



# wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2018 – 09:10 PM EST

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the i symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

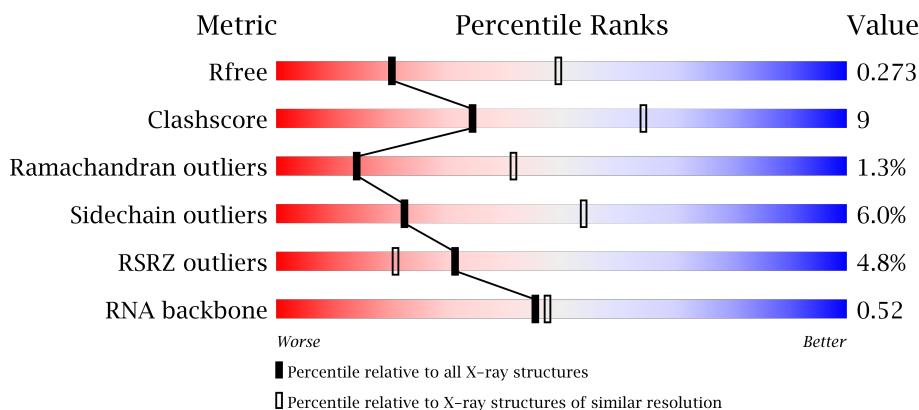
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

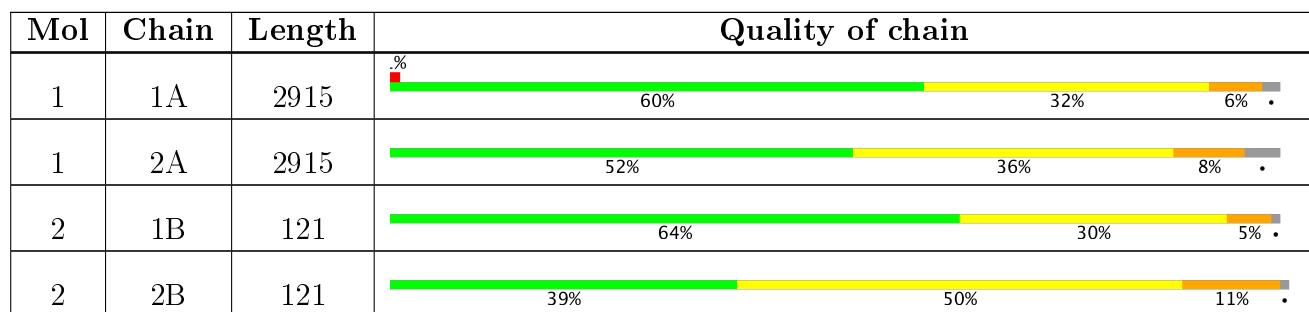
The reported resolution of this entry is 2.80 Å.

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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)
RNA backbone	2435	1007 (3.10-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.



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Mol	Chain	Length	Quality of chain			
3	1D	276	1%	77%	21%	•
3	2D	276		78%	20%	•
4	1E	206		77%	19%	••
4	2E	206	1%	74%	19%	5% •
5	1F	210		70%	23%	••
5	2F	210	1%	64%	29%	••
6	1G	182		73%	24%	•••
6	2G	182	4%	60%	36%	••
7	1H	180		75%	20%	••
7	2H	180	37%	62%	33%	••
8	1I	148		64%	32%	••
8	2I	148	1%	74%	23%	••
9	1N	140		86%	12%	•
9	2N	140	3%	71%	27%	•
10	1O	122		77%	22%	•
10	2O	122		75%	23%	•
11	1P	150		76%	21%	••
11	2P	150	25%	77%	19%	•••
12	1Q	141		72%	27%	•
12	2Q	141	14%	68%	28%	•
13	1R	118		75%	19%	6%
13	2R	118	1%	71%	25%	•
14	1S	112	1%	74%	18%	6% •
14	2S	112	21%	58%	38%	••
15	1T	146		65%	23%	• 10%

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Mol	Chain	Length	Quality of chain				
15	2T	146	3%	60%	27%	•	10%
16	1U	118	.	76%	19%	•	•
16	2U	118	.	71%	27%	•	.
17	1V	101		87%		10%	..
17	2V	101		82%		13%	5%
18	1W	113		83%		16%	•
18	2W	113	.	79%	17%	•	..
19	1X	96		78%		18%	..
19	2X	96		72%		25%	..
20	1Y	110		74%		21%	..
20	2Y	110	2%	75%		18%	•
21	1Z	206	.	58%	16%	25%	
21	2Z	206	19%	47%	28%	•	22%
22	10	85	6%	74%		20%	..
22	20	85	11%	69%		26%	..
23	11	98	.	73%		26%	•
23	21	98	5%	71%		28%	•
24	12	72		72%		25%	•
24	22	72		75%		21%	..
25	13	60		68%		30%	•
25	23	60	17%	68%	23%	7%	•
26	14	71	3%	63%	31%	•	..
26	24	71	4%	46%	48%	•	..
27	15	60	2%	78%		17%	..
27	25	60	2%	72%		25%	..

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Mol	Chain	Length	Quality of chain		
28	16	54	2%	72%	22% ..
28	26	54	11%	65%	31% ..
29	17	49	2%	67%	29% ..
29	27	49		63%	33% ..
30	18	65	2%	65%	32% ..
30	28	65	28%	66%	31% ..
31	19	37		76%	24%
31	29	37	30%	70%	30%
32	1a	1521	.%	82%	16% ..
32	2a	1521	2%	81%	18% ..
33	1b	256	6%	83%	7% 10%
33	2b	256	22%	82%	9% 10%
34	1c	239	9%	82%	• 14%
34	2c	239	26%	81%	5% 14%
35	1d	209	5%	93%	6%
35	2d	209	6%	93%	6%
36	1e	162	3%	85%	6% 9%
36	2e	162	15%	87%	• 9%
37	1f	101		96%	..
37	2f	101	.%	96%	..
38	1g	156	10%	94%	5% •
38	2g	156	12%	92%	8% •
39	1h	138	3%	94%	• ..
39	2h	138	10%	93%	5% ..
40	1i	128	23%	96%	..

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Mol	Chain	Length	Quality of chain			
40	2i	128	54%	96%	..	..
41	1j	105	25%	87%	6%	8%
41	2j	105	35%	83%	9%	9%
42	1k	129	%	84%	.	12%
42	2k	129	5%	82%	6%	12%
43	1l	132		84%	8%	8%
43	2l	132	6%	89%	.	8%
44	1m	126	8%	93%	5%	.
44	2m	126	13%	93%	.	.
45	1n	61	16%	89%	10%	.
45	2n	61	67%	90%	8%	.
46	1o	89	2%	96%	..	..
46	2o	89	%	96%	..	..
47	1p	88	6%	89%	5%	7%
47	2p	88	%	90%	.	7%
48	1q	105	3%	90%	.	6%
48	2q	105	19%	90%	5%	6%
49	1r	88	5%	73%	5%	23%
49	2r	88	2%	75%	.	23%
50	1s	93	%	86%	.	11%
50	2s	93	17%	84%	5%	11%
51	1t	106	13%	83%	8%	9%
51	2t	106	17%	80%	10%	9%
52	1u	27	15%	81%	.	15%
52	2u	27	44%	81%	.	15%

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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	13	101	-	-	-	X
56	MG	15	101	-	-	-	X
56	MG	16	103	-	-	-	X
56	MG	17	103	-	-	-	X
56	MG	18	101	-	-	-	X
56	MG	1A	3030	-	-	-	X
56	MG	1A	3031	-	-	-	X
56	MG	1A	3034	-	-	-	X
56	MG	1A	3037	-	-	-	X
56	MG	1A	3042	-	-	-	X
56	MG	1A	3068	-	-	-	X
56	MG	1A	3087	-	-	-	X
56	MG	1A	3095	-	-	-	X
56	MG	1A	3096	-	-	-	X
56	MG	1A	3102	-	-	-	X
56	MG	1A	3111	-	-	-	X
56	MG	1A	3113	-	-	-	X
56	MG	1A	3140	-	-	-	X
56	MG	1A	3141	-	-	-	X
56	MG	1A	3148	-	-	-	X
56	MG	1A	3154	-	-	-	X
56	MG	1A	3160	-	-	-	X
56	MG	1A	3171	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3173	-	-	-	X
56	MG	1A	3174	-	-	-	X
56	MG	1A	3175	-	-	-	X
56	MG	1A	3178	-	-	-	X
56	MG	1A	3179	-	-	-	X
56	MG	1A	3186	-	-	-	X
56	MG	1A	3199	-	-	-	X
56	MG	1A	3214	-	-	-	X
56	MG	1A	3217	-	-	-	X
56	MG	1A	3221	-	-	-	X
56	MG	1A	3222	-	-	-	X
56	MG	1A	3224	-	-	-	X
56	MG	1A	3252	-	-	-	X
56	MG	1A	3253	-	-	-	X
56	MG	1A	3269	-	-	-	X
56	MG	1A	3302	-	-	-	X
56	MG	1A	3304	-	-	-	X
56	MG	1A	3328	-	-	-	X
56	MG	1A	3337	-	-	-	X
56	MG	1A	3362	-	-	-	X
56	MG	1A	3375	-	-	-	X
56	MG	1A	3377	-	-	-	X
56	MG	1A	3393	-	-	-	X
56	MG	1A	3412	-	-	-	X
56	MG	1A	3422	-	-	-	X
56	MG	1A	3427	-	-	-	X
56	MG	1A	3430	-	-	-	X
56	MG	1A	3451	-	-	-	X
56	MG	1A	3454	-	-	-	X
56	MG	1A	3455	-	-	-	X
56	MG	1A	3456	-	-	-	X
56	MG	1A	3480	-	-	-	X
56	MG	1A	3483	-	-	-	X
56	MG	1A	3485	-	-	-	X
56	MG	1A	3492	-	-	-	X
56	MG	1A	3505	-	-	-	X
56	MG	1A	3526	-	-	-	X
56	MG	1A	3550	-	-	-	X
56	MG	1A	3560	-	-	-	X
56	MG	1A	3567	-	-	-	X
56	MG	1A	3625	-	-	-	X
56	MG	1A	3680	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3685	-	-	-	X
56	MG	1A	3689	-	-	-	X
56	MG	1A	3696	-	-	-	X
56	MG	1A	3704	-	-	-	X
56	MG	1A	3736	-	-	-	X
56	MG	1A	3739	-	-	-	X
56	MG	1A	3749	-	-	-	X
56	MG	1A	3751	-	-	-	X
56	MG	1A	3753	-	-	-	X
56	MG	1A	3756	-	-	-	X
56	MG	1A	3757	-	-	-	X
56	MG	1A	3772	-	-	-	X
56	MG	1A	3783	-	-	-	X
56	MG	1A	3799	-	-	-	X
56	MG	1A	3887	-	-	-	X
56	MG	1A	3932	-	-	-	X
56	MG	1A	3960	-	-	-	X
56	MG	1A	3994	-	-	-	X
56	MG	1A	4008	-	-	-	X
56	MG	1A	4014	-	-	-	X
56	MG	1A	4020	-	-	-	X
56	MG	1A	4023	-	-	-	X
56	MG	1A	4024	-	-	-	X
56	MG	1A	4026	-	-	-	X
56	MG	1A	4031	-	-	-	X
56	MG	1A	4032	-	-	-	X
56	MG	1A	4034	-	-	-	X
56	MG	1A	4036	-	-	-	X
56	MG	1A	4038	-	-	-	X
56	MG	1A	4039	-	-	-	X
56	MG	1A	4040	-	-	-	X
56	MG	1A	4041	-	-	-	X
56	MG	1A	4045	-	-	-	X
56	MG	1A	4046	-	-	-	X
56	MG	1A	4047	-	-	-	X
56	MG	1A	4049	-	-	-	X
56	MG	1A	4050	-	-	-	X
56	MG	1A	4055	-	-	-	X
56	MG	1A	4060	-	-	-	X
56	MG	1A	4061	-	-	-	X
56	MG	1A	4063	-	-	-	X
56	MG	1B	207	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1D	304	-	-	-	X
56	MG	1D	308	-	-	-	X
56	MG	1D	312	-	-	-	X
56	MG	1D	314	-	-	-	X
56	MG	1E	302	-	-	-	X
56	MG	1E	311	-	-	-	X
56	MG	1F	301	-	-	-	X
56	MG	1F	302	-	-	-	X
56	MG	1F	304	-	-	-	X
56	MG	1F	305	-	-	-	X
56	MG	1F	309	-	-	-	X
56	MG	1N	201	-	-	-	X
56	MG	1N	204	-	-	-	X
56	MG	1N	205	-	-	-	X
56	MG	1P	201	-	-	-	X
56	MG	1Q	201	-	-	-	X
56	MG	1R	203	-	-	-	X
56	MG	1R	204	-	-	-	X
56	MG	1Y	503	-	-	-	X
56	MG	1a	3014	-	-	-	X
56	MG	1a	3015	-	-	-	X
56	MG	1a	3038	-	-	-	X
56	MG	1a	3042	-	-	-	X
56	MG	1a	3108	-	-	-	X
56	MG	1a	3214	-	-	-	X
56	MG	1e	201	-	-	-	X
56	MG	1x	102	-	-	-	X
56	MG	25	502	-	-	-	X
56	MG	2A	3024	-	-	-	X
56	MG	2A	3054	-	-	-	X
56	MG	2A	3066	-	-	-	X
56	MG	2A	3072	-	-	-	X
56	MG	2A	3091	-	-	-	X
56	MG	2A	3109	-	-	-	X
56	MG	2A	3125	-	-	-	X
56	MG	2A	3127	-	-	-	X
56	MG	2A	3138	-	-	-	X
56	MG	2A	3180	-	-	-	X
56	MG	2A	3247	-	-	-	X
56	MG	2A	3267	-	-	-	X
56	MG	2A	3271	-	-	-	X
56	MG	2A	3299	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3317	-	-	-	X
56	MG	2A	3323	-	-	-	X
56	MG	2A	3325	-	-	-	X
56	MG	2A	3329	-	-	-	X
56	MG	2A	3343	-	-	-	X
56	MG	2A	3382	-	-	-	X
56	MG	2A	3395	-	-	-	X
56	MG	2A	3398	-	-	-	X
56	MG	2A	3447	-	-	-	X
56	MG	2A	3458	-	-	-	X
56	MG	2A	3464	-	-	-	X
56	MG	2A	3472	-	-	-	X
56	MG	2A	3478	-	-	-	X
56	MG	2A	3495	-	-	-	X
56	MG	2A	3552	-	-	-	X
56	MG	2A	3570	-	-	-	X
56	MG	2A	3583	-	-	-	X
56	MG	2A	3624	-	-	-	X
56	MG	2A	3654	-	-	-	X
56	MG	2A	3661	-	-	-	X
56	MG	2A	3662	-	-	-	X
56	MG	2A	3697	-	-	-	X
56	MG	2A	3732	-	-	-	X
56	MG	2A	3742	-	-	-	X
56	MG	2A	3749	-	-	-	X
56	MG	2A	3755	-	-	-	X
56	MG	2B	3008	-	-	-	X
56	MG	2D	303	-	-	-	X
56	MG	2D	306	-	-	-	X
56	MG	2D	307	-	-	-	X
56	MG	2F	303	-	-	-	X
56	MG	2U	202	-	-	-	X
56	MG	2U	203	-	-	-	X
56	MG	2U	204	-	-	-	X
56	MG	2a	1627	-	-	-	X
56	MG	2a	1655	-	-	-	X
56	MG	2a	1676	-	-	-	X
56	MG	2a	1693	-	-	-	X
56	MG	2a	1694	-	-	-	X
56	MG	2a	1714	-	-	-	X
56	MG	2a	1761	-	-	-	X
56	MG	2a	1822	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	EZG	1A	4030	-	-	-	X
58	EZG	2A	3746	-	-	-	X

## 2 Entry composition (i)

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

15	2T	131	Total C	N	O	S	0	0	0
			1083	675	224	183	1		

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

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

16	2U	116	Total C	N	O	S	0	0	0
			959	608	201	149	1		

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

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

17	2V	101	Total C	N	O	S	0	0	0
			771	495	140	135	1		

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

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

18	2W	112	Total C	N	O	S	0	0	0
			886	557	174	153	2		

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

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

19	2X	95	Total C	N	O	S	0	0	0
			750	488	135	126	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O	S		
26	14	69	552	349	99	99	5	0	0
26	24	69	532	339	97	91	5	0	0

- 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	455	285	89	76	5	0	0
27	25	59	455	285	89	76	5	0	0

- 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	453	281	91	77	4	0	0
28	26	53	449	279	91	75	4	0	0

- 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	418	257	104	55	2	0	0
29	27	48	418	257	104	55	2	0	0

- 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	517	331	102	82	2	0	0
30	28	64	517	331	102	82	2	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total C	N	O	P		0	0	0
			32246	14358	5975	10413	1500			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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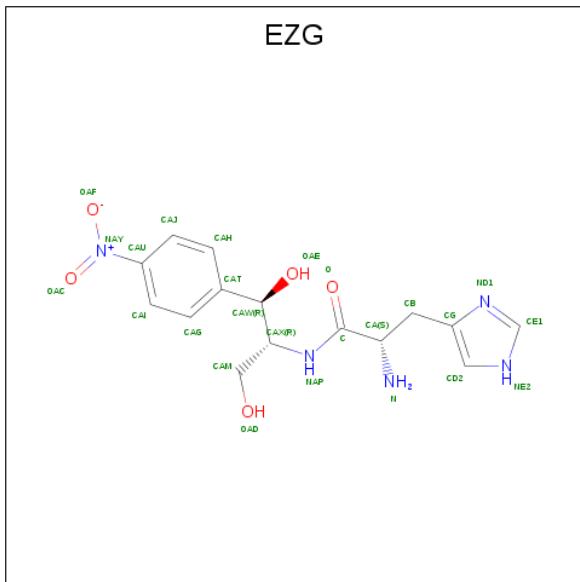
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2q	4	Total Mg 4 4	0	0
56	1U	6	Total Mg 6 6	0	0
56	1O	7	Total Mg 7 7	0	0
56	1r	1	Total Mg 1 1	0	0
56	19	1	Total Mg 1 1	0	0
56	1l	3	Total Mg 3 3	0	0
56	2V	2	Total Mg 2 2	0	0
56	1F	9	Total Mg 9 9	0	0
56	10	5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

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

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

- Molecule 58 is N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]-L-histidinamide (three-letter code: EZG) (formula: C<sub>15</sub>H<sub>19</sub>N<sub>5</sub>O<sub>5</sub>).



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

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

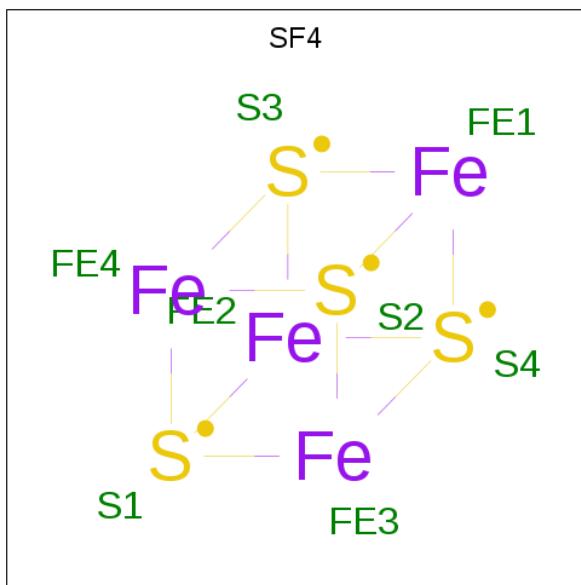
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1Y	1	Total Zn 1 1	0	0
59	14	1	Total Zn 1 1	0	0
59	1n	1	Total Zn 1 1	0	0
59	15	1	Total Zn 1 1	0	0
59	29	1	Total Zn 1 1	0	0
59	19	1	Total Zn 1 1	0	0
59	26	1	Total Zn 1 1	0	0
59	25	1	Total Zn 1 1	0	0

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

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 61 is water.

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

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

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

*Continued on next page...*

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

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

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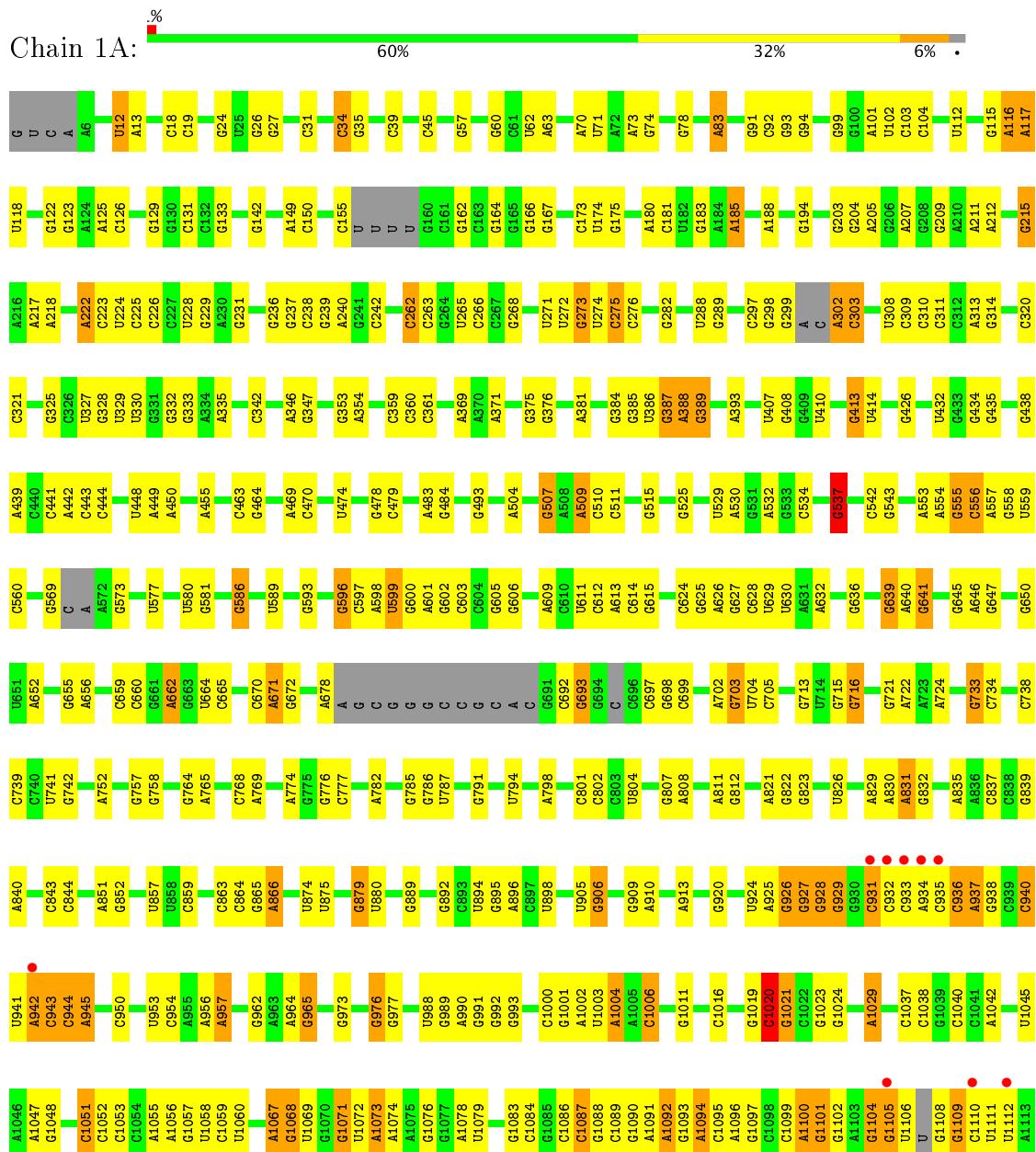
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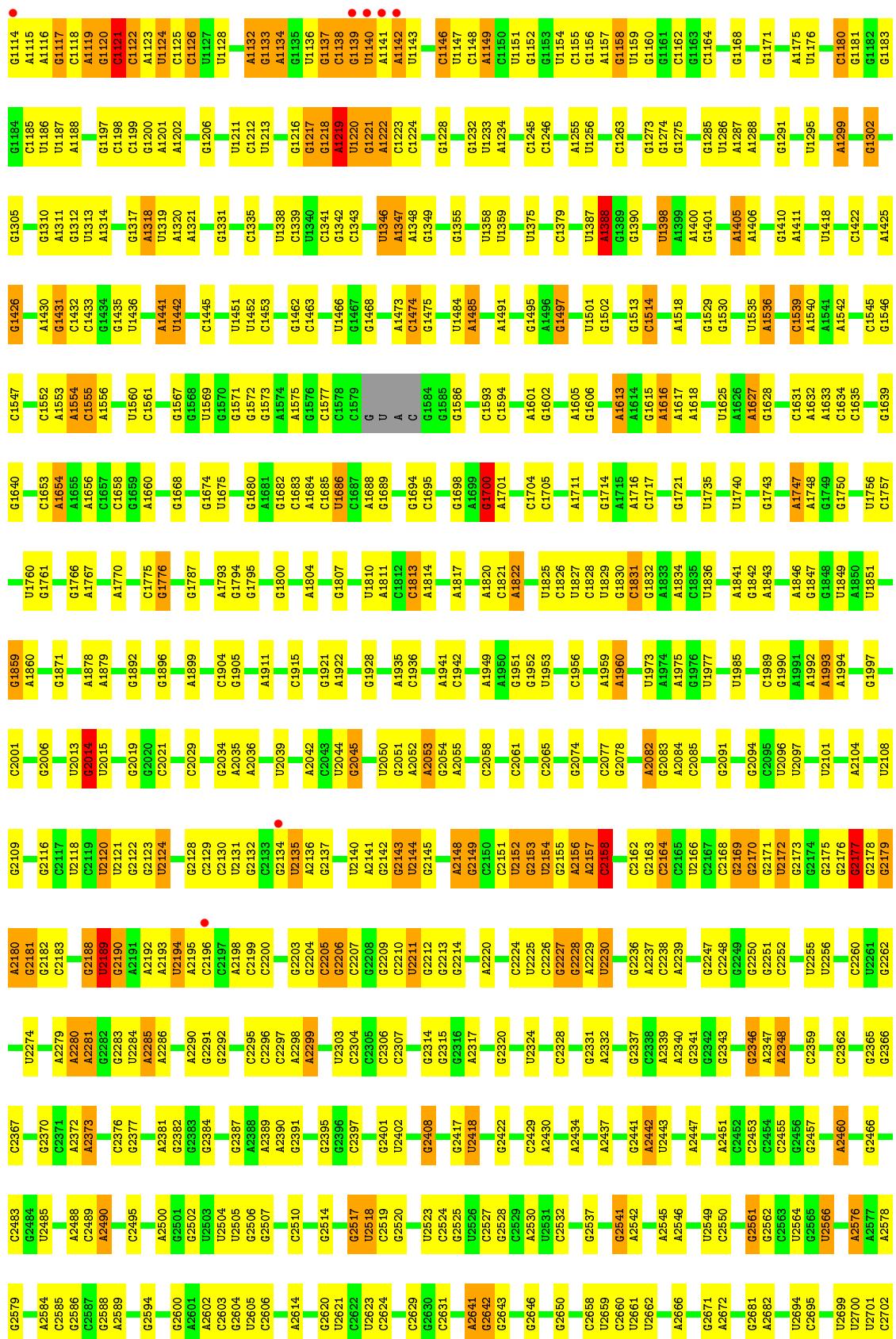
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2y	18	Total      O 18     18	0	0

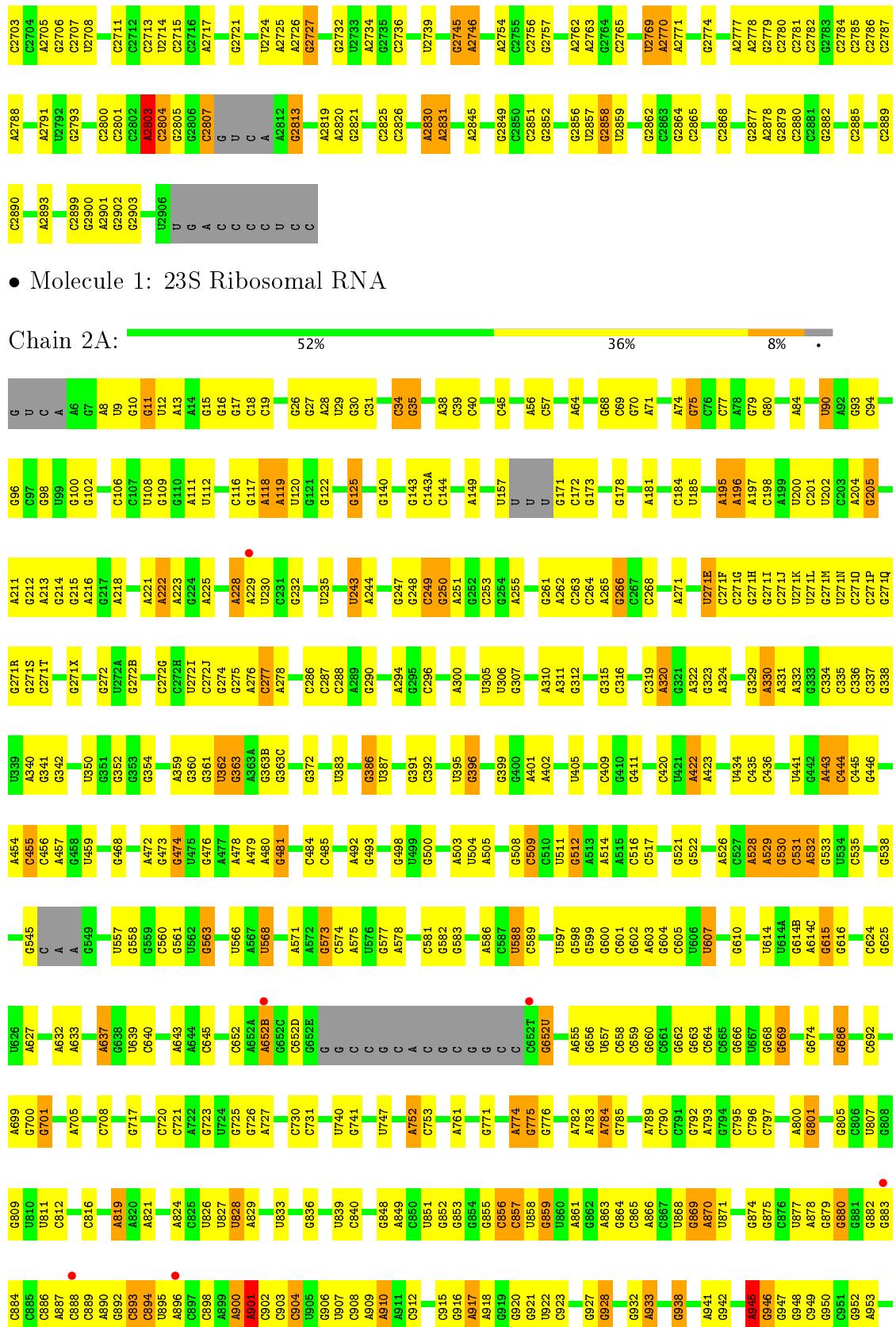
### 3 Residue-property plots

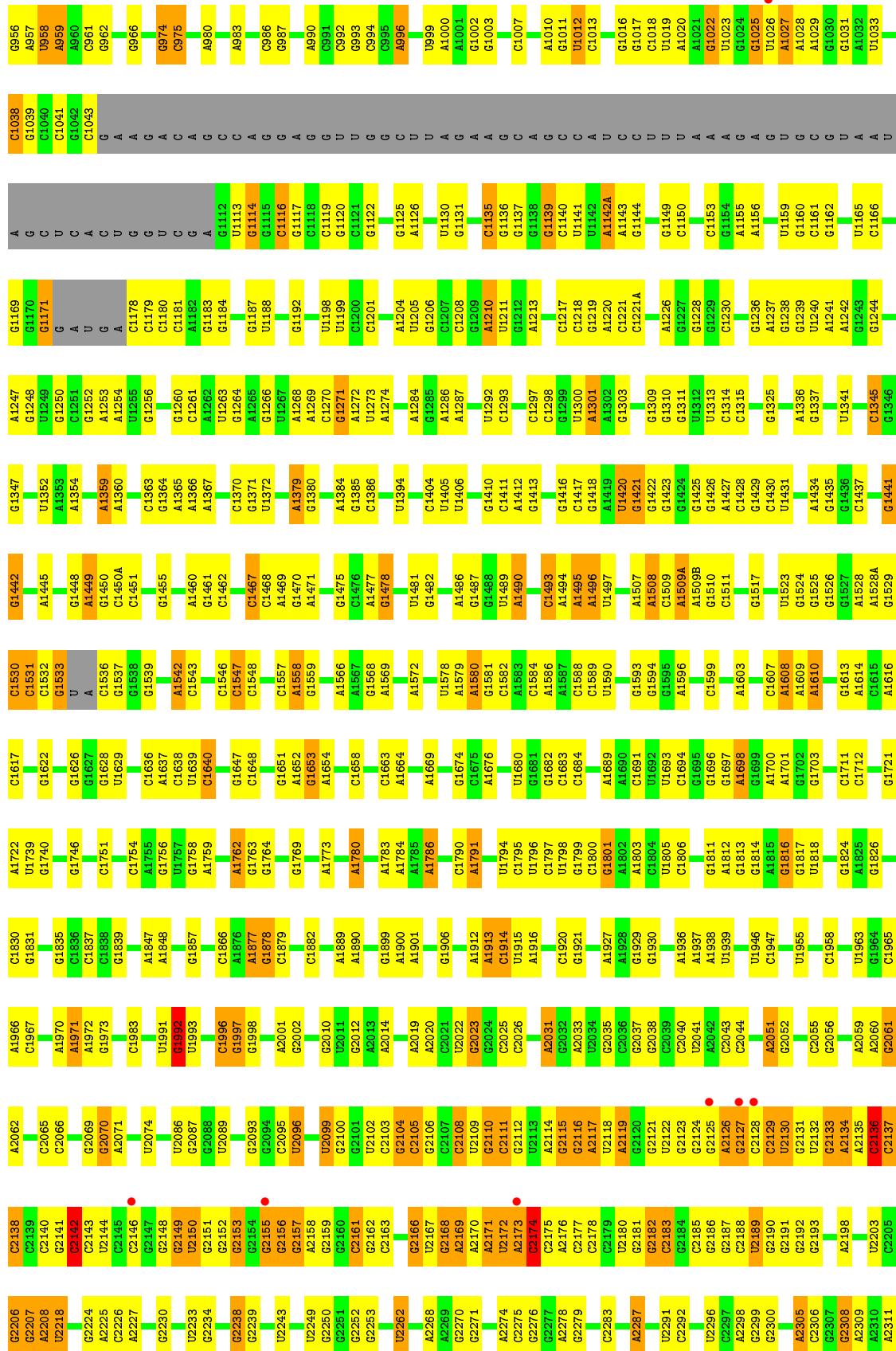
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

