



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 25, 2024 – 02:33 PM EST

PDB ID : 5HCQ  
Title : Crystal structure of antimicrobial peptide Oncocin d15-19 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 : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

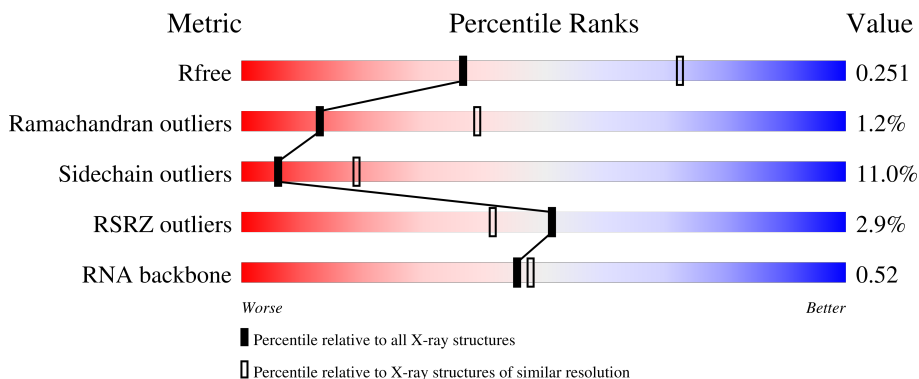
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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
















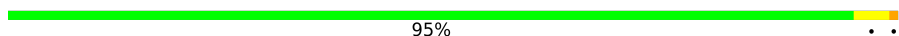




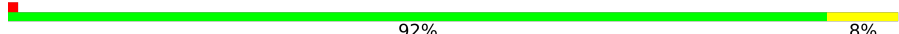






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 2% 77% 15% 6%
1	2A	2915	 2% 76% 18% 2%
2	1B	121	 90% 9% 1%
2	2B	121	 2% 70% 27% 1%
3	1D	276	 89% 11%

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Mol	Chain	Length	Quality of chain
3	2D	276	 91% 9%
4	1E	206	 89% 10%
4	2E	206	 89% 10%
5	1F	210	 88% 9%
5	2F	210	 89% 8%
6	1G	182	 88% 12%
6	2G	182	 86% 13%
7	1H	180	 91% 6%
7	2H	180	 87% 10%
8	1I	148	 84% 15%
8	2I	148	 91% 7%
9	1N	140	 90% 10%
9	2N	140	 91% 9%
10	1O	122	 95%
10	2O	122	 93% 7%
11	1P	150	 90% 9%
11	2P	150	 88% 11%
12	1Q	141	 91% 9%
12	2Q	141	 92% 8%
13	1R	118	 84% 16%
13	2R	118	 85% 15%
14	1S	112	 92% 6%
14	2S	112	 85% 12%
15	1T	146	 80% 9% 10%
15	2T	146	 81% 9% 10%



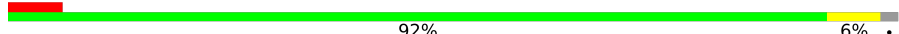



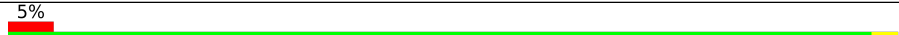
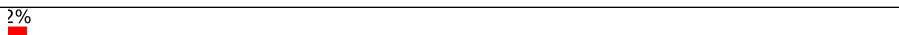
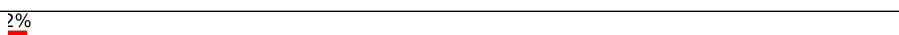
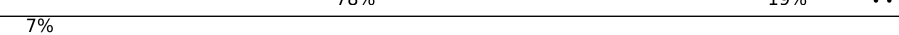
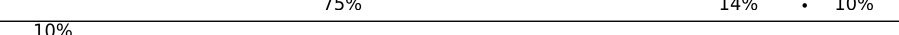
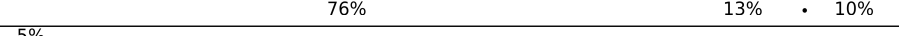












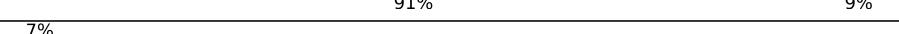
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Mol	Chain	Length	Quality of chain
16	1U	118	91% 7% ..
16	2U	118	90% 8% ..
17	1V	101	88% 11% .
17	2V	101	92% 7% .
18	1W	113	93% 6% .
18	2W	113	91% 8% .
19	1X	96	95% ..
19	2X	96	95% ..
20	1Y	110	91% 5% ..
20	2Y	110	90% 7% .
21	1Z	206	83% 8% 10%
21	2Z	206	82% 8% 10%
22	10	85	81% 6% 12%
22	20	85	84% 5% 12%
23	11	98	92% 6% ..
23	21	98	91% 8% .
24	12	72	89% 8% .
24	22	72	88% 10% .
25	13	60	90% 8% .
25	23	60	92% 7% .
26	14	71	75% 20% ..
26	24	71	79% 17% ..
27	15	60	93% 5% .
27	25	60	92% 7% .
28	16	54	93% 6% .

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Mol	Chain	Length	Quality of chain
28	26	54	 85% 13%
29	17	49	 90% 8%
29	27	49	 92% 6%
30	18	65	 91% 8%
30	28	65	 92% 6%
31	19	37	 97%
31	29	37	 97%
32	1a	1521	 78% 18%
32	2a	1521	 78% 19%
33	1b	256	 75% 14% 10%
33	2b	256	 76% 13% 10%
34	1c	239	 81% 5% 14%
34	2c	239	 79% 8% 14%
35	1d	209	 91% 9%
35	2d	209	 87% 12%
36	1e	162	 80% 11% 9%
36	2e	162	 80% 11% 9%
37	1f	101	 93% 6%
37	2f	101	 91% 8%
38	1g	156	 91% 8%
38	2g	156	 92% 8%
39	1h	138	 88% 12%
39	2h	138	 91% 9%
40	1i	128	 83% 16%
40	2i	128	 85% 12%

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Mol	Chain	Length	Quality of chain
41	1j	105	10% 76% 15% 8%
41	2j	105	16% 79% 12% 9%
42	1k	129	2% 82% 6% 12%
42	2k	129	2% 81% 7% 12%
43	1l	132	2% 88% 8%
43	2l	132	2% 89% 8%
44	1m	126	84% 9% 6%
44	2m	126	6% 85% 6% 8%
45	1n	61	5% 89% 10% 6%
45	2n	61	25% 84% 15% 8%
46	1o	89	2% 90% 9% 8%
46	2o	89	87% 12% 8%
47	1p	88	3% 82% 11% 7%
47	2p	88	2% 84% 9% 7%
48	1q	105	90% 6% 8%
48	2q	105	2% 90% 6% 8%
49	1r	88	5% 65% 11% 23%
49	2r	88	9% 65% 13% 23%
50	1s	93	2% 85% 5% 10%
50	2s	93	26% 77% 12% 11%
51	1t	106	2% 80% 10% 9%
51	2t	106	85% 6% 9%
52	1u	27	4% 81% 15%
52	2u	27	30% 78% 7% 15%
53	1v	24	4% 17% 79%

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Mol	Chain	Length	Quality of chain
53	2v	24	
54	1x	77	
54	2x	77	
55	1z	14	
55	2z	14	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3277	-	-	-	X
56	MG	1A	3285	-	-	-	X
56	MG	1A	3364	-	-	-	X
56	MG	1A	3412	-	-	-	X
56	MG	1A	3451	-	-	-	X
56	MG	1A	3901	-	-	-	X
56	MG	1A	3940	-	-	-	X
56	MG	1A	4015	-	-	-	X
56	MG	1A	4020	-	-	-	X
56	MG	1E	307	-	-	-	X
56	MG	1Z	302	-	-	-	X
56	MG	1a	1642	-	-	-	X
56	MG	1a	1667	-	-	-	X
56	MG	1a	1791	-	-	-	X
56	MG	1a	1824	-	-	-	X
56	MG	2A	3469	-	-	-	X
56	MG	2a	3004	-	-	-	X
56	MG	2a	3034	-	-	-	X
56	MG	2a	3082	-	-	-	X
56	MG	2a	3119	-	-	-	X
56	MG	2a	3149	-	-	-	X

## 2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 288518 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
42	2k	114	829	516	155	155	3	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1m	118	923	569	191	161	2	0	0	0
44	2m	116	903	555	187	159	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	1n	60	482	306	100	72	4	0	0	0
45	2n	60	459	291	93	71	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	1o	88	715	447	140	126	2	0	0	0
46	2o	88	728	456	144	126	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	1p	82	671	424	133	113	1	0	0	0
47	2p	82	677	430	133	113	1	0	0	0



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			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 Oncocin d15-19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	12	Total	C	N	O	0	0	0
			101	67	19	15			
55	2z	12	Total	C	N	O	0	0	0
			101	67	19	15			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1051	Total	Mg	0	0
			1051	1051		
56	1B	26	Total	Mg	0	0
			26	26		
56	1D	17	Total	Mg	0	0
			17	17		
56	1E	10	Total	Mg	0	0
			10	10		
56	1F	7	Total	Mg	0	0
			7	7		
56	1G	3	Total	Mg	0	0
			3	3		
56	1H	4	Total	Mg	0	0
			4	4		
56	1N	8	Total	Mg	0	0
			8	8		
56	1O	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1P	5	Total Mg 5 5	0	0
56	1Q	6	Total Mg 6 6	0	0
56	1R	6	Total Mg 6 6	0	0
56	1T	5	Total Mg 5 5	0	0
56	1U	5	Total Mg 5 5	0	0
56	1V	1	Total Mg 1 1	0	0
56	1W	6	Total Mg 6 6	0	0
56	1X	2	Total Mg 2 2	0	0
56	1Y	1	Total Mg 1 1	0	0
56	1Z	3	Total Mg 3 3	0	0
56	10	7	Total Mg 7 7	0	0
56	11	1	Total Mg 1 1	0	0
56	13	2	Total Mg 2 2	0	0
56	14	1	Total Mg 1 1	0	0
56	15	4	Total Mg 4 4	0	0
56	16	2	Total Mg 2 2	0	0
56	17	4	Total Mg 4 4	0	0
56	18	5	Total Mg 5 5	0	0
56	19	3	Total Mg 3 3	0	0
56	1a	306	Total Mg 306 306	0	0
56	1b	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1c	1	Total Mg 1 1	0	0
56	1d	2	Total Mg 2 2	0	0
56	1e	4	Total Mg 4 4	0	0
56	1f	1	Total Mg 1 1	0	0
56	1h	3	Total Mg 3 3	0	0
56	1k	1	Total Mg 1 1	0	0
56	1l	1	Total Mg 1 1	0	0
56	1n	1	Total Mg 1 1	0	0
56	1o	2	Total Mg 2 2	0	0
56	1q	4	Total Mg 4 4	0	0
56	1r	3	Total Mg 3 3	0	0
56	1t	1	Total Mg 1 1	0	0
56	1x	11	Total Mg 11 11	0	0
56	2A	583	Total Mg 583 583	0	0
56	2B	10	Total Mg 10 10	0	0
56	2D	4	Total Mg 4 4	0	0
56	2E	7	Total Mg 7 7	0	0
56	2F	2	Total Mg 2 2	0	0
56	2G	1	Total Mg 1 1	0	0
56	2N	1	Total Mg 1 1	0	0
56	2O	3	Total Mg 3 3	0	0

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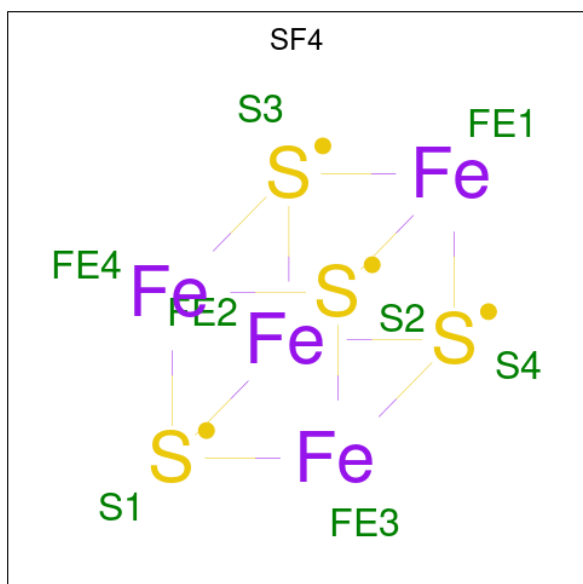
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2P	1	Total Mg 1 1	0	0
56	2Q	5	Total Mg 5 5	0	0
56	2R	1	Total Mg 1 1	0	0
56	2U	2	Total Mg 2 2	0	0
56	2V	1	Total Mg 1 1	0	0
56	2Y	1	Total Mg 1 1	0	0
56	20	1	Total Mg 1 1	0	0
56	25	1	Total Mg 1 1	0	0
56	26	1	Total Mg 1 1	0	0
56	28	1	Total Mg 1 1	0	0
56	2a	244	Total Mg 244 244	0	0
56	2d	2	Total Mg 2 2	0	0
56	2e	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0
56	2k	2	Total Mg 2 2	0	0
56	2l	3	Total Mg 3 3	0	0
56	2n	2	Total Mg 2 2	0	0
56	2p	1	Total Mg 1 1	0	0
56	2q	1	Total Mg 1 1	0	0
56	2t	1	Total Mg 1 1	0	0
56	2x	6	Total Mg 6 6	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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	2110	Total	O	0	0
			2110	2110		
59	1B	42	Total	O	0	0
			42	42		
59	1D	24	Total	O	0	0
			24	24		
59	1E	30	Total	O	0	0
			30	30		
59	1F	16	Total	O	0	0
			16	16		
59	1G	6	Total	O	0	0
			6	6		
59	1H	3	Total	O	0	0
			3	3		
59	1I	1	Total	O	0	0
			1	1		
59	1N	7	Total	O	0	0
			7	7		
59	1O	4	Total	O	0	0
			4	4		
59	1P	21	Total	O	0	0
			21	21		
59	1Q	11	Total	O	0	0
			11	11		
59	1R	16	Total	O	0	0
			16	16		
59	1S	2	Total	O	0	0
			2	2		
59	1T	7	Total	O	0	0
			7	7		
59	1U	14	Total	O	0	0
			14	14		
59	1V	4	Total	O	0	0
			4	4		
59	1W	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1X	4	Total O 4 4	0	0
59	1Y	1	Total O 1 1	0	0
59	1Z	4	Total O 4 4	0	0
59	10	8	Total O 8 8	0	0
59	11	7	Total O 7 7	0	0
59	12	2	Total O 2 2	0	0
59	13	4	Total O 4 4	0	0
59	15	7	Total O 7 7	0	0
59	16	5	Total O 5 5	0	0
59	17	8	Total O 8 8	0	0
59	18	9	Total O 9 9	0	0
59	19	4	Total O 4 4	0	0
59	1a	393	Total O 393 393	0	0
59	1b	1	Total O 1 1	0	0
59	1c	1	Total O 1 1	0	0
59	1d	5	Total O 5 5	0	0
59	1e	3	Total O 3 3	0	0
59	1f	1	Total O 1 1	0	0
59	1h	3	Total O 3 3	0	0
59	1i	1	Total O 1 1	0	0
59	1j	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1k	1	Total 1	O 1	0	0
59	1l	3	Total 3	O 3	0	0
59	1m	1	Total 1	O 1	0	0
59	1o	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	1v	1	Total 1	O 1	0	0
59	1x	8	Total 8	O 8	0	0
59	1z	1	Total 1	O 1	0	0
59	2A	813	Total 813	O 813	0	0
59	2B	10	Total 10	O 10	0	0
59	2D	16	Total 16	O 16	0	0
59	2E	9	Total 9	O 9	0	0
59	2F	5	Total 5	O 5	0	0
59	2N	1	Total 1	O 1	0	0
59	2O	3	Total 3	O 3	0	0
59	2P	9	Total 9	O 9	0	0
59	2Q	2	Total 2	O 2	0	0
59	2R	3	Total 3	O 3	0	0
59	2T	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2U	3	Total O 3 3	0	0
59	2W	1	Total O 1 1	0	0
59	2X	2	Total O 2 2	0	0
59	2Y	1	Total O 1 1	0	0
59	2Z	4	Total O 4 4	0	0
59	20	3	Total O 3 3	0	0
59	21	1	Total O 1 1	0	0
59	23	2	Total O 2 2	0	0
59	26	1	Total O 1 1	0	0
59	27	2	Total O 2 2	0	0
59	28	2	Total O 2 2	0	0
59	2a	321	Total O 321 321	0	0
59	2d	1	Total O 1 1	0	0
59	2e	1	Total O 1 1	0	0
59	2i	2	Total O 2 2	0	0
59	2j	1	Total O 1 1	0	0
59	2l	1	Total O 1 1	0	0
59	2m	3	Total O 3 3	0	0
59	2p	1	Total O 1 1	0	0
59	2q	1	Total O 1 1	0	0
59	2t	4	Total O 4 4	0	0

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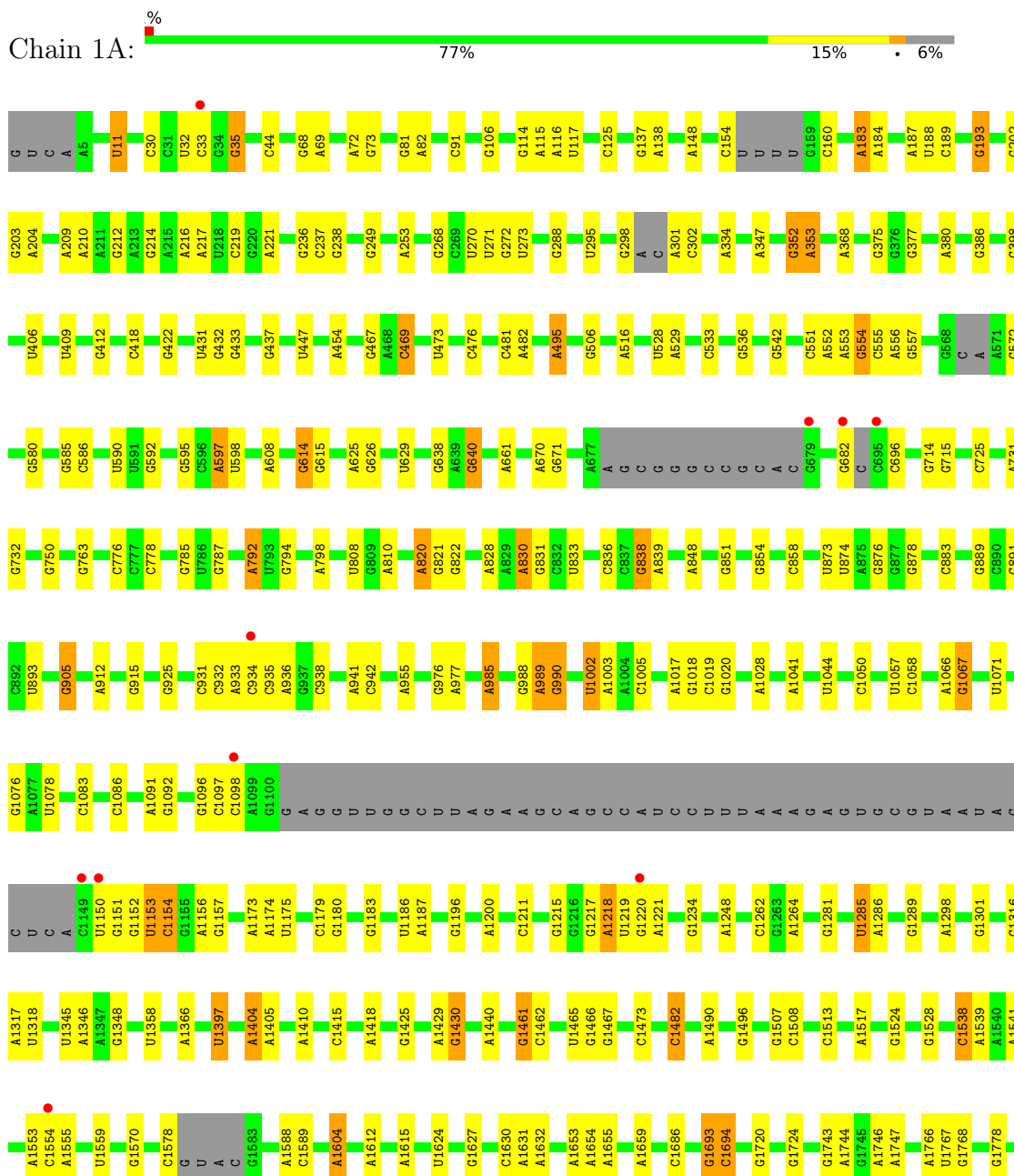
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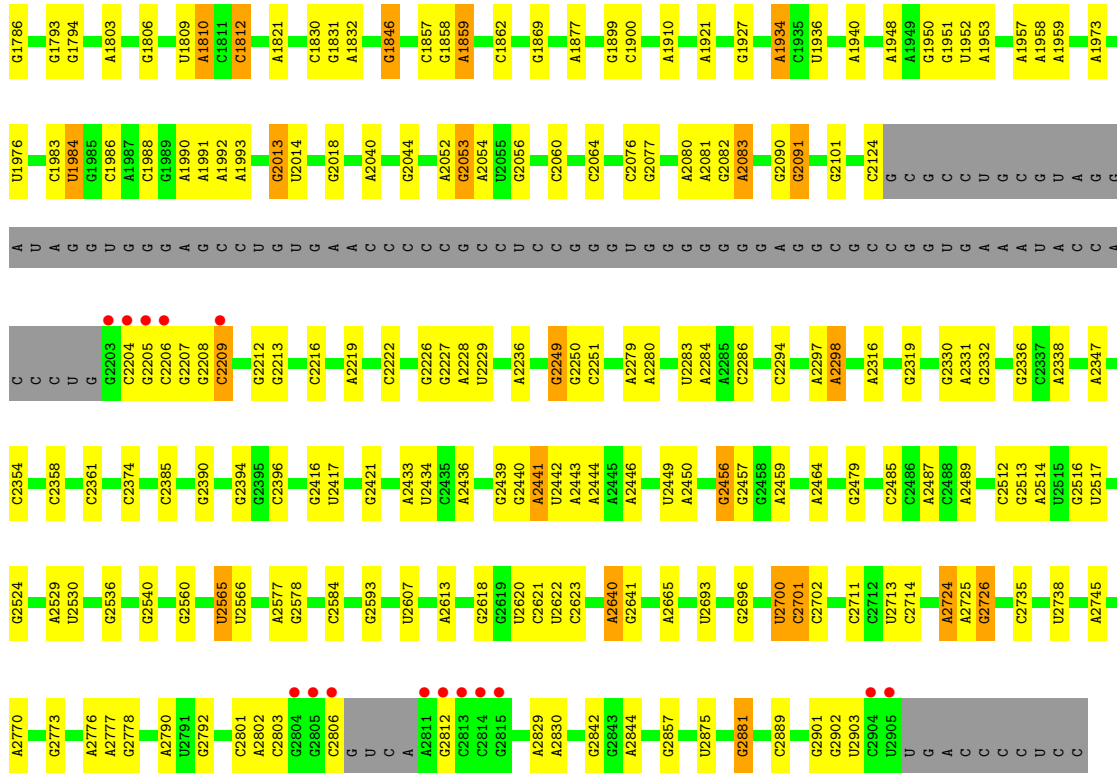
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59	2x	7	Total O 7 7	0	0
59	2z	1	Total O 1 1	0	0

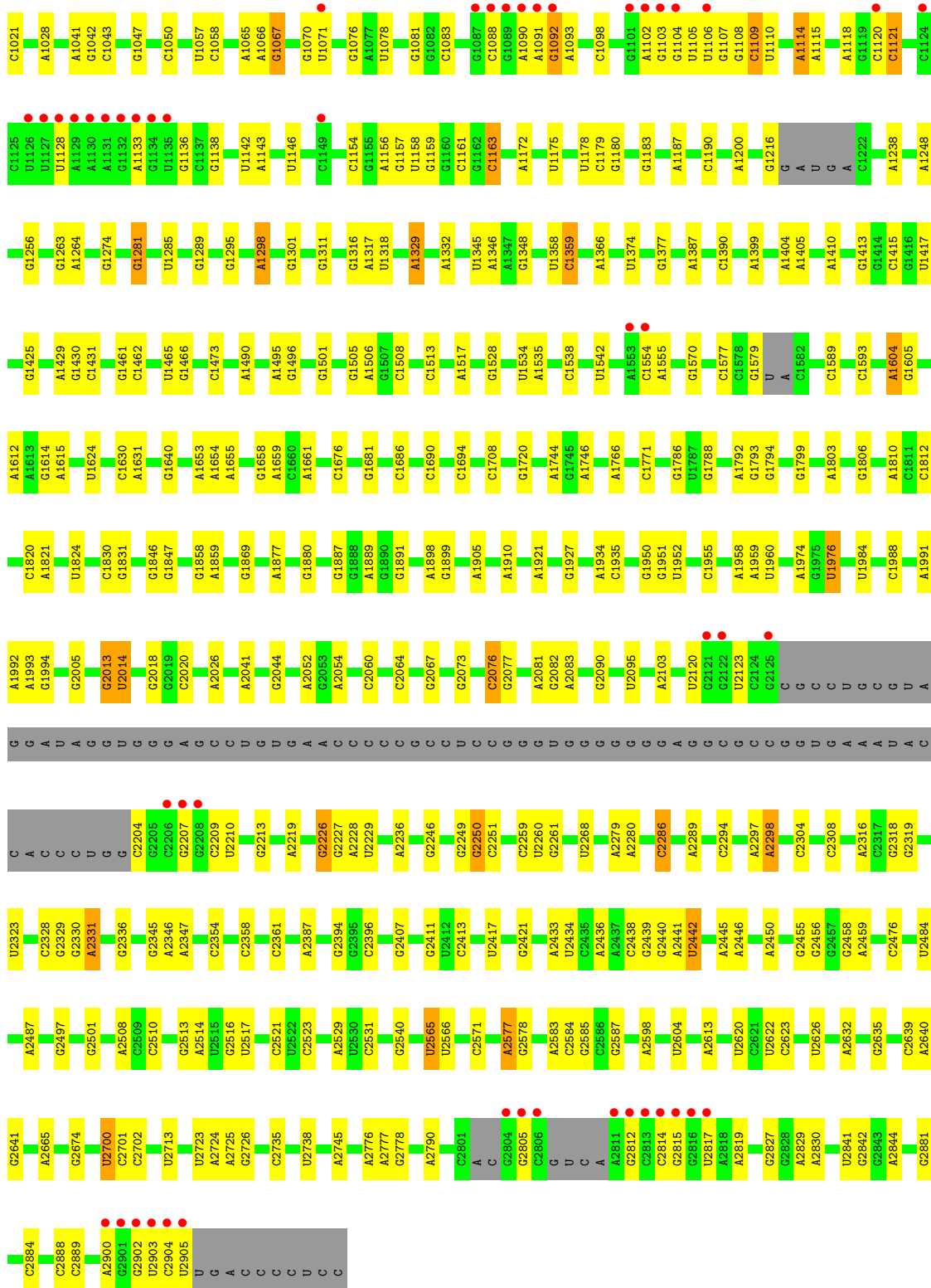
### 3 Residue-property plots [i](#)

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

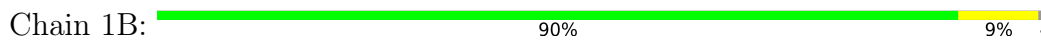
- Molecule 1: 23S Ribosomal RNA







● Molecule 2: 5S Ribosomal RNA





- Molecule 2: 5S Ribosomal RNA



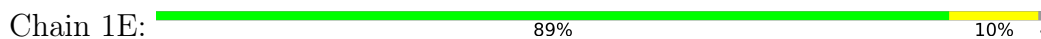
- Molecule 3: 50S ribosomal protein L2



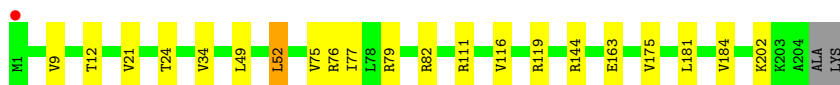
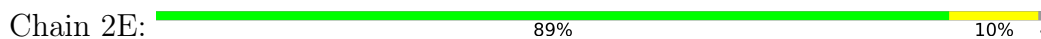
- Molecule 3: 50S ribosomal protein L2



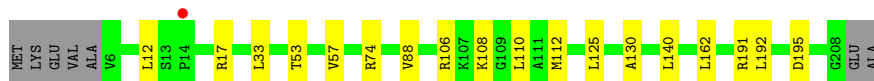
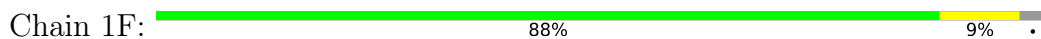
- Molecule 4: 50S ribosomal protein L3



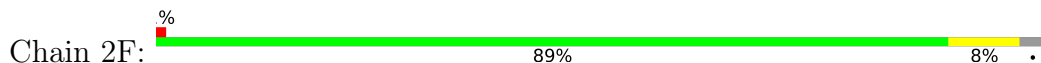
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4

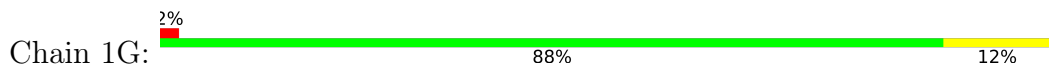


- Molecule 5: 50S ribosomal protein L4

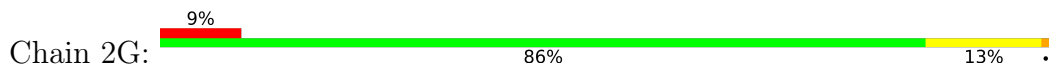




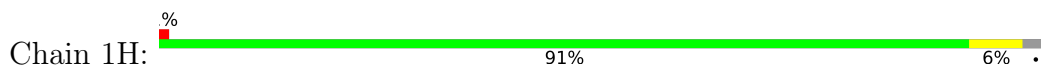
- Molecule 6: 50S ribosomal protein L5



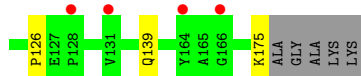
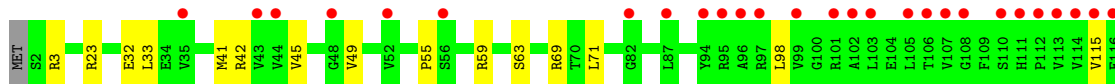
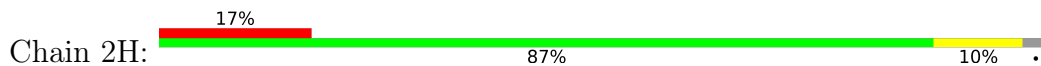
- Molecule 6: 50S ribosomal protein L5



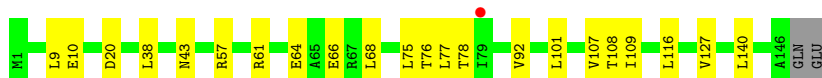
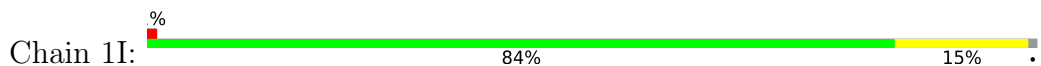
- Molecule 7: 50S ribosomal protein L6



- Molecule 7: 50S ribosomal protein L6

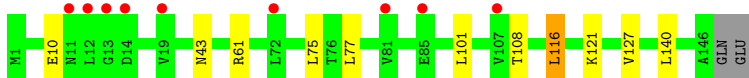
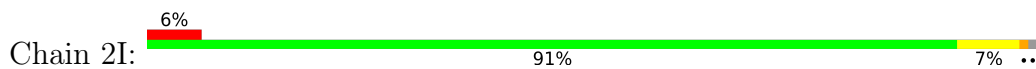


- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9





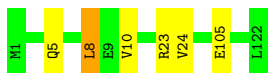
- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13



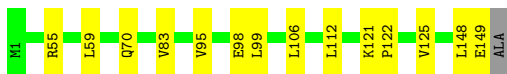
- Molecule 10: 50S ribosomal protein L14



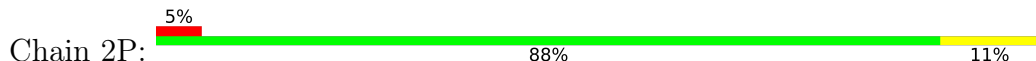
- Molecule 10: 50S ribosomal protein L14



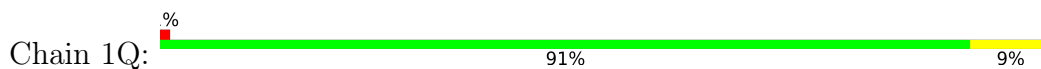
- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15



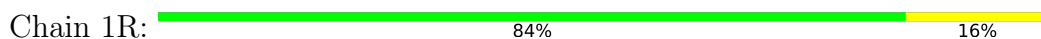
- Molecule 12: 50S ribosomal protein L16



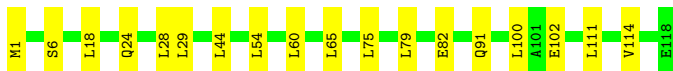
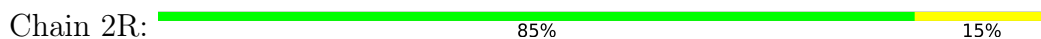
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



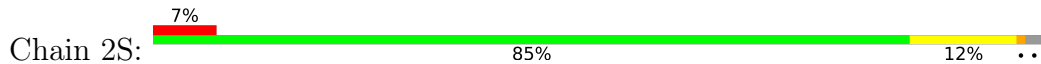
- Molecule 13: 50S ribosomal protein L17



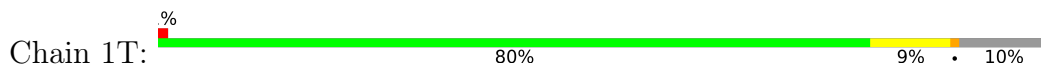
- Molecule 14: 50S ribosomal protein L18




- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19

Chain 2T:  81% 9% 10%




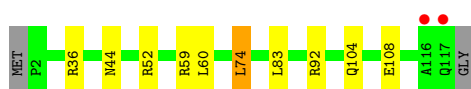
- Molecule 16: 50S ribosomal protein L20

Chain 1U:  91% 7% ..




- Molecule 16: 50S ribosomal protein L20

Chain 2U:  2% 90% 8% ..



- Molecule 17: 50S ribosomal protein L21

Chain 1V:  88% 11% .



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  92% 7% .



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  2% 93% 6% .



- Molecule 18: 50S ribosomal protein L22

Chain 2W:  91% 8% .



