23%)	20,30,33	3.08	6 (30%)
1	5MC	2A	1942	1	15,22,23	1.29	1 (6%)	19,32,35	1.34	2 (10%)
1	PSU	2A	2605	1	17,21,22	1.68	2 (11%)	20,30,33	2.93	6 (30%)
1	5MU	1A	1937	1	15,22,23	1.08	1 (6%)	16,32,35	1.70	1 (6%)
1	4OC	2A	1920	1	15,22,24	0.67	0	17,31,35	1.51	2 (11%)
32	5MC	2a	1400	32	15,22,23	1.45	1 (6%)	19,32,35	1.26	2 (10%)
1	PSU	2A	1917	1	17,21,22	1.58	2 (11%)	20,30,33	3.13	6 (30%)
1	PSU	1A	1939	1	17,21,22	1.54	2 (11%)	20,30,33	3.23	6 (30%)
32	MA6	2a	1519	32	19,26,27	1.01	1 (5%)	18,38,41	1.67	4 (22%)
54	PSU	2y	39	54	17,21,22	1.69	2 (11%)	20,30,33	3.81	7 (35%)
54	5MU	1y	54	54	15,22,23	1.11	2 (13%)	16,32,35	1.91	2 (12%)
55	PSU	1x	55	55	17,21,22	1.63	2 (11%)	20,30,33	3.17	6 (30%)
1	PSU	1A	2617	1,56	17,21,22	1.67	4 (23%)	20,30,33	3.15	6 (30%)
1	2MA	2A	2503	1,56	17,25,26	1.25	2 (11%)	19,37,40	1.94	3 (15%)
54	PSU	1w	39	54	17,21,22	1.60	3 (17%)	20,30,33	3.01	5 (25%)
54	7MG	1w	46	54	22,26,27	1.74	4 (18%)	28,39,42	2.90	8 (28%)
1	5MC	1A	1984	1,56	15,22,23	1.34	1 (6%)	19,32,35	1.24	3 (15%)
54	PSU	1y	32	54	17,21,22	1.50	2 (11%)	20,30,33	3.35	6 (30%)
55	5MC	1x	32	55	15,22,23	1.27	1 (6%)	19,32,35	1.48	4 (21%)
54	7MG	2w	46	54	22,26,27	1.79	4 (18%)	28,39,42	2.64	9 (32%)
55	5MU	1x	54	55,56	15,22,23	1.07	1 (6%)	16,32,35	1.90	2 (12%)
54	7MG	2y	46	54	22,26,27	1.82	3 (13%)	28,39,42	2.92	9 (32%)
32	PSU	2a	516	32	17,21,22	1.44	2 (11%)	20,30,33	3.08	6 (30%)
54	PSU	2w	39	54	17,21,22	1.45	2 (11%)	20,30,33	3.32	6 (30%)
32	UR3	1a	1498	32	14,22,23	0.83	1 (7%)	15,32,35	0.61	0
1	OMG	2A	2251	1,55,56	18,26,27	1.32	2 (11%)	20,38,41	2.09	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	1w	55	54	17,21,22	1.45	2 (11%)	20,30,33	3.43	6 (30%)
32	7MG	2a	527	32,56	22,26,27	1.74	4 (18%)	28,39,42	2.76	9 (32%)
32	5MC	1a	1404	32	15,22,23	1.32	1 (6%)	19,32,35	1.38	2 (10%)
54	4SU	1y	8	54	14,21,22	1.21	1 (7%)	15,30,33	1.67	2 (13%)
32	4OC	2a	1402	32,56	16,23,24	0.63	0	17,32,35	1.31	1 (5%)
54	MIA	2w	37	54	20,27,32	1.71	3 (15%)	22,39,47	1.84	6 (27%)
32	5MC	2a	1404	32	15,22,23	1.31	1 (6%)	19,32,35	1.37	3 (15%)
32	UR3	2a	1498	32	14,22,23	0.84	1 (7%)	15,32,35	0.80	1 (6%)
32	4OC	1a	1402	32	16,23,24	0.68	0	17,32,35	1.14	1 (5%)
54	PSU	2w	55	54	17,21,22	1.46	2 (11%)	20,30,33	3.21	6 (30%)
1	5MC	1A	1964	1	15,22,23	1.29	1 (6%)	19,32,35	1.46	3 (15%)
32	7MG	1a	527	32	22,26,27	1.88	4 (18%)	28,39,42	2.68	8 (28%)
32	5MC	2a	967	32	15,22,23	1.38	1 (6%)	19,32,35	1.29	3 (15%)
32	5MC	1a	1400	32	15,22,23	1.28	1 (6%)	19,32,35	1.52	4 (21%)
1	5MU	1A	1961	1,56	15,22,23	0.97	1 (6%)	16,32,35	1.77	2 (12%)
32	MA6	1a	1519	32	19,26,27	0.99	1 (5%)	18,38,41	1.52	4 (22%)
32	MA6	2a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.62	3 (16%)
54	MIA	2y	37	54	18,24,32	1.11	2 (11%)	18,35,47	1.36	3 (16%)
32	M2G	1a	966	32	20,27,28	1.46	3 (15%)	22,40,43	2.36	7 (31%)
54	MIA	1y	37	54	18,24,32	1.15	2 (11%)	18,35,47	1.27	2 (11%)
54	4SU	2w	8	54	14,21,22	1.27	1 (7%)	15,30,33	1.33	2 (13%)
32	5MC	2a	1407	32	15,22,23	1.26	1 (6%)	19,32,35	1.47	2 (10%)
55	4SU	2x	8	55,56	14,21,22	1.29	2 (14%)	15,30,33	2.37	2 (13%)
54	5MU	2w	54	54	15,22,23	1.09	1 (6%)	16,32,35	2.00	1 (6%)
1	2MU	1A	2564	1,56	14,22,24	0.89	1 (7%)	14,31,36	0.94	1 (7%)
54	PSU	2y	32	54	17,21,22	1.46	3 (17%)	20,30,33	3.16	6 (30%)
54	PSU	2w	32	54	17,21,22	1.48	2 (11%)	20,30,33	3.17	6 (30%)
54	PSU	1y	55	54	17,21,22	1.61	3 (17%)	20,30,33	3.17	7 (35%)
32	PSU	1a	516	32,56	17,21,22	1.50	3 (17%)	20,30,33	3.15	6 (30%)
1	5MU	2A	1939	1,56	15,22,23	1.09	1 (6%)	16,32,35	1.78	2 (12%)
54	PSU	2y	55	54	17,21,22	1.47	3 (17%)	20,30,33	3.32	6 (30%)
1	5MC	2A	1962	1,56	15,22,23	1.27	1 (6%)	19,32,35	1.32	3 (15%)
54	4SU	1w	8	54	14,21,22	1.37	2 (14%)	15,30,33	1.37	2 (13%)
54	PSU	1y	39	54	17,21,22	1.50	3 (17%)	20,30,33	3.23	5 (25%)
32	2MG	1a	1207	32	19,26,27	1.30	2 (10%)	21,38,41	2.27	7 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4OC	1A	1942	1	15,22,24	0.72	0	17,31,35	1.55	2 (11%)
1	PSU	2A	1911	1	17,21,22	1.48	2 (11%)	20,30,33	3.18	7 (35%)
55	4SU	1x	8	55	14,21,22	1.49	2 (14%)	15,30,33	2.53	2 (13%)
32	2MG	2a	1207	32	19,26,27	1.30	2 (10%)	21,38,41	2.46	8 (38%)
1	OMG	1A	2263	1,55,56	18,26,27	1.09	2 (11%)	20,38,41	2.06	6 (30%)
54	PSU	1w	32	54	17,21,22	1.50	2 (11%)	20,30,33	3.12	6 (30%)
54	5MU	1w	54	54	15,22,23	1.13	1 (6%)	16,32,35	1.74	2 (12%)
32	5MC	1a	967	32	15,22,23	1.23	1 (6%)	19,32,35	1.38	2 (10%)
54	MIA	1w	37	54	24,31,32	2.24	4 (16%)	26,44,47	2.48	9 (34%)
43	0TD	1l	92	43	4,9,10	3.15	1 (25%)	3,11,13	3.65	1 (33%)
54	7MG	1y	46	54	22,26,27	1.87	4 (18%)	28,39,42	3.06	10 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	1/7/27/28	0/2/2/2
55	5MC	2x	32	55	-	0/5/25/26	0/2/2/2
1	2MA	1A	2515	1,56	-	2/3/25/26	0/3/3/3
1	5MU	2A	1915	1	-	2/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/3/12/14	-
32	MA6	1a	1518	32	-	3/7/29/30	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	5MU	2y	54	54	-	3/5/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/5/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/5/25/26	0/2/2/2
1	4OC	2A	1920	1	-	1/7/27/30	0/2/2/2
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/5/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	1/7/37/38	0/3/3/3
1	5MC	1A	1984	1,56	-	2/5/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
54	7MG	2w	46	54	-	3/7/37/38	0/3/3/3
55	5MU	1x	54	55,56	-	0/5/25/26	0/2/2/2
54	7MG	2y	46	54	-	2/7/37/38	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
1	OMG	2A	2251	1,55,56	-	0/5/27/28	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	3/7/37/38	0/3/3/3
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
54	4SU	1y	8	54	-	4/5/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
54	MIA	2w	37	54	-	3/7/29/34	0/3/3/3
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	32	-	3/7/37/38	0/3/3/3
32	5MC	2a	967	32	-	1/5/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
1	5MU	1A	1961	1,56	-	0/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
54	MIA	2y	37	54	-	3/3/25/34	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
54	4SU	2w	8	54	-	1/5/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	4SU	2x	8	55,56	-	1/5/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
1	2MU	1A	2564	1,56	-	0/7/27/28	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	1/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/5/25/26	0/2/2/2
54	PSU	2y	55	54	-	5/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	2/5/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	4OC	1A	1942	1	-	0/7/27/30	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	OMG	1A	2263	1,55,56	-	0/5/27/28	0/3/3/3
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/5/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
43	0TD	1l	92	43	-	1/3/12/14	-
54	7MG	1y	46	54	-	3/7/37/38	0/3/3/3

The worst 5 of 149 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C13-C14	7.37	1.53	1.32
54	1w	37	MIA	C2-S10	-6.46	1.70	1.75
54	2w	37	MIA	C2-S10	-6.14	1.70	1.75
43	1l	92	0TD	CB-SB	-6.02	1.69	1.84
43	2l	92	0TD	CB-SB	-5.95	1.69	1.84

The worst 5 of 347 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	46	7MG	N3-C4-N9	10.09	139.87	126.91
54	1w	46	7MG	N3-C4-N9	9.51	139.12	126.91
54	2w	39	PSU	N1-C2-N3	-9.44	120.93	128.43
54	2y	46	7MG	N3-C4-N9	9.37	138.95	126.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	N3-C4-N9	9.19	138.71	126.91

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	1518	MA6	C5-C6-N6-C10
54	2y	54	5MU	C2'-C1'-N1-C6
32	2a	1400	5MC	O4'-C1'-N1-C6

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1915	5MU	1	0
1	2A	1920	4OC	2	0
1	2A	2503	2MA	1	0
1	1A	2564	2MU	2	0
1	2A	1939	5MU	2	0
1	1A	1942	4OC	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2625 ligands modelled in this entry, 2621 are monoatomic - leaving 4 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
60	SF4	1d	501	35	0,12,12	0.00	-	-		
60	SF4	2d	501	35	0,12,12	0.00	-	-		
58	EZG	2A	3746	-	21,26,26	3.67	3 (14%)	26,35,35	1.14	3 (11%)
58	EZG	1A	4030	-	21,26,26	2.80	3 (14%)	26,35,35	1.55	4 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	501	35	-	-	0/6/5/5
58	EZG	1A	4030	-	-	5/24/26/26	0/2/2/2
60	SF4	1d	501	35	-	-	0/6/5/5
58	EZG	2A	3746	-	-	8/24/26/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2A	3746	EZG	OAC-NAY	13.98	1.46	1.22
58	1A	4030	EZG	CAT-CAW	-8.54	1.39	1.51
58	2A	3746	EZG	CAT-CAW	-7.81	1.40	1.51
58	1A	4030	EZG	OAC-NAY	7.73	1.35	1.22
58	1A	4030	EZG	CAU-NAY	-4.83	1.33	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1A	4030	EZG	CAW-CAX-NAP	5.11	119.74	110.05
58	1A	4030	EZG	CAT-CAW-CAX	2.98	116.89	111.64
58	2A	3746	EZG	CAX-NAP-C	-2.97	117.83	123.07
58	1A	4030	EZG	CAI-CAG-CAT	-2.64	118.54	121.20
58	2A	3746	EZG	CAW-CAX-NAP	2.42	114.63	110.05

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	2A	3746	EZG	O-C-CA-CB
58	2A	3746	EZG	NAP-C-CA-CB
58	2A	3746	EZG	NAP-C-CA-N

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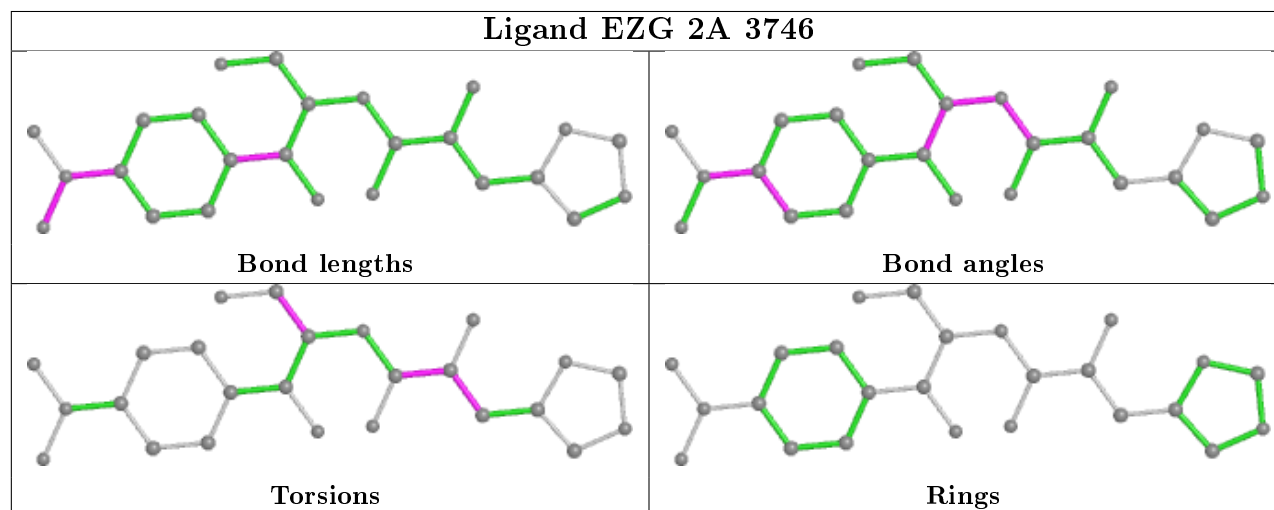
Mol	Chain	Res	Type	Atoms
58	2A	3746	EZG	OAD-CAM-CAX-CAW
58	2A	3746	EZG	OAD-CAM-CAX-NAP

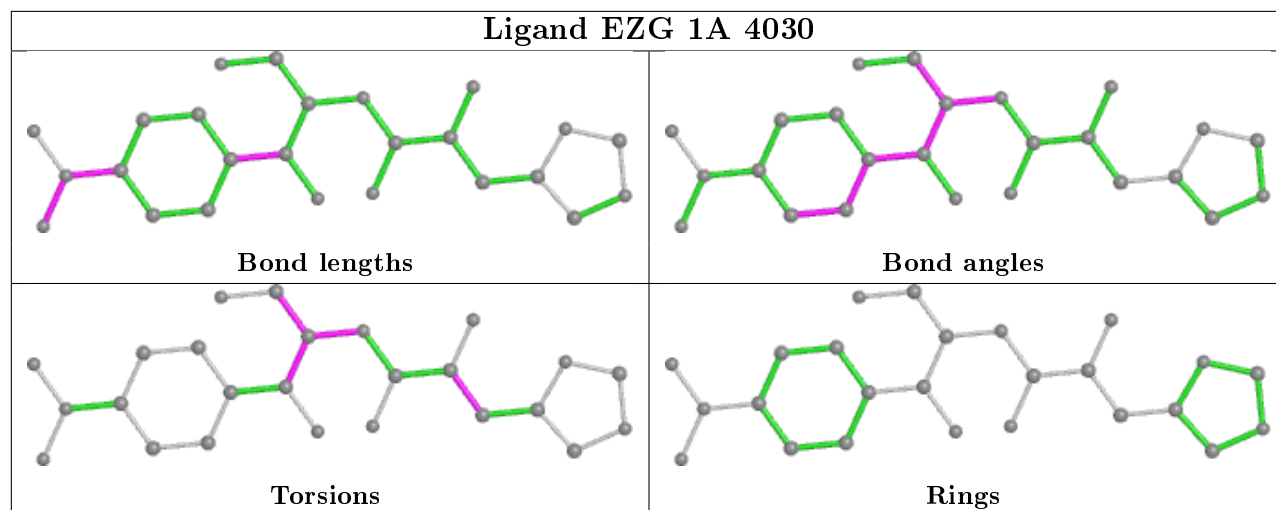
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	2A	3746	EZG	1	0
58	1A	4030	EZG	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.07	15 (0%) 91 88	13, 30, 88, 101	0
1	2A	2789/2915 (95%)	0.07	13 (0%) 91 88	25, 51, 87, 100	0
2	1B	120/121 (99%)	-0.15	0 100 100	23, 43, 57, 85	0
2	2B	120/121 (99%)	-0.15	0 100 100	53, 71, 80, 89	0
3	1D	275/276 (99%)	0.12	2 (0%) 87 84	16, 31, 46, 75	0
3	2D	275/276 (99%)	0.15	0 100 100	23, 43, 56, 66	0
4	1E	204/206 (99%)	0.02	0 100 100	13, 33, 54, 71	0
4	2E	204/206 (99%)	0.25	2 (0%) 82 77	28, 54, 67, 74	0
5	1F	203/210 (96%)	0.00	1 (0%) 91 88	15, 35, 62, 82	0
5	2F	203/210 (96%)	0.18	3 (1%) 73 68	30, 62, 74, 82	0
6	1G	181/182 (99%)	-0.15	0 100 100	35, 51, 69, 78	0
6	2G	181/182 (99%)	0.40	8 (4%) 34 24	56, 72, 78, 83	0
7	1H	174/180 (96%)	-0.13	0 100 100	34, 46, 59, 66	0
7	2H	174/180 (96%)	1.62	67 (38%) 0 0	61, 75, 81, 86	0
8	1I	146/148 (98%)	-0.06	1 (0%) 87 84	39, 67, 75, 81	0
8	2I	146/148 (98%)	0.14	2 (1%) 75 70	50, 66, 77, 81	0
9	1N	140/140 (100%)	-0.09	0 100 100	21, 35, 55, 68	0
9	2N	140/140 (100%)	0.55	4 (2%) 51 41	43, 58, 72, 75	0
10	1O	122/122 (100%)	-0.03	0 100 100	22, 35, 50, 56	0
10	2O	122/122 (100%)	0.33	0 100 100	43, 54, 67, 70	0
11	1P	149/150 (99%)	0.02	0 100 100	14, 40, 62, 66	0
11	2P	149/150 (99%)	1.25	37 (24%) 0 0	30, 61, 75, 83	0
12	1Q	141/141 (100%)	0.17	0 100 100	22, 36, 49, 72	0
12	2Q	141/141 (100%)	1.01	20 (14%) 2 1	41, 60, 70, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.19	0 100 100	18, 29, 44, 54	0
13	2R	118/118 (100%)	0.29	1 (0%) 86 81	33, 46, 55, 66	0
14	1S	110/112 (98%)	-0.12	1 (0%) 84 80	32, 44, 55, 60	0
14	2S	110/112 (98%)	1.33	24 (21%) 0 0	58, 67, 76, 79	0
15	1T	131/146 (89%)	-0.04	0 100 100	25, 39, 61, 71	0
15	2T	131/146 (89%)	0.43	5 (3%) 40 30	46, 58, 69, 75	0
16	1U	116/118 (98%)	0.03	0 100 100	14, 25, 42, 56	0
16	2U	116/118 (98%)	0.31	1 (0%) 84 80	35, 55, 67, 73	0
17	1V	101/101 (100%)	-0.17	0 100 100	19, 34, 53, 69	0
17	2V	101/101 (100%)	0.07	0 100 100	36, 63, 74, 78	0
18	1W	112/113 (99%)	-0.01	0 100 100	21, 26, 48, 71	0
18	2W	112/113 (99%)	0.23	1 (0%) 84 80	33, 44, 59, 85	0
19	1X	95/96 (98%)	-0.09	0 100 100	19, 31, 53, 75	0
19	2X	95/96 (98%)	0.00	0 100 100	40, 53, 64, 72	0
20	1Y	107/110 (97%)	-0.18	0 100 100	29, 43, 61, 72	0
20	2Y	107/110 (97%)	0.33	2 (1%) 66 59	54, 65, 74, 78	0
21	1Z	154/206 (74%)	0.07	3 (1%) 66 59	35, 57, 79, 85	0
21	2Z	160/206 (77%)	1.33	40 (25%) 0 0	61, 75, 84, 91	0
22	10	83/85 (97%)	0.25	5 (6%) 21 14	18, 31, 51, 56	0
22	20	83/85 (97%)	0.72	9 (10%) 5 3	36, 58, 69, 74	0
23	11	97/98 (98%)	0.21	1 (1%) 82 77	20, 38, 62, 70	0
23	21	97/98 (98%)	0.42	5 (5%) 27 18	35, 50, 68, 73	0
24	12	70/72 (97%)	-0.08	0 100 100	29, 41, 53, 64	0
24	22	70/72 (97%)	-0.09	0 100 100	47, 62, 70, 73	0
25	13	59/60 (98%)	-0.11	0 100 100	19, 31, 54, 72	0
25	23	59/60 (98%)	1.12	10 (16%) 1 1	48, 58, 70, 76	0
26	14	69/71 (97%)	-0.00	2 (2%) 51 41	43, 65, 83, 84	0
26	24	69/71 (97%)	-0.02	3 (4%) 35 25	67, 77, 86, 87	0
27	15	59/60 (98%)	-0.02	1 (1%) 70 63	14, 28, 41, 50	0
27	25	59/60 (98%)	0.09	1 (1%) 70 63	32, 46, 56, 64	0
28	16	53/54 (98%)	0.16	1 (1%) 66 59	27, 36, 50, 55	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.90	6 (11%) 5 3	42, 54, 67, 68	0
29	17	48/49 (97%)	0.13	1 (2%) 63 54	16, 21, 50, 60	0
29	27	48/49 (97%)	0.16	0 100 100	24, 35, 51, 60	0
30	18	64/65 (98%)	0.21	1 (1%) 72 66	21, 27, 37, 55	0
30	28	64/65 (98%)	1.63	18 (28%) 0 0	40, 49, 58, 68	0
31	19	37/37 (100%)	0.55	0 100 100	22, 33, 50, 55	0
31	29	37/37 (100%)	1.50	11 (29%) 0 0	53, 62, 71, 75	0
32	1a	1488/1521 (97%)	0.03	9 (0%) 89 86	32, 59, 86, 102	0
32	2a	1491/1521 (98%)	0.13	28 (1%) 66 59	43, 69, 89, 101	0
33	1b	231/256 (90%)	0.59	15 (6%) 18 11	59, 73, 82, 85	0
33	2b	231/256 (90%)	1.30	57 (24%) 0 0	64, 79, 85, 90	0
34	1c	206/239 (86%)	0.63	21 (10%) 6 3	51, 66, 74, 80	0
34	2c	206/239 (86%)	1.46	63 (30%) 0 0	66, 78, 82, 85	0
35	1d	208/209 (99%)	0.50	11 (5%) 26 17	50, 64, 76, 83	0
35	2d	208/209 (99%)	0.60	13 (6%) 20 12	53, 62, 72, 81	0
36	1e	148/162 (91%)	0.40	6 (4%) 37 27	48, 60, 70, 78	0
36	2e	148/162 (91%)	0.97	24 (16%) 1 1	58, 71, 79, 86	0
37	1f	100/101 (99%)	0.10	0 100 100	48, 60, 69, 70	0
37	2f	100/101 (99%)	0.08	1 (1%) 82 77	51, 63, 70, 76	0
38	1g	155/156 (99%)	0.43	16 (10%) 6 3	51, 62, 74, 88	0
38	2g	155/156 (99%)	0.79	19 (12%) 4 2	62, 71, 78, 84	0
39	1h	137/138 (99%)	0.29	4 (2%) 51 41	48, 61, 67, 72	0
39	2h	137/138 (99%)	0.68	14 (10%) 6 3	64, 71, 77, 85	0
40	1i	127/128 (99%)	1.23	29 (22%) 0 0	46, 69, 77, 83	0
40	2i	127/128 (99%)	2.35	69 (54%) 0 0	68, 77, 82, 88	0
41	1j	97/105 (92%)	1.18	25 (25%) 0 0	52, 71, 78, 83	0
41	2j	96/105 (91%)	1.82	37 (38%) 0 0	70, 78, 85, 87	0
42	1k	114/129 (88%)	0.26	1 (0%) 84 80	40, 58, 72, 79	0
42	2k	114/129 (88%)	0.45	7 (6%) 21 13	49, 66, 74, 78	0
43	1l	121/132 (91%)	0.01	0 100 100	33, 47, 59, 66	0
43	2l	121/132 (91%)	0.53	8 (6%) 18 11	53, 61, 71, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.35	9 (7%) 15 8	47, 59, 70, 74	0
44	2m	122/126 (96%)	0.61	17 (13%) 2 1	62, 75, 81, 85	0
45	1n	60/61 (98%)	1.05	10 (16%) 1 1	50, 59, 67, 71	0
45	2n	60/61 (98%)	2.95	41 (68%) 0 0	68, 77, 81, 87	0
46	1o	88/89 (98%)	0.13	2 (2%) 60 51	44, 59, 70, 75	0
46	2o	88/89 (98%)	-0.09	1 (1%) 80 75	53, 65, 74, 75	0
47	1p	82/88 (93%)	0.50	5 (6%) 21 13	51, 61, 70, 75	0
47	2p	82/88 (93%)	0.29	1 (1%) 79 73	55, 62, 71, 75	0
48	1q	99/105 (94%)	0.34	3 (3%) 50 40	47, 59, 72, 75	0
48	2q	99/105 (94%)	0.98	20 (20%) 1 0	55, 65, 73, 75	0
49	1r	68/88 (77%)	0.34	4 (5%) 22 14	48, 61, 71, 73	0
49	2r	68/88 (77%)	0.00	2 (2%) 51 41	57, 63, 73, 77	0
50	1s	83/93 (89%)	0.26	1 (1%) 79 73	49, 64, 73, 77	0
50	2s	83/93 (89%)	0.80	16 (19%) 1 0	71, 78, 84, 87	0
51	1t	96/106 (90%)	0.70	14 (14%) 2 1	50, 64, 73, 78	0
51	2t	96/106 (90%)	1.18	18 (18%) 1 1	52, 63, 76, 79	0
52	1u	23/27 (85%)	1.35	4 (17%) 1 1	52, 59, 63, 70	0
52	2u	23/27 (85%)	2.20	12 (52%) 0 0	67, 73, 80, 80	0
53	1v	13/24 (54%)	1.10	3 (23%) 0 0	42, 56, 81, 90	0
53	2v	13/24 (54%)	1.10	2 (15%) 2 1	59, 74, 91, 97	0
54	1w	67/76 (88%)	0.14	5 (7%) 14 8	32, 82, 93, 96	0
54	1y	67/76 (88%)	0.36	5 (7%) 14 8	28, 88, 96, 100	0
54	2w	65/76 (85%)	0.25	3 (4%) 32 22	54, 87, 95, 99	0
54	2y	66/76 (86%)	0.57	7 (10%) 6 3	49, 90, 94, 97	0
55	1x	72/77 (93%)	-0.08	0 100 100	32, 58, 76, 85	0
55	2x	72/77 (93%)	-0.14	0 100 100	45, 71, 81, 83	0
All	All	20875/21748 (95%)	0.29	1010 (4%) 30 21	13, 57, 83, 102	0

The worst 5 of 1010 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	34	TYR	8.6
44	2m	123	ALA	7.6

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Mol	Chain	Res	Type	RSRZ
40	2i	14	VAL	7.4
38	2g	82	GLY	7.1
44	1m	124	PRO	7.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	PSU	1y	55	20/21	0.76	0.28	85,93,105,123	0
54	5MU	1y	54	21/22	0.78	0.32	79,87,99,114	0
54	4SU	1y	8	20/21	0.80	0.20	91,96,103,105	0
54	PSU	2y	55	20/21	0.80	0.27	85,92,104,109	0
54	7MG	1w	46	24/25	0.82	0.15	76,87,106,118	0
54	5MU	2y	54	21/22	0.82	0.33	84,91,97,115	0
54	7MG	2y	46	24/25	0.83	0.23	83,92,97,112	0
54	7MG	2w	46	24/25	0.83	0.14	78,92,98,107	0
54	7MG	1y	46	24/25	0.84	0.22	86,94,99,108	0
54	4SU	2w	8	20/21	0.85	0.15	85,89,104,109	0
54	4SU	2y	8	20/21	0.85	0.14	83,95,104,112	0
54	MIA	2y	37	22/30	0.86	0.21	69,81,100,111	0
54	PSU	1y	32	20/21	0.88	0.19	71,81,88,90	0
54	PSU	2y	39	20/21	0.88	0.24	77,84,98,102	0
54	PSU	2y	32	20/21	0.88	0.17	69,84,92,94	0
54	MIA	1y	37	22/30	0.90	0.17	70,78,88,93	0
55	PSU	2x	55	20/21	0.91	0.13	67,78,81,81	0
43	0TD	2l	92	10/11	0.91	0.30	58,64,65,80	0
54	4SU	1w	8	20/21	0.91	0.12	74,81,92,95	0
54	PSU	2w	55	20/21	0.91	0.12	75,81,89,94	0
54	5MU	2w	54	21/22	0.92	0.12	68,75,81,83	0
54	PSU	1w	55	20/21	0.92	0.14	61,70,79,80	0
54	PSU	1y	39	20/21	0.92	0.17	70,77,87,90	0
55	5MU	2x	54	21/22	0.92	0.16	77,81,86,94	0
54	PSU	2w	32	20/21	0.93	0.27	67,78,88,89	0
54	PSU	2w	39	20/21	0.93	0.19	60,73,79,81	0
1	5MU	2A	1915	21/22	0.93	0.16	59,64,71,73	0
55	4SU	2x	8	20/21	0.93	0.13	69,73,78,81	0
