



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 01:48 PM EDT

PDB ID : 5HCP / pdb_00005hcp
Title : Crystal structure of antimicrobial peptide Metalnikowin bound to the *Thermus thermophilus* 70S ribosome
Authors : Gagnon, M.G.; Roy, R.N.; Lomakin, I.B.; Florin, T.; Mankin, A.S.; Steitz, T.A.
Deposited on : 2016-01-04
Resolution : 2.89 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

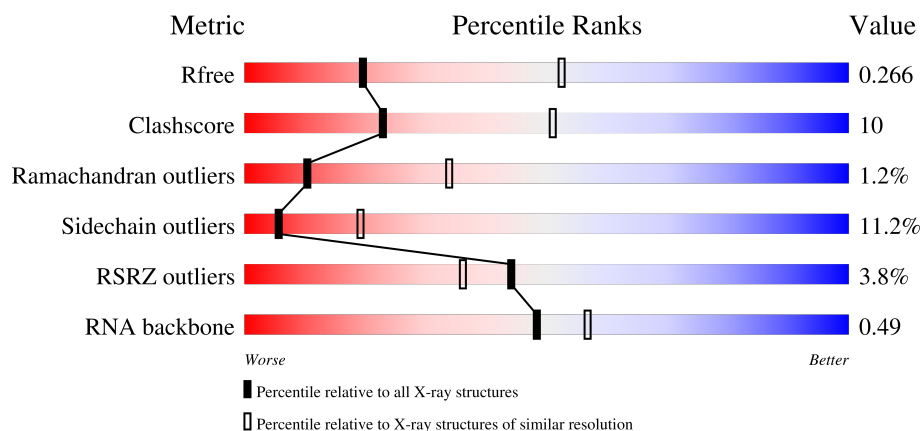
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

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



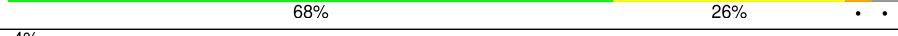
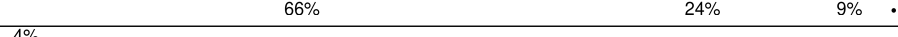
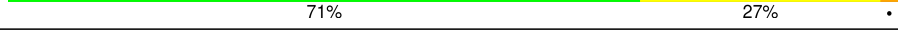
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120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

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

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

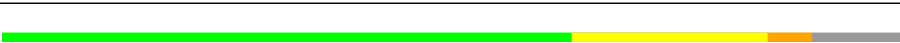
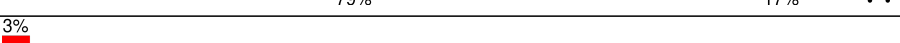
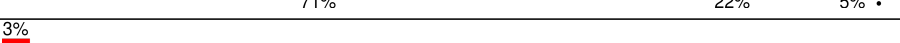
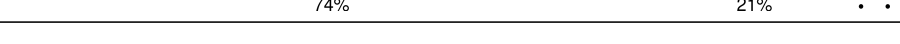
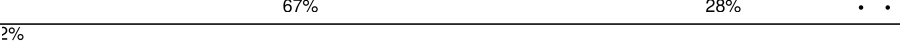
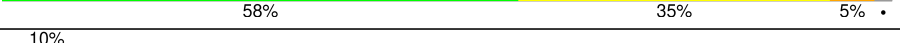
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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118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

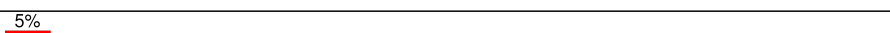
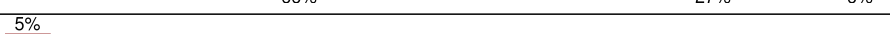
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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25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

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

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

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Mol	Chain	Length	Quality of chain
53	1v	24	4%8%8%79%
53	2v	24	4%8%8%79%
54	1x	77	56%34%9%
54	2x	77	43%45%10%
55	1z	15	13%60%20%20%
55	2z	15	27%53%20%13%13%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 288976 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	2746	Total	C	N	O	P	0	0	0
			59154	26327	11077	19005	2745			
1	2A	2790	Total	C	N	O	P	0	0	0
			60091	26746	11243	19313	2789			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1146	476	831	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2142	1352	426	361	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	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
			1085	693	189	202	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	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			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	186	Total	C	N	O	S	0	0	0
			1470	937	262	269	2			
21	2Z	186	Total	C	N	O	S	0	0	0
			1454	929	256	267	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	75	Total	C	N	O	S	0	0	0
			598	370	127	100	1			
22	20	75	Total	C	N	O	S	0	0	0
			598	370	127	100	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
			558	352	102	99	5			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1477	Total	C	N	O	P	0	0	0
			31750	14131	5883	10259	1477			
32	2a	1483	Total	C	N	O	P	0	0	0
			31877	14188	5905	10301	1483			

- 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
			1786	1136	321	325	4			
33	2b	231	Total	C	N	O	S	0	0	0
			1697	1079	292	321	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
			1480	932	281	266	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1412	883	269	259	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
			1618	1013	312	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1630	1022	321	280	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1095	695	203	193	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
			806	511	143	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			817	516	146	152	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
			1183	732	232	213	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1167	728	220	213	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
			1074	681	202	189	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
			976	620	189	167			
40	2i	127	Total	C	N	O	0	0	0
			932	589	177	166			

- 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
			682	424	130	128			
41	2j	96	Total	C	N	O	0	0	0
			678	424	126	128			

- 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
			826	513	156	154	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			829	516	155	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
			920	579	181	159	1			
43	2l	122	Total	C	N	O	S	0	0	0
			918	576	182	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	118	Total	C	N	O	S	0	0	0
			923	569	191	161	2			
44	2m	116	Total	C	N	O	S	0	0	0
			903	555	187	159	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
			482	306	100	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			459	291	93	71	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
			715	447	140	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
			671	424	133	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
			811	519	148	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	84	Total	C	N	O	S	0	0	0
			642	409	119	112	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
			712	435	152	123	2			
51	2t	96	Total	C	N	O	S	0	0	0
			731	449	156	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
			187	116	42	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			
53	2v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

- Molecule 54 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
54	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 55 is a protein called Metalnikowin-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	12	Total	C	N	O	0	0	0
			105	66	22	17			
55	2z	13	Total	C	N	O	0	0	0
			112	71	23	18			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1090	Total	Mg	0	0
			1090	1090		
56	1B	30	Total	Mg	0	0
			30	30		
56	1D	13	Total	Mg	0	0
			13	13		
56	1E	12	Total	Mg	0	0
			12	12		
56	1F	8	Total	Mg	0	0
			8	8		
56	1G	3	Total	Mg	0	0
			3	3		
56	1H	4	Total	Mg	0	0
			4	4		
56	1N	7	Total	Mg	0	0
			7	7		
56	1O	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1P	6	Total 6	Mg 6	0	0
56	1Q	9	Total 9	Mg 9	0	0
56	1R	6	Total 6	Mg 6	0	0
56	1T	6	Total 6	Mg 6	0	0
56	1U	6	Total 6	Mg 6	0	0
56	1V	2	Total 2	Mg 2	0	0
56	1W	6	Total 6	Mg 6	0	0
56	1X	1	Total 1	Mg 1	0	0
56	1Y	1	Total 1	Mg 1	0	0
56	1Z	2	Total 2	Mg 2	0	0
56	10	6	Total 6	Mg 6	0	0
56	11	3	Total 3	Mg 3	0	0
56	12	1	Total 1	Mg 1	0	0
56	13	2	Total 2	Mg 2	0	0
56	14	1	Total 1	Mg 1	0	0
56	15	3	Total 3	Mg 3	0	0
56	16	4	Total 4	Mg 4	0	0
56	17	2	Total 2	Mg 2	0	0
56	18	3	Total 3	Mg 3	0	0
56	19	5	Total 5	Mg 5	0	0
56	1a	309	Total 309	Mg 309	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1b	1	Total 1	Mg 1	0	0
56	1d	2	Total 2	Mg 2	0	0
56	1e	3	Total 3	Mg 3	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1h	2	Total 2	Mg 2	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1l	2	Total 2	Mg 2	0	0
56	1m	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	1o	3	Total 3	Mg 3	0	0
56	1p	2	Total 2	Mg 2	0	0
56	1q	3	Total 3	Mg 3	0	0
56	1r	3	Total 3	Mg 3	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1u	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	1x	10	Total 10	Mg 10	0	0
56	1z	1	Total 1	Mg 1	0	0
56	2A	561	Total 561	Mg 561	0	0
56	2B	10	Total 10	Mg 10	0	0
56	2D	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	4	Total 4	Mg 4	0	0
56	2F	4	Total 4	Mg 4	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2N	1	Total 1	Mg 1	0	0
56	2O	3	Total 3	Mg 3	0	0
56	2P	1	Total 1	Mg 1	0	0
56	2Q	5	Total 5	Mg 5	0	0
56	2R	2	Total 2	Mg 2	0	0
56	2T	1	Total 1	Mg 1	0	0
56	2U	1	Total 1	Mg 1	0	0
56	2X	1	Total 1	Mg 1	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	1	Total 1	Mg 1	0	0
56	23	1	Total 1	Mg 1	0	0
56	25	1	Total 1	Mg 1	0	0
56	28	3	Total 3	Mg 3	0	0
56	2a	255	Total 255	Mg 255	0	0
56	2d	2	Total 2	Mg 2	0	0
56	2e	2	Total 2	Mg 2	0	0
56	2f	1	Total 1	Mg 1	0	0

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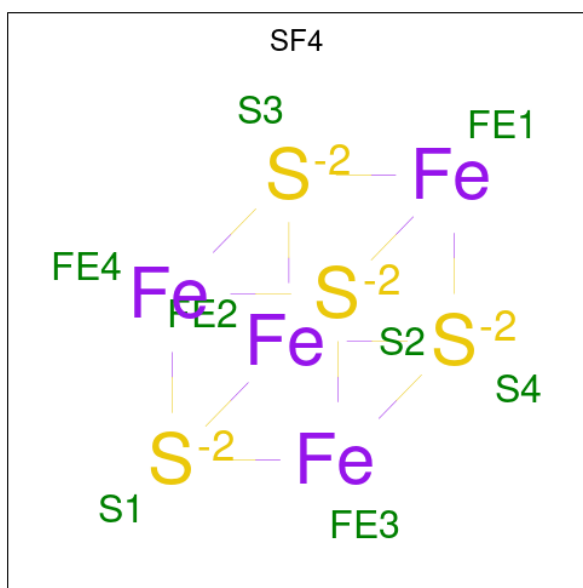
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2l	5	Total 5	Mg 5	0	0
56	2q	3	Total 3	Mg 3	0	0
56	2r	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	1	Total 1	Mg 1	0	0
56	2x	7	Total 7	Mg 7	0	0
56	2z	1	Total 1	Mg 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total 1	Zn 1	0	0
57	14	1	Total 1	Zn 1	0	0
57	15	1	Total 1	Zn 1	0	0
57	16	1	Total 1	Zn 1	0	0
57	19	1	Total 1	Zn 1	0	0
57	1n	1	Total 1	Zn 1	0	0
57	2Y	1	Total 1	Zn 1	0	0
57	24	1	Total 1	Zn 1	0	0
57	25	1	Total 1	Zn 1	0	0
57	26	1	Total 1	Zn 1	0	0
57	29	1	Total 1	Zn 1	0	0
57	2n	1	Total 1	Zn 1	0	0

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



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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	2412	Total	O	0	0
			2412	2412		
59	1B	46	Total	O	0	0
			46	46		
59	1D	25	Total	O	0	0
			25	25		
59	1E	30	Total	O	0	0
			30	30		
59	1F	21	Total	O	0	0
			21	21		
59	1G	8	Total	O	0	0
			8	8		
59	1H	4	Total	O	0	0
			4	4		
59	1I	3	Total	O	0	0
			3	3		
59	1N	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1O	5	Total 5	O 5	0	0
59	1P	25	Total 25	O 25	0	0
59	1Q	13	Total 13	O 13	0	0
59	1R	18	Total 18	O 18	0	0
59	1S	2	Total 2	O 2	0	0
59	1T	13	Total 13	O 13	0	0
59	1U	18	Total 18	O 18	0	0
59	1V	5	Total 5	O 5	0	0
59	1W	14	Total 14	O 14	0	0
59	1X	5	Total 5	O 5	0	0
59	1Y	1	Total 1	O 1	0	0
59	1Z	6	Total 6	O 6	0	0
59	10	8	Total 8	O 8	0	0
59	11	7	Total 7	O 7	0	0
59	12	2	Total 2	O 2	0	0
59	13	3	Total 3	O 3	0	0
59	15	7	Total 7	O 7	0	0
59	16	11	Total 11	O 11	0	0
59	17	9	Total 9	O 9	0	0
59	18	16	Total 16	O 16	0	0
59	19	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1a	394	Total 394	O 394	0	0
59	1b	1	Total 1	O 1	0	0
59	1c	1	Total 1	O 1	0	0
59	1d	3	Total 3	O 3	0	0
59	1e	4	Total 4	O 4	0	0
59	1f	1	Total 1	O 1	0	0
59	1h	2	Total 2	O 2	0	0
59	1j	1	Total 1	O 1	0	0
59	1k	2	Total 2	O 2	0	0
59	1l	3	Total 3	O 3	0	0
59	1m	1	Total 1	O 1	0	0
59	1p	1	Total 1	O 1	0	0
59	1q	1	Total 1	O 1	0	0
59	1s	1	Total 1	O 1	0	0
59	1u	1	Total 1	O 1	0	0
59	1v	3	Total 3	O 3	0	0
59	1x	10	Total 10	O 10	0	0
59	1z	5	Total 5	O 5	0	0
59	2A	824	Total 824	O 824	0	0
59	2B	9	Total 9	O 9	0	0
59	2D	18	Total 18	O 18	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2E	11	Total 11	O 11	0	0
59	2F	6	Total 6	O 6	0	0
59	2N	2	Total 2	O 2	0	0
59	2O	1	Total 1	O 1	0	0
59	2P	6	Total 6	O 6	0	0
59	2R	1	Total 1	O 1	0	0
59	2T	1	Total 1	O 1	0	0
59	2U	3	Total 3	O 3	0	0
59	2W	1	Total 1	O 1	0	0
59	2X	3	Total 3	O 3	0	0
59	2Y	2	Total 2	O 2	0	0
59	2Z	5	Total 5	O 5	0	0
59	20	2	Total 2	O 2	0	0
59	21	1	Total 1	O 1	0	0
59	23	2	Total 2	O 2	0	0
59	25	1	Total 1	O 1	0	0
59	27	1	Total 1	O 1	0	0
59	28	4	Total 4	O 4	0	0
59	2a	329	Total 329	O 329	0	0
59	2c	1	Total 1	O 1	0	0
59	2d	1	Total 1	O 1	0	0

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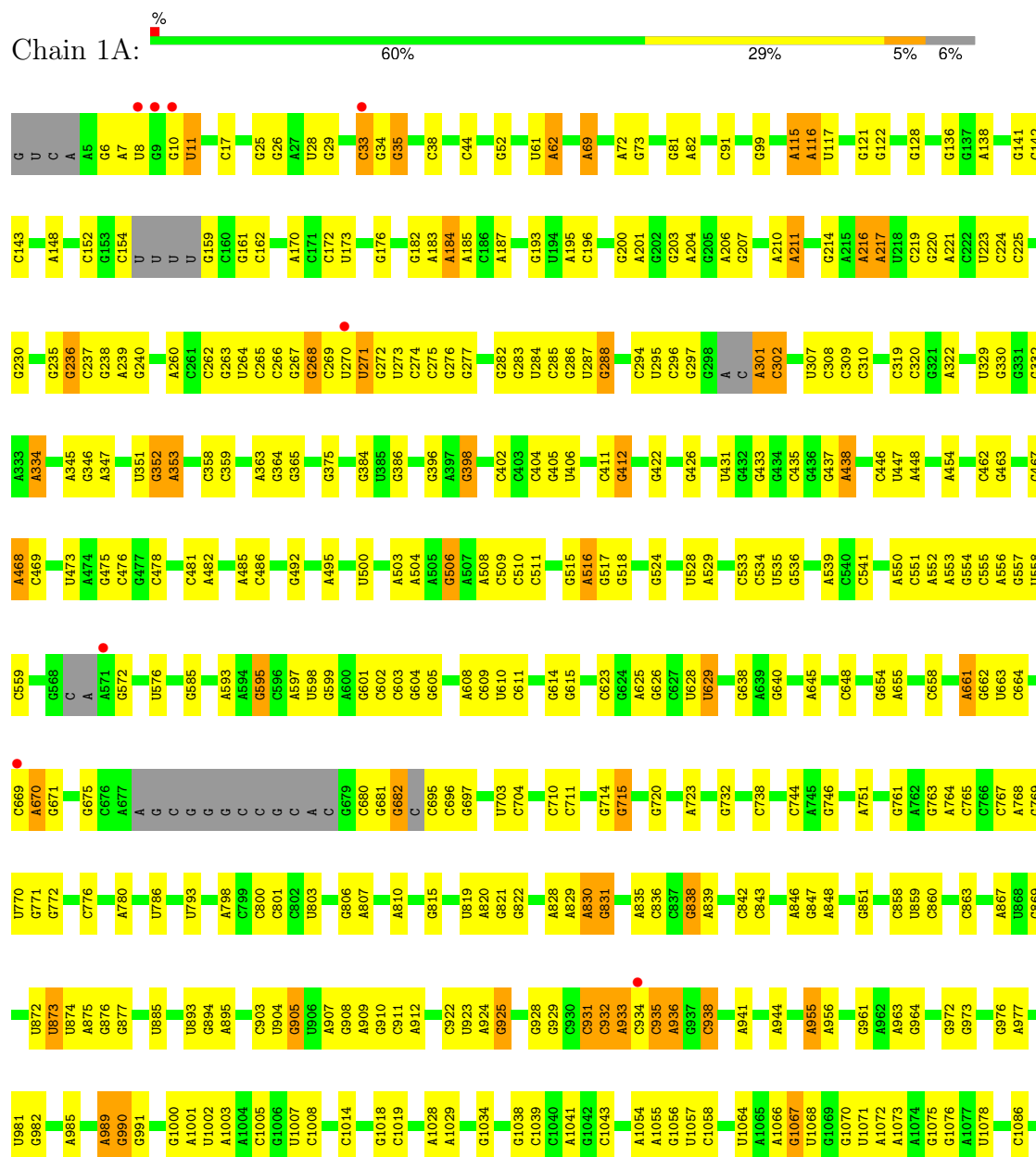
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2e	4	Total 4	O 4	0	0
59	2g	1	Total 1	O 1	0	0
59	2i	2	Total 2	O 2	0	0
59	2l	2	Total 2	O 2	0	0
59	2m	1	Total 1	O 1	0	0
59	2o	1	Total 1	O 1	0	0
59	2p	2	Total 2	O 2	0	0
59	2q	1	Total 1	O 1	0	0
59	2t	4	Total 4	O 4	0	0
59	2u	1	Total 1	O 1	0	0
59	2x	6	Total 6	O 6	0	0
59	2z	2	Total 2	O 2	0	0

3 Residue-property plots

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

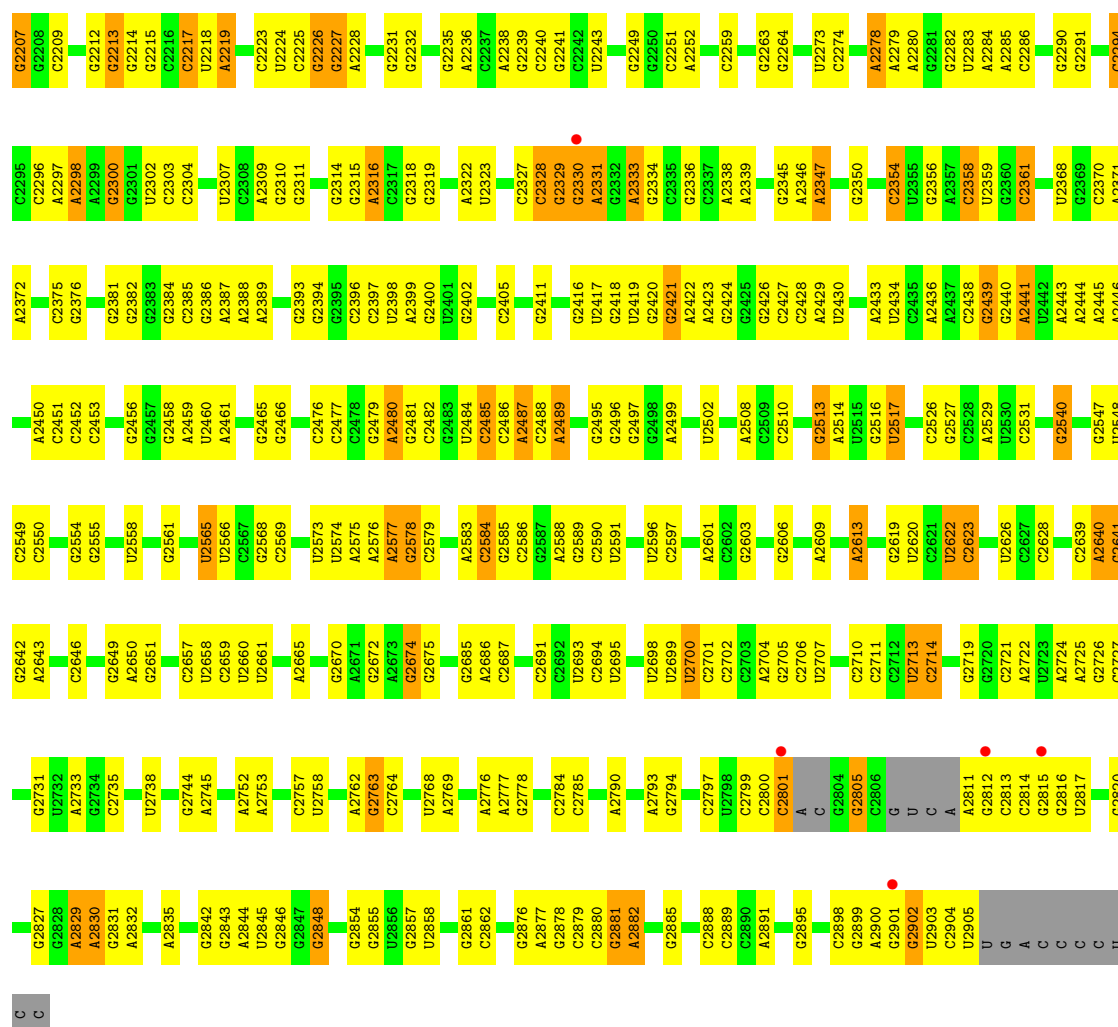
• Molecule 1: 23S Ribosomal RNA



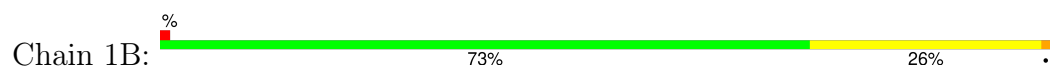








• Molecule 2: 5S Ribosomal RNA



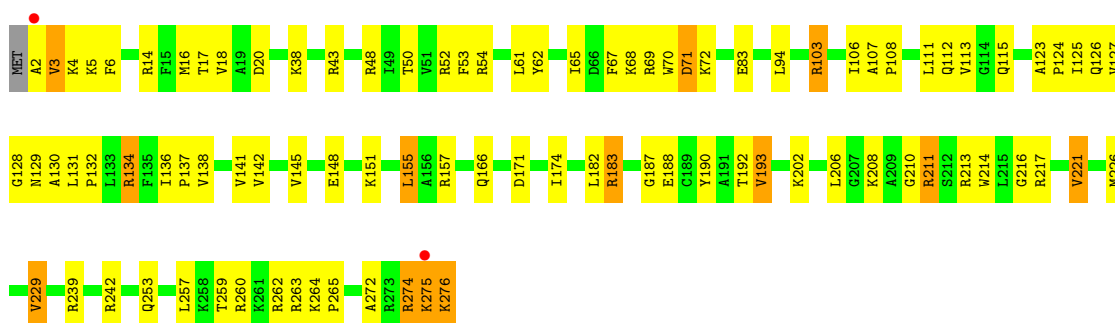
• Molecule 2: 5S Ribosomal RNA



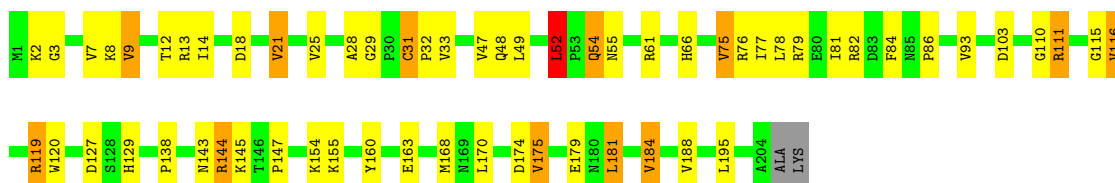
• Molecule 3: 50S ribosomal protein L2

Q253	Q258	Q260	Q270	Q276	V138	V142	V143	V144	V145	V146	V147	V148	K151	L155	T161	Q164	V173	V174	L175	R176	R183	K184	V185	C189	Y190	V193	V205	L206	G207	K208	A209	G210	R211	S212	R213	R217	R218	P219	H220	V221	R222	P228	V229	R239	A240	P241	R242	P249	W250	P132	P131	G128	Q116	L111	P108	A107	I106	R103	K102	E101	L94	N87	P76	D71	W70	R69	L206	K68	Y62	L61	R60	K59	R54	F53	R52	R48	R38	L37	P36	K35	T24	F21	T17	R14	S12	P11	T10	Y9	A2	WET
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	-----

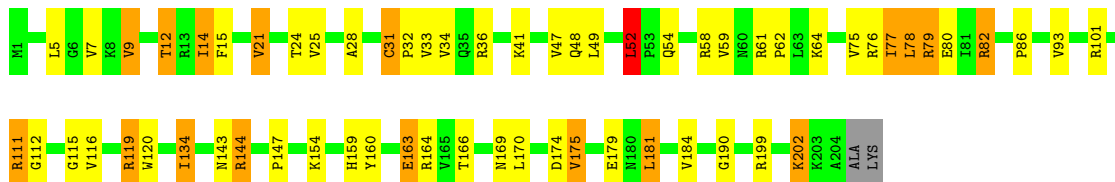
Chain 2D: 66% 29% 5%



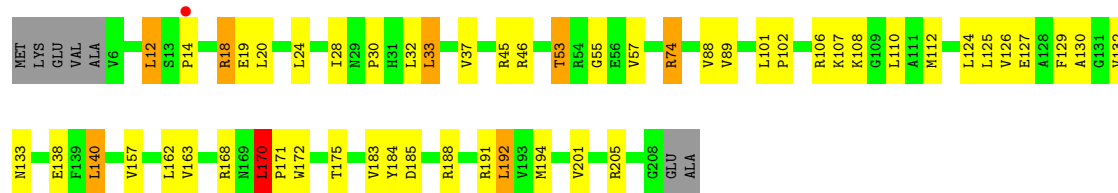
Chain 1E: 69% 23% 6%



Chain 2E: 69% 21% 8%

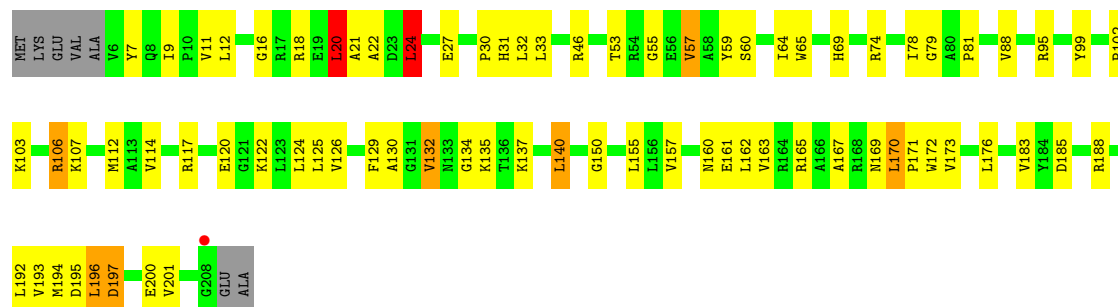


Chain 1F: 71% 21% ..



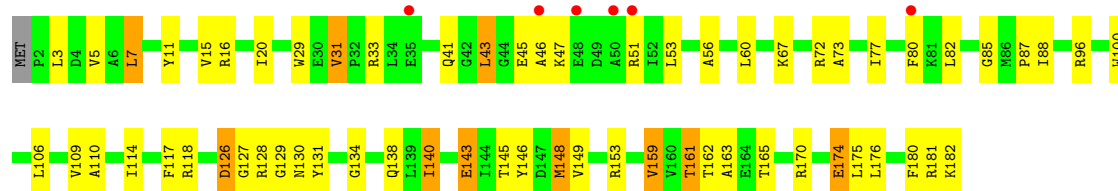
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 60% 32%



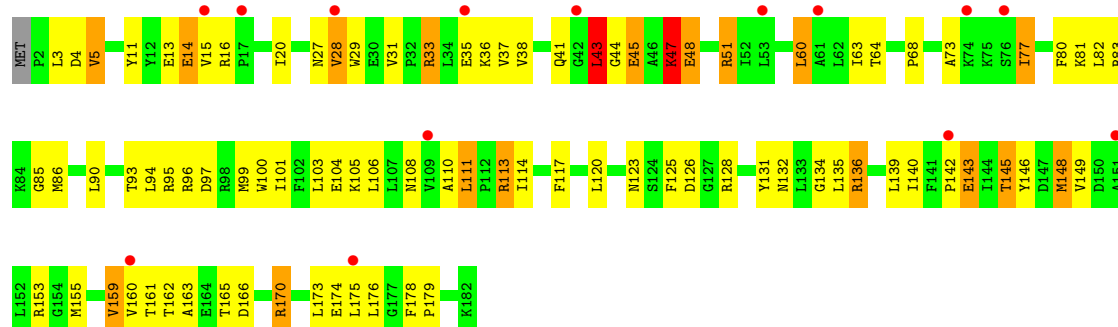
• Molecule 6: 50S ribosomal protein L5

Chain 1G: 3% 65% 29% 5%



• Molecule 6: 50S ribosomal protein L5

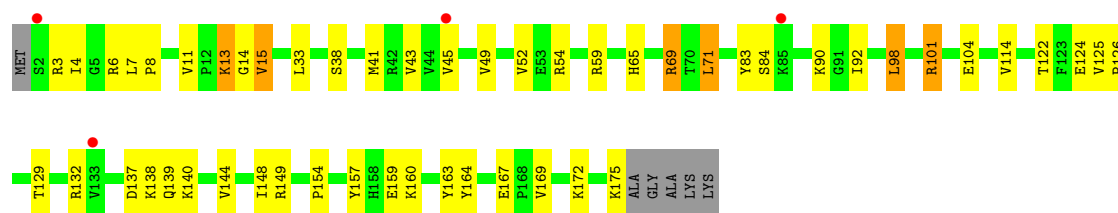
Chain 2G: 8% 50% 39% 9%



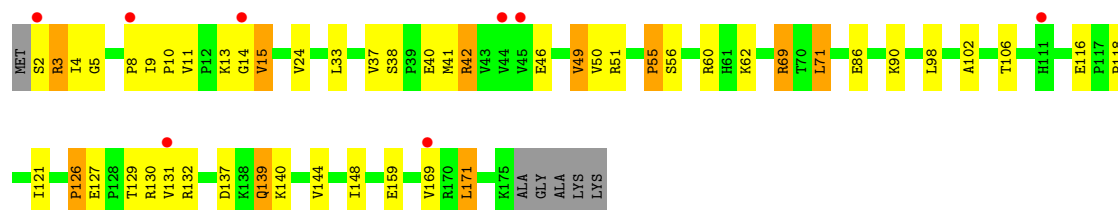
• Molecule 7: 50S ribosomal protein L6

Chain 1H: 2% 68% 26%

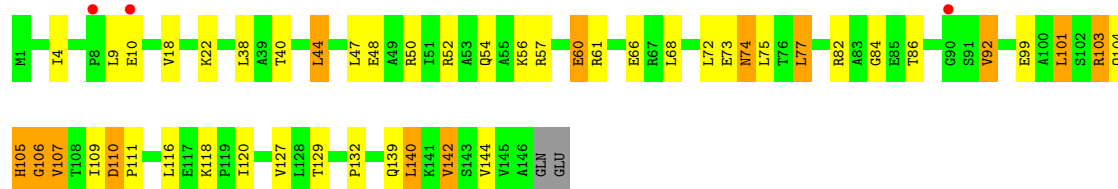




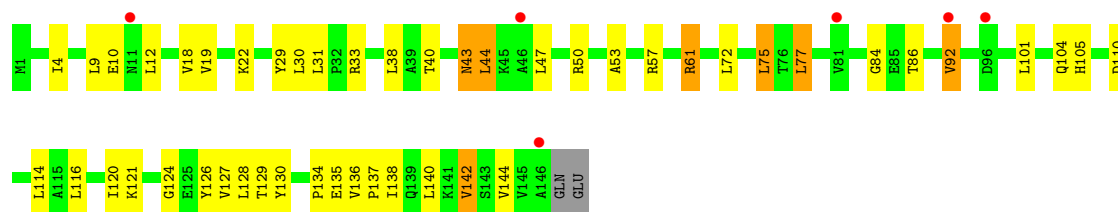
• Molecule 7: 50S ribosomal protein L6



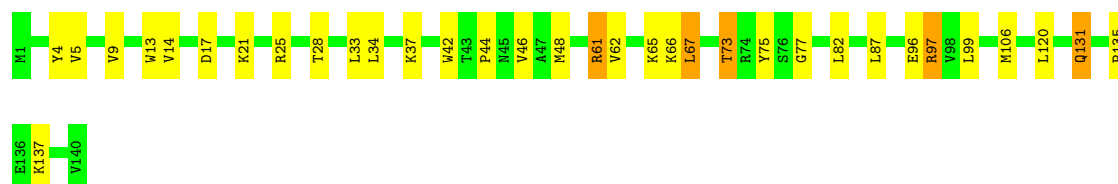
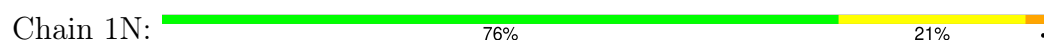
• Molecule 8: 50S ribosomal protein L9



• Molecule 8: 50S ribosomal protein L9

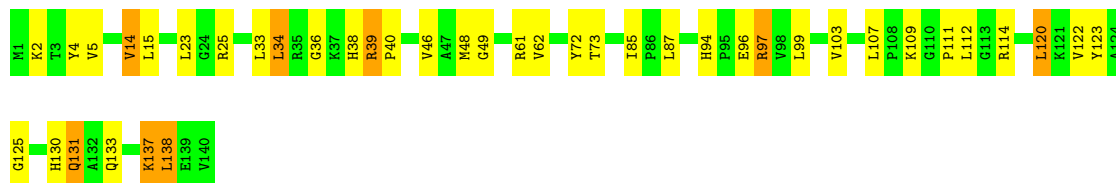


• Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13

Chain 2N:  71% 24% 6%



- Molecule 10: 50S ribosomal protein L14

Chain 1O:  72% 22% 6%



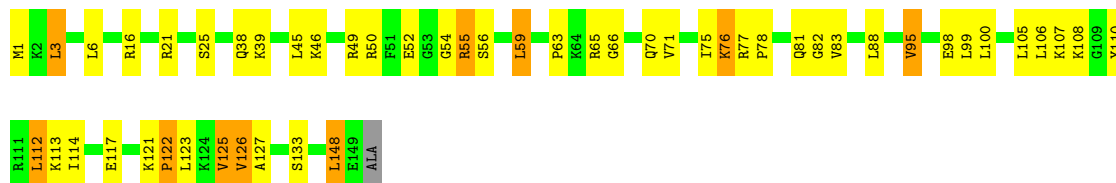
- Molecule 10: 50S ribosomal protein L14

Chain 2O:  71% 27% 2%



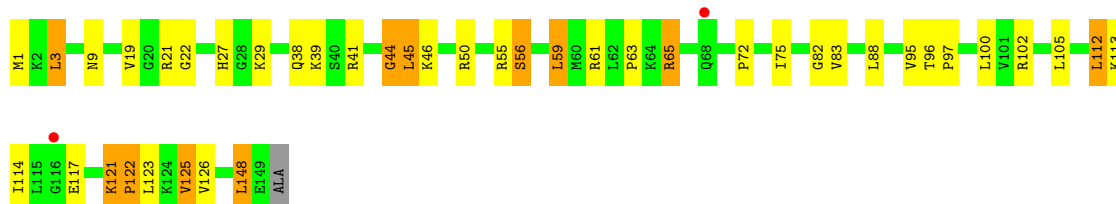
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  65% 27% 7%



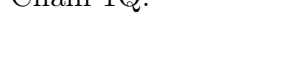
- Molecule 11: 50S ribosomal protein L15

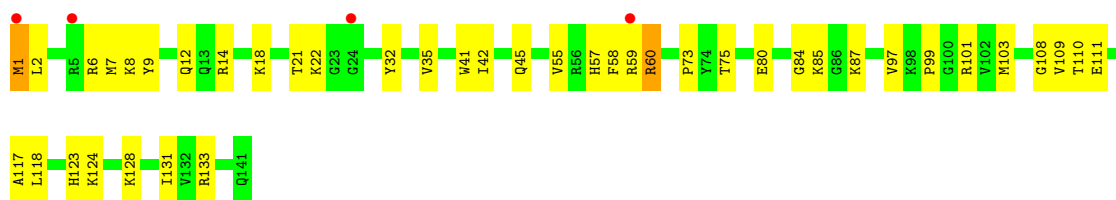
Chain 2P:  71% 21% 7%



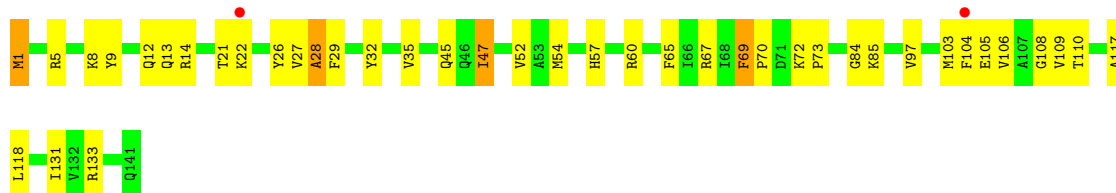
- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  70% 28% 3%

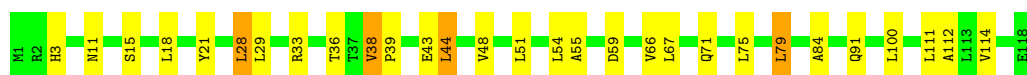
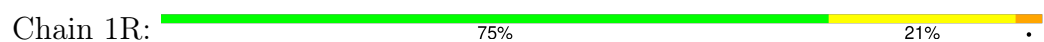




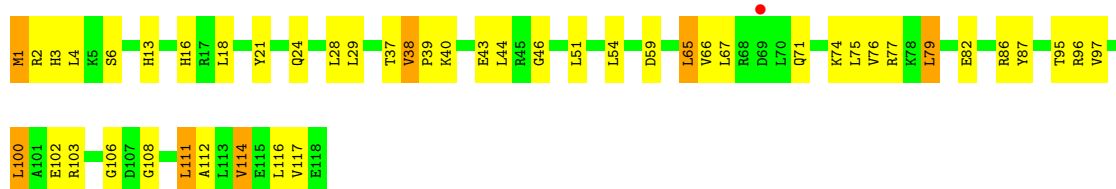
- Molecule 12: 50S ribosomal protein L16



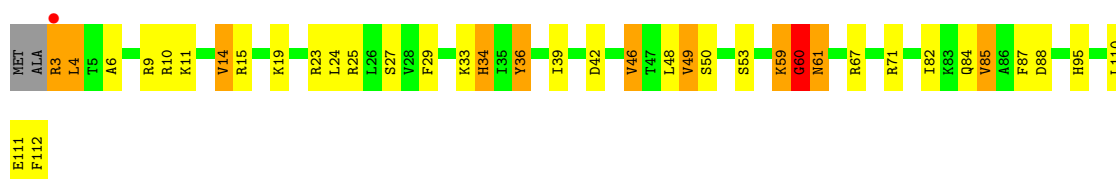
- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17