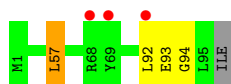
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  95%



- Molecule 19: 50S ribosomal protein L23

Chain 2X:  95%

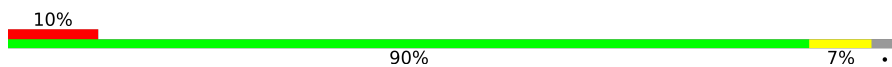


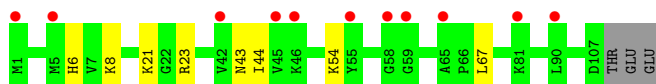
- Molecule 20: 50S ribosomal protein L24

Chain 1Y:  91%




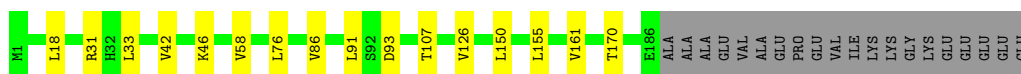
- Molecule 20: 50S ribosomal protein L24

Chain 2Y:  90%




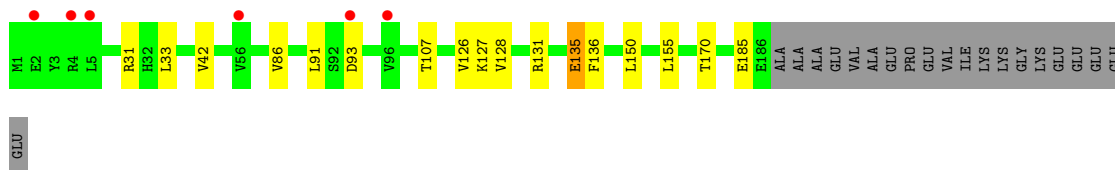
- Molecule 21: 50S ribosomal protein L25

Chain 1Z:  83%




- Molecule 21: 50S ribosomal protein L25

Chain 2Z:  82%

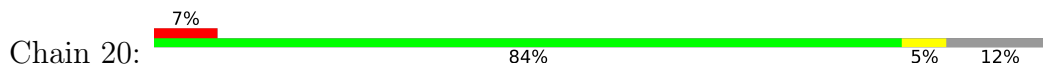


- Molecule 22: 50S ribosomal protein L27

Chain 10:  81%



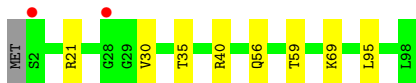
- Molecule 22: 50S ribosomal protein L27



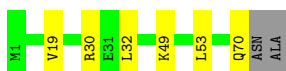
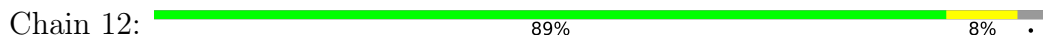
- Molecule 23: 50S ribosomal protein L28



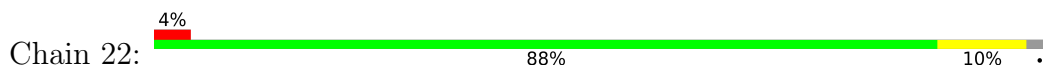
- Molecule 23: 50S ribosomal protein L28



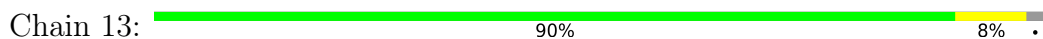
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30

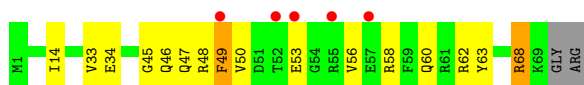
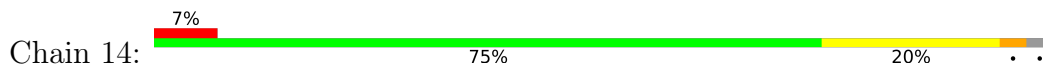


- Molecule 25: 50S ribosomal protein L30

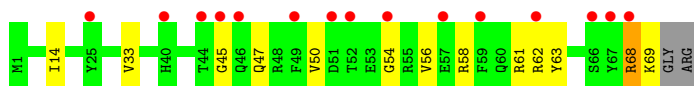
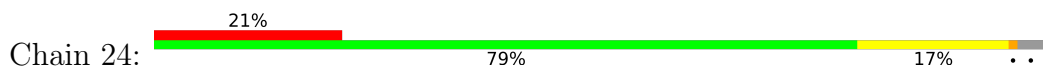




- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



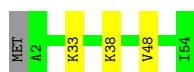
- Molecule 27: 50S ribosomal protein L32



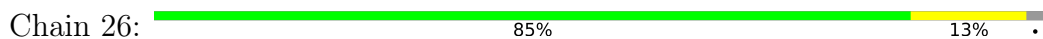
- Molecule 27: 50S ribosomal protein L32



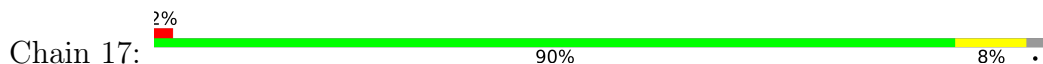
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

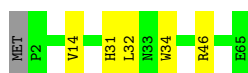




- Molecule 29: 50S ribosomal protein L34



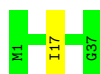
- Molecule 30: 50S ribosomal protein L35



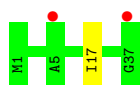
- Molecule 30: 50S ribosomal protein L35



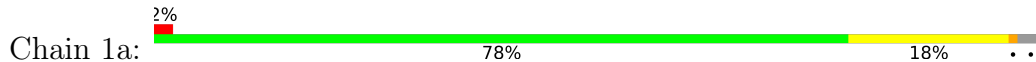
- Molecule 31: 50S ribosomal protein L36

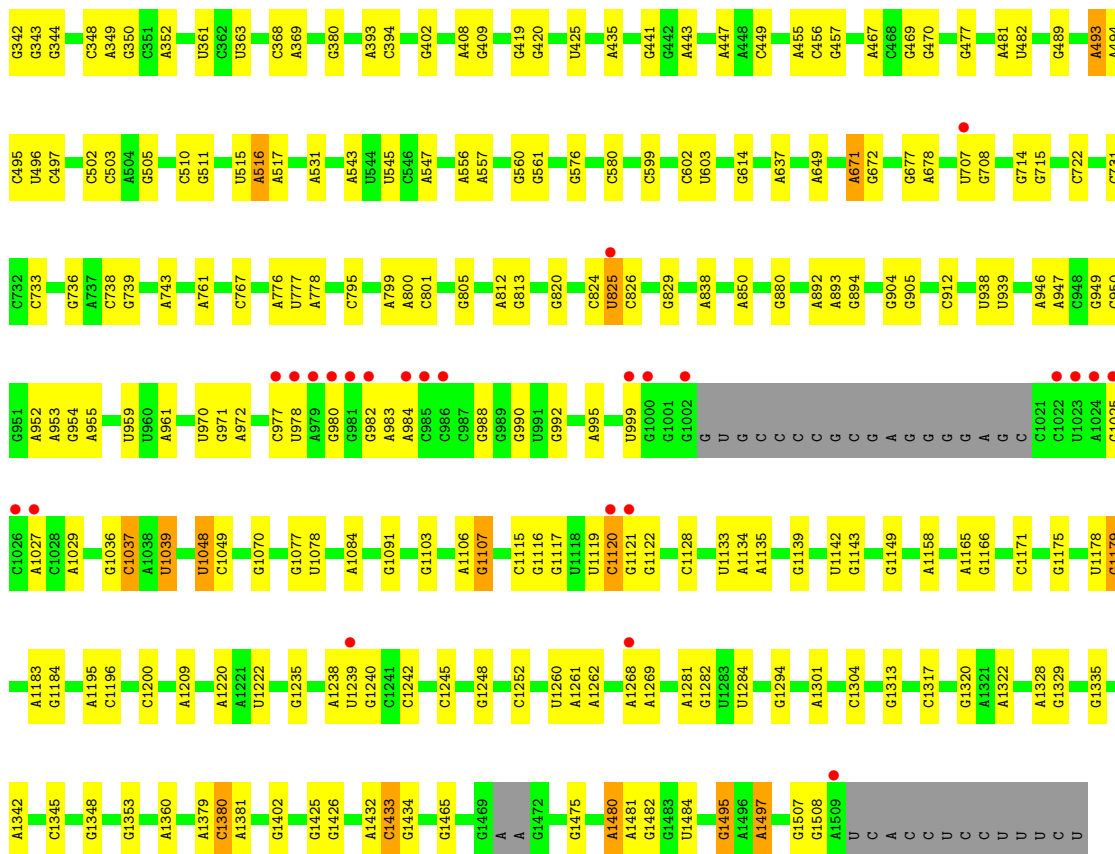


- Molecule 31: 50S ribosomal protein L36

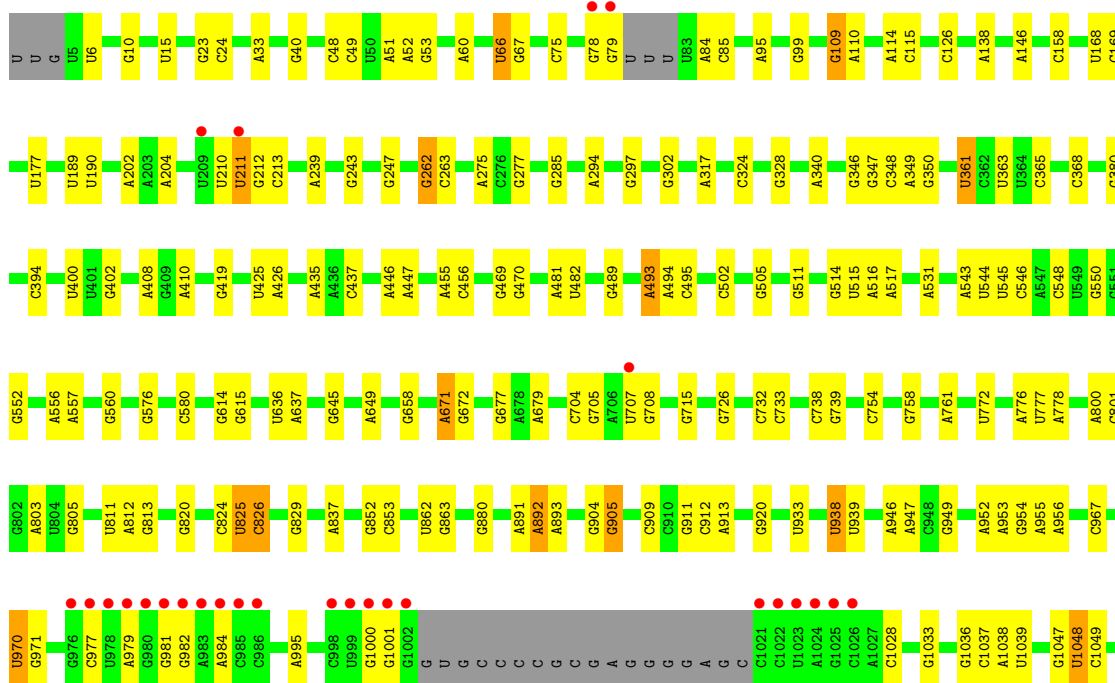
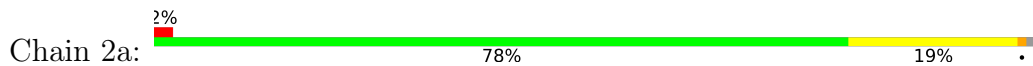


- Molecule 32: 16S Ribosomal RNA

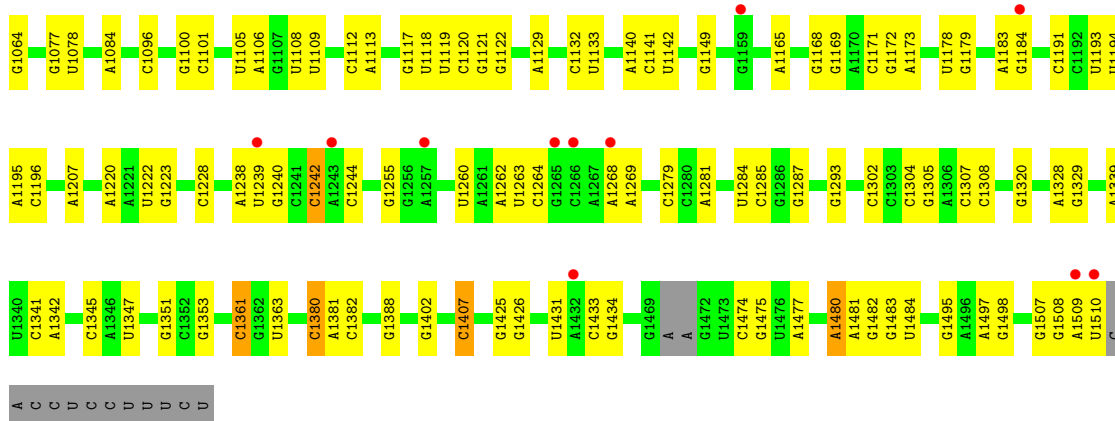




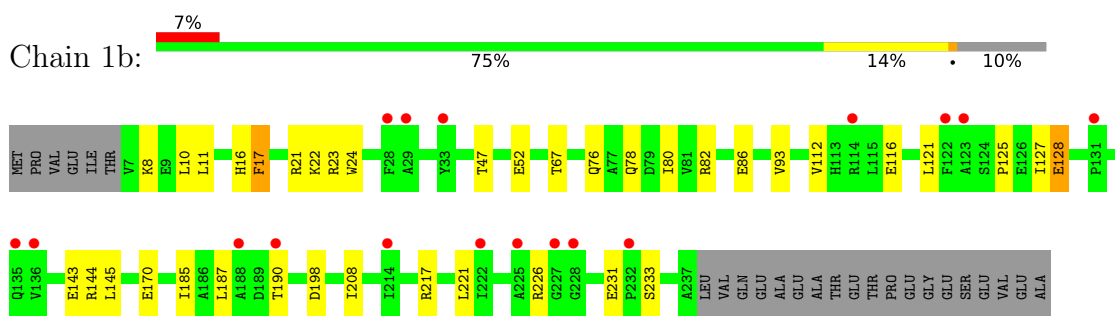
• Molecule 32: 16S Ribosomal RNA



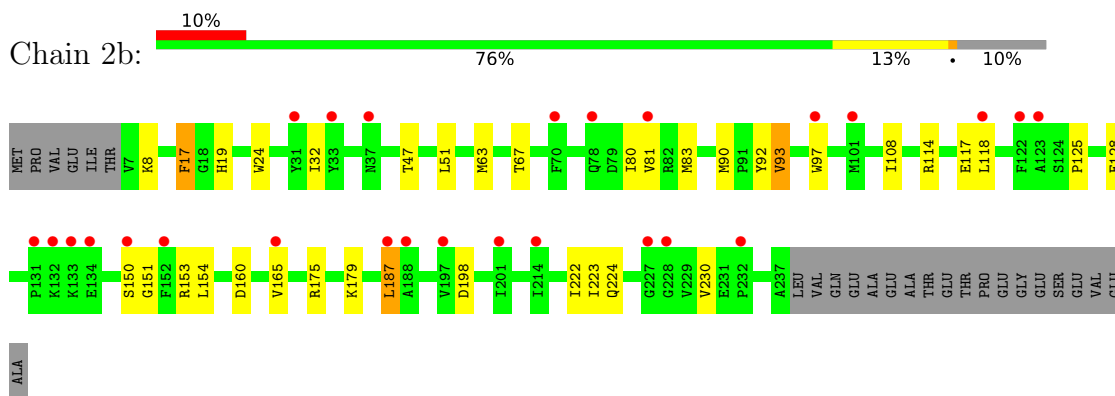




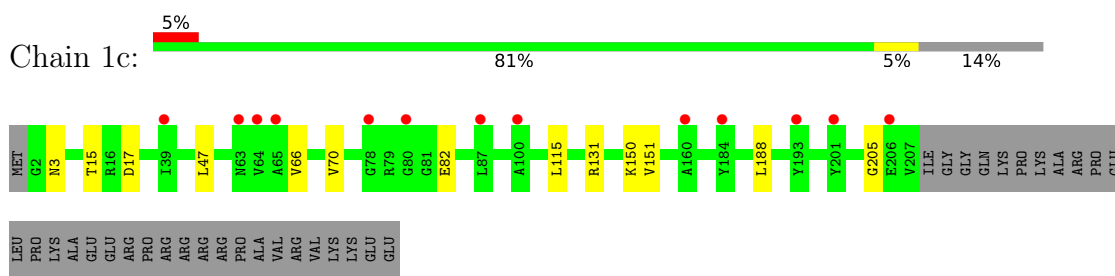
- Molecule 33: 30S ribosomal protein S2



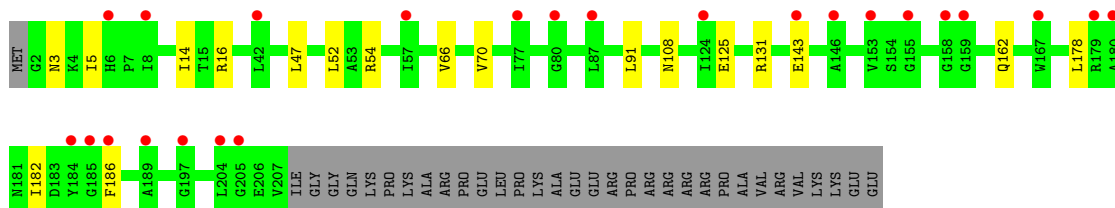
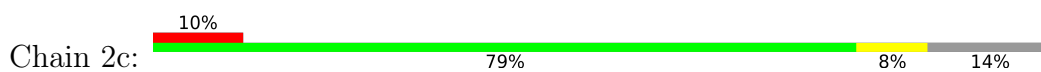
- Molecule 33: 30S ribosomal protein S2



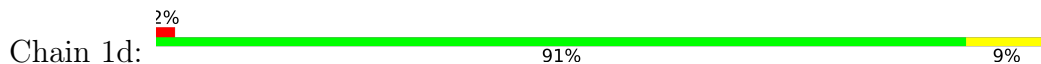
- Molecule 34: 30S ribosomal protein S3



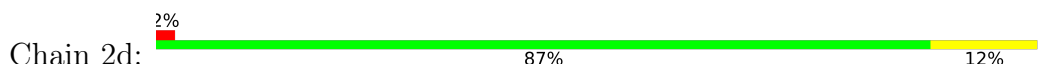
- Molecule 34: 30S ribosomal protein S3



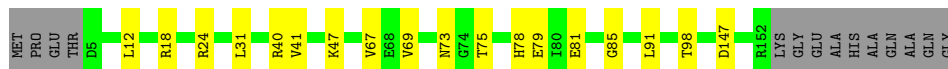
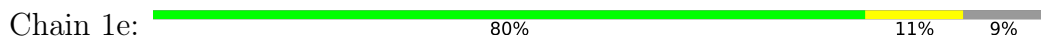
- Molecule 35: 30S ribosomal protein S4



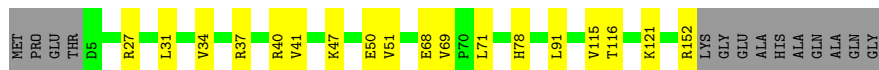
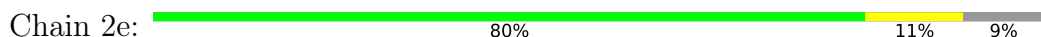
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



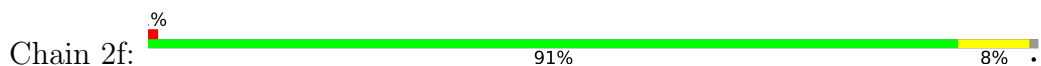
- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6

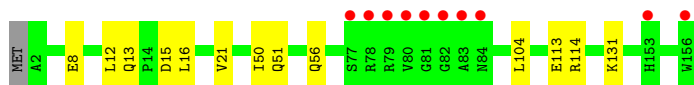
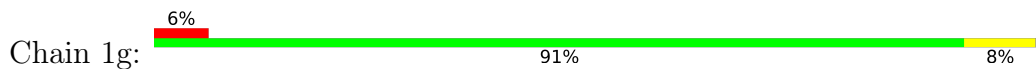


- Molecule 37: 30S ribosomal protein S6

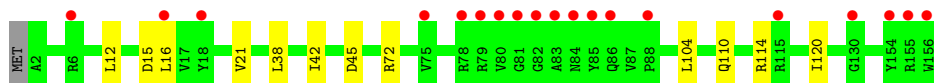
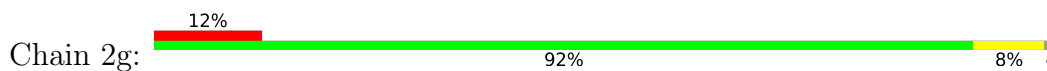




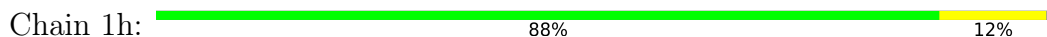
- Molecule 38: 30S ribosomal protein S7



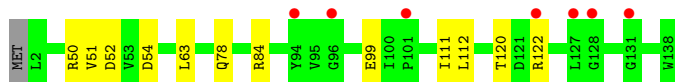
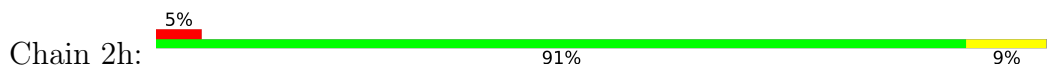
- Molecule 38: 30S ribosomal protein S7



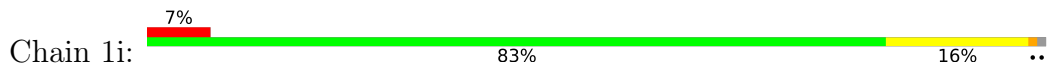
- Molecule 39: 30S ribosomal protein S8



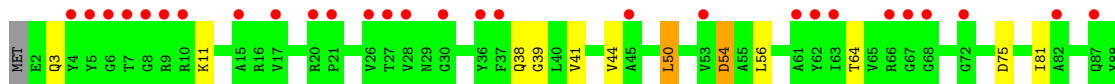
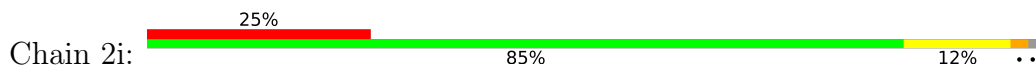
- Molecule 39: 30S ribosomal protein S8

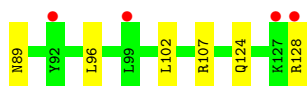


- Molecule 40: 30S ribosomal protein S9

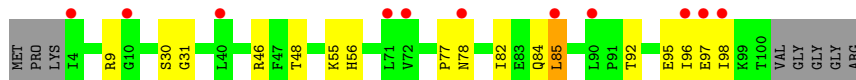
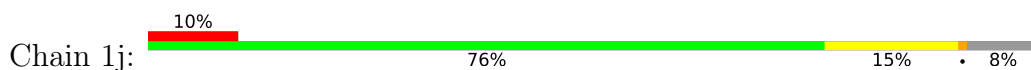


- Molecule 40: 30S ribosomal protein S9

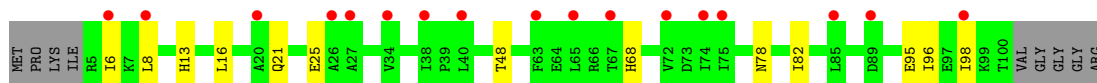
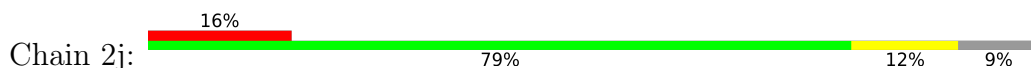




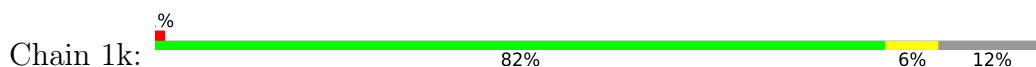
- Molecule 41: 30S ribosomal protein S10



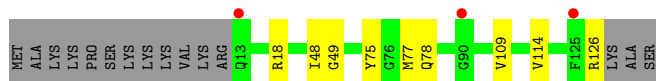
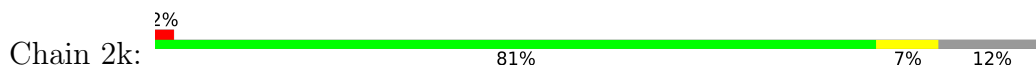
- Molecule 41: 30S ribosomal protein S10



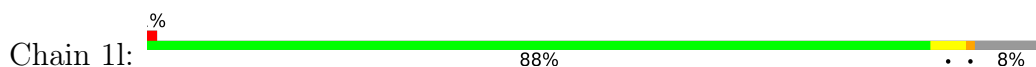
- Molecule 42: 30S ribosomal protein S11



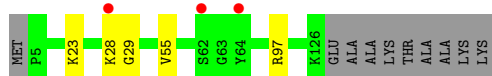
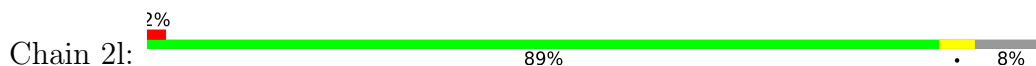
- Molecule 42: 30S ribosomal protein S11




- Molecule 43: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S12




- Molecule 44: 30S ribosomal protein S13

Chain 1m:  84% 9% • 6%




• Molecule 44: 30S ribosomal protein S13

Chain 2m:  6% 85% 6% • 8%




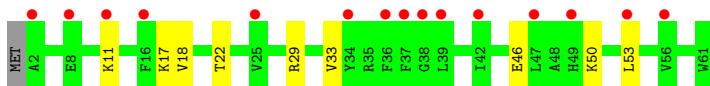
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:  5% 89% 10% •




• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:  25% 84% 15% •




• Molecule 46: 30S ribosomal protein S15

Chain 1o:  2% 90% 9% •




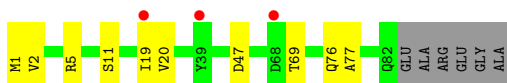
• Molecule 46: 30S ribosomal protein S15

Chain 2o:  87% 12% •

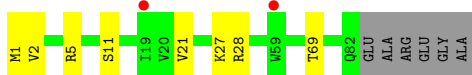
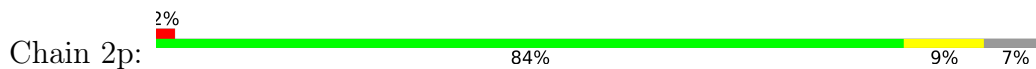


• Molecule 47: 30S ribosomal protein S16

Chain 1p:  3% 82% 11% 7%



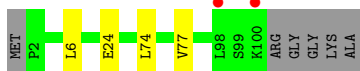
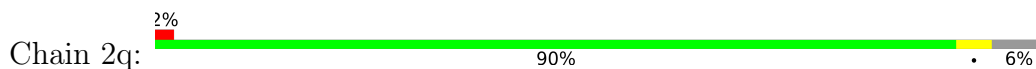
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



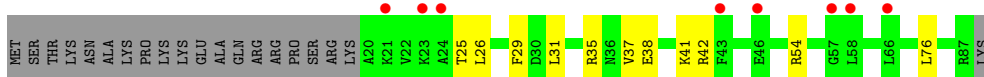
- Molecule 48: 30S ribosomal protein S17



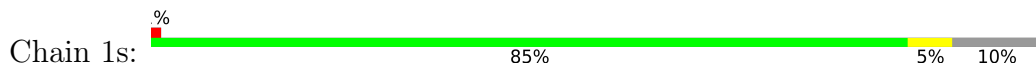
- Molecule 49: 30S ribosomal protein S18



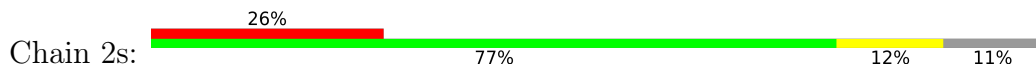
- Molecule 49: 30S ribosomal protein S18

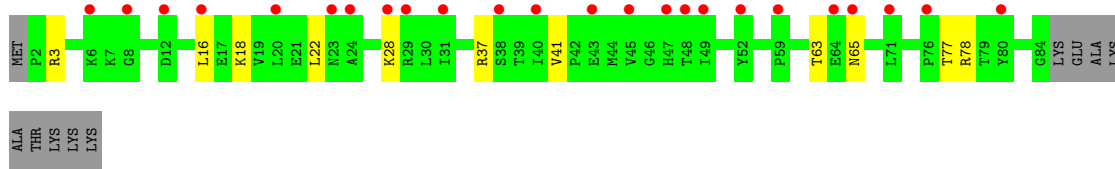


- Molecule 50: 30S ribosomal protein S19

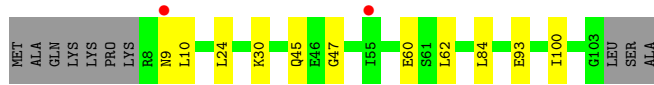
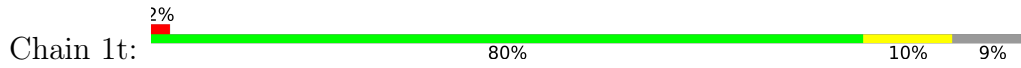


- Molecule 50: 30S ribosomal protein S19

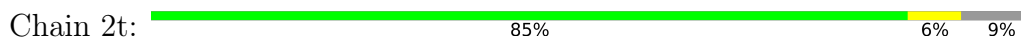




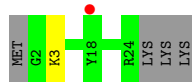
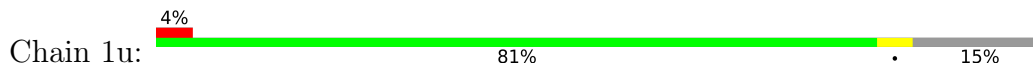
• Molecule 51: 30S ribosomal protein S20



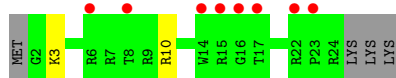
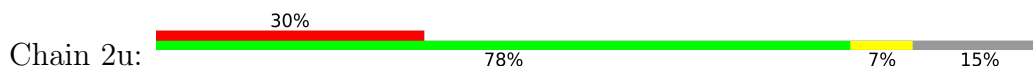
• Molecule 51: 30S ribosomal protein S20



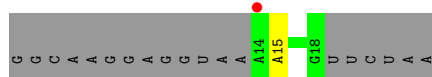
• Molecule 52: 30S ribosomal protein Thx



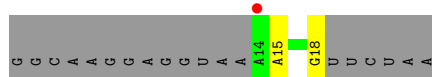
• Molecule 52: 30S ribosomal protein Thx



• Molecule 53: mRNA

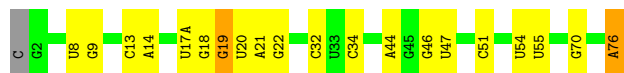


• Molecule 53: mRNA



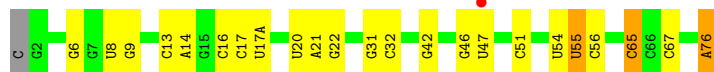
- Molecule 54: P-site tRNA

Chain 1x:  73% 23% ..



- Molecule 54: P-site tRNA

Chain 2x:  % 69% 26% ..



- Molecule 55: Oncocin d15-19

Chain 1z:  57% 21% 7% 14%



- Molecule 55: Oncocin d15-19

Chain 2z:  7% 64% 21% 14%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.05Å 450.75Å 623.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 2.80 49.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.92-2.80) 99.7 (49.92-2.80)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.81Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.200 , 0.251 0.200 , 0.251	Depositor DCC
$R_{free}$ test set	71597 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.7	Xtrriage
Anisotropy	0.179	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 60.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	288518	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, 5MC, MG, ZN, 5MU, SF4, 4SU

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	0.87	14/66249 (0.0%)	1.19	268/103407 (0.3%)
1	2A	0.65	4/67298 (0.0%)	1.16	185/105044 (0.2%)
2	1B	0.64	0/2877	1.02	2/4488 (0.0%)
2	2B	0.81	0/2878	1.22	7/4490 (0.2%)
3	1D	0.55	0/2186	0.65	0/2944
3	2D	0.48	0/2192	0.65	0/2951
4	1E	0.56	0/1592	0.66	0/2149
4	2E	0.47	0/1592	0.66	0/2149
5	1F	0.52	0/1619	0.65	0/2193
5	2F	0.42	0/1615	0.65	0/2188
6	1G	0.40	0/1450	0.62	0/1959
6	2G	0.47	0/1449	0.70	1/1958 (0.1%)
7	1H	0.47	0/1356	0.59	0/1834
7	2H	0.45	0/1356	0.63	0/1834
8	1I	0.41	0/1100	0.63	0/1501
8	2I	0.38	0/1076	0.64	1/1471 (0.1%)
9	1N	0.52	0/1144	0.60	0/1543
9	2N	0.43	0/1144	0.62	0/1543
10	1O	0.54	0/943	0.63	1/1269 (0.1%)
10	2O	0.47	0/943	0.69	1/1269 (0.1%)
11	1P	0.51	0/1156	0.68	0/1537
11	2P	0.45	0/1152	0.67	1/1533 (0.1%)
12	1Q	0.56	0/1143	0.66	0/1527
12	2Q	0.45	0/1143	0.64	0/1527
13	1R	0.54	0/982	0.67	0/1312
13	2R	0.41	0/982	0.66	0/1312
14	1S	0.43	0/887	0.63	0/1180
14	2S	0.51	0/880	0.71	1/1172 (0.1%)
15	1T	0.49	0/1105	0.67	1/1477 (0.1%)
15	2T	0.42	0/1097	0.61	0/1468
16	1U	0.60	0/977	0.66	1/1301 (0.1%)
16	2U	0.49	0/977	0.67	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	1V	0.54	0/782	0.62	0/1049
17	2V	0.48	0/782	0.59	0/1049
18	1W	0.59	0/897	0.67	0/1205
18	2W	0.50	0/897	0.66	0/1205
19	1X	0.53	0/764	0.62	0/1025
19	2X	0.49	0/764	0.63	1/1025 (0.1%)
20	1Y	0.55	0/819	0.67	0/1095
20	2Y	0.46	0/819	0.65	0/1095
21	1Z	0.41	0/1502	0.59	0/2041
21	2Z	0.45	0/1486	0.61	0/2022
22	10	0.53	0/606	0.71	1/808 (0.1%)
22	20	0.38	0/606	0.61	0/808
23	11	0.52	0/762	0.68	2/1014 (0.2%)
23	21	0.46	0/762	0.59	0/1014
24	12	0.47	0/590	0.58	0/781
24	22	0.47	0/590	0.58	0/781
25	13	0.54	0/474	0.63	0/635
25	23	0.42	0/469	0.59	0/630
26	14	0.45	0/571	0.70	0/768
26	24	0.51	0/545	0.76	0/737
27	15	0.57	0/469	0.71	0/635
27	25	0.48	0/469	0.61	0/635
28	16	0.53	0/460	0.61	0/613
28	26	0.48	0/456	0.61	0/608
29	17	0.59	0/426	0.68	0/561
29	27	0.49	0/426	0.68	0/561
30	18	0.56	0/525	0.67	0/691
30	28	0.47	0/525	0.62	0/691
31	19	0.60	0/310	0.65	0/407
31	29	0.46	0/310	0.66	0/407
32	1a	0.56	1/35537 (0.0%)	1.05	68/55456 (0.1%)
32	2a	0.52	0/35680	1.02	51/55681 (0.1%)
33	1b	0.40	0/1820	0.63	0/2468
33	2b	2.74	8/1728 (0.5%)	0.77	4/2352 (0.2%)
34	1c	0.38	0/1504	0.56	0/2047
34	2c	0.42	0/1435	0.62	0/1960
35	1d	0.40	0/1648	0.60	0/2222
35	2d	0.38	0/1659	0.59	0/2230
36	1e	0.39	0/1145	0.62	0/1543
36	2e	0.38	0/1111	0.65	0/1504
37	1f	0.38	0/819	0.60	0/1111
37	2f	0.39	0/830	0.55	0/1125
38	1g	0.36	0/1198	0.56	0/1613

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	2g	0.40	0/1185	0.55	0/1602
39	1h	0.35	0/1108	0.59	0/1494
39	2h	0.35	0/1094	0.57	0/1478
40	1i	0.37	0/995	0.64	0/1339
40	2i	0.43	0/949	0.64	1/1284 (0.1%)
41	1j	0.40	0/695	0.67	1/950 (0.1%)
41	2j	0.42	0/690	0.64	0/943
42	1k	0.38	0/840	0.60	0/1138
42	2k	0.38	0/844	0.57	0/1145
43	1l	0.43	0/936	0.67	1/1263 (0.1%)
43	2l	0.41	0/934	0.66	1/1262 (0.1%)
44	1m	0.37	0/933	0.63	0/1254
44	2m	0.42	0/913	0.58	0/1230
45	1n	0.43	0/491	0.66	0/653
45	2n	0.43	0/467	0.55	0/624
46	1o	0.38	0/726	0.59	0/970
46	2o	0.38	0/739	0.57	0/985
47	1p	0.36	0/686	0.61	0/926
47	2p	0.38	0/693	0.61	0/935
48	1q	0.39	0/824	0.60	1/1105 (0.1%)
48	2q	0.38	0/836	0.55	0/1117
49	1r	0.39	0/560	0.63	1/746 (0.1%)
49	2r	0.38	0/560	0.59	0/746
50	1s	0.36	0/657	0.62	0/890
50	2s	0.40	0/661	0.63	1/893 (0.1%)
51	1t	0.38	0/714	0.66	0/948
51	2t	0.35	0/733	0.58	0/969
52	1u	0.32	0/191	0.57	0/252
52	2u	0.44	0/203	0.58	0/266
53	1v	0.70	0/122	1.30	0/188
53	2v	0.87	0/122	1.35	1/188 (0.5%)
54	1x	0.76	5/1725 (0.3%)	1.40	28/2689 (1.0%)
54	2x	0.65	1/1725 (0.1%)	1.34	24/2689 (0.9%)
55	1z	0.79	0/106	1.00	1/146 (0.7%)
55	2z	0.55	0/106	0.96	0/146
All	All	0.67	33/306280 (0.0%)	1.02	659/458192 (0.1%)