32	5MC	2a	967	21/22	0.93	0.30	62,67,71,73	0
32	PSU	2a	516	20/21	0.93	0.14	50,70,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	7MG	2a	527	24/25	0.94	0.17	46,56,67,71	0
32	M2G	2a	966	25/26	0.94	0.26	60,65,72,79	0
32	5MC	2a	1400	21/22	0.94	0.23	60,67,71,73	0
43	0TD	1l	92	10/11	0.94	0.21	43,48,51,69	0
55	5MC	2x	32	21/22	0.94	0.18	65,68,73,74	0
1	5MU	1A	1937	21/22	0.95	0.17	43,49,54,56	0
32	7MG	1a	527	24/25	0.95	0.18	34,42,51,55	0
54	MIA	2w	37	25/30	0.95	0.17	60,68,74,78	0
32	5MC	2a	1404	21/22	0.95	0.17	47,51,56,61	0
55	PSU	1x	55	20/21	0.95	0.13	53,58,67,72	0
1	PSU	2A	1911	20/21	0.95	0.15	50,60,65,67	0
32	2MG	2a	1207	24/25	0.95	0.15	74,77,86,91	0
54	PSU	1w	32	20/21	0.95	0.19	57,62,68,69	0
54	MIA	1w	37	29/30	0.95	0.23	41,51,60,64	0
1	PSU	2A	1917	20/21	0.95	0.14	55,60,65,69	0
1	4OC	2A	1920	21/23	0.95	0.18	53,58,64,66	0
32	5MC	2a	1407	21/22	0.96	0.19	44,48,55,60	0
32	4OC	2a	1402	22/23	0.96	0.16	52,58,64,67	0
32	2MG	1a	1207	24/25	0.96	0.17	57,62,67,68	0
32	MA6	2a	1518	24/25	0.96	0.19	47,59,63,66	0
55	4SU	1x	8	20/21	0.96	0.15	50,57,65,67	0
1	PSU	1A	1939	20/21	0.96	0.16	38,46,53,54	0
55	5MU	1x	54	21/22	0.96	0.14	55,62,70,76	0
32	MA6	2a	1519	24/25	0.96	0.21	47,56,64,66	0
32	PSU	1a	516	20/21	0.96	0.15	32,49,53,54	0
1	5MC	2A	1942	21/22	0.96	0.17	49,56,62,66	0
1	PSU	1A	1933	20/21	0.97	0.19	30,37,44,45	0
32	5MC	1a	1400	21/22	0.97	0.21	37,47,50,55	0
32	MA6	1a	1519	24/25	0.97	0.20	33,39,43,44	0
32	5MC	1a	1407	21/22	0.97	0.20	28,34,39,40	0
32	5MC	1a	1404	21/22	0.97	0.19	31,38,42,44	0
32	UR3	2a	1498	21/22	0.97	0.18	44,50,54,63	0
54	PSU	1w	39	20/21	0.97	0.17	44,60,69,70	0
54	5MU	1w	54	21/22	0.97	0.17	44,60,67,72	0
32	M2G	1a	966	25/26	0.97	0.22	41,48,56,63	0
1	5MU	2A	1939	21/22	0.97	0.17	34,38,43,44	0
1	2MU	2A	2552	21/23	0.97	0.18	31,41,45,52	0
1	5MC	2A	1962	21/22	0.97	0.17	32,45,48,61	0
32	MA6	1a	1518	24/25	0.98	0.20	31,38,40,40	0
1	OMG	2A	2251	24/25	0.98	0.20	32,37,42,45	0
32	4OC	1a	1402	22/23	0.98	0.18	38,42,47,53	0
1	5MC	1A	1984	21/22	0.98	0.17	24,31,36,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	4OC	1A	1942	21/23	0.98	0.17	32,39,45,47	0
1	5MC	1A	1964	21/22	0.98	0.18	30,39,46,50	0
55	5MC	1x	32	21/22	0.98	0.20	44,50,57,66	0
1	2MU	1A	2564	21/23	0.98	0.19	18,23,28,31	0
1	PSU	2A	2605	20/21	0.98	0.17	27,31,37,38	0
1	PSU	1A	2617	20/21	0.98	0.18	16,20,25,28	0
1	5MU	1A	1961	21/22	0.98	0.18	19,23,26,32	0
1	2MA	2A	2503	23/24	0.98	0.21	24,33,37,46	0
32	5MC	1a	967	21/22	0.98	0.20	45,50,58,64	0
1	2MA	1A	2515	23/24	0.98	0.20	11,16,19,22	0
32	UR3	1a	1498	21/22	0.99	0.19	27,39,42,46	0
1	OMG	1A	2263	24/25	0.99	0.17	14,18,24,25	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2y	3006	1/1	0.34	0.13	88,88,88,88	0
56	MG	2a	1640	1/1	0.36	0.22	62,62,62,62	0
56	MG	2A	3720	1/1	0.47	0.17	97,97,97,97	0
56	MG	1A	3209	1/1	0.52	0.29	61,61,61,61	0
56	MG	1A	3898	1/1	0.56	0.15	71,71,71,71	0
56	MG	1A	3986	1/1	0.60	0.24	67,67,67,67	0
56	MG	1A	3242	1/1	0.63	0.26	59,59,59,59	0
56	MG	2a	1769	1/1	0.63	0.13	75,75,75,75	0
59	ZN	24	501	1/1	0.64	0.09	103,103,103,103	0
56	MG	2A	3258	1/1	0.64	0.17	58,58,58,58	0
56	MG	1A	3414	1/1	0.66	0.28	55,55,55,55	0
56	MG	1A	3201	1/1	0.67	0.51	42,42,42,42	0
56	MG	2a	1750	1/1	0.68	0.09	60,60,60,60	0
56	MG	2A	3383	1/1	0.68	0.22	56,56,56,56	0
56	MG	1a	3129	1/1	0.69	0.15	65,65,65,65	0
56	MG	2A	3615	1/1	0.69	0.34	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	2A	3457	1/1	0.69	0.20	58,58,58,58	0
56	MG	1A	3366	1/1	0.69	0.29	50,50,50,50	0
56	MG	2A	3374	1/1	0.70	0.15	41,41,41,41	0
56	MG	2B	3013	1/1	0.70	0.16	74,74,74,74	0
56	MG	2a	1637	1/1	0.70	0.13	52,52,52,52	0
56	MG	2A	3420	1/1	0.71	0.23	67,67,67,67	0
56	MG	1B	211	1/1	0.71	0.74	45,45,45,45	0
56	MG	2A	3630	1/1	0.71	0.18	55,55,55,55	0
56	MG	1A	3971	1/1	0.71	0.15	65,65,65,65	0
56	MG	1w	110	1/1	0.72	0.19	75,75,75,75	0
56	MG	28	102	1/1	0.72	0.15	64,64,64,64	0
56	MG	2A	3332	1/1	0.72	0.25	56,56,56,56	0
56	MG	1A	3977	1/1	0.72	0.13	44,44,44,44	0
56	MG	2A	3570	1/1	0.73	0.20	56,56,56,56	0
56	MG	1A	3436	1/1	0.73	0.16	62,62,62,62	0
56	MG	1A	3458	1/1	0.73	0.15	68,68,68,68	0
56	MG	2w	106	1/1	0.73	0.33	59,59,59,59	0
56	MG	1Z	3003	1/1	0.73	0.17	52,52,52,52	0
56	MG	2A	3247	1/1	0.73	0.13	63,63,63,63	0
56	MG	2a	1740	1/1	0.73	0.16	60,60,60,60	0
56	MG	2A	3702	1/1	0.74	0.13	59,59,59,59	0
56	MG	2v	3002	1/1	0.74	0.55	67,67,67,67	0
56	MG	2A	3031	1/1	0.74	0.28	57,57,57,57	0
56	MG	2A	3587	1/1	0.74	0.16	55,55,55,55	0
56	MG	1A	3802	1/1	0.74	0.22	54,54,54,54	0
56	MG	2w	109	1/1	0.74	0.13	63,63,63,63	0
56	MG	1A	3907	1/1	0.74	0.21	39,39,39,39	0
56	MG	2A	3353	1/1	0.74	0.16	35,35,35,35	0
56	MG	1X	101	1/1	0.75	0.09	73,73,73,73	0
56	MG	2A	3636	1/1	0.75	0.18	55,55,55,55	0
56	MG	1A	3920	1/1	0.75	0.21	39,39,39,39	0
56	MG	1A	3766	1/1	0.75	0.23	36,36,36,36	0
56	MG	1r	3001	1/1	0.75	0.16	61,61,61,61	0
56	MG	2B	3002	1/1	0.75	0.38	62,62,62,62	0
56	MG	2A	3163	1/1	0.75	0.26	44,44,44,44	0
56	MG	1A	3305	1/1	0.75	0.20	51,51,51,51	0
56	MG	1B	236	1/1	0.75	0.31	65,65,65,65	0
56	MG	2y	3003	1/1	0.76	0.13	59,59,59,59	0
56	MG	2A	3215	1/1	0.76	0.15	58,58,58,58	0
56	MG	1A	3226	1/1	0.76	0.82	49,49,49,49	0
56	MG	1A	3834	1/1	0.76	0.16	51,51,51,51	0
56	MG	2y	3001	1/1	0.76	0.23	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3259	1/1	0.76	0.20	53,53,53,53	0
56	MG	2r	3002	1/1	0.76	0.14	64,64,64,64	0
56	MG	2A	3201	1/1	0.76	0.20	55,55,55,55	0
56	MG	2A	3710	1/1	0.76	0.07	76,76,76,76	0
56	MG	1A	3319	1/1	0.76	0.23	53,53,53,53	0
56	MG	1E	310	1/1	0.77	0.16	60,60,60,60	0
56	MG	2A	3491	1/1	0.77	0.13	75,75,75,75	0
56	MG	2A	3550	1/1	0.77	0.15	58,58,58,58	0
56	MG	2A	3198	1/1	0.77	0.17	43,43,43,43	0
56	MG	2W	202	1/1	0.77	0.54	46,46,46,46	0
56	MG	2a	1656	1/1	0.77	0.14	68,68,68,68	0
56	MG	1D	313	1/1	0.77	0.21	52,52,52,52	0
56	MG	1a	3141	1/1	0.78	0.17	64,64,64,64	0
56	MG	2A	3586	1/1	0.78	0.12	44,44,44,44	0
56	MG	2A	3266	1/1	0.78	0.11	54,54,54,54	0
56	MG	1B	208	1/1	0.78	0.23	59,59,59,59	0
56	MG	1A	3883	1/1	0.78	0.21	59,59,59,59	0
56	MG	2a	1644	1/1	0.78	0.20	62,62,62,62	0
56	MG	2a	1806	1/1	0.78	0.11	76,76,76,76	0
56	MG	1A	3293	1/1	0.78	0.23	51,51,51,51	0
56	MG	1A	3361	1/1	0.78	0.37	57,57,57,57	0
56	MG	2A	3394	1/1	0.78	0.20	29,29,29,29	0
56	MG	1A	3044	1/1	0.78	0.16	37,37,37,37	0
56	MG	2A	3140	1/1	0.78	0.22	60,60,60,60	0
56	MG	2A	3175	1/1	0.78	0.36	43,43,43,43	0
56	MG	1A	3959	1/1	0.79	0.12	76,76,76,76	0
56	MG	2A	3088	1/1	0.79	0.15	40,40,40,40	0
56	MG	2A	3285	1/1	0.79	0.13	58,58,58,58	0
56	MG	1A	3794	1/1	0.79	0.18	18,18,18,18	0
56	MG	2a	1773	1/1	0.79	0.20	70,70,70,70	0
56	MG	1A	3882	1/1	0.79	0.14	62,62,62,62	0
56	MG	2B	3012	1/1	0.79	0.16	75,75,75,75	0
56	MG	2A	3244	1/1	0.79	0.18	47,47,47,47	0
56	MG	1A	3679	1/1	0.79	0.23	14,14,14,14	0
56	MG	2a	1714	1/1	0.79	0.28	68,68,68,68	0
56	MG	1D	301	1/1	0.79	0.28	44,44,44,44	0
56	MG	2v	3003	1/1	0.79	0.20	66,66,66,66	0
56	MG	1A	3459	1/1	0.79	0.20	53,53,53,53	0
56	MG	2y	3005	1/1	0.79	0.09	88,88,88,88	0
56	MG	2a	1799	1/1	0.80	0.12	59,59,59,59	0
56	MG	2G	3001	1/1	0.80	0.10	60,60,60,60	0
56	MG	2A	3093	1/1	0.80	0.13	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	2a	1705	1/1	0.80	0.13	54,54,54,54	0
56	MG	2A	3033	1/1	0.80	0.18	52,52,52,52	0
56	MG	1B	213	1/1	0.80	0.84	55,55,55,55	0
56	MG	2A	3160	1/1	0.80	0.17	47,47,47,47	0
56	MG	1a	3024	1/1	0.80	0.16	52,52,52,52	0
56	MG	2a	1617	1/1	0.80	0.15	73,73,73,73	0
56	MG	2B	3016	1/1	0.80	0.10	54,54,54,54	0
56	MG	1A	3593	1/1	0.80	0.12	30,30,30,30	0
56	MG	1e	201	1/1	0.80	0.38	59,59,59,59	0
56	MG	2x	103	1/1	0.80	0.22	63,63,63,63	0
56	MG	2A	3256	1/1	0.80	0.18	46,46,46,46	0
56	MG	2A	3560	1/1	0.80	0.08	50,50,50,50	0
56	MG	1a	3170	1/1	0.80	0.09	66,66,66,66	0
56	MG	1l	202	1/1	0.81	0.16	85,85,85,85	0
56	MG	2t	3001	1/1	0.81	0.09	53,53,53,53	0
56	MG	2a	1607	1/1	0.81	0.18	73,73,73,73	0
56	MG	27	101	1/1	0.81	0.34	44,44,44,44	0
56	MG	1A	3804	1/1	0.81	0.16	45,45,45,45	0
56	MG	1a	3162	1/1	0.81	0.22	62,62,62,62	0
56	MG	1B	212	1/1	0.81	0.29	46,46,46,46	0
56	MG	2E	305	1/1	0.81	0.14	51,51,51,51	0
56	MG	2A	3128	1/1	0.81	0.26	35,35,35,35	0
56	MG	2a	1662	1/1	0.81	0.11	59,59,59,59	0
56	MG	2a	1772	1/1	0.81	0.17	54,54,54,54	0
56	MG	1A	3408	1/1	0.81	0.30	40,40,40,40	0
56	MG	2A	3723	1/1	0.81	0.31	67,67,67,67	0
56	MG	2a	1603	1/1	0.81	0.17	73,73,73,73	0
56	MG	1a	3175	1/1	0.81	0.09	58,58,58,58	0
56	MG	2A	3046	1/1	0.81	0.15	58,58,58,58	0
56	MG	1a	3049	1/1	0.81	0.16	60,60,60,60	0
56	MG	2A	3536	1/1	0.81	0.14	54,54,54,54	0
56	MG	1Z	3002	1/1	0.81	0.15	46,46,46,46	0
56	MG	1A	3086	1/1	0.81	0.15	55,55,55,55	0
56	MG	1A	3844	1/1	0.81	0.08	23,23,23,23	0
56	MG	2A	3389	1/1	0.81	0.20	35,35,35,35	0
56	MG	28	101	1/1	0.81	0.20	49,49,49,49	0
56	MG	2a	1616	1/1	0.81	0.11	67,67,67,67	0
56	MG	2A	3261	1/1	0.81	0.20	50,50,50,50	0
56	MG	2A	3439	1/1	0.81	0.11	49,49,49,49	0
56	MG	2A	3701	1/1	0.81	0.11	50,50,50,50	0
56	MG	1A	3341	1/1	0.81	0.37	38,38,38,38	0
56	MG	1A	3760	1/1	0.81	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	3149	1/1	0.81	0.54	76,76,76,76	0
56	MG	2A	3058	1/1	0.81	0.20	65,65,65,65	0
56	MG	1A	3523	1/1	0.82	0.12	46,46,46,46	0
56	MG	1A	3230	1/1	0.82	0.19	44,44,44,44	0
56	MG	2A	3229	1/1	0.82	0.24	34,34,34,34	0
56	MG	1A	3367	1/1	0.82	0.22	46,46,46,46	0
56	MG	1B	232	1/1	0.82	0.14	66,66,66,66	0
56	MG	1A	3357	1/1	0.82	0.23	43,43,43,43	0
56	MG	2a	1667	1/1	0.82	0.17	61,61,61,61	0
56	MG	1A	3227	1/1	0.82	0.13	49,49,49,49	0
56	MG	16	103	1/1	0.82	0.53	56,56,56,56	0
56	MG	2A	3524	1/1	0.82	0.12	61,61,61,61	0
56	MG	2A	3196	1/1	0.82	0.19	53,53,53,53	0
56	MG	1A	3795	1/1	0.82	0.17	50,50,50,50	0
56	MG	2a	1651	1/1	0.82	0.08	60,60,60,60	0
56	MG	1A	3166	1/1	0.82	0.37	31,31,31,31	0
56	MG	1A	3914	1/1	0.82	0.21	54,54,54,54	0
56	MG	2A	3747	1/1	0.82	0.17	35,35,35,35	0
56	MG	1A	3363	1/1	0.82	0.17	32,32,32,32	0
56	MG	2a	1738	1/1	0.82	0.12	71,71,71,71	0
56	MG	1a	3069	1/1	0.82	0.15	59,59,59,59	0
56	MG	1A	3248	1/1	0.82	0.14	49,49,49,49	0
56	MG	2a	1829	1/1	0.82	0.30	68,68,68,68	0
56	MG	2A	3558	1/1	0.82	0.28	50,50,50,50	0
56	MG	1V	202	1/1	0.82	0.42	44,44,44,44	0
56	MG	1A	3789	1/1	0.82	0.21	44,44,44,44	0
56	MG	1A	4048	1/1	0.82	0.64	31,31,31,31	0
56	MG	2A	3687	1/1	0.82	0.29	65,65,65,65	0
56	MG	2A	3447	1/1	0.82	0.22	27,27,27,27	0
56	MG	1a	3154	1/1	0.82	0.10	59,59,59,59	0
56	MG	1a	3006	1/1	0.82	0.20	59,59,59,59	0
56	MG	1A	3423	1/1	0.83	0.17	38,38,38,38	0
56	MG	2a	1681	1/1	0.83	0.22	69,69,69,69	0
56	MG	2A	3257	1/1	0.83	0.18	57,57,57,57	0
56	MG	2a	1648	1/1	0.83	0.23	63,63,63,63	0
56	MG	2a	1609	1/1	0.83	0.12	57,57,57,57	0
56	MG	1v	3001	1/1	0.83	0.11	72,72,72,72	0
56	MG	2a	1694	1/1	0.83	0.27	66,66,66,66	0
56	MG	1a	3026	1/1	0.83	0.11	72,72,72,72	0
56	MG	1A	3299	1/1	0.83	0.35	28,28,28,28	0
56	MG	2A	3065	1/1	0.83	0.16	52,52,52,52	0
56	MG	2a	1613	1/1	0.83	0.15	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	3308	1/1	0.83	0.16	49,49,49,49	0
56	MG	2A	3158	1/1	0.83	0.32	49,49,49,49	0
56	MG	1A	3935	1/1	0.83	0.15	43,43,43,43	0
56	MG	1A	3315	1/1	0.83	0.25	37,37,37,37	0
56	MG	1A	3801	1/1	0.83	0.25	71,71,71,71	0
56	MG	1A	4041	1/1	0.83	0.54	35,35,35,35	0
56	MG	2B	3014	1/1	0.83	0.31	71,71,71,71	0
56	MG	2A	3638	1/1	0.83	0.16	66,66,66,66	0
56	MG	1a	3018	1/1	0.83	0.29	55,55,55,55	0
56	MG	2a	1636	1/1	0.83	0.09	66,66,66,66	0
56	MG	2j	8001	1/1	0.83	0.11	66,66,66,66	0
56	MG	1A	3904	1/1	0.83	0.15	71,71,71,71	0
56	MG	2A	3653	1/1	0.83	0.22	37,37,37,37	0
56	MG	2A	3436	1/1	0.83	0.14	62,62,62,62	0
56	MG	2A	3225	1/1	0.83	0.18	53,53,53,53	0
56	MG	2a	1647	1/1	0.84	0.13	80,80,80,80	0
56	MG	1A	3781	1/1	0.84	0.19	51,51,51,51	0
56	MG	2A	3205	1/1	0.84	0.15	55,55,55,55	0
56	MG	2A	3425	1/1	0.84	0.11	59,59,59,59	0
56	MG	1B	210	1/1	0.84	0.15	50,50,50,50	0
56	MG	1A	3672	1/1	0.84	0.22	68,68,68,68	0
56	MG	2T	3001	1/1	0.84	0.26	52,52,52,52	0
56	MG	2A	3087	1/1	0.84	0.08	59,59,59,59	0
56	MG	2a	1722	1/1	0.84	0.18	79,79,79,79	0
56	MG	1w	111	1/1	0.84	0.13	69,69,69,69	0
56	MG	1a	3046	1/1	0.84	0.09	54,54,54,54	0
56	MG	2A	3672	1/1	0.84	0.26	46,46,46,46	0
56	MG	1A	3350	1/1	0.84	0.31	44,44,44,44	0
56	MG	1A	3246	1/1	0.84	0.13	37,37,37,37	0
56	MG	2A	3263	1/1	0.84	0.19	54,54,54,54	0
56	MG	2a	1697	1/1	0.84	0.10	64,64,64,64	0
56	MG	2A	3133	1/1	0.84	0.27	44,44,44,44	0
56	MG	2A	3443	1/1	0.84	0.14	34,34,34,34	0
56	MG	1N	204	1/1	0.84	0.60	46,46,46,46	0
56	MG	2a	1736	1/1	0.84	0.11	82,82,82,82	0
56	MG	2a	1663	1/1	0.84	0.13	48,48,48,48	0
56	MG	1A	3931	1/1	0.84	0.22	47,47,47,47	0
56	MG	2A	3621	1/1	0.84	0.09	49,49,49,49	0
56	MG	1y	103	1/1	0.84	0.26	82,82,82,82	0
56	MG	2a	1788	1/1	0.84	0.12	55,55,55,55	0
56	MG	2a	1802	1/1	0.84	0.23	69,69,69,69	0
56	MG	2a	1604	1/1	0.84	0.16	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3296	1/1	0.84	0.40	54,54,54,54	0
56	MG	2A	3329	1/1	0.84	0.22	46,46,46,46	0
56	MG	1A	3065	1/1	0.84	0.39	62,62,62,62	0
56	MG	2x	104	1/1	0.84	0.13	64,64,64,64	0
56	MG	2a	1751	1/1	0.84	0.12	87,87,87,87	0
56	MG	2q	203	1/1	0.84	0.20	75,75,75,75	0
56	MG	2A	3312	1/1	0.84	0.17	57,57,57,57	0
56	MG	2F	302	1/1	0.84	0.13	50,50,50,50	0
56	MG	1a	3083	1/1	0.85	0.19	54,54,54,54	0
56	MG	1a	3168	1/1	0.85	0.15	63,63,63,63	0
56	MG	1A	3143	1/1	0.85	0.47	37,37,37,37	0
56	MG	1A	3083	1/1	0.85	0.26	55,55,55,55	0
56	MG	1a	3084	1/1	0.85	0.28	54,54,54,54	0
56	MG	1a	3205	1/1	0.85	0.11	69,69,69,69	0
56	MG	2F	304	1/1	0.85	0.10	64,64,64,64	0
56	MG	1A	3960	1/1	0.85	0.23	51,51,51,51	0
56	MG	1a	3014	1/1	0.85	0.39	55,55,55,55	0
56	MG	2a	1605	1/1	0.85	0.13	61,61,61,61	0
56	MG	2a	1615	1/1	0.85	0.22	54,54,54,54	0
56	MG	1A	3137	1/1	0.85	0.42	40,40,40,40	0
56	MG	2U	203	1/1	0.85	0.41	55,55,55,55	0
56	MG	2a	1792	1/1	0.85	0.09	61,61,61,61	0
56	MG	1A	3207	1/1	0.85	0.28	52,52,52,52	0
56	MG	2B	3003	1/1	0.85	0.21	60,60,60,60	0
56	MG	1A	3984	1/1	0.85	0.11	52,52,52,52	0
56	MG	1A	3895	1/1	0.85	0.15	71,71,71,71	0
56	MG	2A	3293	1/1	0.85	0.28	46,46,46,46	0
56	MG	2A	3497	1/1	0.85	0.18	63,63,63,63	0
56	MG	1a	3177	1/1	0.85	0.15	57,57,57,57	0
56	MG	2a	1815	1/1	0.85	0.16	61,61,61,61	0
56	MG	2A	3094	1/1	0.85	0.16	47,47,47,47	0
56	MG	1w	103	1/1	0.85	0.37	68,68,68,68	0
56	MG	2A	3501	1/1	0.85	0.19	53,53,53,53	0
56	MG	1A	3316	1/1	0.85	0.41	34,34,34,34	0
56	MG	2O	8001	1/1	0.85	0.20	56,56,56,56	0
56	MG	2A	3311	1/1	0.85	0.23	50,50,50,50	0
56	MG	1a	3206	1/1	0.85	0.18	51,51,51,51	0
56	MG	2A	3076	1/1	0.85	0.13	45,45,45,45	0
56	MG	2A	3714	1/1	0.85	0.14	50,50,50,50	0
56	MG	2a	1822	1/1	0.85	0.22	52,52,52,52	0
56	MG	2A	3356	1/1	0.85	0.08	42,42,42,42	0
56	MG	2a	1631	1/1	0.85	0.09	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	2a	1791	1/1	0.85	0.12	69,69,69,69	0
56	MG	1x	109	1/1	0.85	0.11	57,57,57,57	0
56	MG	2A	3185	1/1	0.85	0.19	46,46,46,46	0
56	MG	1x	103	1/1	0.85	0.27	54,54,54,54	0
56	MG	2a	1784	1/1	0.85	0.11	66,66,66,66	0
56	MG	2A	3472	1/1	0.85	0.23	42,42,42,42	0
56	MG	1w	108	1/1	0.85	0.16	66,66,66,66	0
56	MG	1A	3640	1/1	0.85	0.16	36,36,36,36	0
56	MG	2D	304	1/1	0.85	0.14	53,53,53,53	0
56	MG	2A	3267	1/1	0.85	0.20	52,52,52,52	0
56	MG	1a	3061	1/1	0.85	0.14	56,56,56,56	0
56	MG	1A	3680	1/1	0.85	0.30	36,36,36,36	0
56	MG	1a	3089	1/1	0.85	0.15	40,40,40,40	0
56	MG	2B	3019	1/1	0.85	0.30	82,82,82,82	0
56	MG	2A	3571	1/1	0.85	0.10	57,57,57,57	0
56	MG	1A	3644	1/1	0.85	0.14	12,12,12,12	0
56	MG	1A	3903	1/1	0.86	0.11	23,23,23,23	0
56	MG	1A	3621	1/1	0.86	0.17	44,44,44,44	0
56	MG	2a	1755	1/1	0.86	0.06	70,70,70,70	0
56	MG	1A	3592	1/1	0.86	0.13	30,30,30,30	0
56	MG	1A	4016	1/1	0.86	0.11	55,55,55,55	0
56	MG	1A	3718	1/1	0.86	0.20	39,39,39,39	0
56	MG	2a	1602	1/1	0.86	0.21	54,54,54,54	0
56	MG	1A	3057	1/1	0.86	0.26	45,45,45,45	0
56	MG	2a	1724	1/1	0.86	0.11	73,73,73,73	0
56	MG	1A	3939	1/1	0.86	0.15	44,44,44,44	0
56	MG	15	107	1/1	0.86	0.21	45,45,45,45	0
56	MG	2A	3002	1/1	0.86	0.13	61,61,61,61	0
56	MG	1A	3590	1/1	0.86	0.22	36,36,36,36	0
56	MG	1A	3480	1/1	0.86	0.64	35,35,35,35	0
56	MG	2a	1732	1/1	0.86	0.11	56,56,56,56	0
56	MG	1Q	204	1/1	0.86	0.17	41,41,41,41	0
56	MG	2A	3468	1/1	0.86	0.11	40,40,40,40	0
56	MG	1A	3416	1/1	0.86	0.15	17,17,17,17	0
56	MG	2a	1612	1/1	0.86	0.11	58,58,58,58	0
56	MG	1a	3161	1/1	0.86	0.08	53,53,53,53	0
56	MG	2A	3650	1/1	0.86	0.09	52,52,52,52	0
56	MG	1A	3951	1/1	0.86	0.12	62,62,62,62	0
56	MG	1A	3691	1/1	0.86	0.30	55,55,55,55	0
56	MG	2A	3220	1/1	0.86	0.13	49,49,49,49	0
56	MG	2A	3083	1/1	0.86	0.10	53,53,53,53	0
56	MG	1A	3455	1/1	0.86	0.51	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3514	1/1	0.86	0.22	56,56,56,56	0
56	MG	2A	3618	1/1	0.86	0.18	71,71,71,71	0
56	MG	1a	3064	1/1	0.86	0.21	54,54,54,54	0
56	MG	1A	3047	1/1	0.86	0.14	50,50,50,50	0
56	MG	2a	1752	1/1	0.86	0.16	62,62,62,62	0
56	MG	1p	101	1/1	0.86	0.24	55,55,55,55	0
56	MG	2w	102	1/1	0.86	0.14	78,78,78,78	0
56	MG	2a	1666	1/1	0.86	0.10	51,51,51,51	0
56	MG	2A	3208	1/1	0.86	0.23	49,49,49,49	0
56	MG	2g	8001	1/1	0.86	0.15	59,59,59,59	0
56	MG	2A	3616	1/1	0.86	0.12	51,51,51,51	0
56	MG	2x	101	1/1	0.86	0.12	52,52,52,52	0
56	MG	2A	3738	1/1	0.86	0.17	63,63,63,63	0
56	MG	1S	3003	1/1	0.86	0.21	61,61,61,61	0
56	MG	2A	3539	1/1	0.86	0.10	59,59,59,59	0
56	MG	2A	3281	1/1	0.86	0.09	60,60,60,60	0
56	MG	2A	3277	1/1	0.86	0.37	54,54,54,54	0
56	MG	2a	1661	1/1	0.86	0.11	63,63,63,63	0
56	MG	2A	3231	1/1	0.86	0.31	49,49,49,49	0