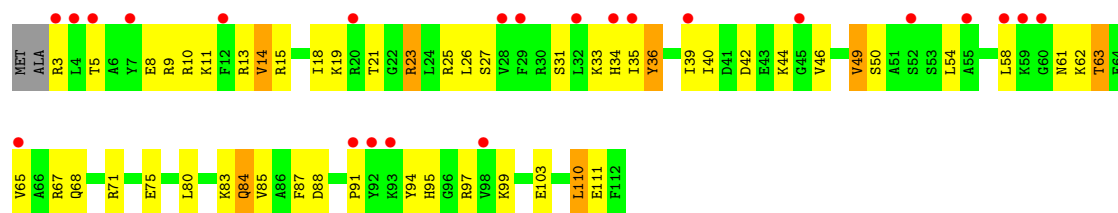


- Molecule 14: 50S ribosomal protein L18

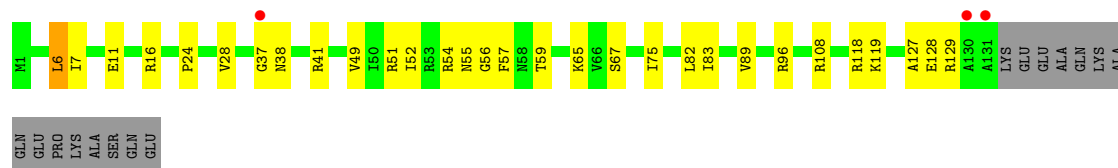


- Molecule 14: 50S ribosomal protein L18





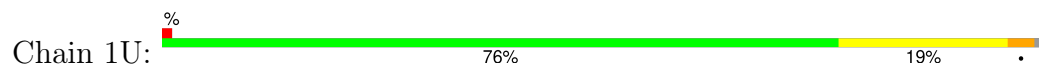
- Molecule 15: 50S ribosomal protein L19



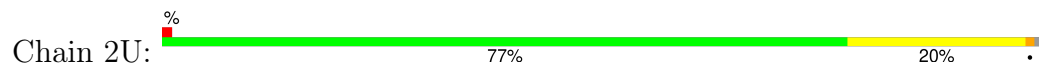
- Molecule 15: 50S ribosomal protein L19



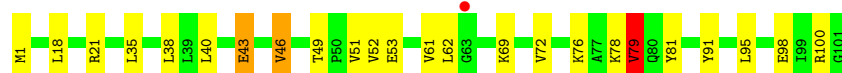
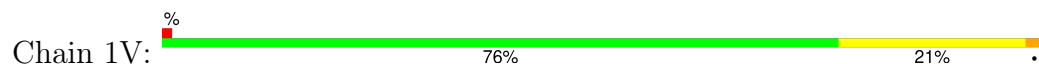
- Molecule 16: 50S ribosomal protein L20



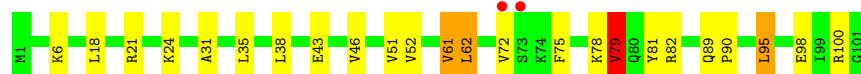
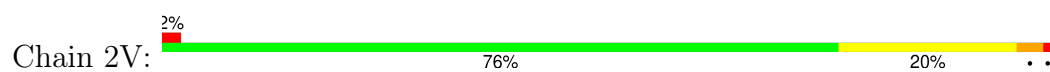
- Molecule 16: 50S ribosomal protein L20



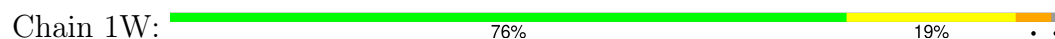
- Molecule 17: 50S ribosomal protein L21



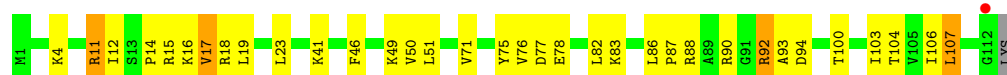
- Molecule 17: 50S ribosomal protein L21



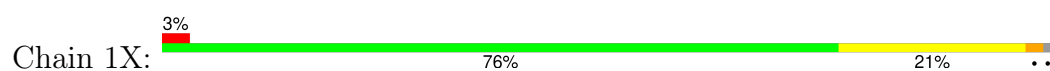
- Molecule 18: 50S ribosomal protein L22



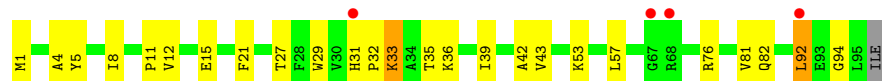
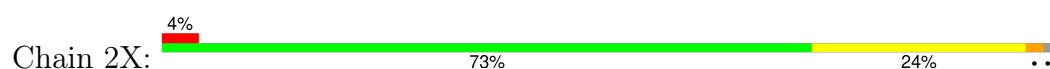
- Molecule 18: 50S ribosomal protein L22



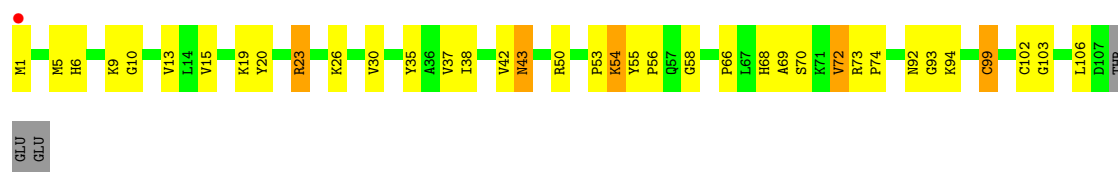
- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24





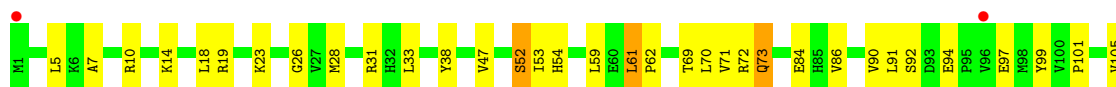
- Molecule 21: 50S ribosomal protein L25

Chain 1Z: 64% 22% 5% 10%



- Molecule 21: 50S ribosomal protein L25

Chain 2Z: 60% 26% 5% 10%



- Molecule 22: 50S ribosomal protein L27

Chain 10: 66% 19% 12%



- Molecule 22: 50S ribosomal protein L27

Chain 20: 66% 21% 12%

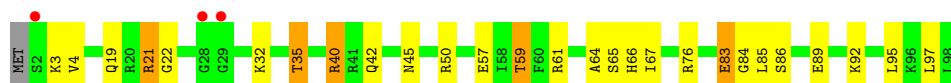


- Molecule 23: 50S ribosomal protein L28

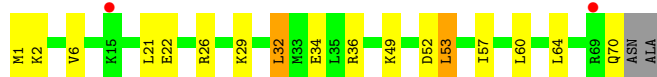
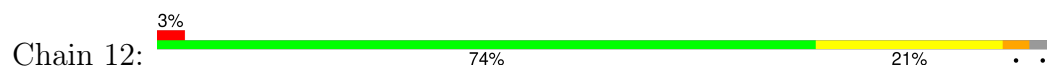
Chain 11: 79% 17% 4%



- Molecule 23: 50S ribosomal protein L28



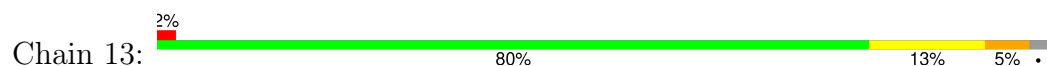
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



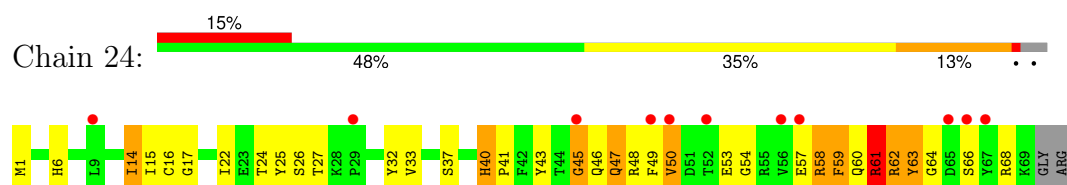
- Molecule 25: 50S ribosomal protein L30



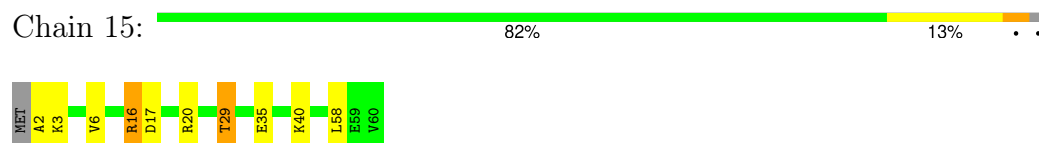
- Molecule 26: 50S ribosomal protein L31



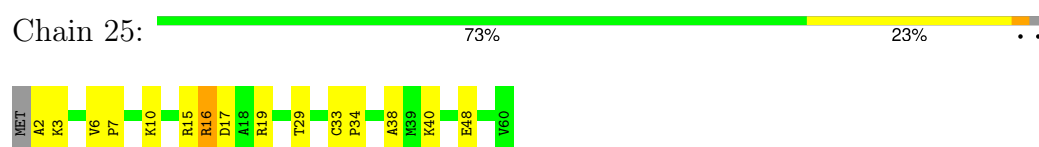
- Molecule 26: 50S ribosomal protein L31



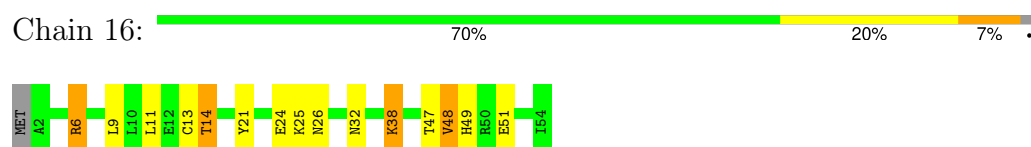
- Molecule 27: 50S ribosomal protein L32



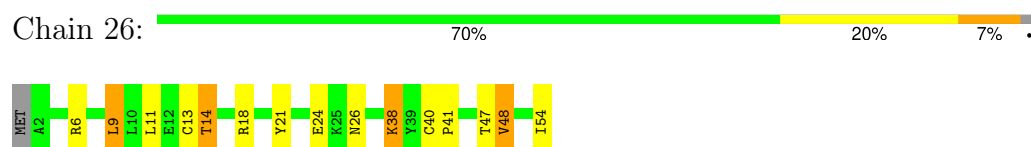
- Molecule 27: 50S ribosomal protein L32



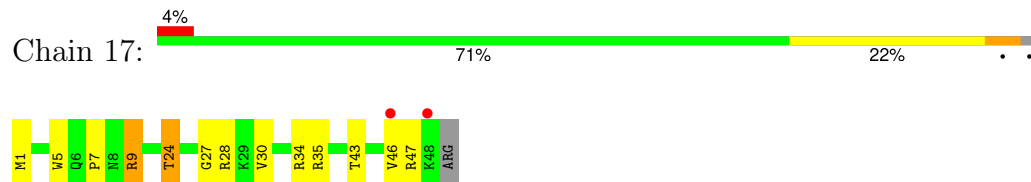
- Molecule 28: 50S ribosomal protein L33



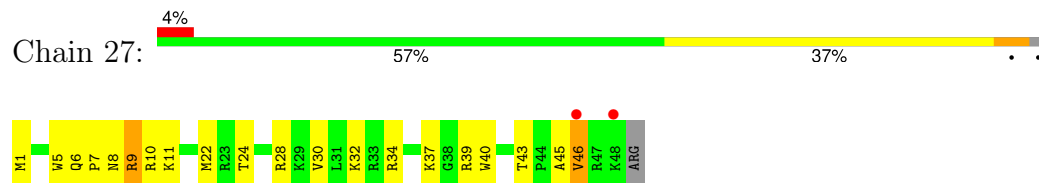
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



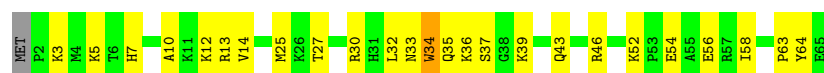
- Molecule 30: 50S ribosomal protein L35

Chain 18:  68% 31% .



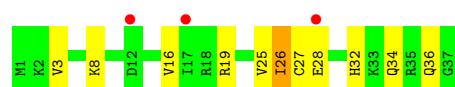
- Molecule 30: 50S ribosomal protein L35

Chain 28:  60% 37% ..



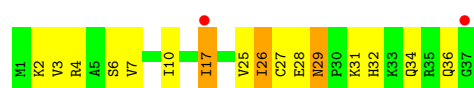
- Molecule 31: 50S ribosomal protein L36

Chain 19:  8% 70% 27% .



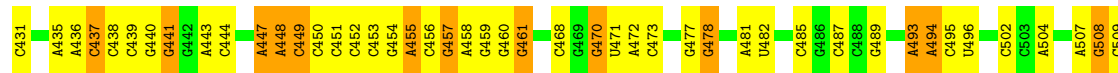
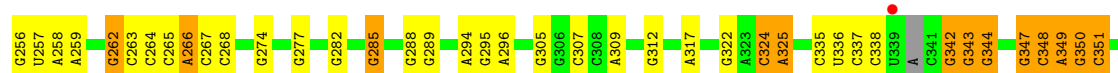
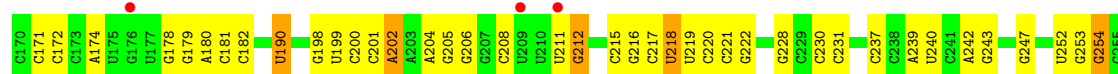
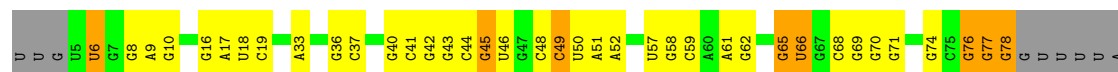
- Molecule 31: 50S ribosomal protein L36

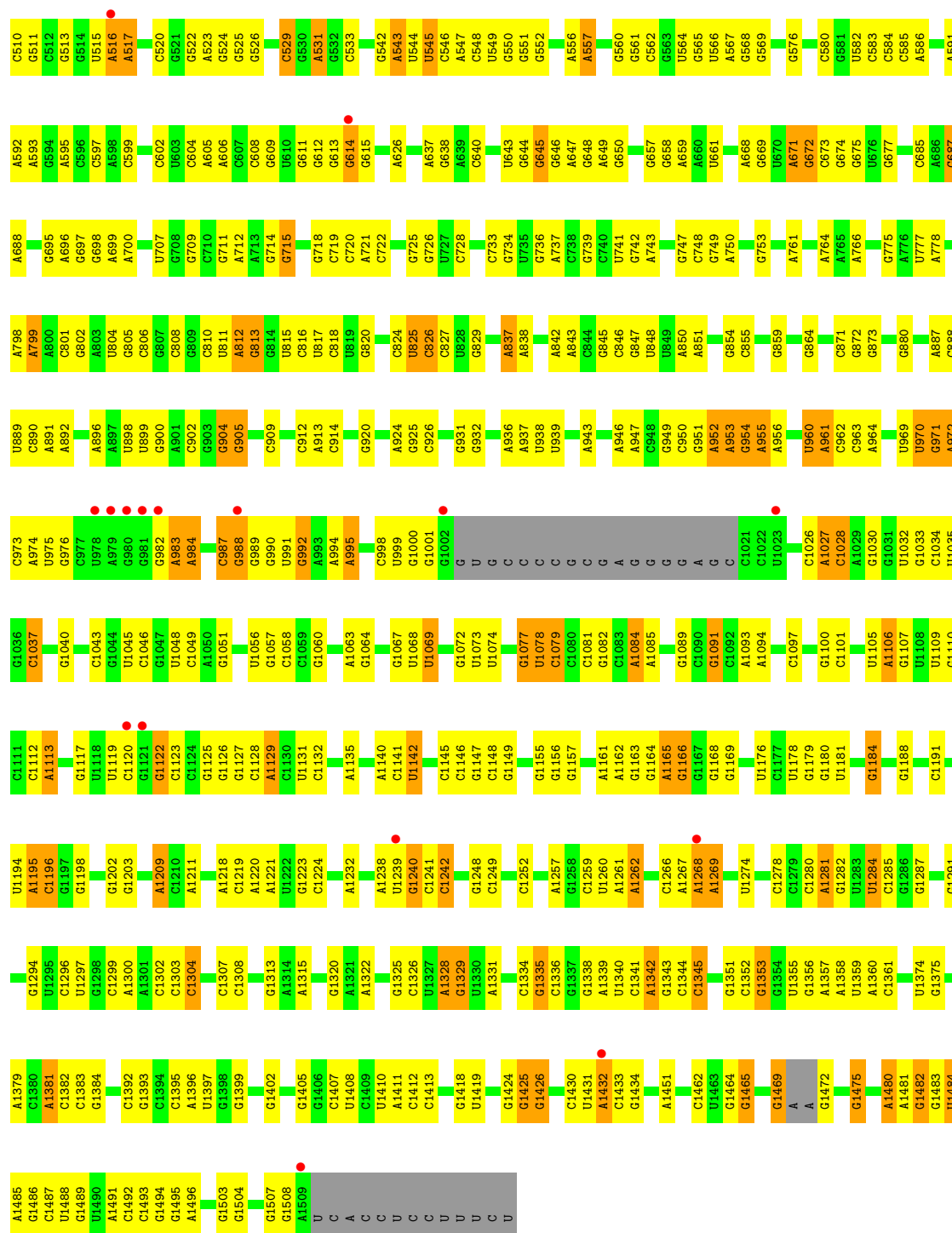
Chain 29:  5% 57% 35% 8%

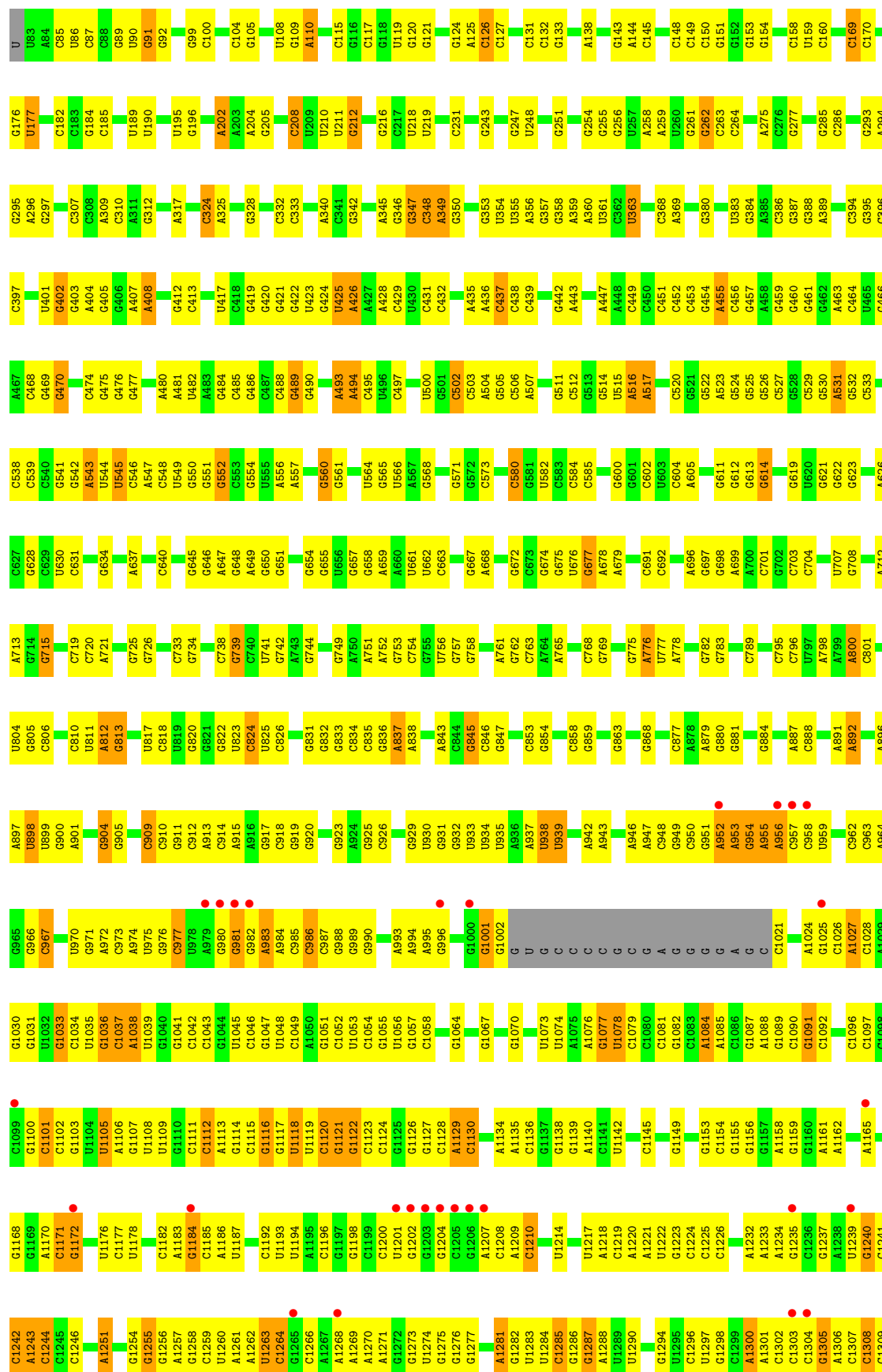


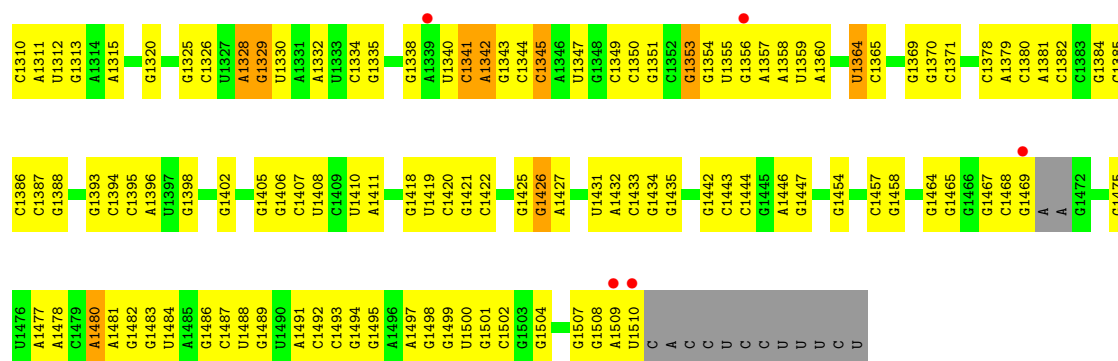
- Molecule 32: 16S Ribosomal RNA

Chain 1a:  2% 50% 38% 9% .

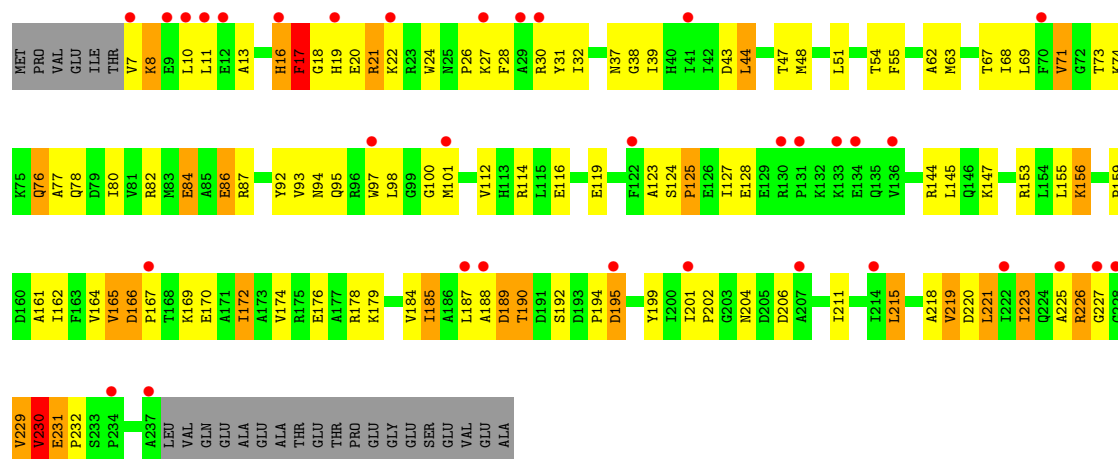




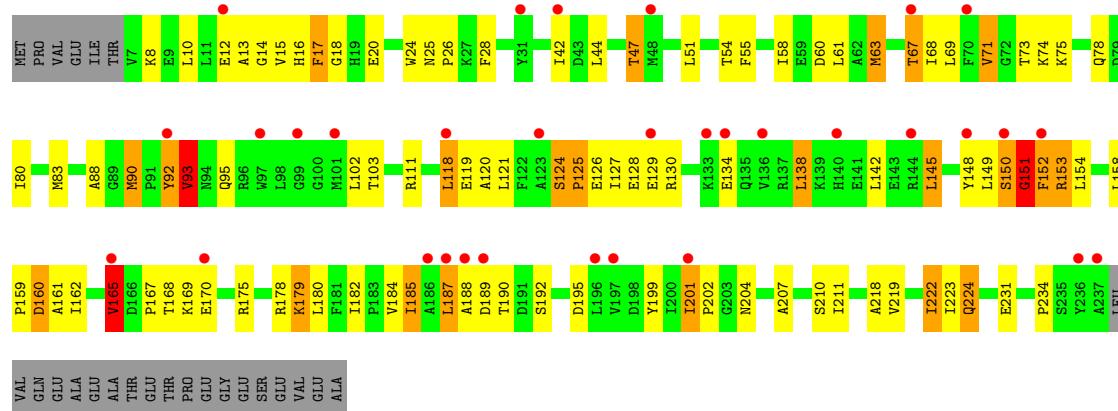




• Molecule 33: 30S ribosomal protein S2

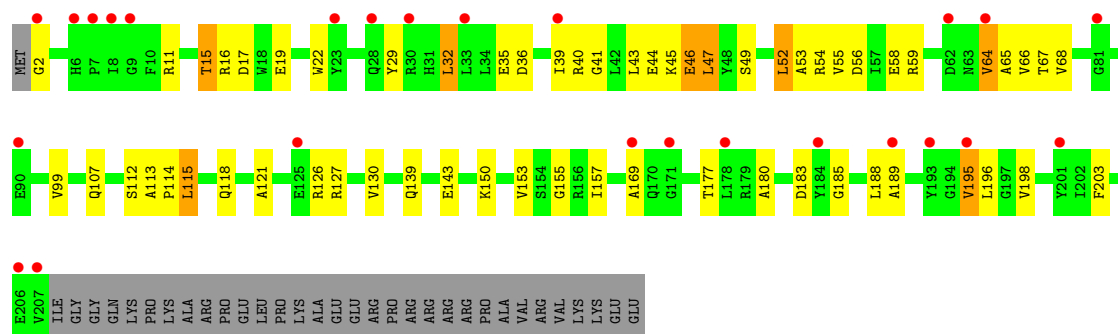


• Molecule 33: 30S ribosomal protein S2

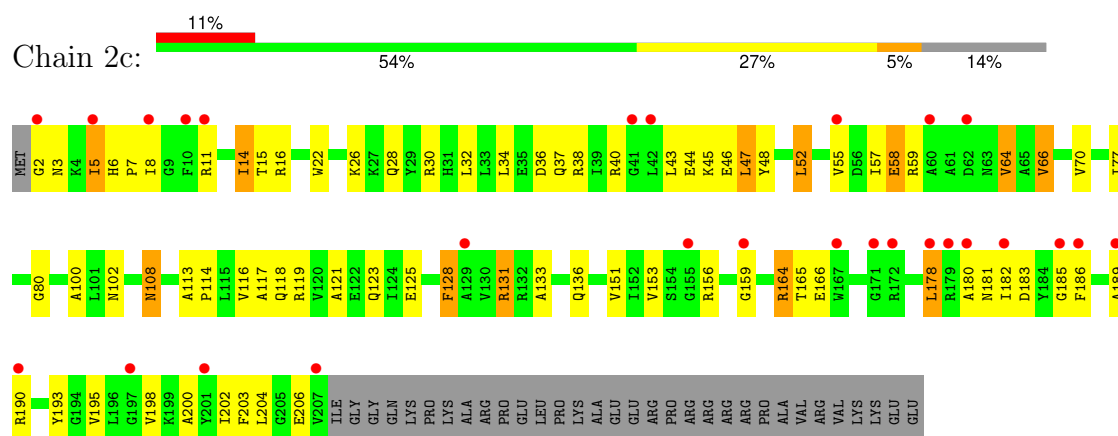


• Molecule 34: 30S ribosomal protein S3

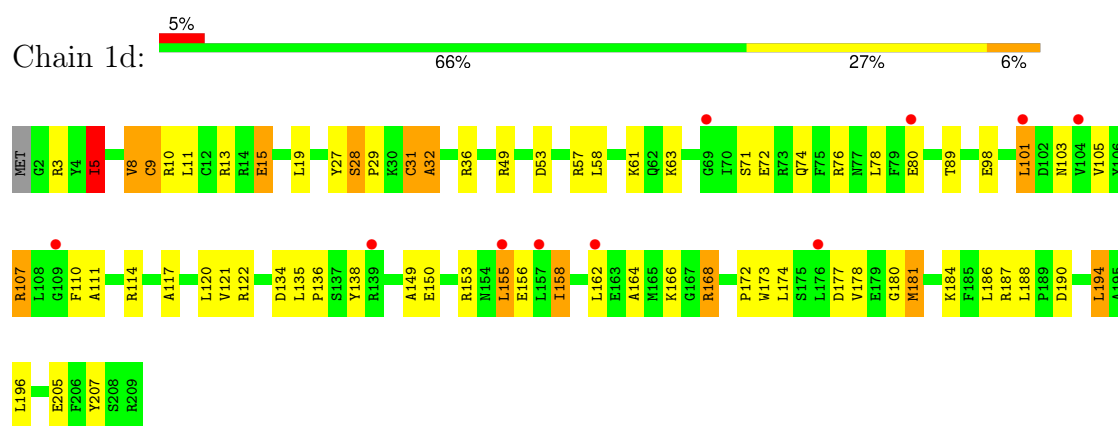




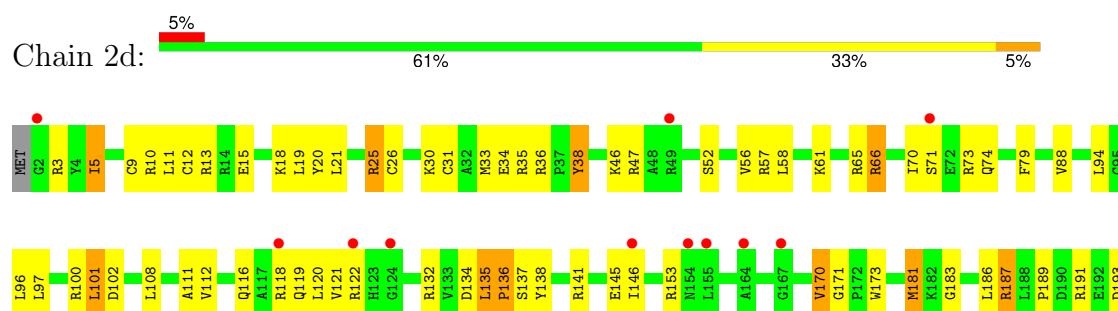
• Molecule 34: 30S ribosomal protein S3



• Molecule 35: 30S ribosomal protein S4

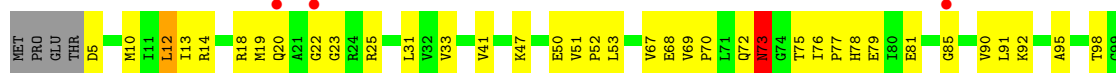


• Molecule 35: 30S ribosomal protein S4





- Molecule 36: 30S ribosomal protein S5



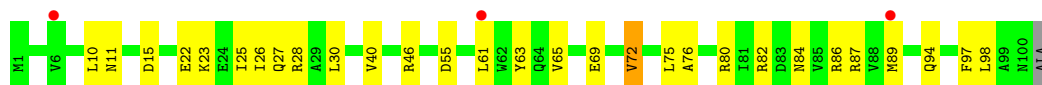
- Molecule 36: 30S ribosomal protein S5



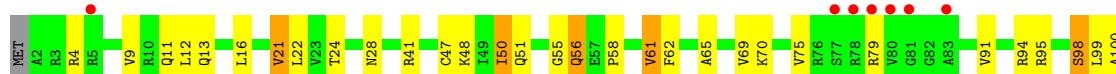
- Molecule 37: 30S ribosomal protein S6



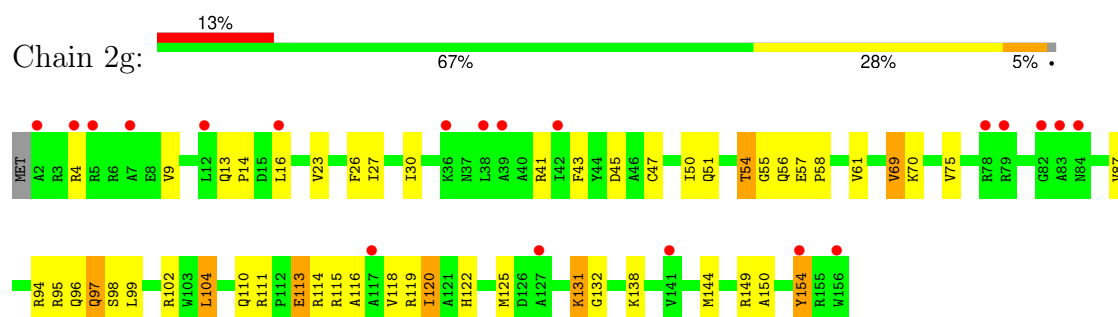
- Molecule 37: 30S ribosomal protein S6



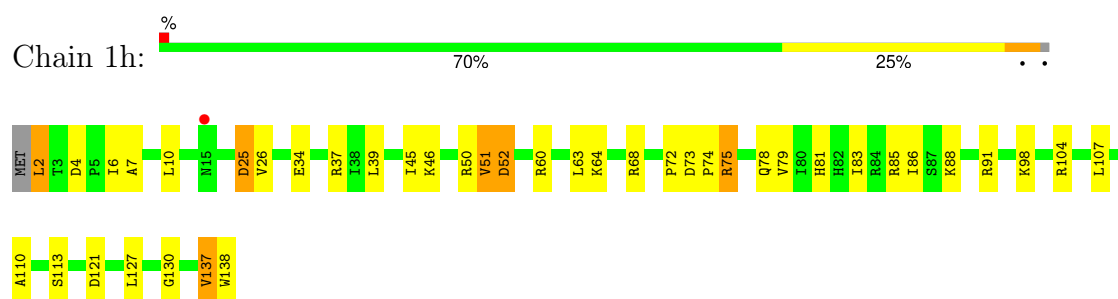
- Molecule 38: 30S ribosomal protein S7



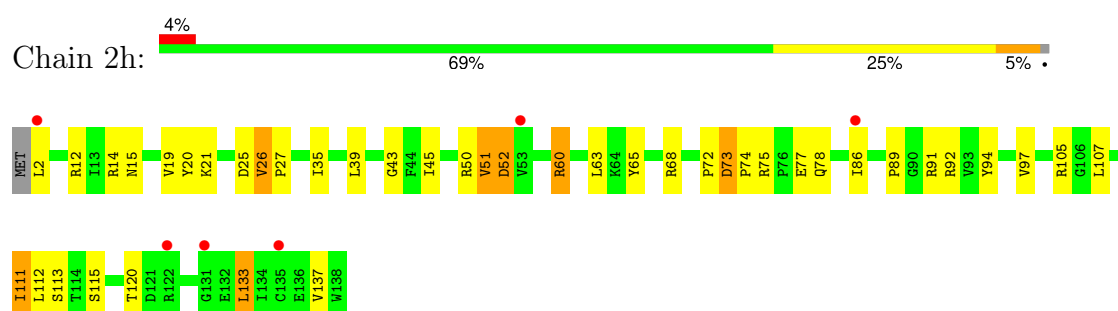
- Molecule 38: 30S ribosomal protein S7



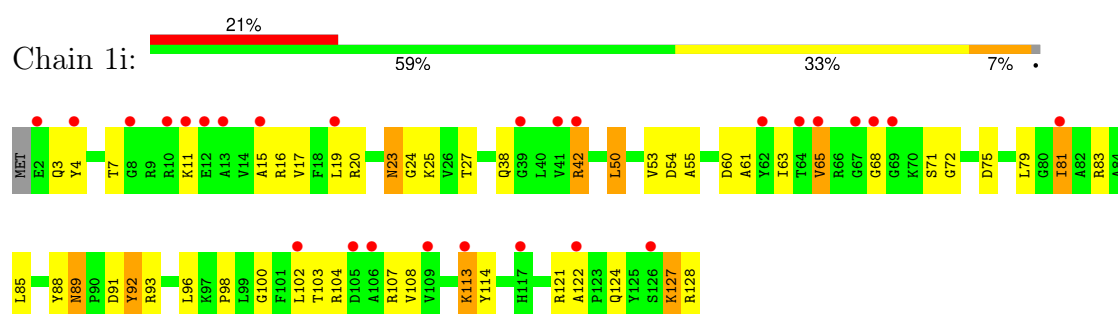
- Molecule 39: 30S ribosomal protein S8



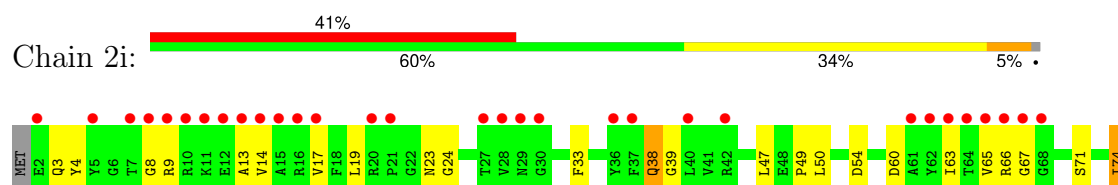
- Molecule 39: 30S ribosomal protein S8

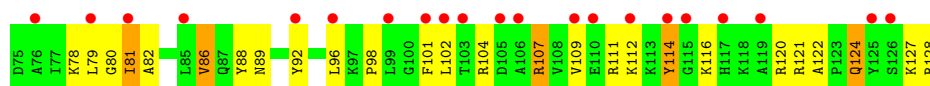


- Molecule 40: 30S ribosomal protein S9

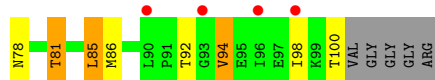


- Molecule 40: 30S ribosomal protein S9

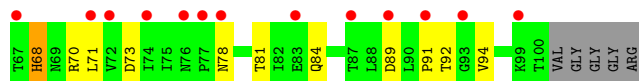
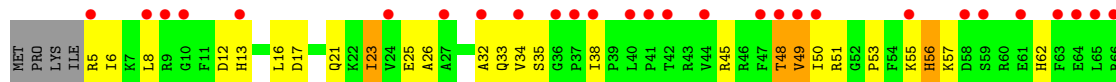
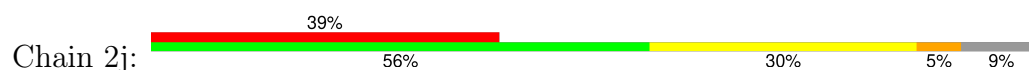




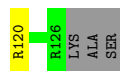
- Molecule 41: 30S ribosomal protein S10



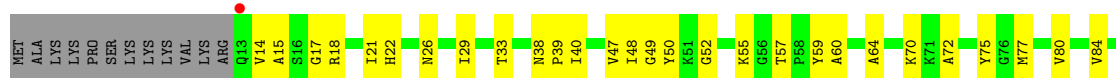
- Molecule 41: 30S ribosomal protein S10