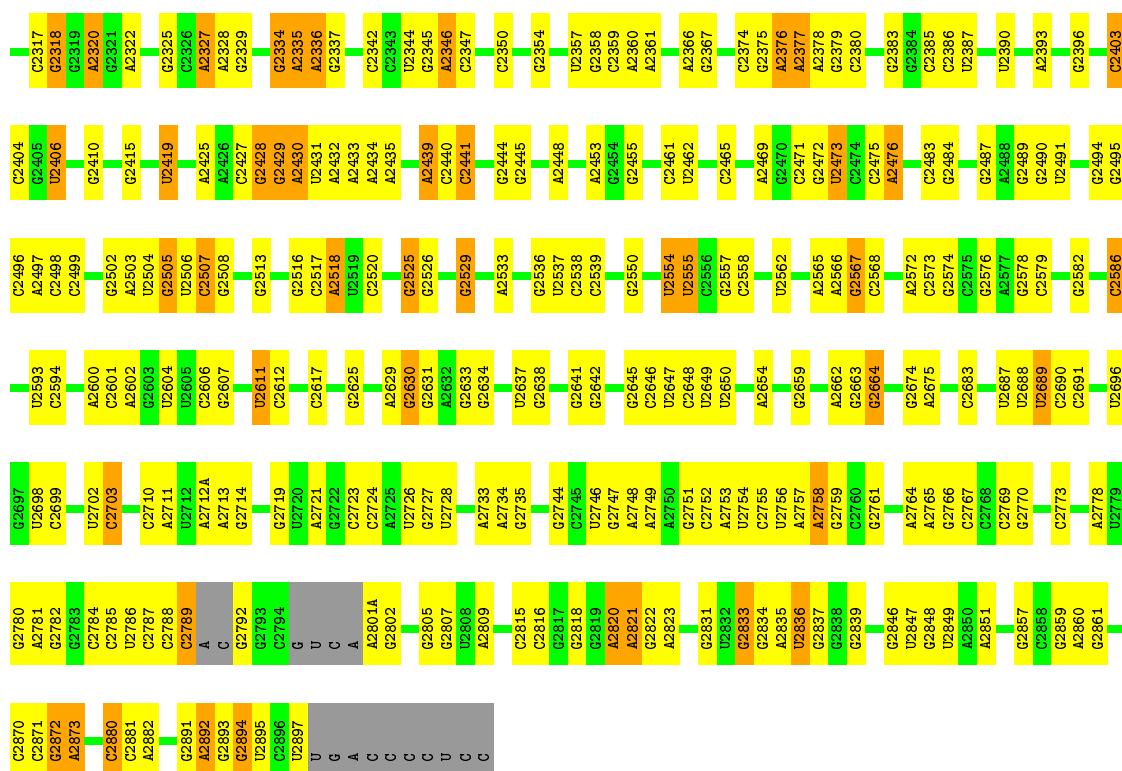
- Molecule 1: 23S Ribosomal RNA





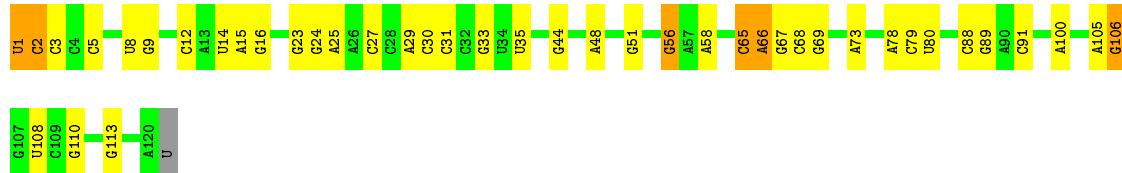






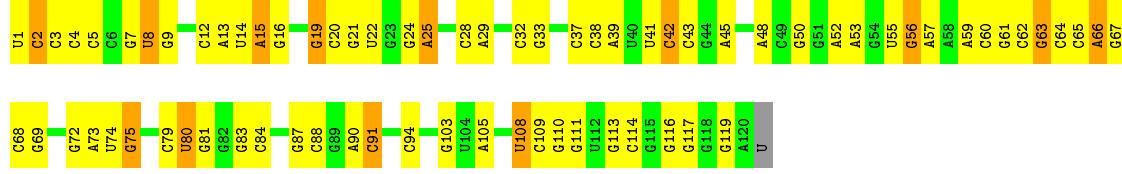
- Molecule 2: 5S Ribosomal RNA

Chain 1B: 64% 30% 5% •



- Molecule 2: 5S Ribosomal RNA

Chain 2B: 39% 50% 11% •



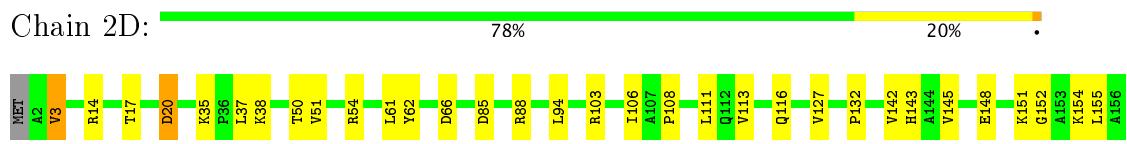
- Molecule 3: 50S ribosomal protein L2

Chain 1D: 77% 21% •

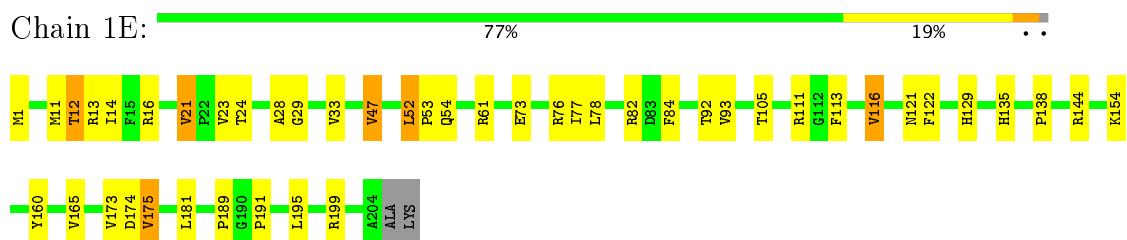




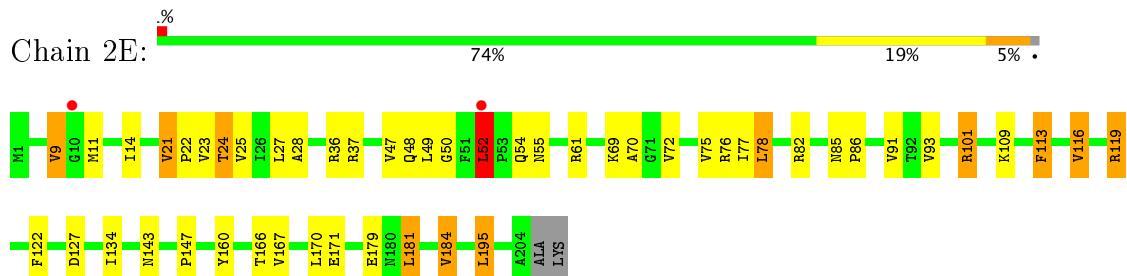
- Molecule 3: 50S ribosomal protein L2



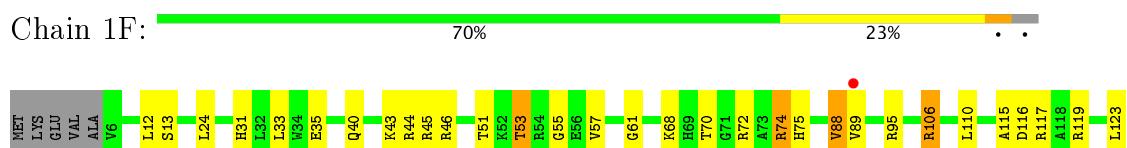
- Molecule 4: 50S ribosomal protein L3



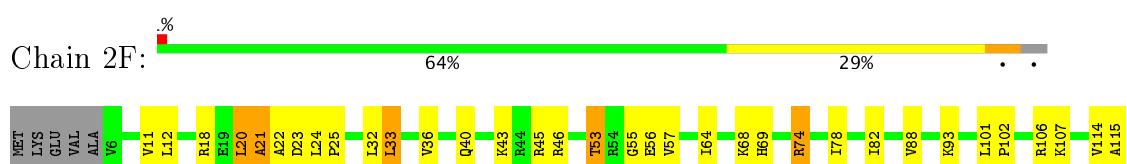
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4



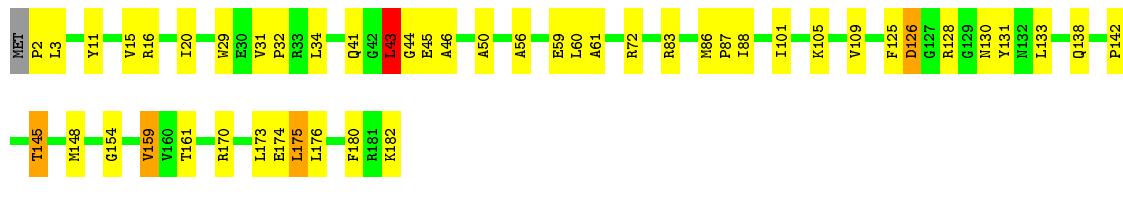
- Molecule 5: 50S ribosomal protein L4





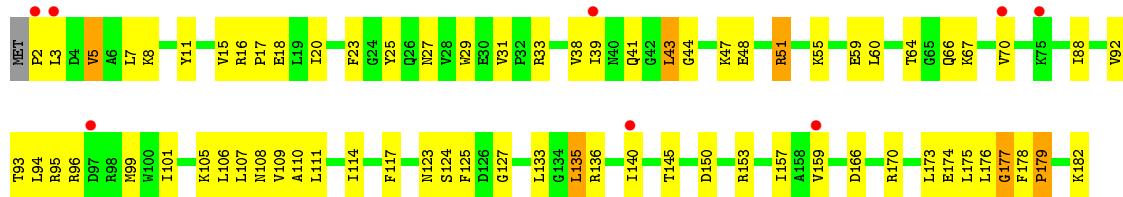
- Molecule 6: 50S ribosomal protein L5

Chain 1G: 73%



- Molecule 6: 50S ribosomal protein L5

Chain 2G: 60%



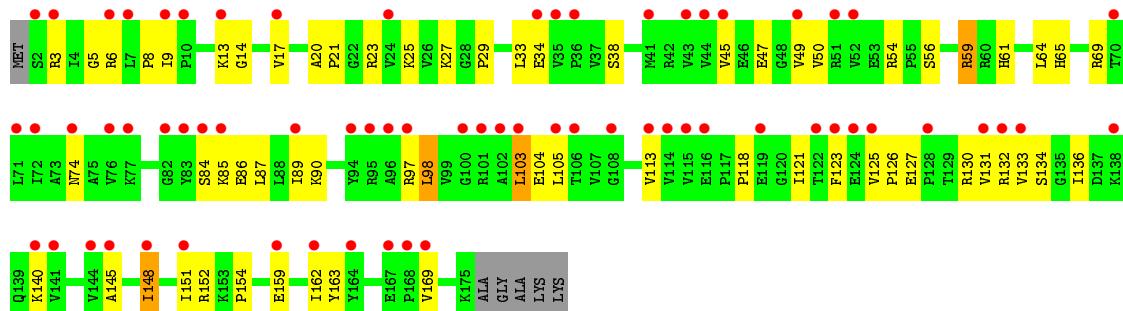
- Molecule 7: 50S ribosomal protein L6

Chain 1H: 75%



- Molecule 7: 50S ribosomal protein L6

Chain 2H: 62%

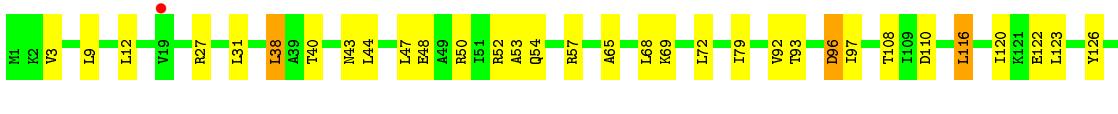
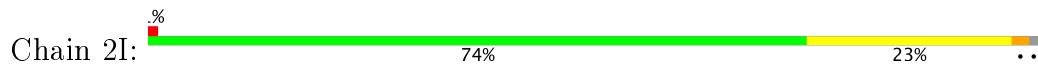


- Molecule 8: 50S ribosomal protein L9

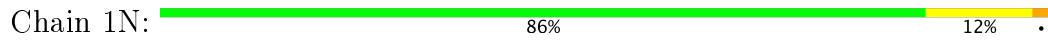
Chain 1I: 64%



- Molecule 8: 50S ribosomal protein L9



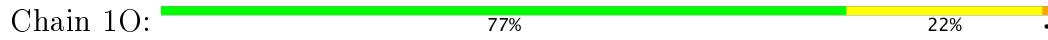
- Molecule 9: 50S ribosomal protein L13



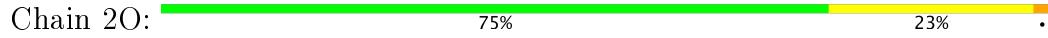
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14

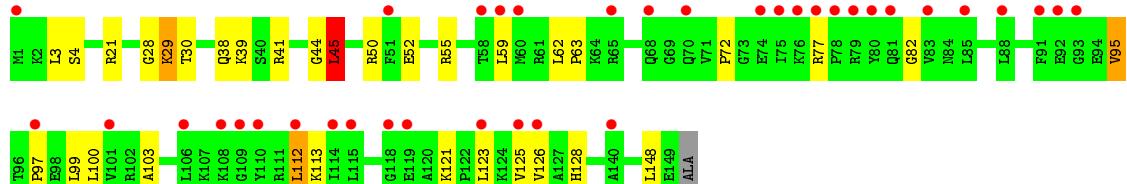
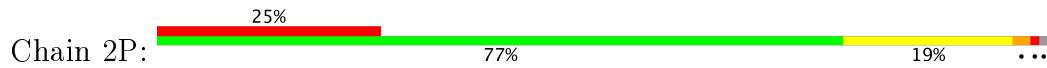


- Molecule 11: 50S ribosomal protein L15





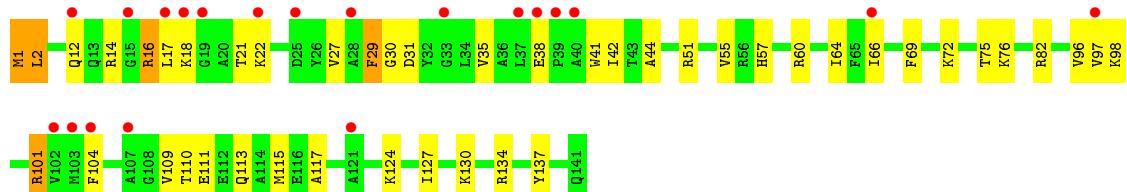
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



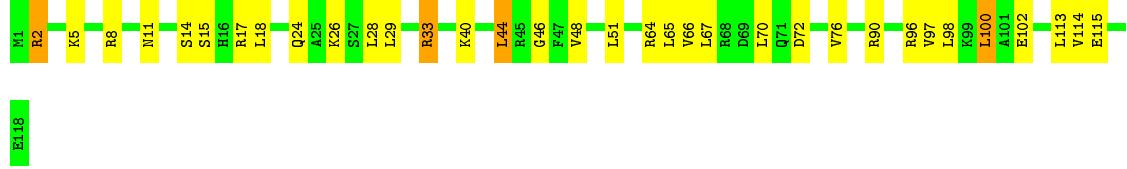
- Molecule 12: 50S ribosomal protein L16



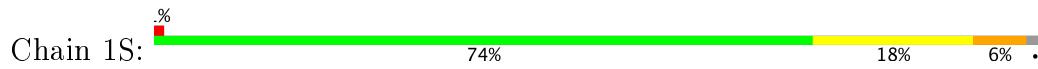
- Molecule 13: 50S ribosomal protein L17



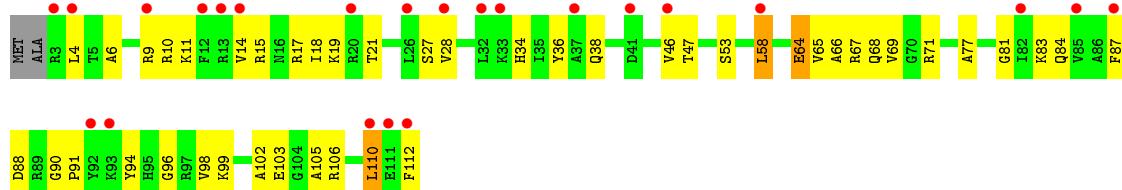
- Molecule 13: 50S ribosomal protein L17



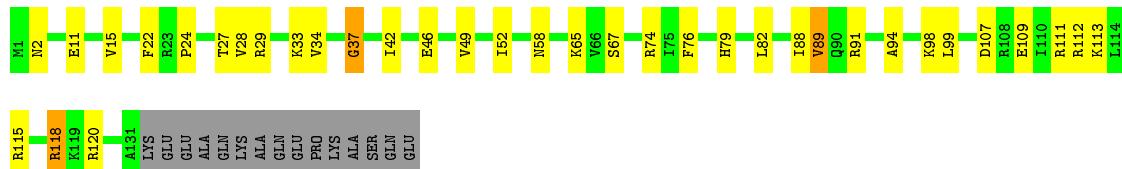
- Molecule 14: 50S ribosomal protein L18



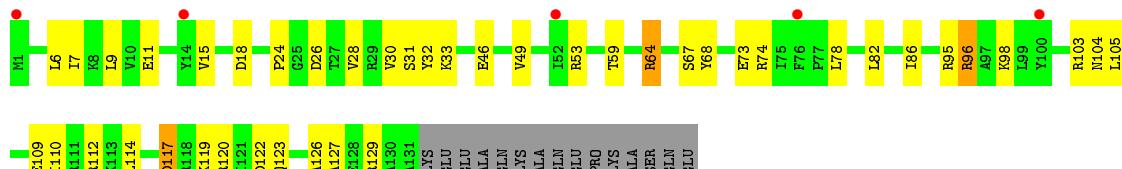
- Molecule 14: 50S ribosomal protein L18



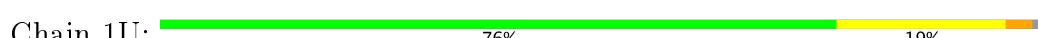
- Molecule 15: 50S ribosomal protein L19



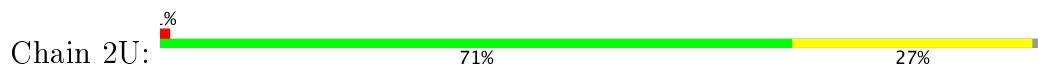
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20





- Molecule 17: 50S ribosomal protein L21

Chain 1V:



- Molecule 17: 50S ribosomal protein L21

Chain 2V:



- Molecule 18: 50S ribosomal protein L22

Chain 1W:



- Molecule 18: 50S ribosomal protein L22

Chain 2W:



- Molecule 19: 50S ribosomal protein L23

Chain 1X:



- Molecule 19: 50S ribosomal protein L23

Chain 2X:

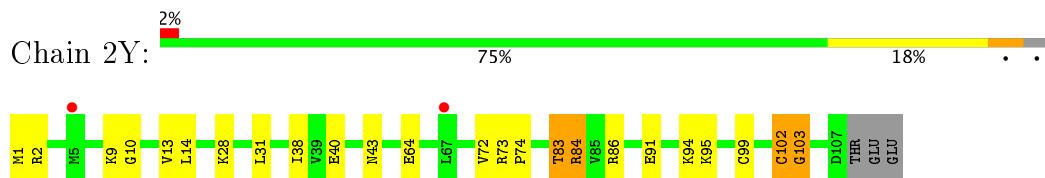


- Molecule 20: 50S ribosomal protein L24

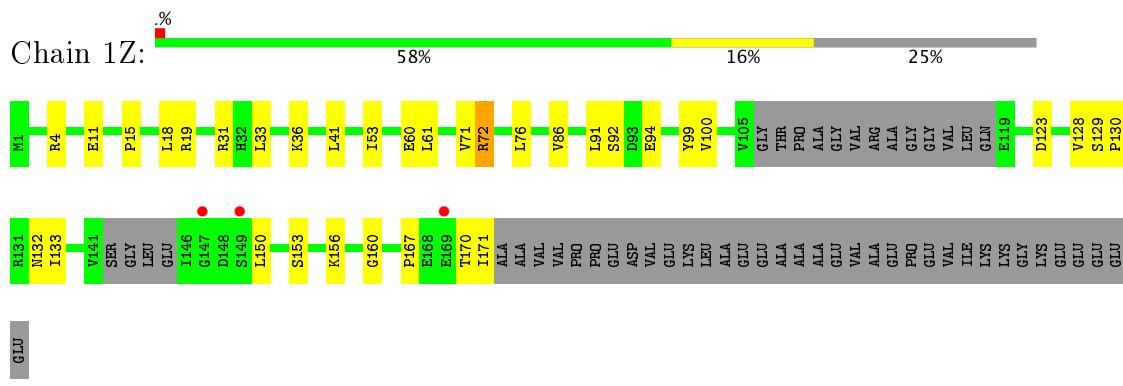
Chain 1Y:



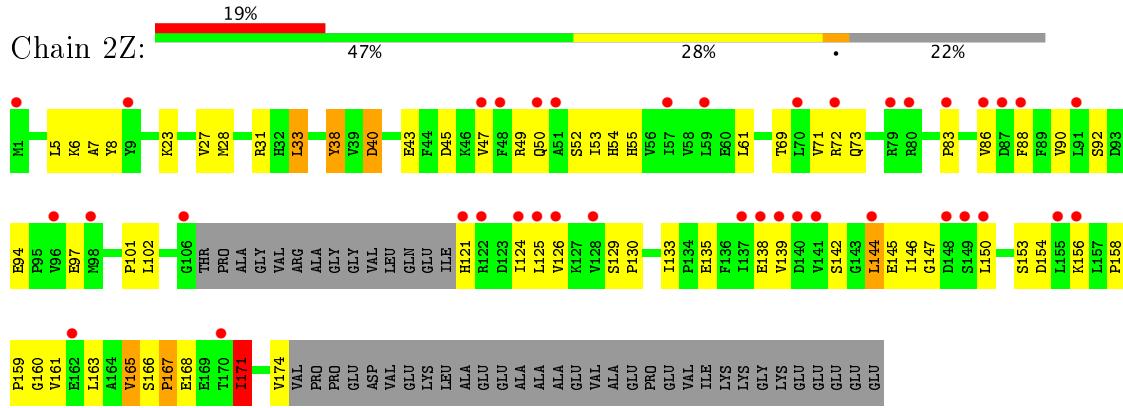
- Molecule 20: 50S ribosomal protein L24



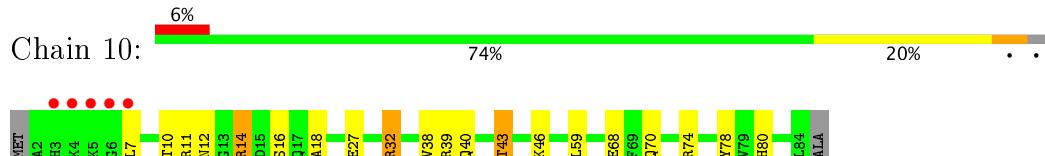
- Molecule 21: 50S ribosomal protein L25



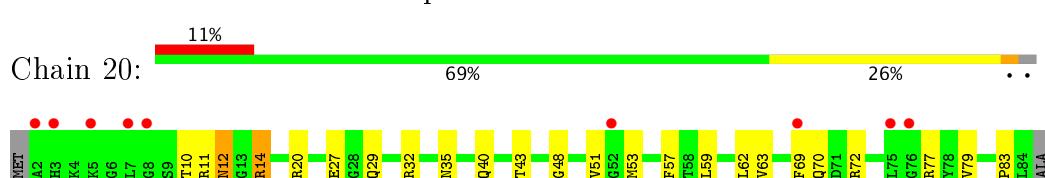
- Molecule 21: 50S ribosomal protein L25



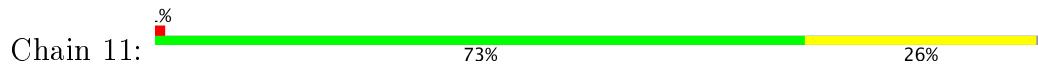
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



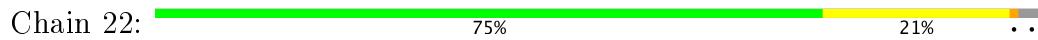
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



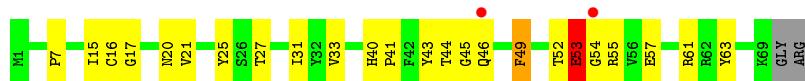
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



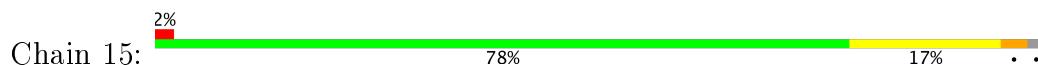
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



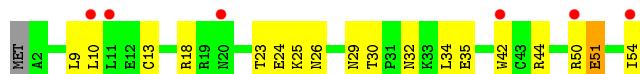
- Molecule 27: 50S ribosomal protein L32



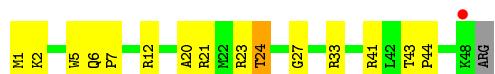
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



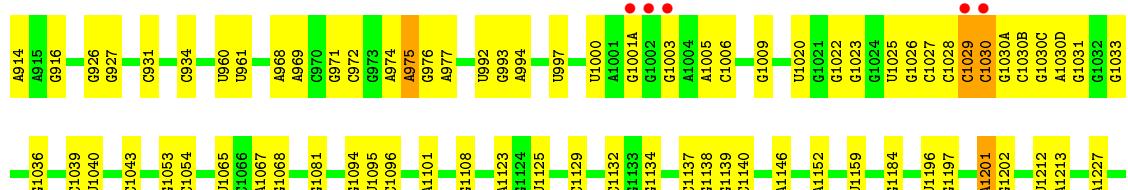
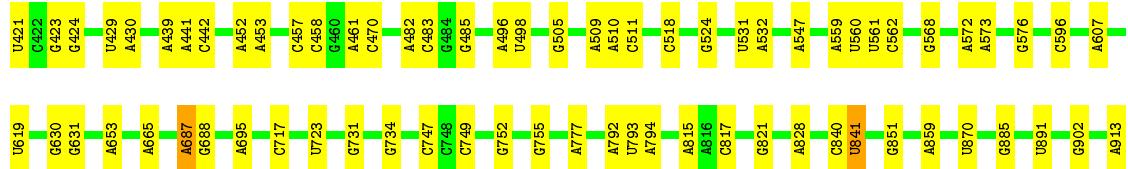
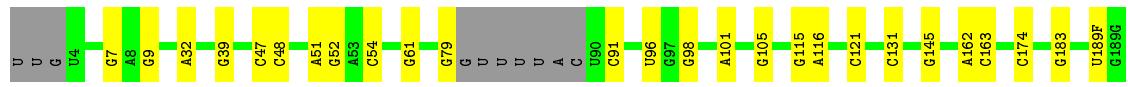
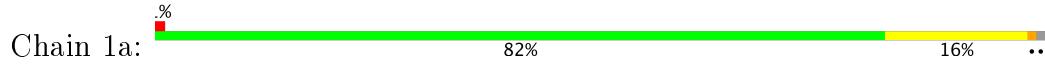
- Molecule 31: 50S ribosomal protein L36

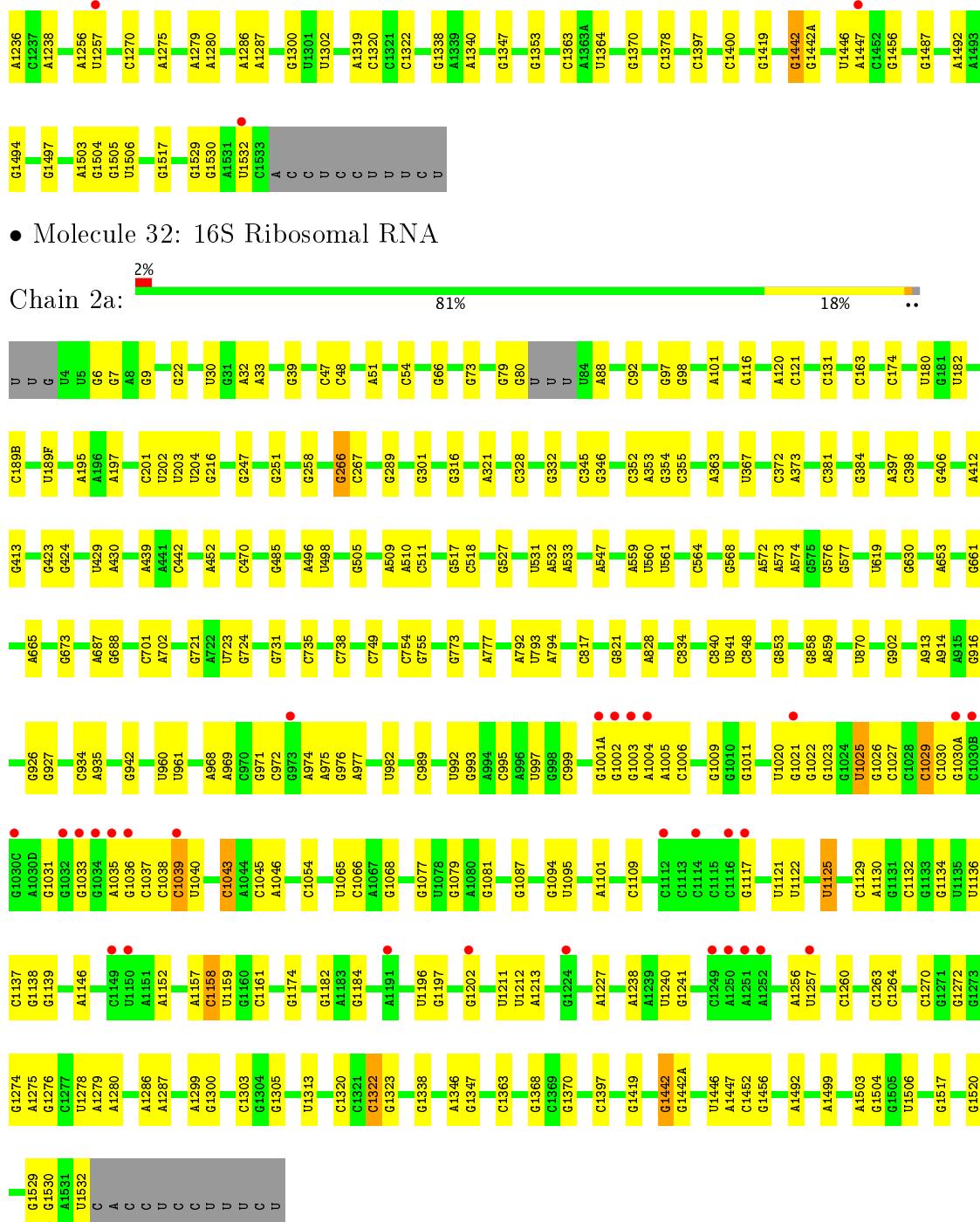


- Molecule 31: 50S ribosomal protein L36

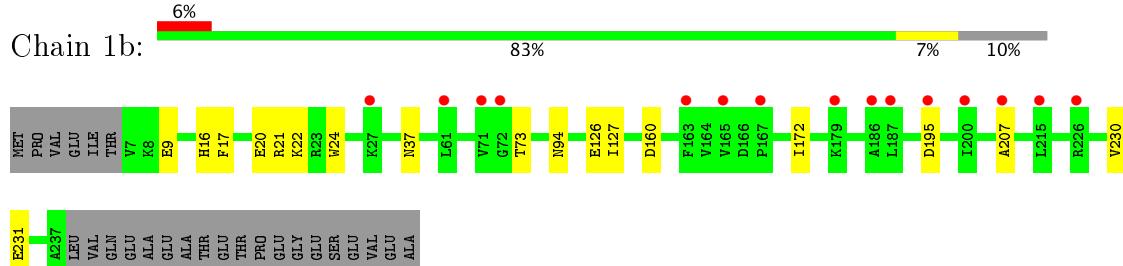


- Molecule 32: 16S Ribosomal RNA

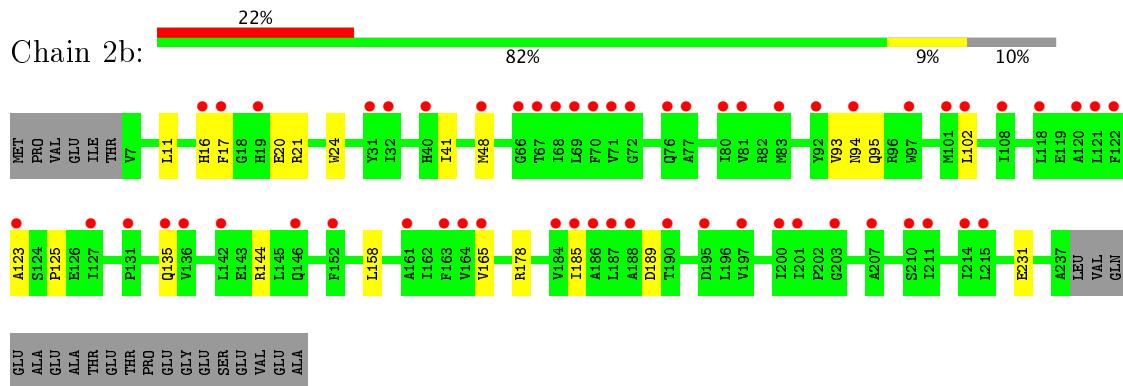




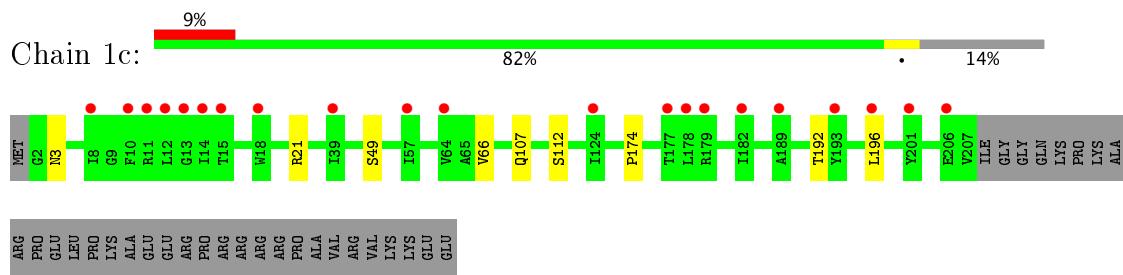
- Molecule 33: 30S ribosomal protein S2



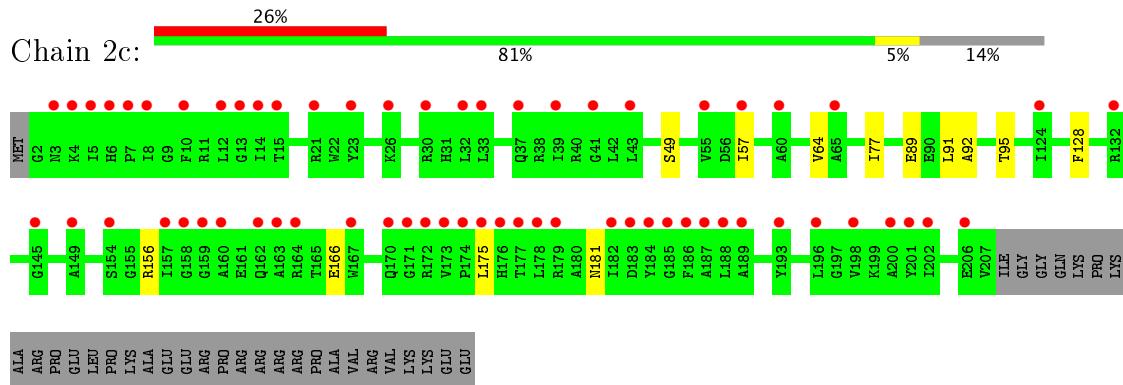
- Molecule 33: 30S ribosomal protein S2



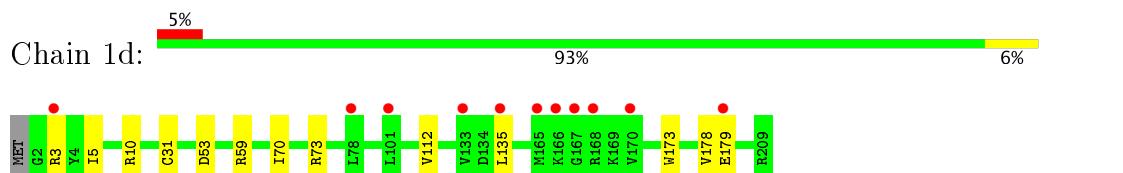
- Molecule 34: 30S ribosomal protein S3



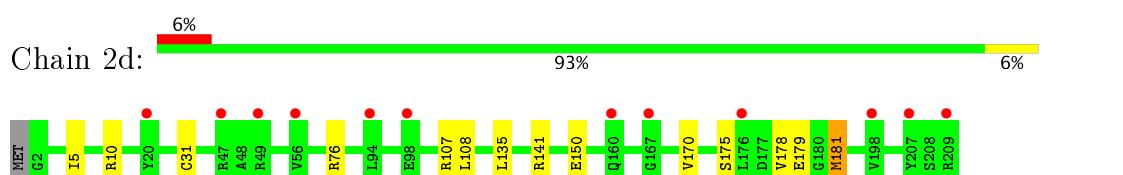
- Molecule 34: 30S ribosomal protein S3



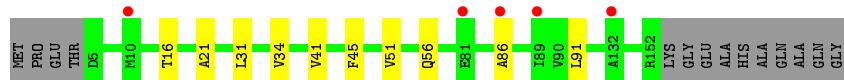
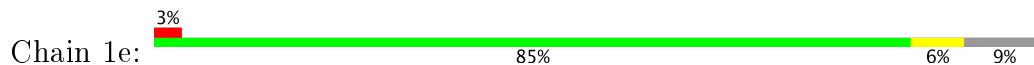
- Molecule 35: 30S ribosomal protein S4



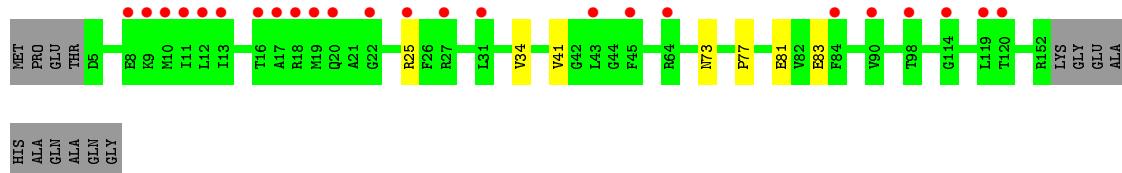
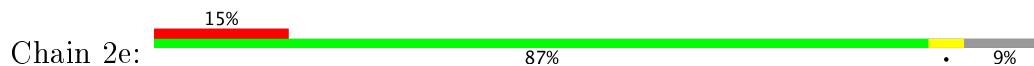
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6



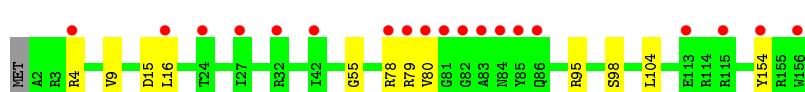
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7