56	MG	1A	3465	1/1	0.86	0.20	55,55,55,55	0
56	MG	2A	3544	1/1	0.86	0.24	30,30,30,30	0
56	MG	2B	3008	1/1	0.86	0.30	59,59,59,59	0
56	MG	1S	3001	1/1	0.86	0.18	47,47,47,47	0
56	MG	2A	3604	1/1	0.86	0.10	58,58,58,58	0
56	MG	2A	3676	1/1	0.86	0.13	79,79,79,79	0
56	MG	2A	3542	1/1	0.86	0.13	36,36,36,36	0
56	MG	2Z	8001	1/1	0.86	0.26	73,73,73,73	0
56	MG	2A	3546	1/1	0.87	0.15	45,45,45,45	0
56	MG	1a	3038	1/1	0.87	0.20	55,55,55,55	0
56	MG	1A	3513	1/1	0.87	0.16	29,29,29,29	0
56	MG	2B	3009	1/1	0.87	0.14	63,63,63,63	0
56	MG	1A	3832	1/1	0.87	0.13	69,69,69,69	0
56	MG	2A	3307	1/1	0.87	0.14	35,35,35,35	0
56	MG	1A	4012	1/1	0.87	0.26	47,47,47,47	0
56	MG	2A	3156	1/1	0.87	0.18	42,42,42,42	0
56	MG	2A	3730	1/1	0.87	0.35	32,32,32,32	0
56	MG	1A	3277	1/1	0.87	0.13	37,37,37,37	0
56	MG	1A	4053	1/1	0.87	0.45	42,42,42,42	0
56	MG	2A	3082	1/1	0.87	0.18	69,69,69,69	0
56	MG	1A	3169	1/1	0.87	0.13	53,53,53,53	0
56	MG	2A	3612	1/1	0.87	0.20	65,65,65,65	0
56	MG	1w	101	1/1	0.87	0.30	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3053	1/1	0.87	0.14	30,30,30,30	0
56	MG	2A	3131	1/1	0.87	0.13	40,40,40,40	0
56	MG	2A	3568	1/1	0.87	0.16	47,47,47,47	0
56	MG	1A	3052	1/1	0.87	0.14	31,31,31,31	0
56	MG	2B	3010	1/1	0.87	0.11	64,64,64,64	0
56	MG	1A	3792	1/1	0.87	0.18	19,19,19,19	0
56	MG	1A	3780	1/1	0.87	0.23	44,44,44,44	0
56	MG	1A	3516	1/1	0.87	0.13	30,30,30,30	0
56	MG	2A	3102	1/1	0.87	0.37	44,44,44,44	0
56	MG	1A	3198	1/1	0.87	0.12	43,43,43,43	0
56	MG	1A	3965	1/1	0.87	0.16	63,63,63,63	0
56	MG	1A	3346	1/1	0.87	0.18	43,43,43,43	0
56	MG	2A	3286	1/1	0.87	0.17	46,46,46,46	0
56	MG	2A	3426	1/1	0.87	0.18	48,48,48,48	0
56	MG	1a	3207	1/1	0.87	0.09	41,41,41,41	0
56	MG	1A	3002	1/1	0.87	0.18	46,46,46,46	0
56	MG	1A	3741	1/1	0.87	0.11	40,40,40,40	0
56	MG	2a	1645	1/1	0.87	0.61	74,74,74,74	0
56	MG	1a	3165	1/1	0.87	0.09	60,60,60,60	0
56	MG	2A	3188	1/1	0.87	0.12	57,57,57,57	0
56	MG	1A	3106	1/1	0.87	0.54	24,24,24,24	0
56	MG	1A	3980	1/1	0.87	0.21	62,62,62,62	0
56	MG	2A	3021	1/1	0.87	0.32	58,58,58,58	0
56	MG	2A	3322	1/1	0.87	0.37	55,55,55,55	0
56	MG	1a	3130	1/1	0.87	0.14	46,46,46,46	0
56	MG	1a	3186	1/1	0.87	0.19	48,48,48,48	0
56	MG	1B	220	1/1	0.87	0.14	57,57,57,57	0
56	MG	2A	3349	1/1	0.87	0.17	30,30,30,30	0
56	MG	1D	307	1/1	0.87	0.17	39,39,39,39	0
56	MG	2A	3715	1/1	0.87	0.09	56,56,56,56	0
56	MG	1A	3989	1/1	0.87	0.10	49,49,49,49	0
56	MG	2Q	3003	1/1	0.87	0.64	52,52,52,52	0
56	MG	2A	3186	1/1	0.87	0.15	51,51,51,51	0
56	MG	2a	1808	1/1	0.87	0.19	58,58,58,58	0
56	MG	2a	1620	1/1	0.87	0.21	64,64,64,64	0
56	MG	1A	3313	1/1	0.87	0.39	35,35,35,35	0
56	MG	1a	3180	1/1	0.87	0.10	62,62,62,62	0
56	MG	2a	1745	1/1	0.87	0.13	64,64,64,64	0
56	MG	2A	3689	1/1	0.87	0.13	56,56,56,56	0
56	MG	1E	308	1/1	0.87	0.17	28,28,28,28	0
56	MG	2A	3193	1/1	0.88	0.12	51,51,51,51	0
56	MG	1A	3373	1/1	0.88	0.12	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	1797	1/1	0.88	0.13	70,70,70,70	0
56	MG	2A	3744	1/1	0.88	0.10	40,40,40,40	0
56	MG	2a	1671	1/1	0.88	0.16	58,58,58,58	0
56	MG	1A	3398	1/1	0.88	0.12	37,37,37,37	0
56	MG	2A	3115	1/1	0.88	0.18	39,39,39,39	0
56	MG	1a	3050	1/1	0.88	0.12	50,50,50,50	0
56	MG	1A	3085	1/1	0.88	0.14	13,13,13,13	0
56	MG	1A	3133	1/1	0.88	0.22	43,43,43,43	0
56	MG	1a	3020	1/1	0.88	0.09	47,47,47,47	0
56	MG	1A	3527	1/1	0.88	0.24	66,66,66,66	0
56	MG	1A	3461	1/1	0.88	0.18	55,55,55,55	0
56	MG	1a	3073	1/1	0.88	0.12	59,59,59,59	0
56	MG	20	3001	1/1	0.88	0.15	52,52,52,52	0
56	MG	21	3001	1/1	0.88	0.54	36,36,36,36	0
56	MG	1A	3309	1/1	0.88	0.14	32,32,32,32	0
56	MG	1A	3843	1/1	0.88	0.10	66,66,66,66	0
56	MG	2A	3045	1/1	0.88	0.14	55,55,55,55	0
56	MG	1A	4065	1/1	0.88	0.12	36,36,36,36	0
56	MG	2A	3606	1/1	0.88	0.12	49,49,49,49	0
56	MG	2A	3202	1/1	0.88	0.14	56,56,56,56	0
56	MG	1A	3368	1/1	0.88	0.39	39,39,39,39	0
56	MG	2A	3213	1/1	0.88	0.11	50,50,50,50	0
56	MG	2A	3117	1/1	0.88	0.21	61,61,61,61	0
56	MG	1A	3297	1/1	0.88	0.13	35,35,35,35	0
56	MG	1A	3425	1/1	0.88	0.14	34,34,34,34	0
56	MG	1A	3549	1/1	0.88	0.11	30,30,30,30	0
56	MG	2A	3433	1/1	0.88	0.19	60,60,60,60	0
56	MG	2w	105	1/1	0.88	0.14	72,72,72,72	0
56	MG	2A	3166	1/1	0.88	0.13	47,47,47,47	0
56	MG	1A	3730	1/1	0.88	0.35	42,42,42,42	0
56	MG	2A	3690	1/1	0.88	0.14	58,58,58,58	0
56	MG	1A	3881	1/1	0.88	0.11	44,44,44,44	0
56	MG	2A	3280	1/1	0.88	0.47	50,50,50,50	0
56	MG	2A	3249	1/1	0.88	0.14	54,54,54,54	0
56	MG	1A	3779	1/1	0.88	0.10	50,50,50,50	0
56	MG	2A	3520	1/1	0.88	0.10	52,52,52,52	0
56	MG	2A	3052	1/1	0.88	0.14	36,36,36,36	0
56	MG	2A	3360	1/1	0.88	0.13	25,25,25,25	0
56	MG	1a	3096	1/1	0.88	0.18	47,47,47,47	0
56	MG	1A	4027	1/1	0.88	0.30	61,61,61,61	0
56	MG	2A	3241	1/1	0.88	0.18	55,55,55,55	0
56	MG	2D	307	1/1	0.88	0.27	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	3506	1/1	0.88	0.09	24,24,24,24	0
56	MG	1A	3283	1/1	0.88	0.33	28,28,28,28	0
56	MG	2y	3007	1/1	0.88	0.14	81,81,81,81	0
56	MG	1t	3001	1/1	0.88	0.20	57,57,57,57	0
56	MG	2A	3737	1/1	0.88	0.26	42,42,42,42	0
56	MG	2A	3071	1/1	0.88	0.08	60,60,60,60	0
56	MG	2A	3321	1/1	0.88	0.21	44,44,44,44	0
56	MG	1A	3967	1/1	0.88	0.27	53,53,53,53	0
56	MG	1A	3282	1/1	0.88	0.21	56,56,56,56	0
56	MG	1E	306	1/1	0.88	0.12	38,38,38,38	0
56	MG	1A	3294	1/1	0.88	0.21	40,40,40,40	0
56	MG	2v	3004	1/1	0.88	0.19	73,73,73,73	0
56	MG	1a	3017	1/1	0.88	0.20	57,57,57,57	0
56	MG	2a	1713	1/1	0.88	0.13	48,48,48,48	0
56	MG	1A	3916	1/1	0.88	0.13	54,54,54,54	0
56	MG	2A	3492	1/1	0.88	0.22	49,49,49,49	0
56	MG	16	101	1/1	0.88	0.17	35,35,35,35	0
56	MG	1x	101	1/1	0.88	0.19	54,54,54,54	0
56	MG	1a	3059	1/1	0.88	0.09	61,61,61,61	0
56	MG	1l	102	1/1	0.88	0.21	72,72,72,72	0
56	MG	2A	3515	1/1	0.88	0.19	44,44,44,44	0
56	MG	1A	3761	1/1	0.88	0.14	48,48,48,48	0
56	MG	2E	307	1/1	0.88	0.20	60,60,60,60	0
56	MG	2A	3376	1/1	0.88	0.17	45,45,45,45	0
56	MG	1A	3944	1/1	0.88	0.13	39,39,39,39	0
56	MG	1A	3321	1/1	0.88	0.41	45,45,45,45	0
56	MG	2A	3441	1/1	0.88	0.14	62,62,62,62	0
56	MG	2a	1610	1/1	0.88	0.81	63,63,63,63	0
56	MG	1A	3135	1/1	0.88	0.27	23,23,23,23	0
56	MG	2a	1639	1/1	0.88	0.21	60,60,60,60	0
56	MG	2A	3174	1/1	0.88	0.24	47,47,47,47	0
56	MG	2a	1770	1/1	0.89	0.17	59,59,59,59	0
56	MG	20	3002	1/1	0.89	0.07	52,52,52,52	0
56	MG	2A	3659	1/1	0.89	0.18	41,41,41,41	0
56	MG	2A	3753	1/1	0.89	0.55	52,52,52,52	0
56	MG	1F	306	1/1	0.89	0.18	36,36,36,36	0
56	MG	1A	3094	1/1	0.89	0.13	56,56,56,56	0
56	MG	2A	3207	1/1	0.89	0.28	40,40,40,40	0
56	MG	1A	3306	1/1	0.89	0.15	43,43,43,43	0
56	MG	2a	1719	1/1	0.89	0.14	55,55,55,55	0
56	MG	2A	3048	1/1	0.89	0.12	57,57,57,57	0
56	MG	1A	3473	1/1	0.89	0.18	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	2a	1701	1/1	0.89	0.10	72,72,72,72	0
56	MG	2A	3223	1/1	0.89	0.13	45,45,45,45	0
56	MG	1A	3759	1/1	0.89	0.13	32,32,32,32	0
56	MG	2a	1800	1/1	0.89	0.23	61,61,61,61	0
56	MG	2q	202	1/1	0.89	0.24	59,59,59,59	0
56	MG	1A	3333	1/1	0.89	0.51	43,43,43,43	0
56	MG	1A	3584	1/1	0.89	0.14	44,44,44,44	0
56	MG	2A	3194	1/1	0.89	0.21	51,51,51,51	0
56	MG	2a	1641	1/1	0.89	0.13	53,53,53,53	0
56	MG	13	102	1/1	0.89	0.13	46,46,46,46	0
56	MG	2A	3682	1/1	0.89	0.13	61,61,61,61	0
56	MG	2B	3001	1/1	0.89	0.55	75,75,75,75	0
56	MG	2A	3547	1/1	0.89	0.25	47,47,47,47	0
56	MG	1a	3027	1/1	0.89	0.24	58,58,58,58	0
56	MG	1w	106	1/1	0.89	0.10	70,70,70,70	0
56	MG	1A	3566	1/1	0.89	0.17	62,62,62,62	0
56	MG	1A	3713	1/1	0.89	0.11	48,48,48,48	0
56	MG	2A	3396	1/1	0.89	0.14	29,29,29,29	0
56	MG	2A	3086	1/1	0.89	0.14	62,62,62,62	0
56	MG	2A	3049	1/1	0.89	0.12	53,53,53,53	0
56	MG	1A	3104	1/1	0.89	0.22	45,45,45,45	0
56	MG	1A	3263	1/1	0.89	0.09	48,48,48,48	0
56	MG	1A	3427	1/1	0.89	0.67	29,29,29,29	0
56	MG	2A	3545	1/1	0.89	0.18	45,45,45,45	0
56	MG	1A	3197	1/1	0.89	0.13	32,32,32,32	0
56	MG	1A	3997	1/1	0.89	0.20	45,45,45,45	0
56	MG	1A	3548	1/1	0.89	0.14	52,52,52,52	0
56	MG	1A	3796	1/1	0.89	0.17	33,33,33,33	0
56	MG	2l	202	1/1	0.89	0.43	66,66,66,66	0
56	MG	1N	202	1/1	0.89	0.13	36,36,36,36	0
56	MG	10	105	1/1	0.89	0.10	50,50,50,50	0
56	MG	1P	203	1/1	0.89	0.42	33,33,33,33	0
56	MG	1A	3947	1/1	0.89	0.14	49,49,49,49	0
56	MG	2A	3044	1/1	0.89	0.08	61,61,61,61	0
56	MG	2a	1626	1/1	0.89	0.08	50,50,50,50	0
56	MG	1A	3711	1/1	0.89	0.15	44,44,44,44	0
56	MG	2A	3507	1/1	0.89	0.10	67,67,67,67	0
56	MG	1B	226	1/1	0.89	0.14	67,67,67,67	0
56	MG	1A	3355	1/1	0.89	0.49	30,30,30,30	0
56	MG	2A	3666	1/1	0.89	0.14	46,46,46,46	0
56	MG	2A	3228	1/1	0.89	0.38	38,38,38,38	0
56	MG	1a	3003	1/1	0.89	0.20	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3592	1/1	0.89	0.12	43,43,43,43	0
56	MG	2a	1826	1/1	0.89	0.12	55,55,55,55	0
56	MG	2a	1824	1/1	0.89	0.18	63,63,63,63	0
56	MG	2A	3338	1/1	0.89	0.26	42,42,42,42	0
56	MG	1B	229	1/1	0.89	0.09	57,57,57,57	0
56	MG	1a	3044	1/1	0.89	0.15	46,46,46,46	0
56	MG	2A	3530	1/1	0.89	0.16	64,64,64,64	0
56	MG	1A	3018	1/1	0.89	0.14	43,43,43,43	0
56	MG	25	504	1/1	0.89	0.36	67,67,67,67	0
56	MG	1A	4047	1/1	0.89	0.39	29,29,29,29	0
56	MG	2a	1708	1/1	0.89	0.14	61,61,61,61	0
56	MG	1A	3697	1/1	0.89	0.20	27,27,27,27	0
56	MG	1A	3339	1/1	0.89	0.26	48,48,48,48	0
56	MG	1a	3192	1/1	0.89	0.09	62,62,62,62	0
56	MG	2A	3015	1/1	0.89	0.15	37,37,37,37	0
56	MG	1A	3317	1/1	0.89	0.47	45,45,45,45	0
56	MG	1A	3586	1/1	0.89	0.19	17,17,17,17	0
56	MG	1A	3735	1/1	0.89	0.14	22,22,22,22	0
56	MG	2A	3067	1/1	0.89	0.22	46,46,46,46	0
56	MG	2A	3731	1/1	0.89	0.11	37,37,37,37	0
56	MG	1A	3609	1/1	0.89	0.08	61,61,61,61	0
56	MG	1O	205	1/1	0.89	0.38	57,57,57,57	0
56	MG	2a	1642	1/1	0.89	0.21	55,55,55,55	0
56	MG	2a	1748	1/1	0.89	0.14	60,60,60,60	0
56	MG	2A	3518	1/1	0.89	0.13	45,45,45,45	0
56	MG	2a	1621	1/1	0.89	0.55	65,65,65,65	0
56	MG	1A	4009	1/1	0.89	0.22	41,41,41,41	0
56	MG	1A	3823	1/1	0.89	0.13	50,50,50,50	0
56	MG	2a	1650	1/1	0.89	0.16	68,68,68,68	0
56	MG	1A	3430	1/1	0.89	0.66	40,40,40,40	0
56	MG	1A	3439	1/1	0.89	0.31	37,37,37,37	0
56	MG	2A	3024	1/1	0.89	0.20	50,50,50,50	0
56	MG	1A	3054	1/1	0.89	0.12	26,26,26,26	0
56	MG	1A	3456	1/1	0.89	0.41	33,33,33,33	0
56	MG	1A	3828	1/1	0.89	0.19	62,62,62,62	0
56	MG	1A	3432	1/1	0.89	0.15	31,31,31,31	0
56	MG	1A	3415	1/1	0.89	0.45	38,38,38,38	0
56	MG	2B	3018	1/1	0.89	0.86	80,80,80,80	0
56	MG	1x	114	1/1	0.89	0.14	67,67,67,67	0
56	MG	1O	207	1/1	0.89	0.10	54,54,54,54	0
56	MG	2A	3695	1/1	0.89	0.25	58,58,58,58	0
56	MG	2a	1633	1/1	0.89	0.11	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	2A	3001	1/1	0.89	0.09	44,44,44,44	0
56	MG	1A	3356	1/1	0.89	0.19	48,48,48,48	0
56	MG	1A	3568	1/1	0.89	0.10	30,30,30,30	0
56	MG	2A	3434	1/1	0.90	0.16	46,46,46,46	0
56	MG	1a	3143	1/1	0.90	0.08	74,74,74,74	0
56	MG	2A	3529	1/1	0.90	0.24	59,59,59,59	0
56	MG	1A	4015	1/1	0.90	0.19	55,55,55,55	0
56	MG	2A	3092	1/1	0.90	0.17	38,38,38,38	0
56	MG	1a	3047	1/1	0.90	0.28	46,46,46,46	0
56	MG	1B	209	1/1	0.90	0.09	53,53,53,53	0
56	MG	25	503	1/1	0.90	0.41	40,40,40,40	0
56	MG	1A	3990	1/1	0.90	0.08	38,38,38,38	0
56	MG	1A	3027	1/1	0.90	0.35	27,27,27,27	0
56	MG	2A	3480	1/1	0.90	0.21	47,47,47,47	0
56	MG	2a	1674	1/1	0.90	0.20	55,55,55,55	0
56	MG	1A	4060	1/1	0.90	0.62	19,19,19,19	0
56	MG	2A	3656	1/1	0.90	0.08	68,68,68,68	0
56	MG	1A	3108	1/1	0.90	0.15	25,25,25,25	0
56	MG	1A	3746	1/1	0.90	0.31	49,49,49,49	0
56	MG	10	104	1/1	0.90	0.12	49,49,49,49	0
56	MG	1A	3171	1/1	0.90	0.24	29,29,29,29	0
56	MG	2a	1820	1/1	0.90	0.21	60,60,60,60	0
56	MG	1E	313	1/1	0.90	0.10	25,25,25,25	0
56	MG	2A	3735	1/1	0.90	0.35	45,45,45,45	0
56	MG	1A	3203	1/1	0.90	0.16	27,27,27,27	0
56	MG	2U	202	1/1	0.90	0.82	55,55,55,55	0
56	MG	1a	3043	1/1	0.90	0.12	50,50,50,50	0
56	MG	2A	3366	1/1	0.90	0.14	67,67,67,67	0
56	MG	1A	3671	1/1	0.90	0.09	14,14,14,14	0
56	MG	1a	3101	1/1	0.90	0.15	42,42,42,42	0
56	MG	2A	3532	1/1	0.90	0.18	62,62,62,62	0
56	MG	2A	3073	1/1	0.90	0.16	38,38,38,38	0
56	MG	1A	3797	1/1	0.90	0.18	33,33,33,33	0
56	MG	2A	3167	1/1	0.90	0.14	42,42,42,42	0
56	MG	1A	3296	1/1	0.90	0.12	37,37,37,37	0
56	MG	2F	303	1/1	0.90	0.88	55,55,55,55	0
56	MG	2A	3354	1/1	0.90	0.14	53,53,53,53	0
56	MG	1A	3815	1/1	0.90	0.08	35,35,35,35	0
56	MG	1A	3998	1/1	0.90	0.13	55,55,55,55	0
56	MG	2w	101	1/1	0.90	0.18	65,65,65,65	0
56	MG	1A	3117	1/1	0.90	0.16	48,48,48,48	0
56	MG	2a	1742	1/1	0.90	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	3271	1/1	0.90	0.14	53,53,53,53	0
56	MG	2a	1762	1/1	0.90	0.13	52,52,52,52	0
56	MG	1A	3839	1/1	0.90	0.14	34,34,34,34	0
56	MG	2A	3183	1/1	0.90	0.20	38,38,38,38	0
56	MG	1A	3314	1/1	0.90	0.34	42,42,42,42	0
56	MG	2B	3017	1/1	0.90	0.20	61,61,61,61	0
56	MG	1A	3803	1/1	0.90	0.34	41,41,41,41	0
56	MG	2A	3252	1/1	0.90	0.16	38,38,38,38	0
56	MG	1x	115	1/1	0.90	0.12	50,50,50,50	0
56	MG	2a	1704	1/1	0.90	0.18	52,52,52,52	0
56	MG	2A	3302	1/1	0.90	0.24	43,43,43,43	0
56	MG	1F	308	1/1	0.90	0.11	42,42,42,42	0
56	MG	2A	3484	1/1	0.90	0.11	70,70,70,70	0
56	MG	2A	3688	1/1	0.90	0.14	57,57,57,57	0
56	MG	2A	3692	1/1	0.90	0.07	52,52,52,52	0
56	MG	1a	3048	1/1	0.90	0.47	43,43,43,43	0
56	MG	2A	3400	1/1	0.90	0.25	72,72,72,72	0
56	MG	1w	102	1/1	0.90	0.10	76,76,76,76	0
56	MG	1A	3170	1/1	0.90	0.08	63,63,63,63	0
56	MG	1A	3453	1/1	0.90	0.38	41,41,41,41	0
56	MG	1A	3534	1/1	0.90	0.13	39,39,39,39	0
56	MG	1a	3030	1/1	0.90	0.18	43,43,43,43	0
56	MG	1a	3109	1/1	0.90	0.17	30,30,30,30	0
56	MG	2A	3035	1/1	0.90	0.15	52,52,52,52	0
56	MG	1A	3531	1/1	0.90	0.13	19,19,19,19	0
56	MG	2A	3582	1/1	0.90	0.15	44,44,44,44	0
56	MG	1a	3076	1/1	0.90	0.17	48,48,48,48	0
56	MG	1A	3411	1/1	0.90	0.12	45,45,45,45	0
56	MG	1A	4006	1/1	0.90	0.20	41,41,41,41	0
56	MG	1A	3721	1/1	0.90	0.26	53,53,53,53	0
56	MG	2A	3177	1/1	0.90	0.31	36,36,36,36	0
56	MG	2E	303	1/1	0.90	0.18	50,50,50,50	0
56	MG	2A	3218	1/1	0.90	0.14	39,39,39,39	0
56	MG	2A	3232	1/1	0.90	0.12	54,54,54,54	0
56	MG	1x	110	1/1	0.90	0.12	59,59,59,59	0
56	MG	1B	231	1/1	0.90	0.24	59,59,59,59	0
56	MG	2T	3002	1/1	0.90	0.25	59,59,59,59	0
56	MG	2A	3375	1/1	0.90	0.11	36,36,36,36	0
56	MG	2A	3318	1/1	0.90	0.34	42,42,42,42	0
56	MG	2A	3429	1/1	0.90	0.22	59,59,59,59	0
56	MG	1N	203	1/1	0.90	0.13	51,51,51,51	0
56	MG	2A	3097	1/1	0.90	0.14	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	3014	1/1	0.90	0.32	27,27,27,27	0
56	MG	2A	3136	1/1	0.90	0.15	36,36,36,36	0
56	MG	2a	1686	1/1	0.90	0.22	67,67,67,67	0
56	MG	1y	102	1/1	0.90	0.09	83,83,83,83	0
56	MG	1A	3495	1/1	0.90	0.10	31,31,31,31	0
56	MG	1A	3332	1/1	0.90	0.11	34,34,34,34	0
56	MG	2A	3613	1/1	0.90	0.11	61,61,61,61	0
56	MG	1G	3001	1/1	0.90	0.14	29,29,29,29	0
56	MG	2A	3170	1/1	0.90	0.21	44,44,44,44	0
56	MG	1A	3941	1/1	0.90	0.09	34,34,34,34	0
56	MG	1A	3859	1/1	0.90	0.12	61,61,61,61	0
56	MG	1A	3565	1/1	0.90	0.19	26,26,26,26	0
56	MG	1O	201	1/1	0.90	0.15	45,45,45,45	0
56	MG	2A	3639	1/1	0.90	0.22	56,56,56,56	0
56	MG	2A	3098	1/1	0.90	0.36	68,68,68,68	0
56	MG	2A	3381	1/1	0.90	0.18	33,33,33,33	0
56	MG	2A	3752	1/1	0.90	0.29	61,61,61,61	0
56	MG	1A	3658	1/1	0.90	0.10	46,46,46,46	0
56	MG	2E	306	1/1	0.90	0.12	43,43,43,43	0
56	MG	2A	3705	1/1	0.90	0.19	64,64,64,64	0
56	MG	1A	3127	1/1	0.90	0.15	37,37,37,37	0
56	MG	1A	3479	1/1	0.90	0.13	30,30,30,30	0
56	MG	1A	3707	1/1	0.90	0.12	45,45,45,45	0
56	MG	2A	3103	1/1	0.90	0.48	46,46,46,46	0
56	MG	2A	3111	1/1	0.90	0.21	36,36,36,36	0
56	MG	1A	3861	1/1	0.90	0.13	58,58,58,58	0
56	MG	1A	3900	1/1	0.90	0.13	44,44,44,44	0
56	MG	1w	107	1/1	0.90	0.30	64,64,64,64	0
56	MG	1A	3775	1/1	0.90	0.13	41,41,41,41	0
56	MG	1a	3092	1/1	0.90	0.11	55,55,55,55	0
56	MG	1A	3121	1/1	0.90	0.39	33,33,33,33	0
56	MG	2A	3646	1/1	0.90	0.13	59,59,59,59	0
56	MG	2a	1700	1/1	0.90	0.28	62,62,62,62	0
56	MG	1A	3937	1/1	0.90	0.10	40,40,40,40	0
56	MG	1A	3377	1/1	0.90	0.45	40,40,40,40	0
56	MG	1A	3619	1/1	0.90	0.16	36,36,36,36	0
56	MG	1F	307	1/1	0.90	0.12	40,40,40,40	0
56	MG	2a	1693	1/1	0.90	0.31	75,75,75,75	0
56	MG	1A	3036	1/1	0.90	0.21	26,26,26,26	0
56	MG	11	104	1/1	0.90	0.10	59,59,59,59	0
56	MG	2a	1709	1/1	0.90	0.12	49,49,49,49	0
56	MG	2A	3008	1/1	0.90	0.14	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3670	1/1	0.90	0.11	43,43,43,43	0
56	MG	1a	3077	1/1	0.90	0.09	42,42,42,42	0
56	MG	1E	301	1/1	0.90	0.59	26,26,26,26	0
56	MG	1A	3968	1/1	0.90	0.20	55,55,55,55	0
56	MG	2l	204	1/1	0.90	0.12	43,43,43,43	0
56	MG	2A	3358	1/1	0.90	0.14	47,47,47,47	0
56	MG	1A	3653	1/1	0.90	0.17	20,20,20,20	0
56	MG	1A	3622	1/1	0.90	0.08	56,56,56,56	0
56	MG	27	102	1/1	0.90	0.17	47,47,47,47	0
56	MG	2A	3245	1/1	0.90	0.11	59,59,59,59	0
56	MG	1A	3288	1/1	0.90	0.08	47,47,47,47	0
56	MG	1A	3431	1/1	0.90	0.40	34,34,34,34	0
56	MG	2A	3347	1/1	0.90	0.10	53,53,53,53	0
56	MG	2A	3191	1/1	0.91	0.14	56,56,56,56	0
56	MG	2a	1710	1/1	0.91	0.15	64,64,64,64	0
56	MG	1A	3262	1/1	0.91	0.11	33,33,33,33	0
56	MG	2a	1691	1/1	0.91	0.36	56,56,56,56	0
56	MG	2A	3195	1/1	0.91	0.28	50,50,50,50	0
56	MG	1A	3175	1/1	0.91	0.44	21,21,21,21	0
56	MG	1A	3426	1/1	0.91	0.22	44,44,44,44	0
56	MG	2a	1646	1/1	0.91	0.14	71,71,71,71	0
56	MG	2a	1759	1/1	0.91	0.17	50,50,50,50	0
56	MG	1A	3331	1/1	0.91	0.21	39,39,39,39	0
56	MG	1A	3243	1/1	0.91	0.29	25,25,25,25	0
56	MG	1A	3438	1/1	0.91	0.10	29,29,29,29	0
56	MG	1A	3345	1/1	0.91	0.17	24,24,24,24	0
56	MG	2a	1796	1/1	0.91	0.15	54,54,54,54	0
56	MG	2a	1657	1/1	0.91	0.16	36,36,36,36	0
56	MG	2A	3392	1/1	0.91	0.13	33,33,33,33	0
56	MG	2A	3313	1/1	0.91	0.19	41,41,41,41	0
56	MG	1A	3349	1/1	0.91	0.13	39,39,39,39	0