- Molecule 42: 30S ribosomal protein S11

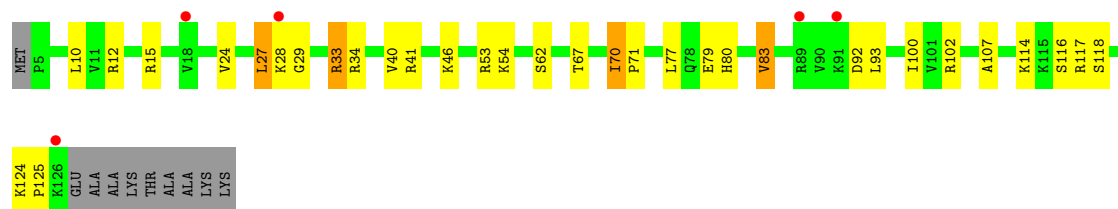


- Molecule 42: 30S ribosomal protein S11

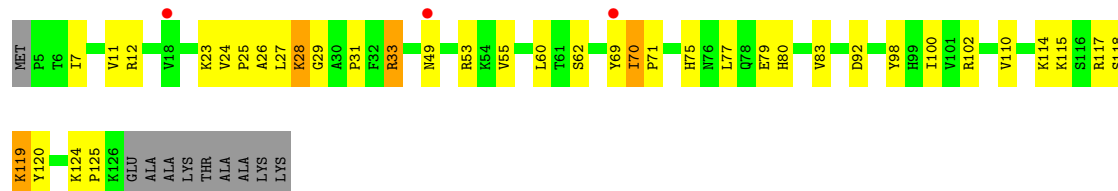


- Molecule 43: 30S ribosomal protein S12

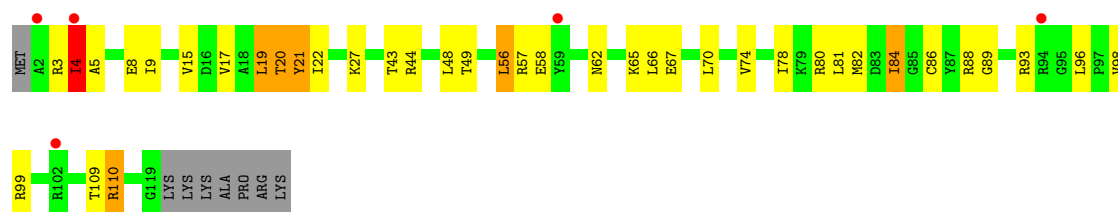




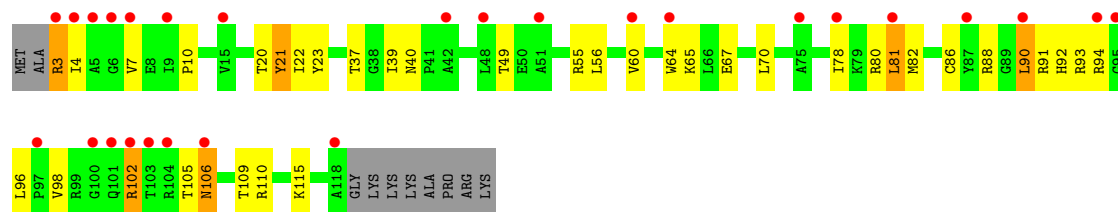
• Molecule 43: 30S ribosomal protein S12



• Molecule 44: 30S ribosomal protein S13



• Molecule 44: 30S ribosomal protein S13

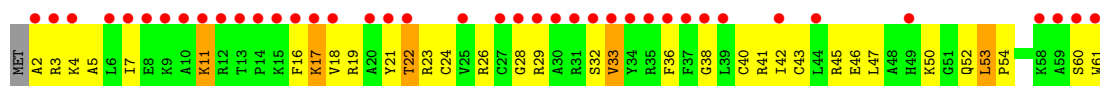


• Molecule 45: 30S ribosomal protein S14 type Z



• Molecule 45: 30S ribosomal protein S14 type Z

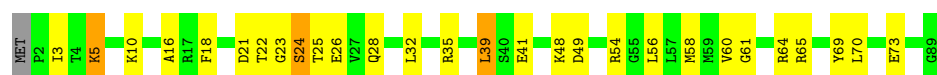




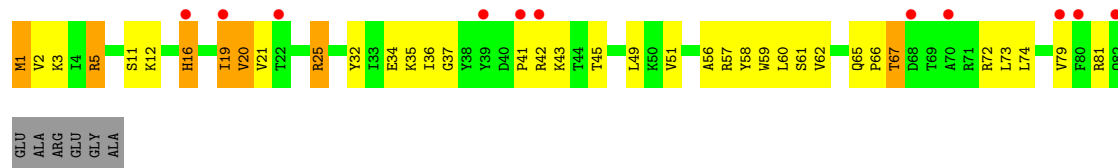
- Molecule 46: 30S ribosomal protein S15



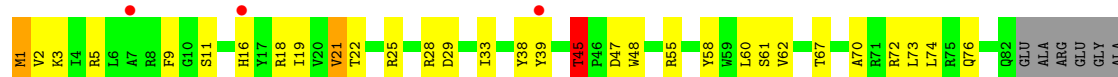
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



LYS
ALA

• Molecule 49: 30S ribosomal protein S18

Chain 1r: 

MET SER THR LYS ASN ALA LYS PRO LYS LYS GLU ALA GLN ARG ARG PRO SER ARG LYS A20 K23 A24 T25 T26 L31 R32 R35 N36 V37 E38 V39 L40 K41 T47 G48 K49 I50 L51 R54 R55 T56 G57 L58 E62 K68 T69 L76 R87 LYS

• Molecule 49: 30S ribosomal protein S18

Chain 2r: 

MET SER THR LYS ASN ALA LYS PRO LYS LYS GLU ALA GLN ARG ARG PRO SER ARG LYS A20 A24 T25 L26 D30 L31 R32 D33 R35 N36 V37 E38 T47 G48 K49 P52 R53 R54 R55 T56 G57 L58 S59 A60 K61 E62 K63 R64 T65 L66 A67 K68 T69 R72 A73

R74 R75 L76 P80 R81 T82 L85 R86 R87 LYS

• Molecule 50: 30S ribosomal protein S19

Chain 1s: 

MET P2 R3 S4 L5 K6 K7 G8 V9 F10 D13 H14 L15 K18 V19 L22 K28 R29 T33 V34 S35 R36 R37 S38 T39 I40 V41 P42 E43 M44 A50 V51 Y52 N53 G54 K55 Q56 H57 V58 P59 V60 Y61 I62 T63 E64 N65 M66 V67 G68 H69 K70 L71 G72 E73

F74 A75 Y80 G82 K85 GLU ALA ALA THR LYS LYS

• Molecule 50: 30S ribosomal protein S19

Chain 2s: 

MET P2 R3 G8 V9 F10 V11 D12 H14 L15 L16 E17 K18 N23 L24 E27 K28 R29 L30 L31 K32 T33 V34 S35 R36 R37 S38 T39 I40 V41 P42 E43 H47 T48 I49 A50 V51 Y52 N53 G54 H57 T63 E64 N65 M66 V67 G68 H69 K70 L71 G72 E73

F74 A75 P76 Y79 Y80 H83 G84 LYS GLU ALA LYS THR LYS LYS

• Molecule 51: 30S ribosomal protein S20

Chain 1t: 

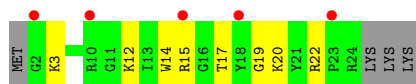
MET ALA GLN LYS LYS PRO LYS R8 R9 L10 S11 A12 L13 K14 R15 H16 R17 Q18 R19 L24 K29 K30 I33 K39 Q42 I43 A44 Q45 E46 C47 K48 E51 I55 M56 R57 E60 S61 L62 A66 A67 K68 G69 S70 T71 K74 R79 R80 K81



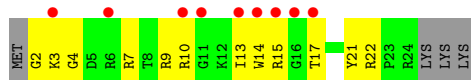
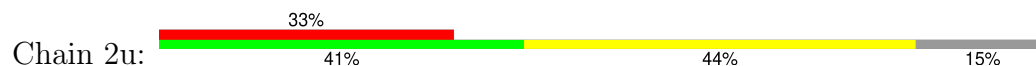
- Molecule 51: 30S ribosomal protein S20



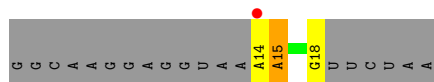
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



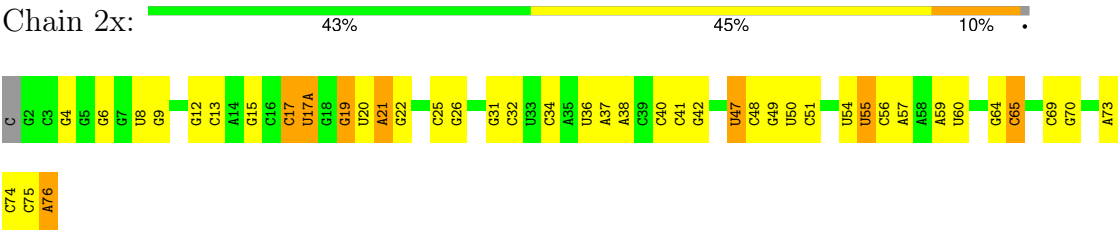
- Molecule 53: mRNA



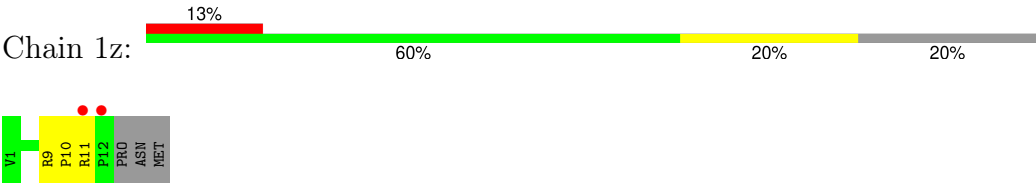
- Molecule 54: P-site tRNA



● Molecule 54: P-site tRNA



● Molecule 55: Metalnikowin-1



● Molecule 55: Metalnikowin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.87Å 450.49Å 623.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 2.89 49.85 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.85-2.89) 98.6 (49.85-2.89)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.212 , 0.268 0.212 , 0.266	Depositor DCC
R_{free} test set	64043 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	288976	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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: ZN, 4SU, PSU, 5MC, MG, SF4, 5MU

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	0.33	0/66249	0.47	1/103407 (0.0%)
1	2A	0.26	0/67298	0.45	1/105044 (0.0%)
2	1B	0.25	0/2877	0.40	0/4488
2	2B	0.28	0/2878	0.44	0/4490
3	1D	0.53	0/2186	0.91	2/2944 (0.1%)
3	2D	0.45	0/2192	0.92	2/2951 (0.1%)
4	1E	0.55	0/1592	0.94	4/2149 (0.2%)
4	2E	0.47	0/1592	0.93	4/2149 (0.2%)
5	1F	0.55	0/1619	0.92	2/2193 (0.1%)
5	2F	0.43	0/1615	0.96	8/2188 (0.4%)
6	1G	0.43	0/1450	0.86	3/1959 (0.2%)
6	2G	0.42	0/1449	0.96	2/1958 (0.1%)
7	1H	0.47	0/1356	0.87	0/1834
7	2H	0.42	0/1356	0.87	0/1834
8	1I	0.42	0/1100	0.95	6/1501 (0.4%)
8	2I	0.42	0/1076	0.93	3/1471 (0.2%)
9	1N	0.54	0/1144	0.86	0/1543
9	2N	0.41	0/1144	0.90	4/1543 (0.3%)
10	1O	0.55	0/943	0.90	2/1269 (0.2%)
10	2O	0.45	0/943	0.88	0/1269
11	1P	0.51	0/1156	0.88	0/1537
11	2P	0.43	0/1152	0.94	4/1533 (0.3%)
12	1Q	0.52	0/1143	0.82	0/1527
12	2Q	0.45	0/1143	0.92	4/1527 (0.3%)
13	1R	0.58	1/982 (0.1%)	0.88	0/1312
13	2R	0.43	0/982	0.81	1/1312 (0.1%)
14	1S	0.46	0/887	0.89	2/1180 (0.2%)
14	2S	0.39	0/880	0.85	0/1172
15	1T	0.51	0/1105	0.85	0/1477
15	2T	0.42	0/1097	0.82	0/1468
16	1U	0.56	0/977	0.85	1/1301 (0.1%)
16	2U	0.42	0/977	0.81	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	1V	0.55	0/782	0.86	1/1049 (0.1%)
17	2V	0.44	0/782	0.86	0/1049
18	1W	0.60	0/897	0.85	0/1205
18	2W	0.47	0/897	0.89	0/1205
19	1X	0.51	0/764	0.83	0/1025
19	2X	0.43	0/764	0.86	0/1025
20	1Y	0.47	0/819	0.91	2/1095 (0.2%)
20	2Y	0.40	0/819	0.85	1/1095 (0.1%)
21	1Z	0.44	0/1502	0.94	3/2041 (0.1%)
21	2Z	0.44	0/1486	1.00	11/2022 (0.5%)
22	10	0.52	0/606	0.89	0/808
22	20	0.41	0/606	0.96	2/808 (0.2%)
23	11	0.53	0/762	0.80	0/1014
23	21	0.44	0/762	0.82	0/1014
24	12	0.50	0/590	0.84	0/781
24	22	0.38	0/590	0.77	0/781
25	13	0.52	0/474	0.85	0/635
25	23	0.41	0/469	0.88	0/630
26	14	0.46	0/571	1.09	3/768 (0.4%)
26	24	0.48	0/545	1.09	6/737 (0.8%)
27	15	0.55	0/469	0.83	0/635
27	25	0.45	0/469	0.85	0/635
28	16	0.49	0/460	0.76	0/613
28	26	0.42	0/456	0.80	0/608
29	17	0.54	0/426	0.86	0/561
29	27	0.50	0/426	0.86	2/561 (0.4%)
30	18	0.57	0/525	0.85	1/691 (0.1%)
30	28	0.47	0/525	0.87	0/691
31	19	0.52	0/310	0.83	0/407
31	29	0.42	0/310	0.93	2/407 (0.5%)
32	1a	0.22	0/35537	0.40	0/55456
32	2a	0.21	0/35680	0.38	0/55681
33	1b	0.41	0/1820	0.95	5/2468 (0.2%)
33	2b	1.62	8/1728 (0.5%)	1.12	9/2352 (0.4%)
34	1c	0.38	0/1504	0.83	0/2047
34	2c	0.45	0/1435	0.92	5/1960 (0.3%)
35	1d	0.40	0/1648	0.89	2/2222 (0.1%)
35	2d	0.40	0/1659	0.89	0/2230
36	1e	0.42	0/1145	0.94	5/1543 (0.3%)
36	2e	0.41	0/1111	0.99	6/1504 (0.4%)
37	1f	0.39	0/819	0.78	0/1111
37	2f	0.42	0/830	0.80	2/1125 (0.2%)
38	1g	0.39	0/1198	0.86	1/1613 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	2g	0.38	0/1185	0.89	1/1602 (0.1%)
39	1h	0.38	0/1108	0.87	0/1494
39	2h	0.36	0/1094	0.85	0/1478
40	1i	0.38	0/995	0.86	2/1339 (0.1%)
40	2i	0.45	0/949	0.87	0/1284
41	1j	0.45	0/695	1.01	3/950 (0.3%)
41	2j	0.41	0/690	0.94	0/943
42	1k	0.40	0/840	0.87	2/1138 (0.2%)
42	2k	0.39	0/844	0.85	3/1145 (0.3%)
43	1l	0.41	0/936	0.81	0/1263
43	2l	0.42	0/934	0.92	3/1262 (0.2%)
44	1m	0.37	0/933	0.88	2/1254 (0.2%)
44	2m	0.41	0/913	0.89	0/1230
45	1n	0.39	0/491	0.88	0/653
45	2n	0.40	0/467	0.90	1/624 (0.2%)
46	1o	0.41	0/726	0.97	3/970 (0.3%)
46	2o	0.38	0/739	0.87	2/985 (0.2%)
47	1p	0.39	0/686	0.88	0/926
47	2p	0.41	0/693	0.84	2/935 (0.2%)
48	1q	0.38	0/824	0.80	0/1105
48	2q	0.36	0/836	0.82	2/1117 (0.2%)
49	1r	0.37	0/560	0.78	2/746 (0.3%)
49	2r	0.37	0/560	0.81	0/746
50	1s	0.38	0/657	0.89	2/890 (0.2%)
50	2s	0.43	0/661	0.97	0/893
51	1t	0.39	0/714	1.02	1/948 (0.1%)
51	2t	0.40	0/733	0.91	1/969 (0.1%)
52	1u	0.32	0/191	0.73	0/252
52	2u	0.34	0/203	0.89	0/266
53	1v	0.29	0/122	0.47	0/188
53	2v	0.31	0/122	0.43	0/188
54	1x	0.29	0/1725	0.46	0/2689
54	2x	0.28	0/1725	0.45	0/2689
55	1z	0.51	0/109	0.95	0/148
55	2z	0.46	0/117	1.46	2/160 (1.2%)
All	All	0.35	9/306294 (0.0%)	0.60	159/458208 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	2F	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2b	92	TYR	CD1-CE1	29.85	2.28	1.38
33	2b	92	TYR	CD2-CE2	26.82	2.19	1.38
33	2b	151	GLY	N-CA	24.08	1.80	1.45
33	2b	92	TYR	CE1-CZ	22.68	1.92	1.38
33	2b	92	TYR	CE2-CZ	22.54	1.92	1.38

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2b	150	SER	CA-C-N	18.01	156.71	121.41
33	2b	150	SER	C-N-CA	18.01	156.71	121.41
33	2b	151	GLY	N-CA-C	9.18	134.95	113.18
22	20	82	ARG	CA-C-N	8.85	129.39	119.92
22	20	82	ARG	C-N-CA	8.85	129.39	119.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	2F	20	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	59154	0	29827	655	0
1	2A	60091	0	30297	880	0
2	1B	2572	0	1306	22	0
2	2B	2573	0	1306	51	0
3	1D	2136	0	2218	61	0
3	2D	2142	0	2229	66	0
4	1E	1559	0	1617	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	2E	1559	0	1618	40	0
5	1F	1584	0	1625	31	0
5	2F	1580	0	1619	45	0
6	1G	1425	0	1443	37	0
6	2G	1424	0	1434	72	0
7	1H	1330	0	1407	32	0
7	2H	1330	0	1407	33	0
8	1I	1085	0	1114	27	0
8	2I	1061	0	1080	26	0
9	1N	1117	0	1184	18	0
9	2N	1117	0	1184	23	0
10	1O	933	0	996	20	0
10	2O	933	0	996	23	0
11	1P	1139	0	1223	39	0
11	2P	1135	0	1212	40	0
12	1Q	1122	0	1178	31	0
12	2Q	1122	0	1179	28	0
13	1R	968	0	1033	14	0
13	2R	968	0	1033	28	0
14	1S	877	0	938	29	0
14	2S	870	0	923	34	0
15	1T	1091	0	1151	20	0
15	2T	1083	0	1136	23	0
16	1U	959	0	1019	19	0
16	2U	959	0	1018	20	0
17	1V	771	0	830	11	0
17	2V	771	0	830	13	0
18	1W	886	0	940	15	0
18	2W	886	0	940	23	0
19	1X	750	0	814	16	0
19	2X	750	0	814	20	0
20	1Y	806	0	881	27	0
20	2Y	806	0	881	26	0
21	1Z	1470	0	1478	29	0
21	2Z	1454	0	1452	36	0
22	10	598	0	614	15	0
22	20	598	0	614	15	0
23	11	755	0	826	15	0
23	21	755	0	826	19	0
24	12	588	0	643	10	0
24	22	588	0	643	15	0
25	13	469	0	518	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	23	464	0	514	15	0
26	14	558	0	544	27	0
26	24	532	0	503	25	0
27	15	455	0	465	9	0
27	25	455	0	465	14	0
28	16	453	0	473	11	0
28	26	449	0	469	11	0
29	17	418	0	467	10	0
29	27	418	0	467	13	0
30	18	517	0	582	15	0
30	28	517	0	582	21	0
31	19	307	0	335	7	0
31	29	307	0	335	11	0
32	1a	31750	0	16028	533	0
32	2a	31877	0	16088	570	0
33	1b	1786	0	1744	69	0
33	2b	1697	0	1574	104	0
34	1c	1480	0	1400	45	0
34	2c	1412	0	1246	56	0
35	1d	1618	0	1579	52	1
35	2d	1630	0	1633	64	0
36	1e	1129	0	1185	31	0
36	2e	1095	0	1124	37	0
37	1f	806	0	793	26	0
37	2f	817	0	808	18	1
38	1g	1183	0	1165	27	0
38	2g	1167	0	1119	33	0
39	1h	1088	0	1126	29	0
39	2h	1074	0	1100	29	0
40	1i	976	0	973	40	0
40	2i	932	0	891	40	0
41	1j	682	0	598	17	0
41	2j	678	0	612	19	0
42	1k	826	0	829	15	0
42	2k	829	0	825	25	0
43	1l	920	0	958	23	0
43	2l	918	0	947	29	0
44	1m	923	0	962	30	0
44	2m	903	0	923	30	0
45	1n	482	0	507	20	0
45	2n	459	0	467	33	0
46	1o	715	0	729	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	2o	728	0	760	20	0
47	1p	671	0	679	28	0
47	2p	677	0	686	19	0
48	1q	811	0	858	21	0
48	2q	823	0	891	22	0
49	1r	555	0	618	15	0
49	2r	555	0	618	19	0
50	1s	642	0	629	34	0
50	2s	646	0	644	28	0
51	1t	712	0	759	20	0
51	2t	731	0	807	17	0
52	1u	187	0	186	6	0
52	2u	199	0	208	10	0
53	1v	109	0	54	2	0
53	2v	109	0	55	3	0
54	1x	1625	0	829	13	0
54	2x	1625	0	829	21	0
55	1z	105	0	108	3	0
55	2z	112	0	115	4	0
56	10	6	0	0	0	0
56	11	3	0	0	0	0
56	12	1	0	0	0	0
56	13	2	0	0	0	0
56	14	1	0	0	0	0
56	15	3	0	0	0	0
56	16	4	0	0	0	0
56	17	2	0	0	0	0
56	18	3	0	0	0	0
56	19	5	0	0	0	0
56	1A	1090	0	0	0	0
56	1B	30	0	0	0	0
56	1D	13	0	0	0	0
56	1E	12	0	0	0	0
56	1F	8	0	0	0	0
56	1G	3	0	0	0	0
56	1H	4	0	0	0	0
56	1N	7	0	0	0	0
56	1O	3	0	0	0	0
56	1P	6	0	0	0	0
56	1Q	9	0	0	0	0
56	1R	6	0	0	0	0
56	1T	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1U	6	0	0	0	0
56	1V	2	0	0	0	0
56	1W	6	0	0	0	0
56	1X	1	0	0	0	0
56	1Y	1	0	0	0	0
56	1Z	2	0	0	0	0
56	1a	309	0	0	0	0
56	1b	1	0	0	0	0
56	1d	2	0	0	0	0
56	1e	3	0	0	0	0
56	1f	1	0	0	0	0
56	1h	2	0	0	0	0
56	1k	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	1	0	0	0	0
56	1n	1	0	0	0	0
56	1o	3	0	0	0	0
56	1p	2	0	0	0	0
56	1q	3	0	0	0	0
56	1r	3	0	0	0	0
56	1t	1	0	0	0	0
56	1u	1	0	0	0	0
56	1v	1	0	0	0	0
56	1x	10	0	0	0	0
56	1z	1	0	0	0	0
56	20	1	0	0	0	0
56	23	1	0	0	0	0
56	25	1	0	0	0	0
56	28	3	0	0	0	0
56	2A	561	0	0	0	0
56	2B	10	0	0	0	0
56	2D	5	0	0	0	0
56	2E	4	0	0	0	0
56	2F	4	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	3	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	5	0	0	0	0
56	2R	2	0	0	0	0
56	2T	1	0	0	0	0
56	2U	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2X	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	255	0	0	0	0
56	2d	2	0	0	0	0
56	2e	2	0	0	0	0
56	2f	1	0	0	0	0
56	2l	5	0	0	0	0
56	2q	3	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	1	0	0	0	0
56	2x	7	0	0	0	0
56	2z	1	0	0	0	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	0	0
58	2d	8	0	0	0	0
59	10	8	0	0	2	0
59	11	7	0	0	0	0
59	12	2	0	0	0	0
59	13	3	0	0	0	0
59	15	7	0	0	1	0
59	16	11	0	0	2	0
59	17	9	0	0	0	0
59	18	16	0	0	0	0
59	19	3	0	0	1	0
59	1A	2412	0	0	134	0
59	1B	46	0	0	5	0
59	1D	25	0	0	2	0
59	1E	30	0	0	5	0
59	1F	21	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1G	8	0	0	0	0
59	1H	4	0	0	0	0
59	1I	3	0	0	2	0
59	1N	8	0	0	0	0
59	1O	5	0	0	0	0
59	1P	25	0	0	3	0
59	1Q	13	0	0	3	0
59	1R	18	0	0	1	0
59	1S	2	0	0	0	0
59	1T	13	0	0	2	0
59	1U	18	0	0	1	0
59	1V	5	0	0	1	0
59	1W	14	0	0	1	0
59	1X	5	0	0	0	0
59	1Y	1	0	0	0	0
59	1Z	6	0	0	1	0
59	1a	394	0	0	34	0
59	1b	1	0	0	0	0
59	1c	1	0	0	0	0
59	1d	3	0	0	1	0
59	1e	4	0	0	1	0
59	1f	1	0	0	0	0
59	1h	2	0	0	0	0
59	1j	1	0	0	0	0
59	1k	2	0	0	1	0
59	1l	3	0	0	1	0
59	1m	1	0	0	0	0
59	1p	1	0	0	0	0
59	1q	1	0	0	0	0
59	1s	1	0	0	1	0
59	1u	1	0	0	0	0
59	1v	3	0	0	1	0
59	1x	10	0	0	0	0
59	1z	5	0	0	0	0
59	20	2	0	0	0	0
59	21	1	0	0	0	0
59	23	2	0	0	0	0
59	25	1	0	0	0	0
59	27	1	0	0	0	0
59	28	4	0	0	0	0
59	2A	824	0	0	85	0
59	2B	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2D	18	0	0	0	0
59	2E	11	0	0	0	0
59	2F	6	0	0	0	0
59	2N	2	0	0	0	0
59	2O	1	0	0	0	0
59	2P	6	0	0	0	0
59	2R	1	0	0	0	0
59	2T	1	0	0	0	0
59	2U	3	0	0	0	0
59	2W	1	0	0	0	0
59	2X	3	0	0	1	0
59	2Y	2	0	0	1	0
59	2Z	5	0	0	1	0
59	2a	329	0	0	38	0
59	2c	1	0	0	1	0
59	2d	1	0	0	0	0
59	2e	4	0	0	1	0
59	2g	1	0	0	0	0
59	2i	2	0	0	0	0
59	2l	2	0	0	0	0
59	2m	1	0	0	0	0
59	2o	1	0	0	0	0
59	2p	2	0	0	0	0
59	2q	1	0	0	1	0
59	2t	4	0	0	1	0
59	2u	1	0	0	0	0
59	2x	6	0	0	1	0
59	2z	2	0	0	0	0
All	All	288976	0	189961	4693	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 4693 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)
33:2b:92:TYR:CD1	33:2b:92:TYR:CG	1.83	1.61
33:2b:92:TYR:CG	33:2b:92:TYR:CD2	1.81	1.57
33:2b:92:TYR:CZ	33:2b:92:TYR:CE2	1.92	1.57
33:2b:92:TYR:CZ	33:2b:92:TYR:CE1	1.92	1.53
33:2b:151:GLY:N	33:2b:151:GLY:CA	1.80	1.43

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:27:TYR:OH	37:2f:15:ASP:OD2[2_655]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	253 (93%)	20 (7%)	0	100	100
3	2D	273/276 (99%)	252 (92%)	19 (7%)	2 (1%)	18	48
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	54
4	2E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	54
5	1F	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	12	39
5	2F	201/210 (96%)	193 (96%)	6 (3%)	2 (1%)	12	39
6	1G	179/182 (98%)	161 (90%)	15 (8%)	3 (2%)	7	26
6	2G	179/182 (98%)	156 (87%)	18 (10%)	5 (3%)	4	15
7	1H	172/180 (96%)	161 (94%)	9 (5%)	2 (1%)	10	34
7	2H	172/180 (96%)	159 (92%)	11 (6%)	2 (1%)	10	34
8	1I	144/148 (97%)	126 (88%)	14 (10%)	4 (3%)	4	15
8	2I	144/148 (97%)	124 (86%)	19 (13%)	1 (1%)	18	48
9	1N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	2N	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	18	48
10	1O	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16	44
10	2O	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16	44
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	48
11	2P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	9	30
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	2Q	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	18	48
13	1R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
13	2R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
14	1S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	14	41
14	2S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	14	41
15	1T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	39
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12	39
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	92 (99%)	0	1 (1%)	11	36
19	2X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	36
20	1Y	105/110 (96%)	93 (89%)	10 (10%)	2 (2%)	6	23
20	2Y	105/110 (96%)	94 (90%)	11 (10%)	0	100	100
21	1Z	184/206 (89%)	169 (92%)	15 (8%)	0	100	100
21	2Z	184/206 (89%)	167 (91%)	15 (8%)	2 (1%)	11	36
22	10	73/85 (86%)	70 (96%)	2 (3%)	1 (1%)	9	30
22	20	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	50 (75%)	8 (12%)	9 (13%)	0	0
26	24	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	2
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	43 (94%)	1 (2%)	2 (4%)	2	8
30	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	190 (83%)	31 (14%)	8 (4%)	3	12
33	2b	229/256 (90%)	188 (82%)	32 (14%)	9 (4%)	2	10
34	1c	204/239 (85%)	178 (87%)	22 (11%)	4 (2%)	6	22
34	2c	204/239 (85%)	173 (85%)	29 (14%)	2 (1%)	12	39
35	1d	206/209 (99%)	188 (91%)	13 (6%)	5 (2%)	4	18
35	2d	206/209 (99%)	188 (91%)	15 (7%)	3 (2%)	8	28
36	1e	146/162 (90%)	126 (86%)	15 (10%)	5 (3%)	3	12
36	2e	146/162 (90%)	129 (88%)	13 (9%)	4 (3%)	4	16
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
38	1g	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	18	48
38	2g	153/156 (98%)	132 (86%)	19 (12%)	2 (1%)	9	32
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	3 (2%)	2 (2%)	8	28
40	1i	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	16	44
40	2i	125/128 (98%)	110 (88%)	13 (10%)	2 (2%)	7	27
41	1j	95/105 (90%)	80 (84%)	8 (8%)	7 (7%)	1	2
41	2j	94/105 (90%)	79 (84%)	13 (14%)	2 (2%)	5	21
42	1k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	6	25
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	6	25
43	1l	120/132 (91%)	115 (96%)	4 (3%)	1 (1%)	16	44
43	2l	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
44	1m	116/126 (92%)	103 (89%)	9 (8%)	4 (3%)	3	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	2m	114/126 (90%)	101 (89%)	11 (10%)	2 (2%)	6	25
45	1n	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	26
45	2n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	1p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	9	32
47	2p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
48	1q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	12	39
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
49	1r	66/88 (75%)	59 (89%)	5 (8%)	2 (3%)	3	14
49	2r	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	8	28
50	1s	82/93 (88%)	72 (88%)	10 (12%)	0	100	100
50	2s	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
51	1t	94/106 (89%)	79 (84%)	12 (13%)	3 (3%)	3	13
51	2t	94/106 (89%)	82 (87%)	8 (8%)	4 (4%)	2	8
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
55	1z	10/15 (67%)	9 (90%)	1 (10%)	0	100	100
55	2z	11/15 (73%)	7 (64%)	3 (27%)	1 (9%)	0	1
All	All	11431/12158 (94%)	10499 (92%)	791 (7%)	141 (1%)	10	34

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	51	ARG
6	1G	126	ASP
7	1H	126	PRO
14	1S	60	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	197 (92%)	18 (8%)	10	31
3	2D	216/218 (99%)	191 (88%)	25 (12%)	5	18
4	1E	164/166 (99%)	143 (87%)	21 (13%)	4	14
4	2E	164/166 (99%)	138 (84%)	26 (16%)	2	8
5	1F	160/166 (96%)	140 (88%)	20 (12%)	4	15
5	2F	159/166 (96%)	141 (89%)	18 (11%)	5	19
6	1G	143/156 (92%)	126 (88%)	17 (12%)	5	16
6	2G	142/156 (91%)	121 (85%)	21 (15%)	3	10
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9	28
7	2H	144/148 (97%)	132 (92%)	12 (8%)	10	32
8	1I	110/124 (89%)	88 (80%)	22 (20%)	1	4
8	2I	104/124 (84%)	91 (88%)	13 (12%)	4	15
9	1N	118/119 (99%)	100 (85%)	18 (15%)	3	9
9	2N	118/119 (99%)	101 (86%)	17 (14%)	3	11
10	1O	100/100 (100%)	92 (92%)	8 (8%)	11	34
10	2O	100/100 (100%)	92 (92%)	8 (8%)	11	34
11	1P	116/116 (100%)	100 (86%)	16 (14%)	3	12
11	2P	115/116 (99%)	102 (89%)	13 (11%)	5	19
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11	33
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16	45
13	1R	101/101 (100%)	87 (86%)	14 (14%)	3	11
13	2R	101/101 (100%)	84 (83%)	17 (17%)	2	7
14	1S	87/88 (99%)	75 (86%)	12 (14%)	3	12
14	2S	85/88 (97%)	71 (84%)	14 (16%)	2	8
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	40
15	2T	113/127 (89%)	105 (93%)	8 (7%)	13	40
16	1U	93/94 (99%)	86 (92%)	7 (8%)	12	37
16	2U	93/94 (99%)	89 (96%)	4 (4%)	26	60
17	1V	80/82 (98%)	68 (85%)	12 (15%)	3	10
17	2V	80/82 (98%)	68 (85%)	12 (15%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	1W	90/92 (98%)	80 (89%)	10 (11%)	6	20
18	2W	90/92 (98%)	83 (92%)	7 (8%)	11	35
19	1X	77/78 (99%)	72 (94%)	5 (6%)	15	44
19	2X	77/78 (99%)	73 (95%)	4 (5%)	21	52
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	13	40
20	2Y	85/91 (93%)	78 (92%)	7 (8%)	10	32
21	1Z	159/179 (89%)	142 (89%)	17 (11%)	6	22
21	2Z	156/179 (87%)	142 (91%)	14 (9%)	9	28
22	10	60/67 (90%)	55 (92%)	5 (8%)	10	32
22	20	60/67 (90%)	57 (95%)	3 (5%)	22	53
23	11	80/83 (96%)	74 (92%)	6 (8%)	12	37
23	21	80/83 (96%)	72 (90%)	8 (10%)	7	24
24	12	65/67 (97%)	60 (92%)	5 (8%)	12	35
24	22	65/67 (97%)	60 (92%)	5 (8%)	12	35
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	12
25	23	50/52 (96%)	43 (86%)	7 (14%)	3	11
26	14	60/63 (95%)	50 (83%)	10 (17%)	2	7
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	10
27	15	50/52 (96%)	45 (90%)	5 (10%)	7	24
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	34
28	16	51/52 (98%)	46 (90%)	5 (10%)	7	25
28	26	50/52 (96%)	46 (92%)	4 (8%)	11	34
29	17	41/42 (98%)	37 (90%)	4 (10%)	7	25
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	16
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	50
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	38
31	19	34/34 (100%)	32 (94%)	2 (6%)	18	48
31	29	34/34 (100%)	30 (88%)	4 (12%)	5	17
33	1b	177/220 (80%)	143 (81%)	34 (19%)	1	5
33	2b	158/220 (72%)	131 (83%)	27 (17%)	2	7
34	1c	127/188 (68%)	117 (92%)	10 (8%)	11	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	2c	108/188 (57%)	93 (86%)	15 (14%)	3	11
35	1d	161/181 (89%)	142 (88%)	19 (12%)	5	17
35	2d	164/181 (91%)	145 (88%)	19 (12%)	5	18
36	1e	113/123 (92%)	103 (91%)	10 (9%)	9	29
36	2e	106/123 (86%)	94 (89%)	12 (11%)	5	19
37	1f	83/90 (92%)	76 (92%)	7 (8%)	10	31
37	2f	86/90 (96%)	81 (94%)	5 (6%)	18	49
38	1g	111/127 (87%)	98 (88%)	13 (12%)	5	17
38	2g	107/127 (84%)	96 (90%)	11 (10%)	7	23
39	1h	114/119 (96%)	100 (88%)	14 (12%)	4	15
39	2h	111/119 (93%)	96 (86%)	15 (14%)	4	12
40	1i	89/99 (90%)	77 (86%)	12 (14%)	4	12
40	2i	80/99 (81%)	67 (84%)	13 (16%)	2	8
41	1j	60/92 (65%)	50 (83%)	10 (17%)	2	7
41	2j	62/92 (67%)	49 (79%)	13 (21%)	1	4
42	1k	82/99 (83%)	75 (92%)	7 (8%)	10	31
42	2k	82/99 (83%)	74 (90%)	8 (10%)	7	25
43	1l	95/109 (87%)	87 (92%)	8 (8%)	10	31
43	2l	94/109 (86%)	89 (95%)	5 (5%)	20	52
44	1m	90/101 (89%)	81 (90%)	9 (10%)	7	24
44	2m	87/101 (86%)	77 (88%)	10 (12%)	5	18
45	1n	47/50 (94%)	42 (89%)	5 (11%)	6	22
45	2n	43/50 (86%)	38 (88%)	5 (12%)	5	18
46	1o	75/80 (94%)	64 (85%)	11 (15%)	3	10
46	2o	78/80 (98%)	70 (90%)	8 (10%)	7	23
47	1p	67/74 (90%)	55 (82%)	12 (18%)	2	6
47	2p	68/74 (92%)	58 (85%)	10 (15%)	3	10
48	1q	91/97 (94%)	82 (90%)	9 (10%)	7	24
48	2q	94/97 (97%)	89 (95%)	5 (5%)	20	52
49	1r	59/77 (77%)	52 (88%)	7 (12%)	5	16
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	1s	65/80 (81%)	57 (88%)	8 (12%)	4	15
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	28
51	1t	66/82 (80%)	57 (86%)	9 (14%)	3	12
51	2t	71/82 (87%)	64 (90%)	7 (10%)	7	24
52	1u	16/22 (73%)	15 (94%)	1 (6%)	16	45
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	50
55	1z	12/15 (80%)	12 (100%)	0	100	100
55	2z	13/15 (87%)	13 (100%)	0	100	100
All	All	9160/10096 (91%)	8138 (89%)	1022 (11%)	6	19

5 of 1022 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	1o	3	ILE
36	2e	51	VAL
5	2F	24	LEU
35	2d	187	ARG
41	2j	84	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 170 such sidechains are listed below:

Mol	Chain	Res	Type
20	2Y	43	ASN
38	2g	97	GLN
25	23	32	GLN
34	2c	28	GLN
40	2i	89	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2737/2915 (93%)	384 (14%)	19 (0%)
1	2A	2781/2915 (95%)	475 (17%)	25 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	119/121 (98%)	22 (18%)	2 (1%)
32	1a	1472/1521 (96%)	257 (17%)	0
32	2a	1479/1521 (97%)	268 (18%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	1v	4/24 (16%)	1 (25%)	0
53	2v	4/24 (16%)	1 (25%)	0
54	1x	75/77 (97%)	18 (24%)	0
54	2x	75/77 (97%)	18 (24%)	0
All	All	8865/9316 (95%)	1453 (16%)	46 (0%)

5 of 1453 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	33	C
1	1A	35	G
1	1A	44	C
1	1A	61	U

5 of 46 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	1071	U
1	2A	1465	U
1	2A	1087	G
1	2A	1238	A
1	2A	1820	C