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
19	1X	0	1
19	2X	0	1
20	1Y	0	1
34	2c	0	1
All	All	0	5

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2b	92	TYR	CD1-CE1	60.02	2.29	1.39
33	2b	92	TYR	CD2-CE2	52.66	2.18	1.39
33	2b	92	TYR	CE1-CZ	41.90	1.93	1.38
33	2b	92	TYR	CE2-CZ	41.41	1.92	1.38
33	2b	92	TYR	CG-CD1	33.83	1.83	1.39

The worst 5 of 659 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2b	150	SER	C-N-CA	16.37	156.68	122.30
1	1A	552	A	C2-N3-C4	-16.26	102.47	110.60
1	1A	1066	A	C2-N3-C4	-14.19	103.50	110.60
54	1x	46	G	C6-N1-C2	-14.02	116.69	125.10
1	1A	353	A	C2-N3-C4	-13.24	103.98	110.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	1X	93	GLU	Peptide
20	1Y	54	LYS	Peptide
5	2F	20	LEU	Peptide
19	2X	93	GLU	Peptide
34	2c	186	PHE	Peptide

## 5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	250 (92%)	21 (8%)	2 (1%)	22	53
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	61
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	61
5	1F	201/210 (96%)	190 (94%)	10 (5%)	1 (0%)	29	61
5	2F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	29	61
6	1G	179/182 (98%)	161 (90%)	14 (8%)	4 (2%)	6	22
6	2G	179/182 (98%)	152 (85%)	22 (12%)	5 (3%)	5	17
7	1H	172/180 (96%)	158 (92%)	13 (8%)	1 (1%)	25	56
7	2H	172/180 (96%)	157 (91%)	13 (8%)	2 (1%)	13	39
8	1I	144/148 (97%)	119 (83%)	24 (17%)	1 (1%)	22	53
8	2I	144/148 (97%)	117 (81%)	26 (18%)	1 (1%)	22	53
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	22	53
10	1O	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	19	49
10	2O	120/122 (98%)	116 (97%)	3 (2%)	1 (1%)	19	49
11	1P	147/150 (98%)	139 (95%)	7 (5%)	1 (1%)	22	53
11	2P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	11	34
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	127 (91%)	10 (7%)	2 (1%)	11	34
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
14	2S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	17	46
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	19	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	1U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	44
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	44
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	41
20	1Y	105/110 (96%)	91 (87%)	12 (11%)	2 (2%)	8	26
20	2Y	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	15	44
21	1Z	184/206 (89%)	170 (92%)	13 (7%)	1 (0%)	29	61
21	2Z	184/206 (89%)	166 (90%)	14 (8%)	4 (2%)	6	22
22	10	73/85 (86%)	69 (94%)	3 (4%)	1 (1%)	11	34
22	20	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
23	21	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	49 (73%)	9 (13%)	9 (13%)	0	0
26	24	67/71 (94%)	49 (73%)	12 (18%)	6 (9%)	1	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
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%)	45 (98%)	0	1 (2%)	6	22
30	18	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	178 (78%)	42 (18%)	9 (4%)	3	10
33	2b	229/256 (90%)	183 (80%)	41 (18%)	5 (2%)	6	22
34	1c	204/239 (85%)	169 (83%)	33 (16%)	2 (1%)	15	44
34	2c	204/239 (85%)	167 (82%)	34 (17%)	3 (2%)	10	33
35	1d	206/209 (99%)	179 (87%)	25 (12%)	2 (1%)	15	44
35	2d	206/209 (99%)	182 (88%)	18 (9%)	6 (3%)	4	15
36	1e	146/162 (90%)	130 (89%)	13 (9%)	3 (2%)	7	23
36	2e	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	11	34
37	1f	98/101 (97%)	91 (93%)	6 (6%)	1 (1%)	15	44
37	2f	98/101 (97%)	92 (94%)	5 (5%)	1 (1%)	15	44
38	1g	153/156 (98%)	136 (89%)	17 (11%)	0	100	100
38	2g	153/156 (98%)	134 (88%)	19 (12%)	0	100	100
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
40	1i	125/128 (98%)	105 (84%)	15 (12%)	5 (4%)	3	9
40	2i	125/128 (98%)	104 (83%)	14 (11%)	7 (6%)	2	5
41	1j	95/105 (90%)	77 (81%)	12 (13%)	6 (6%)	1	3
41	2j	94/105 (90%)	81 (86%)	11 (12%)	2 (2%)	7	23
42	1k	112/129 (87%)	97 (87%)	13 (12%)	2 (2%)	8	28
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	17	46
43	1l	120/132 (91%)	112 (93%)	8 (7%)	0	100	100
43	2l	120/132 (91%)	111 (92%)	9 (8%)	0	100	100
44	1m	116/126 (92%)	100 (86%)	13 (11%)	3 (3%)	5	18
44	2m	114/126 (90%)	96 (84%)	15 (13%)	3 (3%)	5	18
45	1n	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	9	29
45	2n	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
46	1o	86/89 (97%)	75 (87%)	10 (12%)	1 (1%)	13	39
46	2o	86/89 (97%)	77 (90%)	7 (8%)	2 (2%)	6	21
47	1p	80/88 (91%)	67 (84%)	11 (14%)	2 (2%)	5	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	68 (85%)	12 (15%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	15	44
48	2q	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
49	1r	66/88 (75%)	58 (88%)	6 (9%)	2 (3%)	4	15
49	2r	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	10	33
50	1s	82/93 (88%)	70 (85%)	12 (15%)	0	100	100
50	2s	81/93 (87%)	67 (83%)	14 (17%)	0	100	100
51	1t	94/106 (89%)	81 (86%)	11 (12%)	2 (2%)	7	23
51	2t	94/106 (89%)	81 (86%)	10 (11%)	3 (3%)	4	13
52	1u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	7
52	2u	21/27 (78%)	17 (81%)	3 (14%)	1 (5%)	2	7
55	1z	10/14 (71%)	6 (60%)	1 (10%)	3 (30%)	0	0
55	2z	10/14 (71%)	8 (80%)	1 (10%)	1 (10%)	0	1
All	All	11430/12156 (94%)	10379 (91%)	909 (8%)	142 (1%)	13	39

5 of 142 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
6	1G	50	ALA
6	1G	51	ARG
6	1G	126	ASP
7	1H	126	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	186 (86%)	29 (14%)	4	11
3	2D	216/218 (99%)	192 (89%)	24 (11%)	6	19
4	1E	164/166 (99%)	145 (88%)	19 (12%)	5	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	143 (87%)	21 (13%)	4	13
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6	20
5	2F	159/166 (96%)	143 (90%)	16 (10%)	7	22
6	1G	143/156 (92%)	126 (88%)	17 (12%)	5	16
6	2G	142/156 (91%)	121 (85%)	21 (15%)	3	9
7	1H	144/148 (97%)	135 (94%)	9 (6%)	18	46
7	2H	144/148 (97%)	128 (89%)	16 (11%)	6	19
8	1I	110/124 (89%)	89 (81%)	21 (19%)	1	4
8	2I	104/124 (84%)	94 (90%)	10 (10%)	8	24
9	1N	118/119 (99%)	104 (88%)	14 (12%)	5	16
9	2N	118/119 (99%)	106 (90%)	12 (10%)	7	22
10	1O	100/100 (100%)	95 (95%)	5 (5%)	24	56
10	2O	100/100 (100%)	92 (92%)	8 (8%)	12	34
11	1P	116/116 (100%)	103 (89%)	13 (11%)	6	18
11	2P	115/116 (99%)	101 (88%)	14 (12%)	5	15
12	1Q	111/111 (100%)	99 (89%)	12 (11%)	6	19
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11	33
13	1R	101/101 (100%)	82 (81%)	19 (19%)	1	5
13	2R	101/101 (100%)	83 (82%)	18 (18%)	2	5
14	1S	87/88 (99%)	80 (92%)	7 (8%)	12	34
14	2S	85/88 (97%)	71 (84%)	14 (16%)	2	7
15	1T	115/127 (91%)	102 (89%)	13 (11%)	6	18
15	2T	113/127 (89%)	100 (88%)	13 (12%)	5	17
16	1U	93/94 (99%)	84 (90%)	9 (10%)	8	24
16	2U	93/94 (99%)	83 (89%)	10 (11%)	6	19
17	1V	80/82 (98%)	68 (85%)	12 (15%)	3	9
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	22
18	1W	90/92 (98%)	83 (92%)	7 (8%)	12	35
18	2W	90/92 (98%)	81 (90%)	9 (10%)	7	22
19	1X	77/78 (99%)	74 (96%)	3 (4%)	32	66
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	19	49
20	2Y	85/91 (93%)	78 (92%)	7 (8%)	11	33
21	1Z	159/179 (89%)	144 (91%)	15 (9%)	8	26
21	2Z	156/179 (87%)	142 (91%)	14 (9%)	9	28
22	10	60/67 (90%)	55 (92%)	5 (8%)	11	32
22	20	60/67 (90%)	56 (93%)	4 (7%)	16	43
23	11	80/83 (96%)	73 (91%)	7 (9%)	10	29
23	21	80/83 (96%)	72 (90%)	8 (10%)	7	22
24	12	65/67 (97%)	59 (91%)	6 (9%)	9	27
24	22	65/67 (97%)	58 (89%)	7 (11%)	6	19
25	13	51/52 (98%)	46 (90%)	5 (10%)	8	24
25	23	50/52 (96%)	46 (92%)	4 (8%)	12	34
26	14	60/63 (95%)	51 (85%)	9 (15%)	3	9
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	9
27	15	50/52 (96%)	47 (94%)	3 (6%)	19	48
27	25	50/52 (96%)	46 (92%)	4 (8%)	12	34
28	16	51/52 (98%)	48 (94%)	3 (6%)	19	49
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	11
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	24
29	27	41/42 (98%)	39 (95%)	2 (5%)	25	57
30	18	54/55 (98%)	49 (91%)	5 (9%)	9	26
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	37
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	76
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	76
33	1b	177/220 (80%)	146 (82%)	31 (18%)	2	6
33	2b	158/220 (72%)	129 (82%)	29 (18%)	1	5
34	1c	127/188 (68%)	116 (91%)	11 (9%)	10	30
34	2c	108/188 (57%)	94 (87%)	14 (13%)	4	13
35	1d	161/181 (89%)	145 (90%)	16 (10%)	8	23
35	2d	164/181 (91%)	142 (87%)	22 (13%)	4	12
36	1e	113/123 (92%)	98 (87%)	15 (13%)	4	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	106/123 (86%)	90 (85%)	16 (15%)	3	9
37	1f	83/90 (92%)	78 (94%)	5 (6%)	19	48
37	2f	86/90 (96%)	79 (92%)	7 (8%)	11	33
38	1g	111/127 (87%)	98 (88%)	13 (12%)	5	16
38	2g	107/127 (84%)	95 (89%)	12 (11%)	6	18
39	1h	114/119 (96%)	98 (86%)	16 (14%)	3	11
39	2h	111/119 (93%)	99 (89%)	12 (11%)	6	19
40	1i	89/99 (90%)	72 (81%)	17 (19%)	1	4
40	2i	80/99 (81%)	68 (85%)	12 (15%)	3	9
41	1j	60/92 (65%)	49 (82%)	11 (18%)	1	5
41	2j	62/92 (67%)	51 (82%)	11 (18%)	2	5
42	1k	82/99 (83%)	76 (93%)	6 (7%)	14	38
42	2k	82/99 (83%)	74 (90%)	8 (10%)	8	24
43	1l	95/109 (87%)	89 (94%)	6 (6%)	18	46
43	2l	94/109 (86%)	90 (96%)	4 (4%)	29	62
44	1m	90/101 (89%)	80 (89%)	10 (11%)	6	19
44	2m	87/101 (86%)	80 (92%)	7 (8%)	12	34
45	1n	47/50 (94%)	42 (89%)	5 (11%)	6	20
45	2n	43/50 (86%)	34 (79%)	9 (21%)	1	3
46	1o	75/80 (94%)	68 (91%)	7 (9%)	9	26
46	2o	78/80 (98%)	69 (88%)	9 (12%)	5	17
47	1p	67/74 (90%)	59 (88%)	8 (12%)	5	16
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	16
48	1q	91/97 (94%)	88 (97%)	3 (3%)	38	72
48	2q	94/97 (97%)	90 (96%)	4 (4%)	29	62
49	1r	59/77 (77%)	50 (85%)	9 (15%)	2	8
49	2r	59/77 (77%)	49 (83%)	10 (17%)	2	6
50	1s	65/80 (81%)	60 (92%)	5 (8%)	13	35
50	2s	67/80 (84%)	57 (85%)	10 (15%)	3	9
51	1t	66/82 (80%)	57 (86%)	9 (14%)	3	11
51	2t	71/82 (87%)	68 (96%)	3 (4%)	30	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1u	16/22 (73%)	16 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	51
55	1z	12/14 (86%)	11 (92%)	1 (8%)	11	32
55	2z	12/14 (86%)	10 (83%)	2 (17%)	2	6
All	All	9159/10094 (91%)	8156 (89%)	1003 (11%)	6	19

5 of 1003 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	1p	1	MET
38	2g	42	ILE
6	2G	143	GLU
37	2f	46	ARG
44	2m	110	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 133 such sidechains are listed below:

Mol	Chain	Res	Type
38	2g	110	GLN
40	2i	89	ASN
50	2s	69	HIS
40	1i	38	GLN
40	1i	23	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2737/2915 (93%)	392 (14%)	28 (1%)
1	2A	2781/2915 (95%)	470 (16%)	26 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	119/121 (98%)	34 (28%)	2 (1%)
32	1a	1472/1521 (96%)	270 (18%)	0
32	2a	1479/1521 (97%)	281 (18%)	0
53	1v	4/24 (16%)	1 (25%)	0
53	2v	4/24 (16%)	1 (25%)	0
54	1x	75/77 (97%)	12 (16%)	0
54	2x	75/77 (97%)	15 (20%)	0
All	All	8865/9316 (95%)	1485 (16%)	56 (0%)

5 of 1485 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	32	U
1	1A	33	C
1	1A	35	G
1	1A	44	C

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	184	A
2	2B	45	A
1	2A	669	C
2	2B	42	C
1	2A	2013	G

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

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	5MC	2x	32	54	18,22,23	1.07	1 (5%)	26,32,35	1.41	3 (11%)
54	PSU	2x	55	54	18,21,22	1.42	1 (5%)	22,30,33	1.85	3 (13%)
54	5MC	1x	32	54	18,22,23	0.98	2 (11%)	26,32,35	1.29	2 (7%)
54	5MU	1x	54	54	19,22,23	1.46	4 (21%)	28,32,35	1.94	6 (21%)
54	PSU	1x	55	54	18,21,22	1.26	2 (11%)	22,30,33	1.83	4 (18%)
54	4SU	1x	8	54	18,21,22	2.07	5 (27%)	26,30,33	1.59	5 (19%)
54	5MU	2x	54	54	19,22,23	1.41	4 (21%)	28,32,35	1.87	6 (21%)
54	4SU	2x	8	54	18,21,22	1.80	5 (27%)	26,30,33	1.05	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	5MC	2x	32	54	-	2/7/25/26	0/2/2/2
54	PSU	2x	55	54	-	2/7/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/7/25/26	0/2/2/2
54	5MU	1x	54	54	-	0/7/25/26	0/2/2/2
54	PSU	1x	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1x	8	54	-	0/7/25/26	0/2/2/2
54	5MU	2x	54	54	-	0/7/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/7/25/26	0/2/2/2

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	8	4SU	C4-N3	-5.24	1.32	1.37
54	2x	8	4SU	C4-N3	-4.25	1.33	1.37
54	2x	55	PSU	C6-C5	4.23	1.40	1.35
54	1x	8	4SU	C4-S4	-3.98	1.60	1.68
54	1x	8	4SU	C2-N3	-3.89	1.31	1.38

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2x	55	PSU	N1-C2-N3	5.75	121.64	115.13
54	1x	55	PSU	N1-C2-N3	5.25	121.08	115.13
54	1x	54	5MU	C5-C4-N3	4.79	119.40	115.31
54	1x	8	4SU	C6-C5-C4	-4.74	115.84	119.95
54	2x	54	5MU	N3-C2-N1	4.66	121.07	114.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	2x	55	PSU	C3'-C4'-C5'-O5'
54	2x	55	PSU	O4'-C4'-C5'-O5'
54	2x	32	5MC	C2'-C1'-N1-C6
54	2x	32	5MC	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2444 ligands modelled in this entry, 2442 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	301	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	301	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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1A	2746/2915 (94%)	-0.04	25 (0%) 84 80	23, 42, 86, 108	0
1	2A	2790/2915 (95%)	-0.34	58 (2%) 63 54	27, 47, 93, 110	0
2	1B	120/121 (99%)	-0.20	0 100 100	36, 64, 82, 95	0
2	2B	120/121 (99%)	0.06	2 (1%) 70 63	43, 70, 85, 96	0
3	1D	275/276 (99%)	-0.38	0 100 100	21, 41, 57, 80	0
3	2D	275/276 (99%)	-0.50	1 (0%) 92 91	24, 43, 60, 80	0
4	1E	204/206 (99%)	-0.28	0 100 100	20, 44, 67, 83	0
4	2E	204/206 (99%)	-0.31	1 (0%) 91 88	24, 48, 69, 84	0
5	1F	203/210 (96%)	-0.20	1 (0%) 91 88	23, 51, 77, 93	0
5	2F	203/210 (96%)	-0.35	2 (0%) 82 77	27, 55, 79, 94	0
6	1G	181/182 (99%)	-0.24	4 (2%) 62 52	52, 70, 83, 96	0
6	2G	181/182 (99%)	0.51	16 (8%) 10 5	58, 74, 85, 96	0
7	1H	174/180 (96%)	-0.12	1 (0%) 89 86	49, 65, 77, 89	0
7	2H	174/180 (96%)	0.97	31 (17%) 1 1	55, 70, 81, 91	0
8	1I	146/148 (98%)	0.01	1 (0%) 87 84	48, 75, 85, 89	0
8	2I	146/148 (98%)	0.42	9 (6%) 20 13	51, 76, 86, 91	0
9	1N	140/140 (100%)	-0.23	0 100 100	33, 47, 69, 82	0
9	2N	140/140 (100%)	-0.15	0 100 100	36, 52, 71, 84	0
10	1O	122/122 (100%)	-0.32	0 100 100	32, 44, 63, 71	0
10	2O	122/122 (100%)	-0.45	0 100 100	35, 47, 64, 72	0
11	1P	149/150 (99%)	-0.20	0 100 100	24, 54, 76, 85	0
11	2P	149/150 (99%)	0.15	7 (4%) 31 22	27, 58, 78, 88	0
12	1Q	141/141 (100%)	-0.13	1 (0%) 87 84	33, 50, 66, 88	0
12	2Q	141/141 (100%)	-0.43	1 (0%) 87 84	37, 54, 69, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	-0.18	0 100 100	31, 40, 55, 66	0
13	2R	118/118 (100%)	-0.38	0 100 100	34, 44, 56, 69	0
14	1S	110/112 (98%)	-0.21	0 100 100	46, 63, 73, 77	0
14	2S	110/112 (98%)	0.60	8 (7%) 15 8	52, 67, 77, 80	0
15	1T	131/146 (89%)	-0.26	1 (0%) 86 81	37, 50, 75, 86	0
15	2T	131/146 (89%)	-0.41	0 100 100	39, 53, 76, 85	0
16	1U	116/118 (98%)	-0.16	0 100 100	28, 40, 56, 75	0
16	2U	116/118 (98%)	-0.37	2 (1%) 70 63	32, 45, 62, 76	0
17	1V	101/101 (100%)	-0.27	0 100 100	29, 49, 68, 80	0
17	2V	101/101 (100%)	0.01	0 100 100	32, 56, 73, 80	0
18	1W	112/113 (99%)	-0.29	2 (1%) 68 61	27, 37, 57, 91	0
18	2W	112/113 (99%)	-0.42	0 100 100	31, 40, 61, 91	0
19	1X	95/96 (98%)	-0.19	0 100 100	28, 47, 69, 80	0
19	2X	95/96 (98%)	-0.13	3 (3%) 47 37	33, 51, 70, 81	0
20	1Y	107/110 (97%)	-0.00	1 (0%) 84 80	45, 59, 78, 87	0
20	2Y	107/110 (97%)	0.59	11 (10%) 6 3	51, 63, 81, 90	0
21	1Z	186/206 (90%)	-0.39	0 100 100	52, 68, 83, 93	0
21	2Z	186/206 (90%)	0.39	6 (3%) 47 37	55, 72, 85, 94	0
22	10	75/85 (88%)	-0.54	0 100 100	16, 36, 52, 67	0
22	20	75/85 (88%)	0.23	6 (8%) 12 6	40, 64, 77, 80	0
23	11	97/98 (98%)	-0.17	1 (1%) 82 77	30, 48, 75, 79	0
23	21	97/98 (98%)	-0.14	2 (2%) 63 54	34, 51, 76, 81	0
24	12	70/72 (97%)	-0.11	0 100 100	42, 59, 73, 82	0
24	22	70/72 (97%)	0.17	3 (4%) 35 25	47, 63, 76, 80	0
25	13	59/60 (98%)	-0.14	0 100 100	32, 46, 67, 78	0
25	23	59/60 (98%)	0.40	3 (5%) 28 19	37, 51, 71, 82	0
26	14	69/71 (97%)	0.13	5 (7%) 15 8	63, 82, 95, 99	0
26	24	69/71 (97%)	0.86	15 (21%) 0 0	69, 85, 96, 100	0
27	15	59/60 (98%)	-0.38	0 100 100	22, 38, 57, 73	0
27	25	59/60 (98%)	-0.44	0 100 100	27, 42, 61, 74	0
28	16	53/54 (98%)	-0.37	0 100 100	37, 48, 66, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	-0.39	0 100 100	40, 52, 63, 69	0
29	17	48/49 (97%)	-0.18	1 (2%) 63 54	26, 31, 65, 78	0
29	27	48/49 (97%)	-0.12	3 (6%) 20 12	29, 34, 65, 80	0
30	18	64/65 (98%)	-0.12	0 100 100	34, 41, 53, 61	0
30	28	64/65 (98%)	-0.11	0 100 100	37, 45, 57, 64	0
31	19	37/37 (100%)	0.09	0 100 100	40, 49, 69, 74	0
31	29	37/37 (100%)	0.21	2 (5%) 25 17	44, 54, 70, 76	0
32	1a	1477/1521 (97%)	-0.09	37 (2%) 57 47	35, 71, 97, 112	0
32	2a	1483/1521 (97%)	-0.04	38 (2%) 56 46	45, 79, 100, 110	0
33	1b	231/256 (90%)	0.42	17 (7%) 14 8	66, 83, 94, 100	0
33	2b	231/256 (90%)	0.69	26 (11%) 5 3	72, 89, 96, 104	0
34	1c	206/239 (86%)	0.21	13 (6%) 20 12	68, 83, 91, 96	0
34	2c	206/239 (86%)	0.60	24 (11%) 4 2	70, 85, 92, 95	0
35	1d	208/209 (99%)	0.09	4 (1%) 66 59	54, 76, 88, 96	0
35	2d	208/209 (99%)	-0.04	4 (1%) 66 59	62, 75, 86, 92	0
36	1e	148/162 (91%)	-0.29	0 100 100	46, 66, 78, 89	0
36	2e	148/162 (91%)	-0.20	0 100 100	60, 75, 84, 92	0
37	1f	100/101 (99%)	-0.25	0 100 100	58, 74, 83, 90	0
37	2f	100/101 (99%)	-0.31	1 (1%) 82 77	60, 74, 84, 88	0
38	1g	155/156 (99%)	0.26	10 (6%) 18 11	61, 79, 93, 97	0
38	2g	155/156 (99%)	0.78	19 (12%) 4 2	69, 80, 92, 97	0
39	1h	137/138 (99%)	-0.20	0 100 100	54, 69, 79, 86	0
39	2h	137/138 (99%)	0.20	7 (5%) 28 19	65, 77, 86, 91	0
40	1i	127/128 (99%)	0.47	9 (7%) 16 9	64, 86, 93, 96	0
40	2i	127/128 (99%)	1.31	32 (25%) 0 0	64, 88, 95, 96	0
41	1j	97/105 (92%)	0.68	11 (11%) 5 3	63, 86, 95, 98	0
41	2j	96/105 (91%)	1.15	17 (17%) 1 1	76, 91, 99, 101	0
42	1k	114/129 (88%)	-0.21	1 (0%) 84 80	40, 69, 83, 92	0
42	2k	114/129 (88%)	0.11	3 (2%) 56 46	53, 76, 86, 93	0
43	1l	122/132 (92%)	-0.22	1 (0%) 86 81	46, 62, 73, 79	0
43	2l	122/132 (92%)	-0.16	3 (2%) 57 47	56, 69, 78, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	118/126 (93%)	-0.01	0 100 100	65, 80, 87, 92	0
44	2m	116/126 (92%)	0.42	8 (6%) 16 10	70, 83, 89, 93	0
45	1n	60/61 (98%)	0.37	3 (5%) 28 19	63, 75, 88, 89	0
45	2n	60/61 (98%)	1.33	15 (25%) 0 0	76, 87, 92, 96	0
46	1o	88/89 (98%)	-0.01	2 (2%) 60 51	51, 67, 82, 90	0
46	2o	88/89 (98%)	0.02	0 100 100	59, 73, 83, 89	0
47	1p	82/88 (93%)	0.40	3 (3%) 41 31	60, 78, 87, 93	0
47	2p	82/88 (93%)	0.24	2 (2%) 59 49	62, 70, 82, 91	0
48	1q	99/105 (94%)	-0.02	0 100 100	51, 69, 80, 84	0
48	2q	99/105 (94%)	0.10	2 (2%) 65 56	59, 73, 83, 90	0
49	1r	68/88 (77%)	0.33	4 (5%) 22 14	58, 70, 84, 87	0
49	2r	68/88 (77%)	0.56	8 (11%) 4 2	63, 73, 85, 90	0
50	1s	84/93 (90%)	0.42	1 (1%) 79 73	68, 81, 90, 95	0
50	2s	83/93 (89%)	1.67	24 (28%) 0 0	82, 91, 99, 104	0
51	1t	96/106 (90%)	0.21	2 (2%) 63 54	61, 75, 84, 93	0
51	2t	96/106 (90%)	0.11	0 100 100	55, 73, 84, 88	0
52	1u	23/27 (85%)	0.45	1 (4%) 35 25	71, 78, 80, 84	0
52	2u	23/27 (85%)	1.68	8 (34%) 0 0	73, 80, 85, 86	0
53	1v	5/24 (20%)	0.68	1 (20%) 1 0	61, 64, 90, 97	0
53	2v	5/24 (20%)	1.27	1 (20%) 1 0	65, 68, 91, 97	0
54	1x	72/77 (93%)	-0.21	0 100 100	28, 58, 83, 92	0
54	2x	72/77 (93%)	0.11	1 (1%) 75 70	41, 79, 91, 102	0
55	1z	12/14 (85%)	0.29	0 100 100	23, 39, 59, 84	0
55	2z	12/14 (85%)	-0.04	1 (8%) 11 6	26, 42, 64, 85	0
All	All	20520/21472 (95%)	-0.03	600 (2%) 51 41	16, 62, 92, 112	0