56	MG	1A	3291	1/1	0.91	0.21	38,38,38,38	0
56	MG	1A	3397	1/1	0.91	0.15	51,51,51,51	0
56	MG	2A	3238	1/1	0.91	0.14	60,60,60,60	0
56	MG	2A	3489	1/1	0.91	0.14	48,48,48,48	0
56	MG	2d	502	1/1	0.91	0.12	58,58,58,58	0
56	MG	1a	3036	1/1	0.91	0.10	49,49,49,49	0
56	MG	1A	3500	1/1	0.91	0.16	20,20,20,20	0
56	MG	1a	3156	1/1	0.91	0.16	50,50,50,50	0
56	MG	2a	1804	1/1	0.91	0.10	48,48,48,48	0
56	MG	1A	3469	1/1	0.91	0.19	43,43,43,43	0
56	MG	2A	3552	1/1	0.91	0.20	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	3769	1/1	0.91	0.16	15,15,15,15	0
56	MG	2A	3384	1/1	0.91	0.11	27,27,27,27	0
56	MG	2a	1715	1/1	0.91	0.15	50,50,50,50	0
56	MG	2A	3551	1/1	0.91	0.22	48,48,48,48	0
56	MG	2A	3386	1/1	0.91	0.24	43,43,43,43	0
56	MG	1A	3955	1/1	0.91	0.12	32,32,32,32	0
56	MG	2a	1723	1/1	0.91	0.14	57,57,57,57	0
56	MG	1a	3100	1/1	0.91	0.11	61,61,61,61	0
56	MG	2a	1696	1/1	0.91	0.15	48,48,48,48	0
56	MG	2a	1678	1/1	0.91	0.11	65,65,65,65	0
56	MG	2A	3217	1/1	0.91	0.28	51,51,51,51	0
56	MG	1A	3188	1/1	0.91	0.10	12,12,12,12	0
56	MG	2A	3226	1/1	0.91	0.33	42,42,42,42	0
56	MG	1A	3450	1/1	0.91	0.11	40,40,40,40	0
56	MG	2a	1765	1/1	0.91	0.14	64,64,64,64	0
56	MG	2a	1711	1/1	0.91	0.24	67,67,67,67	0
56	MG	1a	3057	1/1	0.91	0.15	43,43,43,43	0
56	MG	1A	3510	1/1	0.91	0.18	50,50,50,50	0
56	MG	1A	3249	1/1	0.91	0.35	31,31,31,31	0
56	MG	1A	4025	1/1	0.91	0.22	24,24,24,24	0
56	MG	1A	3558	1/1	0.91	0.13	16,16,16,16	0
56	MG	1A	3924	1/1	0.91	0.11	34,34,34,34	0
56	MG	2A	3742	1/1	0.91	0.34	52,52,52,52	0
56	MG	2a	1684	1/1	0.91	0.18	49,49,49,49	0
56	MG	1A	3909	1/1	0.91	0.20	46,46,46,46	0
56	MG	1a	3194	1/1	0.91	0.08	59,59,59,59	0
56	MG	1A	3608	1/1	0.91	0.20	54,54,54,54	0
56	MG	2a	1833	1/1	0.91	0.06	62,62,62,62	0
56	MG	19	502	1/1	0.91	0.16	39,39,39,39	0
56	MG	1A	3222	1/1	0.91	0.23	51,51,51,51	0
56	MG	2A	3219	1/1	0.91	0.32	54,54,54,54	0
56	MG	1A	3692	1/1	0.91	0.12	29,29,29,29	0
56	MG	1A	3370	1/1	0.91	0.21	37,37,37,37	0
56	MG	2a	1821	1/1	0.91	0.18	66,66,66,66	0
56	MG	2a	1778	1/1	0.91	0.21	68,68,68,68	0
56	MG	2A	3728	1/1	0.91	0.17	56,56,56,56	0
56	MG	2A	3708	1/1	0.91	0.17	63,63,63,63	0
56	MG	2A	3248	1/1	0.91	0.18	44,44,44,44	0
56	MG	1A	3429	1/1	0.91	0.38	29,29,29,29	0
56	MG	2a	1818	1/1	0.91	0.10	48,48,48,48	0
56	MG	2A	3572	1/1	0.91	0.22	66,66,66,66	0
56	MG	1a	3123	1/1	0.91	0.13	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	3958	1/1	0.91	0.17	32,32,32,32	0
56	MG	1A	3595	1/1	0.91	0.14	40,40,40,40	0
56	MG	1A	3887	1/1	0.91	0.23	16,16,16,16	0
56	MG	2A	3584	1/1	0.91	0.32	50,50,50,50	0
56	MG	17	105	1/1	0.91	0.15	34,34,34,34	0
56	MG	2A	3221	1/1	0.91	0.16	54,54,54,54	0
56	MG	2A	3042	1/1	0.91	0.15	54,54,54,54	0
56	MG	1A	3237	1/1	0.91	0.15	49,49,49,49	0
56	MG	1T	201	1/1	0.91	0.18	42,42,42,42	0
56	MG	1A	4018	1/1	0.91	0.34	24,24,24,24	0
56	MG	1a	3001	1/1	0.91	0.14	52,52,52,52	0
56	MG	1a	3053	1/1	0.91	0.17	56,56,56,56	0
56	MG	1A	3618	1/1	0.91	0.16	55,55,55,55	0
56	MG	1A	3141	1/1	0.91	0.21	38,38,38,38	0
56	MG	2A	3176	1/1	0.91	0.24	41,41,41,41	0
56	MG	2A	3273	1/1	0.91	0.35	57,57,57,57	0
56	MG	1a	3174	1/1	0.91	0.08	51,51,51,51	0
56	MG	2A	3139	1/1	0.91	0.13	41,41,41,41	0
56	MG	2A	3458	1/1	0.91	0.22	40,40,40,40	0
56	MG	1a	3190	1/1	0.91	0.16	51,51,51,51	0
56	MG	2A	3538	1/1	0.91	0.28	49,49,49,49	0
56	MG	1a	3181	1/1	0.91	0.14	41,41,41,41	0
56	MG	1a	3093	1/1	0.91	0.16	49,49,49,49	0
56	MG	2A	3289	1/1	0.91	0.21	53,53,53,53	0
56	MG	2A	3234	1/1	0.91	0.33	47,47,47,47	0
56	MG	1A	3435	1/1	0.91	0.13	56,56,56,56	0
56	MG	1A	3417	1/1	0.91	0.16	42,42,42,42	0
56	MG	1A	3107	1/1	0.91	0.26	24,24,24,24	0
56	MG	1A	3681	1/1	0.91	0.12	23,23,23,23	0
56	MG	2a	1786	1/1	0.91	0.12	66,66,66,66	0
56	MG	2a	1638	1/1	0.91	0.24	49,49,49,49	0
56	MG	1A	3674	1/1	0.91	0.20	56,56,56,56	0
56	MG	1A	3491	1/1	0.91	0.19	17,17,17,17	0
58	EZG	2A	3746	25/25	0.91	0.32	35,43,49,51	0
56	MG	1D	303	1/1	0.91	0.27	26,26,26,26	0
56	MG	1A	3620	1/1	0.91	0.11	49,49,49,49	0
56	MG	1A	3923	1/1	0.91	0.24	39,39,39,39	0
56	MG	1A	3563	1/1	0.91	0.08	35,35,35,35	0
56	MG	1a	3142	1/1	0.91	0.10	64,64,64,64	0
56	MG	2a	1767	1/1	0.91	0.08	39,39,39,39	0
56	MG	2A	3658	1/1	0.91	0.17	36,36,36,36	0
56	MG	1A	3783	1/1	0.91	0.27	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3390	1/1	0.91	0.12	58,58,58,58	0
56	MG	1A	3200	1/1	0.91	0.15	44,44,44,44	0
56	MG	2A	3036	1/1	0.91	0.19	48,48,48,48	0
56	MG	1a	3022	1/1	0.91	0.09	48,48,48,48	0
56	MG	2A	3635	1/1	0.91	0.14	57,57,57,57	0
56	MG	2A	3212	1/1	0.91	0.12	59,59,59,59	0
56	MG	2A	3581	1/1	0.91	0.12	28,28,28,28	0
56	MG	1A	3537	1/1	0.91	0.18	30,30,30,30	0
56	MG	2A	3483	1/1	0.91	0.15	59,59,59,59	0
56	MG	1A	3224	1/1	0.91	0.16	42,42,42,42	0
56	MG	1A	3409	1/1	0.91	0.15	54,54,54,54	0
56	MG	1a	3068	1/1	0.91	0.14	62,62,62,62	0
56	MG	1A	4021	1/1	0.91	0.14	47,47,47,47	0
56	MG	2A	3619	1/1	0.91	0.09	60,60,60,60	0
56	MG	1A	3371	1/1	0.91	0.23	39,39,39,39	0
56	MG	1A	3264	1/1	0.91	0.09	39,39,39,39	0
56	MG	1A	3379	1/1	0.91	0.39	53,53,53,53	0
56	MG	1A	3055	1/1	0.91	0.12	54,54,54,54	0
56	MG	1A	3413	1/1	0.91	0.28	55,55,55,55	0
56	MG	2A	3018	1/1	0.91	0.36	51,51,51,51	0
56	MG	1A	3812	1/1	0.91	0.16	43,43,43,43	0
56	MG	1A	3148	1/1	0.91	0.27	26,26,26,26	0
56	MG	1A	4045	1/1	0.91	0.60	39,39,39,39	0
56	MG	1A	3192	1/1	0.91	0.17	54,54,54,54	0
56	MG	2A	3757	1/1	0.91	0.26	55,55,55,55	0
56	MG	1a	3176	1/1	0.91	0.10	59,59,59,59	0
56	MG	2a	1611	1/1	0.91	0.10	65,65,65,65	0
56	MG	2q	204	1/1	0.91	0.16	65,65,65,65	0
56	MG	2A	3607	1/1	0.91	0.13	48,48,48,48	0
56	MG	1A	3241	1/1	0.91	0.14	58,58,58,58	0
56	MG	1A	3743	1/1	0.91	0.20	42,42,42,42	0
56	MG	1A	3100	1/1	0.91	0.20	38,38,38,38	0
56	MG	2A	3652	1/1	0.92	0.16	38,38,38,38	0
56	MG	2A	3125	1/1	0.92	0.32	32,32,32,32	0
56	MG	1A	3374	1/1	0.92	0.41	40,40,40,40	0
56	MG	23	101	1/1	0.92	0.61	54,54,54,54	0
56	MG	2A	3410	1/1	0.92	0.31	61,61,61,61	0
56	MG	2Q	3002	1/1	0.92	0.21	41,41,41,41	0
56	MG	2A	3159	1/1	0.92	0.14	50,50,50,50	0
56	MG	2A	3025	1/1	0.92	0.26	54,54,54,54	0
56	MG	1G	3005	1/1	0.92	0.08	52,52,52,52	0
56	MG	2a	1764	1/1	0.92	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3482	1/1	0.92	0.28	38,38,38,38	0
56	MG	1A	3304	1/1	0.92	0.43	41,41,41,41	0
56	MG	1A	3376	1/1	0.92	0.23	31,31,31,31	0
56	MG	1A	3991	1/1	0.92	0.14	66,66,66,66	0
56	MG	1A	3445	1/1	0.92	0.10	47,47,47,47	0
56	MG	2a	1634	1/1	0.92	0.11	59,59,59,59	0
56	MG	2A	3685	1/1	0.92	0.14	41,41,41,41	0
56	MG	1A	3464	1/1	0.92	0.17	39,39,39,39	0
56	MG	2A	3022	1/1	0.92	0.18	38,38,38,38	0
56	MG	2A	3147	1/1	0.92	0.28	50,50,50,50	0
56	MG	1A	4036	1/1	0.92	0.56	29,29,29,29	0
56	MG	2a	1614	1/1	0.92	0.09	52,52,52,52	0
56	MG	2A	3206	1/1	0.92	0.34	42,42,42,42	0
56	MG	1a	3063	1/1	0.92	0.16	53,53,53,53	0
56	MG	1n	502	1/1	0.92	0.13	51,51,51,51	0
56	MG	1X	102	1/1	0.92	0.21	35,35,35,35	0
56	MG	1a	3189	1/1	0.92	0.12	53,53,53,53	0
56	MG	20	3003	1/1	0.92	0.11	56,56,56,56	0
56	MG	2a	1780	1/1	0.92	0.07	57,57,57,57	0
56	MG	1A	3217	1/1	0.92	0.29	19,19,19,19	0
56	MG	1A	3238	1/1	0.92	0.16	33,33,33,33	0
56	MG	1A	3025	1/1	0.92	0.27	42,42,42,42	0
56	MG	1A	3110	1/1	0.92	0.17	27,27,27,27	0
56	MG	1T	202	1/1	0.92	0.21	47,47,47,47	0
56	MG	2A	3210	1/1	0.92	0.35	58,58,58,58	0
56	MG	1a	3134	1/1	0.92	0.22	47,47,47,47	0
56	MG	1R	204	1/1	0.92	0.33	33,33,33,33	0
56	MG	2A	3657	1/1	0.92	0.20	41,41,41,41	0
56	MG	1x	111	1/1	0.92	0.15	64,64,64,64	0
56	MG	1q	201	1/1	0.92	0.08	50,50,50,50	0
56	MG	1a	3193	1/1	0.92	0.16	47,47,47,47	0
56	MG	2a	1624	1/1	0.92	0.11	78,78,78,78	0
56	MG	2A	3490	1/1	0.92	0.07	72,72,72,72	0
56	MG	2a	1793	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	3284	1/1	0.92	0.20	42,42,42,42	0
56	MG	1A	3985	1/1	0.92	0.17	60,60,60,60	0
56	MG	2A	3269	1/1	0.92	0.14	36,36,36,36	0
56	MG	1A	3280	1/1	0.92	0.50	26,26,26,26	0
56	MG	1A	3739	1/1	0.92	0.34	29,29,29,29	0
56	MG	2A	3609	1/1	0.92	0.22	36,36,36,36	0
56	MG	2a	1798	1/1	0.92	0.14	60,60,60,60	0
56	MG	1A	3050	1/1	0.92	0.27	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	3889	1/1	0.92	0.14	39,39,39,39	0
56	MG	2A	3478	1/1	0.92	0.60	38,38,38,38	0
56	MG	2A	3562	1/1	0.92	0.10	40,40,40,40	0
56	MG	2A	3279	1/1	0.92	0.10	64,64,64,64	0
56	MG	1A	3876	1/1	0.92	0.21	34,34,34,34	0
56	MG	2A	3644	1/1	0.92	0.14	57,57,57,57	0
56	MG	1a	3150	1/1	0.92	0.11	65,65,65,65	0
56	MG	1A	3292	1/1	0.92	0.17	43,43,43,43	0
56	MG	1A	3700	1/1	0.92	0.09	27,27,27,27	0
56	MG	2A	3691	1/1	0.92	0.11	68,68,68,68	0
56	MG	1A	3071	1/1	0.92	0.14	31,31,31,31	0
56	MG	2A	3590	1/1	0.92	0.15	50,50,50,50	0
56	MG	1a	3111	1/1	0.92	0.17	45,45,45,45	0
56	MG	1A	3744	1/1	0.92	0.12	41,41,41,41	0
56	MG	2A	3300	1/1	0.92	0.20	58,58,58,58	0
56	MG	1A	3878	1/1	0.92	0.11	16,16,16,16	0
56	MG	1A	3302	1/1	0.92	0.78	32,32,32,32	0
56	MG	1A	3648	1/1	0.92	0.10	20,20,20,20	0
56	MG	2A	3402	1/1	0.92	0.15	49,49,49,49	0
56	MG	1A	3831	1/1	0.92	0.13	68,68,68,68	0
56	MG	2A	3017	1/1	0.92	0.11	59,59,59,59	0
56	MG	1a	3203	1/1	0.92	0.20	69,69,69,69	0
56	MG	2A	3733	1/1	0.92	0.17	30,30,30,30	0
56	MG	1A	3179	1/1	0.92	0.37	23,23,23,23	0
56	MG	2A	3187	1/1	0.92	0.26	54,54,54,54	0
56	MG	1A	3219	1/1	0.92	0.29	19,19,19,19	0
56	MG	2A	3588	1/1	0.92	0.09	52,52,52,52	0
56	MG	1A	3511	1/1	0.92	0.22	20,20,20,20	0
56	MG	2A	3204	1/1	0.92	0.15	43,43,43,43	0
56	MG	1A	3380	1/1	0.92	0.29	33,33,33,33	0
56	MG	1A	3420	1/1	0.92	0.13	49,49,49,49	0
56	MG	2A	3155	1/1	0.92	0.09	34,34,34,34	0
56	MG	2F	301	1/1	0.92	0.16	35,35,35,35	0
56	MG	1A	3087	1/1	0.92	0.18	47,47,47,47	0
56	MG	2A	3449	1/1	0.92	0.11	63,63,63,63	0
56	MG	2A	3684	1/1	0.92	0.08	68,68,68,68	0
56	MG	1A	3218	1/1	0.92	0.07	23,23,23,23	0
56	MG	2A	3283	1/1	0.92	0.14	42,42,42,42	0
56	MG	2A	3697	1/1	0.92	0.28	50,50,50,50	0
56	MG	1A	3265	1/1	0.92	0.18	26,26,26,26	0
56	MG	2a	1743	1/1	0.92	0.10	70,70,70,70	0
56	MG	12	3001	1/1	0.92	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3298	1/1	0.92	0.16	40,40,40,40	0
56	MG	1a	3164	1/1	0.92	0.13	58,58,58,58	0
56	MG	1a	3112	1/1	0.92	0.09	48,48,48,48	0
56	MG	2A	3466	1/1	0.92	0.16	41,41,41,41	0
56	MG	2A	3116	1/1	0.92	0.11	55,55,55,55	0
56	MG	1A	3476	1/1	0.92	0.13	27,27,27,27	0
56	MG	2A	3276	1/1	0.92	0.21	58,58,58,58	0
56	MG	1A	3666	1/1	0.92	0.05	50,50,50,50	0
56	MG	2A	3299	1/1	0.92	0.33	43,43,43,43	0
56	MG	2a	1653	1/1	0.92	0.07	67,67,67,67	0
56	MG	1A	4059	1/1	0.92	0.26	22,22,22,22	0
56	MG	2A	3502	1/1	0.92	0.16	42,42,42,42	0
56	MG	1A	3762	1/1	0.92	0.14	12,12,12,12	0
56	MG	1l	203	1/1	0.92	0.17	50,50,50,50	0
56	MG	1A	3708	1/1	0.92	0.10	42,42,42,42	0
56	MG	2A	3620	1/1	0.92	0.09	34,34,34,34	0
56	MG	2a	1819	1/1	0.92	0.08	52,52,52,52	0
56	MG	1A	3505	1/1	0.92	0.22	31,31,31,31	0
56	MG	2A	3446	1/1	0.92	0.14	32,32,32,32	0
56	MG	1A	3970	1/1	0.92	0.05	53,53,53,53	0
56	MG	1A	3460	1/1	0.92	0.10	41,41,41,41	0
56	MG	1A	3072	1/1	0.92	0.31	27,27,27,27	0
56	MG	1A	3921	1/1	0.92	0.21	43,43,43,43	0
56	MG	1A	3024	1/1	0.92	0.12	32,32,32,32	0
56	MG	2A	3477	1/1	0.92	0.13	64,64,64,64	0
56	MG	2A	3640	1/1	0.92	0.24	47,47,47,47	0
56	MG	1A	3786	1/1	0.92	0.11	34,34,34,34	0
56	MG	1A	3466	1/1	0.92	0.17	39,39,39,39	0
56	MG	1A	3261	1/1	0.92	0.10	35,35,35,35	0
56	MG	1A	3945	1/1	0.92	0.34	30,30,30,30	0
56	MG	1A	3698	1/1	0.92	0.12	41,41,41,41	0
56	MG	2A	3250	1/1	0.92	0.15	51,51,51,51	0
56	MG	1A	3922	1/1	0.92	0.09	49,49,49,49	0
56	MG	1D	311	1/1	0.92	0.14	36,36,36,36	0
56	MG	2A	3481	1/1	0.92	0.25	58,58,58,58	0
56	MG	2A	3346	1/1	0.92	0.11	48,48,48,48	0
56	MG	1a	3013	1/1	0.92	0.15	45,45,45,45	0
56	MG	2A	3382	1/1	0.92	0.24	46,46,46,46	0
56	MG	2a	1761	1/1	0.92	0.22	34,34,34,34	0
56	MG	2A	3681	1/1	0.92	0.23	49,49,49,49	0
56	MG	1B	204	1/1	0.92	0.12	29,29,29,29	0
56	MG	2D	306	1/1	0.92	0.66	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3215	1/1	0.92	0.18	54,54,54,54	0
56	MG	2W	203	1/1	0.92	0.12	41,41,41,41	0
56	MG	2A	3211	1/1	0.92	0.11	68,68,68,68	0
56	MG	1A	3145	1/1	0.92	0.62	34,34,34,34	0
56	MG	1A	3194	1/1	0.92	0.21	35,35,35,35	0
56	MG	2A	3316	1/1	0.92	0.16	53,53,53,53	0
56	MG	1a	3055	1/1	0.92	0.14	49,49,49,49	0
56	MG	1Q	205	1/1	0.92	0.11	28,28,28,28	0
56	MG	2a	1664	1/1	0.92	0.17	56,56,56,56	0
56	MG	1A	3641	1/1	0.92	0.18	13,13,13,13	0
56	MG	1A	3849	1/1	0.92	0.27	35,35,35,35	0
56	MG	1A	3190	1/1	0.92	0.08	43,43,43,43	0
56	MG	1a	3011	1/1	0.92	0.14	41,41,41,41	0
56	MG	2A	3075	1/1	0.92	0.16	51,51,51,51	0
56	MG	1A	3837	1/1	0.92	0.19	54,54,54,54	0
56	MG	2A	3743	1/1	0.92	0.19	51,51,51,51	0
56	MG	2A	3591	1/1	0.92	0.12	34,34,34,34	0
56	MG	1A	3152	1/1	0.92	0.17	43,43,43,43	0
56	MG	1A	3938	1/1	0.92	0.26	40,40,40,40	0
56	MG	1A	3183	1/1	0.92	0.09	39,39,39,39	0
56	MG	1A	3512	1/1	0.92	0.08	40,40,40,40	0
56	MG	1A	3472	1/1	0.92	0.14	41,41,41,41	0
56	MG	2a	1783	1/1	0.92	0.11	62,62,62,62	0
56	MG	1A	3838	1/1	0.92	0.11	53,53,53,53	0
56	MG	2a	1747	1/1	0.92	0.12	56,56,56,56	0
56	MG	2a	1775	1/1	0.92	0.15	74,74,74,74	0
56	MG	1Y	502	1/1	0.92	0.10	67,67,67,67	0
56	MG	2a	1729	1/1	0.92	0.10	61,61,61,61	0
56	MG	1A	3825	1/1	0.92	0.47	43,43,43,43	0
56	MG	1A	3195	1/1	0.92	0.49	27,27,27,27	0
56	MG	2A	3134	1/1	0.92	0.08	51,51,51,51	0
56	MG	1A	3749	1/1	0.92	0.23	31,31,31,31	0
56	MG	1A	3231	1/1	0.92	0.27	45,45,45,45	0
56	MG	2A	3698	1/1	0.92	0.16	58,58,58,58	0
56	MG	2A	3408	1/1	0.92	0.09	53,53,53,53	0
56	MG	2R	3001	1/1	0.92	0.50	58,58,58,58	0
56	MG	2A	3006	1/1	0.93	0.08	44,44,44,44	0
56	MG	2a	1739	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3057	1/1	0.93	0.13	47,47,47,47	0
56	MG	2A	3467	1/1	0.93	0.22	28,28,28,28	0
56	MG	2A	3703	1/1	0.93	0.14	50,50,50,50	0
56	MG	2A	3595	1/1	0.93	0.09	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	1A	3386	1/1	0.93	0.10	33,33,33,33	0
56	MG	1A	3424	1/1	0.93	0.56	32,32,32,32	0
56	MG	1A	3444	1/1	0.93	0.14	18,18,18,18	0
56	MG	2A	3305	1/1	0.93	0.15	51,51,51,51	0
56	MG	2A	3503	1/1	0.93	0.16	54,54,54,54	0
56	MG	1a	3099	1/1	0.93	0.10	72,72,72,72	0
56	MG	2a	1807	1/1	0.93	0.11	61,61,61,61	0
56	MG	2A	3013	1/1	0.93	0.13	27,27,27,27	0
56	MG	10	103	1/1	0.93	0.15	54,54,54,54	0
56	MG	2A	3628	1/1	0.93	0.20	40,40,40,40	0
56	MG	2A	3506	1/1	0.93	0.13	48,48,48,48	0
56	MG	1A	3993	1/1	0.93	0.30	44,44,44,44	0
56	MG	1A	3758	1/1	0.93	0.13	32,32,32,32	0
56	MG	1A	3559	1/1	0.93	0.20	15,15,15,15	0
56	MG	2A	3416	1/1	0.93	0.13	40,40,40,40	0
56	MG	1a	3116	1/1	0.93	0.09	35,35,35,35	0
56	MG	1a	3088	1/1	0.93	0.06	57,57,57,57	0
56	MG	2A	3625	1/1	0.93	0.08	52,52,52,52	0
56	MG	1A	3109	1/1	0.93	0.41	50,50,50,50	0
56	MG	2U	204	1/1	0.93	0.83	60,60,60,60	0
56	MG	2A	3565	1/1	0.93	0.12	45,45,45,45	0
56	MG	1B	207	1/1	0.93	0.43	40,40,40,40	0
56	MG	2A	3099	1/1	0.93	0.10	38,38,38,38	0
56	MG	1s	101	1/1	0.93	0.20	62,62,62,62	0
56	MG	1A	3867	1/1	0.93	0.14	19,19,19,19	0
56	MG	1x	102	1/1	0.93	0.26	49,49,49,49	0
56	MG	1A	3628	1/1	0.93	0.13	16,16,16,16	0
56	MG	1A	3182	1/1	0.93	0.20	33,33,33,33	0
56	MG	1a	3166	1/1	0.93	0.08	49,49,49,49	0
56	MG	2A	3486	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	3365	1/1	0.93	0.21	39,39,39,39	0
56	MG	1A	3447	1/1	0.93	0.32	47,47,47,47	0
56	MG	1A	3835	1/1	0.93	0.17	42,42,42,42	0
56	MG	2A	3262	1/1	0.93	0.14	44,44,44,44	0
56	MG	2A	3298	1/1	0.93	0.12	50,50,50,50	0
56	MG	2a	1658	1/1	0.93	0.12	59,59,59,59	0
56	MG	1A	3144	1/1	0.93	0.13	37,37,37,37	0
56	MG	2a	1737	1/1	0.93	0.04	57,57,57,57	0
56	MG	1A	3030	1/1	0.93	0.59	20,20,20,20	0
56	MG	2R	3002	1/1	0.93	0.25	56,56,56,56	0
56	MG	2A	3456	1/1	0.93	0.17	26,26,26,26	0
56	MG	1a	3128	1/1	0.93	0.09	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1695	1/1	0.93	0.16	56,56,56,56	0
56	MG	1A	3441	1/1	0.93	0.07	49,49,49,49	0
56	MG	2A	3216	1/1	0.93	0.15	51,51,51,51	0
56	MG	1S	3002	1/1	0.93	0.20	36,36,36,36	0
56	MG	2A	3050	1/1	0.93	0.14	38,38,38,38	0
56	MG	1a	3032	1/1	0.93	0.19	54,54,54,54	0
56	MG	2A	3331	1/1	0.93	0.16	47,47,47,47	0
56	MG	1A	3060	1/1	0.93	0.08	26,26,26,26	0
56	MG	2a	1702	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3811	1/1	0.93	0.08	32,32,32,32	0
56	MG	1A	3957	1/1	0.93	0.12	55,55,55,55	0
56	MG	1A	3902	1/1	0.93	0.10	55,55,55,55	0
56	MG	2A	3593	1/1	0.93	0.16	47,47,47,47	0
56	MG	2A	3476	1/1	0.93	0.12	44,44,44,44	0
56	MG	1A	3836	1/1	0.93	0.09	56,56,56,56	0
56	MG	1A	3860	1/1	0.93	0.27	54,54,54,54	0
56	MG	1I	3001	1/1	0.93	0.31	64,64,64,64	0
56	MG	2a	1688	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3737	1/1	0.93	0.14	29,29,29,29	0
56	MG	2I	201	1/1	0.93	0.23	51,51,51,51	0
56	MG	1A	3239	1/1	0.93	0.28	38,38,38,38	0
56	MG	1A	3560	1/1	0.93	0.23	26,26,26,26	0
56	MG	1A	3020	1/1	0.93	0.15	18,18,18,18	0
56	MG	1A	3933	1/1	0.93	0.14	54,54,54,54	0
56	MG	2A	3756	1/1	0.93	0.14	33,33,33,33	0
56	MG	1A	3387	1/1	0.93	0.20	37,37,37,37	0
56	MG	1a	3040	1/1	0.93	0.12	41,41,41,41	0
56	MG	2a	1630	1/1	0.93	0.23	57,57,57,57	0
56	MG	2a	1669	1/1	0.93	0.23	56,56,56,56	0
56	MG	2A	3523	1/1	0.93	0.14	37,37,37,37	0
56	MG	1A	3118	1/1	0.93	0.11	29,29,29,29	0
56	MG	1a	3010	1/1	0.93	0.09	45,45,45,45	0
56	MG	1N	201	1/1	0.93	0.54	45,45,45,45	0
56	MG	2A	3603	1/1	0.93	0.11	37,37,37,37	0
56	MG	2A	3361	1/1	0.93	0.11	46,46,46,46	0
56	MG	2a	1643	1/1	0.93	0.21	61,61,61,61	0
56	MG	1A	3705	1/1	0.93	0.17	39,39,39,39	0
56	MG	1A	4014	1/1	0.93	0.34	33,33,33,33	0
56	MG	1a	3105	1/1	0.93	0.11	59,59,59,59	0
56	MG	1A	3798	1/1	0.93	0.26	45,45,45,45	0
56	MG	1a	3103	1/1	0.93	0.07	46,46,46,46	0