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

8 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	$\# Z > 2$
54	PSU	1x	55	54	18,21,22	1.33	2 (11%)	21,30,33	1.87	3 (14%)
54	5MU	1x	54	54	19,22,23	1.54	5 (26%)	27,32,35	1.90	5 (18%)
54	5MU	2x	54	54	19,22,23	1.43	5 (26%)	27,32,35	1.98	6 (22%)
54	5MC	1x	32	54	19,22,23	1.62	3 (15%)	26,32,35	1.16	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	5MC	2x	32	54	19,22,23	1.70	2 (10%)	26,32,35	1.27	3 (11%)
54	PSU	2x	55	54	18,21,22	1.36	2 (11%)	21,30,33	1.95	4 (19%)
54	4SU	2x	8	54	18,21,22	2.00	5 (27%)	25,30,33	1.25	4 (16%)
54	4SU	1x	8	54	18,21,22	2.13	4 (22%)	25,30,33	1.34	4 (16%)

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
54	PSU	1x	55	54	-	2/7/25/26	0/2/2/2
54	5MU	1x	54	54	-	0/7/25/26	0/2/2/2
54	5MU	2x	54	54	-	1/7/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/7/25/26	0/2/2/2
54	5MC	2x	32	54	-	1/7/25/26	0/2/2/2
54	PSU	2x	55	54	-	2/7/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/7/25/26	0/2/2/2
54	4SU	1x	8	54	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2x	32	5MC	C5-C4	5.99	1.48	1.44
54	1x	32	5MC	C5-C4	5.62	1.48	1.44
54	1x	8	4SU	C4-N3	-4.92	1.32	1.37
54	2x	8	4SU	C4-N3	-4.73	1.32	1.37
54	1x	8	4SU	C4-S4	-4.44	1.60	1.68

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2x	55	PSU	N1-C2-N3	6.07	121.57	115.17
54	1x	55	PSU	N1-C2-N3	5.52	120.99	115.17
54	1x	54	5MU	N3-C2-N1	5.25	121.72	114.89
54	2x	54	5MU	N3-C2-N1	4.82	121.16	114.89
54	2x	54	5MU	C4-N3-C2	-4.78	121.07	127.34

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	1x	55	PSU	O4'-C4'-C5'-O5'
54	2x	55	PSU	O4'-C4'-C5'-O5'
54	2x	54	5MU	C3'-C4'-C5'-O5'
54	1x	55	PSU	C3'-C4'-C5'-O5'
54	2x	32	5MC	C2'-C1'-N1-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2x	55	PSU	1	0
54	1x	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2494 ligands modelled in this entry, 2492 are monoatomic - leaving 2 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	$\# Z > 2$
58	SF4	2d	501	35	0,12,12	-	-	-		
58	SF4	1d	501	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	2d	501	35	-	-	0/6/5/5
58	SF4	1d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	2746/2915 (94%)	-0.38	28 (1%) 79 73	22, 41, 87, 114	0
1	2A	2790/2915 (95%)	-0.28	22 (0%) 82 77	25, 46, 93, 111	0
2	1B	120/121 (99%)	0.15	1 (0%) 82 77	36, 65, 80, 91	0
2	2B	120/121 (99%)	0.65	2 (1%) 69 61	41, 70, 83, 92	0
3	1D	275/276 (99%)	-0.21	0 100 100	23, 40, 57, 77	0
3	2D	275/276 (99%)	-0.17	2 (0%) 84 79	24, 43, 59, 78	0
4	1E	204/206 (99%)	-0.12	0 100 100	21, 43, 66, 81	0
4	2E	204/206 (99%)	0.01	0 100 100	23, 45, 67, 82	0
5	1F	203/210 (96%)	0.09	1 (0%) 87 83	22, 50, 75, 90	0
5	2F	203/210 (96%)	0.14	1 (0%) 87 83	24, 54, 76, 93	0
6	1G	181/182 (99%)	0.56	6 (3%) 49 40	50, 70, 83, 98	0
6	2G	181/182 (99%)	1.09	14 (7%) 19 16	54, 73, 85, 100	0
7	1H	174/180 (96%)	0.64	4 (2%) 61 52	48, 64, 77, 82	0
7	2H	174/180 (96%)	0.88	8 (4%) 37 29	56, 69, 81, 83	0
8	1I	146/148 (98%)	0.55	3 (2%) 63 54	45, 75, 84, 89	0
8	2I	146/148 (98%)	0.69	6 (4%) 41 33	47, 76, 85, 92	0
9	1N	140/140 (100%)	0.18	0 100 100	27, 46, 66, 79	0
9	2N	140/140 (100%)	0.16	0 100 100	30, 50, 70, 81	0
10	1O	122/122 (100%)	-0.00	0 100 100	33, 45, 63, 70	0
10	2O	122/122 (100%)	-0.06	0 100 100	34, 47, 63, 73	0
11	1P	149/150 (99%)	0.23	0 100 100	22, 52, 75, 86	0
11	2P	149/150 (99%)	0.30	2 (1%) 75 67	25, 56, 78, 89	0
12	1Q	141/141 (100%)	0.33	4 (2%) 55 46	31, 49, 63, 87	0
12	2Q	141/141 (100%)	0.36	2 (1%) 73 65	35, 52, 66, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.39	0 100 100	19, 30, 47, 57	0
13	2R	118/118 (100%)	0.14	1 (0%) 82 77	35, 51, 65, 76	0
14	1S	110/112 (98%)	-0.06	1 (0%) 81 75	33, 49, 65, 68	0
14	2S	110/112 (98%)	1.33	23 (20%) 2 2	65, 79, 88, 93	0
15	1T	131/146 (89%)	-0.10	3 (2%) 61 52	29, 41, 70, 90	0
15	2T	131/146 (89%)	0.22	0 100 100	47, 58, 78, 90	0
16	1U	116/118 (98%)	-0.58	1 (0%) 81 75	19, 27, 44, 64	0
16	2U	116/118 (98%)	0.34	1 (0%) 81 75	37, 59, 77, 88	0
17	1V	101/101 (100%)	0.08	1 (0%) 79 73	27, 49, 65, 74	0
17	2V	101/101 (100%)	0.20	2 (1%) 65 56	30, 54, 71, 78	0
18	1W	112/113 (99%)	-0.25	0 100 100	23, 35, 55, 84	0
18	2W	112/113 (99%)	-0.20	1 (0%) 81 75	26, 37, 56, 87	0
19	1X	95/96 (98%)	0.29	3 (3%) 50 41	31, 46, 66, 78	0
19	2X	95/96 (98%)	0.44	4 (4%) 40 32	34, 49, 69, 78	0
20	1Y	107/110 (97%)	-0.07	1 (0%) 81 75	29, 47, 68, 85	0
20	2Y	107/110 (97%)	0.88	7 (6%) 25 20	55, 72, 83, 98	0
21	1Z	186/206 (90%)	0.53	1 (0%) 87 83	51, 68, 82, 92	0
21	2Z	186/206 (90%)	0.91	3 (1%) 70 62	55, 71, 84, 93	0
22	10	75/85 (88%)	0.25	1 (1%) 75 67	33, 45, 59, 66	0
22	20	75/85 (88%)	0.51	4 (5%) 32 25	37, 50, 64, 68	0
23	11	97/98 (98%)	0.13	1 (1%) 79 73	28, 47, 71, 78	0
23	21	97/98 (98%)	0.25	3 (3%) 51 42	30, 49, 73, 78	0
24	12	70/72 (97%)	0.47	2 (2%) 53 45	42, 58, 72, 80	0
24	22	70/72 (97%)	0.48	0 100 100	45, 61, 74, 79	0
25	13	59/60 (98%)	0.21	1 (1%) 69 61	32, 45, 65, 78	0
25	23	59/60 (98%)	0.13	1 (1%) 69 61	35, 50, 69, 80	0
26	14	69/71 (97%)	0.66	7 (10%) 12 10	52, 75, 99, 102	0
26	24	69/71 (97%)	1.33	11 (15%) 5 4	78, 93, 98, 103	0
27	15	59/60 (98%)	-0.58	0 100 100	15, 30, 45, 72	0
27	25	59/60 (98%)	-0.09	0 100 100	33, 50, 67, 72	0
28	16	53/54 (98%)	-0.08	0 100 100	38, 48, 59, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.01	0 100 100	42, 51, 62, 72	0
29	17	48/49 (97%)	-0.07	2 (4%) 40 32	24, 31, 64, 81	0
29	27	48/49 (97%)	0.07	2 (4%) 40 32	26, 34, 64, 82	0
30	18	64/65 (98%)	0.07	0 100 100	30, 41, 49, 63	0
30	28	64/65 (98%)	0.17	0 100 100	33, 43, 52, 64	0
31	19	37/37 (100%)	0.45	3 (8%) 18 15	38, 48, 70, 74	0
31	29	37/37 (100%)	0.77	2 (5%) 31 24	43, 53, 71, 77	0
32	1a	1477/1521 (97%)	0.19	23 (1%) 70 62	34, 72, 98, 114	0
32	2a	1483/1521 (97%)	0.38	33 (2%) 62 53	43, 78, 101, 115	0
33	1b	231/256 (90%)	1.04	34 (14%) 6 4	67, 86, 96, 115	0
33	2b	231/256 (90%)	1.16	32 (13%) 6 5	71, 88, 97, 106	0
34	1c	206/239 (86%)	1.07	25 (12%) 8 7	70, 84, 93, 99	0
34	2c	206/239 (86%)	1.34	27 (13%) 7 6	73, 85, 94, 96	0
35	1d	208/209 (99%)	0.89	10 (4%) 35 28	56, 77, 88, 100	0
35	2d	208/209 (99%)	0.82	11 (5%) 32 25	56, 73, 84, 92	0
36	1e	148/162 (91%)	0.30	3 (2%) 65 56	47, 67, 79, 87	0
36	2e	148/162 (91%)	0.67	3 (2%) 65 56	56, 74, 84, 90	0
37	1f	100/101 (99%)	0.44	0 100 100	55, 73, 84, 90	0
37	2f	100/101 (99%)	0.52	3 (3%) 52 43	56, 74, 83, 87	0
38	1g	155/156 (99%)	0.82	9 (5%) 29 22	66, 79, 91, 98	0
38	2g	155/156 (99%)	0.97	20 (12%) 7 6	67, 81, 91, 97	0
39	1h	137/138 (99%)	0.40	1 (0%) 84 79	53, 69, 77, 82	0
39	2h	137/138 (99%)	0.79	6 (4%) 39 30	62, 75, 84, 91	0
40	1i	127/128 (99%)	1.40	27 (21%) 2 2	61, 87, 95, 97	0
40	2i	127/128 (99%)	2.00	52 (40%) 0 0	67, 88, 95, 102	0
41	1j	97/105 (92%)	1.45	21 (21%) 2 2	57, 87, 95, 98	0
41	2j	96/105 (91%)	1.83	41 (42%) 0 0	76, 91, 101, 102	0
42	1k	114/129 (88%)	0.34	2 (1%) 67 59	38, 67, 80, 94	0
42	2k	114/129 (88%)	0.58	6 (5%) 32 25	52, 76, 86, 92	0
43	1l	122/132 (92%)	0.54	5 (4%) 41 33	49, 63, 76, 89	0
43	2l	122/132 (92%)	0.57	3 (2%) 58 48	56, 67, 76, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	118/126 (93%)	0.80	5 (4%) 40 32	58, 80, 87, 92	0
44	2m	116/126 (92%)	1.42	27 (23%) 2 2	70, 83, 89, 96	0
45	1n	60/61 (98%)	1.24	5 (8%) 17 14	60, 77, 86, 92	0
45	2n	60/61 (98%)	2.38	40 (66%) 0 0	77, 88, 94, 96	0
46	1o	88/89 (98%)	0.52	1 (1%) 78 71	50, 65, 82, 86	0
46	2o	88/89 (98%)	0.52	0 100 100	60, 74, 87, 92	0
47	1p	82/88 (93%)	1.22	11 (13%) 7 5	62, 77, 88, 93	0
47	2p	82/88 (93%)	0.89	3 (3%) 45 37	59, 70, 79, 91	0
48	1q	99/105 (94%)	0.66	3 (3%) 52 43	47, 68, 80, 83	0
48	2q	99/105 (94%)	0.57	3 (3%) 52 43	58, 72, 81, 85	0
49	1r	68/88 (77%)	0.50	0 100 100	58, 68, 83, 87	0
49	2r	68/88 (77%)	0.54	2 (2%) 53 45	63, 74, 84, 88	0
50	1s	84/93 (90%)	1.18	10 (11%) 9 7	67, 81, 92, 98	0
50	2s	83/93 (89%)	1.95	32 (38%) 1 0	76, 91, 102, 105	0
51	1t	96/106 (90%)	1.08	12 (12%) 8 7	57, 75, 84, 90	0
51	2t	96/106 (90%)	0.82	10 (10%) 11 10	56, 73, 84, 87	0
52	1u	23/27 (85%)	1.57	5 (21%) 2 2	68, 77, 82, 85	0
52	2u	23/27 (85%)	1.91	9 (39%) 1 0	68, 80, 85, 88	0
53	1v	5/24 (20%)	0.55	1 (20%) 3 2	50, 55, 86, 88	0
53	2v	5/24 (20%)	1.03	1 (20%) 3 2	73, 74, 89, 103	0
54	1x	72/77 (93%)	0.03	0 100 100	34, 68, 85, 99	0
54	2x	72/77 (93%)	0.15	0 100 100	36, 71, 87, 101	0
55	1z	12/15 (80%)	0.42	2 (16%) 4 3	29, 36, 72, 81	0
55	2z	13/15 (86%)	1.47	4 (30%) 1 1	31, 37, 84, 91	0
All	All	20521/21474 (95%)	0.26	782 (3%) 44 36	15, 62, 92, 115	0

The worst 5 of 782 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	2z	13	PRO	7.2
7	1H	2	SER	5.9
55	2z	12	PRO	5.7
38	1g	79	ARG	5.5
29	17	48	LYS	5.2