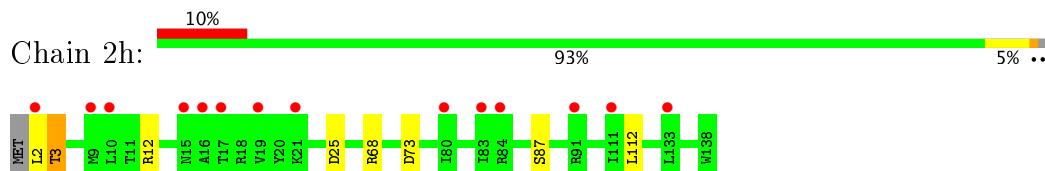


- Molecule 39: 30S ribosomal protein S8

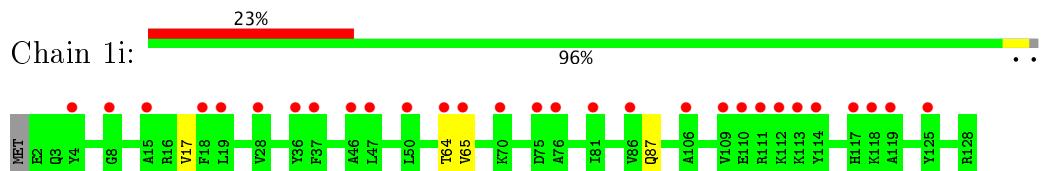




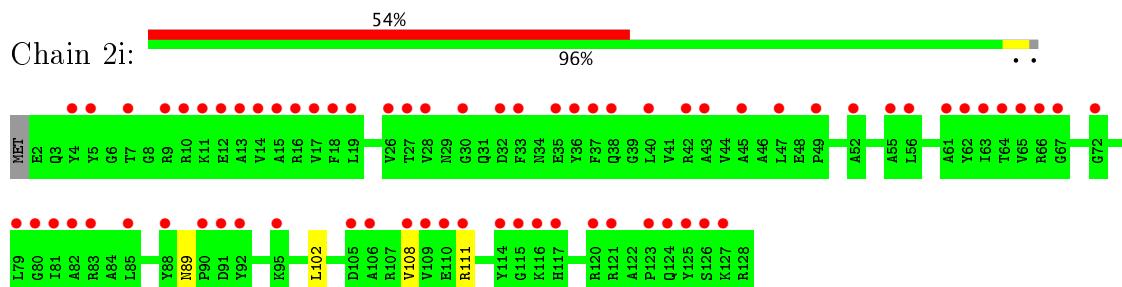
- Molecule 39: 30S ribosomal protein S8



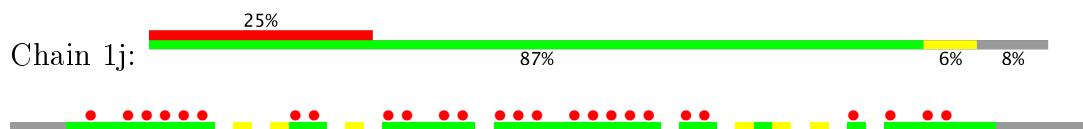
- Molecule 40: 30S ribosomal protein S9



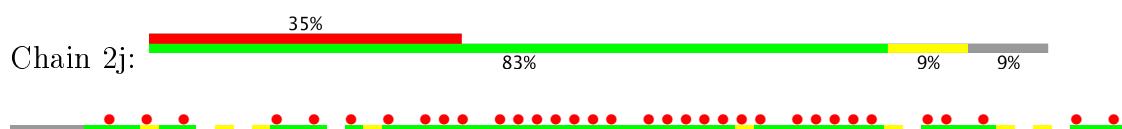
- Molecule 40: 30S ribosomal protein S9



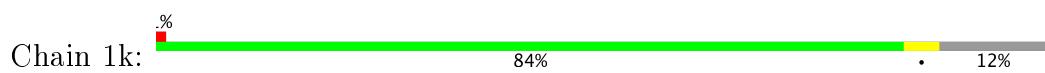
- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10

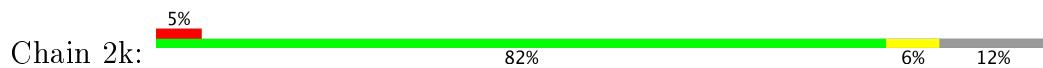


- Molecule 42: 30S ribosomal protein S11

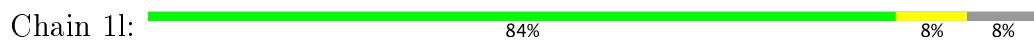




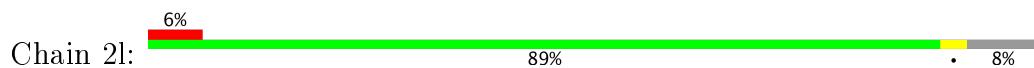
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13



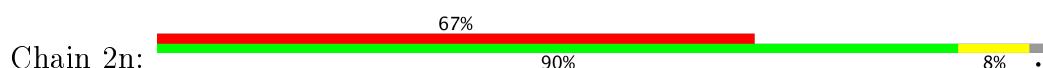
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z





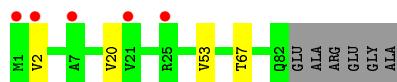
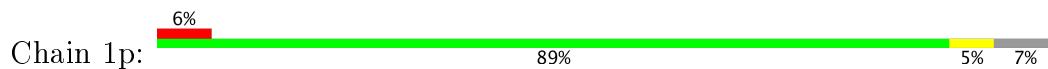
- Molecule 46: 30S ribosomal protein S15



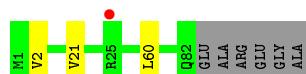
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17

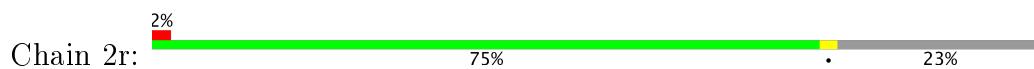


- Molecule 49: 30S ribosomal protein S18

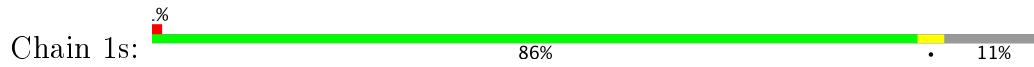




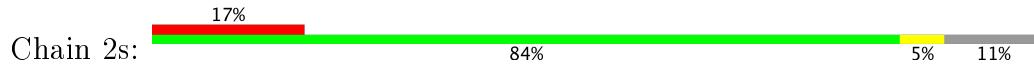
- Molecule 49: 30S ribosomal protein S18



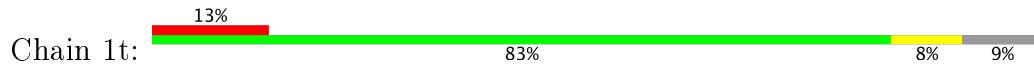
- Molecule 50: 30S ribosomal protein S19



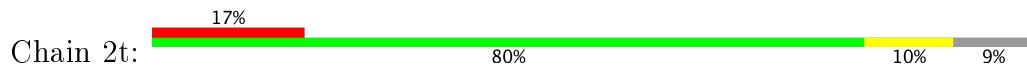
- Molecule 50: 30S ribosomal protein S19



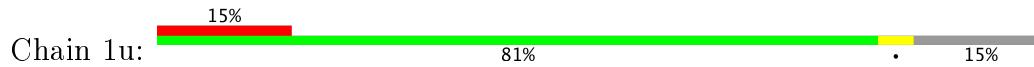
- Molecule 51: 30S ribosomal protein S20



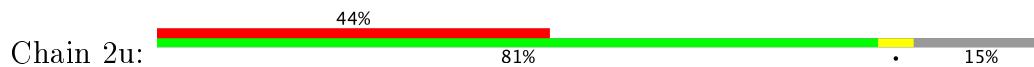
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx

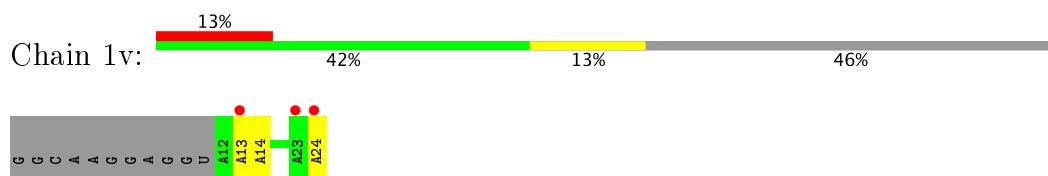


- Molecule 52: 30S ribosomal protein Thx

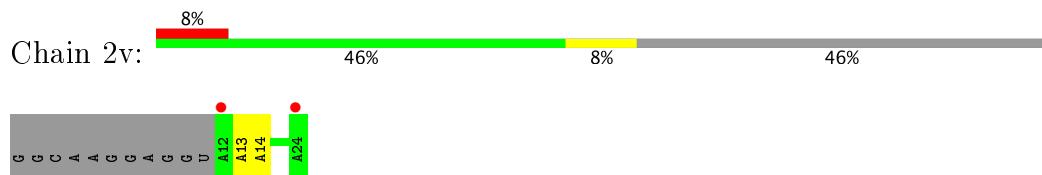




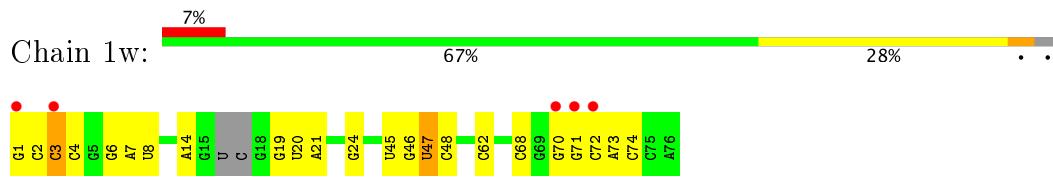
- Molecule 53: mRNA



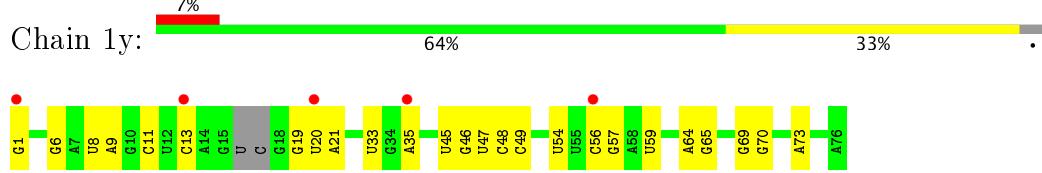
- Molecule 53: mRNA



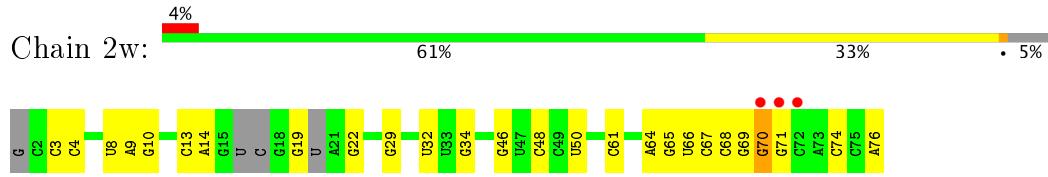
- Molecule 54: A-site and E-site tRNAs



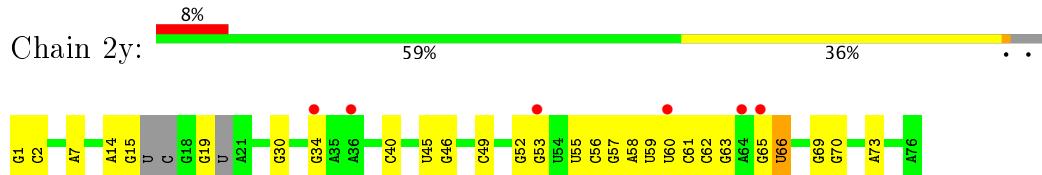
- Molecule 54: A-site and E-site tRNAs



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



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



- Molecule 55: P-site tRNA





- Molecule 55: P-site tRNA

Chain 2x: 83% 16%



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.78 Å    449.83 Å    622.74 Å 90.00°    90.00°    90.00°	Depositor
Resolution (Å)	152.54 – 2.80 181.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.0 (152.54-2.80) 94.0 (181.84-2.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.35 (at 2.82 Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
$R$ , $R_{free}$	0.214 , 0.269 0.221 , 0.273	Depositor DCC
$R_{free}$ test set	67418 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.9	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 60.2	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.41$ , $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	299109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

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

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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

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

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

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

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

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

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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

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

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

*Continued on next page...*

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

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

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

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

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

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

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

The worst 5 of 2479 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2158:C:N4	1:1A:2177:G:H1	1.36	1.21
1:2A:2136:C:N4	1:2A:2155:G:H1	1.46	1.12

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

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	257 (94%)	16 (6%)	0	100 100
3	2D	273/276 (99%)	254 (93%)	18 (7%)	1 (0%)	38 72
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	32 67
4	2E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	32 67
5	1F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	32 67
5	2F	201/210 (96%)	184 (92%)	13 (6%)	4 (2%)	9 28
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	28 62
6	2G	179/182 (98%)	156 (87%)	18 (10%)	5 (3%)	6 19
7	1H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	28 62
7	2H	172/180 (96%)	149 (87%)	20 (12%)	3 (2%)	11 34
8	1I	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	25 59
8	2I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	25 59
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100 100
9	2N	138/140 (99%)	126 (91%)	9 (6%)	3 (2%)	8 26
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100 100
10	2O	120/122 (98%)	111 (92%)	7 (6%)	2 (2%)	11 34
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	2P	147/150 (98%)	134 (91%)	11 (8%)	2 (1%)	13 39
12	1Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	25 59
12	2Q	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	25 59
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100 100
13	2R	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	11 34
14	1S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	20 52
14	2S	108/112 (96%)	100 (93%)	6 (6%)	2 (2%)	9 30
15	1T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	22 55
15	2T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	22 55
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100 100
17	1V	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	18 50
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	18 50
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100 100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100 100
19	2X	93/96 (97%)	84 (90%)	9 (10%)	0	100 100
20	1Y	105/110 (96%)	96 (91%)	8 (8%)	1 (1%)	18 50
20	2Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	9 30
21	1Z	148/206 (72%)	133 (90%)	14 (10%)	1 (1%)	25 59
21	2Z	156/206 (76%)	132 (85%)	19 (12%)	5 (3%)	5 16
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100 100
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	15 44
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100 100
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100 100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
24	22	68/72 (94%)	63 (93%)	4 (6%)	1 (2%)	12 37
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	10 32
26	14	67/71 (94%)	55 (82%)	8 (12%)	4 (6%)	2 5
26	24	67/71 (94%)	50 (75%)	13 (19%)	4 (6%)	2 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
28	26	51/54 (94%)	44 (86%)	7 (14%)	0	100 100
29	17	46/49 (94%)	46 (100%)	0	0	100 100
29	27	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	8 26
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100 100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100 100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
31	29	35/37 (95%)	32 (91%)	3 (9%)	0	100 100
33	1b	229/256 (90%)	192 (84%)	27 (12%)	10 (4%)	3 9
33	2b	229/256 (90%)	200 (87%)	20 (9%)	9 (4%)	3 12
34	1c	204/239 (85%)	190 (93%)	11 (5%)	3 (2%)	12 37
34	2c	204/239 (85%)	173 (85%)	25 (12%)	6 (3%)	5 18
35	1d	206/209 (99%)	190 (92%)	13 (6%)	3 (2%)	12 37
35	2d	206/209 (99%)	187 (91%)	15 (7%)	4 (2%)	9 30
36	1e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	13 39
36	2e	146/162 (90%)	131 (90%)	14 (10%)	1 (1%)	25 59
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
37	2f	98/101 (97%)	91 (93%)	7 (7%)	0	100 100
38	1g	153/156 (98%)	138 (90%)	12 (8%)	3 (2%)	9 28
38	2g	153/156 (98%)	135 (88%)	15 (10%)	3 (2%)	9 28
39	1h	135/138 (98%)	129 (96%)	4 (3%)	2 (2%)	12 37
39	2h	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	12 37
40	1i	125/128 (98%)	110 (88%)	15 (12%)	0	100 100
40	2i	125/128 (98%)	113 (90%)	12 (10%)	0	100 100
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3 10
41	2j	94/105 (90%)	79 (84%)	11 (12%)	4 (4%)	3 10
42	1k	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	20 52
42	2k	112/129 (87%)	103 (92%)	6 (5%)	3 (3%)	6 20
43	1l	119/132 (90%)	110 (92%)	8 (7%)	1 (1%)	22 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
43	2l	119/132 (90%)	103 (87%)	15 (13%)	1 (1%)	22 55
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100 100
44	2m	120/126 (95%)	102 (85%)	15 (12%)	3 (2%)	6 22
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100 100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100 100
46	1o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	15 44
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	15 44
47	1p	80/88 (91%)	69 (86%)	10 (12%)	1 (1%)	14 41
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100 100
48	1q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	18 50
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100 100
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100 100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100 100
50	1s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	15 44
50	2s	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	6 22
51	1t	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	2 7
51	2t	94/106 (89%)	83 (88%)	5 (5%)	6 (6%)	1 4
52	1u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2 8
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
All	All	11370/12128 (94%)	10425 (92%)	802 (7%)	143 (1%)	14 41

5 of 143 Ramachandran outliers are listed below:

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

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

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%)	200 (93%)	15 (7%)	18 45
3	2D	215/218 (99%)	206 (96%)	9 (4%)	34 68
4	1E	164/166 (99%)	152 (93%)	12 (7%)	16 42
4	2E	164/166 (99%)	148 (90%)	16 (10%)	9 27
5	1F	160/166 (96%)	144 (90%)	16 (10%)	9 26
5	2F	159/166 (96%)	144 (91%)	15 (9%)	10 29
6	1G	143/156 (92%)	133 (93%)	10 (7%)	18 45
6	2G	143/156 (92%)	134 (94%)	9 (6%)	21 51
7	1H	144/148 (97%)	138 (96%)	6 (4%)	34 68
7	2H	144/148 (97%)	138 (96%)	6 (4%)	34 68
8	1I	113/124 (91%)	104 (92%)	9 (8%)	14 38
8	2I	105/124 (85%)	99 (94%)	6 (6%)	24 56
9	1N	118/119 (99%)	110 (93%)	8 (7%)	18 47
9	2N	118/119 (99%)	108 (92%)	10 (8%)	12 35
10	1O	100/100 (100%)	97 (97%)	3 (3%)	46 80
10	2O	100/100 (100%)	100 (100%)	0	100 100
11	1P	115/116 (99%)	109 (95%)	6 (5%)	27 60
11	2P	115/116 (99%)	111 (96%)	4 (4%)	41 75
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	26 58
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	14 37
13	1R	101/101 (100%)	90 (89%)	11 (11%)	7 22
13	2R	101/101 (100%)	92 (91%)	9 (9%)	11 32
14	1S	86/88 (98%)	78 (91%)	8 (9%)	10 30
14	2S	85/88 (97%)	78 (92%)	7 (8%)	13 37
15	1T	115/127 (91%)	112 (97%)	3 (3%)	51 83
15	2T	113/127 (89%)	105 (93%)	8 (7%)	17 44
16	1U	93/94 (99%)	85 (91%)	8 (9%)	12 34
16	2U	93/94 (99%)	91 (98%)	2 (2%)	57 87
17	1V	80/82 (98%)	73 (91%)	7 (9%)	12 33
17	2V	80/82 (98%)	71 (89%)	9 (11%)	7 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	1W	90/92 (98%)	87 (97%)	3 (3%)	43 77
18	2W	90/92 (98%)	83 (92%)	7 (8%)	15 39
19	1X	77/78 (99%)	73 (95%)	4 (5%)	27 60
19	2X	77/78 (99%)	74 (96%)	3 (4%)	37 71
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	23 54
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	17 44
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	11 32
21	2Z	137/179 (76%)	128 (93%)	9 (7%)	19 49
22	10	65/67 (97%)	62 (95%)	3 (5%)	31 65
22	20	65/67 (97%)	63 (97%)	2 (3%)	45 79
23	11	80/83 (96%)	77 (96%)	3 (4%)	38 72
23	21	80/83 (96%)	80 (100%)	0	100 100
24	12	65/67 (97%)	62 (95%)	3 (5%)	31 65
24	22	65/67 (97%)	64 (98%)	1 (2%)	70 92
25	13	51/52 (98%)	50 (98%)	1 (2%)	60 88
25	23	50/52 (96%)	45 (90%)	5 (10%)	9 26
26	14	59/63 (94%)	55 (93%)	4 (7%)	18 47
26	24	53/63 (84%)	49 (92%)	4 (8%)	16 41
27	15	50/52 (96%)	44 (88%)	6 (12%)	6 18
27	25	50/52 (96%)	47 (94%)	3 (6%)	22 54
28	16	51/52 (98%)	47 (92%)	4 (8%)	15 39
28	26	50/52 (96%)	45 (90%)	5 (10%)	9 26
29	17	41/42 (98%)	37 (90%)	4 (10%)	9 27
29	27	41/42 (98%)	39 (95%)	2 (5%)	29 62
30	18	54/55 (98%)	49 (91%)	5 (9%)	10 30
30	28	54/55 (98%)	49 (91%)	5 (9%)	10 30
31	19	34/34 (100%)	34 (100%)	0	100 100
31	29	34/34 (100%)	33 (97%)	1 (3%)	48 81
33	1b	192/220 (87%)	184 (96%)	8 (4%)	34 68
33	2b	187/220 (85%)	174 (93%)	13 (7%)	18 45
34	1c	142/188 (76%)	136 (96%)	6 (4%)	34 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	2c	140/188 (74%)	133 (95%)	7 (5%)	28 62
35	1d	169/181 (93%)	159 (94%)	10 (6%)	23 54
35	2d	173/181 (96%)	162 (94%)	11 (6%)	20 50
36	1e	113/123 (92%)	105 (93%)	8 (7%)	17 44
36	2e	114/123 (93%)	108 (95%)	6 (5%)	26 59
37	1f	84/90 (93%)	81 (96%)	3 (4%)	40 74
37	2f	85/90 (94%)	82 (96%)	3 (4%)	41 75
38	1g	119/127 (94%)	114 (96%)	5 (4%)	34 68
38	2g	120/127 (94%)	111 (92%)	9 (8%)	16 41
39	1h	114/119 (96%)	108 (95%)	6 (5%)	26 59
39	2h	114/119 (96%)	107 (94%)	7 (6%)	22 53
40	1i	90/99 (91%)	86 (96%)	4 (4%)	33 67
40	2i	89/99 (90%)	85 (96%)	4 (4%)	32 66
41	1j	66/92 (72%)	64 (97%)	2 (3%)	46 80
41	2j	69/92 (75%)	64 (93%)	5 (7%)	17 43
42	1k	82/99 (83%)	78 (95%)	4 (5%)	29 62
42	2k	83/99 (84%)	78 (94%)	5 (6%)	22 54
43	1l	96/108 (89%)	86 (90%)	10 (10%)	8 24
43	2l	96/108 (89%)	93 (97%)	3 (3%)	45 79
44	1m	93/101 (92%)	87 (94%)	6 (6%)	20 49
44	2m	92/101 (91%)	90 (98%)	2 (2%)	57 87
45	1n	49/50 (98%)	43 (88%)	6 (12%)	6 17
45	2n	49/50 (98%)	44 (90%)	5 (10%)	8 25
46	1o	78/80 (98%)	76 (97%)	2 (3%)	51 83
46	2o	78/80 (98%)	75 (96%)	3 (4%)	38 72
47	1p	69/74 (93%)	66 (96%)	3 (4%)	33 67
47	2p	68/74 (92%)	65 (96%)	3 (4%)	33 67
48	1q	94/97 (97%)	91 (97%)	3 (3%)	44 78
48	2q	94/97 (97%)	89 (95%)	5 (5%)	26 59
49	1r	59/77 (77%)	55 (93%)	4 (7%)	18 47
49	2r	59/77 (77%)	57 (97%)	2 (3%)	42 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
50	1s	69/80 (86%)	67 (97%)	2 (3%)	48 <span style="background-color: blue;">81</span>
50	2s	67/80 (84%)	64 (96%)	3 (4%)	<span style="background-color: pink;">32</span> 66
51	1t	70/82 (85%)	67 (96%)	3 (4%)	<span style="background-color: pink;">33</span> <span style="background-color: blue;">67</span>
51	2t	70/82 (85%)	65 (93%)	5 (7%)	<span style="background-color: red;">17</span> <span style="background-color: pink;">44</span>
52	1u	18/22 (82%)	18 (100%)	0	<span style="background-color: blue;">100</span> <span style="background-color: blue;">100</span>
52	2u	18/22 (82%)	17 (94%)	1 (6%)	<span style="background-color: red;">25</span> <span style="background-color: blue;">57</span>
All	All	9303/10064 (92%)	8749 (94%)	554 (6%)	<span style="background-color: red;">22</span> <span style="background-color: blue;">54</span>

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

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

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

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

### 5.3.3 RNA (i)

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

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

5 of 1650 RNA backbone outliers are listed below:

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

5 of 52 RNA pucker outliers are listed below:

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	1A	1933	1	16,21,22	1.53	3 (18%)	20,30,33	3.54	6 (30%)
1	5MU	1A	1937	1	14,22,23	0.75	0	16,32,35	2.10	2 (12%)
1	PSU	1A	1939	1	16,21,22	1.43	1 (6%)	20,30,33	3.63	7 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4OC	1A	1942	1	15,22,24	0.83	1 (6%)	19,31,35	0.91	1 (5%)
1	5MU	1A	1961	1,56	14,22,23	0.67	0	16,32,35	2.11	3 (18%)
1	5MC	1A	1964	1	15,22,23	1.40	1 (6%)	17,32,35	1.25	2 (11%)
1	5MC	1A	1984	1,56	15,22,23	1.42	1 (6%)	17,32,35	0.99	2 (11%)
1	OMG	1A	2263	1,55,56	18,26,27	1.14	2 (11%)	22,38,41	1.99	6 (27%)
1	2MA	1A	2515	1,56	18,25,26	1.57	4 (22%)	17,37,40	1.69	2 (11%)
1	2MU	1A	2564	1,56	14,22,24	0.95	1 (7%)	18,31,36	2.12	1 (5%)
1	PSU	1A	2617	1,56	16,21,22	1.62	3 (18%)	20,30,33	3.51	7 (35%)
32	2MG	1a	1207	32	19,26,27	1.33	2 (10%)	20,38,41	2.36	7 (35%)
32	5MC	1a	1400	32	15,22,23	1.35	1 (6%)	17,32,35	1.26	2 (11%)
32	4OC	1a	1402	32	16,23,24	0.74	0	19,32,35	1.06	1 (5%)
32	5MC	1a	1404	32	15,22,23	1.45	2 (13%)	17,32,35	1.01	1 (5%)
32	5MC	1a	1407	32	15,22,23	1.35	1 (6%)	17,32,35	1.12	1 (5%)
32	UR3	1a	1498	32	14,22,23	0.86	1 (7%)	16,32,35	0.60	0
32	MA6	1a	1518	32	16,26,27	0.94	1 (6%)	18,38,41	2.45	6 (33%)
32	MA6	1a	1519	32	16,26,27	1.01	1 (6%)	18,38,41	2.21	5 (27%)
32	PSU	1a	516	32,56	16,21,22	1.34	2 (12%)	20,30,33	3.54	6 (30%)
32	7MG	1a	527	32	20,26,27	1.79	2 (10%)	22,39,42	2.70	5 (22%)
32	M2G	1a	966	32	20,27,28	1.48	3 (15%)	21,40,43	2.42	7 (33%)
32	5MC	1a	967	32	15,22,23	1.33	1 (6%)	17,32,35	1.02	1 (5%)
43	0TD	1l	92	43	5,9,10	3.05	2 (40%)	3,11,13	4.01	2 (66%)
54	PSU	1w	32	54	16,21,22	1.31	1 (6%)	20,30,33	3.54	6 (30%)
54	MIA	1w	37	54	23,31,32	1.72	2 (8%)	25,44,47	1.49	5 (20%)
54	PSU	1w	39	54	16,21,22	1.46	1 (6%)	20,30,33	3.44	6 (30%)
54	7MG	1w	46	54	20,26,27	1.54	2 (10%)	22,39,42	2.94	5 (22%)
54	5MU	1w	54	54	14,22,23	0.75	0	16,32,35	2.18	3 (18%)
54	PSU	1w	55	54	16,21,22	1.22	1 (6%)	20,30,33	3.86	6 (30%)
54	4SU	1w	8	54	14,21,22	1.35	2 (14%)	15,30,33	1.39	2 (13%)
55	5MC	1x	32	55	15,22,23	1.39	1 (6%)	17,32,35	1.27	3 (17%)
55	5MU	1x	54	55,56	14,22,23	0.78	0	16,32,35	2.35	3 (18%)
55	PSU	1x	55	55	16,21,22	1.48	1 (6%)	20,30,33	3.65	6 (30%)
55	4SU	1x	8	55	14,21,22	1.49	2 (14%)	15,30,33	2.53	2 (13%)
54	PSU	1y	32	54	16,21,22	1.29	1 (6%)	20,30,33	3.81	6 (30%)
54	MIA	1y	37	54	18,24,32	1.24	2 (11%)	17,35,47	1.85	2 (11%)
54	PSU	1y	39	54	16,21,22	1.30	1 (6%)	20,30,33	3.66	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	7MG	1y	46	54	20,26,27	1.79	3 (15%)	22,39,42	3.17	7 (31%)
54	5MU	1y	54	54	14,22,23	0.75	1 (7%)	16,32,35	2.33	3 (18%)
54	PSU	1y	55	54	16,21,22	1.47	1 (6%)	20,30,33	3.61	7 (35%)
54	4SU	1y	8	54	14,21,22	1.19	1 (7%)	15,30,33	1.62	2 (13%)
1	PSU	2A	1911	1	16,21,22	1.32	1 (6%)	20,30,33	3.60	7 (35%)
1	5MU	2A	1915	1	14,22,23	0.71	0	16,32,35	2.18	3 (18%)
1	PSU	2A	1917	1	16,21,22	1.44	1 (6%)	20,30,33	3.57	7 (35%)
1	4OC	2A	1920	1	15,22,24	0.75	0	19,31,35	0.94	1 (5%)
1	5MU	2A	1939	1,56	14,22,23	0.73	0	16,32,35	2.17	3 (18%)
1	5MC	2A	1942	1	15,22,23	1.39	1 (6%)	17,32,35	1.05	1 (5%)
1	5MC	2A	1962	1,56	15,22,23	1.37	1 (6%)	17,32,35	1.09	2 (11%)
1	OMG	2A	2251	1,55,56	18,26,27	1.36	2 (11%)	22,38,41	2.02	6 (27%)
1	2MA	2A	2503	1,56	18,25,26	1.50	3 (16%)	17,37,40	1.61	2 (11%)
1	2MU	2A	2552	1,56	14,22,24	1.02	1 (7%)	18,31,36	1.98	1 (5%)
1	PSU	2A	2605	1	16,21,22	1.58	1 (6%)	20,30,33	3.28	6 (30%)
32	2MG	2a	1207	32	19,26,27	1.31	2 (10%)	20,38,41	2.54	9 (45%)
32	5MC	2a	1400	32	15,22,23	1.54	1 (6%)	17,32,35	1.03	1 (5%)
32	4OC	2a	1402	32,56	16,23,24	0.70	0	19,32,35	1.21	1 (5%)
32	5MC	2a	1404	32	15,22,23	1.41	1 (6%)	17,32,35	1.18	2 (11%)
32	5MC	2a	1407	32	15,22,23	1.37	1 (6%)	17,32,35	1.21	1 (5%)
32	UR3	2a	1498	32	14,22,23	0.90	1 (7%)	16,32,35	0.77	1 (6%)
32	MA6	2a	1518	32	16,26,27	1.04	1 (6%)	18,38,41	2.33	4 (22%)
32	MA6	2a	1519	32	16,26,27	1.06	1 (6%)	18,38,41	2.22	5 (27%)
32	PSU	2a	516	32	16,21,22	1.23	1 (6%)	20,30,33	3.49	6 (30%)
32	7MG	2a	527	32,56	20,26,27	1.67	2 (10%)	22,39,42	2.73	6 (27%)
32	M2G	2a	966	32	20,27,28	1.44	3 (15%)	21,40,43	2.26	7 (33%)
32	5MC	2a	967	32	15,22,23	1.49	1 (6%)	17,32,35	0.95	2 (11%)
43	0TD	2l	92	43	5,9,10	3.09	2 (40%)	3,11,13	2.73	2 (66%)
54	PSU	2w	32	54	16,21,22	1.19	1 (6%)	20,30,33	3.59	6 (30%)
54	MIA	2w	37	54	20,27,32	1.78	2 (10%)	21,39,47	1.55	5 (23%)
54	PSU	2w	39	54	16,21,22	1.28	1 (6%)	20,30,33	3.71	7 (35%)
54	7MG	2w	46	54	20,26,27	1.69	2 (10%)	22,39,42	2.66	5 (22%)
54	5MU	2w	54	54	14,22,23	0.76	0	16,32,35	2.39	2 (12%)
54	PSU	2w	55	54	16,21,22	1.25	1 (6%)	20,30,33	3.61	6 (30%)
54	4SU	2w	8	54	14,21,22	1.24	1 (7%)	15,30,33	1.33	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
55	5MC	2x	32	55	15,22,23	1.38	1 (6%)	17,32,35	1.22	2 (11%)
55	5MU	2x	54	55	14,22,23	0.75	0	16,32,35	2.10	3 (18%)
55	PSU	2x	55	55	16,21,22	1.33	1 (6%)	20,30,33	3.57	6 (30%)
55	4SU	2x	8	55,56	14,21,22	1.28	2 (14%)	15,30,33	2.39	2 (13%)
54	PSU	2y	32	54	16,21,22	1.27	1 (6%)	20,30,33	3.58	7 (35%)
54	MIA	2y	37	54	18,24,32	1.19	2 (11%)	17,35,47	1.91	2 (11%)
54	PSU	2y	39	54	16,21,22	1.49	1 (6%)	20,30,33	4.24	7 (35%)
54	7MG	2y	46	54	20,26,27	1.71	2 (10%)	22,39,42	2.98	6 (27%)
54	5MU	2y	54	54	14,22,23	0.69	0	16,32,35	2.16	3 (18%)
54	PSU	2y	55	54	16,21,22	1.19	2 (12%)	20,30,33	3.77	7 (35%)
54	4SU	2y	8	54	14,21,22	1.25	1 (7%)	15,30,33	1.30	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/3/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1	-	0/5/27/30	0/2/2/2
1	5MU	1A	1961	1,56	-	0/3/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/3/25/26	0/2/2/2
1	5MC	1A	1984	1,56	-	0/3/25/26	0/2/2/2
1	OMG	1A	2263	1,55,56	-	0/5/27/28	0/3/3/3
1	2MA	1A	2515	1,56	-	0/3/25/26	0/3/3/3
1	2MU	1A	2564	1,56	-	0/5/27/28	0/2/2/2
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	1a	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/7/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32	-	0/7/37/38	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	967	32	-	0/3/25/26	0/2/2/2
43	0TD	1l	92	43	-	0/2/12/14	0/0/0/0
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	0/11/33/34	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	0/7/37/38	0/3/3/3
54	5MU	1w	54	54	-	0/3/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/3/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/3/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/3/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/3/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	0/7/37/38	0/3/3/3
54	5MU	1y	54	54	-	0/3/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	0/3/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/3/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/5/27/30	0/2/2/2
1	5MU	2A	1939	1,56	-	0/3/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/3/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/3/25/26	0/2/2/2
1	OMG	2A	2251	1,55,56	-	0/5/27/28	0/3/3/3
1	2MA	2A	2503	1,56	-	0/3/25/26	0/3/3/3
1	2MU	2A	2552	1,56	-	0/5/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	2a	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	0/7/29/30	0/2/2/2
32	5MC	2a	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	0/7/37/38	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	967	32	-	0/3/25/26	0/2/2/2
43	0TD	2l	92	43	-	0/2/12/14	0/0/0/0
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/7/29/34	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	0/7/37/38	0/3/3/3
54	5MU	2w	54	54	-	0/3/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/3/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/3/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/3/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	0/3/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/3/25/34	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	0/7/37/38	0/3/3/3
54	5MU	2y	54	54	-	0/3/25/26	0/2/2/2
54	PSU	2y	55	54	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/3/25/26	0/2/2/2

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C2-S10	-6.52	1.70	1.75
54	2w	37	MIA	C2-S10	-6.20	1.70	1.75
43	1l	92	0TD	CB-SB	-5.86	1.69	1.84
43	2l	92	0TD	CB-SB	-5.79	1.69	1.84
1	2A	2605	PSU	C5-C1'	-5.09	1.47	1.52

The worst 5 of 328 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	39	PSU	N1-C2-N3	-10.39	120.93	128.40
54	1y	32	PSU	N1-C2-N3	-10.01	121.20	128.40
54	1y	39	PSU	N1-C2-N3	-9.97	121.22	128.40
54	2y	55	PSU	N1-C2-N3	-9.95	121.24	128.40
32	1a	516	PSU	N1-C2-N3	-9.93	121.26	128.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

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

## 5.5 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [\(i\)](#)

Of 2625 ligands modelled in this entry, 2621 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	EZG	1A	4030	-	21,26,26	2.86	3 (14%)	24,35,35	1.23	3 (12%)
60	SF4	1d	501	35	0,12,12	0.00	-	0,24,24	0.00	-
58	EZG	2A	3746	-	21,26,26	3.59	3 (14%)	24,35,35	1.08	2 (8%)
60	SF4	2d	501	35	0,12,12	0.00	-	0,24,24	0.00	-

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	EZG	1A	4030	-	-	0/24/26/26	0/2/2/2
60	SF4	1d	501	35	-	0/0/48/48	0/6/5/5
58	EZG	2A	3746	-	-	0/24/26/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	501	35	-	0/0/48/48	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4030	EZG	CAT-CAW	-8.56	1.39	1.51
58	2A	3746	EZG	CAT-CAW	-7.82	1.40	1.51
58	1A	4030	EZG	CAU-NAY	-6.12	1.33	1.45
58	2A	3746	EZG	CAU-NAY	-5.88	1.34	1.45
58	1A	4030	EZG	OAC-NAY	7.24	1.35	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	2A	3746	EZG	CAX-NAP-C	-2.98	117.83	123.16
58	1A	4030	EZG	CAI-CAG-CAT	-2.62	118.54	121.20
58	1A	4030	EZG	CAM-CAX-NAP	-2.14	105.64	109.38
58	2A	3746	EZG	CAI-CAU-NAY	2.03	120.95	119.41
58	1A	4030	EZG	CAT-CAW-CAX	2.83	116.89	111.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [\(i\)](#)