The worst 5 of 600 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	1a	980	G	8.3
32	2a	980	G	7.8
32	1a	981	G	7.5
1	2A	2812	G	7.0
32	1a	979	A	6.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
54	PSU	2x	55	20/21	0.85	0.14	67,79,90,98	0
54	4SU	2x	8	20/21	0.92	0.11	68,80,91,95	0
54	5MU	2x	54	21/22	0.93	0.18	66,79,92,102	0
54	5MC	2x	32	21/22	0.93	0.20	72,77,87,99	0
54	PSU	1x	55	20/21	0.95	0.15	49,60,75,77	0
54	5MC	1x	32	21/22	0.96	0.16	50,57,66,75	0
54	4SU	1x	8	20/21	0.96	0.13	51,58,69,71	0
54	5MU	1x	54	21/22	0.96	0.13	48,57,75,82	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
56	MG	1a	1791	1/1	0.06	0.74	89,89,89,89	0
56	MG	1A	3893	1/1	0.35	0.28	69,69,69,69	0
56	MG	2a	3137	1/1	0.37	0.23	97,97,97,97	0
56	MG	2a	3149	1/1	0.37	0.77	100,100,100,100	0
56	MG	1a	1780	1/1	0.38	0.25	93,93,93,93	0
56	MG	2a	3004	1/1	0.39	0.69	87,87,87,87	0
56	MG	1A	3277	1/1	0.41	0.53	68,68,68,68	0
56	MG	2G	3001	1/1	0.42	0.19	60,60,60,60	0
56	MG	2B	3002	1/1	0.44	0.17	70,70,70,70	0
57	ZN	24	501	1/1	0.50	0.05	126,126,126,126	0
56	MG	1A	3901	1/1	0.53	0.65	68,68,68,68	0
56	MG	1a	1753	1/1	0.54	0.32	83,83,83,83	0
56	MG	1A	3285	1/1	0.56	1.19	79,79,79,79	0
56	MG	2A	3469	1/1	0.56	0.47	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3138	1/1	0.57	0.20	62,62,62,62	0
56	MG	1A	3847	1/1	0.57	0.14	81,81,81,81	0
56	MG	1A	4015	1/1	0.57	0.53	61,61,61,61	0
56	MG	1B	214	1/1	0.57	0.11	80,80,80,80	0
56	MG	2A	3525	1/1	0.58	0.30	53,53,53,53	0
56	MG	1a	1766	1/1	0.58	0.31	79,79,79,79	0
56	MG	2a	3046	1/1	0.58	0.11	77,77,77,77	0
56	MG	1r	3002	1/1	0.59	0.22	85,85,85,85	0
56	MG	2a	3169	1/1	0.60	0.17	75,75,75,75	0
56	MG	1A	4020	1/1	0.61	0.50	67,67,67,67	0
56	MG	2a	3168	1/1	0.62	0.09	83,83,83,83	0
56	MG	2A	3075	1/1	0.62	0.39	75,75,75,75	0
56	MG	1A	3364	1/1	0.62	0.49	57,57,57,57	0
56	MG	1a	1613	1/1	0.63	0.24	76,76,76,76	0
56	MG	1A	3994	1/1	0.63	0.35	51,51,51,51	0
56	MG	1a	1762	1/1	0.63	0.18	80,80,80,80	0
56	MG	1A	3481	1/1	0.63	0.29	76,76,76,76	0
56	MG	2A	3416	1/1	0.64	0.12	56,56,56,56	0
56	MG	2a	3213	1/1	0.66	0.14	87,87,87,87	0
56	MG	2A	3459	1/1	0.66	0.25	70,70,70,70	0
56	MG	1a	1789	1/1	0.67	0.22	78,78,78,78	0
56	MG	2A	3023	1/1	0.67	0.15	55,55,55,55	0
56	MG	1a	1667	1/1	0.68	0.86	68,68,68,68	0
56	MG	2A	3025	1/1	0.68	0.25	61,61,61,61	0
56	MG	1a	1760	1/1	0.68	0.39	78,78,78,78	0
56	MG	2A	3167	1/1	0.69	0.23	58,58,58,58	0
56	MG	2a	3047	1/1	0.69	0.24	89,89,89,89	0
56	MG	1A	3244	1/1	0.70	0.31	55,55,55,55	0
56	MG	1A	3073	1/1	0.70	0.19	74,74,74,74	0
56	MG	1Z	302	1/1	0.70	0.59	73,73,73,73	0
56	MG	2a	3022	1/1	0.70	0.23	70,70,70,70	0
56	MG	1A	3476	1/1	0.70	0.22	66,66,66,66	0
56	MG	2a	3233	1/1	0.70	0.36	66,66,66,66	0
56	MG	1a	1846	1/1	0.70	0.08	71,71,71,71	0
56	MG	2A	3509	1/1	0.71	0.14	80,80,80,80	0
56	MG	2A	3215	1/1	0.71	0.15	63,63,63,63	0
56	MG	1a	1697	1/1	0.71	0.30	70,70,70,70	0
56	MG	1A	3940	1/1	0.71	0.42	78,78,78,78	0
56	MG	1A	3067	1/1	0.71	0.13	64,64,64,64	0
56	MG	2A	3039	1/1	0.72	0.26	65,65,65,65	0
56	MG	2A	3288	1/1	0.72	0.36	70,70,70,70	0
56	MG	2A	3013	1/1	0.72	0.25	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3109	1/1	0.72	0.11	66,66,66,66	0
56	MG	2A	3460	1/1	0.72	0.14	53,53,53,53	0
56	MG	1A	3268	1/1	0.72	0.36	50,50,50,50	0
56	MG	1A	3351	1/1	0.72	0.39	59,59,59,59	0
56	MG	1A	3515	1/1	0.73	0.23	75,75,75,75	0
56	MG	2a	3014	1/1	0.73	0.22	74,74,74,74	0
56	MG	1b	3001	1/1	0.73	0.24	83,83,83,83	0
56	MG	2A	3137	1/1	0.73	0.11	55,55,55,55	0
56	MG	1A	3503	1/1	0.73	0.29	82,82,82,82	0
56	MG	2A	3001	1/1	0.73	0.39	55,55,55,55	0
56	MG	2A	3096	1/1	0.74	0.29	40,40,40,40	0
56	MG	1A	3098	1/1	0.74	0.22	71,71,71,71	0
56	MG	2a	3186	1/1	0.74	0.14	80,80,80,80	0
56	MG	2a	3119	1/1	0.74	0.57	62,62,62,62	0
56	MG	1a	1638	1/1	0.74	0.23	57,57,57,57	0
56	MG	2a	3027	1/1	0.74	0.17	88,88,88,88	0
56	MG	1A	3499	1/1	0.75	0.16	81,81,81,81	0
56	MG	1A	3459	1/1	0.75	0.35	57,57,57,57	0
56	MG	1A	3859	1/1	0.75	0.10	59,59,59,59	0
56	MG	1B	209	1/1	0.75	0.28	61,61,61,61	0
56	MG	2A	3256	1/1	0.76	0.17	79,79,79,79	0
56	MG	2A	3005	1/1	0.76	0.11	70,70,70,70	0
56	MG	1A	3412	1/1	0.76	0.77	77,77,77,77	0
56	MG	1A	3514	1/1	0.76	0.12	72,72,72,72	0
56	MG	1A	3450	1/1	0.76	0.22	64,64,64,64	0
56	MG	1A	3516	1/1	0.76	0.19	75,75,75,75	0
56	MG	1A	3278	1/1	0.76	0.35	72,72,72,72	0
56	MG	2A	3242	1/1	0.76	0.17	55,55,55,55	0
56	MG	2a	3048	1/1	0.76	0.12	91,91,91,91	0
56	MG	2A	3097	1/1	0.77	0.20	54,54,54,54	0
56	MG	1a	1622	1/1	0.77	0.27	74,74,74,74	0
56	MG	1P	201	1/1	0.77	0.34	55,55,55,55	0
56	MG	2a	3178	1/1	0.77	0.31	75,75,75,75	0
56	MG	2A	3404	1/1	0.77	0.17	69,69,69,69	0
56	MG	1a	1813	1/1	0.77	0.12	99,99,99,99	0
56	MG	1T	205	1/1	0.77	0.16	66,66,66,66	0
56	MG	1a	1891	1/1	0.77	0.26	82,82,82,82	0
56	MG	1h	3001	1/1	0.78	0.13	74,74,74,74	0
56	MG	1a	1735	1/1	0.78	0.10	72,72,72,72	0
56	MG	2A	3202	1/1	0.78	0.19	50,50,50,50	0
56	MG	1E	307	1/1	0.78	0.40	74,74,74,74	0
56	MG	1N	204	1/1	0.78	0.40	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3492	1/1	0.78	0.15	81,81,81,81	0
56	MG	1A	3270	1/1	0.78	0.33	63,63,63,63	0
56	MG	1A	3140	1/1	0.78	0.09	50,50,50,50	0
56	MG	2a	3129	1/1	0.78	0.21	73,73,73,73	0
56	MG	18	104	1/1	0.78	0.32	59,59,59,59	0
56	MG	2A	3068	1/1	0.78	0.22	68,68,68,68	0
56	MG	1A	3068	1/1	0.78	0.10	67,67,67,67	0
56	MG	2A	3088	1/1	0.78	0.20	46,46,46,46	0
56	MG	2a	3171	1/1	0.78	0.13	77,77,77,77	0
56	MG	2A	3500	1/1	0.78	0.21	57,57,57,57	0
56	MG	1A	3451	1/1	0.78	0.42	81,81,81,81	0
56	MG	1A	3251	1/1	0.78	0.23	60,60,60,60	0
56	MG	1A	3313	1/1	0.78	0.28	71,71,71,71	0
56	MG	1A	3069	1/1	0.78	0.17	65,65,65,65	0
56	MG	2a	3034	1/1	0.79	0.48	72,72,72,72	0
56	MG	2a	3040	1/1	0.79	0.36	83,83,83,83	0
56	MG	2A	3290	1/1	0.79	0.17	57,57,57,57	0
56	MG	2A	3093	1/1	0.79	0.30	64,64,64,64	0
56	MG	1A	3758	1/1	0.79	0.12	66,66,66,66	0
56	MG	2a	3072	1/1	0.79	0.10	64,64,64,64	0
56	MG	1A	3805	1/1	0.79	0.12	47,47,47,47	0
56	MG	1a	1769	1/1	0.79	0.10	74,74,74,74	0
56	MG	1A	3259	1/1	0.79	0.24	66,66,66,66	0
56	MG	1A	3501	1/1	0.79	0.31	83,83,83,83	0
56	MG	1A	3862	1/1	0.79	0.18	25,25,25,25	0
56	MG	2A	3190	1/1	0.79	0.39	61,61,61,61	0
56	MG	1A	4027	1/1	0.79	0.30	72,72,72,72	0
56	MG	1a	1824	1/1	0.79	0.51	52,52,52,52	0
56	MG	2a	3182	1/1	0.79	0.15	64,64,64,64	0
56	MG	1a	1750	1/1	0.79	0.22	72,72,72,72	0
56	MG	2A	3246	1/1	0.79	0.18	67,67,67,67	0
56	MG	1A	3009	1/1	0.79	0.31	50,50,50,50	0
56	MG	1a	1609	1/1	0.79	0.28	60,60,60,60	0
56	MG	2a	3058	1/1	0.80	0.18	66,66,66,66	0
56	MG	2A	3206	1/1	0.80	0.09	64,64,64,64	0
56	MG	2a	3082	1/1	0.80	0.42	61,61,61,61	0
56	MG	1A	3402	1/1	0.80	0.24	73,73,73,73	0
56	MG	2a	3126	1/1	0.80	0.37	66,66,66,66	0
56	MG	2A	3529	1/1	0.80	0.13	62,62,62,62	0
56	MG	1A	3090	1/1	0.80	0.32	53,53,53,53	0
56	MG	1F	306	1/1	0.80	0.35	64,64,64,64	0
56	MG	1a	1628	1/1	0.80	0.24	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	3508	1/1	0.80	0.25	64,64,64,64	0
56	MG	1a	1642	1/1	0.80	0.81	68,68,68,68	0
56	MG	1A	3421	1/1	0.80	0.13	65,65,65,65	0
56	MG	1A	3279	1/1	0.80	0.25	46,46,46,46	0
56	MG	1a	1805	1/1	0.80	0.10	70,70,70,70	0
56	MG	1A	3887	1/1	0.80	0.10	29,29,29,29	0
56	MG	1A	3219	1/1	0.80	0.20	63,63,63,63	0
56	MG	2A	3063	1/1	0.80	0.26	56,56,56,56	0
56	MG	1A	3447	1/1	0.81	0.38	75,75,75,75	0
56	MG	1A	3815	1/1	0.81	0.23	52,52,52,52	0
56	MG	2A	3032	1/1	0.81	0.62	50,50,50,50	0
56	MG	2A	3276	1/1	0.81	0.23	58,58,58,58	0
56	MG	1a	1788	1/1	0.81	0.22	81,81,81,81	0
56	MG	1a	1627	1/1	0.81	0.12	68,68,68,68	0
56	MG	1A	3141	1/1	0.81	0.10	56,56,56,56	0
56	MG	1a	1800	1/1	0.81	0.26	84,84,84,84	0
56	MG	2a	3108	1/1	0.81	0.07	79,79,79,79	0
56	MG	1A	3858	1/1	0.81	0.36	52,52,52,52	0
56	MG	1A	3075	1/1	0.81	0.33	60,60,60,60	0
56	MG	1A	3861	1/1	0.81	0.10	68,68,68,68	0
56	MG	1A	3395	1/1	0.81	0.17	59,59,59,59	0
56	MG	2A	3105	1/1	0.81	0.20	55,55,55,55	0
56	MG	1a	1715	1/1	0.81	0.11	76,76,76,76	0
56	MG	1A	3463	1/1	0.81	0.47	53,53,53,53	0
56	MG	1A	3288	1/1	0.81	0.17	70,70,70,70	0
56	MG	2D	303	1/1	0.81	0.17	60,60,60,60	0
56	MG	1A	3303	1/1	0.81	0.48	48,48,48,48	0
56	MG	1x	106	1/1	0.81	0.30	54,54,54,54	0
56	MG	1A	3520	1/1	0.81	0.15	41,41,41,41	0
56	MG	1A	3269	1/1	0.81	0.32	56,56,56,56	0
56	MG	2q	201	1/1	0.81	0.21	71,71,71,71	0
56	MG	1A	4002	1/1	0.81	0.21	71,71,71,71	0
56	MG	1a	1746	1/1	0.82	0.26	60,60,60,60	0
56	MG	1A	3151	1/1	0.82	0.26	49,49,49,49	0
56	MG	1A	3936	1/1	0.82	0.20	39,39,39,39	0
56	MG	1T	203	1/1	0.82	0.20	69,69,69,69	0
56	MG	1A	3167	1/1	0.82	0.19	59,59,59,59	0
56	MG	2a	3041	1/1	0.82	0.25	79,79,79,79	0
56	MG	1A	3975	1/1	0.82	0.14	63,63,63,63	0
56	MG	1A	3984	1/1	0.82	0.18	77,77,77,77	0
56	MG	1A	3262	1/1	0.82	0.21	58,58,58,58	0
56	MG	1A	3999	1/1	0.82	0.27	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3064	1/1	0.82	0.31	56,56,56,56	0
56	MG	2A	3364	1/1	0.82	0.24	55,55,55,55	0
56	MG	2a	3089	1/1	0.82	0.36	75,75,75,75	0
56	MG	2a	3099	1/1	0.82	0.46	63,63,63,63	0
56	MG	1a	1617	1/1	0.82	0.54	74,74,74,74	0
56	MG	1A	3340	1/1	0.82	0.17	56,56,56,56	0
56	MG	2A	3083	1/1	0.82	0.28	66,66,66,66	0
56	MG	1A	3848	1/1	0.82	0.17	57,57,57,57	0
56	MG	1A	3435	1/1	0.82	0.14	62,62,62,62	0
56	MG	2A	3474	1/1	0.82	0.14	58,58,58,58	0
56	MG	2a	3152	1/1	0.82	0.18	89,89,89,89	0
56	MG	2A	3095	1/1	0.82	0.19	48,48,48,48	0
56	MG	1A	3091	1/1	0.82	0.16	61,61,61,61	0
56	MG	1A	3066	1/1	0.82	0.43	63,63,63,63	0
56	MG	1A	3580	1/1	0.82	0.24	68,68,68,68	0
56	MG	2A	3572	1/1	0.82	0.36	61,61,61,61	0
56	MG	2A	3575	1/1	0.82	0.71	47,47,47,47	0
56	MG	2a	3187	1/1	0.82	0.10	56,56,56,56	0
56	MG	1a	1676	1/1	0.82	0.52	51,51,51,51	0
56	MG	1B	215	1/1	0.82	0.15	68,68,68,68	0
56	MG	1A	3635	1/1	0.82	0.24	56,56,56,56	0
56	MG	1A	3745	1/1	0.82	0.32	54,54,54,54	0
56	MG	1N	201	1/1	0.83	0.30	70,70,70,70	0
56	MG	1A	3964	1/1	0.83	0.56	76,76,76,76	0
56	MG	1A	3029	1/1	0.83	0.21	57,57,57,57	0
56	MG	2a	3020	1/1	0.83	0.17	72,72,72,72	0
56	MG	1h	3003	1/1	0.83	0.34	79,79,79,79	0
56	MG	2A	3193	1/1	0.83	0.31	63,63,63,63	0
56	MG	1A	3550	1/1	0.83	0.18	58,58,58,58	0
56	MG	2a	3036	1/1	0.83	0.10	73,73,73,73	0
56	MG	1A	3422	1/1	0.83	0.16	72,72,72,72	0
56	MG	1A	3322	1/1	0.83	0.26	63,63,63,63	0
56	MG	1a	1756	1/1	0.83	0.40	93,93,93,93	0
56	MG	1A	3860	1/1	0.83	0.15	72,72,72,72	0
56	MG	2A	3253	1/1	0.83	0.34	68,68,68,68	0
56	MG	2a	3056	1/1	0.83	1.00	79,79,79,79	0
56	MG	2A	3020	1/1	0.83	0.27	60,60,60,60	0
56	MG	1A	3642	1/1	0.83	0.15	67,67,67,67	0
56	MG	1A	3406	1/1	0.83	0.22	56,56,56,56	0
56	MG	2A	3028	1/1	0.83	0.14	48,48,48,48	0
56	MG	2A	3346	1/1	0.83	0.27	65,65,65,65	0
56	MG	1A	3339	1/1	0.83	0.27	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3109	1/1	0.83	0.41	73,73,73,73	0
56	MG	2a	3110	1/1	0.83	0.15	53,53,53,53	0
56	MG	1A	4031	1/1	0.83	0.63	54,54,54,54	0
56	MG	2a	3125	1/1	0.83	0.22	66,66,66,66	0
56	MG	2A	3058	1/1	0.83	0.14	56,56,56,56	0
56	MG	2A	3446	1/1	0.83	0.12	47,47,47,47	0
56	MG	1a	1781	1/1	0.83	0.18	87,87,87,87	0
56	MG	1a	1625	1/1	0.83	0.09	78,78,78,78	0
56	MG	1A	3798	1/1	0.83	0.14	59,59,59,59	0
56	MG	2a	3162	1/1	0.83	0.15	47,47,47,47	0
56	MG	2a	3164	1/1	0.83	0.25	65,65,65,65	0
56	MG	1A	3413	1/1	0.83	0.17	60,60,60,60	0
56	MG	1A	3519	1/1	0.83	0.25	33,33,33,33	0
56	MG	1a	1803	1/1	0.83	0.21	80,80,80,80	0
56	MG	2a	3175	1/1	0.83	0.17	53,53,53,53	0
56	MG	1A	3829	1/1	0.83	0.08	56,56,56,56	0
56	MG	1a	1663	1/1	0.83	0.22	67,67,67,67	0
56	MG	1A	3943	1/1	0.83	0.31	35,35,35,35	0
56	MG	1a	1843	1/1	0.83	0.40	71,71,71,71	0
56	MG	2a	3191	1/1	0.83	0.26	66,66,66,66	0
56	MG	1G	3002	1/1	0.83	0.16	69,69,69,69	0
56	MG	2B	3006	1/1	0.83	0.17	50,50,50,50	0
56	MG	1a	1847	1/1	0.83	0.25	54,54,54,54	0
56	MG	2E	305	1/1	0.83	0.19	68,68,68,68	0
56	MG	1A	3574	1/1	0.84	0.16	57,57,57,57	0
56	MG	1a	1739	1/1	0.84	0.18	72,72,72,72	0
56	MG	1a	1742	1/1	0.84	0.34	61,61,61,61	0
56	MG	2A	3239	1/1	0.84	0.26	49,49,49,49	0
56	MG	1x	110	1/1	0.84	0.08	78,78,78,78	0
56	MG	1A	3389	1/1	0.84	0.16	50,50,50,50	0
56	MG	2a	3042	1/1	0.84	0.10	78,78,78,78	0
56	MG	1A	3336	1/1	0.84	0.30	61,61,61,61	0
56	MG	2A	3008	1/1	0.84	0.16	59,59,59,59	0
56	MG	1l	101	1/1	0.84	0.28	83,83,83,83	0
56	MG	1A	3205	1/1	0.84	0.11	55,55,55,55	0
56	MG	1a	1604	1/1	0.84	0.27	70,70,70,70	0
56	MG	1A	4018	1/1	0.84	0.38	62,62,62,62	0
56	MG	1a	1763	1/1	0.84	0.11	76,76,76,76	0
56	MG	2A	3373	1/1	0.84	0.10	47,47,47,47	0
56	MG	2A	3388	1/1	0.84	0.20	46,46,46,46	0
56	MG	2A	3395	1/1	0.84	0.12	78,78,78,78	0
56	MG	1A	3247	1/1	0.84	0.32	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3881	1/1	0.84	0.26	63,63,63,63	0
56	MG	2A	3441	1/1	0.84	0.29	51,51,51,51	0
56	MG	1A	3062	1/1	0.84	0.32	57,57,57,57	0
56	MG	1A	3786	1/1	0.84	0.30	67,67,67,67	0
56	MG	1a	1785	1/1	0.84	0.14	66,66,66,66	0
56	MG	1A	3461	1/1	0.84	0.49	46,46,46,46	0
56	MG	1A	3360	1/1	0.84	0.19	61,61,61,61	0
56	MG	1B	221	1/1	0.84	0.16	63,63,63,63	0
56	MG	1A	3240	1/1	0.84	0.42	48,48,48,48	0
56	MG	1A	3368	1/1	0.84	0.28	50,50,50,50	0
56	MG	1a	1664	1/1	0.84	0.14	57,57,57,57	0
56	MG	1A	3486	1/1	0.84	0.20	65,65,65,65	0
56	MG	1a	1823	1/1	0.84	0.22	69,69,69,69	0
56	MG	1a	1670	1/1	0.84	0.41	60,60,60,60	0
56	MG	1a	1673	1/1	0.84	0.10	46,46,46,46	0
56	MG	1A	3968	1/1	0.84	0.28	65,65,65,65	0
56	MG	2E	303	1/1	0.84	0.37	53,53,53,53	0
56	MG	1A	3491	1/1	0.84	0.09	83,83,83,83	0
56	MG	2A	3148	1/1	0.84	0.26	41,41,41,41	0
56	MG	2a	3001	1/1	0.84	0.53	54,54,54,54	0
56	MG	1a	1713	1/1	0.84	0.43	65,65,65,65	0
56	MG	1A	3850	1/1	0.84	0.21	80,80,80,80	0
56	MG	1a	1723	1/1	0.84	0.07	60,60,60,60	0
56	MG	1A	3961	1/1	0.85	0.33	47,47,47,47	0
56	MG	1A	3365	1/1	0.85	0.53	44,44,44,44	0
56	MG	1A	3039	1/1	0.85	0.12	54,54,54,54	0
56	MG	2A	3178	1/1	0.85	0.31	59,59,59,59	0
56	MG	1A	3512	1/1	0.85	0.12	53,53,53,53	0
56	MG	1r	3001	1/1	0.85	0.22	68,68,68,68	0
56	MG	1a	1749	1/1	0.85	0.24	66,66,66,66	0
56	MG	15	105	1/1	0.85	0.20	57,57,57,57	0
56	MG	1x	109	1/1	0.85	0.56	73,73,73,73	0
56	MG	2A	3229	1/1	0.85	0.26	46,46,46,46	0
56	MG	2a	3037	1/1	0.85	0.19	72,72,72,72	0
56	MG	2A	3237	1/1	0.85	0.26	48,48,48,48	0
56	MG	1A	3513	1/1	0.85	0.09	72,72,72,72	0
56	MG	1x	111	1/1	0.85	0.10	80,80,80,80	0
56	MG	1A	3378	1/1	0.85	0.16	53,53,53,53	0
56	MG	2A	3004	1/1	0.85	0.12	55,55,55,55	0
56	MG	1A	3386	1/1	0.85	0.19	51,51,51,51	0
56	MG	2A	3268	1/1	0.85	0.10	63,63,63,63	0
56	MG	1A	4001	1/1	0.85	0.34	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3176	1/1	0.85	0.25	50,50,50,50	0
56	MG	2a	3077	1/1	0.85	0.11	95,95,95,95	0
56	MG	2A	3014	1/1	0.85	0.20	44,44,44,44	0
56	MG	2a	3085	1/1	0.85	0.46	61,61,61,61	0
56	MG	1A	3852	1/1	0.85	0.21	72,72,72,72	0
56	MG	2A	3358	1/1	0.85	0.26	53,53,53,53	0
56	MG	1A	3246	1/1	0.85	0.31	65,65,65,65	0
56	MG	2A	3367	1/1	0.85	0.10	52,52,52,52	0
56	MG	1A	3475	1/1	0.85	0.07	61,61,61,61	0
56	MG	1A	3183	1/1	0.85	0.09	59,59,59,59	0
56	MG	2A	3029	1/1	0.85	0.27	59,59,59,59	0
56	MG	1A	3048	1/1	0.85	0.24	41,41,41,41	0
56	MG	1A	3212	1/1	0.85	0.31	49,49,49,49	0
56	MG	2a	3133	1/1	0.85	0.32	93,93,93,93	0
56	MG	1A	3341	1/1	0.85	0.11	58,58,58,58	0
56	MG	1A	3284	1/1	0.85	0.38	52,52,52,52	0
56	MG	1A	3710	1/1	0.85	0.08	48,48,48,48	0
56	MG	2A	3065	1/1	0.85	0.42	58,58,58,58	0
56	MG	1A	3495	1/1	0.85	0.43	51,51,51,51	0
56	MG	1A	3261	1/1	0.85	0.26	68,68,68,68	0
56	MG	2A	3080	1/1	0.85	0.09	37,37,37,37	0
56	MG	1a	1810	1/1	0.85	0.06	86,86,86,86	0
56	MG	1A	3770	1/1	0.85	0.30	68,68,68,68	0
56	MG	1A	3941	1/1	0.85	0.24	73,73,73,73	0
56	MG	2A	3534	1/1	0.85	0.11	52,52,52,52	0
56	MG	1A	3126	1/1	0.85	0.31	55,55,55,55	0
56	MG	2A	3573	1/1	0.85	0.21	42,42,42,42	0
56	MG	1O	201	1/1	0.85	0.41	54,54,54,54	0
56	MG	2a	3205	1/1	0.85	0.68	78,78,78,78	0
56	MG	1A	3950	1/1	0.85	0.10	55,55,55,55	0
56	MG	2a	3220	1/1	0.85	0.34	87,87,87,87	0
56	MG	1a	1734	1/1	0.85	0.24	66,66,66,66	0
56	MG	2a	3240	1/1	0.85	0.29	65,65,65,65	0
56	MG	1a	1876	1/1	0.85	0.20	61,61,61,61	0
56	MG	1a	1889	1/1	0.85	0.27	64,64,64,64	0
57	ZN	2n	501	1/1	0.85	0.07	105,105,105,105	0
56	MG	1A	3146	1/1	0.86	0.27	43,43,43,43	0
56	MG	1a	1783	1/1	0.86	0.20	75,75,75,75	0
56	MG	2A	3579	1/1	0.86	0.14	42,42,42,42	0
56	MG	1A	3300	1/1	0.86	0.19	51,51,51,51	0
56	MG	2A	3084	1/1	0.86	0.13	51,51,51,51	0
56	MG	1A	3252	1/1	0.86	0.37	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	1618	1/1	0.86	0.27	65,65,65,65	0
56	MG	1A	3271	1/1	0.86	0.10	66,66,66,66	0
56	MG	1A	3384	1/1	0.86	0.14	66,66,66,66	0
56	MG	2N	8001	1/1	0.86	0.07	59,59,59,59	0
56	MG	1A	3527	1/1	0.86	0.19	32,32,32,32	0
56	MG	1A	3319	1/1	0.86	0.11	55,55,55,55	0
56	MG	2a	3013	1/1	0.86	0.22	73,73,73,73	0
56	MG	1A	3275	1/1	0.86	0.29	53,53,53,53	0
56	MG	2a	3018	1/1	0.86	0.29	66,66,66,66	0
56	MG	1A	4033	1/1	0.86	0.14	50,50,50,50	0
56	MG	1a	1643	1/1	0.86	0.21	52,52,52,52	0
56	MG	1B	203	1/1	0.86	0.20	66,66,66,66	0
56	MG	1a	1826	1/1	0.86	0.13	80,80,80,80	0
56	MG	2a	3035	1/1	0.86	0.05	76,76,76,76	0
56	MG	1B	208	1/1	0.86	0.16	61,61,61,61	0
56	MG	1A	3253	1/1	0.86	0.09	81,81,81,81	0
56	MG	1A	3585	1/1	0.86	0.12	68,68,68,68	0
56	MG	1A	3337	1/1	0.86	0.27	48,48,48,48	0
56	MG	1A	3001	1/1	0.86	0.21	45,45,45,45	0
56	MG	2a	3043	1/1	0.86	0.12	85,85,85,85	0
56	MG	1a	1695	1/1	0.86	0.08	77,77,77,77	0
56	MG	1a	1902	1/1	0.86	0.31	59,59,59,59	0
56	MG	1a	1696	1/1	0.86	0.13	67,67,67,67	0
56	MG	1b	3002	1/1	0.86	0.33	87,87,87,87	0
56	MG	1B	223	1/1	0.86	0.14	74,74,74,74	0
56	MG	1A	3647	1/1	0.86	0.25	55,55,55,55	0
56	MG	1a	1714	1/1	0.86	0.22	58,58,58,58	0
56	MG	1A	3900	1/1	0.86	0.39	42,42,42,42	0
56	MG	2A	3257	1/1	0.86	0.14	62,62,62,62	0
56	MG	1x	101	1/1	0.86	0.26	69,69,69,69	0
56	MG	1x	105	1/1	0.86	0.12	57,57,57,57	0
56	MG	2A	3278	1/1	0.86	0.28	65,65,65,65	0
56	MG	1A	3699	1/1	0.86	0.21	17,17,17,17	0
56	MG	1a	1732	1/1	0.86	0.26	53,53,53,53	0
56	MG	1A	3195	1/1	0.86	0.19	45,45,45,45	0
56	MG	1N	202	1/1	0.86	0.68	49,49,49,49	0
56	MG	1a	1736	1/1	0.86	0.33	63,63,63,63	0
56	MG	1A	3716	1/1	0.86	0.22	53,53,53,53	0
56	MG	1a	1741	1/1	0.86	0.54	68,68,68,68	0
56	MG	2A	3007	1/1	0.86	0.14	50,50,50,50	0
56	MG	1A	3012	1/1	0.86	0.31	45,45,45,45	0
56	MG	1a	1745	1/1	0.86	0.19	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3348	1/1	0.86	0.22	63,63,63,63	0
56	MG	2A	3439	1/1	0.86	0.15	54,54,54,54	0
56	MG	1A	3168	1/1	0.86	0.20	41,41,41,41	0
56	MG	1A	3771	1/1	0.86	0.07	54,54,54,54	0
56	MG	2A	3451	1/1	0.86	0.12	63,63,63,63	0
56	MG	2A	3457	1/1	0.86	0.33	55,55,55,55	0
56	MG	1A	3358	1/1	0.86	0.32	54,54,54,54	0
56	MG	10	101	1/1	0.86	0.34	68,68,68,68	0
56	MG	2A	3461	1/1	0.86	0.15	78,78,78,78	0
56	MG	2A	3465	1/1	0.86	0.11	46,46,46,46	0
56	MG	10	105	1/1	0.86	0.20	57,57,57,57	0
56	MG	1A	3442	1/1	0.86	0.85	57,57,57,57	0
56	MG	14	502	1/1	0.86	0.14	79,79,79,79	0
56	MG	1A	3287	1/1	0.86	0.25	57,57,57,57	0
56	MG	2A	3515	1/1	0.86	0.12	63,63,63,63	0
56	MG	1a	1767	1/1	0.86	0.08	84,84,84,84	0
56	MG	1a	1768	1/1	0.86	0.20	90,90,90,90	0
56	MG	2x	3005	1/1	0.86	0.08	70,70,70,70	0
56	MG	1A	3448	1/1	0.86	0.31	58,58,58,58	0
56	MG	1A	3823	1/1	0.86	0.19	39,39,39,39	0
56	MG	2A	3149	1/1	0.87	0.40	59,59,59,59	0
56	MG	1A	3436	1/1	0.87	0.18	68,68,68,68	0
56	MG	1f	3001	1/1	0.87	0.20	66,66,66,66	0
56	MG	2A	3180	1/1	0.87	0.71	52,52,52,52	0
56	MG	2A	3183	1/1	0.87	0.07	58,58,58,58	0
56	MG	2A	3189	1/1	0.87	0.23	61,61,61,61	0
56	MG	1Z	303	1/1	0.87	0.14	64,64,64,64	0
56	MG	2A	3192	1/1	0.87	0.14	45,45,45,45	0
56	MG	2a	3010	1/1	0.87	0.10	83,83,83,83	0
56	MG	2a	3012	1/1	0.87	0.47	69,69,69,69	0
56	MG	1a	1737	1/1	0.87	0.28	66,66,66,66	0
56	MG	2A	3200	1/1	0.87	0.25	41,41,41,41	0
56	MG	1k	3001	1/1	0.87	0.29	65,65,65,65	0
56	MG	1A	3979	1/1	0.87	0.16	59,59,59,59	0
56	MG	1A	3982	1/1	0.87	0.24	74,74,74,74	0
56	MG	2a	3023	1/1	0.87	0.46	74,74,74,74	0
56	MG	2A	3218	1/1	0.87	0.11	64,64,64,64	0
56	MG	2a	3030	1/1	0.87	0.18	59,59,59,59	0
56	MG	1t	3001	1/1	0.87	0.39	64,64,64,64	0
56	MG	1A	3787	1/1	0.87	0.11	45,45,45,45	0
56	MG	1A	3990	1/1	0.87	0.13	64,64,64,64	0
56	MG	2A	3240	1/1	0.87	0.40	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	3097	1/1	0.87	0.22	40,40,40,40	0
56	MG	1A	3159	1/1	0.87	0.26	42,42,42,42	0
56	MG	1a	1601	1/1	0.87	0.16	66,66,66,66	0
56	MG	1A	3366	1/1	0.87	0.31	46,46,46,46	0
56	MG	1A	3072	1/1	0.87	0.18	53,53,53,53	0
56	MG	1A	3323	1/1	0.87	0.11	46,46,46,46	0
56	MG	1A	3326	1/1	0.87	0.07	63,63,63,63	0
56	MG	1A	3331	1/1	0.87	0.15	53,53,53,53	0
56	MG	1A	3058	1/1	0.87	0.06	49,49,49,49	0
56	MG	1A	3264	1/1	0.87	0.21	66,66,66,66	0
56	MG	2A	3293	1/1	0.87	0.18	57,57,57,57	0
56	MG	1A	3396	1/1	0.87	0.13	58,58,58,58	0
56	MG	1A	4036	1/1	0.87	0.49	44,44,44,44	0
56	MG	1a	1771	1/1	0.87	0.19	75,75,75,75	0
56	MG	1A	3397	1/1	0.87	0.12	47,47,47,47	0
56	MG	2a	3101	1/1	0.87	0.32	64,64,64,64	0
56	MG	2A	3027	1/1	0.87	0.14	64,64,64,64	0
56	MG	1B	207	1/1	0.87	0.30	70,70,70,70	0
56	MG	1A	3592	1/1	0.87	0.22	42,42,42,42	0
56	MG	1a	1646	1/1	0.87	0.22	68,68,68,68	0
56	MG	2a	3124	1/1	0.87	0.35	76,76,76,76	0
56	MG	1a	1652	1/1	0.87	0.21	65,65,65,65	0
56	MG	2A	3422	1/1	0.87	0.24	52,52,52,52	0
56	MG	1A	3600	1/1	0.87	0.23	31,31,31,31	0
56	MG	1A	3265	1/1	0.87	0.24	55,55,55,55	0
56	MG	1A	3487	1/1	0.87	0.37	64,64,64,64	0
56	MG	1A	3022	1/1	0.87	0.44	66,66,66,66	0
56	MG	2a	3150	1/1	0.87	0.23	63,63,63,63	0
56	MG	1a	1671	1/1	0.87	0.29	61,61,61,61	0
56	MG	2a	3159	1/1	0.87	0.29	76,76,76,76	0
56	MG	2A	3074	1/1	0.87	0.12	47,47,47,47	0
56	MG	1A	3662	1/1	0.87	0.14	55,55,55,55	0
56	MG	1A	3679	1/1	0.87	0.23	51,51,51,51	0
56	MG	1a	1820	1/1	0.87	0.42	82,82,82,82	0
56	MG	1a	1682	1/1	0.87	0.11	70,70,70,70	0
56	MG	1A	3681	1/1	0.87	0.12	39,39,39,39	0
56	MG	2A	3495	1/1	0.87	0.14	75,75,75,75	0
56	MG	1A	3054	1/1	0.87	0.33	56,56,56,56	0
56	MG	1A	3071	1/1	0.87	0.17	52,52,52,52	0
56	MG	1A	3414	1/1	0.87	0.10	79,79,79,79	0
56	MG	2A	3519	1/1	0.87	0.28	53,53,53,53	0
56	MG	1A	3147	1/1	0.87	0.27	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	3104	1/1	0.87	0.12	42,42,42,42	0
56	MG	1A	3304	1/1	0.87	0.28	74,74,74,74	0
56	MG	1A	3761	1/1	0.87	0.12	52,52,52,52	0