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	2x	55	20/21	0.83	0.11	62,68,78,88	0
54	4SU	2x	8	20/21	0.88	0.10	57,78,89,92	0
54	5MU	2x	54	21/22	0.89	0.10	72,76,86,101	0
54	5MC	2x	32	21/22	0.89	0.14	68,80,88,91	0
54	5MU	1x	54	21/22	0.92	0.10	50,67,76,78	0
54	PSU	1x	55	20/21	0.93	0.09	57,65,79,80	0
54	5MC	1x	32	21/22	0.93	0.12	51,62,76,86	0
54	4SU	1x	8	20/21	0.95	0.09	47,65,79,80	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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(Å ²)	Q<0.9
56	MG	1A	3298	1/1	0.50	0.25	81,81,81,81	0
56	MG	1A	3901	1/1	0.53	0.27	86,86,86,86	0
56	MG	2a	3145	1/1	0.53	0.18	95,95,95,95	0
56	MG	1A	3517	1/1	0.54	0.18	69,69,69,69	0
56	MG	1A	4076	1/1	0.57	0.25	72,72,72,72	0
56	MG	1a	1784	1/1	0.58	0.26	80,80,80,80	0
56	MG	1A	3348	1/1	0.58	0.15	52,52,52,52	0
56	MG	1A	4037	1/1	0.59	0.31	75,75,75,75	0
56	MG	1A	3525	1/1	0.60	0.19	74,74,74,74	0
56	MG	2A	3224	1/1	0.62	0.19	73,73,73,73	0
56	MG	1a	1800	1/1	0.62	0.22	79,79,79,79	0
56	MG	2a	3167	1/1	0.63	0.20	59,59,59,59	0
56	MG	2q	201	1/1	0.63	0.14	58,58,58,58	0
56	MG	1a	1773	1/1	0.64	0.36	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3511	1/1	0.64	0.18	55,55,55,55	0
56	MG	2a	3121	1/1	0.64	0.21	88,88,88,88	0
56	MG	2a	3150	1/1	0.65	0.20	76,76,76,76	0
56	MG	1A	4016	1/1	0.65	0.17	77,77,77,77	0
56	MG	2A	3476	1/1	0.65	0.26	66,66,66,66	0
56	MG	1A	3369	1/1	0.68	0.21	67,67,67,67	0
56	MG	1a	1615	1/1	0.68	0.16	66,66,66,66	0
56	MG	1a	1752	1/1	0.68	0.15	61,61,61,61	0
56	MG	1A	4058	1/1	0.68	0.17	48,48,48,48	0
56	MG	2a	3053	1/1	0.68	0.13	99,99,99,99	0
56	MG	1A	3411	1/1	0.69	0.25	51,51,51,51	0
56	MG	1A	3433	1/1	0.69	0.16	51,51,51,51	0
56	MG	1A	4041	1/1	0.69	0.13	57,57,57,57	0
56	MG	2a	3234	1/1	0.69	0.31	82,82,82,82	0
56	MG	1a	1738	1/1	0.69	0.22	73,73,73,73	0
56	MG	2B	202	1/1	0.70	0.17	55,55,55,55	0
56	MG	1A	3847	1/1	0.70	0.18	55,55,55,55	0
56	MG	1a	1783	1/1	0.70	0.15	73,73,73,73	0
56	MG	1A	3242	1/1	0.70	0.19	67,67,67,67	0
56	MG	2x	107	1/1	0.70	0.17	78,78,78,78	0
56	MG	1m	201	1/1	0.71	0.13	95,95,95,95	0
56	MG	2a	3230	1/1	0.71	0.15	67,67,67,67	0
56	MG	2A	3498	1/1	0.71	0.16	69,69,69,69	0
56	MG	1A	3333	1/1	0.71	0.24	57,57,57,57	0
56	MG	2x	106	1/1	0.71	0.14	82,82,82,82	0
56	MG	2a	3006	1/1	0.71	0.22	77,77,77,77	0
56	MG	2a	3223	1/1	0.72	0.28	77,77,77,77	0
56	MG	1a	1848	1/1	0.72	0.19	77,77,77,77	0
56	MG	1a	1645	1/1	0.72	0.15	78,78,78,78	0
56	MG	2a	3051	1/1	0.73	0.13	91,91,91,91	0
56	MG	1A	3318	1/1	0.73	0.17	65,65,65,65	0
56	MG	2A	3432	1/1	0.73	0.15	55,55,55,55	0
56	MG	2a	3114	1/1	0.74	0.17	77,77,77,77	0
56	MG	2a	3157	1/1	0.74	0.32	108,108,108,108	0
56	MG	1A	4034	1/1	0.74	0.18	72,72,72,72	0
56	MG	2q	202	1/1	0.74	0.18	59,59,59,59	0
56	MG	2a	3168	1/1	0.74	0.23	67,67,67,67	0
56	MG	2A	3456	1/1	0.74	0.31	64,64,64,64	0
56	MG	2a	3162	1/1	0.75	0.18	79,79,79,79	0
56	MG	1A	3510	1/1	0.75	0.12	46,46,46,46	0
56	MG	2a	3146	1/1	0.75	0.16	71,71,71,71	0
56	MG	2a	3049	1/1	0.75	0.15	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3445	1/1	0.75	0.28	74,74,74,74	0
56	MG	1A	3974	1/1	0.76	0.25	59,59,59,59	0
56	MG	1A	4000	1/1	0.76	0.20	69,69,69,69	0
56	MG	2a	3019	1/1	0.76	0.11	72,72,72,72	0
56	MG	2a	3047	1/1	0.76	0.17	79,79,79,79	0
56	MG	2A	3339	1/1	0.76	0.27	63,63,63,63	0
56	MG	2A	3380	1/1	0.76	0.15	59,59,59,59	0
56	MG	1A	3557	1/1	0.76	0.14	71,71,71,71	0
56	MG	2a	3054	1/1	0.76	0.11	96,96,96,96	0
56	MG	1B	214	1/1	0.76	0.16	56,56,56,56	0
56	MG	1Q	206	1/1	0.76	0.17	53,53,53,53	0
56	MG	1A	3408	1/1	0.76	0.32	58,58,58,58	0
56	MG	1A	3493	1/1	0.76	0.10	64,64,64,64	0
56	MG	2A	3404	1/1	0.77	0.21	64,64,64,64	0
56	MG	1A	4027	1/1	0.77	0.17	62,62,62,62	0
56	MG	2a	3039	1/1	0.77	0.22	67,67,67,67	0
56	MG	2A	3443	1/1	0.77	0.26	63,63,63,63	0
56	MG	2A	3197	1/1	0.77	0.12	63,63,63,63	0
56	MG	1F	304	1/1	0.77	0.21	73,73,73,73	0
56	MG	1A	3644	1/1	0.77	0.12	45,45,45,45	0
56	MG	2A	3490	1/1	0.77	0.32	66,66,66,66	0
56	MG	2a	3101	1/1	0.77	0.21	77,77,77,77	0
56	MG	1a	1852	1/1	0.77	0.19	82,82,82,82	0
56	MG	2A	3391	1/1	0.77	0.17	52,52,52,52	0
56	MG	2a	3142	1/1	0.77	0.26	80,80,80,80	0
56	MG	2a	3004	1/1	0.77	0.28	61,61,61,61	0
56	MG	1A	3491	1/1	0.78	0.09	54,54,54,54	0
56	MG	2A	3370	1/1	0.78	0.25	65,65,65,65	0
56	MG	1A	3989	1/1	0.78	0.39	31,31,31,31	0
56	MG	1A	3513	1/1	0.78	0.30	59,59,59,59	0
56	MG	2a	3151	1/1	0.78	0.11	97,97,97,97	0
56	MG	2a	3031	1/1	0.78	0.14	88,88,88,88	0
56	MG	2a	3161	1/1	0.78	0.14	63,63,63,63	0
56	MG	1Z	301	1/1	0.78	0.15	94,94,94,94	0
56	MG	2a	3165	1/1	0.78	0.20	74,74,74,74	0
56	MG	10	106	1/1	0.78	0.19	54,54,54,54	0
56	MG	18	3002	1/1	0.78	0.11	58,58,58,58	0
56	MG	1A	4054	1/1	0.78	0.25	69,69,69,69	0
56	MG	1A	3218	1/1	0.78	0.14	58,58,58,58	0
56	MG	2A	3171	1/1	0.78	0.11	49,49,49,49	0
56	MG	2a	3070	1/1	0.78	0.28	66,66,66,66	0
56	MG	2A	3483	1/1	0.78	0.12	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3465	1/1	0.78	0.11	59,59,59,59	0
56	MG	1a	1747	1/1	0.78	0.17	64,64,64,64	0
56	MG	1a	1782	1/1	0.79	0.13	73,73,73,73	0
56	MG	2A	3194	1/1	0.79	0.17	56,56,56,56	0
56	MG	1H	3002	1/1	0.79	0.11	62,62,62,62	0
56	MG	1l	102	1/1	0.79	0.16	65,65,65,65	0
56	MG	2A	3308	1/1	0.79	0.21	53,53,53,53	0
56	MG	2a	3055	1/1	0.79	0.13	81,81,81,81	0
56	MG	12	3001	1/1	0.79	0.19	57,57,57,57	0
56	MG	2a	3072	1/1	0.79	0.18	65,65,65,65	0
56	MG	2a	3206	1/1	0.79	0.17	56,56,56,56	0
56	MG	2a	3208	1/1	0.79	0.17	65,65,65,65	0
56	MG	2a	3076	1/1	0.79	0.19	65,65,65,65	0
56	MG	1a	1811	1/1	0.79	0.12	66,66,66,66	0
56	MG	1A	4066	1/1	0.79	0.25	35,35,35,35	0
56	MG	1a	1764	1/1	0.79	0.14	59,59,59,59	0
56	MG	1a	1871	1/1	0.79	0.34	69,69,69,69	0
56	MG	1A	3345	1/1	0.79	0.17	63,63,63,63	0
56	MG	2A	3114	1/1	0.79	0.20	50,50,50,50	0
56	MG	1A	3101	1/1	0.80	0.13	50,50,50,50	0
56	MG	1A	3935	1/1	0.80	0.13	52,52,52,52	0
56	MG	1a	1718	1/1	0.80	0.14	75,75,75,75	0
56	MG	1P	204	1/1	0.80	0.15	61,61,61,61	0
56	MG	1A	3138	1/1	0.80	0.17	48,48,48,48	0
56	MG	1T	206	1/1	0.80	0.17	76,76,76,76	0
56	MG	2A	3104	1/1	0.80	0.11	59,59,59,59	0
56	MG	1A	3041	1/1	0.80	0.21	51,51,51,51	0
56	MG	2a	3187	1/1	0.80	0.28	77,77,77,77	0
56	MG	2a	3189	1/1	0.80	0.27	76,76,76,76	0
56	MG	1A	3728	1/1	0.80	0.19	62,62,62,62	0
56	MG	2A	3172	1/1	0.80	0.12	63,63,63,63	0
56	MG	2a	3210	1/1	0.80	0.16	78,78,78,78	0
56	MG	1A	3417	1/1	0.80	0.08	76,76,76,76	0
56	MG	1A	3891	1/1	0.80	0.28	68,68,68,68	0
56	MG	2A	3561	1/1	0.80	0.12	55,55,55,55	0
56	MG	2a	3254	1/1	0.80	0.29	76,76,76,76	0
56	MG	1A	4033	1/1	0.80	0.18	62,62,62,62	0
56	MG	2A	3261	1/1	0.80	0.11	43,43,43,43	0
56	MG	1a	1789	1/1	0.80	0.18	60,60,60,60	0
56	MG	1a	1792	1/1	0.80	0.19	92,92,92,92	0
56	MG	2A	3128	1/1	0.81	0.14	56,56,56,56	0
56	MG	1a	1820	1/1	0.81	0.14	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1786	1/1	0.81	0.20	49,49,49,49	0
56	MG	2A	3433	1/1	0.81	0.14	43,43,43,43	0
56	MG	2a	3193	1/1	0.81	0.12	65,65,65,65	0
56	MG	2a	3138	1/1	0.81	0.20	81,81,81,81	0
56	MG	2a	3141	1/1	0.81	0.14	70,70,70,70	0
56	MG	1A	3019	1/1	0.81	0.22	46,46,46,46	0
56	MG	1a	1791	1/1	0.81	0.28	82,82,82,82	0
56	MG	2a	3226	1/1	0.81	0.16	77,77,77,77	0
56	MG	2a	3229	1/1	0.81	0.17	57,57,57,57	0
56	MG	1a	1872	1/1	0.81	0.12	57,57,57,57	0
56	MG	1a	1880	1/1	0.81	0.20	69,69,69,69	0
56	MG	2A	3278	1/1	0.81	0.14	43,43,43,43	0
56	MG	2l	3002	1/1	0.81	0.25	68,68,68,68	0
56	MG	1A	3368	1/1	0.81	0.17	65,65,65,65	0
56	MG	1o	101	1/1	0.81	0.15	81,81,81,81	0
56	MG	1B	223	1/1	0.81	0.14	65,65,65,65	0
56	MG	14	502	1/1	0.81	0.20	64,64,64,64	0
56	MG	1a	1842	1/1	0.82	0.23	48,48,48,48	0
56	MG	2a	3153	1/1	0.82	0.12	92,92,92,92	0
56	MG	1a	1761	1/1	0.82	0.15	65,65,65,65	0
56	MG	1A	4025	1/1	0.82	0.19	80,80,80,80	0
56	MG	1B	210	1/1	0.82	0.12	56,56,56,56	0
56	MG	2a	3164	1/1	0.82	0.19	80,80,80,80	0
56	MG	1A	3515	1/1	0.82	0.38	41,41,41,41	0
56	MG	1A	3351	1/1	0.82	0.11	46,46,46,46	0
56	MG	1a	1905	1/1	0.82	0.13	67,67,67,67	0
56	MG	1e	201	1/1	0.82	0.14	66,66,66,66	0
56	MG	1E	307	1/1	0.82	0.09	57,57,57,57	0
56	MG	1A	3916	1/1	0.82	0.23	45,45,45,45	0
56	MG	2a	3058	1/1	0.82	0.17	66,66,66,66	0
56	MG	2A	3054	1/1	0.82	0.21	58,58,58,58	0
56	MG	1A	3416	1/1	0.82	0.18	66,66,66,66	0
56	MG	1a	1656	1/1	0.82	0.10	84,84,84,84	0
56	MG	1A	3494	1/1	0.82	0.34	68,68,68,68	0
56	MG	1a	1798	1/1	0.82	0.15	71,71,71,71	0
56	MG	2a	3117	1/1	0.82	0.36	66,66,66,66	0
56	MG	1A	3383	1/1	0.82	0.13	67,67,67,67	0
56	MG	1A	3405	1/1	0.82	0.29	41,41,41,41	0
56	MG	2A	3505	1/1	0.82	0.18	50,50,50,50	0
56	MG	1A	3121	1/1	0.82	0.07	72,72,72,72	0
56	MG	1a	1823	1/1	0.82	0.12	71,71,71,71	0
56	MG	2a	3001	1/1	0.82	0.27	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3230	1/1	0.82	0.18	47,47,47,47	0
56	MG	2A	3087	1/1	0.83	0.11	53,53,53,53	0
56	MG	2A	3093	1/1	0.83	0.18	57,57,57,57	0
56	MG	2A	3486	1/1	0.83	0.11	42,42,42,42	0
56	MG	1A	3550	1/1	0.83	0.18	68,68,68,68	0
56	MG	2a	3149	1/1	0.83	0.13	63,63,63,63	0
56	MG	1H	3004	1/1	0.83	0.10	66,66,66,66	0
56	MG	1a	1668	1/1	0.83	0.15	63,63,63,63	0
56	MG	2a	3152	1/1	0.83	0.16	67,67,67,67	0
56	MG	1A	3456	1/1	0.83	0.10	71,71,71,71	0
56	MG	1a	1732	1/1	0.83	0.27	63,63,63,63	0
56	MG	2a	3158	1/1	0.83	0.24	65,65,65,65	0
56	MG	1A	3366	1/1	0.83	0.11	42,42,42,42	0
56	MG	1a	1739	1/1	0.83	0.14	70,70,70,70	0
56	MG	1a	1827	1/1	0.83	0.19	68,68,68,68	0
56	MG	1A	3056	1/1	0.83	0.10	59,59,59,59	0
56	MG	1A	3747	1/1	0.83	0.21	50,50,50,50	0
56	MG	2a	3032	1/1	0.83	0.15	59,59,59,59	0
56	MG	2a	3169	1/1	0.83	0.25	67,67,67,67	0
56	MG	2a	3170	1/1	0.83	0.21	72,72,72,72	0
56	MG	2A	3272	1/1	0.83	0.19	67,67,67,67	0
56	MG	1A	3444	1/1	0.83	0.17	57,57,57,57	0
56	MG	2a	3191	1/1	0.83	0.10	88,88,88,88	0
56	MG	1A	3881	1/1	0.83	0.14	64,64,64,64	0
56	MG	2a	3197	1/1	0.83	0.13	78,78,78,78	0
56	MG	2a	3198	1/1	0.83	0.16	65,65,65,65	0
56	MG	2A	3336	1/1	0.83	0.15	74,74,74,74	0
56	MG	1A	3451	1/1	0.83	0.12	66,66,66,66	0
56	MG	2A	3364	1/1	0.83	0.11	44,44,44,44	0
56	MG	1a	1781	1/1	0.83	0.11	75,75,75,75	0
56	MG	1B	229	1/1	0.83	0.10	36,36,36,36	0
56	MG	1b	3001	1/1	0.83	0.19	70,70,70,70	0
56	MG	1A	3509	1/1	0.83	0.19	68,68,68,68	0
56	MG	1h	8002	1/1	0.83	0.28	80,80,80,80	0
56	MG	2a	3240	1/1	0.83	0.27	66,66,66,66	0
56	MG	2a	3243	1/1	0.83	0.24	74,74,74,74	0
56	MG	1A	3529	1/1	0.83	0.16	61,61,61,61	0
56	MG	1a	1627	1/1	0.83	0.18	70,70,70,70	0
56	MG	2A	3035	1/1	0.83	0.20	54,54,54,54	0
56	MG	1a	1639	1/1	0.83	0.31	77,77,77,77	0
56	MG	2a	3126	1/1	0.83	0.25	60,60,60,60	0
56	MG	2A	3467	1/1	0.83	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3749	1/1	0.84	0.20	43,43,43,43	0
56	MG	2A	3374	1/1	0.84	0.12	58,58,58,58	0
56	MG	1A	3449	1/1	0.84	0.14	67,67,67,67	0
56	MG	1H	3003	1/1	0.84	0.12	65,65,65,65	0
56	MG	2A	3401	1/1	0.84	0.29	70,70,70,70	0
56	MG	1A	3115	1/1	0.84	0.15	56,56,56,56	0
56	MG	2A	3162	1/1	0.84	0.07	40,40,40,40	0
56	MG	1A	3146	1/1	0.84	0.24	62,62,62,62	0
56	MG	2A	3439	1/1	0.84	0.10	60,60,60,60	0
56	MG	2a	3061	1/1	0.84	0.13	71,71,71,71	0
56	MG	1a	1756	1/1	0.84	0.21	58,58,58,58	0
56	MG	2A	3177	1/1	0.84	0.16	54,54,54,54	0
56	MG	2A	3189	1/1	0.84	0.21	52,52,52,52	0
56	MG	1a	1909	1/1	0.84	0.09	71,71,71,71	0
56	MG	1A	3619	1/1	0.84	0.14	56,56,56,56	0
56	MG	1d	503	1/1	0.84	0.17	77,77,77,77	0
56	MG	1a	1806	1/1	0.84	0.13	51,51,51,51	0
56	MG	2a	3122	1/1	0.84	0.32	71,71,71,71	0
56	MG	2a	3217	1/1	0.84	0.21	68,68,68,68	0
56	MG	2a	3218	1/1	0.84	0.19	67,67,67,67	0
56	MG	2A	3239	1/1	0.84	0.23	59,59,59,59	0
56	MG	2a	3130	1/1	0.84	0.12	50,50,50,50	0
56	MG	2A	3256	1/1	0.84	0.15	43,43,43,43	0
56	MG	1A	3506	1/1	0.84	0.25	75,75,75,75	0
56	MG	1a	1818	1/1	0.84	0.13	81,81,81,81	0
56	MG	2A	3275	1/1	0.84	0.15	51,51,51,51	0
56	MG	2G	3001	1/1	0.84	0.09	56,56,56,56	0
56	MG	2Z	301	1/1	0.84	0.15	70,70,70,70	0
56	MG	2e	3001	1/1	0.84	0.20	74,74,74,74	0
56	MG	1A	3508	1/1	0.84	0.13	68,68,68,68	0
56	MG	1A	3948	1/1	0.84	0.27	41,41,41,41	0
56	MG	1A	3004	1/1	0.84	0.11	54,54,54,54	0
56	MG	2A	3074	1/1	0.84	0.09	54,54,54,54	0
56	MG	1a	1719	1/1	0.84	0.28	68,68,68,68	0
56	MG	2a	3118	1/1	0.85	0.18	60,60,60,60	0
56	MG	1a	1751	1/1	0.85	0.17	64,64,64,64	0
56	MG	1N	3002	1/1	0.85	0.11	48,48,48,48	0
56	MG	1A	3514	1/1	0.85	0.32	59,59,59,59	0
56	MG	1a	1757	1/1	0.85	0.15	69,69,69,69	0
56	MG	1A	3485	1/1	0.85	0.21	57,57,57,57	0
56	MG	1A	3402	1/1	0.85	0.27	60,60,60,60	0
56	MG	1X	3001	1/1	0.85	0.23	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1r	3002	1/1	0.85	0.17	70,70,70,70	0
56	MG	1a	1776	1/1	0.85	0.07	67,67,67,67	0
56	MG	1A	3016	1/1	0.85	0.10	56,56,56,56	0
56	MG	1A	3198	1/1	0.85	0.12	50,50,50,50	0
56	MG	2A	3482	1/1	0.85	0.14	52,52,52,52	0
56	MG	1A	3922	1/1	0.85	0.13	25,25,25,25	0
56	MG	1A	4061	1/1	0.85	0.16	61,61,61,61	0
56	MG	1A	3927	1/1	0.85	0.29	66,66,66,66	0
56	MG	2A	3494	1/1	0.85	0.17	38,38,38,38	0
56	MG	1A	3502	1/1	0.85	0.10	70,70,70,70	0
56	MG	1A	4083	1/1	0.85	0.18	65,65,65,65	0
56	MG	2A	3559	1/1	0.85	0.09	56,56,56,56	0
56	MG	1a	1623	1/1	0.85	0.09	67,67,67,67	0
56	MG	1a	1795	1/1	0.85	0.14	64,64,64,64	0
56	MG	1A	3941	1/1	0.85	0.11	60,60,60,60	0
56	MG	1A	3301	1/1	0.85	0.15	64,64,64,64	0
56	MG	1a	1802	1/1	0.85	0.25	68,68,68,68	0
56	MG	2a	3175	1/1	0.85	0.16	66,66,66,66	0
56	MG	1a	1644	1/1	0.85	0.22	75,75,75,75	0
56	MG	1A	3970	1/1	0.85	0.23	64,64,64,64	0
56	MG	2a	3014	1/1	0.85	0.25	64,64,64,64	0
56	MG	1a	1815	1/1	0.85	0.14	73,73,73,73	0
56	MG	1B	227	1/1	0.85	0.08	69,69,69,69	0
56	MG	1a	1819	1/1	0.85	0.20	73,73,73,73	0
56	MG	2A	3246	1/1	0.85	0.16	55,55,55,55	0
56	MG	2a	3043	1/1	0.85	0.22	78,78,78,78	0
56	MG	2a	3045	1/1	0.85	0.23	68,68,68,68	0
56	MG	1A	3593	1/1	0.85	0.16	62,62,62,62	0
56	MG	2A	3257	1/1	0.85	0.18	67,67,67,67	0
56	MG	1a	1713	1/1	0.85	0.12	66,66,66,66	0
56	MG	1B	230	1/1	0.85	0.08	67,67,67,67	0
56	MG	1a	1831	1/1	0.85	0.15	84,84,84,84	0
56	MG	1A	3453	1/1	0.85	0.11	72,72,72,72	0
56	MG	2a	3057	1/1	0.85	0.21	70,70,70,70	0
56	MG	2A	3298	1/1	0.85	0.12	52,52,52,52	0
56	MG	1A	3087	1/1	0.85	0.15	45,45,45,45	0
56	MG	1A	3384	1/1	0.85	0.32	59,59,59,59	0
56	MG	1A	3473	1/1	0.85	0.17	55,55,55,55	0
56	MG	1a	1744	1/1	0.85	0.32	58,58,58,58	0
56	MG	1a	1746	1/1	0.85	0.16	59,59,59,59	0
56	MG	2a	3111	1/1	0.85	0.22	60,60,60,60	0
56	MG	1a	1899	1/1	0.85	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3479	1/1	0.85	0.11	59,59,59,59	0
56	MG	1T	202	1/1	0.86	0.15	51,51,51,51	0
56	MG	2A	3366	1/1	0.86	0.15	50,50,50,50	0
56	MG	1A	3914	1/1	0.86	0.17	41,41,41,41	0
56	MG	1A	3092	1/1	0.86	0.23	44,44,44,44	0
56	MG	1A	3450	1/1	0.86	0.25	52,52,52,52	0
56	MG	1Z	302	1/1	0.86	0.11	65,65,65,65	0
56	MG	1A	4063	1/1	0.86	0.14	47,47,47,47	0
56	MG	1A	3281	1/1	0.86	0.24	62,62,62,62	0
56	MG	2A	3408	1/1	0.86	0.11	62,62,62,62	0
56	MG	1A	3012	1/1	0.86	0.24	66,66,66,66	0
56	MG	2a	3133	1/1	0.86	0.08	63,63,63,63	0
56	MG	1A	3174	1/1	0.86	0.15	47,47,47,47	0
56	MG	2A	3030	1/1	0.86	0.26	64,64,64,64	0
56	MG	1A	3646	1/1	0.86	0.12	65,65,65,65	0
56	MG	1a	1602	1/1	0.86	0.15	61,61,61,61	0
56	MG	1a	1603	1/1	0.86	0.22	69,69,69,69	0
56	MG	2a	3148	1/1	0.86	0.20	56,56,56,56	0
56	MG	1a	1605	1/1	0.86	0.24	68,68,68,68	0
56	MG	1A	3689	1/1	0.86	0.15	65,65,65,65	0
56	MG	2A	3479	1/1	0.86	0.16	47,47,47,47	0
56	MG	2A	3099	1/1	0.86	0.07	61,61,61,61	0
56	MG	2A	3101	1/1	0.86	0.12	56,56,56,56	0
56	MG	1B	216	1/1	0.86	0.11	70,70,70,70	0
56	MG	1A	3727	1/1	0.86	0.12	49,49,49,49	0
56	MG	2a	3159	1/1	0.86	0.12	58,58,58,58	0
56	MG	1a	1797	1/1	0.86	0.08	73,73,73,73	0
56	MG	2A	3496	1/1	0.86	0.10	35,35,35,35	0
56	MG	2A	3131	1/1	0.86	0.16	56,56,56,56	0
56	MG	1A	3023	1/1	0.86	0.09	55,55,55,55	0
56	MG	2A	3510	1/1	0.86	0.20	61,61,61,61	0
56	MG	2A	3515	1/1	0.86	0.14	55,55,55,55	0
56	MG	1A	3326	1/1	0.86	0.10	62,62,62,62	0
56	MG	1a	1801	1/1	0.86	0.12	65,65,65,65	0
56	MG	1A	3421	1/1	0.86	0.20	38,38,38,38	0
56	MG	2A	3186	1/1	0.86	0.23	59,59,59,59	0
56	MG	1E	301	1/1	0.86	0.31	40,40,40,40	0
56	MG	1E	304	1/1	0.86	0.15	65,65,65,65	0
56	MG	1a	1694	1/1	0.86	0.20	51,51,51,51	0
56	MG	2A	3208	1/1	0.86	0.11	48,48,48,48	0
56	MG	1A	3038	1/1	0.86	0.16	55,55,55,55	0
56	MG	2a	3199	1/1	0.86	0.25	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3876	1/1	0.86	0.10	33,33,33,33	0
56	MG	1F	307	1/1	0.86	0.29	59,59,59,59	0
56	MG	1A	3435	1/1	0.86	0.15	66,66,66,66	0
56	MG	2a	3038	1/1	0.86	0.24	58,58,58,58	0
56	MG	1a	1733	1/1	0.86	0.22	52,52,52,52	0
56	MG	1a	1736	1/1	0.86	0.16	51,51,51,51	0
56	MG	2A	3258	1/1	0.86	0.20	62,62,62,62	0
56	MG	2a	3228	1/1	0.86	0.21	58,58,58,58	0
56	MG	1A	3337	1/1	0.86	0.14	44,44,44,44	0
56	MG	1A	3897	1/1	0.86	0.19	60,60,60,60	0
56	MG	2A	3274	1/1	0.86	0.10	37,37,37,37	0
56	MG	1A	4038	1/1	0.86	0.13	54,54,54,54	0
56	MG	1A	3446	1/1	0.86	0.13	58,58,58,58	0
56	MG	2a	3253	1/1	0.86	0.17	54,54,54,54	0
56	MG	1A	4044	1/1	0.86	0.29	44,44,44,44	0
56	MG	2a	3056	1/1	0.86	0.16	58,58,58,58	0
56	MG	1a	1873	1/1	0.86	0.14	60,60,60,60	0
56	MG	1a	1750	1/1	0.86	0.22	69,69,69,69	0
56	MG	1R	204	1/1	0.86	0.19	70,70,70,70	0
56	MG	2A	3342	1/1	0.86	0.17	61,61,61,61	0
56	MG	2A	3359	1/1	0.86	0.20	57,57,57,57	0
56	MG	1A	3512	1/1	0.87	0.15	50,50,50,50	0
56	MG	1a	1775	1/1	0.87	0.09	65,65,65,65	0
56	MG	1a	1864	1/1	0.87	0.30	69,69,69,69	0
56	MG	1a	1686	1/1	0.87	0.18	62,62,62,62	0
56	MG	1a	1692	1/1	0.87	0.24	64,64,64,64	0
56	MG	2a	3135	1/1	0.87	0.10	73,73,73,73	0
56	MG	1A	3322	1/1	0.87	0.18	53,53,53,53	0
56	MG	2A	3495	1/1	0.87	0.18	60,60,60,60	0
56	MG	2A	3217	1/1	0.87	0.08	41,41,41,41	0
56	MG	1A	3083	1/1	0.87	0.10	45,45,45,45	0
56	MG	1a	1716	1/1	0.87	0.22	54,54,54,54	0
56	MG	1A	3278	1/1	0.87	0.21	50,50,50,50	0
56	MG	1A	3084	1/1	0.87	0.17	53,53,53,53	0
56	MG	2A	3526	1/1	0.87	0.10	50,50,50,50	0
56	MG	2A	3547	1/1	0.87	0.15	52,52,52,52	0
56	MG	1a	1729	1/1	0.87	0.22	75,75,75,75	0
56	MG	19	102	1/1	0.87	0.13	50,50,50,50	0
56	MG	1A	3432	1/1	0.87	0.11	53,53,53,53	0
56	MG	2B	208	1/1	0.87	0.14	58,58,58,58	0
56	MG	2B	210	1/1	0.87	0.15	65,65,65,65	0
56	MG	1e	203	1/1	0.87	0.13	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3265	1/1	0.87	0.12	47,47,47,47	0
56	MG	1a	1796	1/1	0.87	0.10	85,85,85,85	0
56	MG	1A	3050	1/1	0.87	0.10	48,48,48,48	0
56	MG	1A	3024	1/1	0.87	0.15	56,56,56,56	0
56	MG	2a	3009	1/1	0.87	0.14	84,84,84,84	0
56	MG	1a	1608	1/1	0.87	0.10	70,70,70,70	0
56	MG	2A	3009	1/1	0.87	0.12	50,50,50,50	0
56	MG	2a	3020	1/1	0.87	0.19	44,44,44,44	0
56	MG	2a	3022	1/1	0.87	0.16	77,77,77,77	0
56	MG	2A	3011	1/1	0.87	0.08	48,48,48,48	0
56	MG	1a	1610	1/1	0.87	0.16	69,69,69,69	0
56	MG	1A	3758	1/1	0.87	0.19	49,49,49,49	0
56	MG	1A	3237	1/1	0.87	0.12	58,58,58,58	0
56	MG	2a	3042	1/1	0.87	0.13	72,72,72,72	0
56	MG	2A	3073	1/1	0.87	0.08	38,38,38,38	0
56	MG	2a	3203	1/1	0.87	0.15	58,58,58,58	0
56	MG	2a	3044	1/1	0.87	0.12	71,71,71,71	0
56	MG	1A	3865	1/1	0.87	0.14	72,72,72,72	0
56	MG	2A	3077	1/1	0.87	0.12	43,43,43,43	0
56	MG	2a	3212	1/1	0.87	0.14	46,46,46,46	0
56	MG	1a	1813	1/1	0.87	0.18	75,75,75,75	0
56	MG	1a	1814	1/1	0.87	0.14	67,67,67,67	0
56	MG	1A	4048	1/1	0.87	0.13	48,48,48,48	0
56	MG	1a	1640	1/1	0.87	0.27	78,78,78,78	0
56	MG	2A	3102	1/1	0.87	0.11	51,51,51,51	0
56	MG	1a	1643	1/1	0.87	0.15	68,68,68,68	0
56	MG	1D	306	1/1	0.87	0.17	49,49,49,49	0
56	MG	2A	3410	1/1	0.87	0.12	52,52,52,52	0
56	MG	1a	1760	1/1	0.87	0.21	79,79,79,79	0
56	MG	2A	3130	1/1	0.87	0.15	49,49,49,49	0
56	MG	2A	3435	1/1	0.87	0.14	46,46,46,46	0
56	MG	1a	1825	1/1	0.87	0.10	73,73,73,73	0
56	MG	2a	3100	1/1	0.87	0.36	80,80,80,80	0
56	MG	2A	3147	1/1	0.87	0.18	62,62,62,62	0
56	MG	2A	3151	1/1	0.87	0.27	54,54,54,54	0
56	MG	1A	3356	1/1	0.87	0.10	63,63,63,63	0
56	MG	1A	3879	1/1	0.87	0.14	49,49,49,49	0
56	MG	1a	1767	1/1	0.87	0.10	71,71,71,71	0
56	MG	2A	3057	1/1	0.88	0.09	52,52,52,52	0
56	MG	2A	3372	1/1	0.88	0.10	33,33,33,33	0
56	MG	1R	202	1/1	0.88	0.42	55,55,55,55	0
56	MG	1A	3464	1/1	0.88	0.11	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4047	1/1	0.88	0.24	47,47,47,47	0
56	MG	2A	3392	1/1	0.88	0.10	55,55,55,55	0
56	MG	2A	3399	1/1	0.88	0.26	64,64,64,64	0
56	MG	1T	203	1/1	0.88	0.12	75,75,75,75	0
56	MG	2a	3092	1/1	0.88	0.21	62,62,62,62	0
56	MG	2a	3093	1/1	0.88	0.27	66,66,66,66	0
56	MG	1A	3556	1/1	0.88	0.22	58,58,58,58	0
56	MG	1A	3104	1/1	0.88	0.16	52,52,52,52	0
56	MG	2A	3409	1/1	0.88	0.14	64,64,64,64	0
56	MG	1A	3587	1/1	0.88	0.20	42,42,42,42	0
56	MG	2A	3415	1/1	0.88	0.23	57,57,57,57	0
56	MG	2A	3425	1/1	0.88	0.10	48,48,48,48	0
56	MG	1A	3899	1/1	0.88	0.16	77,77,77,77	0
56	MG	1A	3472	1/1	0.88	0.11	53,53,53,53	0
56	MG	1A	3614	1/1	0.88	0.20	57,57,57,57	0
56	MG	2A	3124	1/1	0.88	0.29	65,65,65,65	0
56	MG	1A	3239	1/1	0.88	0.10	50,50,50,50	0
56	MG	1A	3643	1/1	0.88	0.13	49,49,49,49	0
56	MG	1B	208	1/1	0.88	0.25	63,63,63,63	0
56	MG	2A	3463	1/1	0.88	0.18	44,44,44,44	0
56	MG	2A	3135	1/1	0.88	0.11	43,43,43,43	0
56	MG	2A	3141	1/1	0.88	0.21	49,49,49,49	0
56	MG	1B	209	1/1	0.88	0.19	56,56,56,56	0
56	MG	2a	3147	1/1	0.88	0.14	68,68,68,68	0
56	MG	1a	1755	1/1	0.88	0.13	57,57,57,57	0
56	MG	2A	3153	1/1	0.88	0.10	52,52,52,52	0
56	MG	1A	3074	1/1	0.88	0.18	63,63,63,63	0
56	MG	1A	3370	1/1	0.88	0.09	49,49,49,49	0
56	MG	1A	3263	1/1	0.88	0.12	42,42,42,42	0
56	MG	1A	3699	1/1	0.88	0.20	58,58,58,58	0
56	MG	2A	3181	1/1	0.88	0.10	48,48,48,48	0
56	MG	1A	3969	1/1	0.88	0.16	77,77,77,77	0
56	MG	1A	3355	1/1	0.88	0.09	64,64,64,64	0
56	MG	1a	1874	1/1	0.88	0.11	48,48,48,48	0
56	MG	2A	3514	1/1	0.88	0.10	71,71,71,71	0
56	MG	1a	1772	1/1	0.88	0.20	62,62,62,62	0
56	MG	2A	3516	1/1	0.88	0.09	53,53,53,53	0
56	MG	1a	1892	1/1	0.88	0.12	58,58,58,58	0
56	MG	2A	3214	1/1	0.88	0.35	45,45,45,45	0
56	MG	1A	3387	1/1	0.88	0.13	54,54,54,54	0
56	MG	1A	3496	1/1	0.88	0.16	42,42,42,42	0
56	MG	1A	3998	1/1	0.88	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2B	205	1/1	0.88	0.32	59,59,59,59	0
56	MG	1E	302	1/1	0.88	0.17	41,41,41,41	0
56	MG	2A	3244	1/1	0.88	0.21	85,85,85,85	0
56	MG	2a	3192	1/1	0.88	0.18	61,61,61,61	0
56	MG	2D	301	1/1	0.88	0.12	49,49,49,49	0
56	MG	2D	302	1/1	0.88	0.09	57,57,57,57	0
56	MG	1A	3521	1/1	0.88	0.13	46,46,46,46	0
56	MG	1A	3754	1/1	0.88	0.24	39,39,39,39	0
56	MG	1A	3500	1/1	0.88	0.11	53,53,53,53	0
56	MG	1A	3838	1/1	0.88	0.14	64,64,64,64	0
56	MG	2a	3005	1/1	0.88	0.07	72,72,72,72	0
56	MG	2a	3209	1/1	0.88	0.12	53,53,53,53	0
56	MG	1A	3336	1/1	0.88	0.17	58,58,58,58	0
56	MG	1a	1671	1/1	0.88	0.10	77,77,77,77	0
56	MG	2a	3214	1/1	0.88	0.12	73,73,73,73	0
56	MG	2A	3270	1/1	0.88	0.13	59,59,59,59	0
56	MG	1q	202	1/1	0.88	0.17	53,53,53,53	0
56	MG	1a	1678	1/1	0.88	0.18	51,51,51,51	0
56	MG	2a	3225	1/1	0.88	0.15	59,59,59,59	0
56	MG	1x	108	1/1	0.88	0.23	49,49,49,49	0
56	MG	2a	3030	1/1	0.88	0.12	51,51,51,51	0
56	MG	1x	110	1/1	0.88	0.08	73,73,73,73	0
56	MG	2A	3279	1/1	0.88	0.15	51,51,51,51	0
56	MG	2A	3294	1/1	0.88	0.22	50,50,50,50	0
56	MG	2A	3006	1/1	0.88	0.15	59,59,59,59	0
56	MG	1A	3860	1/1	0.88	0.10	38,38,38,38	0
56	MG	2a	3252	1/1	0.88	0.15	67,67,67,67	0
56	MG	2A	3010	1/1	0.88	0.23	68,68,68,68	0
56	MG	1A	3532	1/1	0.88	0.08	62,62,62,62	0
56	MG	2A	3015	1/1	0.88	0.15	57,57,57,57	0
56	MG	2A	3345	1/1	0.88	0.14	60,60,60,60	0
56	MG	1A	3873	1/1	0.88	0.13	41,41,41,41	0
56	MG	1A	4039	1/1	0.88	0.12	56,56,56,56	0
56	MG	1A	3544	1/1	0.88	0.12	61,61,61,61	0
56	MG	2A	3368	1/1	0.88	0.23	48,48,48,48	0
56	MG	1A	3443	1/1	0.89	0.14	72,72,72,72	0
56	MG	1A	3590	1/1	0.89	0.12	51,51,51,51	0
56	MG	2A	3344	1/1	0.89	0.22	59,59,59,59	0
56	MG	2A	3012	1/1	0.89	0.21	71,71,71,71	0
56	MG	2A	3353	1/1	0.89	0.14	41,41,41,41	0
56	MG	1A	3020	1/1	0.89	0.19	40,40,40,40	0
56	MG	2A	3021	1/1	0.89	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3123	1/1	0.89	0.16	49,49,49,49	0
56	MG	1a	1688	1/1	0.89	0.16	61,61,61,61	0
56	MG	2A	3040	1/1	0.89	0.17	57,57,57,57	0
56	MG	1A	3448	1/1	0.89	0.09	56,56,56,56	0
56	MG	1A	3339	1/1	0.89	0.16	56,56,56,56	0
56	MG	2a	3064	1/1	0.89	0.13	79,79,79,79	0
56	MG	2a	3069	1/1	0.89	0.14	65,65,65,65	0
56	MG	2A	3065	1/1	0.89	0.17	55,55,55,55	0
56	MG	2A	3388	1/1	0.89	0.13	55,55,55,55	0
56	MG	1A	3396	1/1	0.89	0.16	55,55,55,55	0
56	MG	1A	3908	1/1	0.89	0.12	51,51,51,51	0
56	MG	2A	3075	1/1	0.89	0.18	48,48,48,48	0
56	MG	1a	1803	1/1	0.89	0.11	66,66,66,66	0
56	MG	2A	3082	1/1	0.89	0.14	57,57,57,57	0
56	MG	2a	3106	1/1	0.89	0.23	52,52,52,52	0
56	MG	1A	3235	1/1	0.89	0.19	53,53,53,53	0
56	MG	1a	1810	1/1	0.89	0.08	59,59,59,59	0
56	MG	1A	3403	1/1	0.89	0.23	50,50,50,50	0
56	MG	1a	1726	1/1	0.89	0.14	68,68,68,68	0
56	MG	1A	3404	1/1	0.89	0.20	54,54,54,54	0
56	MG	1A	4074	1/1	0.89	0.14	47,47,47,47	0
56	MG	1A	3107	1/1	0.89	0.18	53,53,53,53	0
56	MG	2a	3128	1/1	0.89	0.20	62,62,62,62	0
56	MG	10	101	1/1	0.89	0.17	49,49,49,49	0
56	MG	1A	3316	1/1	0.89	0.19	51,51,51,51	0
56	MG	2A	3129	1/1	0.89	0.08	33,33,33,33	0
56	MG	1B	202	1/1	0.89	0.20	63,63,63,63	0
56	MG	2A	3452	1/1	0.89	0.12	60,60,60,60	0
56	MG	1a	1740	1/1	0.89	0.23	63,63,63,63	0
56	MG	2A	3134	1/1	0.89	0.11	44,44,44,44	0
56	MG	1a	1741	1/1	0.89	0.08	48,48,48,48	0
56	MG	2A	3469	1/1	0.89	0.09	49,49,49,49	0
56	MG	2A	3471	1/1	0.89	0.20	63,63,63,63	0
56	MG	1A	3059	1/1	0.89	0.21	32,32,32,32	0
56	MG	1a	1839	1/1	0.89	0.20	53,53,53,53	0
56	MG	2A	3149	1/1	0.89	0.14	63,63,63,63	0
56	MG	1A	3319	1/1	0.89	0.17	75,75,75,75	0
56	MG	2A	3485	1/1	0.89	0.11	56,56,56,56	0
56	MG	1A	3954	1/1	0.89	0.10	16,16,16,16	0
56	MG	1a	1749	1/1	0.89	0.12	64,64,64,64	0
56	MG	1A	3320	1/1	0.89	0.19	70,70,70,70	0
56	MG	1A	3481	1/1	0.89	0.23	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3764	1/1	0.89	0.12	68,68,68,68	0
56	MG	1A	3769	1/1	0.89	0.19	55,55,55,55	0
56	MG	1a	1606	1/1	0.89	0.14	71,71,71,71	0
56	MG	1a	1878	1/1	0.89	0.15	67,67,67,67	0
56	MG	1a	1879	1/1	0.89	0.10	52,52,52,52	0
56	MG	1A	3991	1/1	0.89	0.30	38,38,38,38	0
56	MG	1a	1881	1/1	0.89	0.19	52,52,52,52	0
56	MG	2A	3519	1/1	0.89	0.13	52,52,52,52	0
56	MG	2a	3186	1/1	0.89	0.13	50,50,50,50	0
56	MG	1a	1886	1/1	0.89	0.13	56,56,56,56	0
56	MG	2A	3535	1/1	0.89	0.14	52,52,52,52	0
56	MG	2A	3537	1/1	0.89	0.14	47,47,47,47	0
56	MG	1a	1887	1/1	0.89	0.14	47,47,47,47	0
56	MG	2A	3557	1/1	0.89	0.10	54,54,54,54	0
56	MG	2A	3223	1/1	0.89	0.12	70,70,70,70	0
56	MG	1A	3119	1/1	0.89	0.18	59,59,59,59	0
56	MG	1a	1898	1/1	0.89	0.10	59,59,59,59	0
56	MG	2a	3202	1/1	0.89	0.13	52,52,52,52	0
56	MG	2A	3234	1/1	0.89	0.08	65,65,65,65	0
56	MG	1A	3427	1/1	0.89	0.11	51,51,51,51	0
56	MG	1a	1762	1/1	0.89	0.28	71,71,71,71	0
56	MG	1D	311	1/1	0.89	0.10	51,51,51,51	0
56	MG	2A	3247	1/1	0.89	0.14	59,59,59,59	0
56	MG	1a	1626	1/1	0.89	0.17	68,68,68,68	0
56	MG	2a	3213	1/1	0.89	0.14	71,71,71,71	0
56	MG	1A	3855	1/1	0.89	0.13	48,48,48,48	0
56	MG	1A	3857	1/1	0.89	0.14	51,51,51,51	0
56	MG	1a	1774	1/1	0.89	0.13	62,62,62,62	0
56	MG	1A	3259	1/1	0.89	0.13	53,53,53,53	0
56	MG	1k	201	1/1	0.89	0.10	49,49,49,49	0
56	MG	1A	3187	1/1	0.89	0.23	52,52,52,52	0
56	MG	1a	1777	1/1	0.89	0.12	54,54,54,54	0
56	MG	2a	3017	1/1	0.89	0.19	61,61,61,61	0
56	MG	1A	3868	1/1	0.89	0.10	84,84,84,84	0
56	MG	1A	4036	1/1	0.89	0.10	54,54,54,54	0
56	MG	1a	1650	1/1	0.89	0.26	49,49,49,49	0
56	MG	2a	3023	1/1	0.89	0.17	66,66,66,66	0
56	MG	2a	3025	1/1	0.89	0.18	60,60,60,60	0
56	MG	2A	3281	1/1	0.89	0.09	45,45,45,45	0
56	MG	2A	3288	1/1	0.89	0.09	41,41,41,41	0
56	MG	2d	503	1/1	0.89	0.08	62,62,62,62	0
56	MG	1a	1655	1/1	0.89	0.24	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3036	1/1	0.89	0.09	59,59,59,59	0
56	MG	2A	3003	1/1	0.89	0.10	43,43,43,43	0
56	MG	1A	3373	1/1	0.89	0.14	44,44,44,44	0
56	MG	2t	201	1/1	0.89	0.16	58,58,58,58	0
56	MG	2A	3318	1/1	0.89	0.09	43,43,43,43	0
56	MG	1a	1661	1/1	0.89	0.09	59,59,59,59	0
56	MG	2A	3343	1/1	0.90	0.11	55,55,55,55	0
56	MG	1a	1680	1/1	0.90	0.13	55,55,55,55	0
56	MG	2A	3052	1/1	0.90	0.14	37,37,37,37	0
56	MG	1a	1685	1/1	0.90	0.17	55,55,55,55	0
56	MG	2A	3357	1/1	0.90	0.16	52,52,52,52	0
56	MG	2A	3055	1/1	0.90	0.15	35,35,35,35	0
56	MG	2a	3052	1/1	0.90	0.09	81,81,81,81	0
56	MG	1A	3558	1/1	0.90	0.22	43,43,43,43	0
56	MG	1A	4023	1/1	0.90	0.17	52,52,52,52	0
56	MG	1A	3856	1/1	0.90	0.11	55,55,55,55	0
56	MG	1a	1693	1/1	0.90	0.11	53,53,53,53	0
56	MG	1A	3567	1/1	0.90	0.10	40,40,40,40	0
56	MG	1a	1696	1/1	0.90	0.13	48,48,48,48	0
56	MG	2a	3060	1/1	0.90	0.10	81,81,81,81	0
56	MG	1a	1700	1/1	0.90	0.13	60,60,60,60	0
56	MG	1A	4029	1/1	0.90	0.14	42,42,42,42	0
56	MG	2a	3065	1/1	0.90	0.11	93,93,93,93	0
56	MG	2a	3068	1/1	0.90	0.09	56,56,56,56	0