### 6.1 Protein, DNA and RNA chains [\(i\)](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	2860/2915 (98%)	0.07	16 (0%)	89   86	13, 30, 88, 101	0
1	2A	2789/2915 (95%)	0.07	13 (0%)	90   88	25, 51, 87, 100	0
2	1B	120/121 (99%)	-0.15	0   100	100	23, 43, 57, 85	0
2	2B	120/121 (99%)	-0.14	0   100	100	53, 71, 80, 89	0
3	1D	275/276 (99%)	0.11	2 (0%)	87   83	16, 31, 46, 75	0
3	2D	275/276 (99%)	0.15	0   100	100	23, 43, 56, 66	0
4	1E	204/206 (99%)	0.02	0   100	100	13, 33, 54, 71	0
4	2E	204/206 (99%)	0.24	2 (0%)	82   77	28, 54, 67, 74	0
5	1F	203/210 (96%)	0.00	1 (0%)	90   88	15, 35, 62, 82	0
5	2F	203/210 (96%)	0.17	3 (1%)	74   67	30, 62, 74, 82	0
6	1G	181/182 (99%)	-0.16	0   100	100	35, 51, 69, 78	0
6	2G	181/182 (99%)	0.38	8 (4%)	35   25	56, 72, 78, 83	0
7	1H	174/180 (96%)	-0.13	0   100	100	34, 46, 59, 66	0
7	2H	174/180 (96%)	1.61	67 (38%)	0   0	61, 75, 81, 86	0
8	1I	146/148 (98%)	-0.06	0   100	100	39, 67, 75, 81	0
8	2I	146/148 (98%)	0.13	2 (1%)	75   69	50, 66, 77, 81	0
9	1N	140/140 (100%)	-0.09	0   100	100	21, 35, 55, 68	0
9	2N	140/140 (100%)	0.55	4 (2%)	52   41	43, 58, 72, 75	0
10	1O	122/122 (100%)	-0.03	0   100	100	22, 35, 50, 56	0
10	2O	122/122 (100%)	0.32	0   100	100	43, 54, 67, 70	0
11	1P	149/150 (99%)	0.02	0   100	100	14, 40, 62, 66	0
11	2P	149/150 (99%)	1.23	37 (24%)	1   0	30, 61, 75, 83	0
12	1Q	141/141 (100%)	0.17	0   100	100	22, 36, 49, 72	0
12	2Q	141/141 (100%)	1.00	20 (14%)	3   2	41, 60, 70, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	0.19	0	100	100		18, 29, 44, 54
13	2R	118/118 (100%)	0.29	1 (0%)	86	81		33, 46, 55, 66
14	1S	110/112 (98%)	-0.13	1 (0%)	84	79		32, 44, 55, 60
14	2S	110/112 (98%)	1.33	23 (20%)	1	1		58, 67, 76, 79
15	1T	131/146 (89%)	-0.04	0	100	100		25, 39, 61, 71
15	2T	131/146 (89%)	0.42	5 (3%)	41	30		46, 58, 69, 75
16	1U	116/118 (98%)	0.03	0	100	100		14, 25, 42, 56
16	2U	116/118 (98%)	0.31	1 (0%)	84	79		35, 55, 67, 73
17	1V	101/101 (100%)	-0.17	0	100	100		19, 34, 53, 69
17	2V	101/101 (100%)	0.06	0	100	100		36, 63, 74, 78
18	1W	112/113 (99%)	-0.01	0	100	100		21, 26, 48, 71
18	2W	112/113 (99%)	0.23	1 (0%)	84	79		33, 44, 59, 85
19	1X	95/96 (98%)	-0.09	0	100	100		19, 31, 53, 75
19	2X	95/96 (98%)	0.00	0	100	100		40, 53, 64, 72
20	1Y	107/110 (97%)	-0.18	0	100	100		29, 43, 61, 72
20	2Y	107/110 (97%)	0.33	2 (1%)	67	58		54, 65, 74, 78
21	1Z	154/206 (74%)	0.06	3 (1%)	67	58		35, 57, 79, 85
21	2Z	160/206 (77%)	1.31	39 (24%)	1	1		61, 75, 84, 91
22	10	83/85 (97%)	0.26	5 (6%)	23	14		18, 31, 51, 56
22	20	83/85 (97%)	0.72	9 (10%)	6	3		36, 58, 69, 74
23	11	97/98 (98%)	0.21	1 (1%)	82	77		20, 38, 62, 70
23	21	97/98 (98%)	0.42	5 (5%)	28	19		35, 50, 68, 73
24	12	70/72 (97%)	-0.08	0	100	100		29, 41, 53, 64
24	22	70/72 (97%)	-0.09	0	100	100		47, 62, 70, 73
25	13	59/60 (98%)	-0.11	0	100	100		19, 31, 54, 72
25	23	59/60 (98%)	1.11	10 (16%)	2	1		48, 58, 70, 76
26	14	69/71 (97%)	-0.00	2 (2%)	52	41		43, 65, 83, 84
26	24	69/71 (97%)	-0.03	3 (4%)	36	26		67, 77, 86, 87
27	15	59/60 (98%)	-0.02	1 (1%)	70	63		14, 28, 41, 50
27	25	59/60 (98%)	0.09	1 (1%)	70	63		32, 46, 56, 64
28	16	53/54 (98%)	0.16	1 (1%)	67	58		27, 36, 50, 55

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.90	6 (11%) 6 3	42, 54, 67, 68	0
29	17	48/49 (97%)	0.13	1 (2%) 64 54	16, 21, 50, 60	0
29	27	48/49 (97%)	0.16	0 100 100	24, 35, 51, 60	0
30	18	64/65 (98%)	0.21	1 (1%) 72 65	21, 27, 37, 55	0
30	28	64/65 (98%)	1.63	18 (28%) 1 0	40, 49, 58, 68	0
31	19	37/37 (100%)	0.55	0 100 100	22, 33, 50, 55	0
31	29	37/37 (100%)	1.50	11 (29%) 1 0	53, 62, 71, 75	0
32	1a	1488/1521 (97%)	0.03	9 (0%) 89 86	32, 59, 86, 102	0
32	2a	1491/1521 (98%)	0.13	29 (1%) 67 58	43, 69, 89, 101	0
33	1b	231/256 (90%)	0.58	15 (6%) 20 12	59, 73, 82, 85	0
33	2b	231/256 (90%)	1.29	57 (24%) 1 0	64, 79, 85, 90	0
34	1c	206/239 (86%)	0.62	21 (10%) 7 4	51, 66, 74, 80	0
34	2c	206/239 (86%)	1.44	63 (30%) 0 0	66, 78, 82, 85	0
35	1d	208/209 (99%)	0.48	11 (5%) 27 18	50, 64, 76, 83	0
35	2d	208/209 (99%)	0.58	12 (5%) 24 15	53, 62, 72, 81	0
36	1e	148/162 (91%)	0.39	5 (3%) 46 34	48, 60, 70, 78	0
36	2e	148/162 (91%)	0.96	24 (16%) 2 1	58, 71, 79, 86	0
37	1f	100/101 (99%)	0.09	0 100 100	48, 60, 69, 70	0
37	2f	100/101 (99%)	0.07	1 (1%) 82 77	51, 63, 70, 76	0
38	1g	155/156 (99%)	0.43	16 (10%) 7 4	51, 62, 74, 88	0
38	2g	155/156 (99%)	0.79	19 (12%) 5 2	62, 71, 78, 84	0
39	1h	137/138 (99%)	0.30	4 (2%) 52 41	48, 61, 67, 72	0
39	2h	137/138 (99%)	0.67	14 (10%) 7 4	64, 71, 77, 85	0
40	1i	127/128 (99%)	1.24	29 (22%) 1 1	46, 69, 77, 83	0
40	2i	127/128 (99%)	2.35	69 (54%) 0 0	68, 77, 82, 88	0
41	1j	97/105 (92%)	1.18	26 (26%) 1 0	52, 71, 78, 83	0
41	2j	96/105 (91%)	1.81	37 (38%) 0 0	70, 78, 85, 87	0
42	1k	114/129 (88%)	0.26	1 (0%) 84 79	40, 58, 72, 79	0
42	2k	114/129 (88%)	0.43	7 (6%) 22 14	49, 66, 74, 78	0
43	1l	121/132 (91%)	0.01	0 100 100	33, 47, 59, 66	0
43	2l	121/132 (91%)	0.53	8 (6%) 19 11	53, 61, 71, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	123/126 (97%)	0.36	10 (8%)	13 7	47, 59, 70, 74	0
44	2m	122/126 (96%)	0.60	17 (13%)	3 2	62, 75, 81, 85	0
45	1n	60/61 (98%)	1.05	10 (16%)	2 1	50, 59, 67, 71	0
45	2n	60/61 (98%)	2.94	41 (68%)	0 0	68, 77, 81, 87	0
46	1o	88/89 (98%)	0.12	2 (2%)	61 51	44, 59, 70, 75	0
46	2o	88/89 (98%)	-0.09	1 (1%)	80 74	53, 65, 74, 75	0
47	1p	82/88 (93%)	0.51	5 (6%)	22 14	51, 61, 70, 75	0
47	2p	82/88 (93%)	0.29	1 (1%)	79 72	55, 62, 71, 75	0
48	1q	99/105 (94%)	0.34	3 (3%)	51 39	47, 59, 72, 75	0
48	2q	99/105 (94%)	0.98	20 (20%)	1 1	55, 65, 73, 75	0
49	1r	68/88 (77%)	0.32	4 (5%)	23 15	48, 61, 71, 73	0
49	2r	68/88 (77%)	-0.01	2 (2%)	52 41	57, 63, 73, 77	0
50	1s	83/93 (89%)	0.26	1 (1%)	79 72	49, 64, 73, 77	0
50	2s	83/93 (89%)	0.79	16 (19%)	1 1	71, 78, 84, 87	0
51	1t	96/106 (90%)	0.70	14 (14%)	3 1	50, 64, 73, 78	0
51	2t	96/106 (90%)	1.19	18 (18%)	1 1	52, 63, 76, 79	0
52	1u	23/27 (85%)	1.37	4 (17%)	2 1	52, 59, 63, 70	0
52	2u	23/27 (85%)	2.22	12 (52%)	0 0	67, 73, 80, 80	0
53	1v	13/24 (54%)	1.12	3 (23%)	1 1	42, 56, 81, 90	0
53	2v	13/24 (54%)	1.10	2 (15%)	2 1	59, 74, 91, 97	0
54	1w	67/76 (88%)	0.14	5 (7%)	15 8	32, 82, 93, 96	0
54	1y	67/76 (88%)	0.35	5 (7%)	15 8	28, 88, 96, 100	0
54	2w	65/76 (85%)	0.25	3 (4%)	33 23	54, 87, 95, 99	0
54	2y	66/76 (86%)	0.56	6 (9%)	10 5	49, 90, 94, 97	0
55	1x	72/77 (93%)	-0.07	0	100 100	32, 58, 76, 85	0
55	2x	72/77 (93%)	-0.14	0	100 100	45, 71, 81, 83	0
All	All	20875/21748 (95%)	0.29	1008 (4%)	31 21	13, 57, 83, 102	0

The worst 5 of 1008 RSRZ outliers are listed below:

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

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

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
55	5MU	2x	54	21/22	0.92	0.16	-	77,81,86,94	0
1	2MU	2A	2552	21/23	0.97	0.18	-	31,41,45,52	0
55	5MC	2x	32	21/22	0.94	0.18	-	65,68,73,74	0
1	2MA	1A	2515	23/24	0.98	0.20	-	11,16,19,22	0
1	5MU	2A	1915	21/22	0.93	0.16	-	59,64,71,73	0
32	5MC	1a	1407	21/22	0.97	0.20	-	28,34,39,40	0
43	0TD	2l	92	10/11	0.91	0.30	-	58,64,65,80	0
32	MA6	1a	1518	24/25	0.98	0.20	-	31,38,40,40	0
55	PSU	2x	55	20/21	0.91	0.13	-	67,78,81,81	0
32	M2G	2a	966	25/26	0.94	0.27	-	60,65,72,79	0
54	5MU	2y	54	21/22	0.82	0.33	-	84,91,97,115	0
54	4SU	2y	8	20/21	0.85	0.14	-	83,95,104,112	0
1	PSU	1A	1933	20/21	0.97	0.19	-	30,37,44,45	0
1	5MC	2A	1942	21/22	0.96	0.17	-	49,56,62,66	0
1	PSU	2A	2605	20/21	0.98	0.17	-	27,31,37,38	0
1	5MU	1A	1937	21/22	0.95	0.17	-	43,49,54,56	0
1	4OC	2A	1920	21/23	0.95	0.18	-	53,58,64,66	0
32	5MC	2a	1400	21/22	0.94	0.23	-	60,67,71,73	0
1	PSU	2A	1917	20/21	0.95	0.14	-	55,60,65,69	0
1	PSU	1A	1939	20/21	0.96	0.16	-	38,46,53,54	0
32	MA6	2a	1519	24/25	0.96	0.21	-	47,56,64,66	0
54	PSU	2y	39	20/21	0.88	0.24	-	77,84,98,102	0
54	5MU	1y	54	21/22	0.78	0.32	-	79,87,99,114	0
55	PSU	1x	55	20/21	0.95	0.13	-	53,58,67,72	0
1	PSU	1A	2617	20/21	0.98	0.18	-	16,20,25,28	0
1	2MA	2A	2503	23/24	0.98	0.21	-	24,33,37,46	0
54	PSU	1w	39	20/21	0.97	0.17	-	44,60,69,70	0
54	7MG	1w	46	24/25	0.82	0.15	-	76,87,106,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
1	5MC	1A	1984	21/22	0.98	0.17	-	24,31,36,41	0
55	5MC	1x	32	21/22	0.98	0.20	-	44,50,57,66	0
54	7MG	2w	46	24/25	0.83	0.14	-	78,92,98,107	0
55	5MU	1x	54	21/22	0.96	0.14	-	55,62,70,76	0
54	7MG	2y	46	24/25	0.83	0.23	-	83,92,97,112	0
32	PSU	2a	516	20/21	0.93	0.14	-	50,70,74,75	0
54	PSU	2w	39	20/21	0.93	0.19	-	60,73,79,81	0
32	UR3	1a	1498	21/22	0.99	0.20	-	27,39,42,46	0
1	OMG	2A	2251	24/25	0.98	0.20	-	32,37,42,45	0
54	PSU	2w	55	20/21	0.92	0.12	-	75,81,89,94	0
32	5MC	1a	1404	21/22	0.97	0.19	-	31,38,42,44	0
54	4SU	1y	8	20/21	0.80	0.20	-	91,96,103,105	0
32	7MG	1a	527	24/25	0.95	0.18	-	34,42,51,55	0
32	4OC	2a	1402	22/23	0.96	0.16	-	52,58,64,67	0
32	5MC	1a	967	21/22	0.98	0.20	-	45,50,58,64	0
54	MIA	2w	37	25/30	0.95	0.17	-	60,68,74,78	0
32	5MC	2a	1404	21/22	0.95	0.17	-	47,51,56,61	0
32	UR3	2a	1498	21/22	0.97	0.18	-	44,50,54,63	0
32	4OC	1a	1402	22/23	0.98	0.18	-	38,42,47,53	0
54	MIA	1y	37	22/30	0.90	0.17	-	70,78,88,93	0
1	5MC	1A	1964	21/22	0.98	0.18	-	30,39,46,50	0
54	PSU	1w	55	20/21	0.92	0.14	-	61,70,79,80	0
32	5MC	2a	967	21/22	0.93	0.30	-	62,67,71,73	0
32	5MC	1a	1400	21/22	0.97	0.21	-	37,47,50,55	0
1	5MU	1A	1961	21/22	0.98	0.18	-	19,23,26,32	0
32	MA6	1a	1519	24/25	0.97	0.20	-	33,39,43,44	0
32	MA6	2a	1518	24/25	0.96	0.19	-	47,59,63,66	0
54	MIA	2y	37	22/30	0.86	0.21	-	69,81,100,111	0
32	7MG	2a	527	24/25	0.94	0.17	-	46,56,67,71	0
54	PSU	1y	32	20/21	0.88	0.19	-	71,81,88,90	0
54	4SU	2w	8	20/21	0.85	0.15	-	85,89,104,109	0
32	5MC	2a	1407	21/22	0.96	0.19	-	44,48,55,60	0
55	4SU	2x	8	20/21	0.93	0.13	-	69,73,78,81	0
54	5MU	2w	54	21/22	0.92	0.12	-	68,75,81,83	0
1	2MU	1A	2564	21/23	0.98	0.19	-	18,23,28,31	0
54	PSU	2y	32	20/21	0.88	0.17	-	69,84,92,94	0
54	PSU	2w	32	20/21	0.93	0.27	-	67,78,88,89	0
54	PSU	1y	55	20/21	0.76	0.28	-	85,93,105,123	0
32	PSU	1a	516	20/21	0.96	0.15	-	32,49,53,54	0
1	5MU	2A	1939	21/22	0.97	0.17	-	34,38,43,44	0
54	PSU	2y	55	20/21	0.80	0.27	-	85,92,104,109	0
1	5MC	2A	1962	21/22	0.97	0.17	-	32,45,48,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
54	4SU	1w	8	20/21	0.91	0.12	-	74,81,92,95	0
54	PSU	1y	39	20/21	0.92	0.17	-	70,77,87,90	0
32	2MG	1a	1207	24/25	0.96	0.17	-	57,62,67,68	0
1	4OC	1A	1942	21/23	0.98	0.17	-	32,39,45,47	0
1	PSU	2A	1911	20/21	0.95	0.15	-	50,60,65,67	0
55	4SU	1x	8	20/21	0.96	0.15	-	50,57,65,67	0
32	2MG	2a	1207	24/25	0.95	0.15	-	74,77,86,91	0
1	OMG	1A	2263	24/25	0.99	0.17	-	14,18,24,25	0
54	PSU	1w	32	20/21	0.95	0.19	-	57,62,68,69	0
54	5MU	1w	54	21/22	0.97	0.16	-	44,60,67,72	0
32	M2G	1a	966	25/26	0.97	0.23	-	41,48,56,63	0
54	MIA	1w	37	29/30	0.95	0.24	-	41,51,60,64	0
43	0TD	1l	92	10/11	0.94	0.21	-	43,48,51,69	0
54	7MG	1y	46	24/25	0.84	0.22	-	86,94,99,108	0