56	MG	2A	3132	1/1	0.87	0.12	62,62,62,62	0
56	MG	2a	3244	1/1	0.87	0.10	76,76,76,76	0
56	MG	2l	203	1/1	0.87	0.10	67,67,67,67	0
56	MG	1a	1724	1/1	0.87	0.26	70,70,70,70	0
56	MG	1A	3505	1/1	0.87	0.29	66,66,66,66	0
56	MG	2A	3582	1/1	0.87	0.17	50,50,50,50	0
56	MG	1A	3305	1/1	0.87	0.18	83,83,83,83	0
56	MG	1A	3978	1/1	0.88	0.17	59,59,59,59	0
56	MG	2A	3018	1/1	0.88	0.24	57,57,57,57	0
56	MG	1H	201	1/1	0.88	0.52	54,54,54,54	0
56	MG	2A	3244	1/1	0.88	0.29	73,73,73,73	0
56	MG	2A	3245	1/1	0.88	0.07	78,78,78,78	0
56	MG	1A	3115	1/1	0.88	0.39	40,40,40,40	0
56	MG	1A	3698	1/1	0.88	0.24	46,46,46,46	0
56	MG	1A	3439	1/1	0.88	0.33	50,50,50,50	0
56	MG	1A	3704	1/1	0.88	0.21	34,34,34,34	0
56	MG	1A	3376	1/1	0.88	0.16	60,60,60,60	0
56	MG	2A	3271	1/1	0.88	0.29	36,36,36,36	0
56	MG	2a	3028	1/1	0.88	0.49	61,61,61,61	0
56	MG	1a	1690	1/1	0.88	0.21	82,82,82,82	0
56	MG	1R	204	1/1	0.88	0.18	48,48,48,48	0
56	MG	2A	3052	1/1	0.88	0.39	66,66,66,66	0
56	MG	1a	1812	1/1	0.88	0.27	78,78,78,78	0
56	MG	2A	3062	1/1	0.88	0.25	33,33,33,33	0
56	MG	2A	3305	1/1	0.88	0.29	38,38,38,38	0
56	MG	2A	3320	1/1	0.88	0.19	67,67,67,67	0
56	MG	1A	3227	1/1	0.88	0.10	65,65,65,65	0
56	MG	1A	3409	1/1	0.88	0.65	81,81,81,81	0
56	MG	2A	3359	1/1	0.88	0.15	75,75,75,75	0
56	MG	1A	3870	1/1	0.88	0.06	41,41,41,41	0
56	MG	1A	4006	1/1	0.88	0.23	77,77,77,77	0
56	MG	1A	3569	1/1	0.88	0.25	25,25,25,25	0
56	MG	2A	3386	1/1	0.88	0.26	57,57,57,57	0
56	MG	2a	3071	1/1	0.88	0.18	58,58,58,58	0
56	MG	10	102	1/1	0.88	0.07	56,56,56,56	0
56	MG	2A	3394	1/1	0.88	0.33	61,61,61,61	0
56	MG	1A	3383	1/1	0.88	0.17	51,51,51,51	0
56	MG	1A	3309	1/1	0.88	0.11	65,65,65,65	0
56	MG	2a	3088	1/1	0.88	0.20	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1848	1/1	0.88	0.08	85,85,85,85	0
56	MG	1a	1866	1/1	0.88	0.25	72,72,72,72	0
56	MG	2a	3100	1/1	0.88	0.39	57,57,57,57	0
56	MG	13	102	1/1	0.88	0.27	63,63,63,63	0
56	MG	2a	3102	1/1	0.88	0.17	72,72,72,72	0
56	MG	1A	3291	1/1	0.88	0.22	55,55,55,55	0
56	MG	1A	3416	1/1	0.88	0.21	70,70,70,70	0
56	MG	1a	1897	1/1	0.88	0.11	50,50,50,50	0
56	MG	1A	3507	1/1	0.88	0.38	93,93,93,93	0
56	MG	2a	3120	1/1	0.88	0.23	66,66,66,66	0
56	MG	1A	3607	1/1	0.88	0.16	50,50,50,50	0
56	MG	2A	3108	1/1	0.88	0.22	47,47,47,47	0
56	MG	1A	4041	1/1	0.88	0.28	39,39,39,39	0
56	MG	2A	3121	1/1	0.88	0.25	42,42,42,42	0
56	MG	1a	1607	1/1	0.88	0.29	66,66,66,66	0
56	MG	2a	3134	1/1	0.88	0.48	79,79,79,79	0
56	MG	1A	4042	1/1	0.88	0.22	51,51,51,51	0
56	MG	2a	3147	1/1	0.88	0.07	74,74,74,74	0
56	MG	2A	3480	1/1	0.88	0.11	74,74,74,74	0
56	MG	1A	3419	1/1	0.88	0.30	52,52,52,52	0
56	MG	1B	206	1/1	0.88	0.21	38,38,38,38	0
56	MG	2A	3502	1/1	0.88	0.24	75,75,75,75	0
56	MG	2A	3503	1/1	0.88	0.18	61,61,61,61	0
56	MG	1A	3472	1/1	0.88	0.08	66,66,66,66	0
56	MG	2A	3166	1/1	0.88	0.24	51,51,51,51	0
56	MG	1A	3822	1/1	0.88	0.10	34,34,34,34	0
56	MG	1A	3959	1/1	0.88	0.19	57,57,57,57	0
56	MG	1A	3297	1/1	0.88	0.27	59,59,59,59	0
56	MG	1x	102	1/1	0.88	0.07	69,69,69,69	0
56	MG	2A	3544	1/1	0.88	0.24	61,61,61,61	0
56	MG	1A	3002	1/1	0.88	0.23	43,43,43,43	0
56	MG	1a	1635	1/1	0.88	0.26	64,64,64,64	0
56	MG	1A	3678	1/1	0.88	0.18	67,67,67,67	0
56	MG	2a	3201	1/1	0.88	0.13	83,83,83,83	0
56	MG	2A	3578	1/1	0.88	0.19	58,58,58,58	0
56	MG	1A	3970	1/1	0.88	0.37	53,53,53,53	0
56	MG	2a	3216	1/1	0.88	0.20	57,57,57,57	0
56	MG	2A	3198	1/1	0.88	0.35	53,53,53,53	0
56	MG	1B	225	1/1	0.88	0.16	77,77,77,77	0
56	MG	1A	3057	1/1	0.88	0.33	56,56,56,56	0
56	MG	1F	304	1/1	0.88	0.15	40,40,40,40	0
56	MG	2l	201	1/1	0.88	0.13	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	1772	1/1	0.88	0.28	66,66,66,66	0
56	MG	1a	1653	1/1	0.88	0.09	70,70,70,70	0
56	MG	2t	201	1/1	0.88	0.27	62,62,62,62	0
56	MG	1A	3976	1/1	0.88	0.23	49,49,49,49	0
56	MG	1a	1782	1/1	0.88	0.15	67,67,67,67	0
56	MG	2Q	201	1/1	0.88	0.54	55,55,55,55	0
56	MG	1A	3444	1/1	0.89	0.23	65,65,65,65	0
56	MG	2B	3004	1/1	0.89	0.25	59,59,59,59	0
56	MG	1A	3404	1/1	0.89	0.22	82,82,82,82	0
56	MG	2B	3009	1/1	0.89	0.38	57,57,57,57	0
56	MG	1A	4019	1/1	0.89	0.50	93,93,93,93	0
56	MG	2E	302	1/1	0.89	0.49	63,63,63,63	0
56	MG	2A	3213	1/1	0.89	0.09	67,67,67,67	0
56	MG	2A	3214	1/1	0.89	0.27	49,49,49,49	0
56	MG	18	101	1/1	0.89	0.19	66,66,66,66	0
56	MG	1A	3160	1/1	0.89	0.13	42,42,42,42	0
56	MG	1A	3408	1/1	0.89	0.05	66,66,66,66	0
56	MG	26	101	1/1	0.89	0.15	46,46,46,46	0
56	MG	1A	3868	1/1	0.89	0.17	65,65,65,65	0
56	MG	1A	3700	1/1	0.89	0.26	37,37,37,37	0
56	MG	2A	3002	1/1	0.89	0.23	59,59,59,59	0
56	MG	2a	3011	1/1	0.89	0.71	68,68,68,68	0
56	MG	1a	1758	1/1	0.89	0.08	64,64,64,64	0
56	MG	1A	3043	1/1	0.89	0.16	49,49,49,49	0
56	MG	1A	3289	1/1	0.89	0.39	49,49,49,49	0
56	MG	1A	3074	1/1	0.89	0.28	61,61,61,61	0
56	MG	1a	1765	1/1	0.89	0.13	65,65,65,65	0
56	MG	1A	4049	1/1	0.89	0.26	57,57,57,57	0
56	MG	1a	1621	1/1	0.89	0.36	83,83,83,83	0
56	MG	2A	3267	1/1	0.89	0.22	63,63,63,63	0
56	MG	1A	3723	1/1	0.89	0.21	49,49,49,49	0
56	MG	1A	3728	1/1	0.89	0.18	23,23,23,23	0
56	MG	1A	3902	1/1	0.89	0.14	41,41,41,41	0
56	MG	1A	3916	1/1	0.89	0.19	60,60,60,60	0
56	MG	1A	3462	1/1	0.89	0.25	45,45,45,45	0
56	MG	1A	3342	1/1	0.89	0.13	40,40,40,40	0
56	MG	1A	3415	1/1	0.89	0.09	73,73,73,73	0
56	MG	2A	3304	1/1	0.89	0.18	40,40,40,40	0
56	MG	2A	3037	1/1	0.89	0.29	62,62,62,62	0
56	MG	1A	3474	1/1	0.89	0.34	59,59,59,59	0
56	MG	2A	3328	1/1	0.89	0.13	45,45,45,45	0
56	MG	2A	3331	1/1	0.89	0.20	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3338	1/1	0.89	0.21	54,54,54,54	0
56	MG	2A	3046	1/1	0.89	0.34	62,62,62,62	0
56	MG	2A	3357	1/1	0.89	0.20	75,75,75,75	0
56	MG	1A	3344	1/1	0.89	0.13	54,54,54,54	0
56	MG	2A	3057	1/1	0.89	0.28	50,50,50,50	0
56	MG	1a	1787	1/1	0.89	0.35	70,70,70,70	0
56	MG	2a	3078	1/1	0.89	0.07	49,49,49,49	0
56	MG	2a	3081	1/1	0.89	0.22	69,69,69,69	0
56	MG	1A	3417	1/1	0.89	0.20	60,60,60,60	0
56	MG	2a	3084	1/1	0.89	0.20	75,75,75,75	0
56	MG	1D	306	1/1	0.89	0.20	43,43,43,43	0
56	MG	1a	1654	1/1	0.89	0.17	67,67,67,67	0
56	MG	1A	3296	1/1	0.89	0.08	47,47,47,47	0
56	MG	2A	3390	1/1	0.89	0.26	63,63,63,63	0
56	MG	2A	3066	1/1	0.89	0.15	54,54,54,54	0
56	MG	1F	302	1/1	0.89	0.29	56,56,56,56	0
56	MG	1A	3788	1/1	0.89	0.13	25,25,25,25	0
56	MG	1A	3966	1/1	0.89	0.09	52,52,52,52	0
56	MG	2A	3417	1/1	0.89	0.19	62,62,62,62	0
56	MG	2A	3077	1/1	0.89	0.39	63,63,63,63	0
56	MG	2A	3437	1/1	0.89	0.19	83,83,83,83	0
56	MG	1A	3070	1/1	0.89	0.17	65,65,65,65	0
56	MG	1A	3037	1/1	0.89	0.07	65,65,65,65	0
56	MG	1A	3806	1/1	0.89	0.19	56,56,56,56	0
56	MG	1a	1681	1/1	0.89	0.08	44,44,44,44	0
56	MG	2A	3089	1/1	0.89	0.20	45,45,45,45	0
56	MG	1A	3490	1/1	0.89	0.09	66,66,66,66	0
56	MG	1A	3819	1/1	0.89	0.16	89,89,89,89	0
56	MG	1a	1834	1/1	0.89	0.17	72,72,72,72	0
56	MG	1a	1694	1/1	0.89	0.18	41,41,41,41	0
56	MG	1A	3430	1/1	0.89	0.41	41,41,41,41	0
56	MG	2A	3473	1/1	0.89	0.13	40,40,40,40	0
56	MG	1A	3981	1/1	0.89	0.31	63,63,63,63	0
56	MG	2a	3153	1/1	0.89	0.75	99,99,99,99	0
56	MG	2A	3475	1/1	0.89	0.33	67,67,67,67	0
56	MG	1Q	3005	1/1	0.89	0.16	53,53,53,53	0
56	MG	2A	3486	1/1	0.89	0.10	51,51,51,51	0
56	MG	1a	1699	1/1	0.89	0.24	71,71,71,71	0
56	MG	1a	1700	1/1	0.89	0.20	80,80,80,80	0
56	MG	1a	1884	1/1	0.89	0.29	56,56,56,56	0
56	MG	1A	3256	1/1	0.89	0.16	51,51,51,51	0
56	MG	2A	3504	1/1	0.89	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	3609	1/1	0.89	0.24	28,28,28,28	0
56	MG	1A	3988	1/1	0.89	0.62	38,38,38,38	0
56	MG	1X	3001	1/1	0.89	0.24	44,44,44,44	0
56	MG	2A	3521	1/1	0.89	0.18	59,59,59,59	0
56	MG	2A	3524	1/1	0.89	0.12	33,33,33,33	0
56	MG	1Y	502	1/1	0.89	0.33	59,59,59,59	0
56	MG	1a	1728	1/1	0.89	0.30	55,55,55,55	0
56	MG	1A	3334	1/1	0.89	0.18	55,55,55,55	0
56	MG	1A	3496	1/1	0.89	0.19	68,68,68,68	0
56	MG	2A	3563	1/1	0.89	0.21	58,58,58,58	0
56	MG	2A	3566	1/1	0.89	0.65	58,58,58,58	0
56	MG	1A	3401	1/1	0.89	0.17	67,67,67,67	0
56	MG	2d	503	1/1	0.89	0.12	72,72,72,72	0
56	MG	2k	3001	1/1	0.89	0.38	70,70,70,70	0
56	MG	1A	3440	1/1	0.89	0.16	51,51,51,51	0
56	MG	2A	3574	1/1	0.89	0.29	53,53,53,53	0
56	MG	1q	203	1/1	0.89	0.25	64,64,64,64	0
56	MG	2A	3577	1/1	0.89	0.19	54,54,54,54	0
56	MG	1A	3853	1/1	0.89	0.22	49,49,49,49	0
56	MG	1a	1738	1/1	0.89	0.17	59,59,59,59	0
56	MG	1A	3042	1/1	0.89	0.40	47,47,47,47	0
56	MG	2A	3542	1/1	0.90	0.21	50,50,50,50	0
56	MG	1A	3927	1/1	0.90	0.44	59,59,59,59	0
56	MG	1E	303	1/1	0.90	0.56	51,51,51,51	0
56	MG	2A	3150	1/1	0.90	0.08	56,56,56,56	0
56	MG	2A	3151	1/1	0.90	0.17	45,45,45,45	0
56	MG	1A	3314	1/1	0.90	0.25	57,57,57,57	0
56	MG	1a	1872	1/1	0.90	0.19	67,67,67,67	0
56	MG	1a	1684	1/1	0.90	0.18	58,58,58,58	0
56	MG	1a	1882	1/1	0.90	0.31	55,55,55,55	0
56	MG	1A	3438	1/1	0.90	0.26	62,62,62,62	0
56	MG	2A	3187	1/1	0.90	0.19	53,53,53,53	0
56	MG	2A	3580	1/1	0.90	0.23	51,51,51,51	0
56	MG	1A	3315	1/1	0.90	0.10	51,51,51,51	0
56	MG	1A	3316	1/1	0.90	0.19	81,81,81,81	0
56	MG	1G	3001	1/1	0.90	0.08	47,47,47,47	0
56	MG	1a	1898	1/1	0.90	0.53	65,65,65,65	0
56	MG	2A	3195	1/1	0.90	0.41	58,58,58,58	0
56	MG	1a	1900	1/1	0.90	0.24	62,62,62,62	0
56	MG	1A	3222	1/1	0.90	0.32	38,38,38,38	0
56	MG	1A	3122	1/1	0.90	0.54	60,60,60,60	0
56	MG	1H	202	1/1	0.90	0.18	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	1c	3001	1/1	0.90	0.21	68,68,68,68	0
56	MG	1a	1709	1/1	0.90	0.18	54,54,54,54	0
56	MG	1H	204	1/1	0.90	0.31	62,62,62,62	0
56	MG	1A	3446	1/1	0.90	0.13	52,52,52,52	0
56	MG	28	8001	1/1	0.90	0.39	56,56,56,56	0
56	MG	2A	3219	1/1	0.90	0.36	38,38,38,38	0
56	MG	2a	3003	1/1	0.90	0.53	60,60,60,60	0
56	MG	1A	3228	1/1	0.90	0.22	51,51,51,51	0
56	MG	2a	3006	1/1	0.90	0.10	66,66,66,66	0
56	MG	2a	3009	1/1	0.90	0.15	81,81,81,81	0
56	MG	1A	3393	1/1	0.90	0.26	46,46,46,46	0
56	MG	1A	3325	1/1	0.90	0.10	75,75,75,75	0
56	MG	1A	3124	1/1	0.90	0.31	54,54,54,54	0
56	MG	1A	3456	1/1	0.90	0.13	58,58,58,58	0
56	MG	1A	3457	1/1	0.90	0.29	48,48,48,48	0
56	MG	1A	3808	1/1	0.90	0.39	57,57,57,57	0
56	MG	1A	3004	1/1	0.90	0.43	44,44,44,44	0
56	MG	1A	3571	1/1	0.90	0.10	66,66,66,66	0
56	MG	1A	3245	1/1	0.90	0.22	64,64,64,64	0
56	MG	2a	3024	1/1	0.90	0.26	58,58,58,58	0
56	MG	2a	3026	1/1	0.90	0.80	72,72,72,72	0
56	MG	1A	3983	1/1	0.90	0.17	62,62,62,62	0
56	MG	2A	3259	1/1	0.90	0.19	40,40,40,40	0
56	MG	2A	3261	1/1	0.90	0.17	34,34,34,34	0
56	MG	1A	3173	1/1	0.90	0.29	24,24,24,24	0
56	MG	1A	3985	1/1	0.90	0.21	73,73,73,73	0
56	MG	1A	3828	1/1	0.90	0.16	55,55,55,55	0
56	MG	10	103	1/1	0.90	0.12	69,69,69,69	0
56	MG	2a	3038	1/1	0.90	0.14	85,85,85,85	0
56	MG	1a	1748	1/1	0.90	0.10	61,61,61,61	0
56	MG	1A	3080	1/1	0.90	0.15	52,52,52,52	0
56	MG	1A	3992	1/1	0.90	0.17	50,50,50,50	0
56	MG	2A	3292	1/1	0.90	0.14	60,60,60,60	0
56	MG	1A	3834	1/1	0.90	0.17	58,58,58,58	0
56	MG	2A	3297	1/1	0.90	0.19	49,49,49,49	0
56	MG	1A	3250	1/1	0.90	0.20	42,42,42,42	0
56	MG	1a	1757	1/1	0.90	0.16	64,64,64,64	0
56	MG	2A	3313	1/1	0.90	0.21	49,49,49,49	0
56	MG	1A	3045	1/1	0.90	0.15	53,53,53,53	0
56	MG	2A	3022	1/1	0.90	0.30	63,63,63,63	0
56	MG	1A	3024	1/1	0.90	0.17	52,52,52,52	0
56	MG	1A	3197	1/1	0.90	0.21	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	3339	1/1	0.90	0.14	55,55,55,55	0
56	MG	1A	4010	1/1	0.90	0.38	58,58,58,58	0
56	MG	2a	3083	1/1	0.90	0.14	43,43,43,43	0
56	MG	1A	3616	1/1	0.90	0.17	28,28,28,28	0
56	MG	1A	4016	1/1	0.90	0.19	58,58,58,58	0
56	MG	1A	3854	1/1	0.90	0.07	76,76,76,76	0
56	MG	2A	3361	1/1	0.90	0.05	72,72,72,72	0
56	MG	1A	3477	1/1	0.90	0.24	67,67,67,67	0
56	MG	1A	3479	1/1	0.90	0.20	78,78,78,78	0
56	MG	1A	4025	1/1	0.90	0.20	51,51,51,51	0
56	MG	2A	3377	1/1	0.90	0.18	21,21,21,21	0
56	MG	2A	3380	1/1	0.90	0.17	45,45,45,45	0
56	MG	2A	3382	1/1	0.90	0.14	71,71,71,71	0
56	MG	1A	3255	1/1	0.90	0.25	44,44,44,44	0
56	MG	1a	1774	1/1	0.90	0.46	63,63,63,63	0
56	MG	1a	1779	1/1	0.90	0.12	73,73,73,73	0
56	MG	1A	3200	1/1	0.90	0.16	54,54,54,54	0
56	MG	1A	3671	1/1	0.90	0.17	47,47,47,47	0
56	MG	1A	3257	1/1	0.90	0.39	68,68,68,68	0
56	MG	1A	3204	1/1	0.90	0.07	38,38,38,38	0
56	MG	2a	3131	1/1	0.90	0.06	63,63,63,63	0
56	MG	1a	1784	1/1	0.90	0.11	73,73,73,73	0
56	MG	1a	1629	1/1	0.90	0.24	54,54,54,54	0
56	MG	2A	3429	1/1	0.90	0.24	64,64,64,64	0
56	MG	2a	3138	1/1	0.90	0.18	73,73,73,73	0
56	MG	2a	3142	1/1	0.90	0.13	83,83,83,83	0
56	MG	2a	3143	1/1	0.90	0.13	90,90,90,90	0
56	MG	2A	3430	1/1	0.90	0.24	57,57,57,57	0
56	MG	1A	3871	1/1	0.90	0.16	67,67,67,67	0
56	MG	2A	3438	1/1	0.90	0.20	70,70,70,70	0
56	MG	1A	3873	1/1	0.90	0.20	25,25,25,25	0
56	MG	1a	1641	1/1	0.90	0.25	70,70,70,70	0
56	MG	2A	3443	1/1	0.90	0.17	52,52,52,52	0
56	MG	1A	3359	1/1	0.90	0.52	51,51,51,51	0
56	MG	1a	1794	1/1	0.90	0.30	63,63,63,63	0
56	MG	1a	1795	1/1	0.90	0.22	64,64,64,64	0
56	MG	2A	3085	1/1	0.90	0.25	34,34,34,34	0
56	MG	2A	3087	1/1	0.90	0.13	36,36,36,36	0
56	MG	1A	3050	1/1	0.90	0.23	63,63,63,63	0
56	MG	1a	1644	1/1	0.90	0.11	68,68,68,68	0
56	MG	1A	3493	1/1	0.90	0.20	63,63,63,63	0
56	MG	1A	3899	1/1	0.90	0.26	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	3209	1/1	0.90	0.30	41,41,41,41	0
56	MG	2a	3188	1/1	0.90	0.44	74,74,74,74	0
56	MG	1A	3210	1/1	0.90	0.27	46,46,46,46	0
56	MG	2a	3200	1/1	0.90	0.17	56,56,56,56	0
56	MG	2A	3477	1/1	0.90	0.07	61,61,61,61	0
56	MG	1a	1819	1/1	0.90	0.25	58,58,58,58	0
56	MG	1a	1661	1/1	0.90	0.23	57,57,57,57	0
56	MG	2A	3107	1/1	0.90	0.13	50,50,50,50	0
56	MG	1A	3053	1/1	0.90	0.44	38,38,38,38	0
56	MG	1A	3906	1/1	0.90	0.09	42,42,42,42	0
56	MG	2a	3234	1/1	0.90	0.57	79,79,79,79	0
56	MG	2A	3113	1/1	0.90	0.08	54,54,54,54	0
56	MG	2A	3117	1/1	0.90	0.37	51,51,51,51	0
56	MG	1A	3013	1/1	0.90	0.26	64,64,64,64	0
56	MG	2A	3512	1/1	0.90	0.09	40,40,40,40	0
56	MG	2k	3002	1/1	0.90	0.14	66,66,66,66	0
56	MG	2A	3127	1/1	0.90	0.17	54,54,54,54	0
56	MG	2A	3130	1/1	0.90	0.15	50,50,50,50	0
56	MG	2n	503	1/1	0.90	0.08	64,64,64,64	0
56	MG	2A	3131	1/1	0.90	0.17	48,48,48,48	0
56	MG	1B	224	1/1	0.90	0.18	69,69,69,69	0
56	MG	1A	3921	1/1	0.90	0.12	80,80,80,80	0
56	MG	1D	301	1/1	0.90	0.22	58,58,58,58	0
56	MG	2A	3139	1/1	0.90	0.31	47,47,47,47	0
56	MG	2A	3146	1/1	0.91	0.30	41,41,41,41	0
56	MG	1a	1858	1/1	0.91	0.20	69,69,69,69	0
56	MG	2A	3527	1/1	0.91	0.17	68,68,68,68	0
56	MG	1a	1865	1/1	0.91	0.18	65,65,65,65	0
56	MG	1A	3110	1/1	0.91	0.13	39,39,39,39	0
56	MG	1A	3225	1/1	0.91	0.22	40,40,40,40	0
56	MG	2A	3543	1/1	0.91	0.10	66,66,66,66	0
56	MG	2A	3156	1/1	0.91	0.15	53,53,53,53	0
56	MG	1a	1873	1/1	0.91	0.10	56,56,56,56	0
56	MG	2A	3565	1/1	0.91	0.09	62,62,62,62	0
56	MG	1a	1672	1/1	0.91	0.21	61,61,61,61	0
56	MG	2A	3569	1/1	0.91	0.13	41,41,41,41	0
56	MG	2A	3171	1/1	0.91	0.15	52,52,52,52	0
56	MG	1a	1881	1/1	0.91	0.18	84,84,84,84	0
56	MG	1A	3028	1/1	0.91	0.09	58,58,58,58	0
56	MG	1D	305	1/1	0.91	0.25	58,58,58,58	0
56	MG	1A	3184	1/1	0.91	0.05	61,61,61,61	0
56	MG	2A	3188	1/1	0.91	0.25	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	1A	3081	1/1	0.91	0.34	62,62,62,62	0
56	MG	1a	1894	1/1	0.91	0.45	56,56,56,56	0
56	MG	1A	3346	1/1	0.91	0.36	33,33,33,33	0
56	MG	1A	3241	1/1	0.91	0.22	49,49,49,49	0
56	MG	1A	3454	1/1	0.91	0.43	50,50,50,50	0
56	MG	1A	3954	1/1	0.91	0.19	83,83,83,83	0
56	MG	2B	3008	1/1	0.91	0.15	73,73,73,73	0
56	MG	1A	3764	1/1	0.91	0.14	54,54,54,54	0
56	MG	1A	3405	1/1	0.91	0.08	59,59,59,59	0
56	MG	2A	3204	1/1	0.91	0.12	53,53,53,53	0
56	MG	1a	1698	1/1	0.91	0.27	75,75,75,75	0
56	MG	2A	3210	1/1	0.91	0.18	49,49,49,49	0
56	MG	1A	3518	1/1	0.91	0.36	52,52,52,52	0
56	MG	1A	3783	1/1	0.91	0.16	22,22,22,22	0
56	MG	1a	1701	1/1	0.91	0.24	50,50,50,50	0
56	MG	2Q	203	1/1	0.91	0.12	52,52,52,52	0
56	MG	2Q	205	1/1	0.91	0.26	57,57,57,57	0
56	MG	2U	201	1/1	0.91	0.19	40,40,40,40	0
56	MG	20	8001	1/1	0.91	0.17	72,72,72,72	0
56	MG	1A	3196	1/1	0.91	0.15	45,45,45,45	0
56	MG	1o	3001	1/1	0.91	0.06	77,77,77,77	0
56	MG	2A	3221	1/1	0.91	0.32	35,35,35,35	0
56	MG	2a	3002	1/1	0.91	0.43	68,68,68,68	0
56	MG	2A	3225	1/1	0.91	0.28	42,42,42,42	0
56	MG	1q	202	1/1	0.91	0.31	62,62,62,62	0
56	MG	2A	3230	1/1	0.91	0.49	51,51,51,51	0
56	MG	2A	3231	1/1	0.91	0.17	53,53,53,53	0
56	MG	1A	3158	1/1	0.91	0.18	37,37,37,37	0
56	MG	1A	3972	1/1	0.91	0.13	22,22,22,22	0
56	MG	1A	3523	1/1	0.91	0.16	59,59,59,59	0
56	MG	1N	205	1/1	0.91	0.17	53,53,53,53	0
56	MG	2A	3243	1/1	0.91	0.18	62,62,62,62	0
56	MG	2a	3017	1/1	0.91	0.91	68,68,68,68	0
56	MG	1A	3199	1/1	0.91	0.30	48,48,48,48	0
56	MG	1A	3799	1/1	0.91	0.34	54,54,54,54	0
56	MG	1P	203	1/1	0.91	0.23	67,67,67,67	0
56	MG	1A	3532	1/1	0.91	0.31	43,43,43,43	0
56	MG	1R	201	1/1	0.91	0.25	38,38,38,38	0
56	MG	1A	3410	1/1	0.91	0.17	51,51,51,51	0
56	MG	1R	205	1/1	0.91	0.40	52,52,52,52	0
56	MG	1T	202	1/1	0.91	0.08	43,43,43,43	0
56	MG	1A	3556	1/1	0.91	0.12	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	1T	204	1/1	0.91	0.13	72,72,72,72	0
56	MG	1A	3021	1/1	0.91	0.24	48,48,48,48	0
56	MG	2A	3275	1/1	0.91	0.21	34,34,34,34	0
56	MG	2A	3006	1/1	0.91	0.14	71,71,71,71	0
56	MG	1A	3249	1/1	0.91	0.27	53,53,53,53	0
56	MG	2a	3039	1/1	0.91	0.41	75,75,75,75	0
56	MG	2A	3280	1/1	0.91	0.15	46,46,46,46	0
56	MG	2A	3283	1/1	0.91	0.13	51,51,51,51	0
56	MG	2A	3286	1/1	0.91	0.19	47,47,47,47	0
56	MG	1A	3006	1/1	0.91	0.37	61,61,61,61	0
56	MG	2A	3009	1/1	0.91	0.58	56,56,56,56	0
56	MG	1Z	301	1/1	0.91	0.07	74,74,74,74	0
56	MG	1A	3986	1/1	0.91	0.20	44,44,44,44	0
56	MG	2a	3055	1/1	0.91	0.22	70,70,70,70	0
56	MG	2A	3295	1/1	0.91	0.09	50,50,50,50	0
56	MG	1A	3165	1/1	0.91	0.34	48,48,48,48	0
56	MG	2a	3065	1/1	0.91	0.10	84,84,84,84	0
56	MG	2A	3303	1/1	0.91	0.11	42,42,42,42	0
56	MG	1A	3826	1/1	0.91	0.13	35,35,35,35	0
56	MG	1a	1754	1/1	0.91	0.20	53,53,53,53	0
56	MG	1A	3991	1/1	0.91	0.25	53,53,53,53	0
56	MG	1A	3283	1/1	0.91	0.18	60,60,60,60	0
56	MG	2A	3324	1/1	0.91	0.27	64,64,64,64	0
56	MG	1A	3993	1/1	0.91	0.13	73,73,73,73	0
56	MG	1A	3371	1/1	0.91	0.20	39,39,39,39	0
56	MG	1A	3597	1/1	0.91	0.13	49,49,49,49	0
56	MG	2a	3086	1/1	0.91	0.48	65,65,65,65	0
56	MG	2A	3030	1/1	0.91	0.08	57,57,57,57	0
56	MG	1A	3599	1/1	0.91	0.16	51,51,51,51	0
56	MG	2A	3036	1/1	0.91	0.23	35,35,35,35	0
56	MG	1A	3136	1/1	0.91	0.39	47,47,47,47	0
56	MG	1A	3601	1/1	0.91	0.23	28,28,28,28	0
56	MG	18	103	1/1	0.91	0.12	49,49,49,49	0
56	MG	2a	3105	1/1	0.91	0.29	58,58,58,58	0
56	MG	1A	3604	1/1	0.91	0.19	26,26,26,26	0
56	MG	2A	3053	1/1	0.91	0.40	49,49,49,49	0
56	MG	19	503	1/1	0.91	0.27	61,61,61,61	0
56	MG	1A	3420	1/1	0.91	0.15	50,50,50,50	0
56	MG	2A	3059	1/1	0.91	0.14	50,50,50,50	0
56	MG	2a	3122	1/1	0.91	0.18	69,69,69,69	0
56	MG	2a	3123	1/1	0.91	0.18	57,57,57,57	0
56	MG	1A	3482	1/1	0.91	0.17	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	2A	3383	1/1	0.91	0.15	64,64,64,64	0
56	MG	1a	1606	1/1	0.91	0.12	73,73,73,73	0
56	MG	1A	3484	1/1	0.91	0.12	70,70,70,70	0
56	MG	1A	3626	1/1	0.91	0.10	24,24,24,24	0
56	MG	2A	3392	1/1	0.91	0.36	43,43,43,43	0
56	MG	1A	3631	1/1	0.91	0.15	55,55,55,55	0
56	MG	1a	1614	1/1	0.91	0.16	57,57,57,57	0
56	MG	2A	3073	1/1	0.91	0.30	37,37,37,37	0
56	MG	2A	3410	1/1	0.91	0.24	40,40,40,40	0
56	MG	1A	4021	1/1	0.91	0.23	33,33,33,33	0
56	MG	2a	3146	1/1	0.91	0.16	66,66,66,66	0
56	MG	1A	3038	1/1	0.91	0.10	52,52,52,52	0
56	MG	2A	3076	1/1	0.91	0.47	61,61,61,61	0
56	MG	1A	3638	1/1	0.91	0.24	22,22,22,22	0
56	MG	2a	3151	1/1	0.91	0.09	64,64,64,64	0
56	MG	1A	3640	1/1	0.91	0.09	70,70,70,70	0
56	MG	2A	3082	1/1	0.91	0.16	56,56,56,56	0
56	MG	2a	3154	1/1	0.91	0.20	84,84,84,84	0
56	MG	2a	3155	1/1	0.91	0.35	91,91,91,91	0
56	MG	1A	3869	1/1	0.91	0.22	85,85,85,85	0
56	MG	1A	3379	1/1	0.91	0.19	47,47,47,47	0
56	MG	1A	4037	1/1	0.91	0.26	62,62,62,62	0
56	MG	1A	4039	1/1	0.91	0.27	56,56,56,56	0
56	MG	1A	3489	1/1	0.91	0.33	55,55,55,55	0
56	MG	2A	3447	1/1	0.91	0.15	77,77,77,77	0
56	MG	1a	1637	1/1	0.91	0.17	64,64,64,64	0
56	MG	1A	3658	1/1	0.91	0.21	21,21,21,21	0
56	MG	2a	3181	1/1	0.91	0.15	71,71,71,71	0
56	MG	1A	4046	1/1	0.91	0.17	56,56,56,56	0
56	MG	1a	1807	1/1	0.91	0.19	71,71,71,71	0
56	MG	1a	1809	1/1	0.91	0.17	67,67,67,67	0
56	MG	1A	3876	1/1	0.91	0.22	68,68,68,68	0
56	MG	1a	1811	1/1	0.91	0.30	71,71,71,71	0
56	MG	2a	3194	1/1	0.91	0.43	75,75,75,75	0
56	MG	1A	3425	1/1	0.91	0.15	57,57,57,57	0
56	MG	1A	3381	1/1	0.91	0.16	61,61,61,61	0
56	MG	1A	3433	1/1	0.91	0.18	50,50,50,50	0
56	MG	2A	3110	1/1	0.91	0.30	49,49,49,49	0
56	MG	1a	1648	1/1	0.91	0.23	64,64,64,64	0
56	MG	2A	3482	1/1	0.91	0.21	63,63,63,63	0
56	MG	2a	3222	1/1	0.91	0.17	67,67,67,67	0
56	MG	2a	3224	1/1	0.91	0.12	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3231	1/1	0.91	0.29	79,79,79,79	0
56	MG	1a	1821	1/1	0.91	0.14	77,77,77,77	0
56	MG	2A	3491	1/1	0.91	0.11	39,39,39,39	0
56	MG	2a	3236	1/1	0.91	0.22	67,67,67,67	0
56	MG	1A	3254	1/1	0.91	0.21	32,32,32,32	0
56	MG	2A	3497	1/1	0.91	0.24	49,49,49,49	0
56	MG	2A	3124	1/1	0.91	0.06	62,62,62,62	0
56	MG	1A	3170	1/1	0.91	0.28	32,32,32,32	0
56	MG	1B	211	1/1	0.91	0.30	54,54,54,54	0
56	MG	1A	3005	1/1	0.91	0.27	60,60,60,60	0
56	MG	2A	3507	1/1	0.91	0.12	48,48,48,48	0
56	MG	1A	3221	1/1	0.91	0.27	56,56,56,56	0
56	MG	2A	3135	1/1	0.91	0.16	48,48,48,48	0
56	MG	1A	3390	1/1	0.91	0.09	54,54,54,54	0
56	MG	2A	3518	1/1	0.91	0.17	67,67,67,67	0
56	MG	1a	1666	1/1	0.91	0.14	55,55,55,55	0
56	MG	1A	3907	1/1	0.91	0.17	13,13,13,13	0
56	MG	2O	203	1/1	0.92	0.19	57,57,57,57	0
56	MG	2P	201	1/1	0.92	0.26	33,33,33,33	0
56	MG	1D	315	1/1	0.92	0.32	56,56,56,56	0
56	MG	2A	3291	1/1	0.92	0.45	56,56,56,56	0
56	MG	1a	1645	1/1	0.92	0.11	71,71,71,71	0
56	MG	1A	3971	1/1	0.92	0.22	61,61,61,61	0
56	MG	2A	3294	1/1	0.92	0.28	58,58,58,58	0
56	MG	25	502	1/1	0.92	0.57	56,56,56,56	0
56	MG	1E	305	1/1	0.92	0.24	58,58,58,58	0
56	MG	1A	3185	1/1	0.92	0.09	44,44,44,44	0
56	MG	1E	308	1/1	0.92	0.21	70,70,70,70	0
56	MG	1A	3224	1/1	0.92	0.16	36,36,36,36	0
56	MG	1A	3633	1/1	0.92	0.15	29,29,29,29	0
56	MG	2A	3311	1/1	0.92	0.20	44,44,44,44	0
56	MG	1A	3511	1/1	0.92	0.32	51,51,51,51	0
56	MG	2a	3007	1/1	0.92	0.09	91,91,91,91	0
56	MG	2A	3317	1/1	0.92	0.25	40,40,40,40	0
56	MG	1A	3051	1/1	0.92	0.16	57,57,57,57	0