56	MG	2A	3089	1/1	0.90	0.17	36,36,36,36	0
56	MG	1N	3007	1/1	0.90	0.14	54,54,54,54	0
56	MG	1A	3418	1/1	0.90	0.10	48,48,48,48	0
56	MG	1Q	202	1/1	0.90	0.16	32,32,32,32	0
56	MG	1A	3272	1/1	0.90	0.20	58,58,58,58	0
56	MG	1A	3462	1/1	0.90	0.10	47,47,47,47	0
56	MG	1a	1834	1/1	0.90	0.14	57,57,57,57	0
56	MG	1a	1837	1/1	0.90	0.09	48,48,48,48	0
56	MG	2A	3412	1/1	0.90	0.20	54,54,54,54	0
56	MG	1A	3870	1/1	0.90	0.09	44,44,44,44	0
56	MG	1A	3599	1/1	0.90	0.09	38,38,38,38	0
56	MG	1A	3423	1/1	0.90	0.10	42,42,42,42	0
56	MG	1A	3878	1/1	0.90	0.08	37,37,37,37	0
56	MG	1a	1858	1/1	0.90	0.09	56,56,56,56	0
56	MG	1a	1859	1/1	0.90	0.17	59,59,59,59	0
56	MG	1a	1860	1/1	0.90	0.14	61,61,61,61	0
56	MG	1U	205	1/1	0.90	0.35	41,41,41,41	0
56	MG	1W	3006	1/1	0.90	0.19	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3273	1/1	0.90	0.11	37,37,37,37	0
56	MG	1A	3350	1/1	0.90	0.19	60,60,60,60	0
56	MG	2a	3136	1/1	0.90	0.21	56,56,56,56	0
56	MG	2A	3160	1/1	0.90	0.16	49,49,49,49	0
56	MG	1A	3884	1/1	0.90	0.23	58,58,58,58	0
56	MG	2A	3167	1/1	0.90	0.14	45,45,45,45	0
56	MG	2A	3168	1/1	0.90	0.10	33,33,33,33	0
56	MG	1A	3889	1/1	0.90	0.15	55,55,55,55	0
56	MG	1A	3184	1/1	0.90	0.27	52,52,52,52	0
56	MG	1A	3478	1/1	0.90	0.14	49,49,49,49	0
56	MG	2A	3178	1/1	0.90	0.14	54,54,54,54	0
56	MG	1A	3030	1/1	0.90	0.09	46,46,46,46	0
56	MG	2A	3487	1/1	0.90	0.06	40,40,40,40	0
56	MG	13	101	1/1	0.90	0.15	47,47,47,47	0
56	MG	1A	3436	1/1	0.90	0.19	51,51,51,51	0
56	MG	2A	3192	1/1	0.90	0.19	43,43,43,43	0
56	MG	15	104	1/1	0.90	0.14	53,53,53,53	0
56	MG	1a	1894	1/1	0.90	0.28	63,63,63,63	0
56	MG	2A	3504	1/1	0.90	0.14	42,42,42,42	0
56	MG	2A	3198	1/1	0.90	0.08	56,56,56,56	0
56	MG	2a	3163	1/1	0.90	0.12	94,94,94,94	0
56	MG	1a	1895	1/1	0.90	0.26	59,59,59,59	0
56	MG	1A	3713	1/1	0.90	0.08	61,61,61,61	0
56	MG	1A	3289	1/1	0.90	0.10	61,61,61,61	0
56	MG	2A	3219	1/1	0.90	0.27	56,56,56,56	0
56	MG	2A	3220	1/1	0.90	0.12	72,72,72,72	0
56	MG	2A	3525	1/1	0.90	0.22	36,36,36,36	0
56	MG	2A	3221	1/1	0.90	0.09	39,39,39,39	0
56	MG	1a	1601	1/1	0.90	0.14	63,63,63,63	0
56	MG	1A	4078	1/1	0.90	0.20	65,65,65,65	0
56	MG	1A	3488	1/1	0.90	0.10	43,43,43,43	0
56	MG	2A	3549	1/1	0.90	0.13	49,49,49,49	0
56	MG	1A	3733	1/1	0.90	0.18	49,49,49,49	0
56	MG	2A	3558	1/1	0.90	0.32	43,43,43,43	0
56	MG	1B	206	1/1	0.90	0.15	51,51,51,51	0
56	MG	2A	3241	1/1	0.90	0.14	56,56,56,56	0
56	MG	1A	3926	1/1	0.90	0.14	51,51,51,51	0
56	MG	2a	3200	1/1	0.90	0.12	71,71,71,71	0
56	MG	1A	3094	1/1	0.90	0.10	54,54,54,54	0
56	MG	1A	3335	1/1	0.90	0.34	58,58,58,58	0
56	MG	2a	3204	1/1	0.90	0.08	57,57,57,57	0
56	MG	1A	3936	1/1	0.90	0.18	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3533	1/1	0.90	0.14	56,56,56,56	0
56	MG	1p	3002	1/1	0.90	0.14	77,77,77,77	0
56	MG	1B	221	1/1	0.90	0.10	30,30,30,30	0
56	MG	2O	201	1/1	0.90	0.13	54,54,54,54	0
56	MG	2Q	3001	1/1	0.90	0.12	45,45,45,45	0
56	MG	2X	8001	1/1	0.90	0.11	45,45,45,45	0
56	MG	2a	3216	1/1	0.90	0.14	55,55,55,55	0
56	MG	1a	1628	1/1	0.90	0.13	57,57,57,57	0
56	MG	1x	105	1/1	0.90	0.18	64,64,64,64	0
56	MG	1x	106	1/1	0.90	0.09	42,42,42,42	0
56	MG	1A	3540	1/1	0.90	0.31	48,48,48,48	0
56	MG	1A	3063	1/1	0.90	0.13	57,57,57,57	0
56	MG	1A	3313	1/1	0.90	0.08	42,42,42,42	0
56	MG	2a	3012	1/1	0.90	0.16	58,58,58,58	0
56	MG	1A	3771	1/1	0.90	0.14	55,55,55,55	0
56	MG	2a	3231	1/1	0.90	0.19	59,59,59,59	0
56	MG	2A	3007	1/1	0.90	0.14	77,77,77,77	0
56	MG	2a	3235	1/1	0.90	0.15	73,73,73,73	0
56	MG	2a	3236	1/1	0.90	0.23	83,83,83,83	0
56	MG	1A	3793	1/1	0.90	0.11	55,55,55,55	0
56	MG	1A	3983	1/1	0.90	0.13	31,31,31,31	0
56	MG	2a	3250	1/1	0.90	0.13	63,63,63,63	0
56	MG	1A	3794	1/1	0.90	0.09	19,19,19,19	0
56	MG	2A	3304	1/1	0.90	0.09	66,66,66,66	0
56	MG	1A	3090	1/1	0.90	0.14	47,47,47,47	0
56	MG	2a	3255	1/1	0.90	0.09	57,57,57,57	0
56	MG	2d	502	1/1	0.90	0.31	61,61,61,61	0
56	MG	2a	3027	1/1	0.90	0.16	47,47,47,47	0
56	MG	2A	3314	1/1	0.90	0.11	43,43,43,43	0
56	MG	2A	3316	1/1	0.90	0.11	55,55,55,55	0
56	MG	1A	3845	1/1	0.90	0.42	35,35,35,35	0
56	MG	2A	3329	1/1	0.90	0.15	55,55,55,55	0
56	MG	1A	3999	1/1	0.90	0.17	51,51,51,51	0
56	MG	2v	101	1/1	0.90	0.12	65,65,65,65	0
56	MG	2x	101	1/1	0.90	0.12	72,72,72,72	0
56	MG	2x	104	1/1	0.90	0.22	84,84,84,84	0
56	MG	1F	302	1/1	0.90	0.17	39,39,39,39	0
56	MG	1A	3376	1/1	0.90	0.10	49,49,49,49	0
56	MG	1A	3516	1/1	0.91	0.23	52,52,52,52	0
56	MG	2a	3026	1/1	0.91	0.20	54,54,54,54	0
56	MG	2A	3259	1/1	0.91	0.14	39,39,39,39	0
56	MG	1A	3997	1/1	0.91	0.08	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3162	1/1	0.91	0.21	38,38,38,38	0
56	MG	1A	3397	1/1	0.91	0.09	36,36,36,36	0
56	MG	1R	203	1/1	0.91	0.08	35,35,35,35	0
56	MG	1A	3400	1/1	0.91	0.11	37,37,37,37	0
56	MG	1A	4002	1/1	0.91	0.14	65,65,65,65	0
56	MG	2a	3040	1/1	0.91	0.16	58,58,58,58	0
56	MG	1a	1748	1/1	0.91	0.15	55,55,55,55	0
56	MG	1A	4010	1/1	0.91	0.13	37,37,37,37	0
56	MG	1A	3792	1/1	0.91	0.10	62,62,62,62	0
56	MG	1U	202	1/1	0.91	0.27	51,51,51,51	0
56	MG	1A	3076	1/1	0.91	0.10	51,51,51,51	0
56	MG	1A	3276	1/1	0.91	0.17	51,51,51,51	0
56	MG	2A	3301	1/1	0.91	0.06	42,42,42,42	0
56	MG	1A	4026	1/1	0.91	0.23	63,63,63,63	0
56	MG	1A	3827	1/1	0.91	0.12	30,30,30,30	0
56	MG	2A	3005	1/1	0.91	0.10	59,59,59,59	0
56	MG	1A	3835	1/1	0.91	0.10	47,47,47,47	0
56	MG	1A	3343	1/1	0.91	0.10	55,55,55,55	0
56	MG	2A	3328	1/1	0.91	0.13	70,70,70,70	0
56	MG	10	103	1/1	0.91	0.24	62,62,62,62	0
56	MG	1A	3535	1/1	0.91	0.14	59,59,59,59	0
56	MG	1a	1765	1/1	0.91	0.11	58,58,58,58	0
56	MG	2a	3063	1/1	0.91	0.07	85,85,85,85	0
56	MG	1A	4035	1/1	0.91	0.11	46,46,46,46	0
56	MG	1a	1769	1/1	0.91	0.13	63,63,63,63	0
56	MG	2A	3017	1/1	0.91	0.23	46,46,46,46	0
56	MG	1A	3467	1/1	0.91	0.15	54,54,54,54	0
56	MG	2A	3348	1/1	0.91	0.14	60,60,60,60	0
56	MG	2A	3026	1/1	0.91	0.17	49,49,49,49	0
56	MG	2a	3075	1/1	0.91	0.06	59,59,59,59	0
56	MG	2A	3029	1/1	0.91	0.10	57,57,57,57	0
56	MG	2a	3088	1/1	0.91	0.12	76,76,76,76	0
56	MG	1A	3849	1/1	0.91	0.09	52,52,52,52	0
56	MG	2A	3031	1/1	0.91	0.08	47,47,47,47	0
56	MG	2a	3096	1/1	0.91	0.15	55,55,55,55	0
56	MG	1A	3103	1/1	0.91	0.24	32,32,32,32	0
56	MG	1A	3055	1/1	0.91	0.23	45,45,45,45	0
56	MG	2A	3041	1/1	0.91	0.08	41,41,41,41	0
56	MG	1A	3285	1/1	0.91	0.16	32,32,32,32	0
56	MG	1A	3858	1/1	0.91	0.23	53,53,53,53	0
56	MG	2a	3115	1/1	0.91	0.21	50,50,50,50	0
56	MG	1A	3035	1/1	0.91	0.09	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3206	1/1	0.91	0.23	45,45,45,45	0
56	MG	2a	3119	1/1	0.91	0.10	69,69,69,69	0
56	MG	1A	3866	1/1	0.91	0.17	42,42,42,42	0
56	MG	1A	3114	1/1	0.91	0.13	48,48,48,48	0
56	MG	2a	3124	1/1	0.91	0.15	62,62,62,62	0
56	MG	2A	3396	1/1	0.91	0.14	49,49,49,49	0
56	MG	1A	4060	1/1	0.91	0.08	31,31,31,31	0
56	MG	1A	3579	1/1	0.91	0.13	41,41,41,41	0
56	MG	1A	3486	1/1	0.91	0.07	57,57,57,57	0
56	MG	2A	3081	1/1	0.91	0.18	54,54,54,54	0
56	MG	1a	1611	1/1	0.91	0.07	46,46,46,46	0
56	MG	1A	4064	1/1	0.91	0.15	57,57,57,57	0
56	MG	1a	1619	1/1	0.91	0.07	75,75,75,75	0
56	MG	2A	3091	1/1	0.91	0.12	49,49,49,49	0
56	MG	2A	3092	1/1	0.91	0.19	48,48,48,48	0
56	MG	1a	1620	1/1	0.91	0.17	54,54,54,54	0
56	MG	2A	3098	1/1	0.91	0.13	41,41,41,41	0
56	MG	1a	1622	1/1	0.91	0.08	49,49,49,49	0
56	MG	1A	3588	1/1	0.91	0.13	60,60,60,60	0
56	MG	1A	3877	1/1	0.91	0.13	39,39,39,39	0
56	MG	1A	3419	1/1	0.91	0.21	52,52,52,52	0
56	MG	2A	3106	1/1	0.91	0.11	47,47,47,47	0
56	MG	2A	3107	1/1	0.91	0.14	49,49,49,49	0
56	MG	2a	3155	1/1	0.91	0.14	87,87,87,87	0
56	MG	2A	3457	1/1	0.91	0.15	46,46,46,46	0
56	MG	2A	3109	1/1	0.91	0.18	54,54,54,54	0
56	MG	2A	3466	1/1	0.91	0.09	45,45,45,45	0
56	MG	1A	3229	1/1	0.91	0.13	50,50,50,50	0
56	MG	1a	1629	1/1	0.91	0.17	63,63,63,63	0
56	MG	1a	1633	1/1	0.91	0.07	77,77,77,77	0
56	MG	1A	3422	1/1	0.91	0.08	40,40,40,40	0
56	MG	2A	3478	1/1	0.91	0.10	50,50,50,50	0
56	MG	1A	3367	1/1	0.91	0.10	48,48,48,48	0
56	MG	2A	3481	1/1	0.91	0.10	46,46,46,46	0
56	MG	1a	1641	1/1	0.91	0.21	47,47,47,47	0
56	MG	1B	205	1/1	0.91	0.19	56,56,56,56	0
56	MG	2a	3173	1/1	0.91	0.09	43,43,43,43	0
56	MG	1A	3616	1/1	0.91	0.09	29,29,29,29	0
56	MG	2a	3177	1/1	0.91	0.20	69,69,69,69	0
56	MG	2a	3183	1/1	0.91	0.14	60,60,60,60	0
56	MG	2A	3136	1/1	0.91	0.15	61,61,61,61	0
56	MG	1A	3010	1/1	0.91	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1646	1/1	0.91	0.14	80,80,80,80	0
56	MG	1A	3631	1/1	0.91	0.11	43,43,43,43	0
56	MG	1a	1824	1/1	0.91	0.12	54,54,54,54	0
56	MG	1a	1653	1/1	0.91	0.23	56,56,56,56	0
56	MG	2A	3159	1/1	0.91	0.16	49,49,49,49	0
56	MG	1A	3632	1/1	0.91	0.13	67,67,67,67	0
56	MG	1A	3497	1/1	0.91	0.15	55,55,55,55	0
56	MG	2A	3163	1/1	0.91	0.16	56,56,56,56	0
56	MG	2A	3512	1/1	0.91	0.14	38,38,38,38	0
56	MG	1A	3009	1/1	0.91	0.32	42,42,42,42	0
56	MG	1a	1662	1/1	0.91	0.14	60,60,60,60	0
56	MG	1a	1667	1/1	0.91	0.10	64,64,64,64	0
56	MG	2A	3518	1/1	0.91	0.10	32,32,32,32	0
56	MG	1A	3238	1/1	0.91	0.17	52,52,52,52	0
56	MG	2A	3174	1/1	0.91	0.13	56,56,56,56	0
56	MG	1a	1669	1/1	0.91	0.14	37,37,37,37	0
56	MG	1A	3666	1/1	0.91	0.07	25,25,25,25	0
56	MG	1B	225	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3184	1/1	0.91	0.08	45,45,45,45	0
56	MG	1A	3918	1/1	0.91	0.13	61,61,61,61	0
56	MG	1A	3091	1/1	0.91	0.27	54,54,54,54	0
56	MG	1A	3066	1/1	0.91	0.11	56,56,56,56	0
56	MG	2A	3193	1/1	0.91	0.10	37,37,37,37	0
56	MG	1a	1870	1/1	0.91	0.14	75,75,75,75	0
56	MG	2A	3196	1/1	0.91	0.10	47,47,47,47	0
56	MG	1A	3711	1/1	0.91	0.12	61,61,61,61	0
56	MG	1A	3439	1/1	0.91	0.07	50,50,50,50	0
56	MG	1A	3014	1/1	0.91	0.12	55,55,55,55	0
56	MG	2a	3232	1/1	0.91	0.23	54,54,54,54	0
56	MG	2A	3211	1/1	0.91	0.21	33,33,33,33	0
56	MG	1A	3940	1/1	0.91	0.20	65,65,65,65	0
56	MG	2A	3215	1/1	0.91	0.11	31,31,31,31	0
56	MG	1a	1876	1/1	0.91	0.19	62,62,62,62	0
56	MG	2a	3241	1/1	0.91	0.15	73,73,73,73	0
56	MG	2a	3242	1/1	0.91	0.11	73,73,73,73	0
56	MG	2O	202	1/1	0.91	0.09	37,37,37,37	0
56	MG	2a	3248	1/1	0.91	0.16	56,56,56,56	0
56	MG	1A	3095	1/1	0.91	0.12	46,46,46,46	0
56	MG	2Q	3005	1/1	0.91	0.09	54,54,54,54	0
56	MG	1a	1697	1/1	0.91	0.14	56,56,56,56	0
56	MG	1A	3271	1/1	0.91	0.20	54,54,54,54	0
56	MG	25	502	1/1	0.91	0.31	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1704	1/1	0.91	0.23	48,48,48,48	0
56	MG	1a	1706	1/1	0.91	0.18	52,52,52,52	0
56	MG	2A	3226	1/1	0.91	0.11	42,42,42,42	0
56	MG	1A	3953	1/1	0.91	0.12	38,38,38,38	0
56	MG	1A	3390	1/1	0.91	0.09	52,52,52,52	0
56	MG	1F	306	1/1	0.91	0.20	59,59,59,59	0
56	MG	1A	3963	1/1	0.91	0.09	27,27,27,27	0
56	MG	1A	3391	1/1	0.91	0.10	51,51,51,51	0
56	MG	1A	3750	1/1	0.91	0.08	28,28,28,28	0
56	MG	1A	3751	1/1	0.91	0.14	74,74,74,74	0
56	MG	1A	3753	1/1	0.91	0.09	34,34,34,34	0
56	MG	1A	3395	1/1	0.91	0.12	46,46,46,46	0
56	MG	1A	3027	1/1	0.92	0.13	47,47,47,47	0
56	MG	2A	3255	1/1	0.92	0.13	43,43,43,43	0
56	MG	1A	3156	1/1	0.92	0.17	50,50,50,50	0
56	MG	1l	101	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3623	1/1	0.92	0.13	45,45,45,45	0
56	MG	1A	3329	1/1	0.92	0.20	53,53,53,53	0
56	MG	1r	3001	1/1	0.92	0.12	61,61,61,61	0
56	MG	1A	3120	1/1	0.92	0.10	59,59,59,59	0
56	MG	1r	3003	1/1	0.92	0.06	49,49,49,49	0
56	MG	1t	3001	1/1	0.92	0.17	53,53,53,53	0
56	MG	1x	103	1/1	0.92	0.15	48,48,48,48	0
56	MG	13	102	1/1	0.92	0.07	46,46,46,46	0
56	MG	1a	1754	1/1	0.92	0.20	51,51,51,51	0
56	MG	1A	3077	1/1	0.92	0.13	48,48,48,48	0
56	MG	1A	4050	1/1	0.92	0.26	84,84,84,84	0
56	MG	2A	3002	1/1	0.92	0.09	40,40,40,40	0
56	MG	1A	4053	1/1	0.92	0.29	52,52,52,52	0
56	MG	1a	1759	1/1	0.92	0.36	66,66,66,66	0
56	MG	1A	3372	1/1	0.92	0.10	50,50,50,50	0
56	MG	1A	3175	1/1	0.92	0.24	43,43,43,43	0
56	MG	1A	3375	1/1	0.92	0.08	44,44,44,44	0
56	MG	1A	3007	1/1	0.92	0.15	73,73,73,73	0
56	MG	1A	3378	1/1	0.92	0.14	35,35,35,35	0
56	MG	1A	3701	1/1	0.92	0.05	29,29,29,29	0
56	MG	2A	3320	1/1	0.92	0.17	53,53,53,53	0
56	MG	1A	3890	1/1	0.92	0.13	31,31,31,31	0
56	MG	1A	3704	1/1	0.92	0.08	45,45,45,45	0
56	MG	1A	3706	1/1	0.92	0.07	15,15,15,15	0
56	MG	1A	3476	1/1	0.92	0.20	56,56,56,56	0
56	MG	2a	3059	1/1	0.92	0.07	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1616	1/1	0.92	0.21	55,55,55,55	0
56	MG	1a	1618	1/1	0.92	0.10	77,77,77,77	0
56	MG	1A	3527	1/1	0.92	0.20	69,69,69,69	0
56	MG	1A	4088	1/1	0.92	0.15	45,45,45,45	0
56	MG	1B	201	1/1	0.92	0.09	40,40,40,40	0
56	MG	2a	3066	1/1	0.92	0.19	64,64,64,64	0
56	MG	1A	3716	1/1	0.92	0.10	38,38,38,38	0
56	MG	1a	1625	1/1	0.92	0.06	34,34,34,34	0
56	MG	2A	3358	1/1	0.92	0.08	60,60,60,60	0
56	MG	1A	3719	1/1	0.92	0.09	56,56,56,56	0
56	MG	2a	3073	1/1	0.92	0.16	63,63,63,63	0
56	MG	1a	1787	1/1	0.92	0.13	52,52,52,52	0
56	MG	1A	3722	1/1	0.92	0.13	49,49,49,49	0
56	MG	2a	3087	1/1	0.92	0.18	57,57,57,57	0
56	MG	2A	3064	1/1	0.92	0.27	56,56,56,56	0
56	MG	2A	3369	1/1	0.92	0.15	56,56,56,56	0
56	MG	1A	3477	1/1	0.92	0.20	40,40,40,40	0
56	MG	2A	3371	1/1	0.92	0.12	52,52,52,52	0
56	MG	2A	3070	1/1	0.92	0.17	53,53,53,53	0
56	MG	1A	3920	1/1	0.92	0.15	65,65,65,65	0
56	MG	1a	1632	1/1	0.92	0.11	32,32,32,32	0
56	MG	2a	3109	1/1	0.92	0.23	42,42,42,42	0
56	MG	1A	3186	1/1	0.92	0.16	24,24,24,24	0
56	MG	1A	3425	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3740	1/1	0.92	0.15	68,68,68,68	0
56	MG	2A	3393	1/1	0.92	0.12	56,56,56,56	0
56	MG	2A	3395	1/1	0.92	0.14	47,47,47,47	0
56	MG	1a	1799	1/1	0.92	0.14	57,57,57,57	0
56	MG	2a	3120	1/1	0.92	0.18	62,62,62,62	0
56	MG	2A	3084	1/1	0.92	0.08	26,26,26,26	0
56	MG	1A	3741	1/1	0.92	0.09	63,63,63,63	0
56	MG	2a	3123	1/1	0.92	0.11	39,39,39,39	0
56	MG	1A	3341	1/1	0.92	0.07	53,53,53,53	0
56	MG	1A	3484	1/1	0.92	0.08	45,45,45,45	0
56	MG	1A	3541	1/1	0.92	0.09	56,56,56,56	0
56	MG	1A	3942	1/1	0.92	0.10	91,91,91,91	0
56	MG	1a	1809	1/1	0.92	0.10	54,54,54,54	0
56	MG	2a	3134	1/1	0.92	0.27	55,55,55,55	0
56	MG	1a	1647	1/1	0.92	0.17	53,53,53,53	0
56	MG	2A	3419	1/1	0.92	0.26	61,61,61,61	0
56	MG	2a	3137	1/1	0.92	0.14	62,62,62,62	0
56	MG	2A	3421	1/1	0.92	0.23	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1649	1/1	0.92	0.10	59,59,59,59	0
56	MG	2A	3431	1/1	0.92	0.12	50,50,50,50	0
56	MG	2a	3144	1/1	0.92	0.12	66,66,66,66	0
56	MG	1a	1812	1/1	0.92	0.09	53,53,53,53	0
56	MG	1A	3429	1/1	0.92	0.10	52,52,52,52	0
56	MG	1A	3547	1/1	0.92	0.14	61,61,61,61	0
56	MG	2A	3436	1/1	0.92	0.10	44,44,44,44	0
56	MG	2A	3437	1/1	0.92	0.10	69,69,69,69	0
56	MG	1D	310	1/1	0.92	0.06	42,42,42,42	0
56	MG	1A	3430	1/1	0.92	0.24	41,41,41,41	0
56	MG	1a	1660	1/1	0.92	0.10	23,23,23,23	0
56	MG	2A	3448	1/1	0.92	0.09	62,62,62,62	0
56	MG	2A	3116	1/1	0.92	0.10	54,54,54,54	0
56	MG	2A	3117	1/1	0.92	0.20	46,46,46,46	0
56	MG	2A	3118	1/1	0.92	0.20	52,52,52,52	0
56	MG	2A	3461	1/1	0.92	0.15	53,53,53,53	0
56	MG	2A	3462	1/1	0.92	0.10	46,46,46,46	0
56	MG	1A	3554	1/1	0.92	0.16	65,65,65,65	0
56	MG	1a	1822	1/1	0.92	0.18	56,56,56,56	0
56	MG	1A	3964	1/1	0.92	0.10	50,50,50,50	0
56	MG	1a	1666	1/1	0.92	0.09	72,72,72,72	0
56	MG	1A	3555	1/1	0.92	0.12	61,61,61,61	0
56	MG	2A	3133	1/1	0.92	0.08	35,35,35,35	0
56	MG	1A	3765	1/1	0.92	0.10	45,45,45,45	0
56	MG	1A	3300	1/1	0.92	0.24	41,41,41,41	0
56	MG	1A	3125	1/1	0.92	0.13	52,52,52,52	0
56	MG	1a	1673	1/1	0.92	0.10	46,46,46,46	0
56	MG	2a	3176	1/1	0.92	0.22	50,50,50,50	0
56	MG	1a	1674	1/1	0.92	0.15	62,62,62,62	0
56	MG	2a	3178	1/1	0.92	0.14	55,55,55,55	0
56	MG	2a	3182	1/1	0.92	0.11	78,78,78,78	0
56	MG	1A	3984	1/1	0.92	0.22	32,32,32,32	0
56	MG	1a	1679	1/1	0.92	0.11	45,45,45,45	0
56	MG	1a	1851	1/1	0.92	0.09	56,56,56,56	0
56	MG	2A	3489	1/1	0.92	0.11	52,52,52,52	0
56	MG	2A	3154	1/1	0.92	0.19	42,42,42,42	0
56	MG	1A	3252	1/1	0.92	0.10	56,56,56,56	0
56	MG	1a	1853	1/1	0.92	0.10	70,70,70,70	0
56	MG	1a	1857	1/1	0.92	0.12	71,71,71,71	0
56	MG	1G	3001	1/1	0.92	0.09	50,50,50,50	0
56	MG	2A	3164	1/1	0.92	0.29	51,51,51,51	0
56	MG	1A	3563	1/1	0.92	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1687	1/1	0.92	0.10	42,42,42,42	0
56	MG	1A	3995	1/1	0.92	0.12	54,54,54,54	0
56	MG	2A	3513	1/1	0.92	0.13	26,26,26,26	0
56	MG	1a	1866	1/1	0.92	0.17	73,73,73,73	0
56	MG	2a	3207	1/1	0.92	0.11	59,59,59,59	0
56	MG	1A	3394	1/1	0.92	0.11	42,42,42,42	0
56	MG	1A	3806	1/1	0.92	0.12	38,38,38,38	0
56	MG	1N	3003	1/1	0.92	0.10	38,38,38,38	0
56	MG	1A	3813	1/1	0.92	0.10	48,48,48,48	0
56	MG	2A	3522	1/1	0.92	0.18	43,43,43,43	0
56	MG	1O	3003	1/1	0.92	0.14	60,60,60,60	0
56	MG	1P	201	1/1	0.92	0.14	49,49,49,49	0
56	MG	2A	3528	1/1	0.92	0.14	46,46,46,46	0
56	MG	1a	1702	1/1	0.92	0.13	60,60,60,60	0
56	MG	2a	3222	1/1	0.92	0.13	62,62,62,62	0
56	MG	2A	3190	1/1	0.92	0.15	48,48,48,48	0
56	MG	2A	3539	1/1	0.92	0.18	57,57,57,57	0
56	MG	1A	3826	1/1	0.92	0.09	17,17,17,17	0
56	MG	1A	3575	1/1	0.92	0.18	57,57,57,57	0
56	MG	1A	4007	1/1	0.92	0.12	35,35,35,35	0
56	MG	1a	1882	1/1	0.92	0.27	60,60,60,60	0
56	MG	1A	3578	1/1	0.92	0.10	48,48,48,48	0
56	MG	1A	3837	1/1	0.92	0.09	26,26,26,26	0
56	MG	2a	3233	1/1	0.92	0.13	58,58,58,58	0
56	MG	1a	1888	1/1	0.92	0.18	60,60,60,60	0
56	MG	1a	1889	1/1	0.92	0.06	42,42,42,42	0
56	MG	1A	4017	1/1	0.92	0.12	61,61,61,61	0
56	MG	1A	3188	1/1	0.92	0.12	53,53,53,53	0
56	MG	1A	3585	1/1	0.92	0.10	14,14,14,14	0
56	MG	1a	1896	1/1	0.92	0.21	46,46,46,46	0
56	MG	2F	302	1/1	0.92	0.17	48,48,48,48	0
56	MG	1A	3846	1/1	0.92	0.11	66,66,66,66	0
56	MG	2N	8001	1/1	0.92	0.09	63,63,63,63	0
56	MG	1A	3194	1/1	0.92	0.07	39,39,39,39	0
56	MG	1a	1900	1/1	0.92	0.16	47,47,47,47	0
56	MG	1a	1903	1/1	0.92	0.14	56,56,56,56	0
56	MG	1a	1734	1/1	0.92	0.22	53,53,53,53	0
56	MG	2A	3228	1/1	0.92	0.11	44,44,44,44	0
56	MG	1A	3195	1/1	0.92	0.12	44,44,44,44	0
56	MG	23	101	1/1	0.92	0.16	50,50,50,50	0
56	MG	2A	3233	1/1	0.92	0.07	52,52,52,52	0
56	MG	1A	3005	1/1	0.92	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3236	1/1	0.92	0.07	60,60,60,60	0
56	MG	1A	3504	1/1	0.92	0.13	62,62,62,62	0
56	MG	2A	3240	1/1	0.92	0.11	34,34,34,34	0
56	MG	1A	3358	1/1	0.92	0.07	61,61,61,61	0
56	MG	1A	3610	1/1	0.92	0.08	48,48,48,48	0
56	MG	1A	3362	1/1	0.92	0.11	49,49,49,49	0
56	MG	2a	3015	1/1	0.92	0.14	62,62,62,62	0
56	MG	2z	8001	1/1	0.92	0.17	69,69,69,69	0
56	MG	2A	3235	1/1	0.93	0.10	57,57,57,57	0
56	MG	1A	3992	1/1	0.93	0.09	36,36,36,36	0
56	MG	28	103	1/1	0.93	0.14	56,56,56,56	0
56	MG	1a	1717	1/1	0.93	0.07	47,47,47,47	0
56	MG	1P	202	1/1	0.93	0.17	59,59,59,59	0
56	MG	1A	3360	1/1	0.93	0.26	57,57,57,57	0
56	MG	2A	3243	1/1	0.93	0.08	69,69,69,69	0
56	MG	2a	3008	1/1	0.93	0.09	53,53,53,53	0
56	MG	1a	1720	1/1	0.93	0.16	45,45,45,45	0
56	MG	2a	3010	1/1	0.93	0.17	44,44,44,44	0
56	MG	2a	3011	1/1	0.93	0.21	58,58,58,58	0
56	MG	1A	3996	1/1	0.93	0.10	37,37,37,37	0
56	MG	1a	1727	1/1	0.93	0.09	56,56,56,56	0
56	MG	2A	3252	1/1	0.93	0.09	43,43,43,43	0
56	MG	1Q	204	1/1	0.93	0.10	45,45,45,45	0
56	MG	2a	3018	1/1	0.93	0.07	62,62,62,62	0
56	MG	1A	3307	1/1	0.93	0.10	63,63,63,63	0
56	MG	1Q	209	1/1	0.93	0.13	59,59,59,59	0
56	MG	1A	3228	1/1	0.93	0.12	48,48,48,48	0
56	MG	1A	3026	1/1	0.93	0.10	47,47,47,47	0
56	MG	1A	3420	1/1	0.93	0.09	54,54,54,54	0
56	MG	2A	3262	1/1	0.93	0.06	53,53,53,53	0
56	MG	1A	3772	1/1	0.93	0.17	43,43,43,43	0
56	MG	1A	3777	1/1	0.93	0.10	30,30,30,30	0
56	MG	1A	3562	1/1	0.93	0.07	54,54,54,54	0
56	MG	1a	1742	1/1	0.93	0.21	68,68,68,68	0
56	MG	2a	3033	1/1	0.93	0.29	64,64,64,64	0
56	MG	1A	4015	1/1	0.93	0.15	46,46,46,46	0
56	MG	1A	3157	1/1	0.93	0.16	43,43,43,43	0
56	MG	1V	202	1/1	0.93	0.07	28,28,28,28	0
56	MG	1A	3236	1/1	0.93	0.14	58,58,58,58	0
56	MG	2A	3284	1/1	0.93	0.09	34,34,34,34	0
56	MG	1A	4020	1/1	0.93	0.06	26,26,26,26	0
56	MG	1A	4022	1/1	0.93	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1x	109	1/1	0.93	0.16	66,66,66,66	0
56	MG	1A	3800	1/1	0.93	0.06	32,32,32,32	0
56	MG	1A	3804	1/1	0.93	0.06	66,66,66,66	0
56	MG	1a	1753	1/1	0.93	0.10	48,48,48,48	0
56	MG	2A	3310	1/1	0.93	0.20	55,55,55,55	0
56	MG	2A	3311	1/1	0.93	0.12	41,41,41,41	0
56	MG	1A	3490	1/1	0.93	0.08	57,57,57,57	0
56	MG	1A	3576	1/1	0.93	0.10	65,65,65,65	0
56	MG	2A	3317	1/1	0.93	0.17	36,36,36,36	0
56	MG	1A	3825	1/1	0.93	0.21	45,45,45,45	0
56	MG	1A	4030	1/1	0.93	0.12	43,43,43,43	0
56	MG	1A	3008	1/1	0.93	0.18	51,51,51,51	0
56	MG	1A	3492	1/1	0.93	0.23	47,47,47,47	0
56	MG	1A	3832	1/1	0.93	0.08	34,34,34,34	0
56	MG	2A	3013	1/1	0.93	0.05	60,60,60,60	0
56	MG	1A	3583	1/1	0.93	0.15	49,49,49,49	0
56	MG	15	102	1/1	0.93	0.15	52,52,52,52	0
56	MG	2A	3019	1/1	0.93	0.07	48,48,48,48	0
56	MG	2A	3020	1/1	0.93	0.15	39,39,39,39	0
56	MG	1A	3371	1/1	0.93	0.06	46,46,46,46	0
56	MG	1a	1766	1/1	0.93	0.10	50,50,50,50	0
56	MG	2a	3071	1/1	0.93	0.17	72,72,72,72	0
56	MG	1A	3165	1/1	0.93	0.18	23,23,23,23	0
56	MG	1a	1768	1/1	0.93	0.11	56,56,56,56	0
56	MG	1A	3323	1/1	0.93	0.08	41,41,41,41	0
56	MG	2A	3360	1/1	0.93	0.17	43,43,43,43	0
56	MG	2a	3081	1/1	0.93	0.13	65,65,65,65	0
56	MG	2A	3363	1/1	0.93	0.08	49,49,49,49	0
56	MG	2A	3032	1/1	0.93	0.18	62,62,62,62	0
56	MG	1A	3324	1/1	0.93	0.14	57,57,57,57	0
56	MG	1A	3499	1/1	0.93	0.08	64,64,64,64	0
56	MG	1A	3594	1/1	0.93	0.12	40,40,40,40	0
56	MG	1A	3595	1/1	0.93	0.11	66,66,66,66	0
56	MG	1A	4049	1/1	0.93	0.12	49,49,49,49	0
56	MG	2a	3104	1/1	0.93	0.19	54,54,54,54	0
56	MG	1a	1607	1/1	0.93	0.12	60,60,60,60	0
56	MG	1A	3086	1/1	0.93	0.14	52,52,52,52	0
56	MG	1A	3605	1/1	0.93	0.10	31,31,31,31	0
56	MG	2a	3112	1/1	0.93	0.19	53,53,53,53	0
56	MG	1A	3501	1/1	0.93	0.11	51,51,51,51	0
56	MG	2A	3390	1/1	0.93	0.11	35,35,35,35	0
56	MG	2A	3066	1/1	0.93	0.16	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3029	1/1	0.93	0.05	71,71,71,71	0
56	MG	2A	3071	1/1	0.93	0.09	46,46,46,46	0
56	MG	1A	3861	1/1	0.93	0.05	42,42,42,42	0
56	MG	1A	3331	1/1	0.93	0.15	62,62,62,62	0
56	MG	1a	1788	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3618	1/1	0.93	0.15	68,68,68,68	0
56	MG	2A	3079	1/1	0.93	0.09	50,50,50,50	0
56	MG	2A	3405	1/1	0.93	0.11	46,46,46,46	0
56	MG	2A	3406	1/1	0.93	0.14	55,55,55,55	0
56	MG	2a	3129	1/1	0.93	0.13	60,60,60,60	0
56	MG	2A	3080	1/1	0.93	0.15	59,59,59,59	0
56	MG	1A	3505	1/1	0.93	0.11	49,49,49,49	0
56	MG	1a	1621	1/1	0.93	0.07	57,57,57,57	0
56	MG	1A	3621	1/1	0.93	0.11	40,40,40,40	0
56	MG	1A	4072	1/1	0.93	0.12	48,48,48,48	0
56	MG	1a	1624	1/1	0.93	0.07	80,80,80,80	0
56	MG	1A	3178	1/1	0.93	0.10	37,37,37,37	0
56	MG	2A	3423	1/1	0.93	0.07	53,53,53,53	0
56	MG	1A	4075	1/1	0.93	0.16	61,61,61,61	0
56	MG	2a	3143	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3624	1/1	0.93	0.10	40,40,40,40	0
56	MG	1A	4077	1/1	0.93	0.06	47,47,47,47	0
56	MG	1A	3437	1/1	0.93	0.07	46,46,46,46	0
56	MG	2A	3434	1/1	0.93	0.10	42,42,42,42	0
56	MG	1a	1630	1/1	0.93	0.07	42,42,42,42	0
56	MG	1A	3386	1/1	0.93	0.10	68,68,68,68	0
56	MG	1A	4086	1/1	0.93	0.12	63,63,63,63	0
56	MG	2A	3438	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3633	1/1	0.93	0.10	50,50,50,50	0
56	MG	2A	3440	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	4090	1/1	0.93	0.17	26,26,26,26	0
56	MG	1A	3635	1/1	0.93	0.14	50,50,50,50	0
56	MG	2A	3112	1/1	0.93	0.15	59,59,59,59	0
56	MG	1A	3638	1/1	0.93	0.10	38,38,38,38	0
56	MG	2A	3455	1/1	0.93	0.15	62,62,62,62	0
56	MG	1A	3117	1/1	0.93	0.13	62,62,62,62	0
56	MG	1A	3389	1/1	0.93	0.23	56,56,56,56	0
56	MG	1a	1816	1/1	0.93	0.12	76,76,76,76	0
56	MG	1A	3057	1/1	0.93	0.09	47,47,47,47	0
56	MG	2a	3166	1/1	0.93	0.13	60,60,60,60	0
56	MG	1A	3022	1/1	0.93	0.14	49,49,49,49	0
56	MG	2A	3465	1/1	0.93	0.12	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3670	1/1	0.93	0.10	37,37,37,37	0
56	MG	1A	3393	1/1	0.93	0.14	42,42,42,42	0
56	MG	1a	1651	1/1	0.93	0.10	62,62,62,62	0
56	MG	1A	3691	1/1	0.93	0.08	54,54,54,54	0
56	MG	2A	3474	1/1	0.93	0.10	51,51,51,51	0
56	MG	2A	3475	1/1	0.93	0.08	39,39,39,39	0
56	MG	1A	3338	1/1	0.93	0.09	52,52,52,52	0
56	MG	1A	3017	1/1	0.93	0.10	53,53,53,53	0
56	MG	1a	1829	1/1	0.93	0.07	45,45,45,45	0
56	MG	2A	3138	1/1	0.93	0.11	47,47,47,47	0
56	MG	1a	1830	1/1	0.93	0.18	68,68,68,68	0
56	MG	2A	3142	1/1	0.93	0.22	56,56,56,56	0
56	MG	2A	3484	1/1	0.93	0.11	47,47,47,47	0
56	MG	1A	3452	1/1	0.93	0.13	50,50,50,50	0
56	MG	1B	226	1/1	0.93	0.15	71,71,71,71	0
56	MG	2a	3196	1/1	0.93	0.12	70,70,70,70	0
56	MG	1A	3519	1/1	0.93	0.09	48,48,48,48	0
56	MG	1A	3707	1/1	0.93	0.11	32,32,32,32	0
56	MG	1a	1841	1/1	0.93	0.17	52,52,52,52	0
56	MG	2A	3491	1/1	0.93	0.13	46,46,46,46	0
56	MG	1A	3710	1/1	0.93	0.08	48,48,48,48	0
56	MG	1a	1845	1/1	0.93	0.11	62,62,62,62	0
56	MG	1A	3193	1/1	0.93	0.10	53,53,53,53	0
56	MG	1A	3522	1/1	0.93	0.09	50,50,50,50	0
56	MG	1a	1670	1/1	0.93	0.08	50,50,50,50	0
56	MG	2A	3166	1/1	0.93	0.09	32,32,32,32	0
56	MG	2A	3508	1/1	0.93	0.09	42,42,42,42	0
56	MG	1A	3015	1/1	0.93	0.17	51,51,51,51	0
56	MG	1a	1854	1/1	0.93	0.11	60,60,60,60	0
56	MG	1D	312	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3460	1/1	0.93	0.23	52,52,52,52	0
56	MG	1a	1675	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3039	1/1	0.93	0.10	71,71,71,71	0
56	MG	1A	3025	1/1	0.93	0.14	55,55,55,55	0
56	MG	2a	3221	1/1	0.93	0.24	57,57,57,57	0
56	MG	1a	1865	1/1	0.93	0.15	51,51,51,51	0
56	MG	1A	3204	1/1	0.93	0.23	33,33,33,33	0
56	MG	1a	1867	1/1	0.93	0.16	64,64,64,64	0
56	MG	2A	3187	1/1	0.93	0.17	40,40,40,40	0
56	MG	1a	1682	1/1	0.93	0.07	47,47,47,47	0
56	MG	2A	3529	1/1	0.93	0.24	53,53,53,53	0
56	MG	1a	1684	1/1	0.93	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1E	310	1/1	0.93	0.13	49,49,49,49	0
56	MG	1A	3729	1/1	0.93	0.19	60,60,60,60	0
56	MG	1A	3466	1/1	0.93	0.11	55,55,55,55	0
56	MG	2A	3195	1/1	0.93	0.15	47,47,47,47	0
56	MG	1A	3047	1/1	0.93	0.15	54,54,54,54	0
56	MG	1a	1690	1/1	0.93	0.06	57,57,57,57	0
56	MG	1A	3214	1/1	0.93	0.10	34,34,34,34	0
56	MG	2A	3207	1/1	0.93	0.17	49,49,49,49	0
56	MG	2B	201	1/1	0.93	0.14	57,57,57,57	0
56	MG	1A	3744	1/1	0.93	0.09	43,43,43,43	0
56	MG	1H	3001	1/1	0.93	0.14	35,35,35,35	0
56	MG	1A	3542	1/1	0.93	0.24	63,63,63,63	0
56	MG	2a	3251	1/1	0.93	0.15	43,43,43,43	0
56	MG	2B	209	1/1	0.93	0.31	57,57,57,57	0
56	MG	1a	1885	1/1	0.93	0.12	54,54,54,54	0
56	MG	1A	3215	1/1	0.93	0.11	49,49,49,49	0
56	MG	1A	3410	1/1	0.93	0.07	42,42,42,42	0
56	MG	2E	301	1/1	0.93	0.22	36,36,36,36	0
56	MG	2E	303	1/1	0.93	0.05	60,60,60,60	0
56	MG	2E	304	1/1	0.93	0.04	56,56,56,56	0
56	MG	2I	3001	1/1	0.93	0.10	65,65,65,65	0
56	MG	1A	3549	1/1	0.93	0.14	73,73,73,73	0
56	MG	2I	3004	1/1	0.93	0.10	60,60,60,60	0
56	MG	1A	3987	1/1	0.93	0.11	58,58,58,58	0
56	MG	1a	1891	1/1	0.93	0.14	51,51,51,51	0
56	MG	1A	3153	1/1	0.93	0.14	20,20,20,20	0
56	MG	1a	1707	1/1	0.93	0.09	31,31,31,31	0
56	MG	1a	1710	1/1	0.93	0.13	45,45,45,45	0
56	MG	2x	103	1/1	0.93	0.13	65,65,65,65	0
56	MG	1A	3552	1/1	0.93	0.10	51,51,51,51	0
56	MG	2x	105	1/1	0.93	0.13	52,52,52,52	0
56	MG	1a	1897	1/1	0.93	0.20	84,84,84,84	0
56	MG	2Y	502	1/1	0.93	0.14	51,51,51,51	0
56	MG	1a	1715	1/1	0.93	0.17	50,50,50,50	0
57	ZN	24	501	1/1	0.93	0.08	133,133,133,133	0
56	MG	1A	3169	1/1	0.94	0.07	55,55,55,55	0
56	MG	1A	3447	1/1	0.94	0.08	54,54,54,54	0
56	MG	2R	201	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3093	1/1	0.94	0.07	48,48,48,48	0
56	MG	2A	3249	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3002	1/1	0.94	0.18	38,38,38,38	0
56	MG	1A	3060	1/1	0.94	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1u	8001	1/1	0.94	0.08	53,53,53,53	0
56	MG	28	101	1/1	0.94	0.14	45,45,45,45	0
56	MG	1x	101	1/1	0.94	0.06	64,64,64,64	0
56	MG	1x	102	1/1	0.94	0.16	67,67,67,67	0
56	MG	2a	3003	1/1	0.94	0.18	55,55,55,55	0
56	MG	1A	3634	1/1	0.94	0.10	38,38,38,38	0
56	MG	1x	104	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3098	1/1	0.94	0.13	40,40,40,40	0
56	MG	16	101	1/1	0.94	0.16	55,55,55,55	0
56	MG	2A	3267	1/1	0.94	0.18	38,38,38,38	0
56	MG	2A	3268	1/1	0.94	0.13	44,44,44,44	0
56	MG	17	102	1/1	0.94	0.13	60,60,60,60	0
56	MG	2A	3271	1/1	0.94	0.08	50,50,50,50	0
56	MG	2a	3013	1/1	0.94	0.16	50,50,50,50	0
56	MG	18	3001	1/1	0.94	0.17	50,50,50,50	0
56	MG	1A	3636	1/1	0.94	0.21	49,49,49,49	0
56	MG	1A	3256	1/1	0.94	0.42	44,44,44,44	0
56	MG	2A	3277	1/1	0.94	0.10	44,44,44,44	0
56	MG	19	104	1/1	0.94	0.08	42,42,42,42	0
56	MG	1A	3862	1/1	0.94	0.15	45,45,45,45	0
56	MG	1A	3639	1/1	0.94	0.13	47,47,47,47	0
56	MG	1A	3641	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	3867	1/1	0.94	0.13	60,60,60,60	0
56	MG	2A	3289	1/1	0.94	0.10	37,37,37,37	0
56	MG	1A	3392	1/1	0.94	0.08	33,33,33,33	0
56	MG	2a	3028	1/1	0.94	0.07	38,38,38,38	0
56	MG	1A	3869	1/1	0.94	0.06	40,40,40,40	0