### 6.3 Carbohydrates [\(i\)](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3054	1/1	0.94	0.41	60.37	53,53,53,53	0
56	MG	1A	3739	1/1	0.92	0.34	47.17	29,29,29,29	0
56	MG	1A	3337	1/1	0.97	0.60	42.71	27,27,27,27	0
56	MG	1F	301	1/1	0.98	0.58	37.73	23,23,23,23	0
56	MG	1A	3140	1/1	0.96	0.54	37.39	23,23,23,23	0
56	MG	1A	4032	1/1	0.96	0.49	32.31	30,30,30,30	0
56	MG	1A	3160	1/1	0.95	0.60	28.94	29,29,29,29	0
56	MG	1A	3095	1/1	0.96	0.43	26.12	28,28,28,28	0
56	MG	1A	3199	1/1	0.93	0.52	25.82	32,32,32,32	0
56	MG	1A	3179	1/1	0.92	0.37	25.77	23,23,23,23	0
56	MG	2F	303	1/1	0.90	0.88	24.26	55,55,55,55	0
56	MG	2A	3755	1/1	0.94	0.81	21.97	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	1A	3427	1/1	0.89	0.67	21.76	29,29,29,29	0
56	MG	1A	4034	1/1	0.97	0.58	21.64	28,28,28,28	0
56	MG	1A	3174	1/1	0.94	0.39	20.80	32,32,32,32	0
56	MG	1A	4049	1/1	0.94	0.78	20.22	30,30,30,30	0
56	MG	1A	4041	1/1	0.83	0.54	19.48	35,35,35,35	0
56	MG	1A	4036	1/1	0.92	0.56	17.74	29,29,29,29	0
56	MG	1A	3480	1/1	0.86	0.64	16.52	35,35,35,35	0
56	MG	1A	3377	1/1	0.90	0.45	16.24	40,40,40,40	0
56	MG	1A	3302	1/1	0.92	0.77	15.97	32,32,32,32	0
56	MG	1A	4008	1/1	0.95	0.36	15.52	24,24,24,24	0
56	MG	1A	3422	1/1	0.95	0.49	15.45	43,43,43,43	0
56	MG	1A	3154	1/1	0.98	0.44	15.42	31,31,31,31	0
56	MG	2A	3299	1/1	0.92	0.33	15.25	43,43,43,43	0
56	MG	1N	201	1/1	0.93	0.54	14.17	45,45,45,45	0
56	MG	1A	3704	1/1	0.94	0.25	14.02	28,28,28,28	0
56	MG	1A	3253	1/1	0.96	0.71	13.74	24,24,24,24	0
56	MG	2D	306	1/1	0.92	0.67	13.39	43,43,43,43	0
56	MG	2A	3732	1/1	0.99	0.31	12.99	24,24,24,24	0
56	MG	1a	3015	1/1	0.95	0.31	12.96	48,48,48,48	0
56	MG	1A	4055	1/1	0.95	0.66	12.96	31,31,31,31	0
56	MG	25	502	1/1	0.94	0.59	12.95	47,47,47,47	0
56	MG	2A	3343	1/1	0.98	0.28	12.90	36,36,36,36	0
56	MG	1A	4045	1/1	0.91	0.61	12.89	39,39,39,39	0
56	MG	1A	3037	1/1	0.96	0.26	12.71	22,22,22,22	0
56	MG	1A	4024	1/1	0.98	0.35	12.46	43,43,43,43	0
56	MG	1A	3412	1/1	0.95	0.37	12.04	37,37,37,37	0
56	MG	1P	201	1/1	0.96	0.46	11.87	16,16,16,16	0
56	MG	1A	3252	1/1	0.93	0.29	11.78	32,32,32,32	0
56	MG	1A	3454	1/1	0.97	0.37	11.75	30,30,30,30	0
56	MG	2U	202	1/1	0.90	0.81	11.31	55,55,55,55	0
56	MG	1D	304	1/1	0.97	0.68	11.26	43,43,43,43	0
56	MG	1A	3753	1/1	0.96	0.31	11.21	27,27,27,27	0
56	MG	1A	4023	1/1	0.96	0.56	11.11	21,21,21,21	0
56	MG	1A	4060	1/1	0.90	0.62	10.74	19,19,19,19	0
56	MG	2a	1822	1/1	0.85	0.22	10.31	52,52,52,52	0
56	MG	2A	3495	1/1	0.94	0.28	10.29	60,60,60,60	0
56	MG	13	101	1/1	0.94	0.53	10.21	39,39,39,39	0
56	MG	2A	3125	1/1	0.92	0.33	10.18	32,32,32,32	0
56	MG	1A	3030	1/1	0.92	0.59	10.07	20,20,20,20	0
56	MG	1A	3375	1/1	0.98	0.37	10.05	34,34,34,34	0
56	MG	1A	3783	1/1	0.91	0.27	9.95	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3214	1/1	0.99	0.31	9.82	32,32,32,32	0
56	MG	1R	203	1/1	0.97	0.49	9.75	34,34,34,34	0
56	MG	1A	3680	1/1	0.85	0.30	9.59	36,36,36,36	0
56	MG	1A	3696	1/1	0.99	0.22	9.56	46,46,46,46	0
56	MG	2U	204	1/1	0.93	0.83	9.56	60,60,60,60	0
56	MG	1A	3068	1/1	0.97	0.35	9.49	41,41,41,41	0
56	MG	1B	207	1/1	0.93	0.43	9.34	40,40,40,40	0
56	MG	2A	3072	1/1	0.97	0.30	9.12	32,32,32,32	0
56	MG	1A	3148	1/1	0.90	0.27	9.09	26,26,26,26	0
56	MG	1A	3455	1/1	0.86	0.51	9.06	28,28,28,28	0
56	MG	1a	3014	1/1	0.85	0.39	9.04	55,55,55,55	0
56	MG	1A	3887	1/1	0.91	0.23	8.98	16,16,16,16	0
56	MG	1N	204	1/1	0.84	0.60	8.83	46,46,46,46	0
56	MG	2A	3583	1/1	0.94	0.45	8.78	40,40,40,40	0
56	MG	1F	304	1/1	0.96	0.35	8.78	20,20,20,20	0
56	MG	2A	3382	1/1	0.92	0.24	8.73	46,46,46,46	0
56	MG	2A	3478	1/1	0.92	0.60	8.72	38,38,38,38	0
56	MG	1N	205	1/1	0.97	0.48	8.70	48,48,48,48	0
56	MG	1A	3111	1/1	0.95	0.28	8.69	30,30,30,30	0
56	MG	1A	3689	1/1	0.96	0.39	8.52	20,20,20,20	0
56	MG	1E	302	1/1	0.97	0.37	8.31	16,16,16,16	0
56	MG	1A	3034	1/1	0.97	0.22	8.28	12,12,12,12	0
56	MG	2A	3662	1/1	0.98	0.26	8.25	28,28,28,28	0
56	MG	1A	3560	1/1	0.93	0.23	8.24	26,26,26,26	0
56	MG	1A	3304	1/1	0.92	0.43	8.21	41,41,41,41	0
56	MG	2A	3697	1/1	0.92	0.28	8.20	50,50,50,50	0
56	MG	1A	3175	1/1	0.91	0.44	7.95	21,21,21,21	0
56	MG	1A	3173	1/1	0.97	0.29	7.93	34,34,34,34	0
56	MG	1A	3483	1/1	0.98	0.39	7.85	32,32,32,32	0
56	MG	1F	305	1/1	0.96	0.39	7.58	28,28,28,28	0
56	MG	1A	4040	1/1	0.95	0.47	7.46	34,34,34,34	0
56	MG	2A	3323	1/1	0.97	0.43	7.27	31,31,31,31	0
56	MG	17	103	1/1	0.98	0.47	7.23	33,33,33,33	0
56	MG	2A	3091	1/1	0.97	0.29	7.03	38,38,38,38	0
56	MG	1A	4031	1/1	0.96	0.42	6.98	35,35,35,35	0
56	MG	1A	4039	1/1	0.95	0.45	6.85	33,33,33,33	0
56	MG	1x	102	1/1	0.93	0.26	6.83	49,49,49,49	0
56	MG	2B	3008	1/1	0.85	0.30	6.82	59,59,59,59	0
56	MG	1A	3178	1/1	0.99	0.29	6.82	21,21,21,21	0
56	MG	1A	4063	1/1	0.98	0.39	6.79	31,31,31,31	0
56	MG	1A	4020	1/1	0.97	0.30	6.77	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	4061	1/1	0.95	0.31	6.49	38,38,38,38	0
56	MG	1A	3430	1/1	0.89	0.66	6.43	40,40,40,40	0
56	MG	1A	4014	1/1	0.93	0.34	6.39	33,33,33,33	0
56	MG	1A	4047	1/1	0.89	0.39	6.20	29,29,29,29	0
56	MG	15	101	1/1	0.94	0.38	6.18	27,27,27,27	0
56	MG	1A	3113	1/1	0.96	0.47	6.09	27,27,27,27	0
56	MG	1A	3994	1/1	0.98	0.27	6.07	21,21,21,21	0
56	MG	2A	3271	1/1	0.95	0.25	6.02	45,45,45,45	0
56	MG	1A	3756	1/1	0.94	0.65	5.98	27,27,27,27	0
56	MG	2A	3654	1/1	0.94	0.26	5.93	33,33,33,33	0
56	MG	1A	3751	1/1	0.94	0.32	5.77	23,23,23,23	0
56	MG	1E	311	1/1	0.96	0.46	5.68	36,36,36,36	0
56	MG	1A	3526	1/1	0.94	0.22	5.67	42,42,42,42	0
56	MG	1A	3736	1/1	0.96	0.24	5.58	16,16,16,16	0
56	MG	1A	3102	1/1	0.95	0.27	5.53	31,31,31,31	0
56	MG	2A	3066	1/1	0.96	0.58	5.52	40,40,40,40	0
56	MG	1A	4038	1/1	0.98	0.49	5.50	31,31,31,31	0
56	MG	2A	3127	1/1	0.93	0.22	5.50	56,56,56,56	0
56	MG	1A	3960	1/1	0.85	0.23	5.49	51,51,51,51	0
56	MG	1A	3328	1/1	0.98	0.41	5.36	25,25,25,25	0
56	MG	1A	3625	1/1	0.96	0.26	5.23	10,10,10,10	0
56	MG	2A	3749	1/1	0.96	0.36	5.20	34,34,34,34	0
56	MG	1A	3171	1/1	0.90	0.24	5.14	29,29,29,29	0
56	MG	2A	3464	1/1	0.96	0.25	5.02	29,29,29,29	0
56	MG	2A	3398	1/1	0.96	0.23	4.93	26,26,26,26	0
56	MG	2a	1714	1/1	0.79	0.28	4.91	68,68,68,68	0
56	MG	1A	4026	1/1	0.98	0.52	4.88	35,35,35,35	0
56	MG	2A	3661	1/1	0.98	0.26	4.85	36,36,36,36	0
56	MG	1a	3038	1/1	0.87	0.20	4.84	55,55,55,55	0
56	MG	1A	3031	1/1	0.98	0.31	4.79	34,34,34,34	0
56	MG	1D	314	1/1	0.95	0.30	4.74	29,29,29,29	0
56	MG	2A	3472	1/1	0.85	0.23	4.72	42,42,42,42	0
56	MG	1A	3456	1/1	0.89	0.41	4.72	33,33,33,33	0
56	MG	1e	201	1/1	0.80	0.37	4.68	59,59,59,59	0
56	MG	2a	1655	1/1	0.95	0.17	4.65	67,67,67,67	0
56	MG	1A	3222	1/1	0.91	0.23	4.62	51,51,51,51	0
56	MG	2a	1627	1/1	0.96	0.22	4.61	53,53,53,53	0
56	MG	1A	4046	1/1	0.95	0.44	4.58	20,20,20,20	0
56	MG	2A	3325	1/1	0.98	0.51	4.56	63,63,63,63	0
56	MG	1A	3393	1/1	0.99	0.23	4.52	24,24,24,24	0
56	MG	2A	3624	1/1	0.94	0.22	4.51	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	2A	3180	1/1	0.95	0.24	4.43	33,33,33,33	0
56	MG	1A	3217	1/1	0.92	0.29	4.24	19,19,19,19	0
56	MG	1A	3749	1/1	0.92	0.23	4.17	31,31,31,31	0
56	MG	1R	204	1/1	0.92	0.32	4.15	33,33,33,33	0
56	MG	2A	3395	1/1	0.99	0.21	4.13	33,33,33,33	0
56	MG	1F	309	1/1	0.97	0.33	4.10	50,50,50,50	0
56	MG	2A	3109	1/1	0.97	0.24	4.09	39,39,39,39	0
56	MG	1Y	503	1/1	0.97	0.40	4.04	42,42,42,42	0
56	MG	1A	3087	1/1	0.92	0.18	4.03	47,47,47,47	0
56	MG	1A	3492	1/1	0.95	0.25	4.00	35,35,35,35	0
56	MG	2A	3329	1/1	0.84	0.22	3.98	46,46,46,46	0
56	MG	2A	3138	1/1	0.98	0.23	3.98	34,34,34,34	0
56	MG	16	103	1/1	0.82	0.53	3.92	56,56,56,56	0
56	MG	2D	307	1/1	0.88	0.27	3.88	35,35,35,35	0
56	MG	1A	3799	1/1	0.94	0.23	3.87	29,29,29,29	0
56	MG	1A	3362	1/1	0.96	0.25	3.81	33,33,33,33	0
56	MG	1A	3451	1/1	0.96	0.28	3.65	24,24,24,24	0
56	MG	2a	1694	1/1	0.83	0.28	3.61	66,66,66,66	0
56	MG	1A	3505	1/1	0.92	0.22	3.59	31,31,31,31	0
56	MG	1A	3757	1/1	0.97	0.24	3.28	22,22,22,22	0
56	MG	2a	1693	1/1	0.91	0.31	3.26	75,75,75,75	0
56	MG	18	101	1/1	0.96	0.34	3.26	37,37,37,37	0
56	MG	1A	3772	1/1	0.93	0.20	3.26	22,22,22,22	0
56	MG	1A	3141	1/1	0.91	0.21	3.26	38,38,38,38	0
56	MG	2A	3247	1/1	0.73	0.13	3.24	63,63,63,63	0
56	MG	1A	3550	1/1	0.96	0.19	3.22	26,26,26,26	0
58	EZG	2A	3746	25/25	0.91	0.32	3.21	35,43,49,51	0
56	MG	2a	1761	1/1	0.92	0.22	3.21	34,34,34,34	0
56	MG	1a	3214	1/1	0.93	0.40	3.13	58,58,58,58	0
56	MG	2A	3447	1/1	0.82	0.22	3.11	27,27,27,27	0
56	MG	1A	3685	1/1	0.98	0.21	3.09	21,21,21,21	0
56	MG	2U	203	1/1	0.85	0.41	3.09	55,55,55,55	0
56	MG	2A	3458	1/1	0.91	0.22	3.08	40,40,40,40	0
56	MG	2D	303	1/1	0.96	0.34	3.06	41,41,41,41	0
56	MG	1A	3269	1/1	0.94	0.21	3.06	35,35,35,35	0
56	MG	1Q	201	1/1	0.96	0.36	3.03	33,33,33,33	0
56	MG	1F	302	1/1	0.97	0.32	2.94	30,30,30,30	0
56	MG	1D	312	1/1	0.98	0.25	2.87	27,27,27,27	0
56	MG	2A	3317	1/1	0.96	0.25	2.80	36,36,36,36	0
56	MG	2A	3552	1/1	0.91	0.20	2.80	35,35,35,35	0
56	MG	2A	3742	1/1	0.91	0.33	2.78	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	1A	3221	1/1	0.98	0.28	2.73	21,21,21,21	0
56	MG	1A	3932	1/1	0.98	0.23	2.68	13,13,13,13	0
56	MG	1a	3042	1/1	0.95	0.18	2.54	44,44,44,44	0
56	MG	2a	1676	1/1	0.97	0.19	2.50	48,48,48,48	0
56	MG	2A	3267	1/1	0.85	0.20	2.50	52,52,52,52	0
58	EZG	1A	4030	25/25	0.94	0.27	2.48	19,29,40,41	0
56	MG	1A	3186	1/1	0.97	0.20	2.40	27,27,27,27	0
56	MG	2A	3570	1/1	0.73	0.20	2.29	56,56,56,56	0
56	MG	1A	3567	1/1	0.98	0.21	2.24	13,13,13,13	0
56	MG	1A	3042	1/1	0.99	0.21	2.18	19,19,19,19	0
56	MG	1A	4050	1/1	0.98	0.29	2.14	26,26,26,26	0
56	MG	2A	3024	1/1	0.89	0.20	2.14	50,50,50,50	0
56	MG	1A	3096	1/1	0.95	0.25	2.11	26,26,26,26	0
56	MG	1A	3485	1/1	0.98	0.21	2.09	21,21,21,21	0
56	MG	1a	3108	1/1	0.95	0.21	2.08	40,40,40,40	0
56	MG	1D	308	1/1	0.99	0.32	2.03	26,26,26,26	0
56	MG	1A	3224	1/1	0.91	0.16	2.01	42,42,42,42	0
56	MG	1A	3866	1/1	0.96	0.23	1.99	20,20,20,20	0
56	MG	2A	3752	1/1	0.90	0.29	1.94	61,61,61,61	0
56	MG	1A	3515	1/1	0.98	0.21	1.93	11,11,11,11	0
56	MG	1A	4052	1/1	0.94	0.40	1.93	31,31,31,31	0
56	MG	2V	3001	1/1	0.94	0.39	1.90	46,46,46,46	0
56	MG	1T	202	1/1	0.92	0.21	1.89	47,47,47,47	0
56	MG	2A	3014	1/1	0.94	0.21	1.86	54,54,54,54	0
56	MG	2A	3452	1/1	0.97	0.22	1.82	32,32,32,32	0
56	MG	1A	3465	1/1	0.86	0.20	1.81	55,55,55,55	0
56	MG	1a	3053	1/1	0.91	0.17	1.81	56,56,56,56	0
56	MG	1B	217	1/1	0.97	0.17	1.78	44,44,44,44	0
56	MG	2A	3578	1/1	0.94	0.20	1.76	27,27,27,27	0
56	MG	1a	3206	1/1	0.85	0.18	1.73	51,51,51,51	0
56	MG	1A	3484	1/1	0.96	0.24	1.68	22,22,22,22	0
56	MG	1A	3182	1/1	0.93	0.20	1.67	33,33,33,33	0
56	MG	2a	1683	1/1	0.95	0.20	1.66	33,33,33,33	0
56	MG	2A	3750	1/1	0.97	0.28	1.61	40,40,40,40	0
56	MG	2A	3304	1/1	0.94	0.20	1.57	49,49,49,49	0
56	MG	1A	3503	1/1	0.96	0.18	1.54	22,22,22,22	0
56	MG	2A	3289	1/1	0.91	0.21	1.46	53,53,53,53	0
56	MG	1x	106	1/1	0.94	0.15	1.45	66,66,66,66	0
56	MG	1A	3038	1/1	0.97	0.22	1.43	25,25,25,25	0
56	MG	2a	1681	1/1	0.83	0.22	1.43	69,69,69,69	0
56	MG	1A	4044	1/1	0.97	0.27	1.41	29,29,29,29	0
56	MG	2A	3385	1/1	0.95	0.20	1.39	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3401	1/1	0.97	0.19	1.35	32,32,32,32	0
56	MG	1A	3572	1/1	0.95	0.20	1.35	12,12,12,12	0
56	MG	1U	203	1/1	0.94	0.23	1.34	23,23,23,23	0
56	MG	1P	202	1/1	0.96	0.27	1.33	23,23,23,23	0
56	MG	1A	4066	1/1	0.98	0.23	1.32	35,35,35,35	0
56	MG	1A	3921	1/1	0.92	0.22	1.32	43,43,43,43	0
56	MG	1A	3192	1/1	0.91	0.17	1.32	54,54,54,54	0
56	MG	1A	3649	1/1	0.96	0.19	1.30	16,16,16,16	0
56	MG	15	106	1/1	0.93	0.24	1.25	19,19,19,19	0
56	MG	1U	204	1/1	0.99	0.26	1.25	23,23,23,23	0
56	MG	2A	3757	1/1	0.91	0.26	1.23	55,55,55,55	0
59	ZN	25	501	1/1	0.98	0.18	1.20	45,45,45,45	0
56	MG	1A	3058	1/1	0.93	0.19	1.20	33,33,33,33	0
56	MG	1A	3070	1/1	0.96	0.17	1.18	23,23,23,23	0
56	MG	2A	3359	1/1	0.96	0.20	1.18	52,52,52,52	0
56	MG	1A	4059	1/1	0.92	0.26	1.18	22,22,22,22	0
56	MG	1A	4064	1/1	0.97	0.26	1.15	30,30,30,30	0
56	MG	2A	3568	1/1	0.87	0.16	1.13	47,47,47,47	0
56	MG	1a	3141	1/1	0.78	0.17	1.13	64,64,64,64	0
56	MG	2D	301	1/1	0.95	0.24	1.09	54,54,54,54	0
56	MG	1A	4005	1/1	0.98	0.22	1.08	10,10,10,10	0
56	MG	1A	3640	1/1	0.85	0.16	1.08	36,36,36,36	0
56	MG	1E	303	1/1	0.98	0.24	1.07	22,22,22,22	0
56	MG	2A	3659	1/1	0.89	0.18	1.07	41,41,41,41	0
56	MG	1A	3656	1/1	0.97	0.19	1.06	25,25,25,25	0
56	MG	2A	3501	1/1	0.86	0.18	1.04	53,53,53,53	0
56	MG	2A	3657	1/1	0.92	0.20	1.02	41,41,41,41	0
56	MG	1A	3300	1/1	0.95	0.18	1.02	29,29,29,29	0
56	MG	2A	3060	1/1	0.97	0.20	1.02	32,32,32,32	0
56	MG	1D	305	1/1	0.97	0.24	1.00	28,28,28,28	0
56	MG	1E	305	1/1	0.97	0.23	0.92	50,50,50,50	0
56	MG	1A	4025	1/1	0.91	0.22	0.91	24,24,24,24	0
56	MG	1D	309	1/1	0.95	0.23	0.87	28,28,28,28	0
56	MG	2R	3002	1/1	0.93	0.25	0.87	56,56,56,56	0
56	MG	1A	3674	1/1	0.91	0.20	0.87	56,56,56,56	0
56	MG	1W	3004	1/1	0.99	0.20	0.87	21,21,21,21	0
56	MG	1A	3590	1/1	0.86	0.22	0.86	36,36,36,36	0
56	MG	1A	4057	1/1	0.98	0.21	0.75	27,27,27,27	0
56	MG	2a	1770	1/1	0.89	0.17	0.74	59,59,59,59	0
56	MG	1a	3145	1/1	0.96	0.22	0.73	48,48,48,48	0
56	MG	2A	3740	1/1	0.97	0.21	0.72	37,37,37,37	0
56	MG	1A	3428	1/1	0.95	0.21	0.72	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	1S	3002	1/1	0.93	0.20	0.71	36,36,36,36	0
56	MG	2A	3355	1/1	0.99	0.21	0.67	23,23,23,23	0
59	ZN	15	104	1/1	0.99	0.20	0.64	42,42,42,42	0
56	MG	1X	104	1/1	0.98	0.20	0.62	31,31,31,31	0
56	MG	2A	3110	1/1	0.94	0.18	0.61	37,37,37,37	0
56	MG	1A	3837	1/1	0.92	0.19	0.60	54,54,54,54	0
56	MG	1A	3099	1/1	0.98	0.24	0.60	23,23,23,23	0
56	MG	1A	3537	1/1	0.91	0.18	0.58	30,30,30,30	0
56	MG	2A	3628	1/1	0.93	0.20	0.58	40,40,40,40	0
56	MG	2A	3467	1/1	0.93	0.22	0.57	28,28,28,28	0
56	MG	1A	3565	1/1	0.90	0.19	0.56	26,26,26,26	0
56	MG	1A	3012	1/1	0.98	0.19	0.55	13,13,13,13	0
56	MG	1Q	203	1/1	0.98	0.22	0.53	28,28,28,28	0
56	MG	2A	3244	1/1	0.79	0.18	0.52	47,47,47,47	0
56	MG	1A	3705	1/1	0.93	0.17	0.50	39,39,39,39	0
56	MG	2A	3737	1/1	0.88	0.26	0.47	42,42,42,42	0
56	MG	1F	303	1/1	0.94	0.19	0.47	35,35,35,35	0
56	MG	1A	3971	1/1	0.71	0.14	0.44	65,65,65,65	0
56	MG	2T	3002	1/1	0.90	0.25	0.44	59,59,59,59	0
56	MG	2A	3739	1/1	0.98	0.23	0.43	29,29,29,29	0
56	MG	1A	3792	1/1	0.87	0.18	0.43	19,19,19,19	0
56	MG	2A	3670	1/1	0.96	0.18	0.40	46,46,46,46	0
56	MG	1O	202	1/1	0.97	0.24	0.36	56,56,56,56	0
56	MG	2A	3003	1/1	0.98	0.19	0.35	49,49,49,49	0
56	MG	2A	3485	1/1	0.94	0.22	0.35	56,56,56,56	0
56	MG	1A	3051	1/1	0.97	0.17	0.34	22,22,22,22	0
56	MG	1A	3268	1/1	0.97	0.16	0.33	31,31,31,31	0
56	MG	2A	3630	1/1	0.71	0.18	0.29	55,55,55,55	0
56	MG	2U	205	1/1	0.96	0.23	0.29	49,49,49,49	0
56	MG	2A	3115	1/1	0.88	0.18	0.27	39,39,39,39	0
56	MG	1a	3102	1/1	0.99	0.16	0.26	39,39,39,39	0
56	MG	1A	3116	1/1	0.98	0.17	0.24	26,26,26,26	0
56	MG	1A	3879	1/1	0.95	0.18	0.18	18,18,18,18	0
56	MG	1A	3776	1/1	0.96	0.20	0.14	25,25,25,25	0
56	MG	1A	3579	1/1	0.96	0.18	0.13	31,31,31,31	0
56	MG	2A	3729	1/1	0.96	0.20	0.12	43,43,43,43	0
56	MG	1l	201	1/1	0.94	0.17	0.08	31,31,31,31	0
56	MG	2q	203	1/1	0.84	0.20	0.07	75,75,75,75	0
56	MG	2a	1609	1/1	0.83	0.12	0.05	57,57,57,57	0
56	MG	1p	101	1/1	0.86	0.24	0.01	55,55,55,55	0
56	MG	1A	3310	1/1	0.98	0.17	-0.02	24,24,24,24	0
56	MG	2A	3377	1/1	0.93	0.20	-0.03	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1W	3001	1/1	0.96	0.19	-0.08	34,34,34,34	0
56	MG	1A	3528	1/1	0.95	0.15	-0.08	23,23,23,23	0
56	MG	1A	3794	1/1	0.79	0.18	-0.10	18,18,18,18	0
56	MG	1A	3925	1/1	0.97	0.17	-0.10	12,12,12,12	0
56	MG	2T	3001	1/1	0.84	0.26	-0.10	52,52,52,52	0
56	MG	2A	3444	1/1	0.94	0.20	-0.11	42,42,42,42	0
56	MG	2A	3394	1/1	0.78	0.20	-0.13	29,29,29,29	0
59	ZN	16	102	1/1	0.99	0.17	-0.15	38,38,38,38	0
56	MG	2A	3320	1/1	0.98	0.20	-0.18	17,17,17,17	0
56	MG	2a	1672	1/1	0.94	0.17	-0.18	50,50,50,50	0
56	MG	2a	1710	1/1	0.91	0.15	-0.19	64,64,64,64	0
56	MG	2a	1726	1/1	0.97	0.13	-0.19	64,64,64,64	0
56	MG	2A	3551	1/1	0.91	0.22	-0.22	48,48,48,48	0
56	MG	1a	3074	1/1	0.95	0.16	-0.23	49,49,49,49	0
56	MG	17	101	1/1	0.94	0.19	-0.24	27,27,27,27	0
56	MG	2A	3417	1/1	0.94	0.18	-0.24	35,35,35,35	0
56	MG	1A	3507	1/1	0.98	0.19	-0.25	24,24,24,24	0
59	ZN	2Y	501	1/1	0.97	0.15	-0.26	79,79,79,79	0
56	MG	1A	3641	1/1	0.92	0.18	-0.26	13,13,13,13	0
56	MG	2B	3006	1/1	0.95	0.17	-0.27	65,65,65,65	0
56	MG	2A	3512	1/1	0.96	0.15	-0.28	55,55,55,55	0
56	MG	2A	3381	1/1	0.89	0.18	-0.31	33,33,33,33	0
56	MG	2A	3669	1/1	0.97	0.20	-0.33	27,27,27,27	0
56	MG	1A	3662	1/1	0.98	0.19	-0.34	32,32,32,32	0
56	MG	2A	3124	1/1	0.95	0.18	-0.38	48,48,48,48	0
56	MG	15	102	1/1	0.97	0.19	-0.38	22,22,22,22	0
56	MG	1A	3123	1/1	0.96	0.16	-0.46	21,21,21,21	0
56	MG	1A	3778	1/1	0.97	0.17	-0.46	13,13,13,13	0
56	MG	1U	206	1/1	0.98	0.21	-0.49	16,16,16,16	0
56	MG	1A	3810	1/1	0.98	0.15	-0.49	40,40,40,40	0
56	MG	1A	3928	1/1	0.94	0.17	-0.51	37,37,37,37	0
56	MG	1A	3229	1/1	0.96	0.15	-0.53	28,28,28,28	0
56	MG	2a	1704	1/1	0.90	0.18	-0.53	52,52,52,52	0
56	MG	1a	3139	1/1	0.93	0.21	-0.53	56,56,56,56	0
56	MG	2a	1747	1/1	0.92	0.12	-0.56	56,56,56,56	0
56	MG	1a	3211	1/1	0.95	0.15	-0.56	35,35,35,35	0
56	MG	1A	3771	1/1	0.96	0.18	-0.57	17,17,17,17	0
59	ZN	1Y	501	1/1	0.99	0.14	-0.57	58,58,58,58	0
56	MG	1A	3423	1/1	0.83	0.17	-0.57	38,38,38,38	0
56	MG	1a	3109	1/1	0.90	0.16	-0.58	30,30,30,30	0
56	MG	2A	3754	1/1	0.98	0.26	-0.59	43,43,43,43	0
56	MG	2R	3004	1/1	0.94	0.19	-0.59	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3714	1/1	0.95	0.19	-0.62	26,26,26,26	0
56	MG	2A	3449	1/1	0.92	0.11	-0.64	63,63,63,63	0
56	MG	1A	3474	1/1	0.96	0.17	-0.64	38,38,38,38	0
56	MG	1Q	202	1/1	0.97	0.16	-0.66	28,28,28,28	0
56	MG	16	101	1/1	0.88	0.17	-0.67	35,35,35,35	0
56	MG	1a	3155	1/1	0.94	0.18	-0.68	53,53,53,53	0
56	MG	2a	1740	1/1	0.73	0.16	-0.69	60,60,60,60	0
56	MG	2q	204	1/1	0.91	0.16	-0.72	65,65,65,65	0
56	MG	2A	3378	1/1	0.94	0.16	-0.72	25,25,25,25	0
56	MG	1A	3935	1/1	0.83	0.15	-0.73	43,43,43,43	0
56	MG	1B	220	1/1	0.87	0.14	-0.74	57,57,57,57	0
56	MG	1A	3934	1/1	0.94	0.16	-0.74	22,22,22,22	0
56	MG	2a	1715	1/1	0.91	0.15	-0.75	50,50,50,50	0
56	MG	2A	3307	1/1	0.87	0.14	-0.75	35,35,35,35	0
56	MG	2A	3545	1/1	0.89	0.18	-0.76	45,45,45,45	0
56	MG	2A	3483	1/1	0.91	0.15	-0.78	59,59,59,59	0
56	MG	1a	3025	1/1	0.97	0.16	-0.78	24,24,24,24	0
59	ZN	19	501	1/1	0.98	0.17	-0.78	42,42,42,42	0
56	MG	1A	3562	1/1	0.95	0.16	-0.79	18,18,18,18	0
56	MG	1D	310	1/1	0.96	0.19	-0.79	33,33,33,33	0
56	MG	1A	3519	1/1	0.98	0.17	-0.79	21,21,21,21	0
56	MG	1A	3039	1/1	0.94	0.18	-0.81	26,26,26,26	0
56	MG	1a	3098	1/1	0.97	0.16	-0.82	39,39,39,39	0
56	MG	2A	3463	1/1	0.96	0.16	-0.85	27,27,27,27	0
60	SF4	2d	501	8/8	0.98	0.15	-0.86	58,60,69,79	0
56	MG	1A	3110	1/1	0.91	0.17	-0.86	27,27,27,27	0
56	MG	1D	307	1/1	0.87	0.17	-0.87	39,39,39,39	0
56	MG	2A	3712	1/1	0.98	0.15	-0.87	35,35,35,35	0
56	MG	1A	3677	1/1	0.98	0.17	-0.90	18,18,18,18	0
56	MG	1a	3164	1/1	0.92	0.13	-0.91	58,58,58,58	0
56	MG	2A	3086	1/1	0.89	0.14	-0.93	62,62,62,62	0
60	SF4	1d	501	8/8	0.98	0.16	-0.94	52,54,61,66	0
56	MG	1R	201	1/1	0.96	0.16	-0.94	36,36,36,36	0
59	ZN	24	501	1/1	0.64	0.09	-0.95	103,103,103,103	0
56	MG	1E	312	1/1	0.98	0.15	-0.96	44,44,44,44	0
59	ZN	14	501	1/1	0.99	0.13	-0.99	70,70,70,70	0
56	MG	12	3002	1/1	0.97	0.19	-1.00	35,35,35,35	0
56	MG	1A	3661	1/1	0.98	0.17	-1.00	18,18,18,18	0
56	MG	2A	3713	1/1	0.96	0.18	-1.01	26,26,26,26	0
56	MG	1D	302	1/1	0.94	0.19	-1.02	21,21,21,21	0
56	MG	1E	308	1/1	0.87	0.17	-1.02	28,28,28,28	0
56	MG	1G	3001	1/1	0.89	0.14	-1.03	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	1O	203	1/1	0.98	0.16	-1.04	48,48,48,48	0
56	MG	2A	3046	1/1	0.81	0.15	-1.05	58,58,58,58	0
56	MG	1A	3808	1/1	0.95	0.17	-1.05	34,34,34,34	0
56	MG	1A	3796	1/1	0.89	0.17	-1.06	33,33,33,33	0
56	MG	1a	3210	1/1	0.95	0.14	-1.06	41,41,41,41	0
56	MG	1X	105	1/1	0.96	0.16	-1.07	44,44,44,44	0
56	MG	2A	3431	1/1	0.94	0.17	-1.08	24,24,24,24	0
56	MG	1U	205	1/1	0.95	0.20	-1.10	23,23,23,23	0
56	MG	1A	3890	1/1	0.95	0.15	-1.11	36,36,36,36	0
56	MG	2A	3380	1/1	0.95	0.17	-1.16	25,25,25,25	0
56	MG	2a	1807	1/1	0.93	0.11	-1.17	61,61,61,61	0
56	MG	1B	228	1/1	0.93	0.15	-1.19	24,24,24,24	0
56	MG	1a	3105	1/1	0.93	0.11	-1.19	59,59,59,59	0
56	MG	2A	3453	1/1	0.97	0.18	-1.20	34,34,34,34	0
56	MG	1r	3001	1/1	0.75	0.16	-1.20	61,61,61,61	0
56	MG	2A	3734	1/1	0.96	0.16	-1.20	25,25,25,25	0
56	MG	1A	3524	1/1	0.95	0.16	-1.20	20,20,20,20	0
59	ZN	1n	501	1/1	0.97	0.11	-1.21	51,51,51,51	0
56	MG	2A	3733	1/1	0.92	0.17	-1.21	30,30,30,30	0
56	MG	1A	3646	1/1	0.94	0.16	-1.22	19,19,19,19	0
56	MG	1A	3795	1/1	0.82	0.16	-1.23	50,50,50,50	0
56	MG	2A	3576	1/1	0.95	0.10	-1.27	52,52,52,52	0
56	MG	2e	3001	1/1	0.96	0.11	-1.28	60,60,60,60	0
56	MG	2A	3357	1/1	0.94	0.15	-1.29	21,21,21,21	0
56	MG	2a	1725	1/1	0.95	0.14	-1.30	49,49,49,49	0
56	MG	19	502	1/1	0.90	0.16	-1.32	39,39,39,39	0
56	MG	2A	3727	1/1	0.96	0.12	-1.35	49,49,49,49	0
56	MG	1a	3114	1/1	0.97	0.10	-1.35	68,68,68,68	0
56	MG	2a	1830	1/1	0.97	0.16	-1.35	71,71,71,71	0
56	MG	1A	3653	1/1	0.90	0.17	-1.35	20,20,20,20	0
56	MG	2A	3076	1/1	0.86	0.13	-1.38	45,45,45,45	0
56	MG	2A	3308	1/1	0.93	0.15	-1.38	54,54,54,54	0
56	MG	2A	3748	1/1	0.95	0.14	-1.38	27,27,27,27	0
56	MG	2d	502	1/1	0.91	0.12	-1.40	58,58,58,58	0
56	MG	1D	311	1/1	0.92	0.14	-1.40	36,36,36,36	0
56	MG	2A	3015	1/1	0.89	0.15	-1.40	37,37,37,37	0
56	MG	2a	1671	1/1	0.88	0.16	-1.41	58,58,58,58	0
56	MG	1a	3007	1/1	0.95	0.18	-1.44	50,50,50,50	0
56	MG	1a	3181	1/1	0.91	0.14	-1.46	41,41,41,41	0
56	MG	2A	3020	1/1	0.96	0.15	-1.48	29,29,29,29	0
56	MG	2F	302	1/1	0.84	0.13	-1.50	50,50,50,50	0
59	ZN	29	501	1/1	0.97	0.07	-1.52	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
59	ZN	26	501	1/1	0.98	0.09	-1.53	59,59,59,59	0
56	MG	2a	1736	1/1	0.84	0.11	-1.53	82,82,82,82	0
56	MG	1a	3028	1/1	0.97	0.14	-1.53	37,37,37,37	0
56	MG	1b	3001	1/1	0.97	0.15	-1.55	69,69,69,69	0
56	MG	1t	3001	1/1	0.88	0.20	-1.57	57,57,57,57	0
56	MG	1A	3534	1/1	0.90	0.13	-1.58	39,39,39,39	0
56	MG	2a	1766	1/1	0.98	0.14	-1.58	36,36,36,36	0
59	ZN	2n	501	1/1	0.96	0.05	-1.59	93,93,93,93	0
56	MG	2A	3682	1/1	0.89	0.13	-1.61	61,61,61,61	0
56	MG	2A	3510	1/1	0.96	0.11	-1.62	50,50,50,50	0
56	MG	1A	3676	1/1	0.97	0.17	-1.63	31,31,31,31	0
56	MG	1A	3297	1/1	0.88	0.13	-1.64	35,35,35,35	0
56	MG	1a	3213	1/1	0.99	0.15	-1.65	33,33,33,33	0
56	MG	1a	3013	1/1	0.92	0.15	-1.65	45,45,45,45	0
56	MG	2A	3073	1/1	0.90	0.16	-1.66	38,38,38,38	0
56	MG	1A	3758	1/1	0.93	0.13	-1.66	32,32,32,32	0
56	MG	1a	3120	1/1	0.96	0.08	-1.66	43,43,43,43	0
56	MG	1A	3153	1/1	0.98	0.16	-1.68	29,29,29,29	0
56	MG	2a	1731	1/1	0.98	0.09	-1.68	56,56,56,56	0
56	MG	1B	219	1/1	0.97	0.13	-1.69	27,27,27,27	0
56	MG	2l	203	1/1	0.93	0.17	-1.73	62,62,62,62	0
56	MG	1b	3002	1/1	0.94	0.10	-1.73	53,53,53,53	0
56	MG	1S	3001	1/1	0.86	0.18	-1.75	47,47,47,47	0
56	MG	1A	3627	1/1	0.95	0.13	-1.77	26,26,26,26	0
56	MG	2q	201	1/1	0.98	0.07	-1.78	46,46,46,46	0
56	MG	2A	3392	1/1	0.91	0.13	-1.80	33,33,33,33	0
56	MG	1a	3099	1/1	0.93	0.10	-1.80	72,72,72,72	0
56	MG	1a	3051	1/1	0.94	0.12	-1.81	55,55,55,55	0
56	MG	1w	106	1/1	0.90	0.10	-1.84	70,70,70,70	0
56	MG	1A	3585	1/1	0.99	0.16	-1.86	30,30,30,30	0
56	MG	2A	3646	1/1	0.90	0.13	-1.87	59,59,59,59	0
56	MG	11	105	1/1	0.96	0.11	-1.89	32,32,32,32	0
56	MG	2A	3407	1/1	0.97	0.15	-1.90	35,35,35,35	0
56	MG	1A	3847	1/1	0.96	0.14	-1.90	18,18,18,18	0
56	MG	1a	3031	1/1	0.97	0.06	-1.91	54,54,54,54	0
56	MG	2A	3406	1/1	0.93	0.13	-1.91	40,40,40,40	0
56	MG	1a	3212	1/1	0.94	0.14	-1.91	41,41,41,41	0
56	MG	2A	3571	1/1	0.85	0.10	-1.92	57,57,57,57	0
56	MG	2A	3292	1/1	0.98	0.16	-1.92	31,31,31,31	0
56	MG	1A	3762	1/1	0.92	0.14	-1.93	12,12,12,12	0
56	MG	1A	4062	1/1	0.94	0.13	-1.96	21,21,21,21	0
56	MG	1a	3040	1/1	0.93	0.12	-1.98	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3090	1/1	0.97	0.15	-1.98	32,32,32,32	0
56	MG	2X	3002	1/1	0.96	0.14	-1.99	49,49,49,49	0
56	MG	2a	1796	1/1	0.91	0.15	-2.01	54,54,54,54	0
56	MG	1X	106	1/1	0.97	0.14	-2.01	21,21,21,21	0