56	MG	2A	3322	1/1	0.92	0.14	29,29,29,29	0
56	MG	1a	1816	1/1	0.92	0.21	88,88,88,88	0
56	MG	2A	3327	1/1	0.92	0.10	68,68,68,68	0
56	MG	1a	1665	1/1	0.92	0.18	47,47,47,47	0
56	MG	1A	3077	1/1	0.92	0.22	53,53,53,53	0
56	MG	2A	3333	1/1	0.92	0.08	61,61,61,61	0
56	MG	2a	3019	1/1	0.92	0.17	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3334	1/1	0.92	0.16	44,44,44,44	0
56	MG	2A	3337	1/1	0.92	0.12	41,41,41,41	0
56	MG	1A	3327	1/1	0.92	0.07	64,64,64,64	0
56	MG	1A	3842	1/1	0.92	0.30	55,55,55,55	0
56	MG	2A	3341	1/1	0.92	0.13	39,39,39,39	0
56	MG	1A	3330	1/1	0.92	0.27	62,62,62,62	0
56	MG	2A	3355	1/1	0.92	0.14	42,42,42,42	0
56	MG	1A	3041	1/1	0.92	0.21	56,56,56,56	0
56	MG	2a	3033	1/1	0.92	0.13	76,76,76,76	0
56	MG	1A	3231	1/1	0.92	0.40	42,42,42,42	0
56	MG	1A	3260	1/1	0.92	0.18	49,49,49,49	0
56	MG	2A	3094	1/1	0.92	0.23	48,48,48,48	0
56	MG	1A	3237	1/1	0.92	0.20	52,52,52,52	0
56	MG	1A	3426	1/1	0.92	0.48	67,67,67,67	0
56	MG	1a	1683	1/1	0.92	0.67	56,56,56,56	0
56	MG	2A	3098	1/1	0.92	0.08	53,53,53,53	0
56	MG	1a	1853	1/1	0.92	0.06	56,56,56,56	0
56	MG	1A	3480	1/1	0.92	0.18	75,75,75,75	0
56	MG	1a	1861	1/1	0.92	0.25	68,68,68,68	0
56	MG	2a	3045	1/1	0.92	0.16	81,81,81,81	0
56	MG	1a	1686	1/1	0.92	0.17	53,53,53,53	0
56	MG	2A	3387	1/1	0.92	0.15	51,51,51,51	0
56	MG	1A	3686	1/1	0.92	0.24	58,58,58,58	0
56	MG	2a	3051	1/1	0.92	0.22	76,76,76,76	0
56	MG	1a	1691	1/1	0.92	0.15	50,50,50,50	0
56	MG	1Q	3003	1/1	0.92	0.21	54,54,54,54	0
56	MG	1Q	3004	1/1	0.92	0.43	46,46,46,46	0
56	MG	2a	3063	1/1	0.92	0.13	66,66,66,66	0
56	MG	1a	1878	1/1	0.92	0.09	78,78,78,78	0
56	MG	2A	3396	1/1	0.92	0.15	44,44,44,44	0
56	MG	1a	1879	1/1	0.92	0.20	51,51,51,51	0
56	MG	2a	3076	1/1	0.92	0.39	68,68,68,68	0
56	MG	1A	3692	1/1	0.92	0.18	57,57,57,57	0
56	MG	1A	3997	1/1	0.92	0.11	18,18,18,18	0
56	MG	1A	3338	1/1	0.92	0.09	55,55,55,55	0
56	MG	1a	1885	1/1	0.92	0.20	66,66,66,66	0
56	MG	2A	3134	1/1	0.92	0.15	35,35,35,35	0
56	MG	1a	1888	1/1	0.92	0.20	75,75,75,75	0
56	MG	1A	3546	1/1	0.92	0.17	41,41,41,41	0
56	MG	1A	3162	1/1	0.92	0.38	38,38,38,38	0
56	MG	1A	3552	1/1	0.92	0.29	58,58,58,58	0
56	MG	2A	3440	1/1	0.92	0.16	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	3090	1/1	0.92	0.22	60,60,60,60	0
56	MG	1A	4007	1/1	0.92	0.31	58,58,58,58	0
56	MG	1A	3483	1/1	0.92	0.26	65,65,65,65	0
56	MG	1U	203	1/1	0.92	0.73	40,40,40,40	0
56	MG	1W	3002	1/1	0.92	0.21	47,47,47,47	0
56	MG	2a	3103	1/1	0.92	0.18	59,59,59,59	0
56	MG	1a	1722	1/1	0.92	0.31	60,60,60,60	0
56	MG	1W	3004	1/1	0.92	0.24	43,43,43,43	0
56	MG	1W	3005	1/1	0.92	0.12	41,41,41,41	0
56	MG	1e	204	1/1	0.92	0.10	64,64,64,64	0
56	MG	1a	1726	1/1	0.92	0.26	66,66,66,66	0
56	MG	2A	3462	1/1	0.92	0.41	74,74,74,74	0
56	MG	2A	3173	1/1	0.92	0.22	49,49,49,49	0
56	MG	1W	3006	1/1	0.92	0.40	42,42,42,42	0
56	MG	1h	3002	1/1	0.92	0.22	64,64,64,64	0
56	MG	1A	3036	1/1	0.92	0.24	52,52,52,52	0
56	MG	1A	3720	1/1	0.92	0.31	64,64,64,64	0
56	MG	2a	3127	1/1	0.92	0.28	51,51,51,51	0
56	MG	2a	3128	1/1	0.92	0.43	63,63,63,63	0
56	MG	1A	4017	1/1	0.92	0.28	41,41,41,41	0
56	MG	1A	3134	1/1	0.92	0.15	31,31,31,31	0
56	MG	2a	3132	1/1	0.92	0.13	71,71,71,71	0
56	MG	1A	3055	1/1	0.92	0.19	55,55,55,55	0
56	MG	1A	3883	1/1	0.92	0.09	66,66,66,66	0
56	MG	1A	3731	1/1	0.92	0.18	29,29,29,29	0
56	MG	1r	3003	1/1	0.92	0.07	58,58,58,58	0
56	MG	2a	3139	1/1	0.92	0.20	94,94,94,94	0
56	MG	2a	3140	1/1	0.92	0.19	83,83,83,83	0
56	MG	2a	3141	1/1	0.92	0.18	57,57,57,57	0
56	MG	1A	3739	1/1	0.92	0.18	22,22,22,22	0
56	MG	1A	3575	1/1	0.92	0.11	39,39,39,39	0
56	MG	2A	3201	1/1	0.92	0.20	52,52,52,52	0
56	MG	1a	1743	1/1	0.92	0.99	71,71,71,71	0
56	MG	1A	3751	1/1	0.92	0.19	40,40,40,40	0
56	MG	1A	3577	1/1	0.92	0.10	38,38,38,38	0
56	MG	1x	107	1/1	0.92	0.06	64,64,64,64	0
56	MG	2A	3211	1/1	0.92	0.15	52,52,52,52	0
56	MG	1A	4034	1/1	0.92	0.23	44,44,44,44	0
56	MG	1A	3208	1/1	0.92	0.08	57,57,57,57	0
56	MG	1A	3903	1/1	0.92	0.11	66,66,66,66	0
56	MG	1A	3584	1/1	0.92	0.11	52,52,52,52	0
56	MG	2A	3522	1/1	0.92	0.24	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3523	1/1	0.92	0.19	57,57,57,57	0
56	MG	1A	3306	1/1	0.92	0.26	62,62,62,62	0
56	MG	1a	1755	1/1	0.92	0.33	60,60,60,60	0
56	MG	2A	3224	1/1	0.92	0.15	33,33,33,33	0
56	MG	2A	3528	1/1	0.92	0.08	56,56,56,56	0
56	MG	1A	3020	1/1	0.92	0.26	56,56,56,56	0
56	MG	1A	3778	1/1	0.92	0.17	20,20,20,20	0
56	MG	2A	3540	1/1	0.92	0.31	39,39,39,39	0
56	MG	2a	3185	1/1	0.92	0.21	79,79,79,79	0
56	MG	1a	1602	1/1	0.92	0.24	51,51,51,51	0
56	MG	1A	3924	1/1	0.92	0.11	67,67,67,67	0
56	MG	2A	3236	1/1	0.92	0.28	41,41,41,41	0
56	MG	2A	3550	1/1	0.92	0.45	37,37,37,37	0
56	MG	1a	1761	1/1	0.92	0.23	66,66,66,66	0
56	MG	2a	3195	1/1	0.92	0.12	53,53,53,53	0
56	MG	1B	202	1/1	0.92	0.20	59,59,59,59	0
56	MG	1A	3925	1/1	0.92	0.17	54,54,54,54	0
56	MG	1A	3593	1/1	0.92	0.23	30,30,30,30	0
56	MG	1a	1611	1/1	0.92	0.16	85,85,85,85	0
56	MG	1A	3349	1/1	0.92	0.29	51,51,51,51	0
56	MG	1A	3938	1/1	0.92	0.17	47,47,47,47	0
56	MG	1A	3248	1/1	0.92	0.27	60,60,60,60	0
56	MG	1A	3095	1/1	0.92	0.22	41,41,41,41	0
56	MG	1A	3010	1/1	0.92	0.38	53,53,53,53	0
56	MG	1A	3014	1/1	0.92	0.11	58,58,58,58	0
56	MG	1A	3605	1/1	0.92	0.23	35,35,35,35	0
56	MG	1a	1626	1/1	0.92	0.45	69,69,69,69	0
56	MG	2a	3238	1/1	0.92	0.53	61,61,61,61	0
56	MG	1A	3318	1/1	0.92	0.12	46,46,46,46	0
56	MG	2a	3241	1/1	0.92	0.22	67,67,67,67	0
56	MG	2a	3242	1/1	0.92	0.12	57,57,57,57	0
56	MG	1A	3807	1/1	0.92	0.16	58,58,58,58	0
56	MG	1A	3411	1/1	0.92	0.18	51,51,51,51	0
56	MG	2e	3001	1/1	0.92	0.06	68,68,68,68	0
56	MG	2A	3273	1/1	0.92	0.15	36,36,36,36	0
56	MG	1A	3811	1/1	0.92	0.17	50,50,50,50	0
56	MG	2D	302	1/1	0.92	0.10	57,57,57,57	0
56	MG	1D	303	1/1	0.92	0.23	47,47,47,47	0
56	MG	1A	3040	1/1	0.92	0.24	58,58,58,58	0
56	MG	1a	1639	1/1	0.92	0.08	70,70,70,70	0
56	MG	1A	3816	1/1	0.92	0.10	67,67,67,67	0
56	MG	2x	3001	1/1	0.92	0.06	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	2x	3002	1/1	0.92	0.06	58,58,58,58	0
56	MG	2F	301	1/1	0.92	0.22	63,63,63,63	0
56	MG	2x	3006	1/1	0.92	0.08	78,78,78,78	0
56	MG	1D	309	1/1	0.92	0.12	37,37,37,37	0
56	MG	1D	314	1/1	0.92	0.14	48,48,48,48	0
56	MG	2A	3302	1/1	0.93	0.13	64,64,64,64	0
56	MG	1A	3730	1/1	0.93	0.17	33,33,33,33	0
56	MG	2A	3060	1/1	0.93	0.24	42,42,42,42	0
56	MG	1B	212	1/1	0.93	0.14	47,47,47,47	0
56	MG	2A	3309	1/1	0.93	0.29	44,44,44,44	0
56	MG	1a	1631	1/1	0.93	0.24	44,44,44,44	0
56	MG	1a	1790	1/1	0.93	0.20	33,33,33,33	0
56	MG	1B	213	1/1	0.93	0.41	65,65,65,65	0
56	MG	1A	3573	1/1	0.93	0.10	74,74,74,74	0
56	MG	1A	3732	1/1	0.93	0.12	32,32,32,32	0
56	MG	2A	3323	1/1	0.93	0.14	54,54,54,54	0
56	MG	1A	3738	1/1	0.93	0.22	18,18,18,18	0
56	MG	1a	1801	1/1	0.93	0.19	70,70,70,70	0
56	MG	1A	3088	1/1	0.93	0.17	52,52,52,52	0
56	MG	1A	3061	1/1	0.93	0.51	51,51,51,51	0
56	MG	1A	3154	1/1	0.93	0.40	44,44,44,44	0
56	MG	1a	1808	1/1	0.93	0.41	85,85,85,85	0
56	MG	1A	3276	1/1	0.93	0.22	74,74,74,74	0
56	MG	1A	3428	1/1	0.93	0.10	55,55,55,55	0
56	MG	1A	3485	1/1	0.93	0.11	67,67,67,67	0
56	MG	1A	3765	1/1	0.93	0.14	56,56,56,56	0
56	MG	1a	1651	1/1	0.93	0.13	61,61,61,61	0
56	MG	2A	3353	1/1	0.93	0.21	54,54,54,54	0
56	MG	1a	1815	1/1	0.93	0.09	70,70,70,70	0
56	MG	1A	3590	1/1	0.93	0.16	56,56,56,56	0
56	MG	1D	312	1/1	0.93	0.18	47,47,47,47	0
56	MG	1A	3949	1/1	0.93	0.30	59,59,59,59	0
56	MG	1A	3387	1/1	0.93	0.05	64,64,64,64	0
56	MG	1a	1822	1/1	0.93	0.17	74,74,74,74	0
56	MG	1D	317	1/1	0.93	0.21	69,69,69,69	0
56	MG	2A	3372	1/1	0.93	0.18	62,62,62,62	0
56	MG	1A	3388	1/1	0.93	0.30	42,42,42,42	0
56	MG	1A	3956	1/1	0.93	0.09	69,69,69,69	0
56	MG	1a	1829	1/1	0.93	0.17	73,73,73,73	0
56	MG	1a	1833	1/1	0.93	0.24	47,47,47,47	0
56	MG	1A	3958	1/1	0.93	0.15	46,46,46,46	0
56	MG	1A	3780	1/1	0.93	0.10	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	1668	1/1	0.93	0.06	71,71,71,71	0
56	MG	1A	3488	1/1	0.93	0.15	53,53,53,53	0
56	MG	1F	303	1/1	0.93	0.16	40,40,40,40	0
56	MG	1A	3308	1/1	0.93	0.15	64,64,64,64	0
56	MG	1A	3232	1/1	0.93	0.17	57,57,57,57	0
56	MG	2A	3126	1/1	0.93	0.35	54,54,54,54	0
56	MG	1a	1860	1/1	0.93	0.40	61,61,61,61	0
56	MG	2a	3054	1/1	0.93	0.14	83,83,83,83	0
56	MG	1A	3437	1/1	0.93	0.49	56,56,56,56	0
56	MG	1a	1680	1/1	0.93	0.18	57,57,57,57	0
56	MG	2a	3057	1/1	0.93	0.36	75,75,75,75	0
56	MG	1A	3793	1/1	0.93	0.09	72,72,72,72	0
56	MG	1a	1867	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3391	1/1	0.93	0.26	56,56,56,56	0
56	MG	2A	3426	1/1	0.93	0.24	67,67,67,67	0
56	MG	1A	3311	1/1	0.93	0.14	57,57,57,57	0
56	MG	2a	3074	1/1	0.93	0.12	63,63,63,63	0
56	MG	1A	3801	1/1	0.93	0.14	52,52,52,52	0
56	MG	2A	3432	1/1	0.93	0.21	64,64,64,64	0
56	MG	1A	3394	1/1	0.93	0.10	58,58,58,58	0
56	MG	1a	1688	1/1	0.93	0.25	76,76,76,76	0
56	MG	1A	3977	1/1	0.93	0.30	50,50,50,50	0
56	MG	1A	3343	1/1	0.93	0.28	31,31,31,31	0
56	MG	1A	3236	1/1	0.93	0.26	49,49,49,49	0
56	MG	2A	3442	1/1	0.93	0.17	66,66,66,66	0
56	MG	1A	3623	1/1	0.93	0.35	40,40,40,40	0
56	MG	2a	3087	1/1	0.93	0.45	60,60,60,60	0
56	MG	2A	3154	1/1	0.93	0.34	55,55,55,55	0
56	MG	1A	3624	1/1	0.93	0.19	35,35,35,35	0
56	MG	2A	3161	1/1	0.93	0.32	46,46,46,46	0
56	MG	1A	3445	1/1	0.93	0.13	58,58,58,58	0
56	MG	1A	3627	1/1	0.93	0.20	20,20,20,20	0
56	MG	2A	3168	1/1	0.93	0.46	51,51,51,51	0
56	MG	1A	3817	1/1	0.93	0.27	61,61,61,61	0
56	MG	1A	3155	1/1	0.93	0.27	51,51,51,51	0
56	MG	2A	3174	1/1	0.93	0.42	48,48,48,48	0
56	MG	2A	3468	1/1	0.93	0.13	64,64,64,64	0
56	MG	1A	3025	1/1	0.93	0.11	60,60,60,60	0
56	MG	2A	3471	1/1	0.93	0.25	54,54,54,54	0
56	MG	2a	3112	1/1	0.93	0.11	67,67,67,67	0
56	MG	1R	203	1/1	0.93	0.23	56,56,56,56	0
56	MG	1A	3011	1/1	0.93	0.66	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3449	1/1	0.93	0.21	77,77,77,77	0
56	MG	1A	3317	1/1	0.93	0.23	67,67,67,67	0
56	MG	1A	3121	1/1	0.93	0.42	42,42,42,42	0
56	MG	1d	302	1/1	0.93	0.09	70,70,70,70	0
56	MG	1A	3161	1/1	0.93	0.17	61,61,61,61	0
56	MG	2A	3487	1/1	0.93	0.46	60,60,60,60	0
56	MG	2A	3489	1/1	0.93	0.32	43,43,43,43	0
56	MG	1A	3838	1/1	0.93	0.14	45,45,45,45	0
56	MG	1A	3839	1/1	0.93	0.28	54,54,54,54	0
56	MG	2A	3196	1/1	0.93	0.06	37,37,37,37	0
56	MG	2A	3499	1/1	0.93	0.10	31,31,31,31	0
56	MG	1A	4000	1/1	0.93	0.26	54,54,54,54	0
56	MG	2a	3135	1/1	0.93	0.11	61,61,61,61	0
56	MG	1A	3650	1/1	0.93	0.30	46,46,46,46	0
56	MG	1A	3651	1/1	0.93	0.23	25,25,25,25	0
56	MG	1l	201	1/1	0.93	0.10	62,62,62,62	0
56	MG	2A	3203	1/1	0.93	0.21	58,58,58,58	0
56	MG	1A	3220	1/1	0.93	0.22	43,43,43,43	0
56	MG	1A	3361	1/1	0.93	0.31	59,59,59,59	0
56	MG	1A	3851	1/1	0.93	0.25	42,42,42,42	0
56	MG	1A	4011	1/1	0.93	0.37	48,48,48,48	0
56	MG	1A	3664	1/1	0.93	0.10	57,57,57,57	0
56	MG	1A	3670	1/1	0.93	0.10	56,56,56,56	0
56	MG	1A	3458	1/1	0.93	0.14	72,72,72,72	0
56	MG	1A	3096	1/1	0.93	0.14	40,40,40,40	0
56	MG	1A	3460	1/1	0.93	0.17	51,51,51,51	0
56	MG	1A	3680	1/1	0.93	0.07	71,71,71,71	0
56	MG	2A	3526	1/1	0.93	0.22	54,54,54,54	0
56	MG	1A	3290	1/1	0.93	0.27	47,47,47,47	0
56	MG	13	101	1/1	0.93	0.21	52,52,52,52	0
56	MG	1A	3143	1/1	0.93	0.15	55,55,55,55	0
56	MG	2A	3530	1/1	0.93	0.20	48,48,48,48	0
56	MG	1a	1751	1/1	0.93	0.23	63,63,63,63	0
56	MG	2A	3535	1/1	0.93	0.14	69,69,69,69	0
56	MG	2a	3170	1/1	0.93	0.21	53,53,53,53	0
56	MG	2A	3536	1/1	0.93	0.11	67,67,67,67	0
56	MG	2A	3538	1/1	0.93	0.19	52,52,52,52	0
56	MG	2a	3176	1/1	0.93	0.37	87,87,87,87	0
56	MG	2A	3539	1/1	0.93	0.24	48,48,48,48	0
56	MG	1a	1752	1/1	0.93	0.20	72,72,72,72	0
56	MG	2A	3234	1/1	0.93	0.49	52,52,52,52	0
56	MG	1A	4026	1/1	0.93	0.63	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	15	103	1/1	0.93	0.21	45,45,45,45	0
56	MG	1A	3690	1/1	0.93	0.36	41,41,41,41	0
56	MG	2A	3558	1/1	0.93	0.12	37,37,37,37	0
56	MG	17	104	1/1	0.93	0.32	57,57,57,57	0
56	MG	1A	3691	1/1	0.93	0.27	59,59,59,59	0
56	MG	1A	4032	1/1	0.93	0.62	47,47,47,47	0
56	MG	1a	1759	1/1	0.93	0.10	82,82,82,82	0
56	MG	1A	3367	1/1	0.93	0.33	51,51,51,51	0
56	MG	2a	3203	1/1	0.93	0.10	53,53,53,53	0
56	MG	2a	3204	1/1	0.93	0.20	62,62,62,62	0
56	MG	2A	3010	1/1	0.93	0.43	51,51,51,51	0
56	MG	2a	3207	1/1	0.93	0.14	58,58,58,58	0
56	MG	2a	3208	1/1	0.93	0.12	68,68,68,68	0
56	MG	1A	3528	1/1	0.93	0.45	54,54,54,54	0
56	MG	1A	4035	1/1	0.93	0.10	81,81,81,81	0
56	MG	2A	3576	1/1	0.93	0.49	50,50,50,50	0
56	MG	1A	3468	1/1	0.93	0.15	59,59,59,59	0
56	MG	1A	3875	1/1	0.93	0.17	50,50,50,50	0
56	MG	2a	3225	1/1	0.93	0.49	67,67,67,67	0
56	MG	1a	1605	1/1	0.93	0.12	84,84,84,84	0
56	MG	1A	3292	1/1	0.93	0.10	44,44,44,44	0
56	MG	2A	3024	1/1	0.93	0.12	67,67,67,67	0
56	MG	1A	3878	1/1	0.93	0.23	60,60,60,60	0
56	MG	1A	3701	1/1	0.93	0.14	22,22,22,22	0
56	MG	2a	3239	1/1	0.93	0.43	60,60,60,60	0
56	MG	1a	1770	1/1	0.93	0.15	87,87,87,87	0
56	MG	1A	3702	1/1	0.93	0.10	73,73,73,73	0
56	MG	1A	3369	1/1	0.93	0.22	49,49,49,49	0
56	MG	2B	3010	1/1	0.93	0.26	66,66,66,66	0
56	MG	1B	201	1/1	0.93	0.14	44,44,44,44	0
56	MG	1A	3328	1/1	0.93	0.12	56,56,56,56	0
56	MG	2A	3285	1/1	0.93	0.27	58,58,58,58	0
56	MG	1A	3267	1/1	0.93	0.36	57,57,57,57	0
56	MG	2E	304	1/1	0.93	0.68	74,74,74,74	0
56	MG	1B	204	1/1	0.93	0.13	53,53,53,53	0
56	MG	1A	3567	1/1	0.93	0.25	51,51,51,51	0
56	MG	2A	3050	1/1	0.93	0.09	44,44,44,44	0
56	MG	1A	3198	1/1	0.93	0.42	41,41,41,41	0
56	MG	1A	3724	1/1	0.93	0.34	55,55,55,55	0
56	MG	2A	3054	1/1	0.93	0.09	41,41,41,41	0
56	MG	1A	3123	1/1	0.93	0.27	25,25,25,25	0
56	MG	2A	3296	1/1	0.93	0.21	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2Q	204	1/1	0.93	0.23	46,46,46,46	0
56	MG	1a	1786	1/1	0.93	0.08	83,83,83,83	0
56	MG	2A	3537	1/1	0.94	0.29	59,59,59,59	0
56	MG	2A	3184	1/1	0.94	0.26	59,59,59,59	0
56	MG	1A	3725	1/1	0.94	0.13	39,39,39,39	0
56	MG	1A	3915	1/1	0.94	0.17	38,38,38,38	0
56	MG	1D	302	1/1	0.94	0.18	33,33,33,33	0
56	MG	1a	1877	1/1	0.94	0.29	56,56,56,56	0
56	MG	1A	3186	1/1	0.94	0.15	47,47,47,47	0
56	MG	2A	3547	1/1	0.94	0.34	37,37,37,37	0
56	MG	1A	3917	1/1	0.94	0.25	60,60,60,60	0
56	MG	1A	3920	1/1	0.94	0.13	23,23,23,23	0
56	MG	2A	3562	1/1	0.94	0.24	37,37,37,37	0
56	MG	1D	307	1/1	0.94	0.15	39,39,39,39	0
56	MG	1a	1675	1/1	0.94	0.15	62,62,62,62	0
56	MG	1A	3353	1/1	0.94	0.20	57,57,57,57	0
56	MG	1A	3356	1/1	0.94	0.18	49,49,49,49	0
56	MG	1A	3357	1/1	0.94	0.13	50,50,50,50	0
56	MG	1A	3926	1/1	0.94	0.16	66,66,66,66	0
56	MG	1D	316	1/1	0.94	0.49	76,76,76,76	0
56	MG	1A	3737	1/1	0.94	0.23	29,29,29,29	0
56	MG	2A	3207	1/1	0.94	0.28	23,23,23,23	0
56	MG	2A	3209	1/1	0.94	0.73	49,49,49,49	0
56	MG	1a	1685	1/1	0.94	0.15	23,23,23,23	0
56	MG	1A	3930	1/1	0.94	0.08	23,23,23,23	0
56	MG	1a	1901	1/1	0.94	0.14	46,46,46,46	0
56	MG	1E	304	1/1	0.94	0.21	64,64,64,64	0
56	MG	1a	1904	1/1	0.94	0.10	53,53,53,53	0
56	MG	1a	1906	1/1	0.94	0.14	83,83,83,83	0
56	MG	1A	3931	1/1	0.94	0.30	49,49,49,49	0
56	MG	1A	3188	1/1	0.94	0.23	54,54,54,54	0
56	MG	1A	3307	1/1	0.94	0.10	75,75,75,75	0
56	MG	1A	3939	1/1	0.94	0.24	57,57,57,57	0
56	MG	2A	3226	1/1	0.94	0.64	52,52,52,52	0
56	MG	2A	3227	1/1	0.94	0.41	49,49,49,49	0
56	MG	2A	3228	1/1	0.94	0.34	44,44,44,44	0
56	MG	1e	201	1/1	0.94	0.13	59,59,59,59	0
56	MG	1A	3744	1/1	0.94	0.16	63,63,63,63	0
56	MG	1A	3263	1/1	0.94	0.38	56,56,56,56	0
56	MG	2A	3233	1/1	0.94	0.26	62,62,62,62	0
56	MG	2F	302	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3581	1/1	0.94	0.13	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	1A	3944	1/1	0.94	0.27	19,19,19,19	0
56	MG	1A	3946	1/1	0.94	0.12	51,51,51,51	0
56	MG	1A	3755	1/1	0.94	0.05	65,65,65,65	0
56	MG	1a	1702	1/1	0.94	0.08	67,67,67,67	0
56	MG	1A	3757	1/1	0.94	0.12	41,41,41,41	0
56	MG	1a	1712	1/1	0.94	0.25	65,65,65,65	0
56	MG	1H	203	1/1	0.94	0.20	60,60,60,60	0
56	MG	1A	3952	1/1	0.94	0.24	57,57,57,57	0
56	MG	1A	3230	1/1	0.94	0.11	61,61,61,61	0
56	MG	2A	3249	1/1	0.94	0.15	57,57,57,57	0
56	MG	1a	1718	1/1	0.94	0.14	64,64,64,64	0
56	MG	1a	1719	1/1	0.94	0.21	47,47,47,47	0
56	MG	1A	3418	1/1	0.94	0.39	43,43,43,43	0
56	MG	1A	3588	1/1	0.94	0.12	69,69,69,69	0
56	MG	1x	103	1/1	0.94	0.11	70,70,70,70	0
56	MG	2A	3265	1/1	0.94	0.17	59,59,59,59	0
56	MG	1A	3190	1/1	0.94	0.25	59,59,59,59	0
56	MG	1A	3312	1/1	0.94	0.17	60,60,60,60	0
56	MG	2A	3269	1/1	0.94	0.22	43,43,43,43	0
56	MG	2A	3270	1/1	0.94	0.29	61,61,61,61	0
56	MG	1A	3101	1/1	0.94	0.34	35,35,35,35	0
56	MG	1A	3596	1/1	0.94	0.18	53,53,53,53	0
56	MG	1Q	3001	1/1	0.94	0.41	47,47,47,47	0
56	MG	1A	3131	1/1	0.94	0.12	32,32,32,32	0
56	MG	2a	3015	1/1	0.94	0.28	79,79,79,79	0
56	MG	1A	3782	1/1	0.94	0.12	43,43,43,43	0
56	MG	2A	3279	1/1	0.94	0.34	71,71,71,71	0
56	MG	1A	3103	1/1	0.94	0.42	41,41,41,41	0
56	MG	1A	3239	1/1	0.94	0.16	41,41,41,41	0
56	MG	1A	3974	1/1	0.94	0.20	48,48,48,48	0
56	MG	1A	3370	1/1	0.94	0.35	53,53,53,53	0
56	MG	1A	3135	1/1	0.94	0.27	44,44,44,44	0
56	MG	1T	201	1/1	0.94	0.16	59,59,59,59	0
56	MG	1A	3789	1/1	0.94	0.34	31,31,31,31	0
56	MG	1A	3792	1/1	0.94	0.11	47,47,47,47	0
56	MG	1a	1747	1/1	0.94	0.28	59,59,59,59	0
56	MG	2a	3031	1/1	0.94	0.37	48,48,48,48	0
56	MG	1A	3374	1/1	0.94	0.12	59,59,59,59	0
56	MG	2A	3015	1/1	0.94	0.43	72,72,72,72	0
56	MG	2A	3016	1/1	0.94	0.26	59,59,59,59	0
56	MG	1A	3274	1/1	0.94	0.10	69,69,69,69	0
56	MG	2A	3300	1/1	0.94	0.23	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3109	1/1	0.94	0.15	69,69,69,69	0
56	MG	1W	3001	1/1	0.94	0.28	52,52,52,52	0
56	MG	1A	3612	1/1	0.94	0.22	24,24,24,24	0
56	MG	1A	3243	1/1	0.94	0.34	43,43,43,43	0
56	MG	1A	3620	1/1	0.94	0.16	19,19,19,19	0
56	MG	2A	3026	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3380	1/1	0.94	0.19	39,39,39,39	0
56	MG	1A	3497	1/1	0.94	0.26	56,56,56,56	0
56	MG	1A	3989	1/1	0.94	0.07	70,70,70,70	0
56	MG	1A	3163	1/1	0.94	0.31	43,43,43,43	0
56	MG	1A	3016	1/1	0.94	0.32	49,49,49,49	0
56	MG	1A	3630	1/1	0.94	0.20	50,50,50,50	0
56	MG	2A	3326	1/1	0.94	0.19	34,34,34,34	0
56	MG	1A	3441	1/1	0.94	0.17	50,50,50,50	0
56	MG	1A	3166	1/1	0.94	0.41	47,47,47,47	0
56	MG	1A	3820	1/1	0.94	0.17	50,50,50,50	0
56	MG	2a	3061	1/1	0.94	0.15	72,72,72,72	0
56	MG	2A	3047	1/1	0.94	0.22	46,46,46,46	0
56	MG	2A	3048	1/1	0.94	0.38	57,57,57,57	0
56	MG	2A	3335	1/1	0.94	0.25	52,52,52,52	0
56	MG	10	104	1/1	0.94	0.19	46,46,46,46	0
56	MG	1A	3998	1/1	0.94	0.33	51,51,51,51	0
56	MG	1A	3506	1/1	0.94	0.18	57,57,57,57	0
56	MG	1A	3114	1/1	0.94	0.35	48,48,48,48	0
56	MG	2A	3345	1/1	0.94	0.17	68,68,68,68	0
56	MG	2a	3079	1/1	0.94	0.48	55,55,55,55	0
56	MG	2A	3056	1/1	0.94	0.18	57,57,57,57	0
56	MG	1A	3034	1/1	0.94	0.35	42,42,42,42	0
56	MG	1A	3116	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	4005	1/1	0.94	0.17	31,31,31,31	0
56	MG	1A	3087	1/1	0.94	0.27	32,32,32,32	0
56	MG	2A	3061	1/1	0.94	0.29	44,44,44,44	0
56	MG	1A	3830	1/1	0.94	0.18	54,54,54,54	0
56	MG	2A	3362	1/1	0.94	0.17	54,54,54,54	0
56	MG	1a	1776	1/1	0.94	0.37	76,76,76,76	0
56	MG	1a	1778	1/1	0.94	0.18	78,78,78,78	0
56	MG	2A	3369	1/1	0.94	0.12	65,65,65,65	0
56	MG	2A	3371	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	4008	1/1	0.94	0.11	47,47,47,47	0
56	MG	1A	3215	1/1	0.94	0.21	26,26,26,26	0
56	MG	2A	3375	1/1	0.94	0.18	50,50,50,50	0
56	MG	2a	3104	1/1	0.94	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3836	1/1	0.94	0.11	36,36,36,36	0
56	MG	2a	3106	1/1	0.94	0.18	59,59,59,59	0
56	MG	2A	3378	1/1	0.94	0.15	53,53,53,53	0
56	MG	2A	3069	1/1	0.94	0.18	55,55,55,55	0
56	MG	2A	3071	1/1	0.94	0.52	56,56,56,56	0
56	MG	2A	3072	1/1	0.94	0.23	55,55,55,55	0
56	MG	2a	3113	1/1	0.94	0.27	51,51,51,51	0
56	MG	2a	3114	1/1	0.94	0.14	70,70,70,70	0
56	MG	2a	3115	1/1	0.94	0.25	52,52,52,52	0
56	MG	2A	3385	1/1	0.94	0.19	43,43,43,43	0
56	MG	1A	3837	1/1	0.94	0.30	74,74,74,74	0
56	MG	1A	3217	1/1	0.94	0.29	48,48,48,48	0
56	MG	1A	3654	1/1	0.94	0.24	60,60,60,60	0
56	MG	1A	3046	1/1	0.94	0.07	60,60,60,60	0
56	MG	2A	3391	1/1	0.94	0.31	61,61,61,61	0
56	MG	1A	3846	1/1	0.94	0.13	43,43,43,43	0
56	MG	2A	3393	1/1	0.94	0.18	71,71,71,71	0
56	MG	1A	3660	1/1	0.94	0.28	38,38,38,38	0
56	MG	1A	3179	1/1	0.94	0.15	47,47,47,47	0
56	MG	1a	1608	1/1	0.94	0.12	68,68,68,68	0
56	MG	2A	3399	1/1	0.94	0.16	49,49,49,49	0
56	MG	2A	3403	1/1	0.94	0.12	34,34,34,34	0
56	MG	1A	3452	1/1	0.94	0.25	42,42,42,42	0
56	MG	2A	3407	1/1	0.94	0.13	31,31,31,31	0
56	MG	2A	3408	1/1	0.94	0.16	47,47,47,47	0
56	MG	1A	3665	1/1	0.94	0.07	64,64,64,64	0
56	MG	1a	1792	1/1	0.94	0.18	59,59,59,59	0
56	MG	1a	1793	1/1	0.94	0.59	68,68,68,68	0
56	MG	2A	3420	1/1	0.94	0.29	59,59,59,59	0
56	MG	1A	3667	1/1	0.94	0.16	42,42,42,42	0
56	MG	2A	3425	1/1	0.94	0.45	72,72,72,72	0
56	MG	2a	3145	1/1	0.94	0.12	91,91,91,91	0
56	MG	1A	3182	1/1	0.94	0.07	59,59,59,59	0
56	MG	1a	1799	1/1	0.94	0.27	76,76,76,76	0
56	MG	1A	3294	1/1	0.94	0.18	60,60,60,60	0
56	MG	1A	3674	1/1	0.94	0.11	30,30,30,30	0
56	MG	1a	1619	1/1	0.94	0.26	71,71,71,71	0
56	MG	1a	1804	1/1	0.94	0.12	88,88,88,88	0
56	MG	2A	3099	1/1	0.94	0.51	45,45,45,45	0
56	MG	2A	3100	1/1	0.94	0.35	62,62,62,62	0
56	MG	1A	3152	1/1	0.94	0.34	50,50,50,50	0
56	MG	1A	3526	1/1	0.94	0.14	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	3160	1/1	0.94	0.34	59,59,59,59	0
56	MG	1A	3019	1/1	0.94	0.19	61,61,61,61	0
56	MG	1A	3299	1/1	0.94	0.36	30,30,30,30	0
56	MG	1A	3867	1/1	0.94	0.55	40,40,40,40	0
56	MG	2A	3448	1/1	0.94	0.11	65,65,65,65	0
56	MG	1A	3531	1/1	0.94	0.18	56,56,56,56	0
56	MG	2A	3456	1/1	0.94	0.06	41,41,41,41	0
56	MG	2a	3172	1/1	0.94	0.14	78,78,78,78	0
56	MG	2A	3111	1/1	0.94	0.47	62,62,62,62	0
56	MG	2A	3112	1/1	0.94	0.21	36,36,36,36	0
56	MG	1A	3258	1/1	0.94	0.18	45,45,45,45	0
56	MG	2a	3180	1/1	0.94	0.08	79,79,79,79	0
56	MG	2A	3114	1/1	0.94	0.17	34,34,34,34	0
56	MG	2A	3116	1/1	0.94	0.22	55,55,55,55	0
56	MG	2a	3183	1/1	0.94	0.34	54,54,54,54	0
56	MG	1A	4045	1/1	0.94	0.70	50,50,50,50	0
56	MG	2A	3466	1/1	0.94	0.09	56,56,56,56	0
56	MG	2A	3119	1/1	0.94	0.20	46,46,46,46	0
56	MG	2A	3120	1/1	0.94	0.13	23,23,23,23	0
56	MG	2a	3189	1/1	0.94	0.23	57,57,57,57	0
56	MG	1A	3535	1/1	0.94	0.19	24,24,24,24	0
56	MG	2a	3193	1/1	0.94	0.25	76,76,76,76	0
56	MG	2A	3122	1/1	0.94	0.20	43,43,43,43	0