56	MG	1A	3524	1/1	0.94	0.07	68,68,68,68	0
56	MG	1A	3454	1/1	0.94	0.07	64,64,64,64	0
56	MG	2A	3305	1/1	0.94	0.10	50,50,50,50	0
56	MG	2A	3306	1/1	0.94	0.06	32,32,32,32	0
56	MG	2a	3037	1/1	0.94	0.15	50,50,50,50	0
56	MG	2A	3014	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	3649	1/1	0.94	0.11	26,26,26,26	0
56	MG	1a	1612	1/1	0.94	0.09	57,57,57,57	0
56	MG	2a	3041	1/1	0.94	0.08	50,50,50,50	0
56	MG	2A	3312	1/1	0.94	0.09	38,38,38,38	0
56	MG	1a	1614	1/1	0.94	0.06	66,66,66,66	0
56	MG	1A	3659	1/1	0.94	0.08	17,17,17,17	0
56	MG	1A	3526	1/1	0.94	0.12	47,47,47,47	0
56	MG	2A	3025	1/1	0.94	0.26	55,55,55,55	0
56	MG	1A	3100	1/1	0.94	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3322	1/1	0.94	0.08	49,49,49,49	0
56	MG	1A	3680	1/1	0.94	0.16	44,44,44,44	0
56	MG	1A	3457	1/1	0.94	0.09	61,61,61,61	0
56	MG	2A	3331	1/1	0.94	0.17	45,45,45,45	0
56	MG	1A	3885	1/1	0.94	0.12	54,54,54,54	0
56	MG	1A	3887	1/1	0.94	0.15	45,45,45,45	0
56	MG	2A	3340	1/1	0.94	0.14	52,52,52,52	0
56	MG	2A	3034	1/1	0.94	0.18	44,44,44,44	0
56	MG	1A	3690	1/1	0.94	0.07	21,21,21,21	0
56	MG	1A	3261	1/1	0.94	0.38	68,68,68,68	0
56	MG	1A	3697	1/1	0.94	0.12	41,41,41,41	0
56	MG	2a	3062	1/1	0.94	0.07	81,81,81,81	0
56	MG	2A	3051	1/1	0.94	0.12	35,35,35,35	0
56	MG	2A	3352	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3895	1/1	0.94	0.05	40,40,40,40	0
56	MG	1A	3124	1/1	0.94	0.20	36,36,36,36	0
56	MG	1A	3534	1/1	0.94	0.11	55,55,55,55	0
56	MG	1a	1794	1/1	0.94	0.06	56,56,56,56	0
56	MG	2A	3061	1/1	0.94	0.13	29,29,29,29	0
56	MG	2A	3361	1/1	0.94	0.10	34,34,34,34	0
56	MG	2A	3063	1/1	0.94	0.21	48,48,48,48	0
56	MG	1A	3267	1/1	0.94	0.12	22,22,22,22	0
56	MG	2a	3074	1/1	0.94	0.20	47,47,47,47	0
56	MG	2A	3365	1/1	0.94	0.06	41,41,41,41	0
56	MG	1B	207	1/1	0.94	0.15	52,52,52,52	0
56	MG	2a	3077	1/1	0.94	0.10	51,51,51,51	0
56	MG	2a	3080	1/1	0.94	0.31	55,55,55,55	0
56	MG	1A	3907	1/1	0.94	0.10	50,50,50,50	0
56	MG	2a	3083	1/1	0.94	0.10	49,49,49,49	0
56	MG	2A	3067	1/1	0.94	0.12	49,49,49,49	0
56	MG	2A	3068	1/1	0.94	0.10	52,52,52,52	0
56	MG	2a	3090	1/1	0.94	0.19	47,47,47,47	0
56	MG	1A	3537	1/1	0.94	0.10	53,53,53,53	0
56	MG	1a	1636	1/1	0.94	0.25	53,53,53,53	0
56	MG	2a	3094	1/1	0.94	0.24	55,55,55,55	0
56	MG	2a	3095	1/1	0.94	0.08	41,41,41,41	0
56	MG	2A	3072	1/1	0.94	0.08	29,29,29,29	0
56	MG	2a	3097	1/1	0.94	0.14	55,55,55,55	0
56	MG	2A	3378	1/1	0.94	0.09	41,41,41,41	0
56	MG	1A	3270	1/1	0.94	0.09	41,41,41,41	0
56	MG	1B	212	1/1	0.94	0.25	59,59,59,59	0
56	MG	1B	213	1/1	0.94	0.07	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3076	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3709	1/1	0.94	0.15	38,38,38,38	0
56	MG	1A	3049	1/1	0.94	0.07	37,37,37,37	0
56	MG	2a	3113	1/1	0.94	0.30	50,50,50,50	0
56	MG	1a	1807	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3127	1/1	0.94	0.14	40,40,40,40	0
56	MG	2a	3116	1/1	0.94	0.12	45,45,45,45	0
56	MG	1A	3543	1/1	0.94	0.12	46,46,46,46	0
56	MG	2A	3400	1/1	0.94	0.11	48,48,48,48	0
56	MG	1A	3471	1/1	0.94	0.12	55,55,55,55	0
56	MG	2A	3403	1/1	0.94	0.09	57,57,57,57	0
56	MG	2A	3085	1/1	0.94	0.12	38,38,38,38	0
56	MG	2A	3086	1/1	0.94	0.13	47,47,47,47	0
56	MG	1A	3718	1/1	0.94	0.11	36,36,36,36	0
56	MG	1A	3018	1/1	0.94	0.11	53,53,53,53	0
56	MG	1A	3548	1/1	0.94	0.09	72,72,72,72	0
56	MG	2a	3127	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3139	1/1	0.94	0.12	52,52,52,52	0
56	MG	1a	1654	1/1	0.94	0.07	45,45,45,45	0
56	MG	1D	301	1/1	0.94	0.15	32,32,32,32	0
56	MG	2a	3132	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3417	1/1	0.94	0.08	44,44,44,44	0
56	MG	2A	3418	1/1	0.94	0.13	52,52,52,52	0
56	MG	1D	305	1/1	0.94	0.15	13,13,13,13	0
56	MG	2A	3420	1/1	0.94	0.35	72,72,72,72	0
56	MG	1a	1657	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	3145	1/1	0.94	0.17	38,38,38,38	0
56	MG	2a	3140	1/1	0.94	0.18	49,49,49,49	0
56	MG	1A	3407	1/1	0.94	0.17	40,40,40,40	0
56	MG	1A	3947	1/1	0.94	0.17	42,42,42,42	0
56	MG	1a	1663	1/1	0.94	0.11	52,52,52,52	0
56	MG	1a	1664	1/1	0.94	0.15	62,62,62,62	0
56	MG	1A	3199	1/1	0.94	0.14	44,44,44,44	0
56	MG	1A	3089	1/1	0.94	0.05	52,52,52,52	0
56	MG	1A	3147	1/1	0.94	0.12	28,28,28,28	0
56	MG	1a	1833	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	3483	1/1	0.94	0.12	41,41,41,41	0
56	MG	2A	3122	1/1	0.94	0.20	51,51,51,51	0
56	MG	1A	3414	1/1	0.94	0.15	50,50,50,50	0
56	MG	2A	3442	1/1	0.94	0.06	66,66,66,66	0
56	MG	2A	3125	1/1	0.94	0.15	52,52,52,52	0
56	MG	2A	3127	1/1	0.94	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3559	1/1	0.94	0.07	55,55,55,55	0
56	MG	2A	3449	1/1	0.94	0.08	57,57,57,57	0
56	MG	1a	1672	1/1	0.94	0.17	47,47,47,47	0
56	MG	2A	3454	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3290	1/1	0.94	0.12	30,30,30,30	0
56	MG	1F	303	1/1	0.94	0.35	32,32,32,32	0
56	MG	1A	3972	1/1	0.94	0.08	41,41,41,41	0
56	MG	1a	1850	1/1	0.94	0.13	44,44,44,44	0
56	MG	1A	3297	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3975	1/1	0.94	0.12	44,44,44,44	0
56	MG	1A	3977	1/1	0.94	0.06	31,31,31,31	0
56	MG	1A	3208	1/1	0.94	0.05	55,55,55,55	0
56	MG	1a	1855	1/1	0.94	0.18	48,48,48,48	0
56	MG	2a	3171	1/1	0.94	0.12	46,46,46,46	0
56	MG	2A	3143	1/1	0.94	0.07	41,41,41,41	0
56	MG	1A	3105	1/1	0.94	0.16	47,47,47,47	0
56	MG	2A	3473	1/1	0.94	0.10	41,41,41,41	0
56	MG	1A	3757	1/1	0.94	0.08	49,49,49,49	0
56	MG	1A	3006	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3990	1/1	0.94	0.16	17,17,17,17	0
56	MG	2A	3477	1/1	0.94	0.07	47,47,47,47	0
56	MG	1A	3302	1/1	0.94	0.14	59,59,59,59	0
56	MG	2A	3158	1/1	0.94	0.06	39,39,39,39	0
56	MG	2a	3188	1/1	0.94	0.16	53,53,53,53	0
56	MG	1N	3005	1/1	0.94	0.11	45,45,45,45	0
56	MG	1N	3006	1/1	0.94	0.08	55,55,55,55	0
56	MG	1A	3306	1/1	0.94	0.31	69,69,69,69	0
56	MG	1a	1869	1/1	0.94	0.18	68,68,68,68	0
56	MG	2a	3195	1/1	0.94	0.09	48,48,48,48	0
56	MG	1A	3111	1/1	0.94	0.20	35,35,35,35	0
56	MG	1A	3495	1/1	0.94	0.11	41,41,41,41	0
56	MG	1A	3424	1/1	0.94	0.10	37,37,37,37	0
56	MG	2A	3488	1/1	0.94	0.09	69,69,69,69	0
56	MG	1a	1698	1/1	0.94	0.18	63,63,63,63	0
56	MG	1a	1699	1/1	0.94	0.18	58,58,58,58	0
56	MG	1A	3773	1/1	0.94	0.16	48,48,48,48	0
56	MG	1a	1701	1/1	0.94	0.10	63,63,63,63	0
56	MG	2a	3205	1/1	0.94	0.22	57,57,57,57	0
56	MG	1Q	201	1/1	0.94	0.08	33,33,33,33	0
56	MG	1a	1703	1/1	0.94	0.16	52,52,52,52	0
56	MG	1A	3311	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3499	1/1	0.94	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3501	1/1	0.94	0.08	37,37,37,37	0
56	MG	2a	3211	1/1	0.94	0.16	55,55,55,55	0
56	MG	2A	3182	1/1	0.94	0.05	36,36,36,36	0
56	MG	1A	3786	1/1	0.94	0.13	23,23,23,23	0
56	MG	1A	3589	1/1	0.94	0.12	36,36,36,36	0
56	MG	2A	3509	1/1	0.94	0.07	46,46,46,46	0
56	MG	1A	3426	1/1	0.94	0.09	54,54,54,54	0
56	MG	2A	3188	1/1	0.94	0.12	41,41,41,41	0
56	MG	2a	3219	1/1	0.94	0.13	62,62,62,62	0
56	MG	1A	3161	1/1	0.94	0.22	47,47,47,47	0
56	MG	1A	3315	1/1	0.94	0.10	65,65,65,65	0
56	MG	2A	3191	1/1	0.94	0.16	37,37,37,37	0
56	MG	1A	3802	1/1	0.94	0.14	65,65,65,65	0
56	MG	1R	205	1/1	0.94	0.11	28,28,28,28	0
56	MG	1A	3033	1/1	0.94	0.10	50,50,50,50	0
56	MG	2A	3521	1/1	0.94	0.08	41,41,41,41	0
56	MG	1A	4019	1/1	0.94	0.12	39,39,39,39	0
56	MG	1T	204	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3374	1/1	0.94	0.14	26,26,26,26	0
56	MG	1A	3808	1/1	0.94	0.08	73,73,73,73	0
56	MG	2A	3200	1/1	0.94	0.11	50,50,50,50	0
56	MG	2A	3531	1/1	0.94	0.15	52,52,52,52	0
56	MG	1a	1728	1/1	0.94	0.19	46,46,46,46	0
56	MG	2a	3237	1/1	0.94	0.08	59,59,59,59	0
56	MG	2a	3239	1/1	0.94	0.24	55,55,55,55	0
56	MG	1A	3317	1/1	0.94	0.24	63,63,63,63	0
56	MG	1A	3232	1/1	0.94	0.07	44,44,44,44	0
56	MG	2A	3541	1/1	0.94	0.15	38,38,38,38	0
56	MG	2A	3213	1/1	0.94	0.16	42,42,42,42	0
56	MG	1W	3004	1/1	0.94	0.09	40,40,40,40	0
56	MG	2A	3555	1/1	0.94	0.17	49,49,49,49	0
56	MG	1a	1904	1/1	0.94	0.23	76,76,76,76	0
56	MG	1A	3613	1/1	0.94	0.11	41,41,41,41	0
56	MG	1a	1908	1/1	0.94	0.08	53,53,53,53	0
56	MG	1A	3164	1/1	0.94	0.08	40,40,40,40	0
56	MG	1a	1737	1/1	0.94	0.22	48,48,48,48	0
56	MG	1d	502	1/1	0.94	0.12	82,82,82,82	0
56	MG	2B	204	1/1	0.94	0.29	65,65,65,65	0
56	MG	1A	3379	1/1	0.94	0.27	43,43,43,43	0
56	MG	2f	201	1/1	0.94	0.11	48,48,48,48	0
56	MG	2B	206	1/1	0.94	0.13	37,37,37,37	0
56	MG	1A	3380	1/1	0.94	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1e	202	1/1	0.94	0.12	65,65,65,65	0
56	MG	2A	3229	1/1	0.94	0.17	59,59,59,59	0
56	MG	1A	4031	1/1	0.94	0.20	66,66,66,66	0
56	MG	2q	203	1/1	0.94	0.20	53,53,53,53	0
56	MG	2r	3001	1/1	0.94	0.10	55,55,55,55	0
56	MG	1A	3381	1/1	0.94	0.15	54,54,54,54	0
56	MG	10	105	1/1	0.94	0.10	52,52,52,52	0
56	MG	1l	202	1/1	0.94	0.05	58,58,58,58	0
56	MG	1A	3044	1/1	0.94	0.21	60,60,60,60	0
56	MG	2A	3238	1/1	0.94	0.12	30,30,30,30	0
56	MG	2F	304	1/1	0.94	0.06	41,41,41,41	0
56	MG	1n	102	1/1	0.94	0.08	53,53,53,53	0
56	MG	1a	1745	1/1	0.94	0.06	55,55,55,55	0
56	MG	1o	103	1/1	0.94	0.16	47,47,47,47	0
56	MG	1A	3622	1/1	0.94	0.06	36,36,36,36	0
56	MG	1A	3080	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3937	1/1	0.95	0.13	52,52,52,52	0
56	MG	1a	1906	1/1	0.95	0.18	45,45,45,45	0
56	MG	2F	301	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3938	1/1	0.95	0.07	45,45,45,45	0
56	MG	1F	305	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3939	1/1	0.95	0.11	19,19,19,19	0
56	MG	1A	3568	1/1	0.95	0.11	45,45,45,45	0
56	MG	1A	3569	1/1	0.95	0.06	40,40,40,40	0
56	MG	1G	3003	1/1	0.95	0.06	43,43,43,43	0
56	MG	2P	201	1/1	0.95	0.10	33,33,33,33	0
56	MG	1A	3409	1/1	0.95	0.10	42,42,42,42	0
56	MG	2Q	3002	1/1	0.95	0.15	55,55,55,55	0
56	MG	2Q	3004	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	3489	1/1	0.95	0.08	41,41,41,41	0
56	MG	1h	8001	1/1	0.95	0.07	60,60,60,60	0
56	MG	1a	1714	1/1	0.95	0.14	57,57,57,57	0
56	MG	1A	3257	1/1	0.95	0.15	39,39,39,39	0
56	MG	2A	3245	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3952	1/1	0.95	0.08	40,40,40,40	0
56	MG	1N	3001	1/1	0.95	0.13	44,44,44,44	0
56	MG	1A	3752	1/1	0.95	0.06	63,63,63,63	0
56	MG	2A	3251	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3046	1/1	0.95	0.14	45,45,45,45	0
56	MG	2a	3002	1/1	0.95	0.15	58,58,58,58	0
56	MG	1o	102	1/1	0.95	0.05	72,72,72,72	0
56	MG	1A	3959	1/1	0.95	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1721	1/1	0.95	0.15	45,45,45,45	0
56	MG	1A	3580	1/1	0.95	0.10	36,36,36,36	0
56	MG	2a	3007	1/1	0.95	0.23	40,40,40,40	0
56	MG	1A	3128	1/1	0.95	0.09	50,50,50,50	0
56	MG	1O	3001	1/1	0.95	0.10	39,39,39,39	0
56	MG	1O	3002	1/1	0.95	0.10	47,47,47,47	0
56	MG	2A	3263	1/1	0.95	0.06	42,42,42,42	0
56	MG	1a	1730	1/1	0.95	0.15	44,44,44,44	0
56	MG	2A	3266	1/1	0.95	0.06	41,41,41,41	0
56	MG	1A	3968	1/1	0.95	0.10	26,26,26,26	0
56	MG	1v	3001	1/1	0.95	0.12	41,41,41,41	0
56	MG	1A	3415	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3759	1/1	0.95	0.10	68,68,68,68	0
56	MG	1P	203	1/1	0.95	0.33	28,28,28,28	0
56	MG	1A	3971	1/1	0.95	0.05	27,27,27,27	0
56	MG	1A	3761	1/1	0.95	0.07	67,67,67,67	0
56	MG	1A	3262	1/1	0.95	0.15	28,28,28,28	0
56	MG	2a	3024	1/1	0.95	0.10	78,78,78,78	0
56	MG	1x	107	1/1	0.95	0.23	48,48,48,48	0
56	MG	1A	3129	1/1	0.95	0.07	42,42,42,42	0
56	MG	2A	3280	1/1	0.95	0.09	58,58,58,58	0
56	MG	1A	3976	1/1	0.95	0.14	42,42,42,42	0
56	MG	1A	3766	1/1	0.95	0.12	37,37,37,37	0
56	MG	2A	3001	1/1	0.95	0.07	35,35,35,35	0
56	MG	1A	3979	1/1	0.95	0.11	55,55,55,55	0
56	MG	2A	3290	1/1	0.95	0.09	36,36,36,36	0
56	MG	2a	3034	1/1	0.95	0.09	43,43,43,43	0
56	MG	2A	3293	1/1	0.95	0.09	30,30,30,30	0
56	MG	1A	3982	1/1	0.95	0.09	21,21,21,21	0
56	MG	2A	3296	1/1	0.95	0.17	57,57,57,57	0
56	MG	1A	3768	1/1	0.95	0.07	8,8,8,8	0
56	MG	1A	3265	1/1	0.95	0.14	27,27,27,27	0
56	MG	1A	3136	1/1	0.95	0.10	35,35,35,35	0
56	MG	1A	3013	1/1	0.95	0.23	43,43,43,43	0
56	MG	1A	3085	1/1	0.95	0.12	48,48,48,48	0
56	MG	1A	3774	1/1	0.95	0.09	43,43,43,43	0
56	MG	2A	3309	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3061	1/1	0.95	0.07	51,51,51,51	0
56	MG	2a	3048	1/1	0.95	0.14	66,66,66,66	0
56	MG	1U	204	1/1	0.95	0.15	40,40,40,40	0
56	MG	2a	3050	1/1	0.95	0.06	86,86,86,86	0
56	MG	1A	3779	1/1	0.95	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3313	1/1	0.95	0.14	46,46,46,46	0
56	MG	1A	3780	1/1	0.95	0.09	26,26,26,26	0
56	MG	2A	3016	1/1	0.95	0.09	51,51,51,51	0
56	MG	1W	3001	1/1	0.95	0.14	53,53,53,53	0
56	MG	2A	3018	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3106	1/1	0.95	0.06	48,48,48,48	0
56	MG	2A	3321	1/1	0.95	0.14	26,26,26,26	0
56	MG	1W	3005	1/1	0.95	0.20	42,42,42,42	0
56	MG	1A	3787	1/1	0.95	0.07	26,26,26,26	0
56	MG	1A	3601	1/1	0.95	0.09	36,36,36,36	0
56	MG	1A	3001	1/1	0.95	0.17	31,31,31,31	0
56	MG	2A	3334	1/1	0.95	0.10	53,53,53,53	0
56	MG	2A	3027	1/1	0.95	0.10	56,56,56,56	0
56	MG	2A	3028	1/1	0.95	0.12	53,53,53,53	0
56	MG	1a	1763	1/1	0.95	0.17	55,55,55,55	0
56	MG	2a	3067	1/1	0.95	0.30	57,57,57,57	0
56	MG	1A	3200	1/1	0.95	0.12	39,39,39,39	0
56	MG	1A	4003	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	4005	1/1	0.95	0.10	42,42,42,42	0
56	MG	10	104	1/1	0.95	0.12	47,47,47,47	0
56	MG	1A	4006	1/1	0.95	0.08	35,35,35,35	0
56	MG	2A	3350	1/1	0.95	0.09	62,62,62,62	0
56	MG	2A	3351	1/1	0.95	0.12	49,49,49,49	0
56	MG	1A	3280	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	3201	1/1	0.95	0.07	40,40,40,40	0
56	MG	2A	3043	1/1	0.95	0.13	42,42,42,42	0
56	MG	2a	3078	1/1	0.95	0.16	61,61,61,61	0
56	MG	2A	3045	1/1	0.95	0.15	48,48,48,48	0
56	MG	2A	3046	1/1	0.95	0.30	60,60,60,60	0
56	MG	2a	3082	1/1	0.95	0.21	54,54,54,54	0
56	MG	2A	3048	1/1	0.95	0.07	45,45,45,45	0
56	MG	1A	4014	1/1	0.95	0.10	57,57,57,57	0
56	MG	2A	3362	1/1	0.95	0.11	42,42,42,42	0
56	MG	1A	3361	1/1	0.95	0.12	45,45,45,45	0
56	MG	2a	3091	1/1	0.95	0.14	46,46,46,46	0
56	MG	2A	3053	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	3283	1/1	0.95	0.25	43,43,43,43	0
56	MG	1A	3364	1/1	0.95	0.10	64,64,64,64	0
56	MG	2A	3367	1/1	0.95	0.14	54,54,54,54	0
56	MG	2A	3056	1/1	0.95	0.13	52,52,52,52	0
56	MG	1A	4018	1/1	0.95	0.07	45,45,45,45	0
56	MG	2a	3098	1/1	0.95	0.26	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1779	1/1	0.95	0.07	66,66,66,66	0
56	MG	2A	3062	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3620	1/1	0.95	0.06	55,55,55,55	0
56	MG	2A	3373	1/1	0.95	0.11	48,48,48,48	0
56	MG	1A	3818	1/1	0.95	0.10	59,59,59,59	0
56	MG	2A	3376	1/1	0.95	0.07	19,19,19,19	0
56	MG	1A	3820	1/1	0.95	0.12	71,71,71,71	0
56	MG	1A	3824	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3381	1/1	0.95	0.17	41,41,41,41	0
56	MG	1a	1785	1/1	0.95	0.08	60,60,60,60	0
56	MG	2A	3389	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3202	1/1	0.95	0.15	50,50,50,50	0
56	MG	2A	3069	1/1	0.95	0.21	42,42,42,42	0
56	MG	1A	3286	1/1	0.95	0.10	40,40,40,40	0
56	MG	1A	3150	1/1	0.95	0.24	44,44,44,44	0
56	MG	1A	3828	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	3830	1/1	0.95	0.05	34,34,34,34	0
56	MG	1A	3831	1/1	0.95	0.07	18,18,18,18	0
56	MG	1A	4032	1/1	0.95	0.08	38,38,38,38	0
56	MG	1A	3205	1/1	0.95	0.12	33,33,33,33	0
56	MG	2A	3402	1/1	0.95	0.15	44,44,44,44	0
56	MG	1A	3834	1/1	0.95	0.09	63,63,63,63	0
56	MG	2A	3078	1/1	0.95	0.09	48,48,48,48	0
56	MG	1A	3438	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3836	1/1	0.95	0.05	25,25,25,25	0
56	MG	1a	1609	1/1	0.95	0.12	58,58,58,58	0
56	MG	1A	3152	1/1	0.95	0.08	30,30,30,30	0
56	MG	2A	3083	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3442	1/1	0.95	0.07	39,39,39,39	0
56	MG	2A	3413	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3520	1/1	0.95	0.08	61,61,61,61	0
56	MG	2a	3139	1/1	0.95	0.13	53,53,53,53	0
56	MG	2A	3416	1/1	0.95	0.07	36,36,36,36	0
56	MG	1a	1613	1/1	0.95	0.09	77,77,77,77	0
56	MG	1a	1805	1/1	0.95	0.11	61,61,61,61	0
56	MG	1A	3207	1/1	0.95	0.16	42,42,42,42	0
56	MG	1A	3021	1/1	0.95	0.06	56,56,56,56	0
56	MG	1A	4046	1/1	0.95	0.13	45,45,45,45	0
56	MG	1A	3209	1/1	0.95	0.17	39,39,39,39	0
56	MG	2A	3096	1/1	0.95	0.11	47,47,47,47	0
56	MG	2A	3428	1/1	0.95	0.09	59,59,59,59	0
56	MG	2A	3429	1/1	0.95	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3097	1/1	0.95	0.17	51,51,51,51	0
56	MG	1A	3850	1/1	0.95	0.10	47,47,47,47	0
56	MG	1A	3853	1/1	0.95	0.07	35,35,35,35	0
56	MG	1A	3210	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	4052	1/1	0.95	0.31	33,33,33,33	0
56	MG	2a	3156	1/1	0.95	0.12	50,50,50,50	0
56	MG	2A	3103	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3640	1/1	0.95	0.12	38,38,38,38	0
56	MG	1A	3305	1/1	0.95	0.15	50,50,50,50	0
56	MG	2a	3160	1/1	0.95	0.09	61,61,61,61	0
56	MG	1A	4057	1/1	0.95	0.15	50,50,50,50	0
56	MG	1A	3112	1/1	0.95	0.20	51,51,51,51	0
56	MG	2A	3110	1/1	0.95	0.22	53,53,53,53	0
56	MG	1A	4059	1/1	0.95	0.15	28,28,28,28	0
56	MG	1a	1821	1/1	0.95	0.14	52,52,52,52	0
56	MG	2A	3446	1/1	0.95	0.09	55,55,55,55	0
56	MG	1A	3859	1/1	0.95	0.08	52,52,52,52	0
56	MG	1A	3067	1/1	0.95	0.19	56,56,56,56	0
56	MG	1A	4062	1/1	0.95	0.10	49,49,49,49	0
56	MG	2A	3120	1/1	0.95	0.13	58,58,58,58	0
56	MG	2A	3121	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3530	1/1	0.95	0.06	47,47,47,47	0
56	MG	2a	3174	1/1	0.95	0.11	51,51,51,51	0
56	MG	1a	1826	1/1	0.95	0.09	59,59,59,59	0
56	MG	1A	3648	1/1	0.95	0.07	26,26,26,26	0
56	MG	1a	1828	1/1	0.95	0.08	70,70,70,70	0
56	MG	1a	1634	1/1	0.95	0.24	55,55,55,55	0
56	MG	1A	4065	1/1	0.95	0.07	33,33,33,33	0
56	MG	1a	1638	1/1	0.95	0.07	52,52,52,52	0
56	MG	1a	1832	1/1	0.95	0.10	52,52,52,52	0
56	MG	1A	3863	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	4070	1/1	0.95	0.14	47,47,47,47	0
56	MG	1A	3864	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	3308	1/1	0.95	0.18	49,49,49,49	0
56	MG	1A	3309	1/1	0.95	0.16	59,59,59,59	0
56	MG	1A	3310	1/1	0.95	0.10	52,52,52,52	0
56	MG	1a	1844	1/1	0.95	0.11	56,56,56,56	0
56	MG	1A	3382	1/1	0.95	0.07	53,53,53,53	0
56	MG	2A	3144	1/1	0.95	0.17	41,41,41,41	0
56	MG	1A	3216	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3687	1/1	0.95	0.11	17,17,17,17	0
56	MG	1A	4085	1/1	0.95	0.30	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3871	1/1	0.95	0.07	31,31,31,31	0
56	MG	1a	1652	1/1	0.95	0.25	60,60,60,60	0
56	MG	1A	3539	1/1	0.95	0.07	45,45,45,45	0
56	MG	1A	3312	1/1	0.95	0.12	41,41,41,41	0
56	MG	1A	3217	1/1	0.95	0.10	56,56,56,56	0
56	MG	2A	3161	1/1	0.95	0.08	38,38,38,38	0
56	MG	1A	3314	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3160	1/1	0.95	0.08	46,46,46,46	0
56	MG	2A	3493	1/1	0.95	0.06	39,39,39,39	0
56	MG	1a	1659	1/1	0.95	0.08	52,52,52,52	0
56	MG	2A	3165	1/1	0.95	0.16	42,42,42,42	0
56	MG	1a	1862	1/1	0.95	0.10	35,35,35,35	0
56	MG	2A	3497	1/1	0.95	0.12	46,46,46,46	0
56	MG	1A	3880	1/1	0.95	0.16	38,38,38,38	0
56	MG	1A	3070	1/1	0.95	0.13	48,48,48,48	0
56	MG	1A	3031	1/1	0.95	0.14	60,60,60,60	0
56	MG	1A	3705	1/1	0.95	0.10	59,59,59,59	0
56	MG	1a	1868	1/1	0.95	0.12	44,44,44,44	0
56	MG	2A	3176	1/1	0.95	0.12	38,38,38,38	0
56	MG	1A	3075	1/1	0.95	0.07	46,46,46,46	0
56	MG	1A	3888	1/1	0.95	0.08	43,43,43,43	0
56	MG	2A	3511	1/1	0.95	0.11	40,40,40,40	0
56	MG	2A	3179	1/1	0.95	0.23	29,29,29,29	0
56	MG	1A	3003	1/1	0.95	0.07	44,44,44,44	0
56	MG	1A	3708	1/1	0.95	0.11	59,59,59,59	0
56	MG	2A	3183	1/1	0.95	0.14	46,46,46,46	0
56	MG	1A	3167	1/1	0.95	0.12	25,25,25,25	0
56	MG	1A	3321	1/1	0.95	0.15	33,33,33,33	0
56	MG	1A	3553	1/1	0.95	0.12	63,63,63,63	0
56	MG	1a	1877	1/1	0.95	0.10	52,52,52,52	0
56	MG	1A	3712	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3045	1/1	0.95	0.06	39,39,39,39	0
56	MG	1A	3905	1/1	0.95	0.18	45,45,45,45	0
56	MG	1A	3171	1/1	0.95	0.27	51,51,51,51	0
56	MG	1A	3172	1/1	0.95	0.07	31,31,31,31	0
56	MG	1a	1883	1/1	0.95	0.15	53,53,53,53	0
56	MG	2A	3532	1/1	0.95	0.12	46,46,46,46	0
56	MG	2a	3245	1/1	0.95	0.12	64,64,64,64	0
56	MG	2a	3246	1/1	0.95	0.13	60,60,60,60	0
56	MG	2a	3247	1/1	0.95	0.14	50,50,50,50	0
56	MG	1A	3909	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3912	1/1	0.95	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3241	1/1	0.95	0.12	23,23,23,23	0
56	MG	1D	307	1/1	0.95	0.16	37,37,37,37	0
56	MG	2A	3542	1/1	0.95	0.12	56,56,56,56	0
56	MG	2A	3543	1/1	0.95	0.14	49,49,49,49	0
56	MG	2A	3545	1/1	0.95	0.10	53,53,53,53	0
56	MG	2A	3546	1/1	0.95	0.11	49,49,49,49	0
56	MG	1D	308	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3204	1/1	0.95	0.19	53,53,53,53	0
56	MG	2e	3002	1/1	0.95	0.06	64,64,64,64	0
56	MG	2A	3553	1/1	0.95	0.11	41,41,41,41	0
56	MG	2A	3554	1/1	0.95	0.13	59,59,59,59	0
56	MG	2A	3205	1/1	0.95	0.10	43,43,43,43	0
56	MG	1a	1890	1/1	0.95	0.16	40,40,40,40	0
56	MG	1A	3327	1/1	0.95	0.07	44,44,44,44	0
56	MG	1A	3078	1/1	0.95	0.10	61,61,61,61	0
56	MG	2A	3212	1/1	0.95	0.19	34,34,34,34	0
56	MG	1A	3560	1/1	0.95	0.06	63,63,63,63	0
56	MG	1D	313	1/1	0.95	0.09	39,39,39,39	0
56	MG	2B	203	1/1	0.95	0.13	51,51,51,51	0
56	MG	1A	3921	1/1	0.95	0.06	45,45,45,45	0
56	MG	1A	3561	1/1	0.95	0.09	72,72,72,72	0
56	MG	2A	3218	1/1	0.95	0.21	54,54,54,54	0
56	MG	1A	3099	1/1	0.95	0.15	55,55,55,55	0
56	MG	1E	306	1/1	0.95	0.09	57,57,57,57	0
56	MG	1A	3735	1/1	0.95	0.09	63,63,63,63	0
56	MG	1a	1902	1/1	0.95	0.09	62,62,62,62	0
56	MG	1A	3332	1/1	0.95	0.10	35,35,35,35	0
57	ZN	2n	501	1/1	0.95	0.07	110,110,110,110	0
56	MG	1A	3848	1/1	0.96	0.07	45,45,45,45	0
56	MG	2A	3283	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3656	1/1	0.96	0.09	20,20,20,20	0
56	MG	2A	3287	1/1	0.96	0.12	33,33,33,33	0
56	MG	2A	3033	1/1	0.96	0.22	47,47,47,47	0
56	MG	20	8001	1/1	0.96	0.07	62,62,62,62	0
56	MG	16	102	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3538	1/1	0.96	0.08	39,39,39,39	0
56	MG	2A	3037	1/1	0.96	0.17	42,42,42,42	0
56	MG	2A	3038	1/1	0.96	0.06	45,45,45,45	0
56	MG	2A	3295	1/1	0.96	0.09	38,38,38,38	0
56	MG	2A	3039	1/1	0.96	0.17	38,38,38,38	0
56	MG	2A	3297	1/1	0.96	0.07	40,40,40,40	0
56	MG	1A	3661	1/1	0.96	0.07	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3299	1/1	0.96	0.12	64,64,64,64	0
56	MG	1A	3131	1/1	0.96	0.12	31,31,31,31	0
56	MG	2A	3302	1/1	0.96	0.11	41,41,41,41	0
56	MG	2A	3042	1/1	0.96	0.16	46,46,46,46	0
56	MG	1A	3133	1/1	0.96	0.24	48,48,48,48	0
56	MG	2A	3044	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3672	1/1	0.96	0.12	29,29,29,29	0
56	MG	1A	3676	1/1	0.96	0.11	40,40,40,40	0
56	MG	2A	3047	1/1	0.96	0.12	37,37,37,37	0
56	MG	1A	3679	1/1	0.96	0.06	38,38,38,38	0
56	MG	2A	3049	1/1	0.96	0.12	56,56,56,56	0
56	MG	2a	3016	1/1	0.96	0.27	65,65,65,65	0
56	MG	2A	3050	1/1	0.96	0.29	55,55,55,55	0
56	MG	1a	1790	1/1	0.96	0.09	62,62,62,62	0
56	MG	1A	3463	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3682	1/1	0.96	0.12	29,29,29,29	0
56	MG	2a	3021	1/1	0.96	0.08	58,58,58,58	0
56	MG	1A	3684	1/1	0.96	0.08	50,50,50,50	0
56	MG	2A	3319	1/1	0.96	0.20	51,51,51,51	0
56	MG	1A	3686	1/1	0.96	0.11	28,28,28,28	0
56	MG	1A	3266	1/1	0.96	0.10	18,18,18,18	0
56	MG	1A	3116	1/1	0.96	0.05	52,52,52,52	0
56	MG	2A	3324	1/1	0.96	0.04	43,43,43,43	0
56	MG	2A	3058	1/1	0.96	0.10	51,51,51,51	0
56	MG	2a	3029	1/1	0.96	0.09	66,66,66,66	0
56	MG	2A	3060	1/1	0.96	0.12	40,40,40,40	0
56	MG	1A	3268	1/1	0.96	0.15	23,23,23,23	0
56	MG	1A	3269	1/1	0.96	0.12	53,53,53,53	0
56	MG	1A	3470	1/1	0.96	0.07	51,51,51,51	0
56	MG	2A	3338	1/1	0.96	0.12	46,46,46,46	0
56	MG	2a	3035	1/1	0.96	0.11	59,59,59,59	0
56	MG	1A	3166	1/1	0.96	0.13	35,35,35,35	0
56	MG	1A	3137	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	3051	1/1	0.96	0.28	47,47,47,47	0
56	MG	1A	3872	1/1	0.96	0.08	39,39,39,39	0
56	MG	1a	1617	1/1	0.96	0.18	55,55,55,55	0
56	MG	1A	3474	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3875	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3475	1/1	0.96	0.11	66,66,66,66	0
56	MG	1A	3052	1/1	0.96	0.11	51,51,51,51	0
56	MG	1A	3334	1/1	0.96	0.09	73,73,73,73	0
56	MG	2a	3046	1/1	0.96	0.05	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3140	1/1	0.96	0.08	36,36,36,36	0
56	MG	1A	3141	1/1	0.96	0.09	39,39,39,39	0
56	MG	1A	3279	1/1	0.96	0.20	41,41,41,41	0
56	MG	1A	3406	1/1	0.96	0.13	49,49,49,49	0
56	MG	1A	4068	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3143	1/1	0.96	0.06	34,34,34,34	0
56	MG	1A	4071	1/1	0.96	0.15	44,44,44,44	0
56	MG	1A	3886	1/1	0.96	0.05	42,42,42,42	0
56	MG	1A	3714	1/1	0.96	0.15	49,49,49,49	0
56	MG	1A	3042	1/1	0.96	0.10	42,42,42,42	0
56	MG	1A	3717	1/1	0.96	0.15	55,55,55,55	0
56	MG	1A	3340	1/1	0.96	0.10	59,59,59,59	0
56	MG	1a	1637	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3564	1/1	0.96	0.06	36,36,36,36	0
56	MG	2A	3088	1/1	0.96	0.06	44,44,44,44	0
56	MG	1A	3720	1/1	0.96	0.12	45,45,45,45	0
56	MG	2A	3090	1/1	0.96	0.20	58,58,58,58	0
56	MG	1A	4084	1/1	0.96	0.24	32,32,32,32	0
56	MG	1A	3721	1/1	0.96	0.06	45,45,45,45	0
56	MG	1a	1642	1/1	0.96	0.04	58,58,58,58	0
56	MG	2A	3377	1/1	0.96	0.07	33,33,33,33	0
56	MG	2A	3094	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3565	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	4087	1/1	0.96	0.17	42,42,42,42	0
56	MG	2A	3385	1/1	0.96	0.07	61,61,61,61	0
56	MG	2A	3387	1/1	0.96	0.20	38,38,38,38	0
56	MG	1A	3726	1/1	0.96	0.07	46,46,46,46	0
56	MG	1a	1836	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3903	1/1	0.96	0.18	71,71,71,71	0
56	MG	1A	3487	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3282	1/1	0.96	0.16	54,54,54,54	0
56	MG	1B	203	1/1	0.96	0.11	39,39,39,39	0
56	MG	2a	3079	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3394	1/1	0.96	0.16	54,54,54,54	0
56	MG	1a	1843	1/1	0.96	0.09	55,55,55,55	0
56	MG	1A	3220	1/1	0.96	0.30	41,41,41,41	0
56	MG	1A	3574	1/1	0.96	0.11	37,37,37,37	0
56	MG	2a	3085	1/1	0.96	0.15	48,48,48,48	0
56	MG	2a	3086	1/1	0.96	0.08	50,50,50,50	0
56	MG	1a	1847	1/1	0.96	0.07	53,53,53,53	0
56	MG	2A	3111	1/1	0.96	0.15	36,36,36,36	0
56	MG	1A	3910	1/1	0.96	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1849	1/1	0.96	0.06	38,38,38,38	0
56	MG	2A	3115	1/1	0.96	0.15	41,41,41,41	0
56	MG	1A	3911	1/1	0.96	0.09	30,30,30,30	0
56	MG	1A	3222	1/1	0.96	0.10	19,19,19,19	0
56	MG	2A	3407	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	3913	1/1	0.96	0.06	28,28,28,28	0
56	MG	1A	3739	1/1	0.96	0.13	34,34,34,34	0
56	MG	1a	1658	1/1	0.96	0.10	58,58,58,58	0
56	MG	2A	3411	1/1	0.96	0.04	47,47,47,47	0
56	MG	1A	3915	1/1	0.96	0.14	52,52,52,52	0
56	MG	2a	3102	1/1	0.96	0.12	44,44,44,44	0
56	MG	2A	3123	1/1	0.96	0.19	57,57,57,57	0
56	MG	1A	3223	1/1	0.96	0.14	29,29,29,29	0
56	MG	1A	3917	1/1	0.96	0.04	35,35,35,35	0
56	MG	2A	3126	1/1	0.96	0.26	43,43,43,43	0
56	MG	1A	3577	1/1	0.96	0.11	30,30,30,30	0
56	MG	1A	3349	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3745	1/1	0.96	0.06	57,57,57,57	0
56	MG	1A	3287	1/1	0.96	0.16	38,38,38,38	0
56	MG	2A	3422	1/1	0.96	0.09	73,73,73,73	0
56	MG	1A	3923	1/1	0.96	0.08	40,40,40,40	0
56	MG	1A	3924	1/1	0.96	0.12	52,52,52,52	0
56	MG	2A	3427	1/1	0.96	0.22	54,54,54,54	0
56	MG	1A	3288	1/1	0.96	0.22	42,42,42,42	0
56	MG	1A	3352	1/1	0.96	0.20	57,57,57,57	0
56	MG	2A	3430	1/1	0.96	0.21	50,50,50,50	0
56	MG	1D	302	1/1	0.96	0.13	52,52,52,52	0
56	MG	2A	3137	1/1	0.96	0.08	33,33,33,33	0
56	MG	1D	304	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3928	1/1	0.96	0.11	29,29,29,29	0
56	MG	1A	3929	1/1	0.96	0.07	29,29,29,29	0
56	MG	1A	3930	1/1	0.96	0.09	55,55,55,55	0
56	MG	1a	1676	1/1	0.96	0.07	55,55,55,55	0
56	MG	1a	1875	1/1	0.96	0.08	58,58,58,58	0
56	MG	2A	3148	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3931	1/1	0.96	0.06	32,32,32,32	0
56	MG	2A	3441	1/1	0.96	0.12	55,55,55,55	0
56	MG	2A	3150	1/1	0.96	0.11	30,30,30,30	0
56	MG	1D	309	1/1	0.96	0.14	56,56,56,56	0
56	MG	1A	3932	1/1	0.96	0.10	59,59,59,59	0
56	MG	1a	1681	1/1	0.96	0.12	47,47,47,47	0
56	MG	2A	3155	1/1	0.96	0.17	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3157	1/1	0.96	0.06	31,31,31,31	0
56	MG	2A	3450	1/1	0.96	0.06	56,56,56,56	0
56	MG	1A	3933	1/1	0.96	0.08	46,46,46,46	0
56	MG	2A	3453	1/1	0.96	0.08	31,31,31,31	0
56	MG	1a	1683	1/1	0.96	0.07	58,58,58,58	0
56	MG	1A	3584	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3354	1/1	0.96	0.10	84,84,84,84	0
56	MG	1a	1884	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3179	1/1	0.96	0.16	22,22,22,22	0
56	MG	1A	3498	1/1	0.96	0.09	53,53,53,53	0
56	MG	1A	3048	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3294	1/1	0.96	0.17	55,55,55,55	0