56	MG	1a	3170	1/1	0.80	0.09	-2.02	66,66,66,66	0
56	MG	2D	305	1/1	0.95	0.10	-2.02	29,29,29,29	0
56	MG	1A	3912	1/1	0.95	0.15	-2.03	25,25,25,25	0
56	MG	2A	3719	1/1	0.95	0.14	-2.03	70,70,70,70	0
56	MG	2A	3011	1/1	0.93	0.15	-2.05	54,54,54,54	0
56	MG	2A	3155	1/1	0.92	0.09	-2.06	34,34,34,34	0
56	MG	1W	3005	1/1	0.96	0.14	-2.09	21,21,21,21	0
56	MG	2A	3405	1/1	0.97	0.15	-2.09	35,35,35,35	0
56	MG	2f	3001	1/1	0.95	0.11	-2.10	40,40,40,40	0
56	MG	1A	3812	1/1	0.91	0.16	-2.11	43,43,43,43	0
56	MG	2A	3466	1/1	0.92	0.16	-2.11	41,41,41,41	0
56	MG	2A	3716	1/1	0.95	0.09	-2.12	44,44,44,44	0
56	MG	2A	3650	1/1	0.85	0.09	-2.14	52,52,52,52	0
56	MG	2A	3009	1/1	0.96	0.14	-2.15	29,29,29,29	0
56	MG	2a	1774	1/1	0.96	0.15	-2.15	44,44,44,44	0
56	MG	1a	3115	1/1	0.93	0.13	-2.16	48,48,48,48	0
56	MG	1A	3737	1/1	0.93	0.14	-2.17	29,29,29,29	0
56	MG	2A	3455	1/1	0.97	0.15	-2.17	42,42,42,42	0
56	MG	1A	3476	1/1	0.92	0.13	-2.18	27,27,27,27	0
56	MG	2A	3095	1/1	0.95	0.12	-2.18	52,52,52,52	0
56	MG	2A	3668	1/1	0.98	0.12	-2.19	41,41,41,41	0
56	MG	1a	3113	1/1	0.96	0.14	-2.19	40,40,40,40	0
56	MG	1A	3180	1/1	0.96	0.14	-2.19	42,42,42,42	0
56	MG	2A	3029	1/1	0.97	0.14	-2.21	36,36,36,36	0
56	MG	1A	3652	1/1	0.98	0.15	-2.21	23,23,23,23	0
56	MG	2a	1632	1/1	0.95	0.11	-2.23	67,67,67,67	0
56	MG	1A	3626	1/1	0.94	0.14	-2.23	23,23,23,23	0
56	MG	2Q	3001	1/1	0.95	0.07	-2.23	54,54,54,54	0
56	MG	2G	3001	1/1	0.80	0.10	-2.23	60,60,60,60	0
56	MG	2A	3460	1/1	0.93	0.15	-2.24	39,39,39,39	0
56	MG	2A	3523	1/1	0.93	0.14	-2.25	37,37,37,37	0
56	MG	2a	1832	1/1	0.98	0.13	-2.27	37,37,37,37	0
56	MG	2A	3462	1/1	0.96	0.14	-2.28	54,54,54,54	0
56	MG	1A	3592	1/1	0.86	0.14	-2.32	30,30,30,30	0
56	MG	1A	3032	1/1	0.97	0.14	-2.33	26,26,26,26	0
56	MG	2A	3345	1/1	0.95	0.12	-2.39	63,63,63,63	0
56	MG	2a	1663	1/1	0.84	0.13	-2.40	48,48,48,48	0
56	MG	1a	3122	1/1	0.95	0.11	-2.40	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	2A	3123	1/1	0.94	0.07	-2.40	58,58,58,58	0
56	MG	2a	1759	1/1	0.91	0.17	-2.42	50,50,50,50	0
56	MG	1A	3764	1/1	0.97	0.15	-2.42	24,24,24,24	0
56	MG	1A	3541	1/1	0.97	0.10	-2.43	35,35,35,35	0
56	MG	1G	3003	1/1	0.95	0.11	-2.44	51,51,51,51	0
56	MG	1A	3075	1/1	0.94	0.13	-2.44	34,34,34,34	0
56	MG	1A	3569	1/1	0.95	0.14	-2.45	17,17,17,17	0
56	MG	1a	3215	1/1	0.97	0.07	-2.47	39,39,39,39	0
56	MG	2t	3001	1/1	0.81	0.09	-2.47	53,53,53,53	0
56	MG	2A	3651	1/1	0.94	0.13	-2.50	42,42,42,42	0
56	MG	2A	3074	1/1	0.96	0.15	-2.50	32,32,32,32	0
56	MG	1A	3197	1/1	0.89	0.13	-2.51	32,32,32,32	0
56	MG	1A	3663	1/1	0.97	0.13	-2.53	43,43,43,43	0
56	MG	2a	1734	1/1	0.98	0.11	-2.56	48,48,48,48	0
56	MG	1A	3827	1/1	0.94	0.13	-2.59	47,47,47,47	0
56	MG	2a	1777	1/1	0.95	0.10	-2.60	55,55,55,55	0
56	MG	2a	1658	1/1	0.93	0.12	-2.60	59,59,59,59	0
56	MG	2A	3443	1/1	0.84	0.14	-2.60	34,34,34,34	0
56	MG	2A	3027	1/1	0.95	0.14	-2.63	32,32,32,32	0
56	MG	1A	3009	1/1	0.98	0.11	-2.65	24,24,24,24	0
56	MG	1A	3707	1/1	0.90	0.12	-2.66	45,45,45,45	0
56	MG	1E	306	1/1	0.88	0.12	-2.66	38,38,38,38	0
56	MG	2A	3411	1/1	0.97	0.14	-2.69	27,27,27,27	0
56	MG	1A	3266	1/1	0.98	0.14	-2.70	24,24,24,24	0
56	MG	1A	3553	1/1	0.96	0.14	-2.71	10,10,10,10	0
56	MG	20	3003	1/1	0.92	0.11	-2.76	56,56,56,56	0
56	MG	2a	1661	1/1	0.87	0.11	-2.77	63,63,63,63	0
56	MG	1A	3631	1/1	0.93	0.16	-2.82	32,32,32,32	0
56	MG	1A	3020	1/1	0.93	0.14	-2.83	18,18,18,18	0
56	MG	1N	202	1/1	0.89	0.13	-2.83	36,36,36,36	0
56	MG	10	104	1/1	0.90	0.12	-2.84	49,49,49,49	0
56	MG	1a	3110	1/1	0.96	0.13	-2.85	50,50,50,50	0
56	MG	1n	503	1/1	0.93	0.08	-2.91	38,38,38,38	0
56	MG	1A	3819	1/1	0.93	0.11	-2.94	29,29,29,29	0
56	MG	1a	3036	1/1	0.91	0.10	-2.95	49,49,49,49	0
56	MG	2a	1689	1/1	0.97	0.08	-2.95	57,57,57,57	0
56	MG	2A	3677	1/1	0.94	0.15	-2.98	48,48,48,48	0
56	MG	1A	3648	1/1	0.92	0.10	-3.00	20,20,20,20	0
56	MG	2a	1665	1/1	0.98	0.16	-3.01	49,49,49,49	0
56	MG	1A	3637	1/1	0.95	0.13	-3.02	20,20,20,20	0
56	MG	2E	306	1/1	0.90	0.12	-3.03	43,43,43,43	0
56	MG	2A	3704	1/1	0.97	0.14	-3.04	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	4013	1/1	0.94	0.13	-3.04	21,21,21,21	0
56	MG	1a	3002	1/1	0.97	0.10	-3.09	46,46,46,46	0
56	MG	2A	3520	1/1	0.88	0.10	-3.10	52,52,52,52	0
56	MG	1A	3628	1/1	0.93	0.13	-3.11	16,16,16,16	0
56	MG	2a	1789	1/1	0.95	0.09	-3.20	54,54,54,54	0
56	MG	1A	3444	1/1	0.93	0.14	-3.25	18,18,18,18	0
56	MG	1A	3686	1/1	0.97	0.16	-3.25	18,18,18,18	0
56	MG	2a	1670	1/1	0.94	0.11	-3.26	55,55,55,55	0
56	MG	2A	3717	1/1	0.97	0.11	-3.28	57,57,57,57	0
56	MG	2a	1673	1/1	0.93	0.10	-3.31	57,57,57,57	0
56	MG	1A	3574	1/1	0.95	0.15	-3.31	16,16,16,16	0
56	MG	1A	3644	1/1	0.85	0.14	-3.33	12,12,12,12	0
56	MG	1x	115	1/1	0.90	0.12	-3.33	50,50,50,50	0
56	MG	1a	3143	1/1	0.90	0.08	-3.35	74,74,74,74	0
56	MG	2a	1833	1/1	0.91	0.06	-3.36	62,62,62,62	0
56	MG	1A	3558	1/1	0.91	0.13	-3.38	16,16,16,16	0
56	MG	2A	3715	1/1	0.87	0.09	-3.38	56,56,56,56	0
56	MG	1A	3043	1/1	0.94	0.15	-3.39	19,19,19,19	0
56	MG	2A	3409	1/1	0.94	0.11	-3.39	54,54,54,54	0
56	MG	1A	3481	1/1	0.98	0.12	-3.43	28,28,28,28	0
56	MG	2A	3448	1/1	0.95	0.14	-3.50	33,33,33,33	0
56	MG	2a	1697	1/1	0.84	0.10	-3.52	64,64,64,64	0
56	MG	1A	3668	1/1	0.97	0.14	-3.53	22,22,22,22	0
56	MG	2A	3565	1/1	0.93	0.12	-3.61	45,45,45,45	0
56	MG	1A	3033	1/1	0.96	0.12	-3.63	21,21,21,21	0
56	MG	2E	301	1/1	0.96	0.14	-3.64	33,33,33,33	0
56	MG	2A	3344	1/1	0.97	0.11	-3.67	24,24,24,24	0
56	MG	2A	3143	1/1	0.96	0.13	-3.67	41,41,41,41	0
56	MG	2A	3030	1/1	0.97	0.08	-3.71	25,25,25,25	0
56	MG	2A	3702	1/1	0.74	0.13	-3.73	59,59,59,59	0
56	MG	1a	3019	1/1	0.95	0.10	-3.74	54,54,54,54	0
56	MG	1A	3021	1/1	0.97	0.13	-3.74	29,29,29,29	0
56	MG	1a	3077	1/1	0.90	0.09	-3.74	42,42,42,42	0
56	MG	1A	3184	1/1	0.97	0.14	-3.75	14,14,14,14	0
56	MG	1A	3599	1/1	0.97	0.11	-3.81	15,15,15,15	0
56	MG	2A	3008	1/1	0.90	0.14	-3.82	34,34,34,34	0
56	MG	2A	3144	1/1	0.97	0.10	-3.82	33,33,33,33	0
56	MG	1a	3012	1/1	0.94	0.10	-3.83	41,41,41,41	0
56	MG	2A	3445	1/1	0.93	0.10	-3.90	47,47,47,47	0
56	MG	2A	3606	1/1	0.88	0.12	-3.93	49,49,49,49	0
56	MG	2A	3057	1/1	0.93	0.13	-3.93	47,47,47,47	0
56	MG	1a	3071	1/1	0.97	0.10	-3.96	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	2A	3744	1/1	0.88	0.10	-3.97	40,40,40,40	0
56	MG	1A	3552	1/1	0.97	0.14	-3.97	23,23,23,23	0
56	MG	2A	3562	1/1	0.92	0.10	-3.98	40,40,40,40	0
56	MG	1A	3962	1/1	0.97	0.08	-4.00	23,23,23,23	0
56	MG	2a	1653	1/1	0.92	0.07	-4.03	67,67,67,67	0
56	MG	2A	3301	1/1	0.95	0.14	-4.03	40,40,40,40	0
56	MG	2a	1754	1/1	0.95	0.09	-4.04	61,61,61,61	0
56	MG	1A	3022	1/1	0.97	0.13	-4.05	22,22,22,22	0
56	MG	1a	3126	1/1	0.94	0.12	-4.06	46,46,46,46	0
56	MG	1x	105	1/1	0.95	0.13	-4.06	59,59,59,59	0
56	MG	2A	3360	1/1	0.88	0.13	-4.07	25,25,25,25	0
56	MG	1A	3011	1/1	0.98	0.09	-4.11	20,20,20,20	0
56	MG	1a	3022	1/1	0.91	0.09	-4.12	48,48,48,48	0
56	MG	1A	4035	1/1	0.95	0.10	-4.14	38,38,38,38	0
56	MG	1a	3041	1/1	0.96	0.05	-4.17	51,51,51,51	0
56	MG	2A	3424	1/1	0.99	0.09	-4.18	24,24,24,24	0
56	MG	1a	3039	1/1	0.95	0.10	-4.22	47,47,47,47	0
56	MG	1A	3520	1/1	0.96	0.11	-4.23	11,11,11,11	0
56	MG	2A	3625	1/1	0.93	0.08	-4.24	52,52,52,52	0
56	MG	1A	3807	1/1	0.97	0.11	-4.28	28,28,28,28	0
56	MG	1A	3554	1/1	0.96	0.13	-4.29	14,14,14,14	0
56	MG	2A	3368	1/1	0.97	0.13	-4.32	36,36,36,36	0
56	MG	1a	3205	1/1	0.85	0.12	-4.35	69,69,69,69	0
56	MG	2A	3037	1/1	0.93	0.11	-4.40	61,61,61,61	0
56	MG	2a	1678	1/1	0.91	0.11	-4.46	65,65,65,65	0
56	MG	2A	3535	1/1	0.93	0.14	-4.47	27,27,27,27	0
56	MG	2A	3692	1/1	0.90	0.07	-4.48	52,52,52,52	0
56	MG	2A	3442	1/1	0.94	0.17	-4.49	23,23,23,23	0
56	MG	1A	3634	1/1	0.97	0.12	-4.52	28,28,28,28	0
56	MG	2A	3272	1/1	0.96	0.09	-4.56	33,33,33,33	0
56	MG	2A	3012	1/1	0.96	0.10	-4.60	44,44,44,44	0
56	MG	1U	201	1/1	0.97	0.10	-4.61	20,20,20,20	0
56	MG	1A	3745	1/1	0.97	0.13	-4.67	33,33,33,33	0
56	MG	1A	3605	1/1	0.98	0.09	-4.68	14,14,14,14	0
56	MG	1A	3848	1/1	0.97	0.10	-4.70	34,34,34,34	0
56	MG	1E	313	1/1	0.90	0.10	-4.73	25,25,25,25	0
56	MG	2A	3709	1/1	0.98	0.14	-4.74	40,40,40,40	0
56	MG	2A	3541	1/1	0.96	0.14	-4.79	32,32,32,32	0
56	MG	1A	3670	1/1	0.90	0.11	-4.80	43,43,43,43	0
56	MG	1A	3615	1/1	0.97	0.11	-4.83	12,12,12,12	0
56	MG	1A	3118	1/1	0.93	0.11	-4.85	29,29,29,29	0
56	MG	2A	3077	1/1	0.97	0.10	-4.85	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2a	1788	1/1	0.84	0.12	-4.88	55,55,55,55	0
56	MG	2a	1690	1/1	0.94	0.07	-4.93	57,57,57,57	0
56	MG	2A	3375	1/1	0.89	0.11	-5.02	36,36,36,36	0
56	MG	1B	223	1/1	0.96	0.10	-5.03	51,51,51,51	0
56	MG	1a	3009	1/1	0.96	0.10	-5.04	32,32,32,32	0
56	MG	2A	3063	1/1	0.97	0.14	-5.05	43,43,43,43	0
56	MG	1A	3525	1/1	0.96	0.12	-5.10	9,9,9,9	0
56	MG	2A	3597	1/1	0.96	0.12	-5.12	34,34,34,34	0
56	MG	2A	3354	1/1	0.90	0.14	-5.16	53,53,53,53	0
56	MG	2A	3356	1/1	0.85	0.08	-5.18	42,42,42,42	0
56	MG	1a	3188	1/1	0.95	0.10	-5.19	47,47,47,47	0
56	MG	2A	3521	1/1	0.96	0.07	-5.21	63,63,63,63	0
56	MG	1a	3010	1/1	0.93	0.09	-5.24	45,45,45,45	0
56	MG	2A	3387	1/1	0.97	0.09	-5.24	50,50,50,50	0
56	MG	1a	3169	1/1	0.95	0.09	-5.27	38,38,38,38	0
56	MG	2w	108	1/1	0.98	0.07	-5.28	68,68,68,68	0
56	MG	1A	3888	1/1	0.96	0.14	-5.32	15,15,15,15	0
56	MG	2A	3493	1/1	0.96	0.09	-5.43	28,28,28,28	0
56	MG	1a	3185	1/1	0.99	0.10	-5.44	26,26,26,26	0
56	MG	1A	3660	1/1	0.99	0.09	-5.48	26,26,26,26	0
56	MG	1A	3593	1/1	0.80	0.12	-5.51	30,30,30,30	0
56	MG	2A	3346	1/1	0.92	0.11	-5.52	48,48,48,48	0
56	MG	1a	3158	1/1	0.95	0.06	-5.67	47,47,47,47	0
56	MG	1A	3257	1/1	0.98	0.09	-5.71	34,34,34,34	0
56	MG	1A	3546	1/1	0.96	0.11	-5.74	14,14,14,14	0
56	MG	1A	3942	1/1	0.94	0.10	-5.80	47,47,47,47	0
56	MG	1A	3949	1/1	0.96	0.11	-5.82	18,18,18,18	0
56	MG	1a	3160	1/1	0.96	0.09	-5.83	52,52,52,52	0
56	MG	1A	3196	1/1	0.96	0.12	-5.87	34,34,34,34	0
56	MG	1A	3549	1/1	0.88	0.11	-5.91	30,30,30,30	0
56	MG	1B	206	1/1	0.97	0.07	-5.93	36,36,36,36	0
56	MG	1A	3642	1/1	0.98	0.09	-6.01	34,34,34,34	0
56	MG	2A	3006	1/1	0.93	0.08	-6.05	44,44,44,44	0
56	MG	1A	3288	1/1	0.90	0.08	-6.06	47,47,47,47	0
56	MG	1A	3049	1/1	0.96	0.10	-6.09	21,21,21,21	0
56	MG	2U	201	1/1	0.94	0.08	-6.10	49,49,49,49	0
56	MG	1A	3508	1/1	0.96	0.10	-6.22	26,26,26,26	0
56	MG	1A	3506	1/1	0.88	0.09	-6.30	24,24,24,24	0
56	MG	1A	3701	1/1	0.97	0.10	-6.33	15,15,15,15	0
56	MG	2A	3080	1/1	0.94	0.11	-6.39	28,28,28,28	0
56	MG	1A	3521	1/1	0.94	0.09	-6.48	50,50,50,50	0
56	MG	2A	3486	1/1	0.93	0.12	-6.48	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3535	1/1	0.98	0.09	-6.49	23,23,23,23	0
56	MG	2A	3148	1/1	0.97	0.06	-6.50	34,34,34,34	0
56	MG	1A	3216	1/1	0.96	0.14	-6.52	25,25,25,25	0
56	MG	1A	3671	1/1	0.90	0.09	-6.60	14,14,14,14	0
56	MG	2A	3351	1/1	0.94	0.13	-6.67	43,43,43,43	0
56	MG	1A	3836	1/1	0.92	0.09	-6.72	56,56,56,56	0
56	MG	1A	3815	1/1	0.90	0.08	-6.78	35,35,35,35	0
56	MG	2A	3706	1/1	0.94	0.14	-6.79	42,42,42,42	0
56	MG	1A	3162	1/1	0.97	0.13	-6.80	24,24,24,24	0
56	MG	1A	3441	1/1	0.93	0.07	-6.81	49,49,49,49	0
56	MG	2A	3099	1/1	0.93	0.10	-6.88	38,38,38,38	0
56	MG	2W	203	1/1	0.92	0.12	-6.91	41,41,41,41	0
56	MG	2A	3648	1/1	0.97	0.07	-6.97	46,46,46,46	0
56	MG	1B	224	1/1	0.94	0.09	-7.02	54,54,54,54	0
56	MG	1A	3891	1/1	0.96	0.10	-7.06	33,33,33,33	0
56	MG	2A	3736	1/1	0.97	0.09	-7.13	37,37,37,37	0
56	MG	1A	3885	1/1	0.94	0.12	-7.20	16,16,16,16	0
56	MG	1D	306	1/1	0.96	0.10	-7.29	17,17,17,17	0
56	MG	2A	3026	1/1	0.98	0.10	-7.46	43,43,43,43	0
56	MG	1A	3007	1/1	0.98	0.10	-7.53	12,12,12,12	0
56	MG	2A	3013	1/1	0.93	0.13	-7.65	27,27,27,27	0
56	MG	1A	3941	1/1	0.91	0.09	-7.78	34,34,34,34	0
56	MG	1A	3495	1/1	0.90	0.10	-7.99	31,31,31,31	0
56	MG	1A	3557	1/1	0.99	0.08	-8.00	25,25,25,25	0
56	MG	1A	3060	1/1	0.93	0.08	-8.10	26,26,26,26	0
56	MG	2A	3120	1/1	0.98	0.13	-8.31	38,38,38,38	0
56	MG	2a	1709	1/1	0.90	0.12	-8.50	49,49,49,49	0
56	MG	1A	3188	1/1	0.91	0.10	-8.51	12,12,12,12	0
56	MG	1A	3163	1/1	0.97	0.08	-8.53	24,24,24,24	0
56	MG	1A	3497	1/1	0.98	0.10	-8.98	23,23,23,23	0
56	MG	2A	3540	1/1	0.97	0.09	-9.03	37,37,37,37	0
56	MG	1A	3544	1/1	0.99	0.09	-9.12	12,12,12,12	0
56	MG	1A	3516	1/1	0.87	0.13	-9.70	30,30,30,30	0
56	MG	2A	3473	1/1	0.98	0.10	-9.85	29,29,29,29	0
56	MG	1A	3702	1/1	0.96	0.07	-10.00	23,23,23,23	0
56	MG	1A	3232	1/1	0.95	0.10	-10.57	17,17,17,17	0
56	MG	1A	3937	1/1	0.90	0.10	-10.81	40,40,40,40	0
56	MG	2a	1675	1/1	0.94	0.07	-11.37	53,53,53,53	0
56	MG	2A	3488	1/1	0.96	0.08	-11.45	53,53,53,53	0
56	MG	2A	3504	1/1	0.99	0.08	-12.23	29,29,29,29	0
56	MG	1A	3267	1/1	0.99	0.12	-12.32	24,24,24,24	0
56	MG	2a	1819	1/1	0.92	0.08	-12.83	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3220	1/1	0.97	0.08	-14.13	24,24,24,24	0
56	MG	1A	4000	1/1	0.98	0.07	-	29,29,29,29	0
56	MG	1A	3271	1/1	0.90	0.14	-	53,53,53,53	0
56	MG	1V	202	1/1	0.82	0.42	-	44,44,44,44	0
56	MG	1A	3849	1/1	0.92	0.27	-	35,35,35,35	0
56	MG	1A	3187	1/1	0.95	0.08	-	28,28,28,28	0
56	MG	1A	3712	1/1	0.93	0.25	-	34,34,34,34	0
56	MG	2A	3038	1/1	0.97	0.16	-	33,33,33,33	0
56	MG	1A	3989	1/1	0.87	0.10	-	49,49,49,49	0
56	MG	1A	3321	1/1	0.88	0.41	-	45,45,45,45	0
56	MG	2A	3698	1/1	0.92	0.16	-	58,58,58,58	0
56	MG	2A	3212	1/1	0.91	0.12	-	59,59,59,59	0
56	MG	2A	3186	1/1	0.87	0.14	-	51,51,51,51	0
56	MG	2A	3275	1/1	0.97	0.09	-	37,37,37,37	0
56	MG	2a	1802	1/1	0.84	0.23	-	69,69,69,69	0
56	MG	1A	3017	1/1	0.97	0.11	-	19,19,19,19	0
56	MG	15	107	1/1	0.86	0.21	-	45,45,45,45	0
56	MG	1a	3061	1/1	0.85	0.14	-	56,56,56,56	0
56	MG	1a	3004	1/1	0.94	0.14	-	50,50,50,50	0
56	MG	1A	3978	1/1	0.98	0.08	-	33,33,33,33	0
56	MG	1A	3015	1/1	0.97	0.16	-	37,37,37,37	0
56	MG	1A	3233	1/1	0.96	0.44	-	35,35,35,35	0
56	MG	1A	3364	1/1	0.98	0.14	-	23,23,23,23	0
56	MG	2A	3334	1/1	0.93	0.28	-	58,58,58,58	0
56	MG	2B	3017	1/1	0.90	0.20	-	61,61,61,61	0
56	MG	1a	3127	1/1	0.97	0.08	-	48,48,48,48	0
56	MG	1a	3076	1/1	0.90	0.17	-	48,48,48,48	0
56	MG	2A	3468	1/1	0.86	0.11	-	40,40,40,40	0
56	MG	1a	3176	1/1	0.91	0.10	-	59,59,59,59	0
56	MG	1A	3782	1/1	0.95	0.09	-	34,34,34,34	0
56	MG	2A	3548	1/1	0.97	0.13	-	51,51,51,51	0
56	MG	1a	3104	1/1	0.93	0.17	-	45,45,45,45	0
56	MG	1a	3129	1/1	0.69	0.15	-	65,65,65,65	0
56	MG	2A	3579	1/1	0.95	0.09	-	51,51,51,51	0
56	MG	2A	3195	1/1	0.91	0.28	-	50,50,50,50	0
56	MG	1A	3139	1/1	0.96	0.19	-	21,21,21,21	0
56	MG	2A	3213	1/1	0.88	0.11	-	50,50,50,50	0
56	MG	2A	3494	1/1	0.95	0.26	-	49,49,49,49	0
56	MG	1A	3255	1/1	0.97	0.11	-	36,36,36,36	0
56	MG	1A	3296	1/1	0.90	0.12	-	37,37,37,37	0
56	MG	2a	1703	1/1	0.98	0.12	-	41,41,41,41	0
56	MG	1A	3284	1/1	0.92	0.20	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	1V	203	1/1	0.95	0.21	-	63,63,63,63	0
56	MG	2A	3278	1/1	0.94	0.14	-	57,57,57,57	0
56	MG	1A	3985	1/1	0.92	0.17	-	60,60,60,60	0
56	MG	1A	3667	1/1	0.98	0.18	-	31,31,31,31	0
56	MG	2A	3031	1/1	0.74	0.28	-	57,57,57,57	0
56	MG	2A	3166	1/1	0.88	0.13	-	47,47,47,47	0
56	MG	2g	8001	1/1	0.86	0.15	-	59,59,59,59	0
56	MG	1B	215	1/1	0.94	0.06	-	34,34,34,34	0
56	MG	2x	101	1/1	0.86	0.12	-	52,52,52,52	0
56	MG	2a	1657	1/1	0.91	0.16	-	36,36,36,36	0
56	MG	1A	3595	1/1	0.91	0.14	-	40,40,40,40	0
56	MG	2A	3527	1/1	0.97	0.18	-	52,52,52,52	0
56	MG	1A	3804	1/1	0.81	0.16	-	45,45,45,45	0
56	MG	1A	3645	1/1	0.98	0.11	-	25,25,25,25	0
56	MG	2A	3313	1/1	0.91	0.19	-	41,41,41,41	0
56	MG	2x	104	1/1	0.84	0.13	-	64,64,64,64	0
56	MG	1A	3596	1/1	0.93	0.19	-	44,44,44,44	0
56	MG	2A	3678	1/1	0.94	0.21	-	71,71,71,71	0
56	MG	1A	3874	1/1	0.96	0.16	-	36,36,36,36	0
56	MG	1A	3133	1/1	0.88	0.22	-	43,43,43,43	0
56	MG	1A	3201	1/1	0.67	0.51	-	42,42,42,42	0
56	MG	2A	3116	1/1	0.92	0.11	-	55,55,55,55	0
56	MG	1A	3490	1/1	0.98	0.15	-	26,26,26,26	0
56	MG	2A	3362	1/1	0.97	0.09	-	58,58,58,58	0
56	MG	2A	3157	1/1	0.94	0.11	-	51,51,51,51	0
56	MG	1B	203	1/1	0.94	0.20	-	39,39,39,39	0
56	MG	1A	3904	1/1	0.83	0.15	-	71,71,71,71	0
56	MG	2A	3358	1/1	0.90	0.14	-	47,47,47,47	0
56	MG	2a	1625	1/1	0.96	0.10	-	67,67,67,67	0
56	MG	2A	3168	1/1	0.93	0.11	-	39,39,39,39	0
56	MG	1A	3318	1/1	0.98	0.20	-	46,46,46,46	0
56	MG	1A	3138	1/1	0.97	0.46	-	30,30,30,30	0
56	MG	1A	3538	1/1	0.97	0.06	-	45,45,45,45	0
56	MG	2v	3002	1/1	0.74	0.54	-	67,67,67,67	0
56	MG	1A	3741	1/1	0.87	0.11	-	40,40,40,40	0
56	MG	1A	3858	1/1	0.97	0.17	-	54,54,54,54	0
56	MG	2a	1795	1/1	0.93	0.37	-	64,64,64,64	0
56	MG	1A	3432	1/1	0.89	0.15	-	31,31,31,31	0
56	MG	1A	3672	1/1	0.84	0.22	-	68,68,68,68	0
56	MG	1A	3570	1/1	0.93	0.19	-	57,57,57,57	0
56	MG	1A	3913	1/1	0.95	0.25	-	39,39,39,39	0
56	MG	1a	3044	1/1	0.89	0.15	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	1A	3665	1/1	0.97	0.13	-	12,12,12,12	0
56	MG	2A	3575	1/1	0.97	0.12	-	46,46,46,46	0
56	MG	1A	3027	1/1	0.90	0.36	-	27,27,27,27	0
56	MG	1B	238	1/1	0.97	0.10	-	23,23,23,23	0
56	MG	2A	3112	1/1	0.94	0.12	-	52,52,52,52	0
56	MG	2A	3649	1/1	0.99	0.13	-	21,21,21,21	0
56	MG	1A	3317	1/1	0.89	0.47	-	45,45,45,45	0
56	MG	2A	3340	1/1	0.94	0.19	-	30,30,30,30	0
56	MG	2A	3421	1/1	0.94	0.10	-	39,39,39,39	0
56	MG	1A	3386	1/1	0.93	0.10	-	33,33,33,33	0
56	MG	2a	1825	1/1	0.96	0.17	-	56,56,56,56	0
56	MG	1a	3119	1/1	0.96	0.15	-	52,52,52,52	0
56	MG	1A	3193	1/1	0.95	0.19	-	30,30,30,30	0
56	MG	1A	3700	1/1	0.92	0.09	-	27,27,27,27	0
56	MG	2d	503	1/1	0.94	0.12	-	56,56,56,56	0
56	MG	1A	3244	1/1	0.93	0.24	-	34,34,34,34	0
56	MG	1A	3872	1/1	0.93	0.33	-	27,27,27,27	0
56	MG	1A	3119	1/1	0.96	0.18	-	49,49,49,49	0
56	MG	20	3002	1/1	0.89	0.07	-	52,52,52,52	0
56	MG	1x	101	1/1	0.88	0.19	-	54,54,54,54	0
56	MG	1A	3693	1/1	0.98	0.12	-	40,40,40,40	0
56	MG	2A	3197	1/1	0.94	0.14	-	39,39,39,39	0
56	MG	2A	3096	1/1	0.98	0.09	-	42,42,42,42	0
56	MG	2a	1816	1/1	0.97	0.15	-	48,48,48,48	0
56	MG	2A	3305	1/1	0.93	0.15	-	51,51,51,51	0
56	MG	1a	3130	1/1	0.87	0.14	-	46,46,46,46	0
56	MG	1A	3418	1/1	0.95	0.56	-	30,30,30,30	0
56	MG	2A	3207	1/1	0.89	0.28	-	40,40,40,40	0
56	MG	2A	3316	1/1	0.92	0.15	-	53,53,53,53	0
56	MG	2a	1708	1/1	0.89	0.14	-	61,61,61,61	0
56	MG	1A	3806	1/1	0.96	0.11	-	45,45,45,45	0
56	MG	1A	3166	1/1	0.82	0.37	-	31,31,31,31	0
56	MG	2A	3140	1/1	0.78	0.22	-	60,60,60,60	0
56	MG	1A	3326	1/1	0.94	0.17	-	25,25,25,25	0
56	MG	1A	3939	1/1	0.86	0.15	-	44,44,44,44	0
56	MG	1A	3365	1/1	0.93	0.21	-	39,39,39,39	0
56	MG	2a	1620	1/1	0.87	0.21	-	64,64,64,64	0
56	MG	1A	3743	1/1	0.91	0.20	-	42,42,42,42	0
56	MG	1A	3706	1/1	0.94	0.11	-	27,27,27,27	0
56	MG	2a	1809	1/1	0.95	0.15	-	58,58,58,58	0
56	MG	1a	3154	1/1	0.82	0.10	-	59,59,59,59	0
56	MG	1A	3740	1/1	0.95	0.15	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2B	3019	1/1	0.85	0.30	-	82,82,82,82	0
56	MG	1A	3278	1/1	0.96	0.18	-	40,40,40,40	0
56	MG	2a	1640	1/1	0.36	0.22	-	62,62,62,62	0
56	MG	1A	3360	1/1	0.96	0.18	-	32,32,32,32	0
56	MG	2A	3538	1/1	0.91	0.28	-	49,49,49,49	0
56	MG	2A	3391	1/1	0.96	0.14	-	41,41,41,41	0
56	MG	2A	3582	1/1	0.90	0.14	-	44,44,44,44	0
56	MG	1Q	204	1/1	0.86	0.17	-	41,41,41,41	0
56	MG	2A	3428	1/1	0.97	0.17	-	43,43,43,43	0
56	MG	1A	3832	1/1	0.87	0.13	-	69,69,69,69	0
56	MG	2A	3396	1/1	0.89	0.14	-	29,29,29,29	0
56	MG	1A	3651	1/1	0.98	0.12	-	22,22,22,22	0
56	MG	1A	3770	1/1	0.98	0.16	-	12,12,12,12	0
56	MG	1A	3725	1/1	0.96	0.17	-	30,30,30,30	0
56	MG	1A	3864	1/1	0.98	0.23	-	20,20,20,20	0
56	MG	1A	3429	1/1	0.91	0.38	-	29,29,29,29	0
56	MG	1A	3681	1/1	0.91	0.12	-	23,23,23,23	0
56	MG	1a	3147	1/1	0.94	0.05	-	58,58,58,58	0
56	MG	1a	3085	1/1	0.96	0.21	-	33,33,33,33	0
56	MG	1A	3439	1/1	0.88	0.31	-	37,37,37,37	0
56	MG	2a	1786	1/1	0.91	0.12	-	66,66,66,66	0
56	MG	2a	1634	1/1	0.92	0.11	-	59,59,59,59	0
56	MG	2w	103	1/1	0.96	0.09	-	44,44,44,44	0
56	MG	2A	3022	1/1	0.92	0.18	-	38,38,38,38	0
56	MG	1A	3228	1/1	0.94	0.29	-	40,40,40,40	0
56	MG	1A	3816	1/1	0.96	0.27	-	46,46,46,46	0
56	MG	1A	3239	1/1	0.93	0.28	-	38,38,38,38	0
56	MG	1D	303	1/1	0.91	0.27	-	26,26,26,26	0
56	MG	1A	3620	1/1	0.91	0.11	-	49,49,49,49	0
56	MG	1A	3263	1/1	0.89	0.09	-	48,48,48,48	0
56	MG	2A	3237	1/1	0.95	0.15	-	43,43,43,43	0
56	MG	2r	3002	1/1	0.77	0.14	-	64,64,64,64	0
56	MG	2a	1680	1/1	0.95	0.16	-	45,45,45,45	0
56	MG	2a	1775	1/1	0.92	0.15	-	74,74,74,74	0
56	MG	2E	308	1/1	0.97	0.09	-	49,49,49,49	0
56	MG	2A	3525	1/1	0.96	0.27	-	52,52,52,52	0
56	MG	2y	3003	1/1	0.76	0.13	-	59,59,59,59	0
56	MG	1A	3629	1/1	0.95	0.22	-	60,60,60,60	0
56	MG	2a	1612	1/1	0.86	0.11	-	58,58,58,58	0
56	MG	2A	3584	1/1	0.92	0.32	-	50,50,50,50	0
56	MG	2A	3160	1/1	0.80	0.17	-	47,47,47,47	0
56	MG	1a	3193	1/1	0.92	0.16	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3103	1/1	0.95	0.25	-	33,33,33,33	0
56	MG	1A	3169	1/1	0.87	0.13	-	53,53,53,53	0
56	MG	2A	3036	1/1	0.91	0.19	-	48,48,48,48	0
56	MG	11	103	1/1	0.95	0.08	-	31,31,31,31	0
56	MG	2a	1798	1/1	0.92	0.14	-	60,60,60,60	0
56	MG	2A	3726	1/1	0.95	0.17	-	43,43,43,43	0
56	MG	1A	3636	1/1	0.99	0.16	-	21,21,21,21	0
56	MG	1A	3788	1/1	0.95	0.10	-	25,25,25,25	0
56	MG	2A	3566	1/1	0.95	0.13	-	56,56,56,56	0
56	MG	2a	1735	1/1	0.97	0.18	-	50,50,50,50	0
56	MG	2B	3002	1/1	0.75	0.38	-	62,62,62,62	0
56	MG	2a	1712	1/1	0.96	0.09	-	63,63,63,63	0
56	MG	2A	3623	1/1	0.94	0.27	-	46,46,46,46	0
56	MG	1a	3182	1/1	0.96	0.15	-	45,45,45,45	0
56	MG	2a	1824	1/1	0.89	0.18	-	63,63,63,63	0
56	MG	2A	3249	1/1	0.88	0.14	-	54,54,54,54	0
56	MG	1A	3715	1/1	0.93	0.10	-	23,23,23,23	0
56	MG	2A	3590	1/1	0.92	0.15	-	50,50,50,50	0
56	MG	1A	3742	1/1	0.97	0.14	-	28,28,28,28	0
56	MG	1A	3392	1/1	0.97	0.09	-	38,38,38,38	0
56	MG	1A	4058	1/1	0.95	0.24	-	69,69,69,69	0
56	MG	1x	103	1/1	0.85	0.27	-	54,54,54,54	0
56	MG	2A	3184	1/1	0.93	0.30	-	52,52,52,52	0
56	MG	2A	3025	1/1	0.92	0.26	-	54,54,54,54	0
56	MG	1A	3155	1/1	0.97	0.14	-	29,29,29,29	0
56	MG	1A	3850	1/1	0.97	0.40	-	43,43,43,43	0
56	MG	1A	3859	1/1	0.90	0.12	-	61,61,61,61	0
56	MG	2A	3636	1/1	0.75	0.18	-	55,55,55,55	0
56	MG	1A	3963	1/1	0.96	0.08	-	33,33,33,33	0
56	MG	2A	3427	1/1	0.95	0.08	-	46,46,46,46	0
56	MG	1A	3213	1/1	0.96	0.18	-	36,36,36,36	0
56	MG	1D	313	1/1	0.77	0.21	-	52,52,52,52	0
56	MG	2A	3638	1/1	0.83	0.16	-	66,66,66,66	0
56	MG	1A	3371	1/1	0.91	0.23	-	39,39,39,39	0
56	MG	2A	3664	1/1	0.96	0.21	-	41,41,41,41	0
56	MG	1A	3511	1/1	0.92	0.22	-	20,20,20,20	0
56	MG	1A	3402	1/1	0.96	0.08	-	28,28,28,28	0
56	MG	1A	3247	1/1	0.95	0.23	-	27,27,27,27	0
56	MG	1A	4027	1/1	0.88	0.30	-	61,61,61,61	0
56	MG	1A	3250	1/1	0.98	0.31	-	20,20,20,20	0
56	MG	2B	3020	1/1	0.97	0.14	-	54,54,54,54	0
56	MG	1A	3090	1/1	0.97	0.24	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1a	3107	1/1	0.97	0.20	-	39,39,39,39	0
56	MG	2a	1831	1/1	0.95	0.09	-	53,53,53,53	0
56	MG	1A	3813	1/1	0.96	0.16	-	29,29,29,29	0
56	MG	2A	3673	1/1	0.97	0.17	-	47,47,47,47	0
56	MG	2A	3021	1/1	0.87	0.32	-	58,58,58,58	0
56	MG	2A	3547	1/1	0.89	0.25	-	47,47,47,47	0
56	MG	1A	3339	1/1	0.89	0.26	-	48,48,48,48	0
56	MG	1A	3882	1/1	0.78	0.14	-	62,62,62,62	0
56	MG	2A	3181	1/1	0.94	0.16	-	35,35,35,35	0
56	MG	1a	3088	1/1	0.93	0.06	-	57,57,57,57	0
56	MG	1a	3084	1/1	0.85	0.28	-	54,54,54,54	0
56	MG	2A	3130	1/1	0.94	0.20	-	51,51,51,51	0
56	MG	1A	3873	1/1	0.97	0.17	-	42,42,42,42	0
56	MG	2A	3499	1/1	0.95	0.14	-	41,41,41,41	0
56	MG	1A	3241	1/1	0.91	0.14	-	58,58,58,58	0
56	MG	1A	3078	1/1	0.95	0.39	-	26,26,26,26	0
56	MG	2A	3489	1/1	0.91	0.14	-	48,48,48,48	0
56	MG	2A	3242	1/1	0.94	0.13	-	47,47,47,47	0
56	MG	1O	206	1/1	0.93	0.36	-	60,60,60,60	0
56	MG	2A	3399	1/1	0.96	0.20	-	57,57,57,57	0
56	MG	1A	3920	1/1	0.75	0.21	-	39,39,39,39	0
56	MG	1A	3442	1/1	0.97	0.22	-	36,36,36,36	0
56	MG	2A	3171	1/1	0.99	0.05	-	51,51,51,51	0
56	MG	1A	3024	1/1	0.92	0.12	-	32,32,32,32	0
56	MG	2A	3722	1/1	0.93	0.14	-	47,47,47,47	0
56	MG	25	503	1/1	0.90	0.41	-	40,40,40,40	0
56	MG	2A	3019	1/1	0.99	0.19	-	50,50,50,50	0
56	MG	2A	3231	1/1	0.86	0.31	-	49,49,49,49	0
56	MG	2A	3656	1/1	0.90	0.08	-	68,68,68,68	0
56	MG	2A	3544	1/1	0.86	0.24	-	30,30,30,30	0
56	MG	2A	3537	1/1	0.96	0.15	-	46,46,46,46	0
56	MG	1A	3132	1/1	0.97	0.15	-	37,37,37,37	0
56	MG	1a	3156	1/1	0.91	0.16	-	50,50,50,50	0