56	MG	1A	3538	1/1	0.94	0.21	14,14,14,14	0
56	MG	2a	3197	1/1	0.94	0.08	74,74,74,74	0
56	MG	2a	3199	1/1	0.94	0.34	59,59,59,59	0
56	MG	1a	1818	1/1	0.94	0.20	78,78,78,78	0
56	MG	1A	4050	1/1	0.94	0.24	53,53,53,53	0
56	MG	1A	3693	1/1	0.94	0.14	58,58,58,58	0
56	MG	1A	3695	1/1	0.94	0.15	63,63,63,63	0
56	MG	2A	3483	1/1	0.94	0.16	47,47,47,47	0
56	MG	1A	3696	1/1	0.94	0.10	62,62,62,62	0
56	MG	2A	3133	1/1	0.94	0.09	40,40,40,40	0
56	MG	2a	3210	1/1	0.94	0.22	69,69,69,69	0
56	MG	2a	3212	1/1	0.94	0.34	56,56,56,56	0
56	MG	1A	3877	1/1	0.94	0.21	61,61,61,61	0
56	MG	1A	3541	1/1	0.94	0.15	56,56,56,56	0
56	MG	2A	3136	1/1	0.94	0.16	45,45,45,45	0
56	MG	1a	1825	1/1	0.94	0.35	61,61,61,61	0
56	MG	1A	3301	1/1	0.94	0.24	33,33,33,33	0
56	MG	1a	1827	1/1	0.94	0.30	63,63,63,63	0
56	MG	2a	3228	1/1	0.94	0.07	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3099	1/1	0.94	0.30	42,42,42,42	0
56	MG	1a	1647	1/1	0.94	0.11	58,58,58,58	0
56	MG	1A	3226	1/1	0.94	0.12	53,53,53,53	0
56	MG	2A	3505	1/1	0.94	0.12	48,48,48,48	0
56	MG	1a	1650	1/1	0.94	0.34	72,72,72,72	0
56	MG	1A	3466	1/1	0.94	0.24	48,48,48,48	0
56	MG	2A	3511	1/1	0.94	0.06	50,50,50,50	0
56	MG	1A	3896	1/1	0.94	0.29	32,32,32,32	0
56	MG	1A	3557	1/1	0.94	0.12	44,44,44,44	0
56	MG	2a	3243	1/1	0.94	0.17	58,58,58,58	0
56	MG	2A	3516	1/1	0.94	0.14	38,38,38,38	0
56	MG	2d	502	1/1	0.94	0.56	61,61,61,61	0
56	MG	1A	3561	1/1	0.94	0.27	34,34,34,34	0
56	MG	2A	3162	1/1	0.94	0.14	47,47,47,47	0
56	MG	2A	3165	1/1	0.94	0.12	54,54,54,54	0
56	MG	1a	1655	1/1	0.94	0.14	60,60,60,60	0
56	MG	1a	1656	1/1	0.94	0.10	25,25,25,25	0
56	MG	1A	3562	1/1	0.94	0.20	50,50,50,50	0
56	MG	2n	502	1/1	0.94	0.61	73,73,73,73	0
56	MG	2A	3169	1/1	0.94	0.45	54,54,54,54	0
56	MG	2A	3170	1/1	0.94	0.17	35,35,35,35	0
56	MG	1a	1862	1/1	0.94	0.08	53,53,53,53	0
56	MG	1a	1864	1/1	0.94	0.07	68,68,68,68	0
56	MG	1A	3563	1/1	0.94	0.19	50,50,50,50	0
56	MG	1A	3564	1/1	0.94	0.11	42,42,42,42	0
56	MG	2A	3179	1/1	0.94	0.15	43,43,43,43	0
57	ZN	14	501	1/1	0.94	0.09	102,102,102,102	0
57	ZN	1n	501	1/1	0.94	0.14	86,86,86,86	0
57	ZN	2Y	501	1/1	0.94	0.04	88,88,88,88	0
56	MG	1A	3350	1/1	0.94	0.06	65,65,65,65	0
57	ZN	26	102	1/1	0.94	0.12	68,68,68,68	0
56	MG	1a	1869	1/1	0.94	0.13	63,63,63,63	0
56	MG	2A	3301	1/1	0.95	0.12	48,48,48,48	0
56	MG	1A	3104	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	3734	1/1	0.95	0.17	27,27,27,27	0
56	MG	1A	3128	1/1	0.95	0.37	49,49,49,49	0
56	MG	1A	3108	1/1	0.95	0.49	49,49,49,49	0
56	MG	1a	1634	1/1	0.95	0.39	66,66,66,66	0
56	MG	2A	3081	1/1	0.95	0.06	37,37,37,37	0
56	MG	2Q	202	1/1	0.95	0.16	51,51,51,51	0
56	MG	2A	3312	1/1	0.95	0.23	39,39,39,39	0
56	MG	1A	3133	1/1	0.95	0.07	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	3399	1/1	0.95	0.36	68,68,68,68	0
56	MG	2R	8001	1/1	0.95	0.17	50,50,50,50	0
56	MG	1A	3904	1/1	0.95	0.22	44,44,44,44	0
56	MG	1A	3905	1/1	0.95	0.20	39,39,39,39	0
56	MG	1a	1640	1/1	0.95	0.13	77,77,77,77	0
56	MG	1A	3608	1/1	0.95	0.16	39,39,39,39	0
56	MG	2A	3325	1/1	0.95	0.14	32,32,32,32	0
56	MG	1A	3354	1/1	0.95	0.20	54,54,54,54	0
56	MG	2A	3090	1/1	0.95	0.10	51,51,51,51	0
56	MG	2A	3091	1/1	0.95	0.36	37,37,37,37	0
56	MG	2A	3092	1/1	0.95	0.22	55,55,55,55	0
56	MG	1B	210	1/1	0.95	0.10	45,45,45,45	0
56	MG	1A	3912	1/1	0.95	0.16	49,49,49,49	0
56	MG	1A	3610	1/1	0.95	0.21	33,33,33,33	0
56	MG	1A	3611	1/1	0.95	0.24	28,28,28,28	0
56	MG	1A	3453	1/1	0.95	0.24	49,49,49,49	0
56	MG	1A	3613	1/1	0.95	0.20	30,30,30,30	0
56	MG	1A	3355	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3923	1/1	0.95	0.18	37,37,37,37	0
56	MG	2A	3102	1/1	0.95	0.29	41,41,41,41	0
56	MG	2A	3347	1/1	0.95	0.12	55,55,55,55	0
56	MG	2A	3349	1/1	0.95	0.14	49,49,49,49	0
56	MG	2A	3350	1/1	0.95	0.15	46,46,46,46	0
56	MG	2A	3351	1/1	0.95	0.32	62,62,62,62	0
56	MG	2A	3352	1/1	0.95	0.29	66,66,66,66	0
56	MG	1A	3049	1/1	0.95	0.16	49,49,49,49	0
56	MG	1A	3766	1/1	0.95	0.23	49,49,49,49	0
56	MG	1A	3768	1/1	0.95	0.15	82,82,82,82	0
56	MG	1A	3286	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3191	1/1	0.95	0.13	40,40,40,40	0
56	MG	2a	3029	1/1	0.95	0.24	59,59,59,59	0
56	MG	2A	3360	1/1	0.95	0.06	73,73,73,73	0
56	MG	1a	1657	1/1	0.95	0.11	72,72,72,72	0
56	MG	1a	1660	1/1	0.95	0.38	54,54,54,54	0
56	MG	2A	3363	1/1	0.95	0.25	53,53,53,53	0
56	MG	1A	3777	1/1	0.95	0.22	43,43,43,43	0
56	MG	2A	3366	1/1	0.95	0.21	58,58,58,58	0
56	MG	1a	1850	1/1	0.95	0.29	46,46,46,46	0
56	MG	1a	1852	1/1	0.95	0.15	77,77,77,77	0
56	MG	2A	3115	1/1	0.95	0.34	54,54,54,54	0
56	MG	1A	3934	1/1	0.95	0.13	62,62,62,62	0
56	MG	1a	1855	1/1	0.95	0.29	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3194	1/1	0.95	0.17	41,41,41,41	0
56	MG	1A	3779	1/1	0.95	0.12	45,45,45,45	0
56	MG	1A	3321	1/1	0.95	0.44	52,52,52,52	0
56	MG	1A	3056	1/1	0.95	0.41	49,49,49,49	0
56	MG	1A	3362	1/1	0.95	0.45	42,42,42,42	0
56	MG	1A	3008	1/1	0.95	0.23	51,51,51,51	0
56	MG	2a	3049	1/1	0.95	0.07	91,91,91,91	0
56	MG	1A	3634	1/1	0.95	0.18	19,19,19,19	0
56	MG	2a	3052	1/1	0.95	0.13	73,73,73,73	0
56	MG	2a	3053	1/1	0.95	0.12	83,83,83,83	0
56	MG	2A	3128	1/1	0.95	0.38	61,61,61,61	0
56	MG	1A	3464	1/1	0.95	0.24	43,43,43,43	0
56	MG	1A	3324	1/1	0.95	0.10	66,66,66,66	0
56	MG	1A	3791	1/1	0.95	0.11	60,60,60,60	0
56	MG	1E	306	1/1	0.95	0.22	74,74,74,74	0
56	MG	1a	1677	1/1	0.95	0.47	61,61,61,61	0
56	MG	1a	1678	1/1	0.95	0.15	60,60,60,60	0
56	MG	1A	3467	1/1	0.95	0.21	44,44,44,44	0
56	MG	2a	3068	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	3953	1/1	0.95	0.18	61,61,61,61	0
56	MG	1A	3641	1/1	0.95	0.14	22,22,22,22	0
56	MG	1A	3533	1/1	0.95	0.18	37,37,37,37	0
56	MG	2a	3075	1/1	0.95	0.11	60,60,60,60	0
56	MG	2A	3400	1/1	0.95	0.18	31,31,31,31	0
56	MG	2A	3140	1/1	0.95	0.32	62,62,62,62	0
56	MG	1A	3646	1/1	0.95	0.14	21,21,21,21	0
56	MG	1F	305	1/1	0.95	0.45	28,28,28,28	0
56	MG	1a	1887	1/1	0.95	0.25	66,66,66,66	0
56	MG	2A	3409	1/1	0.95	0.20	59,59,59,59	0
56	MG	1A	3139	1/1	0.95	0.24	28,28,28,28	0
56	MG	2A	3413	1/1	0.95	0.29	44,44,44,44	0
56	MG	2A	3415	1/1	0.95	0.27	43,43,43,43	0
56	MG	1A	3649	1/1	0.95	0.07	28,28,28,28	0
56	MG	2A	3153	1/1	0.95	0.25	42,42,42,42	0
56	MG	2A	3418	1/1	0.95	0.19	62,62,62,62	0
56	MG	2A	3419	1/1	0.95	0.37	51,51,51,51	0
56	MG	1A	3963	1/1	0.95	0.31	54,54,54,54	0
56	MG	2a	3092	1/1	0.95	0.46	65,65,65,65	0
56	MG	2a	3096	1/1	0.95	0.10	72,72,72,72	0
56	MG	1G	3003	1/1	0.95	0.05	59,59,59,59	0
56	MG	2A	3424	1/1	0.95	0.13	50,50,50,50	0
56	MG	1A	3537	1/1	0.95	0.14	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	1A	3018	1/1	0.95	0.49	58,58,58,58	0
56	MG	2A	3427	1/1	0.95	0.23	68,68,68,68	0
56	MG	1A	3967	1/1	0.95	0.15	53,53,53,53	0
56	MG	1A	3473	1/1	0.95	0.06	63,63,63,63	0
56	MG	2A	3431	1/1	0.95	0.24	68,68,68,68	0
56	MG	1A	3545	1/1	0.95	0.17	31,31,31,31	0
56	MG	2A	3434	1/1	0.95	0.07	55,55,55,55	0
56	MG	2A	3436	1/1	0.95	0.37	68,68,68,68	0
56	MG	1A	3813	1/1	0.95	0.22	55,55,55,55	0
56	MG	1A	3814	1/1	0.95	0.17	58,58,58,58	0
56	MG	1A	3659	1/1	0.95	0.35	73,73,73,73	0
56	MG	1N	208	1/1	0.95	0.08	60,60,60,60	0
56	MG	2a	3117	1/1	0.95	0.39	68,68,68,68	0
56	MG	2A	3172	1/1	0.95	0.18	47,47,47,47	0
56	MG	1A	3293	1/1	0.95	0.17	36,36,36,36	0
56	MG	1a	1711	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3175	1/1	0.95	0.09	40,40,40,40	0
56	MG	1A	3549	1/1	0.95	0.11	68,68,68,68	0
56	MG	1P	202	1/1	0.95	0.28	46,46,46,46	0
56	MG	2A	3449	1/1	0.95	0.14	62,62,62,62	0
56	MG	2A	3450	1/1	0.95	0.33	52,52,52,52	0
56	MG	1A	3663	1/1	0.95	0.28	55,55,55,55	0
56	MG	2A	3455	1/1	0.95	0.10	67,67,67,67	0
56	MG	2a	3130	1/1	0.95	0.30	58,58,58,58	0
56	MG	1A	3052	1/1	0.95	0.27	48,48,48,48	0
56	MG	1A	3551	1/1	0.95	0.20	32,32,32,32	0
56	MG	2A	3186	1/1	0.95	0.26	43,43,43,43	0
56	MG	1A	3980	1/1	0.95	0.48	63,63,63,63	0
56	MG	1A	3142	1/1	0.95	0.20	43,43,43,43	0
56	MG	1A	3201	1/1	0.95	0.26	39,39,39,39	0
56	MG	1R	202	1/1	0.95	0.25	68,68,68,68	0
56	MG	1A	3372	1/1	0.95	0.12	56,56,56,56	0
56	MG	1A	3673	1/1	0.95	0.20	52,52,52,52	0
56	MG	1q	204	1/1	0.95	0.10	58,58,58,58	0
56	MG	1A	3558	1/1	0.95	0.22	27,27,27,27	0
56	MG	2A	3197	1/1	0.95	0.09	47,47,47,47	0
56	MG	1R	206	1/1	0.95	0.17	34,34,34,34	0
56	MG	2A	3199	1/1	0.95	0.35	47,47,47,47	0
56	MG	1A	3833	1/1	0.95	0.15	56,56,56,56	0
56	MG	1A	3987	1/1	0.95	0.21	35,35,35,35	0
56	MG	2A	3481	1/1	0.95	0.12	41,41,41,41	0
56	MG	1A	3675	1/1	0.95	0.17	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3835	1/1	0.95	0.24	49,49,49,49	0
56	MG	1A	3677	1/1	0.95	0.24	50,50,50,50	0
56	MG	1x	104	1/1	0.95	0.07	47,47,47,47	0
56	MG	2A	3488	1/1	0.95	0.20	31,31,31,31	0
56	MG	2a	3158	1/1	0.95	0.25	72,72,72,72	0
56	MG	1U	202	1/1	0.95	0.32	43,43,43,43	0
56	MG	2A	3490	1/1	0.95	0.13	30,30,30,30	0
56	MG	1A	3559	1/1	0.95	0.22	36,36,36,36	0
56	MG	2A	3492	1/1	0.95	0.24	45,45,45,45	0
56	MG	2a	3165	1/1	0.95	0.32	50,50,50,50	0
56	MG	1A	3332	1/1	0.95	0.23	61,61,61,61	0
56	MG	1A	3375	1/1	0.95	0.21	59,59,59,59	0
56	MG	1A	3840	1/1	0.95	0.25	67,67,67,67	0
56	MG	1A	3298	1/1	0.95	0.07	52,52,52,52	0
56	MG	1A	3843	1/1	0.95	0.13	37,37,37,37	0
56	MG	2a	3174	1/1	0.95	0.13	56,56,56,56	0
56	MG	2A	3217	1/1	0.95	0.39	45,45,45,45	0
56	MG	1A	3684	1/1	0.95	0.23	41,41,41,41	0
56	MG	1A	3335	1/1	0.95	0.12	43,43,43,43	0
56	MG	2a	3179	1/1	0.95	0.06	47,47,47,47	0
56	MG	1A	3427	1/1	0.95	0.32	41,41,41,41	0
56	MG	1A	3238	1/1	0.95	0.38	53,53,53,53	0
56	MG	2A	3510	1/1	0.95	0.25	62,62,62,62	0
56	MG	1A	4003	1/1	0.95	0.29	24,24,24,24	0
56	MG	1A	4004	1/1	0.95	0.44	31,31,31,31	0
56	MG	2A	3513	1/1	0.95	0.19	38,38,38,38	0
56	MG	1A	3202	1/1	0.95	0.17	50,50,50,50	0
56	MG	1A	3431	1/1	0.95	0.14	14,14,14,14	0
56	MG	1A	3084	1/1	0.95	0.08	25,25,25,25	0
56	MG	1A	3047	1/1	0.95	0.46	46,46,46,46	0
56	MG	2a	3192	1/1	0.95	0.16	56,56,56,56	0
56	MG	2A	3520	1/1	0.95	0.27	75,75,75,75	0
56	MG	10	106	1/1	0.95	0.33	62,62,62,62	0
56	MG	1A	3857	1/1	0.95	0.14	51,51,51,51	0
56	MG	2a	3196	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3576	1/1	0.95	0.30	48,48,48,48	0
56	MG	2a	3198	1/1	0.95	0.23	76,76,76,76	0
56	MG	1A	3171	1/1	0.95	0.20	47,47,47,47	0
56	MG	2A	3021	1/1	0.95	0.34	60,60,60,60	0
56	MG	1A	3385	1/1	0.95	0.16	51,51,51,51	0
56	MG	15	101	1/1	0.95	0.24	43,43,43,43	0
56	MG	1A	3031	1/1	0.95	0.18	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	15	104	1/1	0.95	0.19	49,49,49,49	0
56	MG	1A	3582	1/1	0.95	0.23	44,44,44,44	0
56	MG	2A	3531	1/1	0.95	0.12	58,58,58,58	0
56	MG	16	101	1/1	0.95	0.18	51,51,51,51	0
56	MG	16	103	1/1	0.95	0.14	57,57,57,57	0
56	MG	2A	3247	1/1	0.95	0.26	63,63,63,63	0
56	MG	1A	3703	1/1	0.95	0.05	58,58,58,58	0
56	MG	2a	3217	1/1	0.95	0.24	59,59,59,59	0
56	MG	2A	3251	1/1	0.95	0.36	55,55,55,55	0
56	MG	1A	3149	1/1	0.95	0.19	34,34,34,34	0
56	MG	2A	3255	1/1	0.95	0.13	42,42,42,42	0
56	MG	1a	1773	1/1	0.95	0.20	57,57,57,57	0
56	MG	2a	3226	1/1	0.95	0.41	75,75,75,75	0
56	MG	1A	3150	1/1	0.95	0.24	40,40,40,40	0
56	MG	1a	1775	1/1	0.95	0.36	65,65,65,65	0
56	MG	2a	3232	1/1	0.95	0.14	62,62,62,62	0
56	MG	1A	4023	1/1	0.95	0.24	40,40,40,40	0
56	MG	2A	3263	1/1	0.95	0.23	24,24,24,24	0
56	MG	2A	3552	1/1	0.95	0.34	50,50,50,50	0
56	MG	2A	3045	1/1	0.95	0.15	45,45,45,45	0
56	MG	2A	3266	1/1	0.95	0.19	54,54,54,54	0
56	MG	19	502	1/1	0.95	0.22	46,46,46,46	0
56	MG	1A	3712	1/1	0.95	0.08	58,58,58,58	0
56	MG	19	504	1/1	0.95	0.11	56,56,56,56	0
56	MG	1A	3713	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	3872	1/1	0.95	0.14	46,46,46,46	0
56	MG	1A	3089	1/1	0.95	0.32	44,44,44,44	0
56	MG	2A	3274	1/1	0.95	0.21	47,47,47,47	0
56	MG	1A	3874	1/1	0.95	0.13	45,45,45,45	0
56	MG	2f	3001	1/1	0.95	0.10	58,58,58,58	0
56	MG	1A	3345	1/1	0.95	0.26	64,64,64,64	0
56	MG	2A	3277	1/1	0.95	0.11	36,36,36,36	0
56	MG	1A	3498	1/1	0.95	0.54	50,50,50,50	0
56	MG	1A	3125	1/1	0.95	0.17	49,49,49,49	0
56	MG	1A	3594	1/1	0.95	0.19	62,62,62,62	0
56	MG	1A	3727	1/1	0.95	0.22	25,25,25,25	0
56	MG	1A	4038	1/1	0.95	0.16	66,66,66,66	0
56	MG	1A	3392	1/1	0.95	0.08	55,55,55,55	0
56	MG	1a	1615	1/1	0.95	0.30	83,83,83,83	0
56	MG	1A	4040	1/1	0.95	0.34	35,35,35,35	0
56	MG	1A	3502	1/1	0.95	0.19	77,77,77,77	0
56	MG	1A	3891	1/1	0.95	0.24	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	1a	1798	1/1	0.95	0.29	64,64,64,64	0
56	MG	1A	4043	1/1	0.95	0.11	45,45,45,45	0
56	MG	2A	3070	1/1	0.95	0.46	58,58,58,58	0
56	MG	1A	4044	1/1	0.95	0.61	39,39,39,39	0
56	MG	1A	3892	1/1	0.95	0.33	46,46,46,46	0
57	ZN	29	501	1/1	0.95	0.09	65,65,65,65	0
56	MG	1A	3218	1/1	0.95	0.19	52,52,52,52	0
56	MG	2D	301	1/1	0.96	0.14	54,54,54,54	0
56	MG	1D	311	1/1	0.96	0.11	49,49,49,49	0
56	MG	1A	3117	1/1	0.96	0.15	41,41,41,41	0
56	MG	1A	3965	1/1	0.96	0.17	35,35,35,35	0
56	MG	1A	3714	1/1	0.96	0.17	32,32,32,32	0
56	MG	2A	3310	1/1	0.96	0.08	46,46,46,46	0
56	MG	2A	3078	1/1	0.96	0.12	53,53,53,53	0
56	MG	2E	307	1/1	0.96	0.09	70,70,70,70	0
56	MG	1A	3478	1/1	0.96	0.45	51,51,51,51	0
56	MG	1A	3536	1/1	0.96	0.20	62,62,62,62	0
56	MG	1E	301	1/1	0.96	0.18	58,58,58,58	0
56	MG	2A	3319	1/1	0.96	0.20	57,57,57,57	0
56	MG	2O	201	1/1	0.96	0.14	54,54,54,54	0
56	MG	1a	1649	1/1	0.96	0.25	56,56,56,56	0
56	MG	1A	3969	1/1	0.96	0.12	39,39,39,39	0
56	MG	1A	3722	1/1	0.96	0.22	56,56,56,56	0
56	MG	2A	3086	1/1	0.96	0.15	30,30,30,30	0
56	MG	1A	3382	1/1	0.96	0.24	29,29,29,29	0
56	MG	1A	3844	1/1	0.96	0.13	63,63,63,63	0
56	MG	1A	3845	1/1	0.96	0.20	57,57,57,57	0
56	MG	1A	3007	1/1	0.96	0.23	53,53,53,53	0
56	MG	2A	3329	1/1	0.96	0.15	39,39,39,39	0
56	MG	2V	201	1/1	0.96	0.66	51,51,51,51	0
56	MG	1E	309	1/1	0.96	0.27	32,32,32,32	0
56	MG	1E	310	1/1	0.96	0.12	45,45,45,45	0
56	MG	1F	301	1/1	0.96	0.24	39,39,39,39	0
56	MG	1A	3540	1/1	0.96	0.20	41,41,41,41	0
56	MG	1a	1662	1/1	0.96	0.27	73,73,73,73	0
56	MG	1A	3083	1/1	0.96	0.15	29,29,29,29	0
56	MG	1a	1830	1/1	0.96	0.26	55,55,55,55	0
56	MG	1a	1832	1/1	0.96	0.27	54,54,54,54	0
56	MG	2A	3344	1/1	0.96	0.25	32,32,32,32	0
56	MG	1A	3628	1/1	0.96	0.29	63,63,63,63	0
56	MG	2a	3008	1/1	0.96	0.22	60,60,60,60	0
56	MG	1A	3542	1/1	0.96	0.11	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1839	1/1	0.96	0.23	62,62,62,62	0
56	MG	2A	3103	1/1	0.96	0.12	50,50,50,50	0
56	MG	1a	1840	1/1	0.96	0.13	67,67,67,67	0
56	MG	1a	1841	1/1	0.96	0.15	40,40,40,40	0
56	MG	2A	3106	1/1	0.96	0.38	33,33,33,33	0
56	MG	1A	3273	1/1	0.96	0.54	45,45,45,45	0
56	MG	2A	3354	1/1	0.96	0.17	75,75,75,75	0
56	MG	1a	1844	1/1	0.96	0.07	38,38,38,38	0
56	MG	1a	1845	1/1	0.96	0.26	52,52,52,52	0
56	MG	1A	3632	1/1	0.96	0.24	45,45,45,45	0
56	MG	1A	3733	1/1	0.96	0.13	37,37,37,37	0
56	MG	1A	3856	1/1	0.96	0.20	52,52,52,52	0
56	MG	1a	1849	1/1	0.96	0.19	54,54,54,54	0
56	MG	1A	3148	1/1	0.96	0.39	42,42,42,42	0
56	MG	1a	1851	1/1	0.96	0.17	49,49,49,49	0
56	MG	1A	3310	1/1	0.96	0.07	65,65,65,65	0
56	MG	1A	3211	1/1	0.96	0.43	46,46,46,46	0
56	MG	2A	3118	1/1	0.96	0.30	56,56,56,56	0
56	MG	1a	1854	1/1	0.96	0.22	51,51,51,51	0
56	MG	2a	3032	1/1	0.96	0.07	65,65,65,65	0
56	MG	1A	3636	1/1	0.96	0.20	19,19,19,19	0
56	MG	1A	3637	1/1	0.96	0.22	29,29,29,29	0
56	MG	1A	3044	1/1	0.96	0.20	50,50,50,50	0
56	MG	1A	3866	1/1	0.96	0.28	65,65,65,65	0
56	MG	2A	3376	1/1	0.96	0.26	29,29,29,29	0
56	MG	1A	3749	1/1	0.96	0.16	27,27,27,27	0
56	MG	1A	3750	1/1	0.96	0.19	18,18,18,18	0
56	MG	1A	3214	1/1	0.96	0.37	34,34,34,34	0
56	MG	2A	3381	1/1	0.96	0.32	45,45,45,45	0
56	MG	1A	3753	1/1	0.96	0.10	67,67,67,67	0
56	MG	1A	3995	1/1	0.96	0.26	10,10,10,10	0
56	MG	1A	3554	1/1	0.96	0.17	38,38,38,38	0
56	MG	1a	1870	1/1	0.96	0.09	56,56,56,56	0
56	MG	1A	3100	1/1	0.96	0.17	31,31,31,31	0
56	MG	1A	3352	1/1	0.96	0.41	49,49,49,49	0
56	MG	2A	3389	1/1	0.96	0.11	36,36,36,36	0
56	MG	2a	3050	1/1	0.96	0.28	71,71,71,71	0
56	MG	1a	1874	1/1	0.96	0.15	64,64,64,64	0
56	MG	1A	3759	1/1	0.96	0.07	54,54,54,54	0
56	MG	1A	3085	1/1	0.96	0.19	41,41,41,41	0
56	MG	1a	1692	1/1	0.96	0.09	50,50,50,50	0
56	MG	1a	1693	1/1	0.96	0.17	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3144	1/1	0.96	0.22	53,53,53,53	0
56	MG	2A	3145	1/1	0.96	0.09	50,50,50,50	0
56	MG	2A	3398	1/1	0.96	0.07	57,57,57,57	0
56	MG	2a	3060	1/1	0.96	0.36	63,63,63,63	0
56	MG	1Q	3006	1/1	0.96	0.31	48,48,48,48	0
56	MG	1A	3648	1/1	0.96	0.15	51,51,51,51	0
56	MG	2A	3401	1/1	0.96	0.20	39,39,39,39	0
56	MG	1a	1883	1/1	0.96	0.23	58,58,58,58	0
56	MG	2a	3069	1/1	0.96	0.17	65,65,65,65	0
56	MG	2a	3070	1/1	0.96	0.30	57,57,57,57	0
56	MG	1A	3280	1/1	0.96	0.08	70,70,70,70	0
56	MG	1A	3443	1/1	0.96	0.17	47,47,47,47	0
56	MG	2a	3073	1/1	0.96	0.15	68,68,68,68	0
56	MG	2A	3152	1/1	0.96	0.16	48,48,48,48	0
56	MG	1a	1886	1/1	0.96	0.22	53,53,53,53	0
56	MG	1A	3880	1/1	0.96	0.10	42,42,42,42	0
56	MG	2A	3411	1/1	0.96	0.25	39,39,39,39	0
56	MG	2A	3412	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3282	1/1	0.96	0.46	47,47,47,47	0
56	MG	2A	3157	1/1	0.96	0.27	47,47,47,47	0
56	MG	2A	3160	1/1	0.96	0.17	42,42,42,42	0
56	MG	1A	3882	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	3652	1/1	0.96	0.12	24,24,24,24	0
56	MG	2A	3163	1/1	0.96	0.24	64,64,64,64	0
56	MG	2A	3164	1/1	0.96	0.07	42,42,42,42	0
56	MG	1a	1892	1/1	0.96	0.41	67,67,67,67	0
56	MG	2A	3423	1/1	0.96	0.41	71,71,71,71	0
56	MG	1a	1893	1/1	0.96	0.28	59,59,59,59	0
56	MG	1A	4009	1/1	0.96	0.46	48,48,48,48	0
56	MG	1a	1896	1/1	0.96	0.12	45,45,45,45	0
56	MG	2a	3093	1/1	0.96	0.18	62,62,62,62	0
56	MG	2a	3094	1/1	0.96	0.18	51,51,51,51	0
56	MG	2a	3095	1/1	0.96	0.05	58,58,58,58	0
56	MG	1a	1706	1/1	0.96	0.12	52,52,52,52	0
56	MG	2A	3428	1/1	0.96	0.09	64,64,64,64	0
56	MG	1a	1707	1/1	0.96	0.27	46,46,46,46	0
56	MG	1A	3884	1/1	0.96	0.07	63,63,63,63	0
56	MG	1A	3885	1/1	0.96	0.11	56,56,56,56	0
56	MG	1A	4012	1/1	0.96	0.20	81,81,81,81	0
56	MG	2A	3433	1/1	0.96	0.12	62,62,62,62	0
56	MG	1A	4013	1/1	0.96	0.34	47,47,47,47	0
56	MG	1A	3032	1/1	0.96	0.11	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1U	204	1/1	0.96	0.48	44,44,44,44	0
56	MG	1a	1716	1/1	0.96	0.15	68,68,68,68	0
56	MG	1a	1717	1/1	0.96	0.08	69,69,69,69	0
56	MG	2A	3182	1/1	0.96	0.20	37,37,37,37	0
56	MG	1A	3888	1/1	0.96	0.43	37,37,37,37	0
56	MG	1A	3889	1/1	0.96	0.08	53,53,53,53	0
56	MG	2A	3185	1/1	0.96	0.47	43,43,43,43	0
56	MG	2A	3444	1/1	0.96	0.17	39,39,39,39	0
56	MG	2A	3445	1/1	0.96	0.07	74,74,74,74	0
56	MG	1e	202	1/1	0.96	0.10	66,66,66,66	0
56	MG	1A	3890	1/1	0.96	0.11	62,62,62,62	0
56	MG	1A	3655	1/1	0.96	0.20	56,56,56,56	0
56	MG	1A	3656	1/1	0.96	0.12	56,56,56,56	0
56	MG	1a	1725	1/1	0.96	0.27	59,59,59,59	0
56	MG	1A	3127	1/1	0.96	0.17	50,50,50,50	0
56	MG	2A	3452	1/1	0.96	0.13	59,59,59,59	0
56	MG	2A	3454	1/1	0.96	0.20	58,58,58,58	0
56	MG	1a	1727	1/1	0.96	0.26	39,39,39,39	0
56	MG	2A	3194	1/1	0.96	0.30	45,45,45,45	0
56	MG	1X	3002	1/1	0.96	0.16	37,37,37,37	0
56	MG	2A	3458	1/1	0.96	0.20	31,31,31,31	0
56	MG	1a	1730	1/1	0.96	0.31	49,49,49,49	0
56	MG	1A	3398	1/1	0.96	0.09	47,47,47,47	0
56	MG	1A	3897	1/1	0.96	0.29	33,33,33,33	0
56	MG	1A	3320	1/1	0.96	0.25	49,49,49,49	0
56	MG	1A	3033	1/1	0.96	0.44	47,47,47,47	0
56	MG	1A	4029	1/1	0.96	0.59	40,40,40,40	0
56	MG	2A	3467	1/1	0.96	0.12	58,58,58,58	0
56	MG	1A	4030	1/1	0.96	0.24	41,41,41,41	0
56	MG	1A	3156	1/1	0.96	0.40	49,49,49,49	0
56	MG	1A	3105	1/1	0.96	0.16	39,39,39,39	0
56	MG	2a	3144	1/1	0.96	0.20	75,75,75,75	0
56	MG	1A	3063	1/1	0.96	0.42	52,52,52,52	0
56	MG	1A	3363	1/1	0.96	0.14	42,42,42,42	0
56	MG	2A	3208	1/1	0.96	0.18	49,49,49,49	0
56	MG	10	107	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3407	1/1	0.96	0.07	71,71,71,71	0
56	MG	1A	3578	1/1	0.96	0.09	39,39,39,39	0
56	MG	2A	3212	1/1	0.96	0.43	58,58,58,58	0
56	MG	1A	3065	1/1	0.96	0.27	60,60,60,60	0
56	MG	2A	3485	1/1	0.96	0.08	35,35,35,35	0
56	MG	1A	3911	1/1	0.96	0.20	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	2a	3156	1/1	0.96	0.33	70,70,70,70	0
56	MG	2a	3157	1/1	0.96	0.45	66,66,66,66	0
56	MG	1A	3794	1/1	0.96	0.21	62,62,62,62	0
56	MG	2A	3216	1/1	0.96	0.34	44,44,44,44	0
56	MG	1A	3795	1/1	0.96	0.14	24,24,24,24	0
56	MG	2a	3161	1/1	0.96	0.14	62,62,62,62	0
56	MG	1A	3023	1/1	0.96	0.39	57,57,57,57	0
56	MG	1A	3509	1/1	0.96	0.24	60,60,60,60	0
56	MG	1A	3919	1/1	0.96	0.12	47,47,47,47	0
56	MG	2a	3166	1/1	0.96	0.24	63,63,63,63	0
56	MG	2A	3493	1/1	0.96	0.14	41,41,41,41	0
56	MG	2A	3494	1/1	0.96	0.12	69,69,69,69	0
56	MG	1A	3800	1/1	0.96	0.10	55,55,55,55	0
56	MG	2A	3496	1/1	0.96	0.14	59,59,59,59	0
56	MG	1A	3583	1/1	0.96	0.20	33,33,33,33	0
56	MG	2A	3498	1/1	0.96	0.09	69,69,69,69	0
56	MG	1A	3804	1/1	0.96	0.10	50,50,50,50	0
56	MG	18	102	1/1	0.96	0.20	66,66,66,66	0
56	MG	1A	4047	1/1	0.96	0.25	36,36,36,36	0
56	MG	1A	4048	1/1	0.96	0.09	32,32,32,32	0
56	MG	18	105	1/1	0.96	0.24	43,43,43,43	0
56	MG	1A	3510	1/1	0.96	0.21	39,39,39,39	0
56	MG	2A	3506	1/1	0.96	0.02	34,34,34,34	0
56	MG	1A	3111	1/1	0.96	0.22	39,39,39,39	0
56	MG	2a	3184	1/1	0.96	0.21	56,56,56,56	0
56	MG	2A	3508	1/1	0.96	0.07	61,61,61,61	0
56	MG	1a	1764	1/1	0.96	0.13	67,67,67,67	0
56	MG	2A	3017	1/1	0.96	0.22	52,52,52,52	0
56	MG	1A	3586	1/1	0.96	0.18	32,32,32,32	0
56	MG	2A	3019	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3137	1/1	0.96	0.30	49,49,49,49	0
56	MG	1A	3329	1/1	0.96	0.10	50,50,50,50	0
56	MG	1a	1603	1/1	0.96	0.19	59,59,59,59	0
56	MG	1A	3229	1/1	0.96	0.14	55,55,55,55	0
56	MG	1A	3932	1/1	0.96	0.27	46,46,46,46	0
56	MG	1A	3138	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3112	1/1	0.96	0.20	35,35,35,35	0
56	MG	1A	3517	1/1	0.96	0.49	56,56,56,56	0
56	MG	2A	3250	1/1	0.96	0.12	61,61,61,61	0
56	MG	1A	3093	1/1	0.96	0.23	46,46,46,46	0
56	MG	1A	3818	1/1	0.96	0.19	62,62,62,62	0
56	MG	1A	3233	1/1	0.96	0.60	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	1777	1/1	0.96	0.23	73,73,73,73	0
56	MG	2A	3035	1/1	0.96	0.10	59,59,59,59	0
56	MG	1A	3234	1/1	0.96	0.32	54,54,54,54	0
56	MG	1A	3521	1/1	0.96	0.23	46,46,46,46	0
56	MG	2a	3209	1/1	0.96	0.06	76,76,76,76	0
56	MG	1a	1616	1/1	0.96	0.10	76,76,76,76	0
56	MG	2A	3041	1/1	0.96	0.10	49,49,49,49	0