56	MG	1A	3591	1/1	0.96	0.12	32,32,32,32	0
56	MG	1E	308	1/1	0.96	0.17	35,35,35,35	0
56	MG	2A	3468	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3169	1/1	0.96	0.11	37,37,37,37	0
56	MG	1A	3296	1/1	0.96	0.09	49,49,49,49	0
56	MG	2A	3472	1/1	0.96	0.06	50,50,50,50	0
56	MG	1a	1695	1/1	0.96	0.17	53,53,53,53	0
56	MG	1a	1893	1/1	0.96	0.18	69,69,69,69	0
56	MG	2A	3175	1/1	0.96	0.14	34,34,34,34	0
56	MG	1E	312	1/1	0.96	0.05	44,44,44,44	0
56	MG	1F	301	1/1	0.96	0.19	30,30,30,30	0
56	MG	1A	3944	1/1	0.96	0.20	39,39,39,39	0
56	MG	1A	3945	1/1	0.96	0.17	30,30,30,30	0
56	MG	2A	3180	1/1	0.96	0.09	29,29,29,29	0
56	MG	1A	3946	1/1	0.96	0.13	24,24,24,24	0
56	MG	1A	3231	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	3122	1/1	0.96	0.07	56,56,56,56	0
56	MG	1a	1901	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3949	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3596	1/1	0.96	0.16	44,44,44,44	0
56	MG	1G	3002	1/1	0.96	0.14	52,52,52,52	0
56	MG	1A	3767	1/1	0.96	0.10	33,33,33,33	0
56	MG	1A	3597	1/1	0.96	0.14	71,71,71,71	0
56	MG	1a	1907	1/1	0.96	0.13	36,36,36,36	0
56	MG	2a	3179	1/1	0.96	0.05	58,58,58,58	0
56	MG	1a	1711	1/1	0.96	0.11	62,62,62,62	0
56	MG	1A	3957	1/1	0.96	0.11	34,34,34,34	0
56	MG	2a	3185	1/1	0.96	0.12	57,57,57,57	0
56	MG	1A	3363	1/1	0.96	0.06	49,49,49,49	0
56	MG	1A	3428	1/1	0.96	0.06	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3602	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3603	1/1	0.96	0.14	62,62,62,62	0
56	MG	1A	3507	1/1	0.96	0.06	45,45,45,45	0
56	MG	2A	3500	1/1	0.96	0.06	45,45,45,45	0
56	MG	2A	3199	1/1	0.96	0.12	21,21,21,21	0
56	MG	2a	3194	1/1	0.96	0.16	44,44,44,44	0
56	MG	2A	3503	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3234	1/1	0.96	0.09	46,46,46,46	0
56	MG	1f	3001	1/1	0.96	0.16	57,57,57,57	0
56	MG	2A	3506	1/1	0.96	0.09	51,51,51,51	0
56	MG	1A	3148	1/1	0.96	0.16	51,51,51,51	0
56	MG	1A	3149	1/1	0.96	0.20	32,32,32,32	0
56	MG	1a	1724	1/1	0.96	0.07	62,62,62,62	0
56	MG	1A	3973	1/1	0.96	0.10	50,50,50,50	0
56	MG	1A	3303	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3304	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3791	1/1	0.96	0.19	51,51,51,51	0
56	MG	1A	3097	1/1	0.96	0.15	49,49,49,49	0
56	MG	1a	1731	1/1	0.96	0.10	37,37,37,37	0
56	MG	2A	3517	1/1	0.96	0.06	47,47,47,47	0
56	MG	1p	3001	1/1	0.96	0.21	52,52,52,52	0
56	MG	1A	3151	1/1	0.96	0.08	45,45,45,45	0
56	MG	1q	201	1/1	0.96	0.17	58,58,58,58	0
56	MG	1A	3980	1/1	0.96	0.18	59,59,59,59	0
56	MG	2A	3524	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3110	1/1	0.96	0.10	65,65,65,65	0
56	MG	1A	3799	1/1	0.96	0.06	20,20,20,20	0
56	MG	2A	3225	1/1	0.96	0.16	58,58,58,58	0
56	MG	1A	3197	1/1	0.96	0.06	23,23,23,23	0
56	MG	2A	3227	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3441	1/1	0.96	0.08	49,49,49,49	0
56	MG	2A	3534	1/1	0.96	0.12	39,39,39,39	0
56	MG	2a	3224	1/1	0.96	0.10	60,60,60,60	0
56	MG	1A	3988	1/1	0.96	0.25	39,39,39,39	0
56	MG	1A	3518	1/1	0.96	0.07	51,51,51,51	0
56	MG	2A	3231	1/1	0.96	0.12	57,57,57,57	0
56	MG	2A	3540	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3625	1/1	0.96	0.05	31,31,31,31	0
56	MG	1A	3627	1/1	0.96	0.10	41,41,41,41	0
56	MG	1a	1743	1/1	0.96	0.12	44,44,44,44	0
56	MG	2A	3544	1/1	0.96	0.06	48,48,48,48	0
56	MG	1A	3629	1/1	0.96	0.10	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1T	201	1/1	0.96	0.09	41,41,41,41	0
56	MG	1A	3814	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3072	1/1	0.96	0.10	46,46,46,46	0
56	MG	2A	3550	1/1	0.96	0.06	39,39,39,39	0
56	MG	2A	3551	1/1	0.96	0.08	32,32,32,32	0
56	MG	2A	3552	1/1	0.96	0.13	44,44,44,44	0
56	MG	1A	3819	1/1	0.96	0.05	43,43,43,43	0
56	MG	1T	205	1/1	0.96	0.06	56,56,56,56	0
56	MG	2a	3244	1/1	0.96	0.09	64,64,64,64	0
56	MG	1A	3247	1/1	0.96	0.17	35,35,35,35	0
56	MG	2A	3556	1/1	0.96	0.06	55,55,55,55	0
56	MG	1z	8001	1/1	0.96	0.11	56,56,56,56	0
56	MG	1A	3823	1/1	0.96	0.10	17,17,17,17	0
56	MG	1A	3248	1/1	0.96	0.09	47,47,47,47	0
56	MG	2A	3560	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	4001	1/1	0.96	0.11	35,35,35,35	0
56	MG	1A	3377	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	3154	1/1	0.96	0.21	30,30,30,30	0
56	MG	2A	3253	1/1	0.96	0.06	59,59,59,59	0
56	MG	1A	3255	1/1	0.96	0.06	45,45,45,45	0
56	MG	1A	3126	1/1	0.96	0.10	27,27,27,27	0
56	MG	1A	3829	1/1	0.96	0.06	18,18,18,18	0
56	MG	1A	3079	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	4011	1/1	0.96	0.08	68,68,68,68	0
56	MG	1A	4013	1/1	0.96	0.09	42,42,42,42	0
56	MG	1A	3258	1/1	0.96	0.16	63,63,63,63	0
56	MG	2l	3003	1/1	0.96	0.14	57,57,57,57	0
56	MG	1A	3073	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3260	1/1	0.96	0.12	31,31,31,31	0
56	MG	1A	3385	1/1	0.96	0.14	45,45,45,45	0
56	MG	1A	3645	1/1	0.96	0.07	36,36,36,36	0
56	MG	1A	3203	1/1	0.96	0.28	47,47,47,47	0
56	MG	2A	3269	1/1	0.96	0.13	38,38,38,38	0
56	MG	1A	3081	1/1	0.96	0.15	40,40,40,40	0
56	MG	1a	1771	1/1	0.96	0.06	48,48,48,48	0
56	MG	2x	102	1/1	0.96	0.27	68,68,68,68	0
56	MG	2A	3022	1/1	0.96	0.05	46,46,46,46	0
56	MG	1A	3840	1/1	0.96	0.15	59,59,59,59	0
56	MG	1A	3841	1/1	0.96	0.06	44,44,44,44	0
56	MG	1A	3458	1/1	0.96	0.10	48,48,48,48	0
56	MG	1A	3650	1/1	0.96	0.09	28,28,28,28	0
56	MG	1A	3654	1/1	0.96	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2Q	3003	1/1	0.96	0.15	44,44,44,44	0
56	MG	15	103	1/1	0.96	0.19	28,28,28,28	0
56	MG	2A	3206	1/1	0.97	0.15	50,50,50,50	0
56	MG	1A	3192	1/1	0.97	0.18	46,46,46,46	0
56	MG	1A	3839	1/1	0.97	0.07	18,18,18,18	0
56	MG	2A	3210	1/1	0.97	0.21	31,31,31,31	0
56	MG	2A	3023	1/1	0.97	0.14	45,45,45,45	0
56	MG	2A	3024	1/1	0.97	0.11	55,55,55,55	0
56	MG	1A	3011	1/1	0.97	0.06	47,47,47,47	0
56	MG	1B	228	1/1	0.97	0.07	36,36,36,36	0
56	MG	1a	1635	1/1	0.97	0.08	56,56,56,56	0
56	MG	2A	3216	1/1	0.97	0.08	44,44,44,44	0
56	MG	1A	3455	1/1	0.97	0.06	58,58,58,58	0
56	MG	2A	3444	1/1	0.97	0.08	63,63,63,63	0
56	MG	1A	3274	1/1	0.97	0.15	47,47,47,47	0
56	MG	1A	3275	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3357	1/1	0.97	0.05	54,54,54,54	0
56	MG	1A	3459	1/1	0.97	0.13	49,49,49,49	0
56	MG	1A	3211	1/1	0.97	0.17	37,37,37,37	0
56	MG	1A	3978	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3461	1/1	0.97	0.17	48,48,48,48	0
56	MG	1A	3851	1/1	0.97	0.06	65,65,65,65	0
56	MG	1A	3852	1/1	0.97	0.08	30,30,30,30	0
56	MG	1A	3277	1/1	0.97	0.11	34,34,34,34	0
56	MG	1A	3213	1/1	0.97	0.23	44,44,44,44	0
56	MG	2A	3460	1/1	0.97	0.05	45,45,45,45	0
56	MG	1a	1648	1/1	0.97	0.10	48,48,48,48	0
56	MG	1A	3985	1/1	0.97	0.06	34,34,34,34	0
56	MG	1A	3986	1/1	0.97	0.13	49,49,49,49	0
56	MG	1A	3523	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3053	1/1	0.97	0.10	36,36,36,36	0
56	MG	1E	303	1/1	0.97	0.06	31,31,31,31	0
56	MG	2A	3237	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3243	1/1	0.97	0.10	38,38,38,38	0
56	MG	2A	3470	1/1	0.97	0.05	64,64,64,64	0
56	MG	1A	3412	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3413	1/1	0.97	0.10	60,60,60,60	0
56	MG	1A	3528	1/1	0.97	0.13	42,42,42,42	0
56	MG	2a	3089	1/1	0.97	0.05	46,46,46,46	0
56	MG	2A	3242	1/1	0.97	0.14	22,22,22,22	0
56	MG	1E	309	1/1	0.97	0.05	54,54,54,54	0
56	MG	1A	3724	1/1	0.97	0.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1E	311	1/1	0.97	0.09	40,40,40,40	0
56	MG	1A	3468	1/1	0.97	0.07	39,39,39,39	0
56	MG	1A	3611	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3469	1/1	0.97	0.16	33,33,33,33	0
56	MG	1A	3244	1/1	0.97	0.05	35,35,35,35	0
56	MG	1a	1665	1/1	0.97	0.07	50,50,50,50	0
56	MG	2A	3059	1/1	0.97	0.09	37,37,37,37	0
56	MG	1A	3731	1/1	0.97	0.06	45,45,45,45	0
56	MG	1A	3245	1/1	0.97	0.11	18,18,18,18	0
56	MG	2a	3103	1/1	0.97	0.12	48,48,48,48	0
56	MG	1a	1838	1/1	0.97	0.13	39,39,39,39	0
56	MG	1A	3734	1/1	0.97	0.06	46,46,46,46	0
56	MG	1A	3108	1/1	0.97	0.06	52,52,52,52	0
56	MG	2A	3260	1/1	0.97	0.13	39,39,39,39	0
56	MG	1F	308	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	4004	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	3284	1/1	0.97	0.11	52,52,52,52	0
56	MG	1A	3536	1/1	0.97	0.18	48,48,48,48	0
56	MG	1A	3196	1/1	0.97	0.16	37,37,37,37	0
56	MG	1A	3874	1/1	0.97	0.04	28,28,28,28	0
56	MG	1A	3742	1/1	0.97	0.07	52,52,52,52	0
56	MG	1A	4012	1/1	0.97	0.05	47,47,47,47	0
56	MG	1A	3109	1/1	0.97	0.04	45,45,45,45	0
56	MG	1A	3253	1/1	0.97	0.16	32,32,32,32	0
56	MG	1A	3325	1/1	0.97	0.05	41,41,41,41	0
56	MG	1N	3004	1/1	0.97	0.03	26,26,26,26	0
56	MG	1A	3068	1/1	0.97	0.17	45,45,45,45	0
56	MG	2a	3125	1/1	0.97	0.15	33,33,33,33	0
56	MG	2A	3276	1/1	0.97	0.04	60,60,60,60	0
56	MG	1a	1856	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3219	1/1	0.97	0.10	56,56,56,56	0
56	MG	1A	3480	1/1	0.97	0.08	54,54,54,54	0
56	MG	1A	3882	1/1	0.97	0.12	36,36,36,36	0
56	MG	2a	3131	1/1	0.97	0.29	48,48,48,48	0
56	MG	1A	3883	1/1	0.97	0.09	36,36,36,36	0
56	MG	2A	3282	1/1	0.97	0.06	35,35,35,35	0
56	MG	1A	4021	1/1	0.97	0.09	59,59,59,59	0
56	MG	1A	3630	1/1	0.97	0.08	37,37,37,37	0
56	MG	1a	1691	1/1	0.97	0.05	66,66,66,66	0
56	MG	1A	3054	1/1	0.97	0.15	53,53,53,53	0
56	MG	1A	4024	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3545	1/1	0.97	0.11	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3292	1/1	0.97	0.06	21,21,21,21	0
56	MG	1P	205	1/1	0.97	0.07	53,53,53,53	0
56	MG	1P	206	1/1	0.97	0.13	42,42,42,42	0
56	MG	1A	3546	1/1	0.97	0.09	66,66,66,66	0
56	MG	1A	3330	1/1	0.97	0.13	39,39,39,39	0
56	MG	2A	3527	1/1	0.97	0.07	39,39,39,39	0
56	MG	1A	4028	1/1	0.97	0.14	63,63,63,63	0
56	MG	1A	3291	1/1	0.97	0.17	41,41,41,41	0
56	MG	2A	3530	1/1	0.97	0.19	43,43,43,43	0
56	MG	2A	3095	1/1	0.97	0.07	46,46,46,46	0
56	MG	1Q	207	1/1	0.97	0.17	41,41,41,41	0
56	MG	1A	3293	1/1	0.97	0.10	11,11,11,11	0
56	MG	2A	3303	1/1	0.97	0.11	30,30,30,30	0
56	MG	1A	3637	1/1	0.97	0.06	43,43,43,43	0
56	MG	2a	3154	1/1	0.97	0.10	71,71,71,71	0
56	MG	2A	3538	1/1	0.97	0.12	39,39,39,39	0
56	MG	1A	3892	1/1	0.97	0.06	46,46,46,46	0
56	MG	2A	3100	1/1	0.97	0.05	35,35,35,35	0
56	MG	2A	3307	1/1	0.97	0.15	60,60,60,60	0
56	MG	1A	3102	1/1	0.97	0.22	49,49,49,49	0
56	MG	1A	3551	1/1	0.97	0.10	55,55,55,55	0
56	MG	1a	1708	1/1	0.97	0.10	67,67,67,67	0
56	MG	1R	206	1/1	0.97	0.11	32,32,32,32	0
56	MG	2A	3105	1/1	0.97	0.15	28,28,28,28	0
56	MG	1A	3295	1/1	0.97	0.10	42,42,42,42	0
56	MG	2A	3548	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	3900	1/1	0.97	0.12	39,39,39,39	0
56	MG	2A	3108	1/1	0.97	0.15	52,52,52,52	0
56	MG	1A	3182	1/1	0.97	0.17	32,32,32,32	0
56	MG	1A	3902	1/1	0.97	0.13	42,42,42,42	0
56	MG	1A	3642	1/1	0.97	0.13	38,38,38,38	0
56	MG	1A	4040	1/1	0.97	0.13	32,32,32,32	0
56	MG	1A	3431	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3224	1/1	0.97	0.05	33,33,33,33	0
56	MG	2A	3323	1/1	0.97	0.13	43,43,43,43	0
56	MG	1A	4045	1/1	0.97	0.06	23,23,23,23	0
56	MG	2A	3325	1/1	0.97	0.11	48,48,48,48	0
56	MG	1U	206	1/1	0.97	0.29	38,38,38,38	0
56	MG	1a	1722	1/1	0.97	0.13	47,47,47,47	0
56	MG	2a	3180	1/1	0.97	0.13	46,46,46,46	0
56	MG	2a	3181	1/1	0.97	0.08	58,58,58,58	0
56	MG	2A	3119	1/1	0.97	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3227	1/1	0.97	0.11	26,26,26,26	0
56	MG	2A	3335	1/1	0.97	0.09	35,35,35,35	0
56	MG	1a	1725	1/1	0.97	0.20	51,51,51,51	0
56	MG	1A	3434	1/1	0.97	0.09	50,50,50,50	0
56	MG	1W	3002	1/1	0.97	0.14	35,35,35,35	0
56	MG	1A	3775	1/1	0.97	0.06	31,31,31,31	0
56	MG	1A	3776	1/1	0.97	0.07	31,31,31,31	0
56	MG	1A	3647	1/1	0.97	0.08	19,19,19,19	0
56	MG	1A	3778	1/1	0.97	0.07	19,19,19,19	0
56	MG	1A	3299	1/1	0.97	0.14	59,59,59,59	0
56	MG	2D	304	1/1	0.97	0.06	36,36,36,36	0
56	MG	1A	3183	1/1	0.97	0.13	28,28,28,28	0
56	MG	2A	3349	1/1	0.97	0.06	67,67,67,67	0
56	MG	1A	4055	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	4056	1/1	0.97	0.04	29,29,29,29	0
56	MG	2A	3132	1/1	0.97	0.08	45,45,45,45	0
56	MG	1A	3783	1/1	0.97	0.08	28,28,28,28	0
56	MG	2A	3356	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	3071	1/1	0.97	0.23	37,37,37,37	0
56	MG	1A	3651	1/1	0.97	0.06	14,14,14,14	0
56	MG	1A	3788	1/1	0.97	0.13	30,30,30,30	0
56	MG	2O	203	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3789	1/1	0.97	0.07	14,14,14,14	0
56	MG	1I	103	1/1	0.97	0.06	42,42,42,42	0
56	MG	2A	3140	1/1	0.97	0.14	33,33,33,33	0
56	MG	1A	3790	1/1	0.97	0.09	19,19,19,19	0
56	MG	1A	3230	1/1	0.97	0.14	35,35,35,35	0
56	MG	1A	3388	1/1	0.97	0.07	55,55,55,55	0
56	MG	1A	3925	1/1	0.97	0.13	56,56,56,56	0
56	MG	2T	201	1/1	0.97	0.06	41,41,41,41	0
56	MG	2A	3146	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3658	1/1	0.97	0.04	13,13,13,13	0
56	MG	1A	3440	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	3342	1/1	0.97	0.13	53,53,53,53	0
56	MG	1A	3665	1/1	0.97	0.13	24,24,24,24	0
56	MG	1I	201	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3036	1/1	0.97	0.17	40,40,40,40	0
56	MG	28	102	1/1	0.97	0.15	50,50,50,50	0
56	MG	16	104	1/1	0.97	0.06	53,53,53,53	0
56	MG	2a	3227	1/1	0.97	0.09	62,62,62,62	0
56	MG	16	105	1/1	0.97	0.10	44,44,44,44	0
56	MG	2A	3156	1/1	0.97	0.09	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	17	101	1/1	0.97	0.05	26,26,26,26	0
56	MG	2A	3379	1/1	0.97	0.05	35,35,35,35	0
56	MG	1A	4073	1/1	0.97	0.25	48,48,48,48	0
56	MG	1A	3667	1/1	0.97	0.13	14,14,14,14	0
56	MG	2A	3382	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3805	1/1	0.97	0.08	49,49,49,49	0
56	MG	1a	1758	1/1	0.97	0.14	67,67,67,67	0
56	MG	18	3003	1/1	0.97	0.08	35,35,35,35	0
56	MG	19	101	1/1	0.97	0.14	51,51,51,51	0
56	MG	1q	203	1/1	0.97	0.19	53,53,53,53	0
56	MG	1A	3669	1/1	0.97	0.06	17,17,17,17	0
56	MG	1A	3566	1/1	0.97	0.09	34,34,34,34	0
56	MG	19	106	1/1	0.97	0.07	45,45,45,45	0
56	MG	1A	3812	1/1	0.97	0.04	48,48,48,48	0
56	MG	1A	4080	1/1	0.97	0.23	36,36,36,36	0
56	MG	2A	3170	1/1	0.97	0.06	33,33,33,33	0
56	MG	2A	3398	1/1	0.97	0.07	32,32,32,32	0
56	MG	1A	3344	1/1	0.97	0.07	42,42,42,42	0
56	MG	1a	1604	1/1	0.97	0.08	60,60,60,60	0
56	MG	1A	3675	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3037	1/1	0.97	0.17	40,40,40,40	0
56	MG	1a	1770	1/1	0.97	0.06	70,70,70,70	0
56	MG	1A	3678	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	3503	1/1	0.97	0.07	30,30,30,30	0
56	MG	1A	3570	1/1	0.97	0.13	46,46,46,46	0
56	MG	1A	3571	1/1	0.97	0.12	32,32,32,32	0
56	MG	1A	3445	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3346	1/1	0.97	0.06	55,55,55,55	0
56	MG	1A	3347	1/1	0.97	0.05	56,56,56,56	0
56	MG	1a	1778	1/1	0.97	0.04	48,48,48,48	0
56	MG	2A	3185	1/1	0.97	0.12	32,32,32,32	0
56	MG	1A	3233	1/1	0.97	0.11	36,36,36,36	0
56	MG	1a	1780	1/1	0.97	0.05	56,56,56,56	0
56	MG	1A	3168	1/1	0.97	0.12	35,35,35,35	0
56	MG	1A	3950	1/1	0.97	0.14	64,64,64,64	0
56	MG	1A	3189	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3399	1/1	0.97	0.20	45,45,45,45	0
56	MG	1A	3698	1/1	0.97	0.06	26,26,26,26	0
56	MG	1B	211	1/1	0.97	0.05	39,39,39,39	0
56	MG	1A	3833	1/1	0.97	0.04	50,50,50,50	0
56	MG	1A	3581	1/1	0.97	0.15	54,54,54,54	0
56	MG	1A	3962	1/1	0.97	0.08	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3426	1/1	0.97	0.05	46,46,46,46	0
56	MG	1B	215	1/1	0.97	0.08	74,74,74,74	0
56	MG	1A	3582	1/1	0.97	0.09	25,25,25,25	0
56	MG	1B	218	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3702	1/1	0.97	0.05	20,20,20,20	0
56	MG	1B	222	1/1	0.97	0.09	59,59,59,59	0
57	ZN	29	501	1/1	0.97	0.05	66,66,66,66	0
56	MG	1A	3190	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3809	1/1	0.98	0.09	33,33,33,33	0
56	MG	2a	3105	1/1	0.98	0.10	62,62,62,62	0
56	MG	1A	4089	1/1	0.98	0.10	29,29,29,29	0
56	MG	2a	3108	1/1	0.98	0.10	68,68,68,68	0
56	MG	2A	3383	1/1	0.98	0.08	29,29,29,29	0
56	MG	2a	3110	1/1	0.98	0.07	55,55,55,55	0
56	MG	2A	3384	1/1	0.98	0.05	39,39,39,39	0
56	MG	1A	3810	1/1	0.98	0.04	30,30,30,30	0
56	MG	2A	3386	1/1	0.98	0.09	37,37,37,37	0
56	MG	1A	3811	1/1	0.98	0.11	28,28,28,28	0
56	MG	1V	201	1/1	0.98	0.18	39,39,39,39	0
56	MG	1A	3893	1/1	0.98	0.10	51,51,51,51	0
56	MG	2A	3232	1/1	0.98	0.06	47,47,47,47	0
56	MG	1a	1793	1/1	0.98	0.07	83,83,83,83	0
56	MG	1A	3894	1/1	0.98	0.10	50,50,50,50	0
56	MG	1A	3163	1/1	0.98	0.04	32,32,32,32	0
56	MG	1W	3003	1/1	0.98	0.15	33,33,33,33	0
56	MG	1a	1677	1/1	0.98	0.10	48,48,48,48	0
56	MG	1A	3660	1/1	0.98	0.04	24,24,24,24	0
56	MG	2A	3397	1/1	0.98	0.04	58,58,58,58	0
56	MG	1A	3993	1/1	0.98	0.04	34,34,34,34	0
56	MG	1A	3994	1/1	0.98	0.07	23,23,23,23	0
56	MG	1A	3898	1/1	0.98	0.06	52,52,52,52	0
56	MG	1Y	502	1/1	0.98	0.08	40,40,40,40	0
56	MG	1A	3398	1/1	0.98	0.05	46,46,46,46	0
56	MG	1a	1804	1/1	0.98	0.15	37,37,37,37	0
56	MG	1A	3817	1/1	0.98	0.07	40,40,40,40	0
56	MG	2B	207	1/1	0.98	0.07	67,67,67,67	0
56	MG	1A	3730	1/1	0.98	0.04	34,34,34,34	0
56	MG	10	102	1/1	0.98	0.04	48,48,48,48	0
56	MG	1a	1808	1/1	0.98	0.08	33,33,33,33	0
56	MG	2A	3250	1/1	0.98	0.16	30,30,30,30	0
56	MG	1A	3118	1/1	0.98	0.05	47,47,47,47	0
56	MG	2D	303	1/1	0.98	0.24	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3212	1/1	0.98	0.18	36,36,36,36	0
56	MG	2D	305	1/1	0.98	0.09	29,29,29,29	0
56	MG	1a	1689	1/1	0.98	0.08	48,48,48,48	0
56	MG	2A	3254	1/1	0.98	0.06	30,30,30,30	0
56	MG	1A	3904	1/1	0.98	0.07	17,17,17,17	0
56	MG	2A	3414	1/1	0.98	0.20	50,50,50,50	0
56	MG	1A	3821	1/1	0.98	0.06	21,21,21,21	0
56	MG	2F	303	1/1	0.98	0.09	52,52,52,52	0
56	MG	1A	3906	1/1	0.98	0.07	53,53,53,53	0
56	MG	1B	219	1/1	0.98	0.08	62,62,62,62	0
56	MG	1B	220	1/1	0.98	0.04	42,42,42,42	0
56	MG	1A	3617	1/1	0.98	0.12	13,13,13,13	0
56	MG	1A	3130	1/1	0.98	0.11	21,21,21,21	0
56	MG	1A	3240	1/1	0.98	0.07	32,32,32,32	0
56	MG	1B	224	1/1	0.98	0.06	58,58,58,58	0
56	MG	1A	3572	1/1	0.98	0.06	52,52,52,52	0
56	MG	2A	3424	1/1	0.98	0.07	63,63,63,63	0
56	MG	1A	4009	1/1	0.98	0.07	47,47,47,47	0
56	MG	1A	3673	1/1	0.98	0.04	25,25,25,25	0
56	MG	1A	3674	1/1	0.98	0.05	24,24,24,24	0
56	MG	1A	3032	1/1	0.98	0.16	44,44,44,44	0
56	MG	2R	202	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3132	1/1	0.98	0.08	33,33,33,33	0
56	MG	2U	201	1/1	0.98	0.11	49,49,49,49	0
56	MG	1A	3746	1/1	0.98	0.05	46,46,46,46	0
56	MG	1A	3677	1/1	0.98	0.05	39,39,39,39	0
56	MG	2A	3008	1/1	0.98	0.05	51,51,51,51	0
56	MG	1D	303	1/1	0.98	0.11	38,38,38,38	0
56	MG	1a	1709	1/1	0.98	0.14	61,61,61,61	0
56	MG	1A	3748	1/1	0.98	0.05	13,13,13,13	0
56	MG	1A	3058	1/1	0.98	0.10	45,45,45,45	0
56	MG	2A	3139	1/1	0.98	0.14	35,35,35,35	0
56	MG	1a	1712	1/1	0.98	0.07	40,40,40,40	0
56	MG	1a	1835	1/1	0.98	0.06	51,51,51,51	0
56	MG	1A	3919	1/1	0.98	0.06	51,51,51,51	0
56	MG	1A	3043	1/1	0.98	0.07	55,55,55,55	0
56	MG	1A	3170	1/1	0.98	0.07	25,25,25,25	0
56	MG	2A	3285	1/1	0.98	0.07	33,33,33,33	0
56	MG	2A	3286	1/1	0.98	0.13	47,47,47,47	0
56	MG	2A	3145	1/1	0.98	0.09	25,25,25,25	0
56	MG	1A	3626	1/1	0.98	0.10	45,45,45,45	0
56	MG	2A	3447	1/1	0.98	0.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1840	1/1	0.98	0.10	27,27,27,27	0
56	MG	1A	3683	1/1	0.98	0.04	42,42,42,42	0
56	MG	2a	3184	1/1	0.98	0.17	53,53,53,53	0
56	MG	2A	3291	1/1	0.98	0.06	37,37,37,37	0
56	MG	2A	3451	1/1	0.98	0.07	59,59,59,59	0
56	MG	1A	3069	1/1	0.98	0.07	39,39,39,39	0
56	MG	1A	3755	1/1	0.98	0.03	26,26,26,26	0
56	MG	1A	3628	1/1	0.98	0.12	43,43,43,43	0
56	MG	2a	3190	1/1	0.98	0.04	47,47,47,47	0
56	MG	1A	3842	1/1	0.98	0.06	54,54,54,54	0
56	MG	1A	3843	1/1	0.98	0.12	53,53,53,53	0
56	MG	1A	3028	1/1	0.98	0.07	50,50,50,50	0
56	MG	2A	3458	1/1	0.98	0.05	54,54,54,54	0
56	MG	1A	3249	1/1	0.98	0.04	20,20,20,20	0
56	MG	1E	305	1/1	0.98	0.08	14,14,14,14	0
56	MG	1A	3250	1/1	0.98	0.08	22,22,22,22	0
56	MG	1A	3763	1/1	0.98	0.06	42,42,42,42	0
56	MG	2A	3464	1/1	0.98	0.06	35,35,35,35	0
56	MG	1A	3251	1/1	0.98	0.09	31,31,31,31	0
56	MG	2a	3201	1/1	0.98	0.04	66,66,66,66	0
56	MG	1A	3934	1/1	0.98	0.06	35,35,35,35	0
56	MG	1A	3692	1/1	0.98	0.05	18,18,18,18	0
56	MG	1A	3693	1/1	0.98	0.05	25,25,25,25	0
56	MG	1A	3694	1/1	0.98	0.05	28,28,28,28	0
56	MG	2A	3036	1/1	0.98	0.12	30,30,30,30	0
56	MG	1A	3695	1/1	0.98	0.06	13,13,13,13	0
56	MG	1a	1735	1/1	0.98	0.07	45,45,45,45	0
56	MG	1A	3854	1/1	0.98	0.10	42,42,42,42	0
56	MG	1A	3696	1/1	0.98	0.12	32,32,32,32	0
56	MG	1a	1863	1/1	0.98	0.12	42,42,42,42	0
56	MG	1A	3770	1/1	0.98	0.05	50,50,50,50	0
56	MG	2A	3315	1/1	0.98	0.07	39,39,39,39	0
56	MG	1A	3221	1/1	0.98	0.18	28,28,28,28	0
56	MG	2A	3173	1/1	0.98	0.11	27,27,27,27	0
56	MG	1A	4042	1/1	0.98	0.13	44,44,44,44	0
56	MG	1A	4043	1/1	0.98	0.09	26,26,26,26	0
56	MG	1A	3943	1/1	0.98	0.11	44,44,44,44	0
56	MG	2a	3220	1/1	0.98	0.11	85,85,85,85	0
56	MG	1A	3040	1/1	0.98	0.08	36,36,36,36	0
56	MG	1A	3062	1/1	0.98	0.05	56,56,56,56	0
56	MG	1A	3700	1/1	0.98	0.06	31,31,31,31	0
56	MG	1A	3176	1/1	0.98	0.07	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3226	1/1	0.98	0.09	23,23,23,23	0
56	MG	2A	3326	1/1	0.98	0.09	43,43,43,43	0
56	MG	1A	3703	1/1	0.98	0.07	18,18,18,18	0
56	MG	1A	3177	1/1	0.98	0.04	33,33,33,33	0
56	MG	2A	3492	1/1	0.98	0.12	67,67,67,67	0
56	MG	1a	1631	1/1	0.98	0.11	44,44,44,44	0
56	MG	1A	3951	1/1	0.98	0.08	36,36,36,36	0
56	MG	1A	3082	1/1	0.98	0.04	33,33,33,33	0
56	MG	1A	3158	1/1	0.98	0.15	32,32,32,32	0
56	MG	2A	3337	1/1	0.98	0.06	59,59,59,59	0
56	MG	1A	3782	1/1	0.98	0.05	19,19,19,19	0
56	MG	1A	3955	1/1	0.98	0.05	21,21,21,21	0
56	MG	1A	3180	1/1	0.98	0.06	34,34,34,34	0
56	MG	2a	3238	1/1	0.98	0.05	57,57,57,57	0
56	MG	1A	3958	1/1	0.98	0.09	40,40,40,40	0
56	MG	1A	3784	1/1	0.98	0.10	20,20,20,20	0
56	MG	1A	3785	1/1	0.98	0.06	26,26,26,26	0
56	MG	1A	3292	1/1	0.98	0.10	62,62,62,62	0
56	MG	2A	3346	1/1	0.98	0.04	69,69,69,69	0
56	MG	1A	3181	1/1	0.98	0.16	38,38,38,38	0
56	MG	1A	3967	1/1	0.98	0.11	57,57,57,57	0
56	MG	1A	3159	1/1	0.98	0.13	36,36,36,36	0
56	MG	1A	3598	1/1	0.98	0.08	30,30,30,30	0
56	MG	1A	3359	1/1	0.98	0.07	37,37,37,37	0
56	MG	2a	3249	1/1	0.98	0.07	36,36,36,36	0
56	MG	1A	3600	1/1	0.98	0.06	56,56,56,56	0
56	MG	2A	3354	1/1	0.98	0.04	48,48,48,48	0
56	MG	2A	3355	1/1	0.98	0.10	45,45,45,45	0
56	MG	2A	3201	1/1	0.98	0.13	47,47,47,47	0
56	MG	2A	3202	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3264	1/1	0.98	0.18	27,27,27,27	0
56	MG	1A	3034	1/1	0.98	0.12	49,49,49,49	0
56	MG	2A	3520	1/1	0.98	0.07	37,37,37,37	0
56	MG	1Q	203	1/1	0.98	0.10	41,41,41,41	0
56	MG	1A	3144	1/1	0.98	0.09	48,48,48,48	0
56	MG	2A	3523	1/1	0.98	0.13	34,34,34,34	0
56	MG	1A	3064	1/1	0.98	0.07	48,48,48,48	0
56	MG	2A	3209	1/1	0.98	0.28	54,54,54,54	0
56	MG	2a	3084	1/1	0.98	0.10	50,50,50,50	0
56	MG	1A	3652	1/1	0.98	0.07	24,24,24,24	0
56	MG	2l	3005	1/1	0.98	0.09	44,44,44,44	0
56	MG	1A	3801	1/1	0.98	0.06	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1R	201	1/1	0.98	0.03	32,32,32,32	0
56	MG	1A	3653	1/1	0.98	0.12	48,48,48,48	0
56	MG	1A	3803	1/1	0.98	0.06	22,22,22,22	0
56	MG	1A	4079	1/1	0.98	0.11	33,33,33,33	0
56	MG	1A	3608	1/1	0.98	0.10	26,26,26,26	0
56	MG	2A	3533	1/1	0.98	0.10	47,47,47,47	0
56	MG	1A	4081	1/1	0.98	0.12	42,42,42,42	0
56	MG	1A	4082	1/1	0.98	0.06	66,66,66,66	0
56	MG	2A	3536	1/1	0.98	0.10	42,42,42,42	0
56	MG	1A	3981	1/1	0.98	0.11	42,42,42,42	0
56	MG	1A	3609	1/1	0.98	0.09	38,38,38,38	0
56	MG	1A	3657	1/1	0.98	0.04	34,34,34,34	0
56	MG	2A	3222	1/1	0.98	0.08	62,62,62,62	0
57	ZN	14	501	1/1	0.98	0.04	103,103,103,103	0
57	ZN	1n	101	1/1	0.98	0.04	83,83,83,83	0
57	ZN	2Y	501	1/1	0.98	0.04	99,99,99,99	0
56	MG	1A	3807	1/1	0.98	0.05	46,46,46,46	0
57	ZN	26	501	1/1	0.98	0.03	61,61,61,61	0
56	MG	1A	3531	1/1	0.98	0.06	45,45,45,45	0
56	MG	1U	201	1/1	0.98	0.04	26,26,26,26	0
58	SF4	1d	501	8/8	0.98	0.06	64,72,77,86	0
56	MG	1A	3715	1/1	0.99	0.04	9,9,9,9	0
56	MG	1A	4067	1/1	0.99	0.04	21,21,21,21	0
56	MG	2a	3107	1/1	0.99	0.03	57,57,57,57	0
56	MG	1A	3185	1/1	0.99	0.08	38,38,38,38	0
56	MG	1A	4069	1/1	0.99	0.04	47,47,47,47	0
56	MG	1A	3482	1/1	0.99	0.05	12,12,12,12	0
56	MG	1A	3096	1/1	0.99	0.16	40,40,40,40	0
56	MG	1A	3762	1/1	0.99	0.03	39,39,39,39	0
56	MG	1A	3960	1/1	0.99	0.03	28,28,28,28	0
56	MG	1A	3961	1/1	0.99	0.03	40,40,40,40	0
56	MG	2A	3375	1/1	0.99	0.09	46,46,46,46	0
56	MG	2A	3459	1/1	0.99	0.04	29,29,29,29	0
56	MG	1A	3685	1/1	0.99	0.05	16,16,16,16	0
56	MG	1A	3328	1/1	0.99	0.04	27,27,27,27	0
56	MG	2A	3004	1/1	0.99	0.05	59,59,59,59	0
56	MG	1A	3088	1/1	0.99	0.05	53,53,53,53	0
56	MG	1U	203	1/1	0.99	0.08	29,29,29,29	0
56	MG	1A	3965	1/1	0.99	0.06	36,36,36,36	0
56	MG	1a	1817	1/1	0.99	0.04	54,54,54,54	0
56	MG	2a	3215	1/1	0.99	0.08	53,53,53,53	0
56	MG	1A	3966	1/1	0.99	0.05	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3300	1/1	0.99	0.03	38,38,38,38	0
56	MG	1A	3688	1/1	0.99	0.06	8,8,8,8	0
56	MG	2A	3152	1/1	0.99	0.14	30,30,30,30	0
56	MG	1A	3723	1/1	0.99	0.03	29,29,29,29	0
56	MG	1A	3655	1/1	0.99	0.05	24,24,24,24	0
56	MG	1A	3815	1/1	0.99	0.04	20,20,20,20	0
56	MG	1A	3816	1/1	0.99	0.04	51,51,51,51	0
56	MG	1A	3725	1/1	0.99	0.03	18,18,18,18	0
56	MG	1A	3604	1/1	0.99	0.06	36,36,36,36	0
56	MG	1A	3113	1/1	0.99	0.05	35,35,35,35	0
56	MG	1A	3606	1/1	0.99	0.05	28,28,28,28	0
56	MG	1A	3246	1/1	0.99	0.04	23,23,23,23	0
56	MG	2A	3480	1/1	0.99	0.05	21,21,21,21	0
56	MG	1A	3822	1/1	0.99	0.06	21,21,21,21	0
56	MG	1A	3134	1/1	0.99	0.07	23,23,23,23	0
56	MG	1A	3155	1/1	0.99	0.15	39,39,39,39	0
56	MG	1A	3732	1/1	0.99	0.05	26,26,26,26	0
56	MG	1B	204	1/1	0.99	0.04	49,49,49,49	0
56	MG	1A	3662	1/1	0.99	0.06	30,30,30,30	0
56	MG	1A	3663	1/1	0.99	0.02	19,19,19,19	0
56	MG	1A	3664	1/1	0.99	0.07	19,19,19,19	0
56	MG	1A	3737	1/1	0.99	0.03	18,18,18,18	0
56	MG	1a	1705	1/1	0.99	0.09	58,58,58,58	0
56	MG	2E	302	1/1	0.99	0.17	36,36,36,36	0
56	MG	1A	3781	1/1	0.99	0.04	24,24,24,24	0
56	MG	1A	3365	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3612	1/1	0.99	0.07	23,23,23,23	0
56	MG	2A	3248	1/1	0.99	0.06	35,35,35,35	0
56	MG	1A	3191	1/1	0.99	0.12	28,28,28,28	0
56	MG	2A	3327	1/1	0.99	0.06	44,44,44,44	0
56	MG	1A	3401	1/1	0.99	0.09	30,30,30,30	0
56	MG	1A	3743	1/1	0.99	0.04	30,30,30,30	0
56	MG	2A	3330	1/1	0.99	0.06	40,40,40,40	0
56	MG	1A	3615	1/1	0.99	0.04	39,39,39,39	0
56	MG	2A	3333	1/1	0.99	0.04	35,35,35,35	0
56	MG	2A	3502	1/1	0.99	0.03	37,37,37,37	0
56	MG	1a	1846	1/1	0.99	0.03	25,25,25,25	0
56	MG	1A	3671	1/1	0.99	0.08	27,27,27,27	0
56	MG	1B	217	1/1	0.99	0.03	38,38,38,38	0
56	MG	1A	3225	1/1	0.99	0.03	21,21,21,21	0
56	MG	2A	3507	1/1	0.99	0.03	38,38,38,38	0
56	MG	1A	3135	1/1	0.99	0.16	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3592	1/1	0.99	0.07	25,25,25,25	0
56	MG	2A	3113	1/1	0.99	0.12	29,29,29,29	0
56	MG	2A	3341	1/1	0.99	0.06	51,51,51,51	0
56	MG	1A	4051	1/1	0.99	0.13	15,15,15,15	0
56	MG	1A	3173	1/1	0.99	0.04	40,40,40,40	0
56	MG	2a	3172	1/1	0.99	0.05	42,42,42,42	0
56	MG	1A	3353	1/1	0.99	0.06	40,40,40,40	0
56	MG	1A	3573	1/1	0.99	0.10	41,41,41,41	0
56	MG	2A	3264	1/1	0.99	0.06	29,29,29,29	0
56	MG	2A	3347	1/1	0.99	0.05	56,56,56,56	0
56	MG	1A	3795	1/1	0.99	0.08	13,13,13,13	0
56	MG	1a	1723	1/1	0.99	0.07	62,62,62,62	0
56	MG	1A	3796	1/1	0.99	0.09	24,24,24,24	0
56	MG	1A	3896	1/1	0.99	0.04	72,72,72,72	0
56	MG	1A	3797	1/1	0.99	0.03	28,28,28,28	0
56	MG	1a	1861	1/1	0.99	0.07	51,51,51,51	0
56	MG	1A	3798	1/1	0.99	0.04	19,19,19,19	0
56	MG	1A	3142	1/1	0.99	0.03	20,20,20,20	0
56	MG	2A	3273	1/1	0.99	0.06	53,53,53,53	0
56	MG	19	105	1/1	0.99	0.13	34,34,34,34	0
56	MG	1Q	205	1/1	0.99	0.03	40,40,40,40	0
57	ZN	1Y	501	1/1	0.99	0.02	62,62,62,62	0
56	MG	1A	3254	1/1	0.99	0.08	41,41,41,41	0
57	ZN	15	101	1/1	0.99	0.07	54,54,54,54	0
57	ZN	16	103	1/1	0.99	0.07	45,45,45,45	0
56	MG	1A	3065	1/1	0.99	0.03	39,39,39,39	0
56	MG	2a	3099	1/1	0.99	0.18	41,41,41,41	0
56	MG	1Q	208	1/1	0.99	0.02	37,37,37,37	0
56	MG	2A	3203	1/1	0.99	0.08	43,43,43,43	0
56	MG	1A	3681	1/1	0.99	0.04	19,19,19,19	0
56	MG	1A	4008	1/1	0.99	0.03	20,20,20,20	0
56	MG	1A	3756	1/1	0.99	0.06	30,30,30,30	0
58	SF4	2d	501	8/8	0.99	0.04	58,72,80,87	0
56	MG	1A	3844	1/1	1.00	0.03	18,18,18,18	0
57	ZN	19	103	1/1	1.00	0.05	47,47,47,47	0
56	MG	1A	3760	1/1	1.00	0.02	34,34,34,34	0
56	MG	1A	3586	1/1	1.00	0.08	33,33,33,33	0
56	MG	1A	3736	1/1	1.00	0.06	15,15,15,15	0
57	ZN	25	501	1/1	1.00	0.03	50,50,50,50	0
56	MG	1A	3607	1/1	1.00	0.07	26,26,26,26	0
56	MG	1A	3738	1/1	1.00	0.05	17,17,17,17	0
56	MG	1A	3668	1/1	1.00	0.04	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3956	1/1	1.00	0.06	12,12,12,12	0
56	MG	2A	3332	1/1	1.00	0.02	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.