56	MG	1A	3943	1/1	0.94	0.16	-	38,38,38,38	0
56	MG	2v	3004	1/1	0.88	0.19	-	73,73,73,73	0
56	MG	1A	3106	1/1	0.87	0.54	-	24,24,24,24	0
56	MG	2A	3261	1/1	0.81	0.20	-	50,50,50,50	0
56	MG	1A	3301	1/1	0.93	0.12	-	39,39,39,39	0
56	MG	1A	3194	1/1	0.92	0.21	-	35,35,35,35	0
56	MG	2a	1739	1/1	0.93	0.14	-	57,57,57,57	0
56	MG	2A	3725	1/1	0.95	0.13	-	47,47,47,47	0
56	MG	1A	3769	1/1	0.92	0.16	-	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3217	1/1	0.91	0.28	-	51,51,51,51	0
56	MG	1A	3602	1/1	0.98	0.09	-	48,48,48,48	0
56	MG	1A	3327	1/1	0.95	0.18	-	10,10,10,10	0
56	MG	1a	3148	1/1	0.94	0.09	-	55,55,55,55	0
56	MG	2A	3700	1/1	0.96	0.06	-	61,61,61,61	0
56	MG	2A	3016	1/1	0.97	0.20	-	32,32,32,32	0
56	MG	1A	3600	1/1	0.95	0.26	-	50,50,50,50	0
56	MG	2A	3152	1/1	0.94	0.18	-	45,45,45,45	0
56	MG	1A	3004	1/1	0.94	0.16	-	21,21,21,21	0
56	MG	2A	3557	1/1	0.98	0.24	-	27,27,27,27	0
56	MG	2a	1785	1/1	0.94	0.15	-	63,63,63,63	0
56	MG	2A	3532	1/1	0.90	0.18	-	62,62,62,62	0
56	MG	1A	3415	1/1	0.89	0.46	-	38,38,38,38	0
56	MG	1A	3013	1/1	0.98	0.10	-	14,14,14,14	0
56	MG	2A	3205	1/1	0.84	0.15	-	55,55,55,55	0
56	MG	1A	3610	1/1	0.97	0.17	-	45,45,45,45	0
56	MG	1A	3997	1/1	0.89	0.20	-	45,45,45,45	0
56	MG	2A	3413	1/1	0.95	0.16	-	55,55,55,55	0
56	MG	1A	3348	1/1	0.98	0.13	-	44,44,44,44	0
56	MG	1A	3500	1/1	0.91	0.16	-	20,20,20,20	0
56	MG	2A	3695	1/1	0.89	0.25	-	58,58,58,58	0
56	MG	1A	3367	1/1	0.82	0.22	-	46,46,46,46	0
56	MG	2a	1781	1/1	0.96	0.10	-	67,67,67,67	0
56	MG	1A	3467	1/1	0.95	0.27	-	49,49,49,49	0
56	MG	2A	3004	1/1	0.94	0.14	-	37,37,37,37	0
56	MG	1A	3790	1/1	0.94	0.37	-	27,27,27,27	0
56	MG	2a	1648	1/1	0.83	0.23	-	63,63,63,63	0
56	MG	11	101	1/1	0.97	0.12	-	28,28,28,28	0
56	MG	2A	3111	1/1	0.90	0.21	-	36,36,36,36	0
56	MG	2A	3753	1/1	0.89	0.55	-	52,52,52,52	0
56	MG	1A	3066	1/1	0.96	0.06	-	22,22,22,22	0
56	MG	17	102	1/1	0.93	0.30	-	31,31,31,31	0
56	MG	2A	3286	1/1	0.87	0.17	-	46,46,46,46	0
56	MG	1a	3072	1/1	0.93	0.09	-	54,54,54,54	0
56	MG	1A	3834	1/1	0.76	0.16	-	51,51,51,51	0
56	MG	2a	1667	1/1	0.82	0.16	-	61,61,61,61	0
56	MG	1A	3727	1/1	0.98	0.05	-	42,42,42,42	0
56	MG	1A	3185	1/1	0.95	0.15	-	26,26,26,26	0
57	K	2A	3327	1/1	0.97	0.11	-	29,29,29,29	0
56	MG	2A	3274	1/1	0.94	0.29	-	45,45,45,45	0
56	MG	2A	3534	1/1	0.98	0.11	-	53,53,53,53	0
56	MG	1a	3162	1/1	0.81	0.22	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1B	209	1/1	0.90	0.09	-	53,53,53,53	0
56	MG	1a	3166	1/1	0.93	0.08	-	49,49,49,49	0
56	MG	1A	3494	1/1	0.95	0.11	-	35,35,35,35	0
56	MG	1A	3064	1/1	0.98	0.11	-	12,12,12,12	0
56	MG	2A	3400	1/1	0.90	0.25	-	72,72,72,72	0
56	MG	1A	3044	1/1	0.78	0.16	-	37,37,37,37	0
56	MG	1A	3170	1/1	0.90	0.08	-	63,63,63,63	0
56	MG	2a	1821	1/1	0.91	0.18	-	66,66,66,66	0
56	MG	2a	1737	1/1	0.93	0.04	-	57,57,57,57	0
56	MG	1A	3453	1/1	0.90	0.38	-	41,41,41,41	0
56	MG	2A	3154	1/1	0.94	0.32	-	51,51,51,51	0
56	MG	1A	3246	1/1	0.84	0.13	-	37,37,37,37	0
57	K	1A	4028	1/1	0.96	0.10	-	40,40,40,40	0
56	MG	2A	3626	1/1	0.94	0.16	-	46,46,46,46	0
56	MG	1A	3529	1/1	0.98	0.09	-	34,34,34,34	0
56	MG	1A	3445	1/1	0.92	0.10	-	47,47,47,47	0
56	MG	2a	1810	1/1	0.96	0.15	-	81,81,81,81	0
56	MG	1A	3612	1/1	0.99	0.09	-	24,24,24,24	0
56	MG	2A	3708	1/1	0.91	0.17	-	63,63,63,63	0
56	MG	1B	213	1/1	0.80	0.85	-	55,55,55,55	0
56	MG	1A	3688	1/1	0.96	0.20	-	21,21,21,21	0
56	MG	2A	3149	1/1	0.97	0.27	-	57,57,57,57	0
56	MG	1A	3352	1/1	0.94	0.18	-	36,36,36,36	0
56	MG	2A	3422	1/1	0.96	0.19	-	49,49,49,49	0
56	MG	1a	3195	1/1	0.96	0.06	-	45,45,45,45	0
56	MG	1R	205	1/1	0.94	0.10	-	34,34,34,34	0
56	MG	2A	3714	1/1	0.85	0.14	-	50,50,50,50	0
56	MG	1A	3958	1/1	0.91	0.17	-	32,32,32,32	0
56	MG	1A	3149	1/1	0.96	0.60	-	28,28,28,28	0
56	MG	1A	3332	1/1	0.90	0.11	-	34,34,34,34	0
56	MG	1a	3020	1/1	0.88	0.09	-	47,47,47,47	0
56	MG	1A	3713	1/1	0.89	0.11	-	48,48,48,48	0
56	MG	1A	3860	1/1	0.93	0.27	-	54,54,54,54	0
56	MG	1A	3025	1/1	0.92	0.27	-	42,42,42,42	0
56	MG	2A	3747	1/1	0.82	0.17	-	35,35,35,35	0
56	MG	1A	3953	1/1	0.93	0.15	-	40,40,40,40	0
56	MG	1A	3270	1/1	0.97	0.09	-	31,31,31,31	0
56	MG	1A	3584	1/1	0.89	0.14	-	44,44,44,44	0
56	MG	2A	3491	1/1	0.77	0.13	-	75,75,75,75	0
56	MG	2A	3319	1/1	0.95	0.13	-	62,62,62,62	0
56	MG	2A	3266	1/1	0.78	0.11	-	54,54,54,54	0
56	MG	2A	3256	1/1	0.79	0.18	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1B	233	1/1	0.95	0.13	-	50,50,50,50	0
56	MG	1A	3295	1/1	0.96	0.11	-	38,38,38,38	0
56	MG	2B	3001	1/1	0.89	0.56	-	75,75,75,75	0
56	MG	2A	3505	1/1	0.99	0.08	-	42,42,42,42	0
56	MG	2a	1669	1/1	0.93	0.23	-	56,56,56,56	0
56	MG	1A	3190	1/1	0.92	0.08	-	43,43,43,43	0
56	MG	1A	3797	1/1	0.90	0.19	-	33,33,33,33	0
56	MG	2A	3490	1/1	0.92	0.07	-	72,72,72,72	0
56	MG	1a	3173	1/1	0.96	0.18	-	39,39,39,39	0
56	MG	1A	3983	1/1	0.98	0.16	-	32,32,32,32	0
56	MG	18	103	1/1	0.95	0.23	-	41,41,41,41	0
56	MG	1A	3833	1/1	0.95	0.14	-	58,58,58,58	0
56	MG	2A	3679	1/1	0.95	0.15	-	49,49,49,49	0
56	MG	1a	3163	1/1	0.95	0.17	-	47,47,47,47	0
56	MG	1A	3883	1/1	0.78	0.21	-	59,59,59,59	0
56	MG	2A	3117	1/1	0.88	0.21	-	61,61,61,61	0
56	MG	2A	3613	1/1	0.90	0.11	-	61,61,61,61	0
56	MG	2A	3581	1/1	0.91	0.12	-	28,28,28,28	0
56	MG	1a	3159	1/1	0.93	0.14	-	41,41,41,41	0
56	MG	2A	3170	1/1	0.90	0.21	-	44,44,44,44	0
56	MG	1A	3131	1/1	0.98	0.12	-	35,35,35,35	0
56	MG	1A	3292	1/1	0.92	0.17	-	43,43,43,43	0
56	MG	2A	3663	1/1	0.93	0.17	-	47,47,47,47	0
56	MG	1A	3400	1/1	0.96	0.17	-	33,33,33,33	0
56	MG	2A	3263	1/1	0.83	0.19	-	54,54,54,54	0
56	MG	1A	3358	1/1	0.97	0.13	-	44,44,44,44	0
56	MG	2a	1617	1/1	0.80	0.15	-	73,73,73,73	0
56	MG	1A	3290	1/1	0.96	0.10	-	46,46,46,46	0
56	MG	2A	3705	1/1	0.90	0.19	-	64,64,64,64	0
56	MG	1A	3509	1/1	0.97	0.18	-	31,31,31,31	0
56	MG	2A	3531	1/1	0.94	0.11	-	60,60,60,60	0
56	MG	1A	3654	1/1	0.98	0.14	-	37,37,37,37	0
56	MG	1A	3127	1/1	0.90	0.15	-	37,37,37,37	0
56	MG	2A	3310	1/1	0.96	0.11	-	58,58,58,58	0
56	MG	2A	3690	1/1	0.88	0.14	-	58,58,58,58	0
56	MG	1A	3172	1/1	0.93	0.40	-	44,44,44,44	0
56	MG	1A	3003	1/1	0.98	0.20	-	19,19,19,19	0
56	MG	2A	3674	1/1	0.98	0.22	-	23,23,23,23	0
56	MG	1A	3001	1/1	0.98	0.09	-	32,32,32,32	0
56	MG	1a	3149	1/1	0.81	0.55	-	76,76,76,76	0
56	MG	2A	3441	1/1	0.88	0.14	-	62,62,62,62	0
56	MG	2A	3416	1/1	0.93	0.13	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1B	235	1/1	0.95	0.17	-	55,55,55,55	0
56	MG	2a	1639	1/1	0.88	0.21	-	60,60,60,60	0
56	MG	1A	3722	1/1	0.95	0.14	-	29,29,29,29	0
56	MG	2A	3616	1/1	0.85	0.12	-	51,51,51,51	0
56	MG	2A	3517	1/1	0.93	0.09	-	51,51,51,51	0
56	MG	1a	3087	1/1	0.95	0.18	-	44,44,44,44	0
56	MG	2a	1760	1/1	0.93	0.24	-	60,60,60,60	0
56	MG	1A	3695	1/1	0.94	0.21	-	50,50,50,50	0
56	MG	1A	3306	1/1	0.89	0.15	-	43,43,43,43	0
56	MG	1A	3407	1/1	0.94	0.08	-	45,45,45,45	0
56	MG	1a	3052	1/1	0.93	0.10	-	58,58,58,58	0
56	MG	2A	3741	1/1	0.99	0.11	-	39,39,39,39	0
56	MG	2a	1817	1/1	0.95	0.16	-	51,51,51,51	0
56	MG	2A	3224	1/1	0.93	0.16	-	54,54,54,54	0
56	MG	1A	3684	1/1	0.96	0.12	-	44,44,44,44	0
56	MG	2A	3347	1/1	0.90	0.10	-	53,53,53,53	0
56	MG	1f	3001	1/1	0.97	0.11	-	31,31,31,31	0
56	MG	1A	3731	1/1	0.95	0.22	-	16,16,16,16	0
56	MG	2F	301	1/1	0.92	0.16	-	35,35,35,35	0
56	MG	25	504	1/1	0.89	0.36	-	67,67,67,67	0
56	MG	1A	3235	1/1	0.96	0.14	-	22,22,22,22	0
56	MG	2A	3529	1/1	0.90	0.24	-	59,59,59,59	0
56	MG	1A	4015	1/1	0.89	0.19	-	55,55,55,55	0
56	MG	1A	3970	1/1	0.92	0.05	-	53,53,53,53	0
56	MG	2A	3386	1/1	0.91	0.24	-	43,43,43,43	0
56	MG	2A	3652	1/1	0.92	0.16	-	38,38,38,38	0
56	MG	2A	3450	1/1	0.99	0.14	-	37,37,37,37	0
56	MG	2a	1790	1/1	0.98	0.21	-	50,50,50,50	0
56	MG	1a	3047	1/1	0.90	0.28	-	46,46,46,46	0
56	MG	2a	1641	1/1	0.89	0.13	-	53,53,53,53	0
56	MG	1a	3128	1/1	0.93	0.09	-	50,50,50,50	0
56	MG	2A	3549	1/1	0.95	0.15	-	43,43,43,43	0
56	MG	1A	3789	1/1	0.82	0.21	-	44,44,44,44	0
56	MG	1A	3283	1/1	0.88	0.33	-	28,28,28,28	0
56	MG	1A	3487	1/1	0.94	0.13	-	34,34,34,34	0
56	MG	1A	4021	1/1	0.90	0.14	-	47,47,47,47	0
56	MG	1A	4010	1/1	0.97	0.13	-	23,23,23,23	0
56	MG	2y	3007	1/1	0.88	0.14	-	81,81,81,81	0
56	MG	2A	3601	1/1	0.94	0.09	-	53,53,53,53	0
56	MG	2A	3291	1/1	0.98	0.12	-	55,55,55,55	0
56	MG	17	104	1/1	0.98	0.08	-	27,27,27,27	0
56	MG	1A	3159	1/1	0.94	0.34	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1a	3117	1/1	0.93	0.09	-	27,27,27,27	0
56	MG	1A	3732	1/1	0.98	0.07	-	45,45,45,45	0
56	MG	1A	3518	1/1	0.97	0.11	-	41,41,41,41	0
56	MG	2A	3480	1/1	0.90	0.21	-	47,47,47,47	0
56	MG	2A	3561	1/1	0.97	0.18	-	56,56,56,56	0
56	MG	1A	3901	1/1	0.95	0.30	-	44,44,44,44	0
56	MG	2a	1815	1/1	0.85	0.16	-	61,61,61,61	0
56	MG	2a	1765	1/1	0.91	0.14	-	64,64,64,64	0
56	MG	15	103	1/1	0.96	0.46	-	25,25,25,25	0
56	MG	2A	3079	1/1	0.93	0.09	-	57,57,57,57	0
56	MG	1A	3587	1/1	0.98	0.10	-	12,12,12,12	0
56	MG	2A	3088	1/1	0.79	0.15	-	40,40,40,40	0
56	MG	2A	3614	1/1	0.93	0.12	-	51,51,51,51	0
56	MG	2a	1753	1/1	0.96	0.15	-	45,45,45,45	0
56	MG	2A	3556	1/1	0.98	0.20	-	46,46,46,46	0
56	MG	2a	1823	1/1	0.95	0.09	-	53,53,53,53	0
56	MG	1w	103	1/1	0.85	0.36	-	68,68,68,68	0
56	MG	1a	3165	1/1	0.87	0.09	-	60,60,60,60	0
56	MG	1A	4048	1/1	0.82	0.64	-	31,31,31,31	0
56	MG	2A	3735	1/1	0.90	0.35	-	45,45,45,45	0
56	MG	2A	3199	1/1	0.93	0.12	-	53,53,53,53	0
56	MG	1l	202	1/1	0.81	0.16	-	85,85,85,85	0
56	MG	1A	3752	1/1	0.96	0.44	-	36,36,36,36	0
56	MG	2A	3675	1/1	0.94	0.09	-	62,62,62,62	0
56	MG	2A	3574	1/1	0.95	0.07	-	46,46,46,46	0
56	MG	1A	3073	1/1	0.94	0.48	-	42,42,42,42	0
56	MG	2r	3001	1/1	0.97	0.15	-	56,56,56,56	0
56	MG	27	101	1/1	0.81	0.34	-	44,44,44,44	0
56	MG	1A	3690	1/1	0.97	0.10	-	42,42,42,42	0
56	MG	1A	3992	1/1	0.94	0.18	-	49,49,49,49	0
56	MG	2A	3671	1/1	0.97	0.18	-	29,29,29,29	0
56	MG	1A	3324	1/1	0.95	0.13	-	33,33,33,33	0
56	MG	1A	3319	1/1	0.76	0.23	-	53,53,53,53	0
56	MG	1A	3896	1/1	0.98	0.20	-	42,42,42,42	0
56	MG	1A	3916	1/1	0.88	0.13	-	54,54,54,54	0
56	MG	1B	230	1/1	0.94	0.31	-	42,42,42,42	0
56	MG	1A	3899	1/1	0.95	0.09	-	35,35,35,35	0
56	MG	2A	3106	1/1	0.93	0.08	-	50,50,50,50	0
56	MG	2A	3257	1/1	0.83	0.18	-	57,57,57,57	0
56	MG	1A	3452	1/1	0.97	0.28	-	30,30,30,30	0
56	MG	1A	3387	1/1	0.93	0.20	-	37,37,37,37	0
56	MG	2A	3696	1/1	0.96	0.09	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2B	3018	1/1	0.89	0.85	-	80,80,80,80	0
56	MG	1x	114	1/1	0.89	0.14	-	67,67,67,67	0
56	MG	2A	3743	1/1	0.92	0.19	-	51,51,51,51	0
56	MG	1A	3936	1/1	0.96	0.08	-	49,49,49,49	0
56	MG	1A	3275	1/1	0.97	0.14	-	25,25,25,25	0
56	MG	1A	3738	1/1	0.98	0.09	-	32,32,32,32	0
56	MG	2A	3415	1/1	0.98	0.18	-	47,47,47,47	0
56	MG	2A	3423	1/1	0.97	0.12	-	22,22,22,22	0
56	MG	1A	3956	1/1	0.95	0.07	-	67,67,67,67	0
56	MG	2A	3370	1/1	1.00	0.17	-	44,44,44,44	0
56	MG	1a	3157	1/1	0.93	0.13	-	58,58,58,58	0
56	MG	2A	3496	1/1	0.96	0.11	-	37,37,37,37	0
56	MG	2A	3192	1/1	0.96	0.29	-	54,54,54,54	0
56	MG	2Z	8001	1/1	0.86	0.25	-	73,73,73,73	0
56	MG	1A	3307	1/1	0.94	0.10	-	49,49,49,49	0
56	MG	10	103	1/1	0.93	0.15	-	54,54,54,54	0
56	MG	2E	307	1/1	0.87	0.20	-	60,60,60,60	0
56	MG	2A	3128	1/1	0.81	0.26	-	35,35,35,35	0
56	MG	2A	3644	1/1	0.92	0.14	-	57,57,57,57	0
56	MG	2a	1729	1/1	0.92	0.10	-	61,61,61,61	0
56	MG	1F	308	1/1	0.90	0.11	-	42,42,42,42	0
56	MG	2x	103	1/1	0.80	0.22	-	63,63,63,63	0
56	MG	1A	3718	1/1	0.86	0.20	-	39,39,39,39	0
56	MG	1a	3065	1/1	0.95	0.15	-	41,41,41,41	0
56	MG	1A	3972	1/1	0.98	0.15	-	49,49,49,49	0
56	MG	28	102	1/1	0.73	0.14	-	64,64,64,64	0
56	MG	2A	3082	1/1	0.87	0.18	-	69,69,69,69	0
56	MG	2A	3403	1/1	0.96	0.26	-	29,29,29,29	0
56	MG	1A	3613	1/1	0.95	0.10	-	30,30,30,30	0
56	MG	1A	3128	1/1	0.97	0.31	-	27,27,27,27	0
56	MG	1a	3197	1/1	0.94	0.10	-	39,39,39,39	0
56	MG	1B	201	1/1	0.95	0.10	-	49,49,49,49	0
56	MG	1A	3227	1/1	0.82	0.13	-	49,49,49,49	0
56	MG	2a	1724	1/1	0.86	0.11	-	73,73,73,73	0
56	MG	2A	3010	1/1	0.95	0.18	-	31,31,31,31	0
56	MG	1A	4012	1/1	0.87	0.27	-	47,47,47,47	0
56	MG	2A	3189	1/1	0.95	0.07	-	38,38,38,38	0
56	MG	1B	221	1/1	0.95	0.10	-	36,36,36,36	0
56	MG	1a	3050	1/1	0.88	0.12	-	50,50,50,50	0
56	MG	1a	3100	1/1	0.91	0.11	-	61,61,61,61	0
56	MG	1A	3840	1/1	0.97	0.17	-	32,32,32,32	0
56	MG	2A	3528	1/1	0.94	0.08	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3035	1/1	0.90	0.15	-	52,52,52,52	0
56	MG	2A	3065	1/1	0.83	0.16	-	52,52,52,52	0
56	MG	1a	3171	1/1	0.96	0.07	-	55,55,55,55	0
56	MG	2a	1718	1/1	0.95	0.14	-	55,55,55,55	0
56	MG	1A	4053	1/1	0.87	0.45	-	42,42,42,42	0
56	MG	2a	1811	1/1	0.93	0.14	-	71,71,71,71	0
56	MG	2a	1711	1/1	0.91	0.24	-	67,67,67,67	0
56	MG	1a	3060	1/1	0.94	0.07	-	50,50,50,50	0
56	MG	2A	3262	1/1	0.93	0.15	-	44,44,44,44	0
56	MG	2a	1608	1/1	0.94	0.14	-	47,47,47,47	0
56	MG	2A	3147	1/1	0.92	0.28	-	50,50,50,50	0
56	MG	1A	3607	1/1	0.98	0.13	-	19,19,19,19	0
56	MG	2A	3364	1/1	0.97	0.08	-	45,45,45,45	0
56	MG	1A	3594	1/1	0.96	0.32	-	46,46,46,46	0
56	MG	1A	3540	1/1	0.96	0.11	-	46,46,46,46	0
56	MG	2a	1698	1/1	0.98	0.07	-	60,60,60,60	0
56	MG	2a	1666	1/1	0.87	0.10	-	51,51,51,51	0
56	MG	2A	3206	1/1	0.92	0.33	-	42,42,42,42	0
56	MG	1A	3664	1/1	0.95	0.19	-	43,43,43,43	0
56	MG	1A	3536	1/1	0.94	0.08	-	25,25,25,25	0
56	MG	1a	3073	1/1	0.88	0.12	-	59,59,59,59	0
56	MG	1n	502	1/1	0.92	0.13	-	51,51,51,51	0
56	MG	1A	3924	1/1	0.91	0.11	-	34,34,34,34	0
56	MG	1A	3384	1/1	0.94	0.08	-	38,38,38,38	0
56	MG	1A	3855	1/1	0.98	0.04	-	49,49,49,49	0
56	MG	1A	4006	1/1	0.90	0.20	-	41,41,41,41	0
56	MG	1A	3608	1/1	0.91	0.20	-	54,54,54,54	0
56	MG	1A	3176	1/1	0.98	0.44	-	25,25,25,25	0
56	MG	1A	3556	1/1	0.97	0.15	-	20,20,20,20	0
56	MG	2A	3352	1/1	0.96	0.10	-	50,50,50,50	0
56	MG	2a	1756	1/1	0.94	0.13	-	43,43,43,43	0
56	MG	2a	1728	1/1	0.94	0.09	-	46,46,46,46	0
56	MG	1w	111	1/1	0.83	0.13	-	69,69,69,69	0
56	MG	1A	3164	1/1	0.97	0.17	-	12,12,12,12	0
56	MG	1A	3678	1/1	0.97	0.16	-	22,22,22,22	0
56	MG	2A	3350	1/1	0.95	0.13	-	50,50,50,50	0
56	MG	2A	3158	1/1	0.83	0.32	-	49,49,49,49	0
56	MG	1A	3370	1/1	0.91	0.22	-	37,37,37,37	0
56	MG	2A	3287	1/1	0.94	0.25	-	47,47,47,47	0
56	MG	1A	3841	1/1	0.94	0.14	-	33,33,33,33	0
56	MG	1A	3842	1/1	0.97	0.07	-	34,34,34,34	0
56	MG	1A	3589	1/1	0.97	0.12	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1X	103	1/1	0.94	0.25	-	29,29,29,29	0
56	MG	18	102	1/1	0.94	0.12	-	29,29,29,29	0
56	MG	1A	3987	1/1	0.99	0.23	-	36,36,36,36	0
56	MG	2A	3373	1/1	0.94	0.17	-	25,25,25,25	0
56	MG	1A	3914	1/1	0.82	0.21	-	54,54,54,54	0
56	MG	2A	3723	1/1	0.81	0.31	-	67,67,67,67	0
56	MG	1A	3425	1/1	0.88	0.14	-	34,34,34,34	0
56	MG	1A	3219	1/1	0.92	0.29	-	19,19,19,19	0
56	MG	1A	4002	1/1	0.95	0.15	-	32,32,32,32	0
56	MG	2A	3269	1/1	0.92	0.14	-	36,36,36,36	0
56	MG	1A	3274	1/1	0.94	0.22	-	40,40,40,40	0
56	MG	1a	3187	1/1	0.95	0.06	-	43,43,43,43	0
56	MG	1a	3097	1/1	0.95	0.08	-	62,62,62,62	0
56	MG	1A	3933	1/1	0.93	0.14	-	54,54,54,54	0
56	MG	1m	201	1/1	0.94	0.10	-	57,57,57,57	0
56	MG	1A	3754	1/1	0.98	0.22	-	22,22,22,22	0
56	MG	1y	104	1/1	0.95	0.13	-	44,44,44,44	0
56	MG	2A	3572	1/1	0.91	0.22	-	66,66,66,66	0
56	MG	1A	3050	1/1	0.92	0.27	-	45,45,45,45	0
56	MG	1A	3889	1/1	0.92	0.14	-	39,39,39,39	0
56	MG	1A	3504	1/1	0.94	0.08	-	48,48,48,48	0
56	MG	2A	3273	1/1	0.91	0.35	-	57,57,57,57	0
56	MG	1a	3174	1/1	0.91	0.08	-	51,51,51,51	0
56	MG	2A	3279	1/1	0.92	0.10	-	64,64,64,64	0
56	MG	1a	3070	1/1	0.98	0.05	-	30,30,30,30	0
56	MG	2a	1659	1/1	0.97	0.12	-	47,47,47,47	0
56	MG	1A	3475	1/1	0.95	0.27	-	28,28,28,28	0
56	MG	1A	3502	1/1	0.97	0.33	-	20,20,20,20	0
56	MG	2a	1603	1/1	0.81	0.17	-	73,73,73,73	0
56	MG	2A	3433	1/1	0.88	0.19	-	60,60,60,60	0
56	MG	2A	3522	1/1	0.97	0.08	-	49,49,49,49	0
56	MG	2A	3594	1/1	0.98	0.12	-	54,54,54,54	0
56	MG	1A	3514	1/1	0.94	0.17	-	21,21,21,21	0
56	MG	1A	3399	1/1	0.96	0.14	-	42,42,42,42	0
56	MG	2R	3003	1/1	0.96	0.15	-	48,48,48,48	0
56	MG	1A	3829	1/1	0.97	0.17	-	43,43,43,43	0
56	MG	1A	3951	1/1	0.86	0.12	-	62,62,62,62	0
56	MG	1B	236	1/1	0.75	0.30	-	65,65,65,65	0
56	MG	2A	3691	1/1	0.92	0.11	-	68,68,68,68	0
56	MG	1A	4033	1/1	0.96	0.60	-	25,25,25,25	0
56	MG	1A	3391	1/1	0.93	0.16	-	46,46,46,46	0
56	MG	1A	3071	1/1	0.92	0.14	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3069	1/1	0.95	0.23	-	39,39,39,39	0
56	MG	2A	3414	1/1	0.94	0.14	-	49,49,49,49	0
56	MG	1a	3190	1/1	0.91	0.16	-	51,51,51,51	0
56	MG	1A	3545	1/1	0.95	0.15	-	25,25,25,25	0
56	MG	1A	3691	1/1	0.86	0.30	-	55,55,55,55	0
56	MG	1A	3878	1/1	0.92	0.11	-	16,16,16,16	0
56	MG	1A	3982	1/1	0.94	0.23	-	46,46,46,46	0
56	MG	1A	3499	1/1	0.98	0.13	-	23,23,23,23	0
56	MG	2A	3145	1/1	0.93	0.15	-	48,48,48,48	0
56	MG	1a	3168	1/1	0.85	0.15	-	63,63,63,63	0
56	MG	1A	4022	1/1	0.95	0.14	-	46,46,46,46	0
56	MG	2A	3440	1/1	0.98	0.13	-	51,51,51,51	0
56	MG	2a	1660	1/1	0.97	0.13	-	59,59,59,59	0
56	MG	2X	3001	1/1	0.94	0.14	-	46,46,46,46	0
56	MG	2A	3042	1/1	0.91	0.15	-	54,54,54,54	0
56	MG	1A	3548	1/1	0.89	0.14	-	52,52,52,52	0
56	MG	1A	3618	1/1	0.91	0.16	-	55,55,55,55	0
56	MG	2A	3083	1/1	0.86	0.10	-	53,53,53,53	0
56	MG	1a	3046	1/1	0.84	0.09	-	54,54,54,54	0
56	MG	2A	3236	1/1	0.97	0.21	-	49,49,49,49	0
56	MG	1P	203	1/1	0.89	0.42	-	33,33,33,33	0
56	MG	2a	1738	1/1	0.81	0.12	-	71,71,71,71	0
56	MG	2A	3228	1/1	0.89	0.39	-	38,38,38,38	0
56	MG	2O	8001	1/1	0.85	0.20	-	56,56,56,56	0
56	MG	1A	3900	1/1	0.90	0.13	-	44,44,44,44	0
56	MG	1A	3682	1/1	0.95	0.09	-	55,55,55,55	0
56	MG	1A	3200	1/1	0.91	0.15	-	44,44,44,44	0
56	MG	2A	3393	1/1	0.98	0.19	-	44,44,44,44	0
56	MG	1A	3305	1/1	0.75	0.20	-	51,51,51,51	0
56	MG	1A	3931	1/1	0.84	0.22	-	47,47,47,47	0
56	MG	1A	3669	1/1	0.99	0.11	-	35,35,35,35	0
56	MG	1A	3573	1/1	0.98	0.09	-	24,24,24,24	0
56	MG	1w	105	1/1	0.95	0.12	-	64,64,64,64	0
56	MG	11	104	1/1	0.90	0.10	-	59,59,59,59	0
56	MG	2A	3229	1/1	0.82	0.24	-	34,34,34,34	0
56	MG	2A	3241	1/1	0.88	0.18	-	55,55,55,55	0
56	MG	2y	3004	1/1	0.96	0.17	-	36,36,36,36	0
56	MG	1A	3947	1/1	0.89	0.14	-	49,49,49,49	0
56	MG	1A	3409	1/1	0.91	0.15	-	54,54,54,54	0
56	MG	2A	3208	1/1	0.86	0.23	-	49,49,49,49	0
56	MG	1A	3335	1/1	0.94	0.44	-	33,33,33,33	0
56	MG	1A	3694	1/1	0.95	0.08	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3034	1/1	0.96	0.16	-	56,56,56,56	0
56	MG	1A	3069	1/1	0.98	0.26	-	27,27,27,27	0
56	MG	1A	3666	1/1	0.92	0.05	-	50,50,50,50	0
56	MG	1A	3838	1/1	0.92	0.11	-	53,53,53,53	0
56	MG	1A	4019	1/1	0.97	0.27	-	26,26,26,26	0
56	MG	2A	3434	1/1	0.90	0.16	-	46,46,46,46	0
56	MG	2A	3264	1/1	0.95	0.41	-	47,47,47,47	0
56	MG	1A	3635	1/1	0.99	0.22	-	25,25,25,25	0
56	MG	1A	3563	1/1	0.91	0.08	-	35,35,35,35	0
56	MG	1A	3146	1/1	0.95	0.56	-	23,23,23,23	0
56	MG	1A	3272	1/1	0.94	0.12	-	34,34,34,34	0
56	MG	2w	104	1/1	0.95	0.15	-	83,83,83,83	0
56	MG	1A	3437	1/1	0.96	0.11	-	52,52,52,52	0
56	MG	1A	3436	1/1	0.73	0.16	-	62,62,62,62	0
56	MG	1A	3084	1/1	0.98	0.10	-	35,35,35,35	0
56	MG	2D	302	1/1	0.93	0.16	-	39,39,39,39	0
56	MG	1A	3045	1/1	0.97	0.17	-	13,13,13,13	0
56	MG	2a	1705	1/1	0.80	0.13	-	54,54,54,54	0
56	MG	2A	3608	1/1	0.97	0.13	-	48,48,48,48	0
56	MG	2A	3156	1/1	0.87	0.18	-	42,42,42,42	0
56	MG	1A	3460	1/1	0.92	0.10	-	41,41,41,41	0
56	MG	1a	3208	1/1	0.98	0.11	-	42,42,42,42	0
56	MG	1a	3135	1/1	0.94	0.12	-	52,52,52,52	0
56	MG	1A	3421	1/1	0.95	0.46	-	37,37,37,37	0
56	MG	1A	3372	1/1	0.95	0.13	-	35,35,35,35	0
56	MG	2A	3268	1/1	0.96	0.10	-	47,47,47,47	0
56	MG	2A	3225	1/1	0.83	0.18	-	53,53,53,53	0
56	MG	1A	3165	1/1	0.97	0.07	-	31,31,31,31	0
56	MG	2A	3314	1/1	0.94	0.37	-	40,40,40,40	0
56	MG	1A	4051	1/1	0.96	0.22	-	13,13,13,13	0
56	MG	1A	3906	1/1	0.97	0.17	-	60,60,60,60	0
56	MG	1W	3003	1/1	0.95	0.10	-	33,33,33,33	0
56	MG	1A	3826	1/1	0.94	0.16	-	27,27,27,27	0
56	MG	1A	3406	1/1	0.96	0.28	-	48,48,48,48	0
56	MG	2A	3092	1/1	0.90	0.17	-	38,38,38,38	0
56	MG	1A	3823	1/1	0.89	0.13	-	50,50,50,50	0
56	MG	1A	3434	1/1	0.93	0.17	-	47,47,47,47	0
56	MG	1A	3586	1/1	0.89	0.19	-	17,17,17,17	0
56	MG	2a	1604	1/1	0.84	0.16	-	48,48,48,48	0
56	MG	2a	1769	1/1	0.63	0.13	-	75,75,75,75	0
56	MG	2A	3388	1/1	0.97	0.18	-	25,25,25,25	0
56	MG	1A	3466	1/1	0.93	0.17	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	2A	3309	1/1	0.93	0.15	-	52,52,52,52	0
56	MG	1A	3168	1/1	0.94	0.19	-	43,43,43,43	0
56	MG	2A	3043	1/1	0.98	0.10	-	40,40,40,40	0
56	MG	1A	3251	1/1	0.92	0.42	-	25,25,25,25	0
56	MG	2a	1748	1/1	0.89	0.14	-	60,60,60,60	0
56	MG	2A	3185	1/1	0.85	0.19	-	46,46,46,46	0
56	MG	1A	3098	1/1	0.93	0.51	-	36,36,36,36	0
56	MG	1A	3617	1/1	0.96	0.10	-	45,45,45,45	0
56	MG	1A	3080	1/1	0.94	0.24	-	41,41,41,41	0
56	MG	1A	3551	1/1	0.95	0.15	-	17,17,17,17	0
56	MG	2y	3002	1/1	0.98	0.14	-	51,51,51,51	0
56	MG	2a	1674	1/1	0.90	0.20	-	55,55,55,55	0
56	MG	1a	3021	1/1	0.95	0.15	-	40,40,40,40	0
56	MG	1A	3844	1/1	0.81	0.08	-	23,23,23,23	0
56	MG	2a	1784	1/1	0.85	0.11	-	66,66,66,66	0
57	K	1A	3486	1/1	0.98	0.07	-	19,19,19,19	0
56	MG	1a	3017	1/1	0.88	0.20	-	57,57,57,57	0
56	MG	2A	3589	1/1	0.97	0.26	-	45,45,45,45	0
56	MG	2A	3107	1/1	0.95	0.17	-	27,27,27,27	0
56	MG	1A	3828	1/1	0.89	0.19	-	62,62,62,62	0
56	MG	2a	1637	1/1	0.71	0.13	-	52,52,52,52	0
56	MG	1a	3063	1/1	0.92	0.16	-	53,53,53,53	0
56	MG	2A	3153	1/1	0.93	0.16	-	49,49,49,49	0
56	MG	2A	3330	1/1	0.98	0.20	-	42,42,42,42	0
56	MG	2A	3546	1/1	0.87	0.15	-	45,45,45,45	0
56	MG	1A	3242	1/1	0.63	0.26	-	59,59,59,59	0
56	MG	2A	3683	1/1	0.93	0.28	-	42,42,42,42	0
56	MG	2A	3312	1/1	0.84	0.17	-	57,57,57,57	0
56	MG	1A	3405	1/1	0.93	0.60	-	46,46,46,46	0
56	MG	2a	1664	1/1	0.91	0.17	-	56,56,56,56	0
56	MG	1a	3132	1/1	0.95	0.08	-	34,34,34,34	0
56	MG	2A	3190	1/1	0.96	0.13	-	44,44,44,44	0
56	MG	2y	3006	1/1	0.34	0.13	-	88,88,88,88	0
56	MG	1a	3006	1/1	0.82	0.20	-	59,59,59,59	0
56	MG	2A	3078	1/1	0.97	0.10	-	54,54,54,54	0
56	MG	2A	3751	1/1	0.97	0.78	-	44,44,44,44	0
56	MG	1w	102	1/1	0.90	0.10	-	76,76,76,76	0
56	MG	2A	3332	1/1	0.72	0.24	-	56,56,56,56	0
56	MG	1A	3606	1/1	0.94	0.18	-	61,61,61,61	0
56	MG	1A	3851	1/1	0.93	0.18	-	44,44,44,44	0
56	MG	2A	3369	1/1	0.98	0.14	-	53,53,53,53	0
56	MG	2A	3121	1/1	0.94	0.15	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3262	1/1	0.91	0.11	-	33,33,33,33	0
56	MG	2A	3001	1/1	0.89	0.09	-	44,44,44,44	0
56	MG	1A	3675	1/1	0.96	0.15	-	66,66,66,66	0
56	MG	2a	1679	1/1	0.98	0.15	-	44,44,44,44	0
56	MG	1A	3472	1/1	0.92	0.14	-	41,41,41,41	0
56	MG	2a	1645	1/1	0.87	0.61	-	74,74,74,74	0
56	MG	1A	3401	1/1	0.95	0.10	-	38,38,38,38	0
56	MG	2A	3100	1/1	0.95	0.15	-	59,59,59,59	0
56	MG	1B	210	1/1	0.84	0.15	-	50,50,50,50	0
56	MG	1A	3236	1/1	0.97	0.21	-	35,35,35,35	0
56	MG	1A	3730	1/1	0.88	0.35	-	42,42,42,42	0
56	MG	1A	3917	1/1	0.98	0.14	-	31,31,31,31	0
56	MG	1A	3809	1/1	0.98	0.09	-	30,30,30,30	0
56	MG	2a	1646	1/1	0.91	0.13	-	71,71,71,71	0
56	MG	2A	3617	1/1	0.96	0.24	-	43,43,43,43	0
56	MG	2A	3379	1/1	0.98	0.09	-	41,41,41,41	0
56	MG	2a	1742	1/1	0.90	0.08	-	70,70,70,70	0
56	MG	2A	3376	1/1	0.88	0.17	-	45,45,45,45	0
56	MG	1A	3825	1/1	0.92	0.48	-	43,43,43,43	0
56	MG	1A	3424	1/1	0.93	0.56	-	32,32,32,32	0
56	MG	2a	1762	1/1	0.90	0.13	-	52,52,52,52	0
56	MG	1A	3231	1/1	0.92	0.27	-	45,45,45,45	0
56	MG	1A	3839	1/1	0.90	0.14	-	34,34,34,34	0
56	MG	2a	1629	1/1	0.95	0.18	-	73,73,73,73	0
56	MG	1A	3621	1/1	0.86	0.17	-	44,44,44,44	0
56	MG	1A	3314	1/1	0.90	0.34	-	42,42,42,42	0
56	MG	1A	3877	1/1	0.96	0.20	-	28,28,28,28	0
56	MG	1A	3632	1/1	0.98	0.29	-	27,27,27,27	0
56	MG	2A	3064	1/1	0.94	0.45	-	44,44,44,44	0
56	MG	2A	3506	1/1	0.93	0.13	-	48,48,48,48	0
56	MG	2a	1755	1/1	0.86	0.06	-	70,70,70,70	0
56	MG	2A	3119	1/1	0.97	0.12	-	41,41,41,41	0
56	MG	1a	3134	1/1	0.92	0.23	-	47,47,47,47	0
56	MG	1A	3359	1/1	0.96	0.12	-	32,32,32,32	0
56	MG	1A	3144	1/1	0.93	0.13	-	37,37,37,37	0
56	MG	1R	202	1/1	0.96	0.08	-	30,30,30,30	0
56	MG	2a	1610	1/1	0.89	0.81	-	63,63,63,63	0
56	MG	2A	3432	1/1	0.94	0.30	-	56,56,56,56	0
56	MG	1a	3116	1/1	0.93	0.09	-	35,35,35,35	0
56	MG	1a	3090	1/1	0.94	0.07	-	41,41,41,41	0
56	MG	2a	1601	1/1	0.98	0.24	-	46,46,46,46	0