56	MG	1A	3340	1/1	0.93	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	1B	228	1/1	0.93	0.15	24,24,24,24	0
56	MG	1A	3101	1/1	0.93	0.44	28,28,28,28	0
56	MG	1A	3603	1/1	0.93	0.16	43,43,43,43	0
56	MG	2a	1757	1/1	0.93	0.12	48,48,48,48	0
56	MG	2A	3334	1/1	0.93	0.28	58,58,58,58	0
56	MG	1A	3391	1/1	0.93	0.16	46,46,46,46	0
56	MG	1A	3048	1/1	0.93	0.45	42,42,42,42	0
56	MG	1a	3214	1/1	0.93	0.40	58,58,58,58	0
56	MG	1a	3159	1/1	0.93	0.14	41,41,41,41	0
56	MG	1n	503	1/1	0.93	0.08	38,38,38,38	0
56	MG	1A	3336	1/1	0.93	0.25	35,35,35,35	0
56	MG	2T	3003	1/1	0.93	0.11	41,41,41,41	0
56	MG	1A	3463	1/1	0.93	0.38	38,38,38,38	0
56	MG	2A	3145	1/1	0.93	0.15	48,48,48,48	0
56	MG	15	106	1/1	0.93	0.24	19,19,19,19	0
56	MG	2A	3308	1/1	0.93	0.15	54,54,54,54	0
56	MG	2A	3663	1/1	0.93	0.17	47,47,47,47	0
56	MG	1A	3329	1/1	0.93	0.10	41,41,41,41	0
56	MG	2A	3222	1/1	0.93	0.16	44,44,44,44	0
56	MG	1A	3712	1/1	0.93	0.25	34,34,34,34	0
56	MG	1A	3819	1/1	0.93	0.11	29,29,29,29	0
56	MG	1a	3104	1/1	0.93	0.17	45,45,45,45	0
56	MG	2a	1673	1/1	0.93	0.10	57,57,57,57	0
56	MG	1A	3715	1/1	0.93	0.10	23,23,23,23	0
56	MG	2A	3471	1/1	0.93	0.20	37,37,37,37	0
56	MG	1A	3383	1/1	0.93	0.18	42,42,42,42	0
56	MG	1A	3172	1/1	0.93	0.40	44,44,44,44	0
56	MG	1A	3105	1/1	0.93	0.24	30,30,30,30	0
56	MG	1A	3287	1/1	0.93	0.13	30,30,30,30	0
56	MG	2A	3011	1/1	0.93	0.15	54,54,54,54	0
56	MG	2A	3535	1/1	0.93	0.14	27,27,27,27	0
56	MG	1a	3091	1/1	0.93	0.22	46,46,46,46	0
56	MG	2A	3460	1/1	0.93	0.15	39,39,39,39	0
56	MG	2A	3517	1/1	0.93	0.09	51,51,51,51	0
56	MG	2a	1760	1/1	0.93	0.24	60,60,60,60	0
56	MG	1a	3052	1/1	0.93	0.10	58,58,58,58	0
56	MG	2l	203	1/1	0.93	0.17	62,62,62,62	0
56	MG	1A	3631	1/1	0.93	0.16	32,32,32,32	0
56	MG	2A	3179	1/1	0.93	0.17	45,45,45,45	0
56	MG	2A	3224	1/1	0.93	0.16	54,54,54,54	0
56	MG	1V	201	1/1	0.93	0.10	40,40,40,40	0
56	MG	2A	3445	1/1	0.93	0.10	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	3037	1/1	0.93	0.11	61,61,61,61	0
56	MG	1a	3072	1/1	0.93	0.09	54,54,54,54	0
56	MG	1a	3029	1/1	0.93	0.10	49,49,49,49	0
56	MG	2D	302	1/1	0.93	0.16	39,39,39,39	0
56	MG	2a	1811	1/1	0.93	0.15	71,71,71,71	0
56	MG	1A	3772	1/1	0.93	0.20	22,22,22,22	0
56	MG	2A	3108	1/1	0.93	0.30	49,49,49,49	0
56	MG	1a	3157	1/1	0.93	0.13	58,58,58,58	0
56	MG	1A	3953	1/1	0.93	0.15	40,40,40,40	0
56	MG	1A	3434	1/1	0.93	0.17	47,47,47,47	0
56	MG	2a	1685	1/1	0.93	0.10	53,53,53,53	0
56	MG	1a	3139	1/1	0.93	0.20	56,56,56,56	0
56	MG	2A	3135	1/1	0.93	0.25	49,49,49,49	0
56	MG	1a	3115	1/1	0.93	0.13	48,48,48,48	0
56	MG	1A	3493	1/1	0.93	0.32	23,23,23,23	0
56	MG	1A	3596	1/1	0.93	0.19	44,44,44,44	0
56	MG	2a	1730	1/1	0.93	0.11	65,65,65,65	0
56	MG	1A	3817	1/1	0.93	0.13	20,20,20,20	0
56	MG	1Z	3001	1/1	0.93	0.26	42,42,42,42	0
56	MG	2A	3309	1/1	0.93	0.15	52,52,52,52	0
56	MG	1A	3251	1/1	0.93	0.42	25,25,25,25	0
56	MG	1a	3117	1/1	0.93	0.09	27,27,27,27	0
56	MG	1A	3199	1/1	0.93	0.52	32,32,32,32	0
56	MG	1A	3098	1/1	0.93	0.51	36,36,36,36	0
56	MG	1B	218	1/1	0.93	0.19	40,40,40,40	0
56	MG	1A	3093	1/1	0.93	0.09	31,31,31,31	0
56	MG	2A	3254	1/1	0.93	0.17	34,34,34,34	0
56	MG	2A	3377	1/1	0.93	0.20	37,37,37,37	0
56	MG	1A	3330	1/1	0.93	0.17	28,28,28,28	0
56	MG	1E	307	1/1	0.93	0.55	50,50,50,50	0
56	MG	2a	1707	1/1	0.93	0.22	68,68,68,68	0
56	MG	1A	3897	1/1	0.93	0.14	44,44,44,44	0
56	MG	2a	1682	1/1	0.93	0.08	48,48,48,48	0
56	MG	1O	206	1/1	0.93	0.36	60,60,60,60	0
56	MG	2A	3184	1/1	0.93	0.31	52,52,52,52	0
56	MG	2A	3118	1/1	0.93	0.19	42,42,42,42	0
56	MG	2A	3079	1/1	0.93	0.09	57,57,57,57	0
56	MG	2A	3161	1/1	0.93	0.36	46,46,46,46	0
56	MG	2A	3614	1/1	0.93	0.12	51,51,51,51	0
56	MG	2A	3153	1/1	0.93	0.16	49,49,49,49	0
56	MG	2A	3253	1/1	0.93	0.54	68,68,68,68	0
56	MG	2A	3722	1/1	0.93	0.14	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	1A	3347	1/1	0.93	0.14	42,42,42,42	0
56	MG	2A	3683	1/1	0.93	0.28	42,42,42,42	0
56	MG	2A	3168	1/1	0.93	0.11	39,39,39,39	0
56	MG	1A	3202	1/1	0.93	0.29	27,27,27,27	0
56	MG	1A	3405	1/1	0.93	0.60	46,46,46,46	0
56	MG	1A	3244	1/1	0.93	0.24	34,34,34,34	0
56	MG	2A	3233	1/1	0.93	0.26	42,42,42,42	0
56	MG	2A	3178	1/1	0.93	0.17	44,44,44,44	0
56	MG	2A	3127	1/1	0.93	0.22	56,56,56,56	0
56	MG	2A	3199	1/1	0.93	0.12	53,53,53,53	0
56	MG	2a	1795	1/1	0.93	0.37	64,64,64,64	0
56	MG	1A	3252	1/1	0.93	0.29	32,32,32,32	0
56	MG	1A	3555	1/1	0.93	0.09	29,29,29,29	0
56	MG	1a	3146	1/1	0.93	0.16	64,64,64,64	0
56	MG	1A	3851	1/1	0.93	0.18	44,44,44,44	0
56	MG	2A	3406	1/1	0.93	0.13	40,40,40,40	0
56	MG	1A	3344	1/1	0.93	0.37	31,31,31,31	0
56	MG	1A	3019	1/1	0.93	0.16	32,32,32,32	0
56	MG	1A	3869	1/1	0.93	0.19	19,19,19,19	0
56	MG	2A	3255	1/1	0.93	0.22	54,54,54,54	0
56	MG	1A	3872	1/1	0.93	0.33	27,27,27,27	0
56	MG	1A	3570	1/1	0.93	0.19	57,57,57,57	0
56	MG	2A	3126	1/1	0.93	0.17	50,50,50,50	0
56	MG	2A	3106	1/1	0.93	0.08	50,50,50,50	0
56	MG	1A	3301	1/1	0.93	0.12	39,39,39,39	0
56	MG	1A	3058	1/1	0.93	0.19	33,33,33,33	0
56	MG	17	102	1/1	0.94	0.30	31,31,31,31	0
56	MG	2j	8002	1/1	0.94	0.05	62,62,62,62	0
56	MG	2A	3197	1/1	0.94	0.14	39,39,39,39	0
56	MG	1A	3885	1/1	0.94	0.12	16,16,16,16	0
56	MG	2U	201	1/1	0.94	0.08	49,49,49,49	0
56	MG	1A	3335	1/1	0.94	0.43	33,33,33,33	0
56	MG	1A	3606	1/1	0.94	0.18	61,61,61,61	0
56	MG	1A	3638	1/1	0.94	0.15	56,56,56,56	0
56	MG	1A	3307	1/1	0.94	0.10	49,49,49,49	0
56	MG	2A	3121	1/1	0.94	0.15	31,31,31,31	0
56	MG	1A	3029	1/1	0.94	0.36	17,17,17,17	0
56	MG	1a	3209	1/1	0.94	0.20	60,60,60,60	0
56	MG	1A	4013	1/1	0.94	0.13	21,21,21,21	0
56	MG	2V	3002	1/1	0.94	0.13	56,56,56,56	0
56	MG	2A	3304	1/1	0.94	0.20	49,49,49,49	0
56	MG	2A	3678	1/1	0.94	0.21	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	3039	1/1	0.94	0.18	26,26,26,26	0
56	MG	2a	1690	1/1	0.94	0.07	57,57,57,57	0
56	MG	2A	3123	1/1	0.94	0.07	58,58,58,58	0
56	MG	2A	3242	1/1	0.94	0.13	47,47,47,47	0
56	MG	1A	3449	1/1	0.94	0.19	52,52,52,52	0
56	MG	1A	3326	1/1	0.94	0.17	25,25,25,25	0
56	MG	2A	3314	1/1	0.94	0.37	40,40,40,40	0
56	MG	1A	3273	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3687	1/1	0.94	0.11	33,33,33,33	0
56	MG	1A	3312	1/1	0.94	0.24	42,42,42,42	0
56	MG	2A	3130	1/1	0.94	0.20	51,51,51,51	0
56	MG	2A	3563	1/1	0.94	0.19	55,55,55,55	0
56	MG	2a	1622	1/1	0.94	0.40	39,39,39,39	0
56	MG	2A	3154	1/1	0.94	0.32	51,51,51,51	0
56	MG	1A	3488	1/1	0.94	0.12	23,23,23,23	0
56	MG	2A	3626	1/1	0.94	0.16	46,46,46,46	0
56	MG	2A	3528	1/1	0.94	0.08	58,58,58,58	0
56	MG	2A	3485	1/1	0.94	0.22	56,56,56,56	0
56	MG	2A	3357	1/1	0.94	0.15	21,21,21,21	0
56	MG	2A	3409	1/1	0.94	0.11	54,54,54,54	0
56	MG	2A	3531	1/1	0.94	0.11	60,60,60,60	0
56	MG	1A	3382	1/1	0.94	0.12	41,41,41,41	0
56	MG	2A	3064	1/1	0.94	0.44	44,44,44,44	0
56	MG	1A	3934	1/1	0.94	0.16	22,22,22,22	0
56	MG	1A	3352	1/1	0.94	0.18	36,36,36,36	0
56	MG	1A	3626	1/1	0.94	0.14	23,23,23,23	0
56	MG	2A	3554	1/1	0.94	0.14	24,24,24,24	0
56	MG	2A	3654	1/1	0.94	0.26	33,33,33,33	0
56	MG	1B	214	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	4007	1/1	0.94	0.66	39,39,39,39	0
56	MG	1a	3124	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3432	1/1	0.94	0.30	56,56,56,56	0
56	MG	1A	3369	1/1	0.94	0.11	38,38,38,38	0
56	MG	2a	1608	1/1	0.94	0.14	47,47,47,47	0
56	MG	1a	3090	1/1	0.94	0.07	41,41,41,41	0
56	MG	1A	3407	1/1	0.94	0.08	45,45,45,45	0
56	MG	1A	3487	1/1	0.94	0.13	34,34,34,34	0
56	MG	2a	1727	1/1	0.94	0.12	87,87,87,87	0
56	MG	1a	3144	1/1	0.94	0.19	66,66,66,66	0
56	MG	2a	1670	1/1	0.94	0.11	55,55,55,55	0
56	MG	1A	3751	1/1	0.94	0.32	23,23,23,23	0
56	MG	1A	3536	1/1	0.94	0.08	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	3147	1/1	0.94	0.05	58,58,58,58	0
56	MG	1A	4011	1/1	0.94	0.21	37,37,37,37	0
56	MG	1A	3269	1/1	0.94	0.21	35,35,35,35	0
56	MG	1F	303	1/1	0.94	0.19	35,35,35,35	0
56	MG	2a	1628	1/1	0.94	0.30	49,49,49,49	0
56	MG	2A	3146	1/1	0.94	0.15	50,50,50,50	0
56	MG	2A	3055	1/1	0.94	0.16	44,44,44,44	0
56	MG	1A	3384	1/1	0.94	0.08	38,38,38,38	0
56	MG	2A	3442	1/1	0.94	0.17	23,23,23,23	0
56	MG	2A	3435	1/1	0.94	0.11	47,47,47,47	0
56	MG	1A	3174	1/1	0.94	0.39	32,32,32,32	0
56	MG	2A	3573	1/1	0.94	0.30	37,37,37,37	0
56	MG	1A	3228	1/1	0.94	0.29	40,40,40,40	0
56	MG	2A	3706	1/1	0.94	0.14	42,42,42,42	0
56	MG	2a	1785	1/1	0.94	0.15	63,63,63,63	0
56	MG	2a	1756	1/1	0.94	0.13	43,43,43,43	0
56	MG	2a	1654	1/1	0.94	0.27	58,58,58,58	0
56	MG	2A	3675	1/1	0.94	0.09	62,62,62,62	0
56	MG	1A	3443	1/1	0.94	0.15	32,32,32,32	0
56	MG	1A	3805	1/1	0.94	0.20	60,60,60,60	0
56	MG	2A	3574	1/1	0.94	0.07	46,46,46,46	0
56	MG	2a	1672	1/1	0.94	0.17	50,50,50,50	0
56	MG	2a	1652	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3827	1/1	0.94	0.13	47,47,47,47	0
56	MG	1A	3396	1/1	0.94	0.28	44,44,44,44	0
56	MG	2A	3061	1/1	0.94	0.17	30,30,30,30	0
56	MG	1A	3787	1/1	0.94	0.14	36,36,36,36	0
56	MG	1A	3303	1/1	0.94	0.16	44,44,44,44	0
56	MG	1a	3155	1/1	0.94	0.18	53,53,53,53	0
56	MG	2A	3287	1/1	0.94	0.25	47,47,47,47	0
56	MG	2a	1623	1/1	0.94	0.14	46,46,46,46	0
56	MG	1A	3378	1/1	0.94	0.40	27,27,27,27	0
56	MG	1A	3092	1/1	0.94	0.17	44,44,44,44	0
56	MG	1A	3076	1/1	0.94	0.25	26,26,26,26	0
56	MG	1A	3790	1/1	0.94	0.36	27,27,27,27	0
56	MG	2B	3007	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3709	1/1	0.94	0.17	30,30,30,30	0
56	MG	18	102	1/1	0.94	0.12	29,29,29,29	0
56	MG	2A	3373	1/1	0.94	0.17	25,25,25,25	0
56	MG	2A	3707	1/1	0.94	0.15	47,47,47,47	0
56	MG	1A	3756	1/1	0.94	0.65	27,27,27,27	0
56	MG	1A	3089	1/1	0.94	0.15	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2R	3004	1/1	0.94	0.19	49,49,49,49	0
56	MG	1A	4049	1/1	0.94	0.77	30,30,30,30	0
56	MG	1a	3178	1/1	0.94	0.06	54,54,54,54	0
56	MG	1A	4042	1/1	0.94	0.13	40,40,40,40	0
56	MG	1A	3457	1/1	0.94	0.14	32,32,32,32	0
56	MG	1A	4054	1/1	0.94	0.47	37,37,37,37	0
56	MG	1a	3012	1/1	0.94	0.10	41,41,41,41	0
56	MG	1A	3706	1/1	0.94	0.11	27,27,27,27	0
56	MG	1A	3134	1/1	0.94	0.46	30,30,30,30	0
56	MG	1A	3311	1/1	0.94	0.19	37,37,37,37	0
56	MG	2A	3182	1/1	0.94	0.64	43,43,43,43	0
56	MG	1x	108	1/1	0.94	0.13	61,61,61,61	0
56	MG	1A	4029	1/1	0.94	0.33	36,36,36,36	0
56	MG	1a	3004	1/1	0.94	0.14	50,50,50,50	0
56	MG	1A	3281	1/1	0.94	0.34	29,29,29,29	0
56	MG	1m	201	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3294	1/1	0.94	0.28	45,45,45,45	0
56	MG	1A	3919	1/1	0.94	0.15	42,42,42,42	0
56	MG	1A	3581	1/1	0.94	0.19	19,19,19,19	0
56	MG	2A	3543	1/1	0.94	0.13	45,45,45,45	0
56	MG	1A	3026	1/1	0.94	0.13	30,30,30,30	0
56	MG	1A	3276	1/1	0.94	0.16	40,40,40,40	0
56	MG	1A	3571	1/1	0.94	0.12	17,17,17,17	0
56	MG	2A	3718	1/1	0.94	0.10	56,56,56,56	0
56	MG	2A	3559	1/1	0.94	0.16	61,61,61,61	0
56	MG	1a	3062	1/1	0.94	0.08	36,36,36,36	0
56	MG	2A	3624	1/1	0.94	0.22	62,62,62,62	0
56	MG	2A	3444	1/1	0.94	0.20	42,42,42,42	0
56	MG	2A	3623	1/1	0.94	0.27	46,46,46,46	0
56	MG	2A	3142	1/1	0.94	0.13	46,46,46,46	0
56	MG	1a	3008	1/1	0.94	0.17	51,51,51,51	0
56	MG	2A	3431	1/1	0.94	0.17	24,24,24,24	0
56	MG	1a	3212	1/1	0.94	0.13	41,41,41,41	0
56	MG	1a	3051	1/1	0.94	0.12	55,55,55,55	0
56	MG	13	101	1/1	0.94	0.53	39,39,39,39	0
56	MG	2A	3632	1/1	0.94	0.32	62,62,62,62	0
56	MG	2a	1677	1/1	0.94	0.15	55,55,55,55	0
56	MG	1a	3167	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3208	1/1	0.94	0.14	29,29,29,29	0
56	MG	1D	302	1/1	0.94	0.19	21,21,21,21	0
56	MG	1a	3197	1/1	0.94	0.10	39,39,39,39	0
56	MG	1R	205	1/1	0.94	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3521	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3583	1/1	0.94	0.45	40,40,40,40	0
56	MG	2A	3378	1/1	0.94	0.16	25,25,25,25	0
56	MG	1B	224	1/1	0.94	0.09	54,54,54,54	0
56	MG	1A	3468	1/1	0.94	0.08	37,37,37,37	0
56	MG	1A	3646	1/1	0.94	0.16	19,19,19,19	0
56	MG	1a	3023	1/1	0.94	0.15	44,44,44,44	0
56	MG	1A	4043	1/1	0.94	0.45	23,23,23,23	0
56	MG	2W	201	1/1	0.94	0.16	50,50,50,50	0
56	MG	2A	3339	1/1	0.94	0.10	58,58,58,58	0
56	MG	1A	3256	1/1	0.94	0.10	33,33,33,33	0
56	MG	1a	3060	1/1	0.94	0.07	50,50,50,50	0
56	MG	1A	4001	1/1	0.94	0.11	45,45,45,45	0
56	MG	2A	3414	1/1	0.94	0.14	49,49,49,49	0
56	MG	2A	3278	1/1	0.94	0.14	57,57,57,57	0
56	MG	2A	3251	1/1	0.94	0.20	49,49,49,49	0
56	MG	2A	3007	1/1	0.94	0.10	32,32,32,32	0
56	MG	1A	3982	1/1	0.94	0.23	46,46,46,46	0
56	MG	2A	3417	1/1	0.94	0.18	35,35,35,35	0
56	MG	2A	3282	1/1	0.94	0.10	51,51,51,51	0
56	MG	2X	3001	1/1	0.94	0.14	46,46,46,46	0
56	MG	1a	3126	1/1	0.94	0.13	46,46,46,46	0
56	MG	2A	3056	1/1	0.94	0.09	52,52,52,52	0
56	MG	2A	3014	1/1	0.94	0.21	54,54,54,54	0
56	MG	2A	3113	1/1	0.94	0.21	48,48,48,48	0
56	MG	1l	201	1/1	0.94	0.17	31,31,31,31	0
56	MG	1A	3410	1/1	0.94	0.12	45,45,45,45	0
56	MG	2A	3070	1/1	0.94	0.15	33,33,33,33	0
56	MG	2a	1728	1/1	0.94	0.09	46,46,46,46	0
56	MG	1A	3462	1/1	0.94	0.31	22,22,22,22	0
56	MG	2A	3181	1/1	0.94	0.16	35,35,35,35	0
56	MG	2a	1720	1/1	0.94	0.18	66,66,66,66	0
56	MG	1A	3799	1/1	0.94	0.23	29,29,29,29	0
56	MG	2A	3667	1/1	0.94	0.11	63,63,63,63	0
56	MG	1A	3043	1/1	0.94	0.15	19,19,19,19	0
56	MG	2A	3470	1/1	0.94	0.22	53,53,53,53	0
56	MG	1A	4062	1/1	0.94	0.13	21,21,21,21	0
56	MG	1A	3841	1/1	0.94	0.14	33,33,33,33	0
56	MG	2A	3755	1/1	0.94	0.81	48,48,48,48	0
56	MG	1A	3564	1/1	0.94	0.21	36,36,36,36	0
56	MG	1X	103	1/1	0.94	0.25	29,29,29,29	0
56	MG	2A	3054	1/1	0.94	0.41	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	1B	215	1/1	0.94	0.06	34,34,34,34	0
56	MG	2A	3580	1/1	0.94	0.15	39,39,39,39	0
56	MG	1A	4037	1/1	0.94	0.55	28,28,28,28	0
56	MG	2A	3605	1/1	0.94	0.13	42,42,42,42	0
56	MG	1B	203	1/1	0.94	0.20	39,39,39,39	0
56	MG	1A	3274	1/1	0.94	0.22	40,40,40,40	0
56	MG	1A	3673	1/1	0.94	0.13	54,54,54,54	0
56	MG	1a	3191	1/1	0.94	0.08	53,53,53,53	0
56	MG	2A	3601	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3704	1/1	0.94	0.25	28,28,28,28	0
56	MG	2A	3101	1/1	0.94	0.17	30,30,30,30	0
58	EZG	1A	4030	25/25	0.94	0.27	19,29,40,41	0
56	MG	1A	3159	1/1	0.94	0.34	36,36,36,36	0
56	MG	1A	3272	1/1	0.94	0.12	34,34,34,34	0
56	MG	1A	3158	1/1	0.94	0.17	31,31,31,31	0
56	MG	1A	3747	1/1	0.94	0.08	31,31,31,31	0
56	MG	2a	1675	1/1	0.94	0.07	53,53,53,53	0
56	MG	2A	3655	1/1	0.94	0.15	53,53,53,53	0
56	MG	2A	3265	1/1	0.94	0.17	46,46,46,46	0
56	MG	1A	3526	1/1	0.94	0.22	42,42,42,42	0
56	MG	1A	3988	1/1	0.94	0.09	34,34,34,34	0
56	MG	1a	3067	1/1	0.94	0.16	46,46,46,46	0
56	MG	2V	3001	1/1	0.94	0.39	46,46,46,46	0
56	MG	1A	3943	1/1	0.94	0.16	38,38,38,38	0
56	MG	1A	3514	1/1	0.94	0.17	21,21,21,21	0
56	MG	1A	3857	1/1	0.94	0.16	32,32,32,32	0
56	MG	1a	3135	1/1	0.94	0.12	52,52,52,52	0
56	MG	25	502	1/1	0.94	0.59	47,47,47,47	0
56	MG	1A	4004	1/1	0.94	0.27	55,55,55,55	0
56	MG	1B	225	1/1	0.94	0.17	57,57,57,57	0
56	MG	17	101	1/1	0.94	0.19	27,27,27,27	0
56	MG	1A	3826	1/1	0.94	0.16	27,27,27,27	0
56	MG	1A	3940	1/1	0.94	0.10	29,29,29,29	0
56	MG	2A	3651	1/1	0.94	0.13	42,42,42,42	0
56	MG	2A	3157	1/1	0.94	0.11	51,51,51,51	0
56	MG	1a	3148	1/1	0.94	0.09	55,55,55,55	0
56	MG	1G	3004	1/1	0.94	0.11	38,38,38,38	0
56	MG	2A	3152	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	3004	1/1	0.94	0.16	21,21,21,21	0
56	MG	1A	3928	1/1	0.94	0.17	37,37,37,37	0
56	MG	1A	3981	1/1	0.94	0.12	30,30,30,30	0
56	MG	1A	3504	1/1	0.94	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	3196	1/1	0.94	0.07	46,46,46,46	0
56	MG	15	101	1/1	0.94	0.38	27,27,27,27	0
56	MG	2A	3110	1/1	0.94	0.18	37,37,37,37	0
56	MG	1A	3695	1/1	0.94	0.21	50,50,50,50	0
56	MG	2a	1716	1/1	0.94	0.18	43,43,43,43	0
56	MG	1A	3168	1/1	0.94	0.19	43,43,43,43	0
56	MG	1U	203	1/1	0.94	0.23	23,23,23,23	0
56	MG	2A	3461	1/1	0.94	0.15	45,45,45,45	0
56	MG	1B	202	1/1	0.94	0.24	42,42,42,42	0
56	MG	2A	3112	1/1	0.94	0.12	52,52,52,52	0
56	MG	1A	3075	1/1	0.94	0.13	34,34,34,34	0
56	MG	2A	3578	1/1	0.94	0.20	27,27,27,27	0
56	MG	1A	3073	1/1	0.94	0.48	42,42,42,42	0
56	MG	1A	3624	1/1	0.94	0.13	26,26,26,26	0
56	MG	1A	3061	1/1	0.94	0.11	39,39,39,39	0
56	MG	2A	3677	1/1	0.94	0.15	48,48,48,48	0
56	MG	1A	3080	1/1	0.94	0.24	41,41,41,41	0
56	MG	2O	8002	1/1	0.94	0.12	52,52,52,52	0
56	MG	1A	3845	1/1	0.94	0.30	42,42,42,42	0
56	MG	1A	3710	1/1	0.94	0.20	28,28,28,28	0
56	MG	1A	3942	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	3992	1/1	0.94	0.18	49,49,49,49	0
56	MG	1A	3005	1/1	0.94	0.13	36,36,36,36	0
56	MG	2A	3340	1/1	0.94	0.19	30,30,30,30	0
56	MG	1A	3389	1/1	0.94	0.21	34,34,34,34	0
56	MG	2A	3104	1/1	0.94	0.12	51,51,51,51	0
56	MG	2A	3326	1/1	0.94	0.11	48,48,48,48	0
56	MG	1A	3210	1/1	0.94	0.42	25,25,25,25	0
56	MG	2A	3421	1/1	0.94	0.11	39,39,39,39	0
56	MG	1B	230	1/1	0.94	0.31	42,42,42,42	0
56	MG	2d	503	1/1	0.94	0.12	56,56,56,56	0
56	MG	2A	3004	1/1	0.94	0.14	37,37,37,37	0
56	MG	1A	3323	1/1	0.94	0.22	19,19,19,19	0
56	MG	2A	3495	1/1	0.94	0.28	60,60,60,60	0
56	MG	2A	3080	1/1	0.94	0.11	28,28,28,28	0
56	MG	2A	3351	1/1	0.94	0.13	43,43,43,43	0
56	MG	1b	3002	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3478	1/1	0.94	0.20	47,47,47,47	0
56	MG	1A	4052	1/1	0.94	0.40	31,31,31,31	0
56	MG	1A	3205	1/1	0.94	0.59	28,28,28,28	0
56	MG	1A	3572	1/1	0.95	0.20	12,12,12,12	0
56	MG	1A	3102	1/1	0.95	0.27	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3327	1/1	0.95	0.18	10,10,10,10	0
56	MG	2B	3006	1/1	0.95	0.17	65,65,65,65	0
56	MG	2A	3643	1/1	0.95	0.08	43,43,43,43	0
56	MG	2A	3487	1/1	0.95	0.20	62,62,62,62	0
56	MG	2A	3180	1/1	0.95	0.24	33,33,33,33	0