56	MG	2A	3042	1/1	0.96	0.30	50,50,50,50	0
56	MG	2A	3043	1/1	0.96	0.23	58,58,58,58	0
56	MG	2A	3044	1/1	0.96	0.11	46,46,46,46	0
56	MG	2a	3219	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3945	1/1	0.96	0.32	30,30,30,30	0
56	MG	1B	216	1/1	0.96	0.09	47,47,47,47	0
56	MG	1B	220	1/1	0.96	0.14	27,27,27,27	0
56	MG	2A	3541	1/1	0.96	0.09	67,67,67,67	0
56	MG	2A	3272	1/1	0.96	0.25	61,61,61,61	0
56	MG	1A	3522	1/1	0.96	0.18	62,62,62,62	0
56	MG	1B	222	1/1	0.96	0.12	58,58,58,58	0
56	MG	2A	3051	1/1	0.96	0.17	49,49,49,49	0
56	MG	2A	3548	1/1	0.96	0.16	42,42,42,42	0
56	MG	1a	1623	1/1	0.96	0.23	79,79,79,79	0
56	MG	1a	1624	1/1	0.96	0.30	65,65,65,65	0
56	MG	2a	3237	1/1	0.96	0.25	69,69,69,69	0
56	MG	2A	3555	1/1	0.96	0.08	43,43,43,43	0
56	MG	2A	3557	1/1	0.96	0.27	45,45,45,45	0
56	MG	1A	3824	1/1	0.96	0.14	31,31,31,31	0
56	MG	2A	3561	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3825	1/1	0.96	0.12	33,33,33,33	0
56	MG	1A	3035	1/1	0.96	0.07	58,58,58,58	0
56	MG	2A	3281	1/1	0.96	0.34	50,50,50,50	0
56	MG	2A	3282	1/1	0.96	0.10	31,31,31,31	0
56	MG	2A	3567	1/1	0.96	0.20	54,54,54,54	0
56	MG	2A	3568	1/1	0.96	0.34	43,43,43,43	0
56	MG	1B	226	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3377	1/1	0.96	0.41	67,67,67,67	0
56	MG	1A	3266	1/1	0.96	0.17	78,78,78,78	0
56	MG	1a	1632	1/1	0.96	0.25	53,53,53,53	0
56	MG	1A	3203	1/1	0.96	0.82	47,47,47,47	0
56	MG	1a	1796	1/1	0.96	0.17	50,50,50,50	0
56	MG	1a	1797	1/1	0.96	0.19	42,42,42,42	0
56	MG	1D	304	1/1	0.96	0.46	50,50,50,50	0
56	MG	1a	1636	1/1	0.96	0.22	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3529	1/1	0.96	0.05	62,62,62,62	0
56	MG	2A	3581	1/1	0.96	0.14	51,51,51,51	0
56	MG	1A	3706	1/1	0.96	0.09	38,38,38,38	0
56	MG	2B	3001	1/1	0.96	0.28	65,65,65,65	0
56	MG	1a	1802	1/1	0.96	0.10	77,77,77,77	0
56	MG	2A	3298	1/1	0.96	0.07	45,45,45,45	0
56	MG	2A	3299	1/1	0.96	0.17	44,44,44,44	0
56	MG	2B	3007	1/1	0.96	0.13	55,55,55,55	0
56	MG	1A	3424	1/1	0.96	0.15	62,62,62,62	0
56	MG	1A	3017	1/1	0.96	0.24	47,47,47,47	0
56	MG	1D	310	1/1	0.96	0.26	33,33,33,33	0
56	MG	2A	3040	1/1	0.97	0.11	43,43,43,43	0
56	MG	1A	3189	1/1	0.97	0.41	28,28,28,28	0
56	MG	1A	3434	1/1	0.97	0.40	41,41,41,41	0
56	MG	1A	4024	1/1	0.97	0.16	29,29,29,29	0
56	MG	1a	1679	1/1	0.97	0.15	52,52,52,52	0
56	MG	2A	3220	1/1	0.97	0.49	50,50,50,50	0
56	MG	1A	3400	1/1	0.97	0.15	48,48,48,48	0
56	MG	2A	3222	1/1	0.97	0.30	45,45,45,45	0
56	MG	1A	3235	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3908	1/1	0.97	0.15	20,20,20,20	0
56	MG	1A	3909	1/1	0.97	0.14	25,25,25,25	0
56	MG	2A	3049	1/1	0.97	0.21	33,33,33,33	0
56	MG	1A	3705	1/1	0.97	0.32	35,35,35,35	0
56	MG	1U	201	1/1	0.97	0.15	38,38,38,38	0
56	MG	1A	3809	1/1	0.97	0.25	40,40,40,40	0
56	MG	1a	1687	1/1	0.97	0.18	54,54,54,54	0
56	MG	1a	1831	1/1	0.97	0.23	63,63,63,63	0
56	MG	2A	3055	1/1	0.97	0.61	46,46,46,46	0
56	MG	1A	3913	1/1	0.97	0.08	41,41,41,41	0
56	MG	1A	3914	1/1	0.97	0.23	22,22,22,22	0
56	MG	2A	3238	1/1	0.97	0.40	48,48,48,48	0
56	MG	1U	205	1/1	0.97	0.42	43,43,43,43	0
56	MG	1a	1836	1/1	0.97	0.27	59,59,59,59	0
56	MG	2A	3241	1/1	0.97	0.24	56,56,56,56	0
56	MG	1a	1837	1/1	0.97	0.33	50,50,50,50	0
56	MG	1A	3810	1/1	0.97	0.19	63,63,63,63	0
56	MG	1A	3079	1/1	0.97	0.17	31,31,31,31	0
56	MG	1W	3003	1/1	0.97	0.23	37,37,37,37	0
56	MG	1A	3812	1/1	0.97	0.15	54,54,54,54	0
56	MG	1A	3707	1/1	0.97	0.18	40,40,40,40	0
56	MG	1A	3708	1/1	0.97	0.18	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	2A	3067	1/1	0.97	0.17	57,57,57,57	0
56	MG	1A	3709	1/1	0.97	0.19	54,54,54,54	0
56	MG	2A	3252	1/1	0.97	0.51	56,56,56,56	0
56	MG	1A	3922	1/1	0.97	0.09	75,75,75,75	0
56	MG	1A	3213	1/1	0.97	0.12	23,23,23,23	0
56	MG	1A	3711	1/1	0.97	0.12	45,45,45,45	0
56	MG	2A	3463	1/1	0.97	0.12	58,58,58,58	0
56	MG	2A	3464	1/1	0.97	0.11	53,53,53,53	0
56	MG	1A	3092	1/1	0.97	0.24	40,40,40,40	0
56	MG	2A	3258	1/1	0.97	0.20	32,32,32,32	0
56	MG	1A	3572	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3193	1/1	0.97	0.22	20,20,20,20	0
56	MG	1a	1708	1/1	0.97	0.14	61,61,61,61	0
56	MG	2A	3470	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3821	1/1	0.97	0.11	26,26,26,26	0
56	MG	2A	3472	1/1	0.97	0.13	54,54,54,54	0
56	MG	1a	1710	1/1	0.97	0.23	54,54,54,54	0
56	MG	2a	3080	1/1	0.97	0.52	61,61,61,61	0
56	MG	1a	1856	1/1	0.97	0.12	70,70,70,70	0
56	MG	1a	1857	1/1	0.97	0.16	47,47,47,47	0
56	MG	1A	3216	1/1	0.97	0.17	66,66,66,66	0
56	MG	2A	3478	1/1	0.97	0.07	47,47,47,47	0
56	MG	2A	3479	1/1	0.97	0.11	31,31,31,31	0
56	MG	1a	1859	1/1	0.97	0.28	72,72,72,72	0
56	MG	1A	3717	1/1	0.97	0.17	44,44,44,44	0
56	MG	1A	3347	1/1	0.97	0.16	41,41,41,41	0
56	MG	1A	3026	1/1	0.97	0.35	36,36,36,36	0
56	MG	1a	1863	1/1	0.97	0.23	47,47,47,47	0
56	MG	2a	3091	1/1	0.97	0.24	63,63,63,63	0
56	MG	1A	3242	1/1	0.97	0.32	48,48,48,48	0
56	MG	1A	3827	1/1	0.97	0.10	27,27,27,27	0
56	MG	1A	3129	1/1	0.97	0.15	35,35,35,35	0
56	MG	1A	3643	1/1	0.97	0.20	22,22,22,22	0
56	MG	1B	205	1/1	0.97	0.12	49,49,49,49	0
56	MG	1a	1721	1/1	0.97	0.16	65,65,65,65	0
56	MG	1a	1871	1/1	0.97	0.18	58,58,58,58	0
56	MG	1A	3726	1/1	0.97	0.19	29,29,29,29	0
56	MG	1A	3644	1/1	0.97	0.15	38,38,38,38	0
56	MG	2A	3284	1/1	0.97	0.22	65,65,65,65	0
56	MG	1A	3579	1/1	0.97	0.19	49,49,49,49	0
56	MG	1a	1875	1/1	0.97	0.36	65,65,65,65	0
56	MG	2A	3287	1/1	0.97	0.10	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	2a	3107	1/1	0.97	0.11	63,63,63,63	0
56	MG	1A	3130	1/1	0.97	0.66	48,48,48,48	0
56	MG	2A	3289	1/1	0.97	0.37	44,44,44,44	0
56	MG	2A	3501	1/1	0.97	0.06	43,43,43,43	0
56	MG	2a	3111	1/1	0.97	0.20	46,46,46,46	0
56	MG	1A	3295	1/1	0.97	0.12	63,63,63,63	0
56	MG	1A	3172	1/1	0.97	0.29	32,32,32,32	0
56	MG	2A	3101	1/1	0.97	0.06	60,60,60,60	0
56	MG	17	101	1/1	0.97	0.36	34,34,34,34	0
56	MG	2a	3116	1/1	0.97	0.42	51,51,51,51	0
56	MG	1a	1880	1/1	0.97	0.21	50,50,50,50	0
56	MG	1a	1729	1/1	0.97	0.57	57,57,57,57	0
56	MG	1A	3157	1/1	0.97	0.29	30,30,30,30	0
56	MG	2a	3121	1/1	0.97	0.38	57,57,57,57	0
56	MG	1A	3530	1/1	0.97	0.17	29,29,29,29	0
56	MG	1A	3736	1/1	0.97	0.16	30,30,30,30	0
56	MG	1A	3955	1/1	0.97	0.20	47,47,47,47	0
56	MG	1A	3841	1/1	0.97	0.24	41,41,41,41	0
56	MG	1B	217	1/1	0.97	0.14	36,36,36,36	0
56	MG	1B	219	1/1	0.97	0.15	53,53,53,53	0
56	MG	1A	3118	1/1	0.97	0.26	20,20,20,20	0
56	MG	1a	1890	1/1	0.97	0.48	58,58,58,58	0
56	MG	1a	1740	1/1	0.97	0.10	57,57,57,57	0
56	MG	1A	3272	1/1	0.97	0.11	70,70,70,70	0
56	MG	1A	3960	1/1	0.97	0.12	41,41,41,41	0
56	MG	1A	3587	1/1	0.97	0.36	42,42,42,42	0
56	MG	1a	1895	1/1	0.97	0.12	56,56,56,56	0
56	MG	1A	3962	1/1	0.97	0.10	34,34,34,34	0
56	MG	2a	3136	1/1	0.97	0.25	72,72,72,72	0
56	MG	2A	3314	1/1	0.97	0.19	28,28,28,28	0
56	MG	2A	3315	1/1	0.97	0.20	40,40,40,40	0
56	MG	2A	3316	1/1	0.97	0.35	43,43,43,43	0
56	MG	1A	3740	1/1	0.97	0.17	13,13,13,13	0
56	MG	2A	3318	1/1	0.97	0.47	64,64,64,64	0
56	MG	1A	3742	1/1	0.97	0.39	60,60,60,60	0
56	MG	1A	3743	1/1	0.97	0.09	60,60,60,60	0
56	MG	2A	3532	1/1	0.97	0.16	56,56,56,56	0
56	MG	2A	3321	1/1	0.97	0.17	53,53,53,53	0
56	MG	1A	3177	1/1	0.97	0.14	56,56,56,56	0
56	MG	2A	3125	1/1	0.97	0.18	43,43,43,43	0
56	MG	2a	3148	1/1	0.97	0.05	77,77,77,77	0
56	MG	1A	3657	1/1	0.97	0.12	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3748	1/1	0.97	0.10	36,36,36,36	0
56	MG	1a	1610	1/1	0.97	0.06	52,52,52,52	0
56	MG	2A	3129	1/1	0.97	0.07	55,55,55,55	0
56	MG	1A	3589	1/1	0.97	0.15	65,65,65,65	0
56	MG	1A	3534	1/1	0.97	0.31	65,65,65,65	0
56	MG	1A	3591	1/1	0.97	0.13	45,45,45,45	0
56	MG	2A	3332	1/1	0.97	0.17	50,50,50,50	0
56	MG	2A	3546	1/1	0.97	0.13	42,42,42,42	0
56	MG	1D	308	1/1	0.97	0.20	13,13,13,13	0
56	MG	1d	303	1/1	0.97	0.23	62,62,62,62	0
56	MG	2A	3549	1/1	0.97	0.23	43,43,43,43	0
56	MG	1A	3855	1/1	0.97	0.23	15,15,15,15	0
56	MG	2A	3551	1/1	0.97	0.57	55,55,55,55	0
56	MG	2a	3163	1/1	0.97	0.15	55,55,55,55	0
56	MG	2A	3336	1/1	0.97	0.24	49,49,49,49	0
56	MG	1A	3973	1/1	0.97	0.18	49,49,49,49	0
56	MG	1A	3752	1/1	0.97	0.14	55,55,55,55	0
56	MG	2a	3167	1/1	0.97	0.20	40,40,40,40	0
56	MG	1A	3661	1/1	0.97	0.07	51,51,51,51	0
56	MG	2A	3560	1/1	0.97	0.14	41,41,41,41	0
56	MG	2A	3340	1/1	0.97	0.34	51,51,51,51	0
56	MG	1a	1620	1/1	0.97	0.10	79,79,79,79	0
56	MG	2A	3343	1/1	0.97	0.25	60,60,60,60	0
56	MG	2A	3564	1/1	0.97	0.46	34,34,34,34	0
56	MG	1D	313	1/1	0.97	0.38	44,44,44,44	0
56	MG	1A	3754	1/1	0.97	0.18	20,20,20,20	0
56	MG	1A	3145	1/1	0.97	0.14	37,37,37,37	0
56	MG	1A	3059	1/1	0.97	0.06	46,46,46,46	0
56	MG	1n	502	1/1	0.97	0.09	47,47,47,47	0
56	MG	2A	3570	1/1	0.97	0.12	50,50,50,50	0
56	MG	1A	3494	1/1	0.97	0.48	58,58,58,58	0
56	MG	1o	3002	1/1	0.97	0.18	55,55,55,55	0
56	MG	1q	201	1/1	0.97	0.68	68,68,68,68	0
56	MG	1A	3455	1/1	0.97	0.33	52,52,52,52	0
56	MG	1A	3865	1/1	0.97	0.19	32,32,32,32	0
56	MG	1A	3760	1/1	0.97	0.17	42,42,42,42	0
56	MG	1A	3102	1/1	0.97	0.28	37,37,37,37	0
56	MG	1a	1630	1/1	0.97	0.14	38,38,38,38	0
56	MG	2a	3190	1/1	0.97	0.11	67,67,67,67	0
56	MG	2A	3158	1/1	0.97	0.21	52,52,52,52	0
56	MG	2A	3159	1/1	0.97	0.28	31,31,31,31	0
56	MG	1A	3762	1/1	0.97	0.12	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	3583	1/1	0.97	0.29	42,42,42,42	0
56	MG	1A	3668	1/1	0.97	0.26	84,84,84,84	0
56	MG	1A	3669	1/1	0.97	0.13	55,55,55,55	0
56	MG	1A	3076	1/1	0.97	0.22	42,42,42,42	0
56	MG	2B	3005	1/1	0.97	0.24	51,51,51,51	0
56	MG	1A	3423	1/1	0.97	0.13	62,62,62,62	0
56	MG	1A	3769	1/1	0.97	0.22	37,37,37,37	0
56	MG	2A	3368	1/1	0.97	0.23	63,63,63,63	0
56	MG	1A	3543	1/1	0.97	0.19	41,41,41,41	0
56	MG	1A	3602	1/1	0.97	0.21	41,41,41,41	0
56	MG	1A	3772	1/1	0.97	0.09	61,61,61,61	0
56	MG	1A	3603	1/1	0.97	0.13	26,26,26,26	0
56	MG	2A	3374	1/1	0.97	0.21	57,57,57,57	0
56	MG	1A	3544	1/1	0.97	0.14	30,30,30,30	0
56	MG	1F	307	1/1	0.97	0.39	49,49,49,49	0
56	MG	1A	3879	1/1	0.97	0.09	24,24,24,24	0
56	MG	1A	3333	1/1	0.97	0.07	51,51,51,51	0
56	MG	2a	3214	1/1	0.97	0.16	75,75,75,75	0
56	MG	2E	306	1/1	0.97	0.41	43,43,43,43	0
56	MG	2A	3379	1/1	0.97	0.25	42,42,42,42	0
56	MG	2A	3003	1/1	0.97	0.09	58,58,58,58	0
56	MG	1A	3606	1/1	0.97	0.20	43,43,43,43	0
56	MG	2a	3221	1/1	0.97	0.19	57,57,57,57	0
56	MG	1A	3113	1/1	0.97	0.14	42,42,42,42	0
56	MG	1A	3548	1/1	0.97	0.15	65,65,65,65	0
56	MG	1A	3784	1/1	0.97	0.22	31,31,31,31	0
56	MG	1A	3785	1/1	0.97	0.09	57,57,57,57	0
56	MG	1A	3886	1/1	0.97	0.17	42,42,42,42	0
56	MG	2a	3229	1/1	0.97	0.29	66,66,66,66	0
56	MG	1A	3206	1/1	0.97	0.11	51,51,51,51	0
56	MG	2A	3012	1/1	0.97	0.10	52,52,52,52	0
56	MG	1A	3164	1/1	0.97	0.41	51,51,51,51	0
56	MG	1A	3687	1/1	0.97	0.20	21,21,21,21	0
56	MG	2a	3235	1/1	0.97	0.38	64,64,64,64	0
56	MG	1N	206	1/1	0.97	0.06	34,34,34,34	0
56	MG	1A	3504	1/1	0.97	0.21	52,52,52,52	0
56	MG	1A	3281	1/1	0.97	0.19	59,59,59,59	0
56	MG	1a	1658	1/1	0.97	0.09	68,68,68,68	0
56	MG	2Y	502	1/1	0.97	0.12	57,57,57,57	0
56	MG	1a	1659	1/1	0.97	0.16	60,60,60,60	0
56	MG	2A	3397	1/1	0.97	0.24	64,64,64,64	0
56	MG	1O	202	1/1	0.97	0.12	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	1A	3429	1/1	0.97	0.29	53,53,53,53	0
56	MG	1A	3187	1/1	0.97	0.10	54,54,54,54	0
56	MG	1A	3894	1/1	0.97	0.24	58,58,58,58	0
56	MG	2A	3402	1/1	0.97	0.23	55,55,55,55	0
56	MG	1P	205	1/1	0.97	0.44	49,49,49,49	0
56	MG	2a	3005	1/1	0.97	0.43	51,51,51,51	0
56	MG	1A	3694	1/1	0.97	0.12	43,43,43,43	0
56	MG	2A	3405	1/1	0.97	0.30	45,45,45,45	0
56	MG	2I	202	1/1	0.97	0.31	57,57,57,57	0
56	MG	1Q	3002	1/1	0.97	0.33	38,38,38,38	0
56	MG	1A	3617	1/1	0.97	0.20	28,28,28,28	0
56	MG	1A	3898	1/1	0.97	0.18	36,36,36,36	0
56	MG	1A	3060	1/1	0.97	0.14	51,51,51,51	0
56	MG	1A	3432	1/1	0.97	0.41	44,44,44,44	0
56	MG	2A	3205	1/1	0.97	0.05	62,62,62,62	0
56	MG	2A	3031	1/1	0.97	0.23	55,55,55,55	0
56	MG	2x	3003	1/1	0.97	0.18	51,51,51,51	0
56	MG	2x	3004	1/1	0.97	0.06	74,74,74,74	0
56	MG	1A	3471	1/1	0.97	0.11	66,66,66,66	0
56	MG	2A	3033	1/1	0.97	0.23	55,55,55,55	0
56	MG	2A	3034	1/1	0.97	0.11	61,61,61,61	0
56	MG	1A	3560	1/1	0.97	0.27	24,24,24,24	0
56	MG	1a	1814	1/1	0.97	0.22	63,63,63,63	0
56	MG	1a	1674	1/1	0.97	0.11	57,57,57,57	0
56	MG	2A	3038	1/1	0.97	0.27	50,50,50,50	0
56	MG	1A	3803	1/1	0.97	0.14	33,33,33,33	0
56	MG	2a	3025	1/1	0.97	0.10	58,58,58,58	0
56	MG	2A	3330	1/1	0.98	0.13	58,58,58,58	0
56	MG	1A	3719	1/1	0.98	0.21	7,7,7,7	0
56	MG	1A	3553	1/1	0.98	0.10	38,38,38,38	0
56	MG	2a	3118	1/1	0.98	0.25	68,68,68,68	0
56	MG	1A	3721	1/1	0.98	0.13	45,45,45,45	0
56	MG	1A	3223	1/1	0.98	0.16	55,55,55,55	0
56	MG	2D	304	1/1	0.98	0.40	34,34,34,34	0
56	MG	2E	301	1/1	0.98	0.12	24,24,24,24	0
56	MG	1A	3831	1/1	0.98	0.08	54,54,54,54	0
56	MG	1A	3773	1/1	0.98	0.19	22,22,22,22	0
56	MG	1A	3895	1/1	0.98	0.31	38,38,38,38	0
56	MG	1A	3775	1/1	0.98	0.22	22,22,22,22	0
56	MG	1A	3776	1/1	0.98	0.22	44,44,44,44	0
56	MG	2A	3223	1/1	0.98	0.27	39,39,39,39	0
56	MG	1A	3153	1/1	0.98	0.13	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	2A	3342	1/1	0.98	0.31	46,46,46,46	0
56	MG	1A	3030	1/1	0.98	0.44	52,52,52,52	0
56	MG	1A	3175	1/1	0.98	0.23	36,36,36,36	0
56	MG	1N	203	1/1	0.98	0.28	46,46,46,46	0
56	MG	1A	3094	1/1	0.98	0.25	24,24,24,24	0
56	MG	1a	1868	1/1	0.98	0.18	49,49,49,49	0
56	MG	2A	3348	1/1	0.98	0.12	72,72,72,72	0
56	MG	1A	3781	1/1	0.98	0.14	28,28,28,28	0
56	MG	2A	3476	1/1	0.98	0.10	45,45,45,45	0
56	MG	1A	3682	1/1	0.98	0.06	59,59,59,59	0
56	MG	2A	3232	1/1	0.98	0.26	38,38,38,38	0
56	MG	1a	1689	1/1	0.98	0.07	60,60,60,60	0
56	MG	1N	207	1/1	0.98	0.49	45,45,45,45	0
56	MG	2U	202	1/1	0.98	0.17	45,45,45,45	0
56	MG	2A	3235	1/1	0.98	0.72	55,55,55,55	0
56	MG	1A	3015	1/1	0.98	0.27	40,40,40,40	0
56	MG	2A	3356	1/1	0.98	0.15	37,37,37,37	0
56	MG	1A	3729	1/1	0.98	0.16	22,22,22,22	0
56	MG	1A	3685	1/1	0.98	0.20	47,47,47,47	0
56	MG	1a	1612	1/1	0.98	0.05	63,63,63,63	0
56	MG	1A	3645	1/1	0.98	0.07	32,32,32,32	0
56	MG	1A	3373	1/1	0.98	0.23	49,49,49,49	0
56	MG	1A	3688	1/1	0.98	0.19	23,23,23,23	0
56	MG	1A	3910	1/1	0.98	0.25	34,34,34,34	0
56	MG	1A	3082	1/1	0.98	0.14	28,28,28,28	0
56	MG	1A	3849	1/1	0.98	0.09	55,55,55,55	0
56	MG	1A	3790	1/1	0.98	0.14	21,21,21,21	0
56	MG	1A	3735	1/1	0.98	0.16	27,27,27,27	0
56	MG	2A	3248	1/1	0.98	0.18	56,56,56,56	0
56	MG	2A	3370	1/1	0.98	0.05	62,62,62,62	0
56	MG	1a	1703	1/1	0.98	0.12	48,48,48,48	0
56	MG	1a	1704	1/1	0.98	0.20	40,40,40,40	0
56	MG	2A	3142	1/1	0.98	0.28	39,39,39,39	0
56	MG	2A	3143	1/1	0.98	0.34	51,51,51,51	0
56	MG	1A	3403	1/1	0.98	0.20	49,49,49,49	0
56	MG	1A	3614	1/1	0.98	0.07	26,26,26,26	0
56	MG	1A	3615	1/1	0.98	0.17	57,57,57,57	0
56	MG	2A	3147	1/1	0.98	0.20	33,33,33,33	0
56	MG	1A	3500	1/1	0.98	0.13	51,51,51,51	0
56	MG	2a	3021	1/1	0.98	0.16	78,78,78,78	0
56	MG	1A	3796	1/1	0.98	0.56	42,42,42,42	0
56	MG	2A	3260	1/1	0.98	0.18	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	3797	1/1	0.98	0.13	73,73,73,73	0
56	MG	2A	3262	1/1	0.98	0.17	55,55,55,55	0
56	MG	2A	3384	1/1	0.98	0.28	47,47,47,47	0
56	MG	1A	3192	1/1	0.98	0.18	50,50,50,50	0
56	MG	2A	3264	1/1	0.98	0.22	65,65,65,65	0
56	MG	2A	3514	1/1	0.98	0.09	58,58,58,58	0
56	MG	1A	3741	1/1	0.98	0.20	32,32,32,32	0
56	MG	1B	218	1/1	0.98	0.17	60,60,60,60	0
56	MG	2A	3517	1/1	0.98	0.07	47,47,47,47	0
56	MG	1A	3996	1/1	0.98	0.12	29,29,29,29	0
56	MG	2A	3155	1/1	0.98	0.14	33,33,33,33	0
56	MG	1A	3618	1/1	0.98	0.17	40,40,40,40	0
56	MG	1A	3619	1/1	0.98	0.15	16,16,16,16	0
56	MG	1a	1899	1/1	0.98	0.08	50,50,50,50	0
56	MG	1a	1806	1/1	0.98	0.31	67,67,67,67	0
56	MG	1a	1633	1/1	0.98	0.14	52,52,52,52	0
56	MG	1A	3802	1/1	0.98	0.16	64,64,64,64	0
56	MG	1a	1720	1/1	0.98	0.33	43,43,43,43	0
56	MG	1a	1905	1/1	0.98	0.10	83,83,83,83	0
56	MG	1A	3863	1/1	0.98	0.23	49,49,49,49	0
56	MG	2a	3044	1/1	0.98	0.23	95,95,95,95	0
56	MG	1A	3929	1/1	0.98	0.16	27,27,27,27	0
56	MG	1A	3568	1/1	0.98	0.13	51,51,51,51	0
56	MG	1A	3621	1/1	0.98	0.11	24,24,24,24	0
56	MG	1A	3746	1/1	0.98	0.15	15,15,15,15	0
56	MG	2A	3533	1/1	0.98	0.08	47,47,47,47	0
56	MG	1V	201	1/1	0.98	0.36	45,45,45,45	0
56	MG	1A	3933	1/1	0.98	0.24	54,54,54,54	0
56	MG	2a	3202	1/1	0.98	0.12	70,70,70,70	0
56	MG	2A	3406	1/1	0.98	0.23	49,49,49,49	0
56	MG	1a	1817	1/1	0.98	0.13	49,49,49,49	0
56	MG	1e	203	1/1	0.98	0.33	76,76,76,76	0
56	MG	1A	3747	1/1	0.98	0.18	28,28,28,28	0
56	MG	1A	3622	1/1	0.98	0.14	21,21,21,21	0
56	MG	1A	3937	1/1	0.98	0.54	51,51,51,51	0
56	MG	2A	3176	1/1	0.98	0.28	44,44,44,44	0
56	MG	2a	3211	1/1	0.98	0.21	60,60,60,60	0
56	MG	2a	3059	1/1	0.98	0.13	58,58,58,58	0
56	MG	2A	3177	1/1	0.98	0.37	40,40,40,40	0
56	MG	2A	3414	1/1	0.98	0.20	39,39,39,39	0
56	MG	2a	3062	1/1	0.98	0.11	66,66,66,66	0
56	MG	2A	3545	1/1	0.98	0.09	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	3064	1/1	0.98	0.45	51,51,51,51	0
56	MG	1a	1731	1/1	0.98	0.10	55,55,55,55	0
56	MG	2a	3066	1/1	0.98	0.10	50,50,50,50	0
56	MG	1A	3465	1/1	0.98	0.33	36,36,36,36	0
56	MG	2a	3223	1/1	0.98	0.21	57,57,57,57	0
56	MG	1A	3570	1/1	0.98	0.20	18,18,18,18	0
56	MG	2A	3181	1/1	0.98	0.30	43,43,43,43	0
56	MG	1A	3625	1/1	0.98	0.24	30,30,30,30	0
56	MG	2a	3227	1/1	0.98	0.32	81,81,81,81	0
56	MG	1A	3181	1/1	0.98	0.39	46,46,46,46	0
56	MG	2A	3421	1/1	0.98	0.04	50,50,50,50	0
56	MG	2a	3230	1/1	0.98	0.10	70,70,70,70	0
56	MG	2A	3553	1/1	0.98	0.26	35,35,35,35	0
56	MG	2A	3554	1/1	0.98	0.15	44,44,44,44	0
56	MG	1A	3942	1/1	0.98	0.40	34,34,34,34	0
56	MG	2A	3556	1/1	0.98	0.20	41,41,41,41	0
56	MG	2A	3079	1/1	0.98	0.25	51,51,51,51	0
56	MG	1A	4014	1/1	0.98	0.12	51,51,51,51	0
56	MG	2A	3559	1/1	0.98	0.04	61,61,61,61	0
56	MG	1a	1828	1/1	0.98	0.26	67,67,67,67	0
56	MG	1A	3595	1/1	0.98	0.33	47,47,47,47	0
56	MG	1A	3119	1/1	0.98	0.24	35,35,35,35	0
56	MG	1A	3629	1/1	0.98	0.27	58,58,58,58	0
56	MG	2A	3191	1/1	0.98	0.20	45,45,45,45	0
56	MG	1A	3525	1/1	0.98	0.07	60,60,60,60	0
56	MG	2A	3306	1/1	0.98	0.16	26,26,26,26	0
56	MG	2A	3307	1/1	0.98	0.12	32,32,32,32	0
56	MG	1A	3598	1/1	0.98	0.08	21,21,21,21	0
56	MG	1A	3120	1/1	0.98	0.18	37,37,37,37	0
56	MG	2A	3435	1/1	0.98	0.12	53,53,53,53	0
56	MG	2A	3571	1/1	0.98	0.35	43,43,43,43	0
56	MG	1a	1835	1/1	0.98	0.19	34,34,34,34	0
56	MG	1A	3951	1/1	0.98	0.16	31,31,31,31	0
56	MG	1E	302	1/1	0.98	0.19	19,19,19,19	0
56	MG	1a	1838	1/1	0.98	0.22	62,62,62,62	0
56	MG	2a	3097	1/1	0.98	0.31	47,47,47,47	0
56	MG	1A	4022	1/1	0.98	0.43	66,66,66,66	0
56	MG	2p	101	1/1	0.98	0.30	68,68,68,68	0
56	MG	1A	3469	1/1	0.98	0.15	47,47,47,47	0
56	MG	1A	3470	1/1	0.98	0.07	57,57,57,57	0
56	MG	1a	1842	1/1	0.98	0.18	61,61,61,61	0
56	MG	1A	3672	1/1	0.98	0.10	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	1A	3763	1/1	0.98	0.18	46,46,46,46	0
56	MG	1A	3715	1/1	0.98	0.14	49,49,49,49	0
56	MG	1A	4028	1/1	0.98	0.12	68,68,68,68	0
56	MG	1A	3957	1/1	0.98	0.18	44,44,44,44	0
56	MG	1A	3027	1/1	0.98	0.19	60,60,60,60	0
56	MG	2B	3003	1/1	0.98	0.20	64,64,64,64	0
56	MG	1A	3144	1/1	0.98	0.17	22,22,22,22	0
56	MG	1a	1669	1/1	0.98	0.30	62,62,62,62	0
56	MG	1A	3767	1/1	0.98	0.24	21,21,21,21	0
56	MG	1A	3718	1/1	0.98	0.23	18,18,18,18	0
56	MG	17	103	1/1	0.98	0.07	53,53,53,53	0
56	MG	1A	3666	1/1	0.99	0.09	9,9,9,9	0
56	MG	2a	3215	1/1	0.99	0.35	80,80,80,80	0
56	MG	1A	3180	1/1	0.99	0.13	50,50,50,50	0
56	MG	1A	3003	1/1	0.99	0.10	58,58,58,58	0
56	MG	2a	3218	1/1	0.99	0.23	55,55,55,55	0
56	MG	1A	3918	1/1	0.99	0.21	25,25,25,25	0
56	MG	1A	3078	1/1	0.99	0.15	21,21,21,21	0
56	MG	1A	3774	1/1	0.99	0.22	21,21,21,21	0
56	MG	1P	204	1/1	0.99	0.38	31,31,31,31	0
56	MG	1A	3064	1/1	0.99	0.14	41,41,41,41	0
56	MG	1A	3832	1/1	0.99	0.22	68,68,68,68	0
56	MG	1A	3302	1/1	0.99	0.21	33,33,33,33	0
56	MG	2A	3484	1/1	0.99	0.05	37,37,37,37	0
56	MG	1A	3697	1/1	0.99	0.05	44,44,44,44	0
56	MG	1A	3864	1/1	0.99	0.08	15,15,15,15	0
56	MG	1A	3524	1/1	0.99	0.22	24,24,24,24	0
56	MG	1A	3555	1/1	0.99	0.12	39,39,39,39	0
56	MG	2a	3173	1/1	0.99	0.19	57,57,57,57	0
56	MG	1A	3928	1/1	0.99	0.21	51,51,51,51	0
56	MG	2a	3067	1/1	0.99	0.17	56,56,56,56	0
56	MG	1A	3539	1/1	0.99	0.13	26,26,26,26	0
56	MG	2a	3177	1/1	0.99	0.22	52,52,52,52	0
56	MG	2a	3016	1/1	0.99	0.14	58,58,58,58	0
56	MG	1A	3653	1/1	0.99	0.12	10,10,10,10	0
56	MG	1A	3676	1/1	0.99	0.13	23,23,23,23	0
56	MG	2A	3254	1/1	0.99	0.34	60,60,60,60	0
56	MG	1A	3106	1/1	0.99	0.24	26,26,26,26	0
56	MG	1a	1733	1/1	0.99	0.51	53,53,53,53	0
56	MG	1A	3756	1/1	0.99	0.17	46,46,46,46	0
56	MG	1A	3207	1/1	0.99	0.23	40,40,40,40	0
56	MG	2A	3123	1/1	0.99	0.13	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	1A	3935	1/1	0.99	0.10	20,20,20,20	0
56	MG	1A	3174	1/1	0.99	0.24	40,40,40,40	0
56	MG	2A	3308	1/1	0.99	0.25	41,41,41,41	0
56	MG	1A	3107	1/1	0.99	0.48	50,50,50,50	0
56	MG	2A	3453	1/1	0.99	0.19	83,83,83,83	0
56	MG	1x	108	1/1	0.99	0.21	57,57,57,57	0
56	MG	1A	3132	1/1	0.99	0.39	17,17,17,17	0
56	MG	17	102	1/1	0.99	0.15	33,33,33,33	0
56	MG	1A	3086	1/1	0.99	0.14	31,31,31,31	0
56	MG	1A	3683	1/1	0.99	0.15	40,40,40,40	0
56	MG	1a	1903	1/1	0.99	0.31	56,56,56,56	0
56	MG	2O	202	1/1	0.99	0.16	53,53,53,53	0
56	MG	1A	3639	1/1	0.99	0.14	11,11,11,11	0
56	MG	1a	1744	1/1	0.99	0.16	80,80,80,80	0
56	MG	2A	3365	1/1	0.99	0.15	44,44,44,44	0
56	MG	1a	1705	1/1	0.99	0.10	64,64,64,64	0
56	MG	1A	3178	1/1	0.99	0.27	50,50,50,50	0
56	MG	1A	3547	1/1	0.99	0.14	38,38,38,38	0
56	MG	1A	3565	1/1	0.99	0.18	17,17,17,17	0
56	MG	2a	3206	1/1	0.99	0.42	62,62,62,62	0
57	ZN	1Y	501	1/1	0.99	0.09	63,63,63,63	0
56	MG	1A	3566	1/1	0.99	0.19	42,42,42,42	0
57	ZN	15	102	1/1	0.99	0.13	43,43,43,43	0
57	ZN	16	102	1/1	0.99	0.13	45,45,45,45	0
57	ZN	19	501	1/1	0.99	0.12	44,44,44,44	0
56	MG	1A	3689	1/1	0.99	0.19	14,14,14,14	0
56	MG	2A	3141	1/1	0.99	0.34	35,35,35,35	0
56	MG	2A	3011	1/1	0.99	0.34	42,42,42,42	0
57	ZN	25	501	1/1	0.99	0.10	49,49,49,49	0
56	MG	1A	3947	1/1	0.99	0.06	37,37,37,37	0
56	MG	1A	3948	1/1	0.99	0.11	18,18,18,18	0
56	MG	1A	3169	1/1	0.99	0.26	41,41,41,41	0
58	SF4	1d	301	8/8	0.99	0.13	64,69,73,86	0
58	SF4	2d	501	8/8	0.99	0.11	58,77,81,90	0
56	MG	1A	4051	1/1	1.00	0.15	44,44,44,44	0
56	MG	2a	3098	1/1	1.00	0.16	49,49,49,49	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.