56	MG	1A	3532	1/1	0.95	0.16	29,29,29,29	0
56	MG	1a	3138	1/1	0.95	0.16	66,66,66,66	0
56	MG	2B	3004	1/1	0.95	0.16	60,60,60,60	0
56	MG	1A	3418	1/1	0.95	0.56	30,30,30,30	0
56	MG	1A	3204	1/1	0.95	0.29	39,39,39,39	0
56	MG	2A	3333	1/1	0.95	0.12	25,25,25,25	0
56	MG	1A	3185	1/1	0.95	0.15	26,26,26,26	0
56	MG	2A	3596	1/1	0.95	0.15	32,32,32,32	0
56	MG	1A	3682	1/1	0.95	0.09	55,55,55,55	0
56	MG	1A	3901	1/1	0.95	0.30	44,44,44,44	0
56	MG	2A	3719	1/1	0.95	0.14	70,70,70,70	0
56	MG	1A	3422	1/1	0.95	0.50	43,43,43,43	0
56	MG	2A	3585	1/1	0.95	0.20	34,34,34,34	0
56	MG	1A	3582	1/1	0.95	0.12	26,26,26,26	0
56	MG	2A	3413	1/1	0.95	0.16	55,55,55,55	0
56	MG	1w	105	1/1	0.95	0.12	64,64,64,64	0
56	MG	1A	3016	1/1	0.95	0.20	40,40,40,40	0
56	MG	2a	1823	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3637	1/1	0.95	0.13	20,20,20,20	0
56	MG	1a	3039	1/1	0.95	0.10	47,47,47,47	0
56	MG	2A	3023	1/1	0.95	0.12	41,41,41,41	0
56	MG	1A	3177	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	3494	1/1	0.95	0.11	35,35,35,35	0
56	MG	2A	3430	1/1	0.95	0.11	53,53,53,53	0
56	MG	1x	104	1/1	0.95	0.22	54,54,54,54	0
56	MG	1A	3056	1/1	0.95	0.14	50,50,50,50	0
56	MG	10	102	1/1	0.95	0.23	25,25,25,25	0
56	MG	1A	3597	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	4035	1/1	0.95	0.10	38,38,38,38	0
56	MG	1A	3300	1/1	0.95	0.18	29,29,29,29	0
56	MG	1A	3576	1/1	0.95	0.15	15,15,15,15	0
56	MG	1A	3694	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3234	1/1	0.95	0.11	43,43,43,43	0
56	MG	1a	3056	1/1	0.95	0.11	50,50,50,50	0
56	MG	1x	112	1/1	0.95	0.16	45,45,45,45	0
56	MG	1A	3125	1/1	0.95	0.28	19,19,19,19	0
56	MG	2a	1683	1/1	0.95	0.20	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3467	1/1	0.95	0.27	49,49,49,49	0
56	MG	2a	1632	1/1	0.95	0.11	67,67,67,67	0
56	MG	1A	3412	1/1	0.95	0.37	37,37,37,37	0
56	MG	1A	3146	1/1	0.95	0.55	23,23,23,23	0
56	MG	1a	3151	1/1	0.95	0.20	62,62,62,62	0
56	MG	1A	3187	1/1	0.95	0.08	28,28,28,28	0
56	MG	2a	1692	1/1	0.95	0.32	60,60,60,60	0
56	MG	1a	3188	1/1	0.95	0.10	47,47,47,47	0
56	MG	1a	3200	1/1	0.95	0.15	41,41,41,41	0
56	MG	1U	205	1/1	0.95	0.20	23,23,23,23	0
56	MG	1A	3720	1/1	0.95	0.14	41,41,41,41	0
56	MG	2A	3372	1/1	0.95	0.23	42,42,42,42	0
56	MG	1A	3879	1/1	0.95	0.18	18,18,18,18	0
56	MG	1A	3740	1/1	0.95	0.15	46,46,46,46	0
56	MG	1A	3569	1/1	0.95	0.14	17,17,17,17	0
56	MG	1A	3079	1/1	0.95	0.16	32,32,32,32	0
56	MG	2a	1746	1/1	0.95	0.08	67,67,67,67	0
56	MG	1A	3533	1/1	0.95	0.10	47,47,47,47	0
56	MG	1a	3033	1/1	0.95	0.07	57,57,57,57	0
56	MG	1A	3324	1/1	0.95	0.13	33,33,33,33	0
56	MG	2A	3290	1/1	0.95	0.19	39,39,39,39	0
56	MG	1A	3112	1/1	0.95	0.16	40,40,40,40	0
56	MG	1A	3912	1/1	0.95	0.15	25,25,25,25	0
56	MG	1A	3428	1/1	0.95	0.21	26,26,26,26	0
56	MG	1A	3059	1/1	0.95	0.20	36,36,36,36	0
56	MG	2A	3107	1/1	0.95	0.17	27,27,27,27	0
56	MG	1A	3421	1/1	0.95	0.46	37,37,37,37	0
56	MG	1A	3129	1/1	0.95	0.36	27,27,27,27	0
56	MG	1A	3905	1/1	0.95	0.07	54,54,54,54	0
56	MG	1A	3062	1/1	0.95	0.11	12,12,12,12	0
56	MG	1A	3285	1/1	0.95	0.14	34,34,34,34	0
56	MG	1W	3003	1/1	0.95	0.10	33,33,33,33	0
56	MG	1A	3899	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	3247	1/1	0.95	0.23	27,27,27,27	0
56	MG	1A	3659	1/1	0.95	0.20	40,40,40,40	0
56	MG	1a	3037	1/1	0.95	0.14	61,61,61,61	0
56	MG	1A	3160	1/1	0.95	0.60	29,29,29,29	0
56	MG	2A	3274	1/1	0.95	0.29	45,45,45,45	0
56	MG	1A	3616	1/1	0.95	0.16	58,58,58,58	0
56	MG	1A	3322	1/1	0.95	0.36	38,38,38,38	0
56	MG	1A	4008	1/1	0.95	0.36	24,24,24,24	0
56	MG	1A	3808	1/1	0.95	0.17	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3419	1/1	0.95	0.07	55,55,55,55	0
56	MG	2A	3040	1/1	0.95	0.34	39,39,39,39	0
56	MG	1A	3232	1/1	0.95	0.10	17,17,17,17	0
56	MG	1A	3726	1/1	0.95	0.06	35,35,35,35	0
56	MG	2A	3526	1/1	0.95	0.11	49,49,49,49	0
56	MG	2a	1789	1/1	0.95	0.09	54,54,54,54	0
56	MG	2D	305	1/1	0.95	0.10	29,29,29,29	0
56	MG	1A	3714	1/1	0.95	0.19	26,26,26,26	0
56	MG	1A	3979	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3777	1/1	0.95	0.10	36,36,36,36	0
56	MG	2A	3227	1/1	0.95	0.09	40,40,40,40	0
56	MG	1a	3042	1/1	0.95	0.18	44,44,44,44	0
56	MG	1A	3647	1/1	0.95	0.16	16,16,16,16	0
56	MG	1a	3132	1/1	0.95	0.08	34,34,34,34	0
56	MG	1A	3956	1/1	0.95	0.07	67,67,67,67	0
56	MG	1x	106	1/1	0.95	0.15	66,66,66,66	0
56	MG	1A	3767	1/1	0.95	0.10	41,41,41,41	0
56	MG	1A	3782	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	3551	1/1	0.95	0.15	17,17,17,17	0
56	MG	1A	3528	1/1	0.95	0.15	23,23,23,23	0
56	MG	1a	3021	1/1	0.95	0.14	40,40,40,40	0
56	MG	1a	3210	1/1	0.95	0.14	41,41,41,41	0
56	MG	2A	3100	1/1	0.95	0.15	59,59,59,59	0
56	MG	2A	3579	1/1	0.95	0.09	51,51,51,51	0
56	MG	2A	3237	1/1	0.95	0.15	43,43,43,43	0
56	MG	2A	3365	1/1	0.95	0.11	38,38,38,38	0
56	MG	1a	3118	1/1	0.95	0.09	65,65,65,65	0
56	MG	2a	1680	1/1	0.95	0.16	45,45,45,45	0
56	MG	2A	3301	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3629	1/1	0.95	0.23	60,60,60,60	0
56	MG	2a	1828	1/1	0.95	0.22	64,64,64,64	0
56	MG	1a	3065	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	4040	1/1	0.95	0.47	34,34,34,34	0
56	MG	2a	1831	1/1	0.95	0.09	53,53,53,53	0
56	MG	1a	3122	1/1	0.95	0.11	40,40,40,40	0
56	MG	2A	3494	1/1	0.95	0.26	49,49,49,49	0
56	MG	1A	3613	1/1	0.95	0.10	30,30,30,30	0
56	MG	2A	3173	1/1	0.95	0.14	45,45,45,45	0
56	MG	2A	3005	1/1	0.95	0.11	42,42,42,42	0
56	MG	1B	201	1/1	0.95	0.10	49,49,49,49	0
56	MG	2A	3010	1/1	0.95	0.18	31,31,31,31	0
56	MG	1A	3703	1/1	0.95	0.22	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3319	1/1	0.95	0.13	62,62,62,62	0
56	MG	1V	203	1/1	0.95	0.21	63,63,63,63	0
56	MG	2A	3132	1/1	0.95	0.07	58,58,58,58	0
56	MG	2A	3189	1/1	0.95	0.07	38,38,38,38	0
56	MG	1B	221	1/1	0.95	0.10	36,36,36,36	0
56	MG	1A	3926	1/1	0.95	0.16	18,18,18,18	0
56	MG	1A	3750	1/1	0.95	0.08	31,31,31,31	0
56	MG	2A	3380	1/1	0.95	0.17	25,25,25,25	0
56	MG	1I	103	1/1	0.95	0.08	31,31,31,31	0
56	MG	1A	3785	1/1	0.95	0.20	35,35,35,35	0
56	MG	2a	1809	1/1	0.95	0.15	58,58,58,58	0
56	MG	2A	3726	1/1	0.95	0.17	43,43,43,43	0
56	MG	2a	1718	1/1	0.95	0.14	55,55,55,55	0
56	MG	2A	3348	1/1	0.95	0.13	47,47,47,47	0
56	MG	2B	3011	1/1	0.95	0.14	69,69,69,69	0
56	MG	2A	3337	1/1	0.95	0.27	27,27,27,27	0
56	MG	2A	3599	1/1	0.95	0.09	61,61,61,61	0
56	MG	1A	3401	1/1	0.95	0.10	38,38,38,38	0
56	MG	2a	1771	1/1	0.95	0.11	62,62,62,62	0
56	MG	1B	237	1/1	0.95	0.16	46,46,46,46	0
56	MG	2A	3566	1/1	0.95	0.13	56,56,56,56	0
56	MG	1B	233	1/1	0.95	0.13	50,50,50,50	0
56	MG	2a	1779	1/1	0.95	0.11	60,60,60,60	0
56	MG	1A	3833	1/1	0.95	0.14	58,58,58,58	0
56	MG	2A	3600	1/1	0.95	0.11	56,56,56,56	0
56	MG	1A	3381	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3471	1/1	0.95	0.23	45,45,45,45	0
56	MG	1A	4046	1/1	0.95	0.44	20,20,20,20	0
56	MG	1a	3005	1/1	0.95	0.11	41,41,41,41	0
56	MG	1A	3279	1/1	0.95	0.18	41,41,41,41	0
56	MG	1a	3163	1/1	0.95	0.17	47,47,47,47	0
56	MG	1A	3724	1/1	0.95	0.10	44,44,44,44	0
56	MG	1A	3664	1/1	0.95	0.19	43,43,43,43	0
56	MG	2A	3499	1/1	0.95	0.15	41,41,41,41	0
56	MG	1a	3183	1/1	0.95	0.10	51,51,51,51	0
56	MG	2D	301	1/1	0.95	0.24	54,54,54,54	0
56	MG	1A	4058	1/1	0.95	0.24	69,69,69,69	0
56	MG	2a	1782	1/1	0.95	0.14	58,58,58,58	0
56	MG	18	103	1/1	0.95	0.22	41,41,41,41	0
56	MG	2A	3748	1/1	0.95	0.14	27,27,27,27	0
56	MG	2a	1629	1/1	0.95	0.18	73,73,73,73	0
56	MG	2A	3498	1/1	0.95	0.06	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	1D	314	1/1	0.95	0.30	29,29,29,29	0
56	MG	1A	3524	1/1	0.95	0.16	20,20,20,20	0
56	MG	1A	3111	1/1	0.95	0.28	30,30,30,30	0
56	MG	2a	1744	1/1	0.95	0.11	67,67,67,67	0
56	MG	2A	3214	1/1	0.95	0.08	49,49,49,49	0
56	MG	2A	3564	1/1	0.95	0.17	42,42,42,42	0
56	MG	2w	104	1/1	0.95	0.14	83,83,83,83	0
56	MG	2A	3297	1/1	0.95	0.24	51,51,51,51	0
56	MG	2A	3427	1/1	0.95	0.08	46,46,46,46	0
56	MG	1a	3097	1/1	0.95	0.08	62,62,62,62	0
56	MG	1A	4039	1/1	0.95	0.45	33,33,33,33	0
56	MG	2A	3479	1/1	0.95	0.15	34,34,34,34	0
56	MG	1A	3611	1/1	0.95	0.19	45,45,45,45	0
56	MG	2A	3645	1/1	0.95	0.15	33,33,33,33	0
56	MG	2A	3385	1/1	0.95	0.21	27,27,27,27	0
56	MG	1A	3151	1/1	0.95	0.21	36,36,36,36	0
56	MG	1A	3354	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3562	1/1	0.95	0.16	18,18,18,18	0
56	MG	2A	3350	1/1	0.95	0.13	50,50,50,50	0
56	MG	1x	105	1/1	0.95	0.13	59,59,59,59	0
56	MG	2f	3001	1/1	0.95	0.11	40,40,40,40	0
56	MG	1G	3003	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3975	1/1	0.95	0.08	51,51,51,51	0
56	MG	2a	1777	1/1	0.95	0.10	55,55,55,55	0
56	MG	1A	3973	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	3627	1/1	0.95	0.13	26,26,26,26	0
56	MG	2A	3725	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	3763	1/1	0.95	0.15	22,22,22,22	0
56	MG	1A	3342	1/1	0.95	0.32	21,21,21,21	0
56	MG	2A	3027	1/1	0.95	0.14	32,32,32,32	0
56	MG	1A	3372	1/1	0.95	0.13	35,35,35,35	0
56	MG	1A	3575	1/1	0.95	0.12	11,11,11,11	0
56	MG	2A	3577	1/1	0.95	0.21	45,45,45,45	0
56	MG	1A	3788	1/1	0.95	0.10	25,25,25,25	0
56	MG	2A	3240	1/1	0.95	0.12	51,51,51,51	0
56	MG	1A	3600	1/1	0.95	0.26	50,50,50,50	0
56	MG	1A	3961	1/1	0.95	0.10	36,36,36,36	0
56	MG	2a	1635	1/1	0.95	0.15	39,39,39,39	0
56	MG	1A	3492	1/1	0.95	0.25	35,35,35,35	0
56	MG	2A	3454	1/1	0.95	0.14	52,52,52,52	0
56	MG	2a	1725	1/1	0.95	0.14	49,49,49,49	0
56	MG	2A	3665	1/1	0.95	0.11	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	2A	3448	1/1	0.95	0.14	33,33,33,33	0
56	MG	2a	1794	1/1	0.95	0.15	58,58,58,58	0
56	MG	1a	3133	1/1	0.95	0.15	47,47,47,47	0
56	MG	1A	3351	1/1	0.95	0.11	34,34,34,34	0
56	MG	1A	3103	1/1	0.95	0.25	33,33,33,33	0
56	MG	1A	4003	1/1	0.95	0.10	32,32,32,32	0
56	MG	2A	3699	1/1	0.95	0.11	39,39,39,39	0
56	MG	1A	3650	1/1	0.95	0.17	34,34,34,34	0
56	MG	1A	4002	1/1	0.95	0.15	32,32,32,32	0
56	MG	1a	3007	1/1	0.95	0.17	50,50,50,50	0
56	MG	2a	1721	1/1	0.95	0.04	73,73,73,73	0
56	MG	2A	3141	1/1	0.95	0.13	40,40,40,40	0
56	MG	1A	3542	1/1	0.95	0.16	44,44,44,44	0
56	MG	1a	3187	1/1	0.95	0.06	43,43,43,43	0
56	MG	1B	235	1/1	0.95	0.16	55,55,55,55	0
56	MG	1A	3722	1/1	0.95	0.14	29,29,29,29	0
56	MG	1A	3078	1/1	0.95	0.39	26,26,26,26	0
56	MG	1A	3969	1/1	0.95	0.13	41,41,41,41	0
56	MG	1y	104	1/1	0.95	0.13	44,44,44,44	0
56	MG	1A	4061	1/1	0.95	0.31	38,38,38,38	0
56	MG	1A	3768	1/1	0.95	0.06	33,33,33,33	0
56	MG	2A	3438	1/1	0.95	0.10	36,36,36,36	0
56	MG	1A	3913	1/1	0.95	0.25	39,39,39,39	0
56	MG	1a	3087	1/1	0.95	0.19	44,44,44,44	0
56	MG	1D	309	1/1	0.95	0.23	28,28,28,28	0
56	MG	1a	3108	1/1	0.95	0.21	40,40,40,40	0
56	MG	2A	3474	1/1	0.95	0.15	35,35,35,35	0
56	MG	1A	3890	1/1	0.95	0.15	36,36,36,36	0
56	MG	1A	3683	1/1	0.95	0.28	41,41,41,41	0
56	MG	2A	3610	1/1	0.95	0.12	47,47,47,47	0
56	MG	1A	3259	1/1	0.95	0.16	45,45,45,45	0
56	MG	2a	1754	1/1	0.95	0.09	61,61,61,61	0
56	MG	2A	3230	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3124	1/1	0.95	0.18	48,48,48,48	0
56	MG	2a	1817	1/1	0.95	0.16	51,51,51,51	0
56	MG	1a	3158	1/1	0.95	0.06	47,47,47,47	0
56	MG	2A	3295	1/1	0.95	0.26	43,43,43,43	0
56	MG	2Q	3001	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3345	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3475	1/1	0.95	0.27	28,28,28,28	0
56	MG	1A	3731	1/1	0.95	0.21	16,16,16,16	0
56	MG	2A	3598	1/1	0.95	0.14	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	3211	1/1	0.95	0.15	35,35,35,35	0
56	MG	2B	3015	1/1	0.95	0.14	51,51,51,51	0
56	MG	2a	1803	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3950	1/1	0.95	0.14	54,54,54,54	0
56	MG	1A	3388	1/1	0.95	0.19	30,30,30,30	0
56	MG	2A	3264	1/1	0.95	0.40	47,47,47,47	0
56	MG	1A	3193	1/1	0.95	0.18	30,30,30,30	0
56	MG	1A	4055	1/1	0.95	0.66	31,31,31,31	0
56	MG	1A	3574	1/1	0.95	0.15	16,16,16,16	0
56	MG	1a	3169	1/1	0.95	0.09	38,38,38,38	0
56	MG	2A	3069	1/1	0.95	0.23	39,39,39,39	0
56	MG	1a	3019	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3271	1/1	0.95	0.25	45,45,45,45	0
56	MG	2A	3081	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3096	1/1	0.95	0.25	26,26,26,26	0
56	MG	1a	3066	1/1	0.95	0.10	58,58,58,58	0
56	MG	2a	1618	1/1	0.95	0.43	51,51,51,51	0
56	MG	2a	1655	1/1	0.95	0.17	67,67,67,67	0
56	MG	2A	3200	1/1	0.95	0.24	50,50,50,50	0
56	MG	1a	3074	1/1	0.95	0.16	49,49,49,49	0
56	MG	2A	3513	1/1	0.95	0.11	52,52,52,52	0
56	MG	2A	3567	1/1	0.95	0.10	44,44,44,44	0
56	MG	1A	3545	1/1	0.95	0.15	25,25,25,25	0
56	MG	1A	3976	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3549	1/1	0.95	0.15	43,43,43,43	0
56	MG	2A	3576	1/1	0.95	0.10	52,52,52,52	0
56	MG	2A	3533	1/1	0.95	0.34	52,52,52,52	0
56	MG	1A	3818	1/1	0.95	0.05	21,21,21,21	0
56	MG	2A	3716	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3082	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	4022	1/1	0.95	0.14	46,46,46,46	0
56	MG	2A	3095	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3190	1/1	0.96	0.13	44,44,44,44	0
56	MG	2A	3012	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3733	1/1	0.96	0.07	55,55,55,55	0
56	MG	2A	3342	1/1	0.96	0.18	49,49,49,49	0
56	MG	1w	104	1/1	0.96	0.07	36,36,36,36	0
56	MG	1a	3171	1/1	0.96	0.07	55,55,55,55	0
56	MG	1A	3191	1/1	0.96	0.21	24,24,24,24	0
56	MG	1U	202	1/1	0.96	0.11	30,30,30,30	0
56	MG	1A	3474	1/1	0.96	0.17	38,38,38,38	0
56	MG	1A	3253	1/1	0.96	0.72	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3852	1/1	0.96	0.15	55,55,55,55	0
56	MG	1A	3508	1/1	0.96	0.10	26,26,26,26	0
56	MG	1R	201	1/1	0.96	0.16	36,36,36,36	0
56	MG	1A	3963	1/1	0.96	0.08	33,33,33,33	0
56	MG	1A	3216	1/1	0.96	0.14	25,25,25,25	0
56	MG	1A	3550	1/1	0.96	0.19	26,26,26,26	0
56	MG	2A	3637	1/1	0.96	0.10	53,53,53,53	0
56	MG	2A	3028	1/1	0.96	0.17	42,42,42,42	0
56	MG	2A	3727	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3081	1/1	0.96	0.17	24,24,24,24	0
56	MG	1A	3212	1/1	0.96	0.18	50,50,50,50	0
56	MG	1A	3594	1/1	0.96	0.32	46,46,46,46	0
56	MG	1A	3675	1/1	0.96	0.15	66,66,66,66	0
56	MG	2A	3066	1/1	0.96	0.57	40,40,40,40	0
56	MG	1X	105	1/1	0.96	0.16	44,44,44,44	0
56	MG	2A	3679	1/1	0.96	0.15	49,49,49,49	0
56	MG	2a	1625	1/1	0.96	0.10	67,67,67,67	0
56	MG	1A	3213	1/1	0.96	0.18	36,36,36,36	0
56	MG	2A	3749	1/1	0.96	0.36	34,34,34,34	0
56	MG	1A	3138	1/1	0.96	0.46	30,30,30,30	0
56	MG	1A	3362	1/1	0.96	0.25	33,33,33,33	0
56	MG	2A	3617	1/1	0.96	0.24	43,43,43,43	0
56	MG	2A	3317	1/1	0.96	0.25	36,36,36,36	0
56	MG	2A	3664	1/1	0.96	0.21	41,41,41,41	0
56	MG	1A	3847	1/1	0.96	0.14	18,18,18,18	0
56	MG	1A	3402	1/1	0.96	0.08	28,28,28,28	0
56	MG	1A	3400	1/1	0.96	0.17	33,33,33,33	0
56	MG	1A	3290	1/1	0.96	0.10	46,46,46,46	0
56	MG	1a	3120	1/1	0.96	0.08	43,43,43,43	0
56	MG	2A	3352	1/1	0.96	0.10	50,50,50,50	0
56	MG	1A	3278	1/1	0.96	0.18	40,40,40,40	0
56	MG	1A	3546	1/1	0.96	0.11	14,14,14,14	0
56	MG	2a	1606	1/1	0.96	0.07	43,43,43,43	0
56	MG	2e	3001	1/1	0.96	0.11	60,60,60,60	0
56	MG	1y	101	1/1	0.96	0.10	35,35,35,35	0
56	MG	1A	3765	1/1	0.96	0.20	19,19,19,19	0
56	MG	2R	3003	1/1	0.96	0.15	48,48,48,48	0
56	MG	2A	3642	1/1	0.96	0.12	43,43,43,43	0
56	MG	1A	4023	1/1	0.96	0.56	21,21,21,21	0
56	MG	1A	3813	1/1	0.96	0.16	29,29,29,29	0
56	MG	1A	3877	1/1	0.96	0.20	28,28,28,28	0
56	MG	2x	102	1/1	0.96	0.19	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	3167	1/1	0.96	0.22	47,47,47,47	0
56	MG	2A	3537	1/1	0.96	0.15	46,46,46,46	0
56	MG	1F	305	1/1	0.96	0.39	28,28,28,28	0
56	MG	1A	3503	1/1	0.96	0.18	22,22,22,22	0
56	MG	1a	3081	1/1	0.96	0.09	67,67,67,67	0
56	MG	1A	3929	1/1	0.96	0.33	35,35,35,35	0
56	MG	2A	3464	1/1	0.96	0.25	29,29,29,29	0
56	MG	1a	3145	1/1	0.96	0.22	48,48,48,48	0
56	MG	1B	227	1/1	0.96	0.12	36,36,36,36	0
56	MG	1a	3152	1/1	0.96	0.10	60,60,60,60	0
56	MG	1A	3547	1/1	0.96	0.13	22,22,22,22	0
56	MG	2A	3680	1/1	0.96	0.08	62,62,62,62	0
56	MG	1A	3359	1/1	0.96	0.12	32,32,32,32	0
56	MG	1R	202	1/1	0.96	0.08	30,30,30,30	0
56	MG	2A	3510	1/1	0.96	0.11	50,50,50,50	0
56	MG	2A	3310	1/1	0.96	0.11	58,58,58,58	0
56	MG	1A	3771	1/1	0.96	0.18	17,17,17,17	0
56	MG	2a	1774	1/1	0.96	0.15	44,44,44,44	0
56	MG	1W	3001	1/1	0.96	0.19	34,34,34,34	0
59	ZN	2n	501	1/1	0.96	0.05	93,93,93,93	0
56	MG	2a	1825	1/1	0.96	0.17	56,56,56,56	0
56	MG	2A	3105	1/1	0.96	0.22	34,34,34,34	0
56	MG	1a	3075	1/1	0.96	0.11	46,46,46,46	0
56	MG	1A	3630	1/1	0.96	0.24	38,38,38,38	0
56	MG	1a	3119	1/1	0.96	0.15	52,52,52,52	0
56	MG	1P	201	1/1	0.96	0.46	16,16,16,16	0
56	MG	1A	3360	1/1	0.96	0.18	32,32,32,32	0
56	MG	2A	3399	1/1	0.96	0.19	57,57,57,57	0
56	MG	1a	3110	1/1	0.96	0.13	50,50,50,50	0
56	MG	1A	3719	1/1	0.96	0.08	47,47,47,47	0
56	MG	2A	3670	1/1	0.96	0.18	46,46,46,46	0
56	MG	2A	3493	1/1	0.96	0.09	28,28,28,28	0
56	MG	1A	3888	1/1	0.96	0.14	15,15,15,15	0
56	MG	2A	3246	1/1	0.96	0.24	48,48,48,48	0
56	MG	1A	3113	1/1	0.96	0.48	27,27,27,27	0
56	MG	1A	3598	1/1	0.96	0.34	48,48,48,48	0
56	MG	1P	202	1/1	0.96	0.27	23,23,23,23	0
56	MG	1A	3684	1/1	0.96	0.12	44,44,44,44	0
56	MG	1A	3886	1/1	0.96	0.10	24,24,24,24	0
56	MG	2A	3391	1/1	0.96	0.14	41,41,41,41	0
56	MG	1A	3591	1/1	0.96	0.16	30,30,30,30	0
56	MG	1A	3063	1/1	0.96	0.31	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3119	1/1	0.96	0.18	49,49,49,49	0
56	MG	1A	3440	1/1	0.96	0.33	28,28,28,28	0
56	MG	1A	3553	1/1	0.96	0.14	10,10,10,10	0
56	MG	2a	1768	1/1	0.96	0.05	55,55,55,55	0
56	MG	1A	3235	1/1	0.96	0.14	22,22,22,22	0
56	MG	1A	3853	1/1	0.96	0.07	38,38,38,38	0
56	MG	2A	3074	1/1	0.96	0.15	32,32,32,32	0
56	MG	2A	3039	1/1	0.96	0.15	25,25,25,25	0
56	MG	1a	3137	1/1	0.96	0.15	51,51,51,51	0
56	MG	2B	3005	1/1	0.96	0.10	55,55,55,55	0
56	MG	1A	3123	1/1	0.96	0.16	21,21,21,21	0
56	MG	1a	3140	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3403	1/1	0.96	0.23	33,33,33,33	0
56	MG	1A	3399	1/1	0.96	0.14	42,42,42,42	0
56	MG	2A	3724	1/1	0.96	0.15	66,66,66,66	0
56	MG	2A	3371	1/1	0.96	0.19	22,22,22,22	0
56	MG	1a	3113	1/1	0.96	0.14	40,40,40,40	0
56	MG	2A	3169	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3649	1/1	0.96	0.19	16,16,16,16	0
56	MG	1F	304	1/1	0.96	0.34	20,20,20,20	0
56	MG	2A	3034	1/1	0.96	0.16	56,56,56,56	0
56	MG	1A	3806	1/1	0.96	0.11	45,45,45,45	0
56	MG	2U	205	1/1	0.96	0.23	49,49,49,49	0
56	MG	1A	4033	1/1	0.96	0.60	25,25,25,25	0
56	MG	2a	1627	1/1	0.96	0.22	53,53,53,53	0
56	MG	1A	3774	1/1	0.96	0.11	56,56,56,56	0
56	MG	2A	3569	1/1	0.96	0.03	63,63,63,63	0
56	MG	1A	3816	1/1	0.96	0.27	46,46,46,46	0
56	MG	1a	3094	1/1	0.96	0.26	40,40,40,40	0
56	MG	2A	3137	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3140	1/1	0.96	0.54	23,23,23,23	0
56	MG	1D	310	1/1	0.96	0.20	33,33,33,33	0
56	MG	1a	3009	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	3484	1/1	0.96	0.24	22,22,22,22	0
56	MG	2A	3020	1/1	0.96	0.15	29,29,29,29	0
56	MG	1A	3891	1/1	0.96	0.10	33,33,33,33	0
56	MG	1A	3006	1/1	0.96	0.10	33,33,33,33	0
56	MG	1A	3245	1/1	0.96	0.46	28,28,28,28	0
56	MG	2A	3512	1/1	0.96	0.15	55,55,55,55	0
56	MG	1A	3070	1/1	0.96	0.17	23,23,23,23	0
56	MG	11	105	1/1	0.96	0.11	32,32,32,32	0
56	MG	1A	3554	1/1	0.96	0.13	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3553	1/1	0.96	0.09	57,57,57,57	0
56	MG	1A	3753	1/1	0.96	0.31	27,27,27,27	0
56	MG	1A	3240	1/1	0.96	0.15	38,38,38,38	0
56	MG	2X	3002	1/1	0.96	0.14	49,49,49,49	0
56	MG	2A	3700	1/1	0.96	0.06	61,61,61,61	0
56	MG	2U	206	1/1	0.96	0.13	42,42,42,42	0
56	MG	2A	3516	1/1	0.96	0.13	62,62,62,62	0
56	MG	16	104	1/1	0.96	0.14	38,38,38,38	0
56	MG	1A	3446	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3046	1/1	0.96	0.26	50,50,50,50	0
56	MG	1A	3037	1/1	0.96	0.26	22,22,22,22	0
56	MG	2A	3463	1/1	0.96	0.16	27,27,27,27	0
56	MG	2A	3272	1/1	0.96	0.09	33,33,33,33	0
56	MG	2A	3239	1/1	0.96	0.44	64,64,64,64	0
56	MG	1A	3525	1/1	0.96	0.13	9,9,9,9	0
56	MG	1a	3015	1/1	0.96	0.31	48,48,48,48	0
56	MG	15	103	1/1	0.96	0.46	25,25,25,25	0
56	MG	2A	3488	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3862	1/1	0.96	0.11	52,52,52,52	0
56	MG	2a	1805	1/1	0.96	0.05	53,53,53,53	0
56	MG	2A	3729	1/1	0.96	0.20	43,43,43,43	0
56	MG	1A	3147	1/1	0.96	0.07	50,50,50,50	0
56	MG	2a	1753	1/1	0.96	0.15	45,45,45,45	0
56	MG	2a	1733	1/1	0.96	0.12	56,56,56,56	0
56	MG	1A	3866	1/1	0.96	0.23	20,20,20,20	0
56	MG	1A	3028	1/1	0.96	0.34	20,20,20,20	0
56	MG	1A	3498	1/1	0.96	0.15	39,39,39,39	0
56	MG	2a	1781	1/1	0.96	0.10	67,67,67,67	0
56	MG	1a	3041	1/1	0.96	0.05	51,51,51,51	0
56	MG	2A	3622	1/1	0.96	0.11	55,55,55,55	0
56	MG	2a	1619	1/1	0.96	0.34	53,53,53,53	0
56	MG	1A	3295	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3477	1/1	0.96	0.23	32,32,32,32	0
56	MG	2A	3084	1/1	0.96	0.18	29,29,29,29	0
56	MG	1A	3702	1/1	0.96	0.07	23,23,23,23	0
56	MG	1A	3773	1/1	0.96	0.10	15,15,15,15	0
56	MG	2A	3398	1/1	0.96	0.24	26,26,26,26	0
56	MG	2A	3359	1/1	0.96	0.20	52,52,52,52	0
56	MG	1A	3752	1/1	0.96	0.45	36,36,36,36	0
56	MG	2y	3004	1/1	0.96	0.17	36,36,36,36	0
56	MG	1A	3725	1/1	0.96	0.17	30,30,30,30	0
56	MG	2A	3260	1/1	0.96	0.16	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3066	1/1	0.96	0.06	22,22,22,22	0
56	MG	2D	303	1/1	0.96	0.34	41,41,41,41	0
56	MG	1A	3233	1/1	0.96	0.43	35,35,35,35	0
56	MG	2A	3541	1/1	0.96	0.14	32,32,32,32	0
56	MG	1A	3539	1/1	0.96	0.07	20,20,20,20	0
56	MG	1a	3085	1/1	0.96	0.21	33,33,33,33	0
56	MG	1A	3736	1/1	0.96	0.24	16,16,16,16	0
56	MG	1A	3579	1/1	0.96	0.18	31,31,31,31	0
56	MG	2a	1717	1/1	0.96	0.08	66,66,66,66	0
56	MG	1A	3949	1/1	0.96	0.11	18,18,18,18	0
56	MG	1A	3206	1/1	0.96	0.13	30,30,30,30	0
56	MG	1W	3005	1/1	0.96	0.14	21,21,21,21	0
56	MG	2w	103	1/1	0.96	0.09	44,44,44,44	0
57	K	1A	4028	1/1	0.96	0.10	40,40,40,40	0
56	MG	1a	3195	1/1	0.96	0.06	45,45,45,45	0
56	MG	1A	3437	1/1	0.96	0.11	52,52,52,52	0
56	MG	1A	4032	1/1	0.96	0.49	30,30,30,30	0
56	MG	2A	3009	1/1	0.96	0.14	29,29,29,29	0
56	MG	2A	3341	1/1	0.96	0.17	39,39,39,39	0
56	MG	2A	3713	1/1	0.96	0.18	26,26,26,26	0
56	MG	1A	3126	1/1	0.96	0.48	21,21,21,21	0
56	MG	1D	306	1/1	0.96	0.10	17,17,17,17	0
56	MG	1A	3320	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	3822	1/1	0.96	0.10	45,45,45,45	0
56	MG	2A	3203	1/1	0.96	0.12	53,53,53,53	0
56	MG	2A	3403	1/1	0.96	0.26	29,29,29,29	0
56	MG	2A	3162	1/1	0.96	0.08	54,54,54,54	0
56	MG	2A	3711	1/1	0.96	0.07	37,37,37,37	0
56	MG	1B	206	1/1	0.96	0.07	36,36,36,36	0
56	MG	1A	3910	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	3010	1/1	0.96	0.21	33,33,33,33	0
56	MG	1A	3875	1/1	0.96	0.17	43,43,43,43	0
56	MG	2A	3284	1/1	0.96	0.08	37,37,37,37	0
56	MG	1A	3936	1/1	0.96	0.08	49,49,49,49	0
56	MG	2A	3451	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3268	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	3489	1/1	0.96	0.22	30,30,30,30	0
56	MG	18	101	1/1	0.96	0.34	37,37,37,37	0
56	MG	1Q	201	1/1	0.96	0.36	33,33,33,33	0
56	MG	2A	3597	1/1	0.96	0.12	34,34,34,34	0
56	MG	1B	223	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3419	1/1	0.96	0.14	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	3999	1/1	0.96	0.17	25,25,25,25	0
56	MG	2E	301	1/1	0.96	0.14	33,33,33,33	0
56	MG	2A	3525	1/1	0.96	0.27	52,52,52,52	0
56	MG	1A	3122	1/1	0.96	0.13	32,32,32,32	0
56	MG	1A	4051	1/1	0.96	0.22	13,13,13,13	0
56	MG	1A	3588	1/1	0.96	0.16	32,32,32,32	0
56	MG	2A	3150	1/1	0.96	0.21	49,49,49,49	0
56	MG	1A	3229	1/1	0.96	0.15	28,28,28,28	0
56	MG	1A	3974	1/1	0.96	0.11	50,50,50,50	0
56	MG	1a	3080	1/1	0.96	0.23	46,46,46,46	0
56	MG	1A	3406	1/1	0.96	0.28	48,48,48,48	0
56	MG	1A	3033	1/1	0.96	0.12	21,21,21,21	0
56	MG	2A	3734	1/1	0.96	0.16	25,25,25,25	0
56	MG	2A	3496	1/1	0.96	0.11	37,37,37,37	0
56	MG	2A	3192	1/1	0.96	0.30	54,54,54,54	0
56	MG	1a	3125	1/1	0.96	0.12	42,42,42,42	0
56	MG	1a	3172	1/1	0.96	0.07	46,46,46,46	0
56	MG	1A	3157	1/1	0.96	0.08	50,50,50,50	0
56	MG	2A	3462	1/1	0.96	0.14	54,54,54,54	0
56	MG	2a	1810	1/1	0.96	0.15	81,81,81,81	0
56	MG	1A	3008	1/1	0.96	0.16	18,18,18,18	0
56	MG	2A	3165	1/1	0.96	0.18	40,40,40,40	0
56	MG	1A	3049	1/1	0.96	0.10	21,21,21,21	0
56	MG	1A	3139	1/1	0.96	0.19	21,21,21,21	0
56	MG	1a	3160	1/1	0.96	0.09	52,52,52,52	0
56	MG	1A	3688	1/1	0.96	0.20	21,21,21,21	0
56	MG	1A	3540	1/1	0.96	0.11	46,46,46,46	0
56	MG	1A	3717	1/1	0.96	0.10	45,45,45,45	0
56	MG	2a	1763	1/1	0.96	0.10	72,72,72,72	0
56	MG	1a	3082	1/1	0.96	0.47	41,41,41,41	0
56	MG	2A	3422	1/1	0.96	0.19	49,49,49,49	0
56	MG	2A	3143	1/1	0.96	0.13	41,41,41,41	0
56	MG	1A	3617	1/1	0.96	0.10	45,45,45,45	0
56	MG	2A	3303	1/1	0.96	0.17	35,35,35,35	0
56	MG	1A	3689	1/1	0.96	0.39	20,20,20,20	0
56	MG	1A	3180	1/1	0.96	0.14	42,42,42,42	0
56	MG	1A	3520	1/1	0.96	0.11	11,11,11,11	0
56	MG	1A	3394	1/1	0.96	0.23	37,37,37,37	0
56	MG	1a	3198	1/1	0.96	0.25	46,46,46,46	0
56	MG	2A	3418	1/1	0.96	0.06	46,46,46,46	0
56	MG	1A	3451	1/1	0.96	0.28	24,24,24,24	0
56	MG	1A	3149	1/1	0.96	0.60	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4031	1/1	0.96	0.42	35,35,35,35	0
56	MG	2A	3412	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3196	1/1	0.96	0.12	34,34,34,34	0
56	MG	2A	3405	1/1	0.96	0.15	35,35,35,35	0
56	MG	1A	3776	1/1	0.96	0.20	25,25,25,25	0
56	MG	2A	3508	1/1	0.96	0.18	57,57,57,57	0
56	MG	1E	311	1/1	0.96	0.46	36,36,36,36	0
56	MG	1A	3124	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3067	1/1	0.96	0.08	22,22,22,22	0
56	MG	1A	3095	1/1	0.96	0.43	28,28,28,28	0
56	MG	2a	1712	1/1	0.96	0.09	63,63,63,63	0
56	MG	2a	1668	1/1	0.96	0.17	55,55,55,55	0
56	MG	1A	3501	1/1	0.96	0.21	30,30,30,30	0
56	MG	1A	3543	1/1	0.96	0.14	20,20,20,20	0
56	MG	1a	3182	1/1	0.96	0.15	45,45,45,45	0
56	MG	2A	3521	1/1	0.96	0.07	63,63,63,63	0
56	MG	1a	3153	1/1	0.96	0.10	52,52,52,52	0
56	MG	1a	3173	1/1	0.96	0.18	39,39,39,39	0
56	MG	1A	3946	1/1	0.96	0.11	46,46,46,46	0
56	MG	2A	3270	1/1	0.96	0.33	34,34,34,34	0
56	MG	1A	3625	1/1	0.96	0.26	10,10,10,10	0
56	MG	1A	3874	1/1	0.96	0.16	36,36,36,36	0
56	MG	2A	3602	1/1	0.96	0.19	62,62,62,62	0
56	MG	1A	3930	1/1	0.96	0.23	33,33,33,33	0
56	MG	2A	3696	1/1	0.96	0.09	39,39,39,39	0
56	MG	1E	309	1/1	0.97	0.16	15,15,15,15	0
56	MG	2A	3072	1/1	0.97	0.29	32,32,32,32	0
56	MG	2A	3172	1/1	0.97	0.32	48,48,48,48	0
56	MG	1U	201	1/1	0.97	0.10	20,20,20,20	0
56	MG	1A	3676	1/1	0.97	0.17	31,31,31,31	0
56	MG	1A	3275	1/1	0.97	0.14	25,25,25,25	0
56	MG	1A	3268	1/1	0.97	0.16	31,31,31,31	0
56	MG	1A	4019	1/1	0.97	0.27	26,26,26,26	0
56	MG	1a	3031	1/1	0.97	0.06	54,54,54,54	0
56	MG	1a	3086	1/1	0.97	0.07	60,60,60,60	0
56	MG	1A	3567	1/1	0.97	0.21	13,13,13,13	0
56	MG	1Q	202	1/1	0.97	0.16	28,28,28,28	0
56	MG	2A	3368	1/1	0.97	0.13	36,36,36,36	0
56	MG	1A	3155	1/1	0.97	0.14	29,29,29,29	0
56	MG	2A	3453	1/1	0.97	0.18	34,34,34,34	0
56	MG	2A	3077	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3742	1/1	0.97	0.14	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3392	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3040	1/1	0.97	0.06	30,30,30,30	0
56	MG	1A	3068	1/1	0.97	0.35	41,41,41,41	0
56	MG	1O	204	1/1	0.97	0.10	45,45,45,45	0
56	MG	2A	3235	1/1	0.97	0.18	40,40,40,40	0
56	MG	2A	3608	1/1	0.97	0.13	48,48,48,48	0
59	ZN	2Y	501	1/1	0.97	0.15	79,79,79,79	0
56	MG	2A	3519	1/1	0.97	0.14	35,35,35,35	0
56	MG	1A	3538	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3336	1/1	0.97	0.14	58,58,58,58	0
56	MG	2A	3016	1/1	0.97	0.20	32,32,32,32	0
56	MG	1A	3270	1/1	0.97	0.09	31,31,31,31	0
56	MG	1G	3002	1/1	0.97	0.15	39,39,39,39	0
56	MG	1a	3002	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3184	1/1	0.97	0.14	14,14,14,14	0
56	MG	1a	3058	1/1	0.97	0.07	58,58,58,58	0
56	MG	2A	3627	1/1	0.97	0.14	50,50,50,50	0
56	MG	2A	3648	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3850	1/1	0.97	0.40	43,43,43,43	0
56	MG	1A	3734	1/1	0.97	0.08	42,42,42,42	0
56	MG	1A	3870	1/1	0.97	0.09	55,55,55,55	0
56	MG	1b	3001	1/1	0.97	0.15	69,69,69,69	0
56	MG	1A	3454	1/1	0.97	0.37	30,30,30,30	0
56	MG	1A	3165	1/1	0.97	0.07	31,31,31,31	0
56	MG	1A	3927	1/1	0.97	0.29	37,37,37,37	0
56	MG	1Z	3004	1/1	0.97	0.14	41,41,41,41	0
56	MG	1O	202	1/1	0.97	0.24	56,56,56,56	0
56	MG	1A	3723	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	4017	1/1	0.97	0.41	37,37,37,37	0
56	MG	1A	3824	1/1	0.97	0.13	33,33,33,33	0
56	MG	1A	3906	1/1	0.97	0.17	60,60,60,60	0
56	MG	2A	3387	1/1	0.97	0.09	50,50,50,50	0
56	MG	2a	1660	1/1	0.97	0.13	59,59,59,59	0
56	MG	1A	3128	1/1	0.97	0.31	27,27,27,27	0
56	MG	2A	3063	1/1	0.97	0.14	43,43,43,43	0
56	MG	2A	3164	1/1	0.97	0.37	53,53,53,53	0
56	MG	1a	3202	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3047	1/1	0.97	0.14	60,60,60,60	0
56	MG	1A	3663	1/1	0.97	0.13	43,43,43,43	0
56	MG	1A	3665	1/1	0.97	0.13	12,12,12,12	0
56	MG	2A	3575	1/1	0.97	0.12	46,46,46,46	0
56	MG	1A	3045	1/1	0.97	0.17	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3388	1/1	0.97	0.17	25,25,25,25	0
56	MG	1A	3583	1/1	0.97	0.18	22,22,22,22	0
56	MG	1B	238	1/1	0.97	0.10	23,23,23,23	0
56	MG	2a	1787	1/1	0.97	0.06	53,53,53,53	0
56	MG	2E	302	1/1	0.97	0.09	44,44,44,44	0
56	MG	1D	304	1/1	0.97	0.68	43,43,43,43	0
56	MG	1A	3840	1/1	0.97	0.17	32,32,32,32	0
56	MG	2B	3020	1/1	0.97	0.14	54,54,54,54	0
56	MG	15	105	1/1	0.97	0.46	33,33,33,33	0
56	MG	1A	3552	1/1	0.97	0.14	23,23,23,23	0
59	ZN	1n	501	1/1	0.97	0.11	51,51,51,51	0
56	MG	1A	3220	1/1	0.97	0.08	24,24,24,24	0
56	MG	1A	3996	1/1	0.97	0.17	49,49,49,49	0
56	MG	1a	3035	1/1	0.97	0.22	49,49,49,49	0
56	MG	1A	3604	1/1	0.97	0.11	28,28,28,28	0
56	MG	1A	3716	1/1	0.97	0.10	45,45,45,45	0
56	MG	2A	3673	1/1	0.97	0.17	47,47,47,47	0
56	MG	2A	3647	1/1	0.97	0.11	51,51,51,51	0
56	MG	1A	3032	1/1	0.97	0.14	26,26,26,26	0
56	MG	1A	3863	1/1	0.97	0.11	56,56,56,56	0
56	MG	1f	3001	1/1	0.97	0.11	31,31,31,31	0
56	MG	1A	3656	1/1	0.97	0.19	25,25,25,25	0
56	MG	2a	1827	1/1	0.97	0.19	58,58,58,58	0
56	MG	1A	3077	1/1	0.97	0.44	21,21,21,21	0
56	MG	1A	3830	1/1	0.97	0.26	39,39,39,39	0
56	MG	2A	3144	1/1	0.97	0.10	33,33,33,33	0
56	MG	2A	3109	1/1	0.97	0.25	39,39,39,39	0
56	MG	1A	3856	1/1	0.97	0.06	62,62,62,62	0
56	MG	1A	3846	1/1	0.97	0.10	48,48,48,48	0
56	MG	2A	3589	1/1	0.97	0.26	45,45,45,45	0
56	MG	2A	3686	1/1	0.97	0.15	40,40,40,40	0
56	MG	2A	3540	1/1	0.97	0.09	37,37,37,37	0
56	MG	2A	3364	1/1	0.97	0.08	45,45,45,45	0
56	MG	2A	3511	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3130	1/1	0.97	0.23	10,10,10,10	0
56	MG	1A	3358	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3655	1/1	0.97	0.14	11,11,11,11	0
56	MG	1A	3163	1/1	0.97	0.08	24,24,24,24	0
56	MG	1A	3173	1/1	0.97	0.29	34,34,34,34	0
56	MG	2a	1699	1/1	0.97	0.05	58,58,58,58	0
56	MG	1A	3821	1/1	0.97	0.11	32,32,32,32	0
56	MG	1a	3098	1/1	0.97	0.16	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3873	1/1	0.97	0.17	42,42,42,42	0
56	MG	1B	222	1/1	0.97	0.22	48,48,48,48	0
56	MG	2A	3694	1/1	0.97	0.09	54,54,54,54	0
56	MG	1A	3643	1/1	0.97	0.40	29,29,29,29	0
56	MG	2A	3704	1/1	0.97	0.14	37,37,37,37	0
56	MG	1A	3728	1/1	0.97	0.12	39,39,39,39	0
56	MG	1A	3090	1/1	0.97	0.24	18,18,18,18	0
56	MG	1A	3518	1/1	0.97	0.11	41,41,41,41	0
56	MG	1A	3541	1/1	0.97	0.10	35,35,35,35	0
56	MG	1A	3868	1/1	0.97	0.14	24,24,24,24	0
56	MG	2a	1816	1/1	0.97	0.15	48,48,48,48	0
56	MG	2A	3633	1/1	0.97	0.13	66,66,66,66	0
56	MG	1D	305	1/1	0.97	0.24	28,28,28,28	0
56	MG	1A	3911	1/1	0.97	0.10	29,29,29,29	0
56	MG	2A	3078	1/1	0.97	0.11	54,54,54,54	0
56	MG	2A	3751	1/1	0.97	0.78	44,44,44,44	0
56	MG	1A	3442	1/1	0.97	0.22	36,36,36,36	0
56	MG	1A	3556	1/1	0.97	0.15	20,20,20,20	0
56	MG	1F	309	1/1	0.97	0.33	50,50,50,50	0
56	MG	1a	3215	1/1	0.97	0.07	39,39,39,39	0
56	MG	1A	3686	1/1	0.97	0.16	18,18,18,18	0
56	MG	2A	3068	1/1	0.97	0.04	35,35,35,35	0
56	MG	2A	3038	1/1	0.97	0.16	33,33,33,33	0
56	MG	1A	3764	1/1	0.97	0.15	24,24,24,24	0
56	MG	1A	3433	1/1	0.97	0.08	50,50,50,50	0
56	MG	2P	201	1/1	0.97	0.13	54,54,54,54	0
56	MG	1A	3678	1/1	0.97	0.16	22,22,22,22	0
56	MG	1X	106	1/1	0.97	0.15	21,21,21,21	0
56	MG	1a	3184	1/1	0.97	0.08	49,49,49,49	0
56	MG	1A	3962	1/1	0.97	0.08	23,23,23,23	0
56	MG	1A	3633	1/1	0.97	0.10	52,52,52,52	0
56	MG	2A	3344	1/1	0.97	0.11	24,24,24,24	0
56	MG	1A	3614	1/1	0.97	0.15	15,15,15,15	0
56	MG	1A	3236	1/1	0.97	0.21	35,35,35,35	0
56	MG	1A	3385	1/1	0.97	0.30	29,29,29,29	0
56	MG	1A	3496	1/1	0.97	0.09	35,35,35,35	0
56	MG	2A	3323	1/1	0.97	0.43	31,31,31,31	0
56	MG	1a	3054	1/1	0.97	0.06	46,46,46,46	0
56	MG	1a	3107	1/1	0.97	0.20	39,39,39,39	0
56	MG	1A	3964	1/1	0.97	0.27	45,45,45,45	0
56	MG	1A	3842	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3589	1/1	0.97	0.12	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1N	205	1/1	0.97	0.49	48,48,48,48	0
56	MG	12	3002	1/1	0.97	0.19	35,35,35,35	0
56	MG	1A	4064	1/1	0.97	0.26	30,30,30,30	0
56	MG	2A	3275	1/1	0.97	0.09	37,37,37,37	0
56	MG	2a	1830	1/1	0.97	0.16	71,71,71,71	0
56	MG	1A	3162	1/1	0.97	0.13	24,24,24,24	0
56	MG	2a	1689	1/1	0.97	0.08	57,57,57,57	0
56	MG	1A	4034	1/1	0.97	0.58	28,28,28,28	0
56	MG	1a	3079	1/1	0.97	0.14	47,47,47,47	0
56	MG	1A	3778	1/1	0.97	0.17	13,13,13,13	0
56	MG	2A	3148	1/1	0.97	0.06	34,34,34,34	0
56	MG	1R	203	1/1	0.97	0.49	34,34,34,34	0
56	MG	1A	3517	1/1	0.97	0.15	28,28,28,28	0
56	MG	1A	3017	1/1	0.97	0.11	19,19,19,19	0
56	MG	2a	1676	1/1	0.97	0.19	48,48,48,48	0
56	MG	2A	3029	1/1	0.97	0.14	36,36,36,36	0
56	MG	2A	3041	1/1	0.97	0.12	46,46,46,46	0
56	MG	1A	3022	1/1	0.97	0.13	22,22,22,22	0
56	MG	1A	3578	1/1	0.97	0.14	23,23,23,23	0
56	MG	1A	3729	1/1	0.97	0.18	49,49,49,49	0
56	MG	1a	3025	1/1	0.97	0.16	24,24,24,24	0
56	MG	2A	3209	1/1	0.97	0.08	35,35,35,35	0
56	MG	1A	3343	1/1	0.97	0.24	30,30,30,30	0
56	MG	1A	3164	1/1	0.97	0.17	12,12,12,12	0
56	MG	1A	3015	1/1	0.97	0.16	37,37,37,37	0
56	MG	2A	3119	1/1	0.97	0.12	41,41,41,41	0
56	MG	2a	1741	1/1	0.97	0.09	57,57,57,57	0
56	MG	2A	3693	1/1	0.97	0.05	68,68,68,68	0
56	MG	2A	3367	1/1	0.97	0.13	28,28,28,28	0
56	MG	1B	217	1/1	0.97	0.17	44,44,44,44	0
56	MG	2A	3091	1/1	0.97	0.30	38,38,38,38	0
56	MG	2A	3306	1/1	0.97	0.22	47,47,47,47	0
56	MG	1E	305	1/1	0.97	0.23	50,50,50,50	0
56	MG	2A	3428	1/1	0.97	0.17	43,43,43,43	0
56	MG	1A	3097	1/1	0.97	0.09	24,24,24,24	0
56	MG	15	102	1/1	0.97	0.19	22,22,22,22	0
59	ZN	29	501	1/1	0.97	0.07	63,63,63,63	0
56	MG	2a	1659	1/1	0.97	0.12	47,47,47,47	0
56	MG	1a	3127	1/1	0.97	0.08	48,48,48,48	0
56	MG	1A	3530	1/1	0.97	0.22	25,25,25,25	0
56	MG	2A	3060	1/1	0.97	0.20	32,32,32,32	0
56	MG	1A	3745	1/1	0.97	0.13	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3502	1/1	0.97	0.33	20,20,20,20	0
56	MG	1A	3610	1/1	0.97	0.17	45,45,45,45	0
56	MG	1A	3404	1/1	0.97	0.26	28,28,28,28	0
56	MG	1a	3028	1/1	0.97	0.14	37,37,37,37	0
56	MG	1A	3615	1/1	0.97	0.11	12,12,12,12	0
56	MG	1A	3908	1/1	0.97	0.14	27,27,27,27	0
56	MG	2A	3611	1/1	0.97	0.13	47,47,47,47	0
56	MG	1B	219	1/1	0.97	0.12	27,27,27,27	0
56	MG	2A	3522	1/1	0.97	0.08	49,49,49,49	0
56	MG	1E	302	1/1	0.97	0.37	16,16,16,16	0
56	MG	1a	3078	1/1	0.97	0.11	48,48,48,48	0
56	MG	1a	3071	1/1	0.97	0.10	43,43,43,43	0
56	MG	1A	3829	1/1	0.97	0.17	43,43,43,43	0
56	MG	1A	3623	1/1	0.97	0.15	41,41,41,41	0
56	MG	1A	4020	1/1	0.97	0.30	50,50,50,50	0
56	MG	1A	3701	1/1	0.97	0.10	15,15,15,15	0
56	MG	2A	3548	1/1	0.97	0.13	51,51,51,51	0
56	MG	1A	3814	1/1	0.97	0.14	8,8,8,8	0
56	MG	1a	3106	1/1	0.97	0.13	52,52,52,52	0
56	MG	1A	3893	1/1	0.97	0.27	27,27,27,27	0
56	MG	2A	3407	1/1	0.97	0.15	35,35,35,35	0
56	MG	2A	3149	1/1	0.97	0.27	57,57,57,57	0
56	MG	2A	3423	1/1	0.97	0.12	22,22,22,22	0
56	MG	1A	3668	1/1	0.97	0.14	22,22,22,22	0
56	MG	1Y	503	1/1	0.97	0.40	42,42,42,42	0
56	MG	1a	3016	1/1	0.97	0.12	38,38,38,38	0
56	MG	1A	3260	1/1	0.97	0.15	18,18,18,18	0
56	MG	2A	3455	1/1	0.97	0.15	42,42,42,42	0
56	MG	2A	3717	1/1	0.97	0.11	57,57,57,57	0
56	MG	11	101	1/1	0.97	0.11	28,28,28,28	0
56	MG	2E	304	1/1	0.97	0.20	49,49,49,49	0
56	MG	1E	304	1/1	0.97	0.33	22,22,22,22	0
56	MG	1A	3757	1/1	0.97	0.23	22,22,22,22	0
56	MG	2A	3362	1/1	0.97	0.09	58,58,58,58	0
56	MG	1A	3848	1/1	0.97	0.10	34,34,34,34	0
56	MG	2A	3085	1/1	0.97	0.18	48,48,48,48	0
56	MG	1A	3255	1/1	0.97	0.11	36,36,36,36	0
56	MG	2A	3452	1/1	0.97	0.22	32,32,32,32	0
56	MG	1x	107	1/1	0.97	0.20	46,46,46,46	0
56	MG	1A	3509	1/1	0.97	0.18	31,31,31,31	0
56	MG	1A	3021	1/1	0.97	0.13	29,29,29,29	0
56	MG	1A	3925	1/1	0.97	0.17	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3411	1/1	0.97	0.14	27,27,27,27	0
56	MG	2A	3750	1/1	0.97	0.28	40,40,40,40	0
56	MG	2E	308	1/1	0.97	0.09	49,49,49,49	0
57	K	2A	3327	1/1	0.97	0.11	29,29,29,29	0
56	MG	1F	302	1/1	0.97	0.32	30,30,30,30	0
56	MG	2A	3324	1/1	0.97	0.06	40,40,40,40	0
56	MG	1A	3034	1/1	0.97	0.22	12,12,12,12	0
56	MG	1A	3561	1/1	0.97	0.11	17,17,17,17	0
56	MG	2A	3669	1/1	0.97	0.20	27,27,27,27	0
56	MG	1a	3121	1/1	0.97	0.15	54,54,54,54	0
56	MG	2A	3151	1/1	0.97	0.09	47,47,47,47	0
56	MG	2r	3001	1/1	0.97	0.15	56,56,56,56	0
56	MG	1A	3634	1/1	0.97	0.12	28,28,28,28	0
56	MG	2E	310	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3657	1/1	0.97	0.13	23,23,23,23	0
56	MG	1A	3784	1/1	0.97	0.12	57,57,57,57	0
56	MG	1A	3690	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	4010	1/1	0.97	0.13	23,23,23,23	0
56	MG	2A	3671	1/1	0.97	0.18	29,29,29,29	0
56	MG	1a	3114	1/1	0.97	0.10	68,68,68,68	0
56	MG	1A	3918	1/1	0.97	0.11	33,33,33,33	0
56	MG	1A	3337	1/1	0.97	0.60	27,27,27,27	0
56	MG	10	101	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3225	1/1	0.97	0.12	40,40,40,40	0
56	MG	1A	4044	1/1	0.97	0.27	29,29,29,29	0
56	MG	2A	3561	1/1	0.97	0.18	56,56,56,56	0
56	MG	1A	3186	1/1	0.97	0.20	27,27,27,27	0
56	MG	1A	3114	1/1	0.97	0.32	22,22,22,22	0
56	MG	1A	3051	1/1	0.97	0.17	22,22,22,22	0
56	MG	1A	3952	1/1	0.97	0.14	50,50,50,50	0
56	MG	2a	1726	1/1	0.97	0.13	64,64,64,64	0
56	MG	2A	3527	1/1	0.97	0.18	52,52,52,52	0
56	MG	2A	3090	1/1	0.97	0.15	32,32,32,32	0
56	MG	2A	3062	1/1	0.97	0.14	47,47,47,47	0
56	MG	1A	3755	1/1	0.97	0.20	21,21,21,21	0
56	MG	2B	3021	1/1	0.97	0.18	59,59,59,59	0
56	MG	1A	3748	1/1	0.97	0.10	38,38,38,38	0
56	MG	2A	3122	1/1	0.97	0.15	26,26,26,26	0
56	MG	1A	3452	1/1	0.97	0.28	30,30,30,30	0
56	MG	1A	3954	1/1	0.97	0.15	53,53,53,53	0
56	MG	2A	3401	1/1	0.97	0.19	32,32,32,32	0
57	K	2A	3745	1/1	0.97	0.08	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	2A	3634	1/1	0.97	0.21	48,48,48,48	0
56	MG	1A	3132	1/1	0.97	0.15	37,37,37,37	0
56	MG	2A	3740	1/1	0.97	0.22	37,37,37,37	0
56	MG	2A	3500	1/1	0.97	0.13	49,49,49,49	0
56	MG	1a	3136	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3448	1/1	0.97	0.18	37,37,37,37	0
56	MG	2A	3736	1/1	0.97	0.09	37,37,37,37	0
56	MG	1A	3038	1/1	0.97	0.22	25,25,25,25	0
56	MG	1A	3858	1/1	0.97	0.17	54,54,54,54	0
56	MG	2a	1735	1/1	0.97	0.18	50,50,50,50	0
56	MG	1A	3599	1/1	0.97	0.11	15,15,15,15	0
56	MG	2A	3030	1/1	0.97	0.08	25,25,25,25	0
56	MG	1A	3871	1/1	0.97	0.05	59,59,59,59	0
56	MG	2A	3509	1/1	0.97	0.20	52,52,52,52	0
56	MG	1F	301	1/1	0.98	0.58	23,23,23,23	0
56	MG	2a	1703	1/1	0.98	0.12	41,41,41,41	0
56	MG	1A	3483	1/1	0.98	0.39	32,32,32,32	0
56	MG	1A	3577	1/1	0.98	0.13	54,54,54,54	0
56	MG	1A	4005	1/1	0.98	0.22	10,10,10,10	0
56	MG	2A	3712	1/1	0.98	0.15	35,35,35,35	0
56	MG	1A	3738	1/1	0.98	0.09	32,32,32,32	0
56	MG	2A	3032	1/1	0.98	0.12	41,41,41,41	0
56	MG	1A	3661	1/1	0.98	0.17	18,18,18,18	0
56	MG	2a	1665	1/1	0.98	0.15	49,49,49,49	0
56	MG	2a	1832	1/1	0.98	0.13	37,37,37,37	0
56	MG	1A	3685	1/1	0.98	0.22	21,21,21,21	0
56	MG	2A	3668	1/1	0.98	0.12	41,41,41,41	0
56	MG	1A	3667	1/1	0.98	0.18	31,31,31,31	0
56	MG	1a	3045	1/1	0.98	0.11	52,52,52,52	0
56	MG	1A	3654	1/1	0.98	0.14	37,37,37,37	0
56	MG	1A	3535	1/1	0.98	0.09	23,23,23,23	0
56	MG	1O	203	1/1	0.98	0.16	48,48,48,48	0
56	MG	1a	3070	1/1	0.98	0.05	30,30,30,30	0
56	MG	1A	3009	1/1	0.98	0.11	24,24,24,24	0
56	MG	1A	3917	1/1	0.98	0.14	31,31,31,31	0
57	K	1A	3486	1/1	0.98	0.07	19,19,19,19	0
56	MG	1A	3353	1/1	0.98	0.43	35,35,35,35	0
60	SF4	2d	501	8/8	0.98	0.15	58,60,69,79	0
56	MG	2A	3379	1/1	0.98	0.09	41,41,41,41	0
56	MG	1a	3095	1/1	0.98	0.11	55,55,55,55	0
56	MG	1a	3204	1/1	0.98	0.11	44,44,44,44	0
56	MG	1A	3632	1/1	0.98	0.29	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4050	1/1	0.98	0.28	26,26,26,26	0
56	MG	2A	3674	1/1	0.98	0.22	23,23,23,23	0
56	MG	2A	3594	1/1	0.98	0.12	54,54,54,54	0
56	MG	1A	3662	1/1	0.98	0.19	32,32,32,32	0
56	MG	1A	3001	1/1	0.98	0.09	32,32,32,32	0
56	MG	2A	3330	1/1	0.98	0.20	42,42,42,42	0
56	MG	2v	3005	1/1	0.98	0.15	56,56,56,56	0
56	MG	2a	1812	1/1	0.98	0.11	64,64,64,64	0
56	MG	2A	3120	1/1	0.98	0.13	38,38,38,38	0
56	MG	1A	3580	1/1	0.98	0.07	18,18,18,18	0
56	MG	1A	3031	1/1	0.98	0.31	34,34,34,34	0
56	MG	1E	303	1/1	0.98	0.24	22,22,22,22	0
56	MG	1A	3507	1/1	0.98	0.19	24,24,24,24	0
56	MG	1A	3865	1/1	0.98	0.18	18,18,18,18	0
56	MG	2a	1649	1/1	0.98	0.22	41,41,41,41	0
56	MG	2A	3721	1/1	0.98	0.07	50,50,50,50	0
56	MG	1A	3645	1/1	0.98	0.11	25,25,25,25	0
56	MG	1A	3896	1/1	0.98	0.20	42,42,42,42	0
56	MG	1A	4026	1/1	0.98	0.52	35,35,35,35	0
56	MG	1A	3855	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	3131	1/1	0.98	0.12	35,35,35,35	0
56	MG	2a	1758	1/1	0.98	0.07	52,52,52,52	0
56	MG	2A	3003	1/1	0.98	0.19	49,49,49,49	0
56	MG	2A	3475	1/1	0.98	0.20	37,37,37,37	0
56	MG	1A	3266	1/1	0.98	0.14	24,24,24,24	0
56	MG	1Q	203	1/1	0.98	0.22	28,28,28,28	0
56	MG	1A	3250	1/1	0.98	0.31	20,20,20,20	0
56	MG	2A	3631	1/1	0.98	0.11	53,53,53,53	0
56	MG	1A	3791	1/1	0.98	0.34	23,23,23,23	0
56	MG	2a	1731	1/1	0.98	0.09	56,56,56,56	0
56	MG	1A	3289	1/1	0.98	0.15	41,41,41,41	0
56	MG	2A	3459	1/1	0.98	0.08	50,50,50,50	0
56	MG	2A	3315	1/1	0.98	0.20	42,42,42,42	0
56	MG	1A	3142	1/1	0.98	0.12	17,17,17,17	0
56	MG	2a	1814	1/1	0.98	0.14	63,63,63,63	0
56	MG	1A	3642	1/1	0.98	0.09	34,34,34,34	0
56	MG	2a	1801	1/1	0.98	0.09	63,63,63,63	0
56	MG	1A	3972	1/1	0.98	0.15	49,49,49,49	0
56	MG	1A	3994	1/1	0.98	0.27	21,21,21,21	0
56	MG	1A	3390	1/1	0.98	0.10	43,43,43,43	0
56	MG	1A	3966	1/1	0.98	0.08	41,41,41,41	0
56	MG	1A	3156	1/1	0.98	0.26	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4056	1/1	0.98	0.32	33,33,33,33	0
56	MG	1A	3328	1/1	0.98	0.41	25,25,25,25	0
56	MG	1A	3007	1/1	0.98	0.10	12,12,12,12	0
56	MG	1A	3727	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3854	1/1	0.98	0.12	46,46,46,46	0
56	MG	2A	3369	1/1	0.98	0.14	53,53,53,53	0
56	MG	1A	3153	1/1	0.98	0.16	29,29,29,29	0
56	MG	1A	3499	1/1	0.98	0.14	23,23,23,23	0
56	MG	1A	3810	1/1	0.98	0.15	40,40,40,40	0
56	MG	1A	3310	1/1	0.98	0.17	24,24,24,24	0
56	MG	2A	3415	1/1	0.98	0.18	47,47,47,47	0
56	MG	2A	3236	1/1	0.98	0.21	49,49,49,49	0
56	MG	2a	1679	1/1	0.98	0.14	44,44,44,44	0
56	MG	1A	3490	1/1	0.98	0.15	26,26,26,26	0
56	MG	2A	3440	1/1	0.98	0.13	51,51,51,51	0
56	MG	1A	3651	1/1	0.98	0.12	22,22,22,22	0
56	MG	2A	3363	1/1	0.98	0.15	43,43,43,43	0
56	MG	1A	3770	1/1	0.98	0.16	12,12,12,12	0
56	MG	2A	3325	1/1	0.98	0.51	63,63,63,63	0
56	MG	1E	312	1/1	0.98	0.15	44,44,44,44	0
56	MG	1D	312	1/1	0.98	0.25	27,27,27,27	0
56	MG	1A	3864	1/1	0.98	0.23	20,20,20,20	0
56	MG	1A	3809	1/1	0.98	0.09	30,30,30,30	0
56	MG	1A	3364	1/1	0.98	0.14	23,23,23,23	0
56	MG	1A	3519	1/1	0.98	0.17	21,21,21,21	0
56	MG	2A	3059	1/1	0.98	0.16	35,35,35,35	0
56	MG	2A	3534	1/1	0.98	0.11	53,53,53,53	0
56	MG	1A	3257	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3325	1/1	0.98	0.14	33,33,33,33	0
56	MG	1A	3035	1/1	0.98	0.20	24,24,24,24	0
56	MG	1A	3091	1/1	0.98	0.18	31,31,31,31	0
56	MG	1a	3131	1/1	0.98	0.10	38,38,38,38	0
56	MG	1A	3995	1/1	0.98	0.10	32,32,32,32	0
56	MG	2A	3292	1/1	0.98	0.16	31,31,31,31	0
56	MG	1A	3652	1/1	0.98	0.15	23,23,23,23	0
56	MG	1A	3529	1/1	0.98	0.09	34,34,34,34	0
56	MG	1A	3023	1/1	0.98	0.16	43,43,43,43	0
56	MG	2a	1790	1/1	0.98	0.21	50,50,50,50	0
56	MG	2A	3709	1/1	0.98	0.14	40,40,40,40	0
56	MG	2A	3393	1/1	0.98	0.19	44,44,44,44	0
56	MG	1A	3318	1/1	0.98	0.20	46,46,46,46	0
56	MG	1A	4024	1/1	0.98	0.35	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1734	1/1	0.98	0.11	48,48,48,48	0
56	MG	17	103	1/1	0.98	0.47	33,33,33,33	0
56	MG	1A	3573	1/1	0.98	0.09	24,24,24,24	0
56	MG	1A	3041	1/1	0.98	0.11	32,32,32,32	0
56	MG	1A	4000	1/1	0.98	0.07	29,29,29,29	0
60	SF4	1d	501	8/8	0.98	0.16	52,54,61,66	0
56	MG	1A	3003	1/1	0.98	0.20	19,19,19,19	0
56	MG	1A	3064	1/1	0.98	0.11	12,12,12,12	0
56	MG	2a	1687	1/1	0.98	0.05	40,40,40,40	0
56	MG	1A	3607	1/1	0.98	0.13	19,19,19,19	0
56	MG	1A	3892	1/1	0.98	0.20	33,33,33,33	0
56	MG	2A	3404	1/1	0.98	0.18	39,39,39,39	0
56	MG	1A	3807	1/1	0.98	0.11	28,28,28,28	0
56	MG	2x	105	1/1	0.98	0.14	47,47,47,47	0
56	MG	1A	3120	1/1	0.98	0.33	29,29,29,29	0
56	MG	2A	3291	1/1	0.98	0.12	55,55,55,55	0
56	MG	2A	3641	1/1	0.98	0.13	50,50,50,50	0
56	MG	1x	113	1/1	0.98	0.12	58,58,58,58	0
56	MG	1A	3884	1/1	0.98	0.08	30,30,30,30	0
56	MG	2a	1698	1/1	0.98	0.07	60,60,60,60	0
56	MG	1A	3375	1/1	0.98	0.37	34,34,34,34	0
56	MG	1A	3481	1/1	0.98	0.12	28,28,28,28	0
56	MG	1A	3069	1/1	0.98	0.26	27,27,27,27	0
56	MG	1A	3485	1/1	0.98	0.22	21,21,21,21	0
56	MG	2a	1601	1/1	0.98	0.24	46,46,46,46	0
56	MG	1A	3497	1/1	0.98	0.10	23,23,23,23	0
56	MG	1A	3221	1/1	0.98	0.28	21,21,21,21	0
56	MG	1A	3732	1/1	0.98	0.07	45,45,45,45	0
56	MG	1a	3034	1/1	0.98	0.14	44,44,44,44	0
56	MG	1A	3211	1/1	0.98	0.23	30,30,30,30	0
59	ZN	25	501	1/1	0.98	0.18	45,45,45,45	0
56	MG	1A	3515	1/1	0.98	0.21	11,11,11,11	0
56	MG	1A	3605	1/1	0.98	0.09	14,14,14,14	0
56	MG	1a	3199	1/1	0.98	0.19	47,47,47,47	0
56	MG	1A	3978	1/1	0.98	0.08	33,33,33,33	0
56	MG	2a	1813	1/1	0.98	0.05	54,54,54,54	0
59	ZN	19	501	1/1	0.98	0.17	42,42,42,42	0
56	MG	2A	3320	1/1	0.98	0.20	17,17,17,17	0
56	MG	2v	3001	1/1	0.98	0.07	49,49,49,49	0
56	MG	2w	107	1/1	0.98	0.14	55,55,55,55	0
56	MG	1A	3084	1/1	0.98	0.10	35,35,35,35	0
56	MG	2w	108	1/1	0.98	0.08	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	3587	1/1	0.98	0.10	12,12,12,12	0
56	MG	1B	216	1/1	0.98	0.17	42,42,42,42	0
56	MG	1a	3201	1/1	0.98	0.06	44,44,44,44	0
56	MG	1B	234	1/1	0.98	0.06	41,41,41,41	0
56	MG	2A	3739	1/1	0.98	0.23	29,29,29,29	0
56	MG	2A	3661	1/1	0.98	0.26	36,36,36,36	0
56	MG	2A	3328	1/1	0.98	0.23	45,45,45,45	0
56	MG	1A	3880	1/1	0.98	0.26	23,23,23,23	0
56	MG	1X	104	1/1	0.98	0.20	31,31,31,31	0
56	MG	1A	3088	1/1	0.98	0.20	32,32,32,32	0
59	ZN	26	501	1/1	0.98	0.09	59,59,59,59	0
56	MG	2A	3343	1/1	0.98	0.28	36,36,36,36	0
56	MG	2A	3556	1/1	0.98	0.20	46,46,46,46	0
56	MG	1A	3948	1/1	0.98	0.09	14,14,14,14	0
56	MG	2A	3662	1/1	0.98	0.26	28,28,28,28	0
56	MG	1a	3208	1/1	0.98	0.11	42,42,42,42	0
56	MG	2A	3469	1/1	0.98	0.29	39,39,39,39	0
56	MG	2A	3473	1/1	0.98	0.10	29,29,29,29	0
56	MG	1A	3181	1/1	0.98	0.08	43,43,43,43	0
56	MG	1A	3334	1/1	0.98	0.21	22,22,22,22	0
56	MG	1A	3223	1/1	0.98	0.20	34,34,34,34	0
56	MG	1A	3154	1/1	0.98	0.44	31,31,31,31	0
56	MG	1U	206	1/1	0.98	0.21	16,16,16,16	0
56	MG	1A	3099	1/1	0.98	0.24	23,23,23,23	0
56	MG	2a	1776	1/1	0.98	0.11	47,47,47,47	0
56	MG	1A	3011	1/1	0.98	0.09	20,20,20,20	0
56	MG	1A	3602	1/1	0.98	0.09	48,48,48,48	0
56	MG	2A	3335	1/1	0.98	0.11	49,49,49,49	0
56	MG	1A	4038	1/1	0.98	0.49	31,31,31,31	0
56	MG	1A	3915	1/1	0.98	0.07	34,34,34,34	0
56	MG	1A	3176	1/1	0.98	0.44	25,25,25,25	0
56	MG	2a	1766	1/1	0.98	0.14	36,36,36,36	0
56	MG	2y	3002	1/1	0.98	0.14	51,51,51,51	0
56	MG	1A	3395	1/1	0.98	0.14	33,33,33,33	0
56	MG	1A	3074	1/1	0.98	0.32	24,24,24,24	0
56	MG	2A	3089	1/1	0.98	0.16	40,40,40,40	0
56	MG	1A	3053	1/1	0.98	0.07	43,43,43,43	0
56	MG	1A	3983	1/1	0.98	0.17	32,32,32,32	0
56	MG	1A	4063	1/1	0.98	0.40	31,31,31,31	0
56	MG	1A	3286	1/1	0.98	0.15	34,34,34,34	0
56	MG	1A	3348	1/1	0.98	0.13	44,44,44,44	0
56	MG	1A	3693	1/1	0.98	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3136	1/1	0.98	0.08	21,21,21,21	0
56	MG	2A	3754	1/1	0.98	0.26	43,43,43,43	0
56	MG	2A	3397	1/1	0.98	0.12	37,37,37,37	0
56	MG	2A	3557	1/1	0.98	0.24	27,27,27,27	0
56	MG	1A	3699	1/1	0.98	0.08	25,25,25,25	0
56	MG	2A	3243	1/1	0.98	0.18	49,49,49,49	0
56	MG	2A	3096	1/1	0.98	0.09	42,42,42,42	0
56	MG	1A	3677	1/1	0.98	0.17	18,18,18,18	0
56	MG	2A	3026	1/1	0.98	0.09	43,43,43,43	0
56	MG	2A	3555	1/1	0.98	0.15	38,38,38,38	0
56	MG	2A	3437	1/1	0.98	0.24	39,39,39,39	0
56	MG	17	104	1/1	0.98	0.08	27,27,27,27	0
56	MG	1A	4057	1/1	0.98	0.21	27,27,27,27	0
56	MG	1A	4066	1/1	0.98	0.23	35,35,35,35	0
56	MG	1A	3013	1/1	0.98	0.10	14,14,14,14	0
56	MG	2A	3138	1/1	0.98	0.23	34,34,34,34	0
56	MG	1A	3116	1/1	0.98	0.17	26,26,26,26	0
56	MG	1A	3012	1/1	0.98	0.19	13,13,13,13	0
56	MG	2q	201	1/1	0.98	0.07	46,46,46,46	0
56	MG	1A	3932	1/1	0.98	0.23	13,13,13,13	0
56	MG	1A	3470	1/1	0.98	0.17	33,33,33,33	0
56	MG	2a	1706	1/1	0.98	0.05	54,54,54,54	0
56	MG	1A	3601	1/1	0.98	0.08	24,24,24,24	0
56	MG	2A	3043	1/1	0.98	0.10	40,40,40,40	0
56	MG	2A	3629	1/1	0.98	0.18	62,62,62,62	0
56	MG	1A	3754	1/1	0.98	0.22	22,22,22,22	0
56	MG	1A	3820	1/1	0.98	0.12	35,35,35,35	0
56	MG	2A	3051	1/1	0.99	0.05	46,46,46,46	0
56	MG	1W	3002	1/1	0.99	0.16	29,29,29,29	0
56	MG	1A	3800	1/1	0.99	0.20	54,54,54,54	0
56	MG	2A	3288	1/1	0.99	0.25	30,30,30,30	0
56	MG	1A	3267	1/1	0.99	0.12	24,24,24,24	0
56	MG	2a	1749	1/1	0.99	0.05	55,55,55,55	0
56	MG	1A	3585	1/1	0.99	0.16	30,30,30,30	0
56	MG	1A	3669	1/1	0.99	0.11	35,35,35,35	0
56	MG	2A	3114	1/1	0.99	0.28	29,29,29,29	0
56	MG	2A	3465	1/1	0.99	0.28	42,42,42,42	0
56	MG	1A	3635	1/1	0.99	0.22	25,25,25,25	0
56	MG	1A	3612	1/1	0.99	0.09	24,24,24,24	0
56	MG	1A	3639	1/1	0.99	0.09	39,39,39,39	0
56	MG	2A	3355	1/1	0.99	0.21	23,23,23,23	0
56	MG	1A	3254	1/1	0.99	0.29	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3150	1/1	0.99	0.25	27,27,27,27	0
56	MG	2A	3395	1/1	0.99	0.21	33,33,33,33	0
56	MG	1W	3004	1/1	0.99	0.20	21,21,21,21	0
56	MG	1a	3185	1/1	0.99	0.10	26,26,26,26	0
56	MG	1a	3102	1/1	0.99	0.16	39,39,39,39	0
56	MG	2E	309	1/1	0.99	0.06	41,41,41,41	0
56	MG	1B	205	1/1	0.99	0.30	45,45,45,45	0
56	MG	1A	3696	1/1	0.99	0.23	46,46,46,46	0
56	MG	1A	3544	1/1	0.99	0.08	12,12,12,12	0
56	MG	1A	3793	1/1	0.99	0.25	26,26,26,26	0
56	MG	1D	308	1/1	0.99	0.32	26,26,26,26	0
59	ZN	14	501	1/1	0.99	0.13	70,70,70,70	0
56	MG	1A	3557	1/1	0.99	0.08	25,25,25,25	0
56	MG	2A	3450	1/1	0.99	0.14	37,37,37,37	0
56	MG	1A	3161	1/1	0.99	0.24	20,20,20,20	0
59	ZN	1Y	501	1/1	0.99	0.14	58,58,58,58	0
56	MG	2A	3504	1/1	0.99	0.08	29,29,29,29	0
56	MG	1A	3522	1/1	0.99	0.15	30,30,30,30	0
56	MG	1A	3660	1/1	0.99	0.09	26,26,26,26	0
59	ZN	15	104	1/1	0.99	0.20	42,42,42,42	0
56	MG	2A	3129	1/1	0.99	0.19	54,54,54,54	0
56	MG	2A	3482	1/1	0.99	0.17	38,38,38,38	0
56	MG	1A	3214	1/1	0.99	0.31	32,32,32,32	0
56	MG	1a	3179	1/1	0.99	0.13	39,39,39,39	0
56	MG	1A	3258	1/1	0.99	0.20	33,33,33,33	0
56	MG	1A	3042	1/1	0.99	0.21	19,19,19,19	0
56	MG	1A	3115	1/1	0.99	0.20	39,39,39,39	0
56	MG	1U	204	1/1	0.99	0.26	23,23,23,23	0
56	MG	2A	3732	1/1	0.99	0.31	24,24,24,24	0
56	MG	2A	3505	1/1	0.99	0.08	42,42,42,42	0
56	MG	1w	109	1/1	0.99	0.41	37,37,37,37	0
56	MG	1A	3178	1/1	0.99	0.29	21,21,21,21	0
56	MG	2A	3171	1/1	0.99	0.05	51,51,51,51	0
56	MG	2A	3424	1/1	0.99	0.09	24,24,24,24	0
56	MG	1A	3393	1/1	0.99	0.22	24,24,24,24	0
56	MG	2A	3741	1/1	0.99	0.12	39,39,39,39	0
56	MG	2A	3649	1/1	0.99	0.13	21,21,21,21	0
56	MG	1A	3636	1/1	0.99	0.16	21,21,21,21	0
56	MG	1A	3894	1/1	0.99	0.09	37,37,37,37	0
56	MG	2A	3019	1/1	0.99	0.19	50,50,50,50	0
56	MG	2A	3660	1/1	0.99	0.13	37,37,37,37	0
56	MG	1A	3987	1/1	0.99	0.22	36,36,36,36	0

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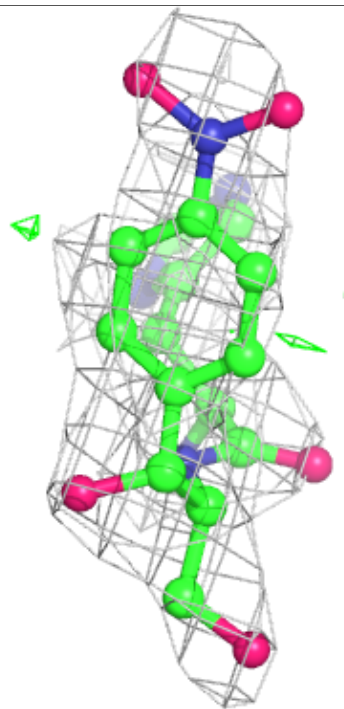
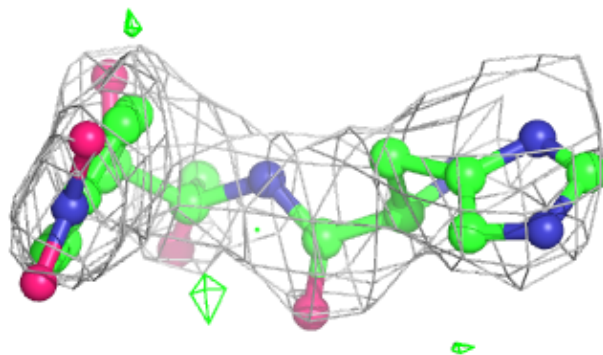
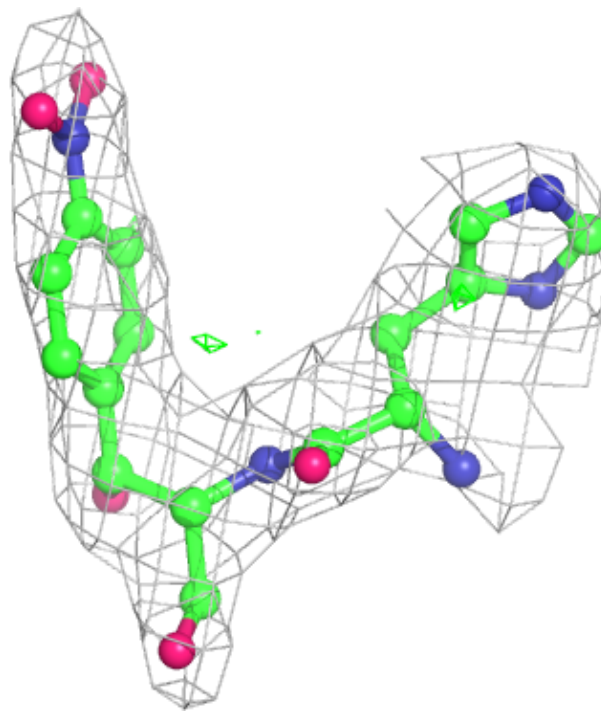
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3338	1/1	0.99	0.22	19,19,19,19	0
59	ZN	16	102	1/1	0.99	0.17	38,38,38,38	0
56	MG	1a	3213	1/1	0.99	0.15	33,33,33,33	0
56	MG	2A	3370	1/1	1.00	0.17	44,44,44,44	0
56	MG	1A	3189	1/1	1.00	0.11	23,23,23,23	0

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

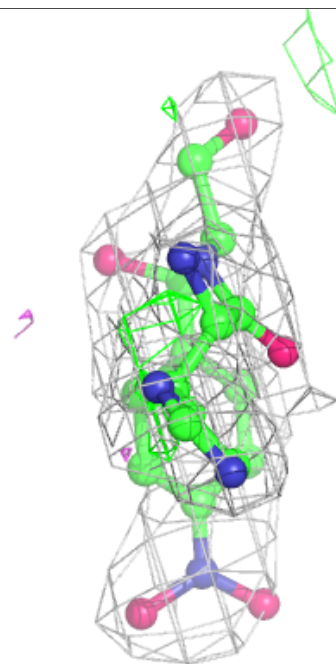
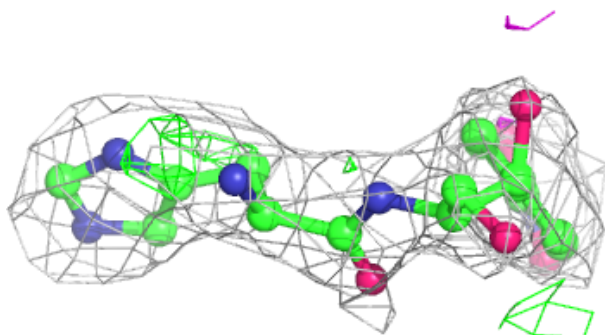
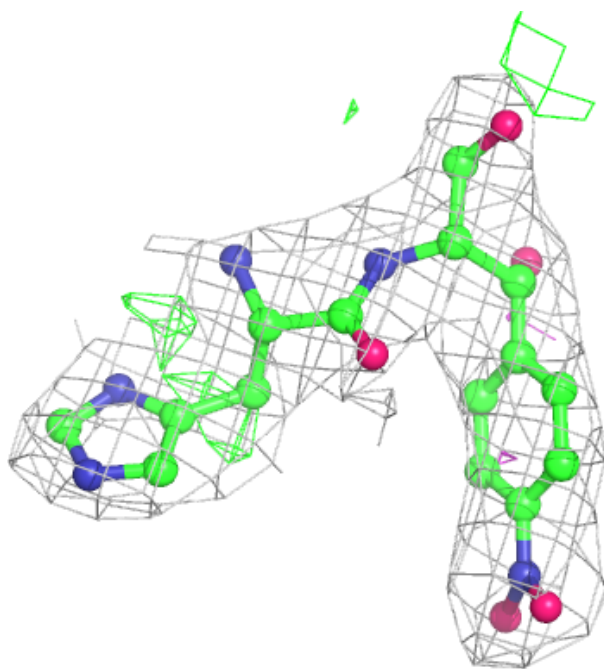
Electron density around EZG 2A 3746:

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



Electron density around EZG 1A 4030:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.