56	MG	1a	3083	1/1	0.85	0.19	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3530	1/1	0.97	0.22	-	25,25,25,25	0
56	MG	1a	3034	1/1	0.98	0.14	-	44,44,44,44	0
56	MG	1G	3005	1/1	0.92	0.08	-	52,52,52,52	0
56	MG	2a	1727	1/1	0.94	0.12	-	87,87,87,87	0
56	MG	1A	3230	1/1	0.82	0.19	-	44,44,44,44	0
56	MG	1A	3482	1/1	0.92	0.28	-	38,38,38,38	0
56	MG	2a	1813	1/1	0.98	0.06	-	54,54,54,54	0
56	MG	1A	3143	1/1	0.85	0.47	-	37,37,37,37	0
56	MG	1A	3376	1/1	0.92	0.23	-	31,31,31,31	0
56	MG	1A	3991	1/1	0.92	0.14	-	66,66,66,66	0
56	MG	2A	3454	1/1	0.95	0.14	-	52,52,52,52	0
56	MG	2A	3665	1/1	0.94	0.11	-	36,36,36,36	0
56	MG	2A	3055	1/1	0.94	0.16	-	44,44,44,44	0
56	MG	1A	3893	1/1	0.97	0.27	-	27,27,27,27	0
56	MG	1A	3591	1/1	0.96	0.16	-	30,30,30,30	0
56	MG	1A	4003	1/1	0.95	0.10	-	32,32,32,32	0
56	MG	1A	3650	1/1	0.95	0.17	-	34,34,34,34	0
56	MG	1A	3345	1/1	0.91	0.17	-	24,24,24,24	0
56	MG	1w	110	1/1	0.72	0.19	-	75,75,75,75	0
56	MG	1A	3996	1/1	0.97	0.17	-	49,49,49,49	0
56	MG	2a	1791	1/1	0.85	0.12	-	69,69,69,69	0
56	MG	1A	3750	1/1	0.95	0.08	-	31,31,31,31	0
56	MG	2A	3141	1/1	0.95	0.13	-	40,40,40,40	0
56	MG	1A	3473	1/1	0.89	0.18	-	42,42,42,42	0
56	MG	1a	3172	1/1	0.96	0.07	-	46,46,46,46	0
56	MG	2B	3005	1/1	0.96	0.10	-	55,55,55,55	0
56	MG	1A	3780	1/1	0.87	0.23	-	44,44,44,44	0
56	MG	1A	3469	1/1	0.91	0.19	-	43,43,43,43	0
56	MG	1x	107	1/1	0.97	0.20	-	46,46,46,46	0
56	MG	1A	3396	1/1	0.94	0.28	-	44,44,44,44	0
56	MG	2a	1614	1/1	0.92	0.09	-	52,52,52,52	0
56	MG	1A	3303	1/1	0.94	0.16	-	44,44,44,44	0
56	MG	1A	3308	1/1	0.83	0.16	-	49,49,49,49	0
56	MG	2q	202	1/1	0.89	0.24	-	59,59,59,59	0
56	MG	2A	3555	1/1	0.98	0.15	-	38,38,38,38	0
56	MG	2A	3610	1/1	0.95	0.12	-	47,47,47,47	0
56	MG	1A	3902	1/1	0.93	0.10	-	55,55,55,55	0
56	MG	2A	3230	1/1	0.95	0.10	-	41,41,41,41	0
56	MG	2a	1652	1/1	0.94	0.09	-	55,55,55,55	0
56	MG	1A	3835	1/1	0.93	0.17	-	42,42,42,42	0
56	MG	2a	1779	1/1	0.95	0.11	-	60,60,60,60	0
56	MG	1A	3470	1/1	0.98	0.17	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	2A	3085	1/1	0.97	0.18	-	48,48,48,48	0
56	MG	2a	1750	1/1	0.68	0.09	-	60,60,60,60	0
56	MG	1A	3208	1/1	0.94	0.14	-	29,29,29,29	0
56	MG	1A	3115	1/1	0.99	0.20	-	39,39,39,39	0
56	MG	1A	3006	1/1	0.96	0.10	-	33,33,33,33	0
56	MG	10	101	1/1	0.97	0.06	-	41,41,41,41	0
56	MG	1a	3175	1/1	0.81	0.09	-	58,58,58,58	0
56	MG	1A	3225	1/1	0.97	0.12	-	40,40,40,40	0
56	MG	1A	3461	1/1	0.88	0.18	-	55,55,55,55	0
56	MG	2B	3015	1/1	0.95	0.14	-	51,51,51,51	0
56	MG	1A	3531	1/1	0.90	0.13	-	19,19,19,19	0
56	MG	1A	3311	1/1	0.94	0.19	-	37,37,37,37	0
56	MG	20	3001	1/1	0.88	0.15	-	52,52,52,52	0
56	MG	2A	3586	1/1	0.78	0.12	-	44,44,44,44	0
56	MG	1A	4065	1/1	0.88	0.12	-	36,36,36,36	0
56	MG	1A	3748	1/1	0.97	0.10	-	38,38,38,38	0
56	MG	1A	3089	1/1	0.94	0.15	-	21,21,21,21	0
56	MG	1A	3249	1/1	0.91	0.35	-	31,31,31,31	0
56	MG	16	104	1/1	0.96	0.14	-	38,38,38,38	0
56	MG	1a	3203	1/1	0.92	0.20	-	69,69,69,69	0
56	MG	1A	3046	1/1	0.96	0.26	-	50,50,50,50	0
56	MG	2B	3003	1/1	0.85	0.20	-	60,60,60,60	0
56	MG	2A	3513	1/1	0.95	0.11	-	52,52,52,52	0
56	MG	2A	3131	1/1	0.87	0.13	-	40,40,40,40	0
56	MG	2A	3331	1/1	0.93	0.16	-	47,47,47,47	0
56	MG	1E	309	1/1	0.97	0.16	-	15,15,15,15	0
56	MG	2a	1688	1/1	0.93	0.13	-	53,53,53,53	0
56	MG	1A	3368	1/1	0.88	0.39	-	39,39,39,39	0
56	MG	1A	3862	1/1	0.96	0.11	-	52,52,52,52	0
56	MG	2E	303	1/1	0.90	0.18	-	50,50,50,50	0
56	MG	1A	3281	1/1	0.94	0.35	-	29,29,29,29	0
56	MG	2A	3218	1/1	0.90	0.15	-	39,39,39,39	0
56	MG	2A	3543	1/1	0.94	0.13	-	45,45,45,45	0
56	MG	1A	3498	1/1	0.96	0.15	-	39,39,39,39	0
56	MG	2A	3293	1/1	0.85	0.28	-	46,46,46,46	0
56	MG	2A	3609	1/1	0.92	0.22	-	36,36,36,36	0
56	MG	2A	3177	1/1	0.90	0.31	-	36,36,36,36	0
56	MG	1A	3289	1/1	0.98	0.15	-	41,41,41,41	0
56	MG	2A	3559	1/1	0.94	0.16	-	61,61,61,61	0
56	MG	2A	3084	1/1	0.96	0.18	-	29,29,29,29	0
56	MG	2A	3429	1/1	0.90	0.22	-	59,59,59,59	0
56	MG	1A	3773	1/1	0.96	0.10	-	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3156	1/1	0.98	0.26	-	27,27,27,27	0
56	MG	1A	3894	1/1	0.99	0.09	-	37,37,37,37	0
56	MG	1I	3001	1/1	0.93	0.31	-	64,64,64,64	0
56	MG	2B	3004	1/1	0.95	0.15	-	60,60,60,60	0
56	MG	1a	3008	1/1	0.94	0.18	-	51,51,51,51	0
56	MG	2A	3033	1/1	0.80	0.18	-	52,52,52,52	0
56	MG	1A	3416	1/1	0.86	0.15	-	17,17,17,17	0
56	MG	1G	3002	1/1	0.97	0.15	-	39,39,39,39	0
56	MG	2A	3596	1/1	0.95	0.15	-	32,32,32,32	0
56	MG	1a	3058	1/1	0.97	0.07	-	58,58,58,58	0
56	MG	2A	3627	1/1	0.97	0.14	-	50,50,50,50	0
56	MG	28	101	1/1	0.81	0.20	-	49,49,49,49	0
56	MG	1A	3870	1/1	0.97	0.09	-	55,55,55,55	0
56	MG	2A	3497	1/1	0.85	0.18	-	63,63,63,63	0
56	MG	2A	3618	1/1	0.86	0.18	-	71,71,71,71	0
56	MG	1Z	3004	1/1	0.97	0.14	-	41,41,41,41	0
56	MG	1A	3468	1/1	0.94	0.08	-	37,37,37,37	0
56	MG	2A	3136	1/1	0.90	0.15	-	36,36,36,36	0
56	MG	1A	3980	1/1	0.87	0.21	-	62,62,62,62	0
56	MG	1A	3206	1/1	0.96	0.13	-	30,30,30,30	0
56	MG	1A	3254	1/1	0.99	0.29	-	11,11,11,11	0
56	MG	2A	3580	1/1	0.94	0.15	-	39,39,39,39	0
56	MG	2A	3756	1/1	0.93	0.14	-	33,33,33,33	0
56	MG	1A	3334	1/1	0.98	0.21	-	22,22,22,22	0
56	MG	1B	229	1/1	0.89	0.09	-	57,57,57,57	0
56	MG	2A	3672	1/1	0.84	0.26	-	46,46,46,46	0
56	MG	2A	3430	1/1	0.95	0.11	-	53,53,53,53	0
56	MG	1x	104	1/1	0.95	0.21	-	54,54,54,54	0
56	MG	2A	3248	1/1	0.91	0.18	-	44,44,44,44	0
56	MG	2W	201	1/1	0.94	0.16	-	50,50,50,50	0
56	MG	2A	3339	1/1	0.94	0.10	-	58,58,58,58	0
56	MG	2A	3203	1/1	0.96	0.12	-	53,53,53,53	0
56	MG	1A	3256	1/1	0.94	0.10	-	33,33,33,33	0
56	MG	2A	3162	1/1	0.96	0.08	-	54,54,54,54	0
56	MG	1A	3010	1/1	0.96	0.21	-	33,33,33,33	0
56	MG	1A	3072	1/1	0.92	0.31	-	27,27,27,27	0
56	MG	2A	3477	1/1	0.92	0.13	-	64,64,64,64	0
56	MG	2w	105	1/1	0.88	0.14	-	72,72,72,72	0
56	MG	1A	3316	1/1	0.85	0.42	-	34,34,34,34	0
56	MG	1A	3346	1/1	0.87	0.18	-	43,43,43,43	0
56	MG	2A	3113	1/1	0.94	0.21	-	48,48,48,48	0
56	MG	2A	3641	1/1	0.98	0.14	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3746	1/1	0.90	0.31	-	49,49,49,49	0
56	MG	1A	3522	1/1	0.99	0.15	-	30,30,30,30	0
56	MG	1a	3111	1/1	0.92	0.17	-	45,45,45,45	0
56	MG	1A	3744	1/1	0.92	0.12	-	41,41,41,41	0
56	MG	1A	3077	1/1	0.97	0.44	-	21,21,21,21	0
56	MG	2A	3374	1/1	0.70	0.15	-	41,41,41,41	0
56	MG	1B	226	1/1	0.89	0.14	-	67,67,67,67	0
56	MG	2A	3282	1/1	0.94	0.10	-	51,51,51,51	0
56	MG	2A	3349	1/1	0.87	0.17	-	30,30,30,30	0
56	MG	2a	1643	1/1	0.93	0.21	-	61,61,61,61	0
56	MG	2a	1797	1/1	0.88	0.13	-	70,70,70,70	0
56	MG	1A	3817	1/1	0.93	0.13	-	20,20,20,20	0
56	MG	1A	3655	1/1	0.97	0.14	-	11,11,11,11	0
56	MG	2A	3175	1/1	0.78	0.36	-	43,43,43,43	0
56	MG	1a	3125	1/1	0.96	0.12	-	42,42,42,42	0
56	MG	1A	3183	1/1	0.92	0.09	-	39,39,39,39	0
56	MG	2A	3017	1/1	0.91	0.11	-	59,59,59,59	0
56	MG	1A	3603	1/1	0.93	0.16	-	43,43,43,43	0
56	MG	1A	3643	1/1	0.97	0.40	-	29,29,29,29	0
56	MG	1A	3129	1/1	0.95	0.36	-	27,27,27,27	0
56	MG	1A	3658	1/1	0.90	0.10	-	46,46,46,46	0
56	MG	2A	3328	1/1	0.98	0.23	-	45,45,45,45	0
56	MG	1S	3003	1/1	0.86	0.21	-	61,61,61,61	0
56	MG	2A	3553	1/1	0.96	0.09	-	57,57,57,57	0
56	MG	1a	3003	1/1	0.89	0.20	-	56,56,56,56	0
56	MG	1a	3192	1/1	0.89	0.09	-	62,62,62,62	0
56	MG	2A	3667	1/1	0.94	0.11	-	63,63,63,63	0
56	MG	2U	206	1/1	0.96	0.13	-	42,42,42,42	0
56	MG	2A	3588	1/1	0.92	0.09	-	52,52,52,52	0
56	MG	1a	3138	1/1	0.95	0.16	-	66,66,66,66	0
56	MG	1A	3616	1/1	0.95	0.16	-	58,58,58,58	0
56	MG	1a	3001	1/1	0.91	0.14	-	52,52,52,52	0
56	MG	2a	1826	1/1	0.89	0.12	-	55,55,55,55	0
56	MG	2A	3465	1/1	0.99	0.28	-	42,42,42,42	0
56	MG	1A	3350	1/1	0.84	0.31	-	44,44,44,44	0
56	MG	2A	3068	1/1	0.97	0.04	-	35,35,35,35	0
56	MG	2A	3103	1/1	0.90	0.48	-	46,46,46,46	0
56	MG	1A	3074	1/1	0.98	0.32	-	24,24,24,24	0
56	MG	1A	3433	1/1	0.97	0.08	-	50,50,50,50	0
56	MG	17	105	1/1	0.91	0.15	-	34,34,34,34	0
56	MG	1A	3979	1/1	0.95	0.10	-	56,56,56,56	0
56	MG	2a	1607	1/1	0.81	0.18	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	2A	3684	1/1	0.92	0.08	-	68,68,68,68	0
56	MG	2A	3605	1/1	0.94	0.13	-	42,42,42,42	0
56	MG	1A	3218	1/1	0.92	0.07	-	23,23,23,23	0
56	MG	2A	3550	1/1	0.77	0.15	-	58,58,58,58	0
56	MG	1A	3673	1/1	0.94	0.13	-	54,54,54,54	0
56	MG	2a	1743	1/1	0.92	0.10	-	70,70,70,70	0
56	MG	12	3001	1/1	0.92	0.15	-	44,44,44,44	0
56	MG	2A	3101	1/1	0.94	0.17	-	30,30,30,30	0
56	MG	2A	3602	1/1	0.96	0.19	-	62,62,62,62	0
56	MG	2A	3052	1/1	0.88	0.14	-	36,36,36,36	0
56	MG	1A	3959	1/1	0.79	0.12	-	76,76,76,76	0
56	MG	1A	3105	1/1	0.93	0.24	-	30,30,30,30	0
56	MG	2A	3342	1/1	0.96	0.18	-	49,49,49,49	0
56	MG	1A	3158	1/1	0.94	0.17	-	31,31,31,31	0
56	MG	1A	3820	1/1	0.98	0.12	-	35,35,35,35	0
56	MG	1A	3578	1/1	0.97	0.14	-	23,23,23,23	0
56	MG	2A	3585	1/1	0.95	0.20	-	34,34,34,34	0
56	MG	2A	3365	1/1	0.95	0.11	-	38,38,38,38	0
56	MG	2A	3198	1/1	0.77	0.17	-	43,43,43,43	0
56	MG	1A	3142	1/1	0.98	0.12	-	17,17,17,17	0
56	MG	1A	3016	1/1	0.95	0.20	-	40,40,40,40	0
56	MG	2a	1828	1/1	0.95	0.23	-	64,64,64,64	0
56	MG	2A	3402	1/1	0.92	0.15	-	49,49,49,49	0
56	MG	1A	3619	1/1	0.90	0.16	-	36,36,36,36	0
56	MG	1F	307	1/1	0.90	0.12	-	40,40,40,40	0
56	MG	1A	3344	1/1	0.93	0.36	-	31,31,31,31	0
56	MG	1A	3417	1/1	0.91	0.16	-	42,42,42,42	0
56	MG	2A	3173	1/1	0.95	0.14	-	45,45,45,45	0
56	MG	2w	102	1/1	0.86	0.14	-	78,78,78,78	0
56	MG	1O	205	1/1	0.89	0.37	-	57,57,57,57	0
56	MG	1A	3703	1/1	0.95	0.22	-	24,24,24,24	0
56	MG	1A	3491	1/1	0.91	0.19	-	17,17,17,17	0
56	MG	2A	3045	1/1	0.88	0.14	-	55,55,55,55	0
56	MG	1A	3777	1/1	0.95	0.10	-	36,36,36,36	0
56	MG	2A	3132	1/1	0.95	0.07	-	58,58,58,58	0
56	MG	1A	3035	1/1	0.98	0.20	-	24,24,24,24	0
56	MG	2A	3446	1/1	0.92	0.14	-	32,32,32,32	0
56	MG	1A	3926	1/1	0.95	0.16	-	18,18,18,18	0
56	MG	1A	3404	1/1	0.97	0.26	-	28,28,28,28	0
56	MG	1A	3923	1/1	0.92	0.23	-	39,39,39,39	0
56	MG	2l	204	1/1	0.90	0.12	-	43,43,43,43	0
56	MG	1A	3981	1/1	0.94	0.12	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	2v	3003	1/1	0.79	0.20	-	66,66,66,66	0
56	MG	1A	3083	1/1	0.85	0.26	-	55,55,55,55	0
56	MG	1A	3865	1/1	0.98	0.18	-	18,18,18,18	0
56	MG	1O	207	1/1	0.89	0.10	-	54,54,54,54	0
56	MG	1A	3623	1/1	0.97	0.15	-	41,41,41,41	0
56	MG	2a	1716	1/1	0.94	0.18	-	43,43,43,43	0
56	MG	1y	101	1/1	0.96	0.10	-	35,35,35,35	0
56	MG	2a	1717	1/1	0.96	0.08	-	66,66,66,66	0
56	MG	2A	3642	1/1	0.96	0.12	-	43,43,43,43	0
56	MG	1B	202	1/1	0.94	0.24	-	42,42,42,42	0
56	MG	27	102	1/1	0.90	0.17	-	47,47,47,47	0
56	MG	1A	3167	1/1	0.96	0.22	-	47,47,47,47	0
56	MG	1A	3209	1/1	0.52	0.29	-	61,61,61,61	0
56	MG	1A	3929	1/1	0.96	0.33	-	35,35,35,35	0
56	MG	2a	1806	1/1	0.78	0.11	-	76,76,76,76	0
56	MG	1A	3390	1/1	0.98	0.10	-	43,43,43,43	0
56	MG	1B	227	1/1	0.96	0.12	-	36,36,36,36	0
56	MG	2A	3067	1/1	0.89	0.22	-	46,46,46,46	0
56	MG	1A	3854	1/1	0.98	0.12	-	46,46,46,46	0
56	MG	2E	304	1/1	0.97	0.20	-	49,49,49,49	0
56	MG	2A	3600	1/1	0.95	0.11	-	56,56,56,56	0
56	MG	1x	109	1/1	0.85	0.11	-	57,57,57,57	0
56	MG	1a	3209	1/1	0.94	0.20	-	60,60,60,60	0
56	MG	1A	3471	1/1	0.95	0.23	-	45,45,45,45	0
56	MG	1A	3998	1/1	0.90	0.13	-	55,55,55,55	0
56	MG	1A	3945	1/1	0.92	0.34	-	30,30,30,30	0
56	MG	2a	1730	1/1	0.93	0.11	-	65,65,65,65	0
56	MG	2A	3341	1/1	0.96	0.17	-	39,39,39,39	0
56	MG	1A	3210	1/1	0.94	0.42	-	25,25,25,25	0
56	MG	1A	3065	1/1	0.84	0.39	-	62,62,62,62	0
56	MG	2A	3363	1/1	0.98	0.15	-	43,43,43,43	0
56	MG	2A	3621	1/1	0.84	0.09	-	49,49,49,49	0
56	MG	2A	3071	1/1	0.88	0.08	-	60,60,60,60	0
56	MG	1A	3277	1/1	0.88	0.13	-	37,37,37,37	0
56	MG	1A	3907	1/1	0.74	0.21	-	39,39,39,39	0
56	MG	1A	3408	1/1	0.81	0.30	-	40,40,40,40	0
56	MG	1A	3026	1/1	0.94	0.13	-	30,30,30,30	0
56	MG	1B	218	1/1	0.93	0.19	-	40,40,40,40	0
56	MG	1a	3121	1/1	0.97	0.15	-	54,54,54,54	0
56	MG	1A	3449	1/1	0.94	0.19	-	52,52,52,52	0
56	MG	1A	3126	1/1	0.96	0.48	-	21,21,21,21	0
56	MG	2A	3214	1/1	0.95	0.08	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3093	1/1	0.93	0.09	-	31,31,31,31	0
56	MG	1A	3995	1/1	0.98	0.10	-	32,32,32,32	0
56	MG	1a	3018	1/1	0.83	0.30	-	55,55,55,55	0
56	MG	1A	3886	1/1	0.96	0.10	-	24,24,24,24	0
56	MG	2A	3097	1/1	0.90	0.14	-	42,42,42,42	0
56	MG	1a	3080	1/1	0.96	0.23	-	46,46,46,46	0
56	MG	1E	307	1/1	0.93	0.55	-	50,50,50,50	0
56	MG	1A	3611	1/1	0.95	0.19	-	45,45,45,45	0
56	MG	2A	3681	1/1	0.91	0.23	-	49,49,49,49	0
56	MG	2A	3615	1/1	0.69	0.34	-	66,66,66,66	0
56	MG	1A	3952	1/1	0.97	0.14	-	50,50,50,50	0
56	MG	1y	102	1/1	0.90	0.09	-	83,83,83,83	0
56	MG	2A	3211	1/1	0.92	0.12	-	68,68,68,68	0
56	MG	2A	3062	1/1	0.97	0.14	-	47,47,47,47	0
56	MG	2A	3687	1/1	0.82	0.29	-	65,65,65,65	0
56	MG	1A	3223	1/1	0.98	0.20	-	34,34,34,34	0
56	MG	1A	3975	1/1	0.95	0.08	-	51,51,51,51	0
56	MG	2a	1622	1/1	0.94	0.40	-	39,39,39,39	0
56	MG	1A	3954	1/1	0.97	0.15	-	53,53,53,53	0
56	MG	1a	3140	1/1	0.96	0.10	-	38,38,38,38	0
56	MG	1A	3884	1/1	0.98	0.08	-	30,30,30,30	0
56	MG	2A	3634	1/1	0.97	0.21	-	48,48,48,48	0
56	MG	2A	3457	1/1	0.69	0.19	-	58,58,58,58	0
56	MG	2A	3253	1/1	0.93	0.54	-	68,68,68,68	0
56	MG	2A	3371	1/1	0.96	0.19	-	22,22,22,22	0
56	MG	2a	1719	1/1	0.89	0.14	-	55,55,55,55	0
56	MG	1A	3055	1/1	0.91	0.12	-	54,54,54,54	0
56	MG	1A	3575	1/1	0.95	0.12	-	11,11,11,11	0
56	MG	1A	3029	1/1	0.94	0.36	-	17,17,17,17	0
56	MG	1A	3211	1/1	0.98	0.23	-	30,30,30,30	0
56	MG	2A	3509	1/1	0.97	0.20	-	52,52,52,52	0
56	MG	1A	3150	1/1	0.99	0.25	-	27,27,27,27	0
56	MG	1A	3108	1/1	0.90	0.15	-	25,25,25,25	0
56	MG	2V	3002	1/1	0.94	0.13	-	56,56,56,56	0
56	MG	2A	3298	1/1	0.93	0.12	-	50,50,50,50	0
56	MG	1A	3961	1/1	0.95	0.10	-	36,36,36,36	0
56	MG	2A	3569	1/1	0.96	0.03	-	63,63,63,63	0
56	MG	1A	3279	1/1	0.95	0.18	-	41,41,41,41	0
56	MG	2A	3137	1/1	0.96	0.08	-	50,50,50,50	0
56	MG	1A	3299	1/1	0.83	0.35	-	28,28,28,28	0
56	MG	1A	3202	1/1	0.93	0.29	-	27,27,27,27	0
56	MG	2a	1800	1/1	0.89	0.23	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3639	1/1	0.99	0.09	-	39,39,39,39	0
56	MG	1a	3133	1/1	0.95	0.15	-	47,47,47,47	0
56	MG	1A	3088	1/1	0.98	0.20	-	32,32,32,32	0
56	MG	2a	1628	1/1	0.94	0.30	-	49,49,49,49	0
56	MG	1A	3380	1/1	0.91	0.29	-	33,33,33,33	0
56	MG	1A	3040	1/1	0.97	0.06	-	30,30,30,30	0
56	MG	2y	3001	1/1	0.76	0.23	-	64,64,64,64	0
56	MG	1A	3245	1/1	0.96	0.46	-	28,28,28,28	0
56	MG	2A	3235	1/1	0.97	0.18	-	40,40,40,40	0
56	MG	1a	3059	1/1	0.88	0.09	-	61,61,61,61	0
56	MG	2A	3216	1/1	0.93	0.16	-	51,51,51,51	0
56	MG	1A	3601	1/1	0.98	0.08	-	24,24,24,24	0
56	MG	1A	3512	1/1	0.92	0.08	-	40,40,40,40	0
56	MG	2a	1611	1/1	0.92	0.10	-	65,65,65,65	0
56	MG	1A	3161	1/1	0.99	0.24	-	20,20,20,20	0
56	MG	1A	3333	1/1	0.89	0.51	-	43,43,43,43	0
56	MG	2A	3335	1/1	0.98	0.11	-	49,49,49,49	0
56	MG	2A	3607	1/1	0.91	0.13	-	48,48,48,48	0
56	MG	1A	3240	1/1	0.96	0.16	-	38,38,38,38	0
56	MG	2A	3563	1/1	0.94	0.19	-	55,55,55,55	0
56	MG	15	105	1/1	0.97	0.46	-	33,33,33,33	0
56	MG	2A	3366	1/1	0.90	0.14	-	67,67,67,67	0
56	MG	1A	3969	1/1	0.95	0.14	-	41,41,41,41	0
56	MG	2A	3126	1/1	0.93	0.17	-	50,50,50,50	0
56	MG	2A	3438	1/1	0.95	0.10	-	36,36,36,36	0
56	MG	1A	3927	1/1	0.97	0.29	-	37,37,37,37	0
56	MG	2A	3191	1/1	0.91	0.14	-	56,56,56,56	0
56	MG	1A	3699	1/1	0.98	0.08	-	25,25,25,25	0
56	MG	2A	3587	1/1	0.74	0.16	-	55,55,55,55	0
56	MG	1A	3723	1/1	0.97	0.10	-	34,34,34,34	0
56	MG	1l	203	1/1	0.92	0.17	-	50,50,50,50	0
56	MG	1A	3191	1/1	0.96	0.21	-	24,24,24,24	0
56	MG	2a	1827	1/1	0.97	0.19	-	58,58,58,58	0
56	MG	2A	3215	1/1	0.76	0.15	-	58,58,58,58	0
56	MG	1A	3683	1/1	0.95	0.28	-	41,41,41,41	0
56	MG	2l	201	1/1	0.93	0.23	-	51,51,51,51	0
56	MG	2a	1812	1/1	0.98	0.11	-	64,64,64,64	0
56	MG	2a	1691	1/1	0.91	0.36	-	56,56,56,56	0
56	MG	1a	3101	1/1	0.90	0.15	-	42,42,42,42	0
56	MG	2a	1733	1/1	0.96	0.12	-	56,56,56,56	0
56	MG	2R	3001	1/1	0.92	0.50	-	58,58,58,58	0
56	MG	1A	3028	1/1	0.96	0.34	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3821	1/1	0.97	0.11	-	32,32,32,32	0
56	MG	1A	3766	1/1	0.75	0.23	-	36,36,36,36	0
56	MG	1A	3583	1/1	0.97	0.18	-	22,22,22,22	0
56	MG	2A	3418	1/1	0.96	0.06	-	46,46,46,46	0
56	MG	1A	3067	1/1	0.96	0.08	-	22,22,22,22	0
56	MG	2A	3633	1/1	0.97	0.13	-	66,66,66,66	0
56	MG	2A	3032	1/1	0.98	0.12	-	41,41,41,41	0
56	MG	1A	3081	1/1	0.96	0.17	-	24,24,24,24	0
56	MG	2A	3410	1/1	0.92	0.31	-	61,61,61,61	0
56	MG	1A	3974	1/1	0.96	0.11	-	50,50,50,50	0
56	MG	1A	3477	1/1	0.96	0.23	-	32,32,32,32	0
56	MG	2a	1803	1/1	0.95	0.08	-	51,51,51,51	0
56	MG	1A	4007	1/1	0.94	0.66	-	39,39,39,39	0
56	MG	1A	3426	1/1	0.91	0.22	-	44,44,44,44	0
56	MG	1a	3124	1/1	0.94	0.13	-	54,54,54,54	0
56	MG	1A	3761	1/1	0.88	0.14	-	48,48,48,48	0
56	MG	2A	3167	1/1	0.90	0.14	-	42,42,42,42	0
56	MG	1a	3035	1/1	0.97	0.22	-	49,49,49,49	0
56	MG	1A	3198	1/1	0.87	0.12	-	43,43,43,43	0
56	MG	1A	3438	1/1	0.91	0.10	-	29,29,29,29	0
56	MG	2A	3240	1/1	0.95	0.12	-	51,51,51,51	0
56	MG	2A	3133	1/1	0.84	0.27	-	44,44,44,44	0
56	MG	1A	3614	1/1	0.97	0.15	-	15,15,15,15	0
56	MG	1A	3863	1/1	0.97	0.11	-	56,56,56,56	0
56	MG	2a	1799	1/1	0.80	0.12	-	59,59,59,59	0
56	MG	2A	3390	1/1	0.91	0.12	-	58,58,58,58	0
56	MG	2a	1613	1/1	0.83	0.15	-	60,60,60,60	0
56	MG	1A	3993	1/1	0.93	0.30	-	44,44,44,44	0
56	MG	1F	306	1/1	0.89	0.18	-	36,36,36,36	0
56	MG	1A	4011	1/1	0.94	0.21	-	37,37,37,37	0
56	MG	1A	3846	1/1	0.97	0.10	-	48,48,48,48	0
56	MG	2B	3021	1/1	0.97	0.18	-	59,59,59,59	0
56	MG	1A	3559	1/1	0.93	0.20	-	15,15,15,15	0
56	MG	1a	3207	1/1	0.87	0.09	-	41,41,41,41	0
56	MG	1A	3130	1/1	0.97	0.23	-	10,10,10,10	0
56	MG	2a	1649	1/1	0.98	0.22	-	41,41,41,41	0
56	MG	1A	3117	1/1	0.90	0.16	-	48,48,48,48	0
56	MG	1A	3397	1/1	0.91	0.15	-	51,51,51,51	0
56	MG	1A	3464	1/1	0.92	0.17	-	39,39,39,39	0
56	MG	1E	310	1/1	0.77	0.15	-	60,60,60,60	0
56	MG	2a	1630	1/1	0.93	0.23	-	57,57,57,57	0
56	MG	2A	3603	1/1	0.93	0.11	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3542	1/1	0.95	0.16	-	44,44,44,44	0
56	MG	1A	3547	1/1	0.96	0.13	-	22,22,22,22	0
56	MG	2A	3487	1/1	0.95	0.20	-	62,62,62,62	0
56	MG	1Z	3002	1/1	0.81	0.15	-	46,46,46,46	0
56	MG	2A	3193	1/1	0.88	0.12	-	51,51,51,51	0
56	MG	2a	1801	1/1	0.98	0.09	-	63,63,63,63	0
56	MG	2A	3048	1/1	0.89	0.12	-	57,57,57,57	0
56	MG	1B	208	1/1	0.78	0.23	-	59,59,59,59	0
56	MG	1X	102	1/1	0.92	0.21	-	35,35,35,35	0
56	MG	1A	3966	1/1	0.98	0.08	-	41,41,41,41	0
56	MG	1A	3443	1/1	0.94	0.15	-	32,32,32,32	0
56	MG	1A	4056	1/1	0.98	0.32	-	33,33,33,33	0
56	MG	1A	3354	1/1	0.95	0.08	-	39,39,39,39	0
56	MG	2F	304	1/1	0.85	0.10	-	64,64,64,64	0
56	MG	2A	3223	1/1	0.89	0.13	-	45,45,45,45	0
56	MG	1A	3489	1/1	0.96	0.22	-	30,30,30,30	0
56	MG	2a	1780	1/1	0.92	0.07	-	57,57,57,57	0
56	MG	1A	3721	1/1	0.90	0.26	-	53,53,53,53	0
56	MG	2A	3361	1/1	0.93	0.11	-	46,46,46,46	0
56	MG	2a	1702	1/1	0.93	0.14	-	56,56,56,56	0
56	MG	1A	3582	1/1	0.95	0.12	-	26,26,26,26	0
56	MG	2A	3061	1/1	0.94	0.17	-	30,30,30,30	0
56	MG	1A	3315	1/1	0.83	0.25	-	37,37,37,37	0
56	MG	2A	3252	1/1	0.90	0.16	-	38,38,38,38	0
56	MG	2A	3660	1/1	0.99	0.13	-	37,37,37,37	0
56	MG	2a	1602	1/1	0.86	0.21	-	54,54,54,54	0
56	MG	1A	3786	1/1	0.92	0.11	-	34,34,34,34	0
56	MG	2A	3210	1/1	0.92	0.35	-	58,58,58,58	0
56	MG	1A	3177	1/1	0.95	0.09	-	34,34,34,34	0
56	MG	1A	3378	1/1	0.94	0.40	-	27,27,27,27	0
56	MG	1A	3496	1/1	0.97	0.09	-	35,35,35,35	0
56	MG	1A	3331	1/1	0.91	0.21	-	39,39,39,39	0
56	MG	1a	3054	1/1	0.97	0.06	-	46,46,46,46	0
56	MG	1A	3076	1/1	0.94	0.25	-	26,26,26,26	0
56	MG	1A	3964	1/1	0.97	0.27	-	45,45,45,45	0
56	MG	1X	101	1/1	0.76	0.09	-	73,73,73,73	0
56	MG	10	102	1/1	0.95	0.23	-	25,25,25,25	0
56	MG	2A	3456	1/1	0.93	0.17	-	26,26,26,26	0
56	MG	1A	3329	1/1	0.93	0.10	-	41,41,41,41	0
56	MG	2A	3420	1/1	0.71	0.23	-	67,67,67,67	0
56	MG	2a	1644	1/1	0.78	0.20	-	62,62,62,62	0
56	MG	1A	3576	1/1	0.95	0.15	-	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3643	1/1	0.95	0.08	-	43,43,43,43	0
56	MG	2A	3302	1/1	0.90	0.24	-	43,43,43,43	0
56	MG	1a	3056	1/1	0.95	0.11	-	50,50,50,50	0
56	MG	2A	3536	1/1	0.81	0.14	-	54,54,54,54	0
56	MG	1x	112	1/1	0.95	0.16	-	45,45,45,45	0
56	MG	2a	1763	1/1	0.96	0.10	-	72,72,72,72	0
56	MG	2A	3707	1/1	0.94	0.15	-	47,47,47,47	0
56	MG	1x	111	1/1	0.92	0.15	-	64,64,64,64	0
56	MG	2A	3129	1/1	0.99	0.19	-	54,54,54,54	0
56	MG	1A	3294	1/1	0.88	0.21	-	40,40,40,40	0
56	MG	2A	3041	1/1	0.97	0.12	-	46,46,46,46	0
56	MG	2A	3303	1/1	0.96	0.17	-	35,35,35,35	0
56	MG	2y	3005	1/1	0.79	0.09	-	88,88,88,88	0
56	MG	1A	3410	1/1	0.94	0.12	-	45,45,45,45	0
56	MG	2A	3209	1/1	0.97	0.08	-	35,35,35,35	0
56	MG	1a	3198	1/1	0.96	0.25	-	46,46,46,46	0
56	MG	1a	3178	1/1	0.94	0.06	-	54,54,54,54	0
56	MG	1a	3151	1/1	0.95	0.20	-	62,62,62,62	0
56	MG	1A	3189	1/1	1.00	0.11	-	23,23,23,23	0
56	MG	1A	4042	1/1	0.94	0.13	-	40,40,40,40	0
56	MG	1A	3457	1/1	0.94	0.14	-	32,32,32,32	0
56	MG	2A	3194	1/1	0.89	0.21	-	51,51,51,51	0
56	MG	1A	3720	1/1	0.95	0.14	-	41,41,41,41	0
56	MG	2A	3384	1/1	0.91	0.10	-	27,27,27,27	0
56	MG	1A	3984	1/1	0.85	0.11	-	52,52,52,52	0
56	MG	2A	3542	1/1	0.86	0.13	-	36,36,36,36	0
56	MG	1A	3097	1/1	0.97	0.09	-	24,24,24,24	0
56	MG	1A	3755	1/1	0.97	0.20	-	21,21,21,21	0
56	MG	1A	3687	1/1	0.94	0.11	-	33,33,33,33	0
56	MG	2a	1746	1/1	0.95	0.08	-	67,67,67,67	0
56	MG	1A	3450	1/1	0.91	0.11	-	40,40,40,40	0
56	MG	1a	3033	1/1	0.95	0.07	-	57,57,57,57	0
56	MG	1A	3955	1/1	0.91	0.13	-	32,32,32,32	0
56	MG	1x	108	1/1	0.94	0.13	-	61,61,61,61	0
56	MG	2A	3290	1/1	0.95	0.19	-	39,39,39,39	0
56	MG	1A	3716	1/1	0.97	0.10	-	45,45,45,45	0
56	MG	1A	3112	1/1	0.95	0.16	-	40,40,40,40	0
56	MG	2v	3001	1/1	0.98	0.07	-	49,49,49,49	0
56	MG	1A	3802	1/1	0.74	0.22	-	54,54,54,54	0
56	MG	1A	3147	1/1	0.96	0.07	-	50,50,50,50	0
56	MG	1a	3048	1/1	0.90	0.47	-	43,43,43,43	0
56	MG	2A	3622	1/1	0.96	0.11	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3533	1/1	0.95	0.10	-	47,47,47,47	0
56	MG	1a	3057	1/1	0.91	0.15	-	43,43,43,43	0
56	MG	1A	3880	1/1	0.98	0.26	-	23,23,23,23	0
56	MG	1A	3510	1/1	0.91	0.18	-	50,50,50,50	0
56	MG	1A	3733	1/1	0.96	0.07	-	55,55,55,55	0
56	MG	1A	3905	1/1	0.95	0.07	-	54,54,54,54	0
56	MG	1a	3106	1/1	0.97	0.13	-	52,52,52,52	0
56	MG	1w	104	1/1	0.96	0.07	-	36,36,36,36	0
56	MG	1A	3895	1/1	0.85	0.15	-	71,71,71,71	0
56	MG	2a	1616	1/1	0.81	0.11	-	67,67,67,67	0
56	MG	1A	3571	1/1	0.94	0.12	-	17,17,17,17	0
56	MG	2A	3134	1/1	0.92	0.08	-	51,51,51,51	0
56	MG	1A	3062	1/1	0.95	0.11	-	12,12,12,12	0
56	MG	1a	3027	1/1	0.89	0.24	-	58,58,58,58	0
56	MG	1A	3852	1/1	0.96	0.14	-	55,55,55,55	0
56	MG	1A	3285	1/1	0.95	0.14	-	34,34,34,34	0
56	MG	1a	3037	1/1	0.95	0.15	-	61,61,61,61	0
56	MG	2A	3028	1/1	0.96	0.17	-	42,42,42,42	0
56	MG	11	102	1/1	0.88	0.21	-	72,72,72,72	0
56	MG	1a	3030	1/1	0.90	0.17	-	43,43,43,43	0
56	MG	1A	3212	1/1	0.96	0.18	-	50,50,50,50	0
56	MG	1A	3915	1/1	0.98	0.07	-	34,34,34,34	0
56	MG	2A	3142	1/1	0.94	0.13	-	46,46,46,46	0
56	MG	1A	3309	1/1	0.88	0.14	-	32,32,32,32	0
56	MG	1A	3909	1/1	0.91	0.20	-	46,46,46,46	0
56	MG	2A	3089	1/1	0.98	0.16	-	40,40,40,40	0
56	MG	2A	3040	1/1	0.95	0.34	-	39,39,39,39	0
56	MG	1W	3002	1/1	0.99	0.16	-	29,29,29,29	0
56	MG	1A	3726	1/1	0.95	0.06	-	35,35,35,35	0
56	MG	1A	3286	1/1	0.98	0.15	-	34,34,34,34	0
56	MG	1A	3824	1/1	0.97	0.13	-	33,33,33,33	0
56	MG	1a	3150	1/1	0.92	0.11	-	65,65,65,65	0
56	MG	2A	3114	1/1	0.99	0.28	-	29,29,29,29	0
56	MG	1a	3194	1/1	0.91	0.08	-	59,59,59,59	0
56	MG	1A	3843	1/1	0.88	0.10	-	66,66,66,66	0
56	MG	2A	3419	1/1	0.95	0.07	-	55,55,55,55	0
56	MG	2A	3243	1/1	0.98	0.17	-	49,49,49,49	0
56	MG	1a	3177	1/1	0.85	0.16	-	57,57,57,57	0
56	MG	2A	3196	1/1	0.82	0.19	-	53,53,53,53	0
56	MG	2A	3437	1/1	0.98	0.24	-	39,39,39,39	0
56	MG	2A	3701	1/1	0.81	0.11	-	50,50,50,50	0
56	MG	1A	3561	1/1	0.97	0.11	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1a	3202	1/1	0.97	0.06	-	45,45,45,45	0
56	MG	2A	3300	1/1	0.92	0.20	-	58,58,58,58	0
56	MG	1A	3341	1/1	0.81	0.36	-	38,38,38,38	0
56	MG	1A	3977	1/1	0.72	0.13	-	44,44,44,44	0
56	MG	2E	310	1/1	0.97	0.09	-	50,50,50,50	0
56	MG	2a	1706	1/1	0.98	0.06	-	54,54,54,54	0
56	MG	2l	202	1/1	0.88	0.43	-	66,66,66,66	0
56	MG	1A	4043	1/1	0.94	0.45	-	23,23,23,23	0
56	MG	1x	110	1/1	0.90	0.12	-	59,59,59,59	0
56	MG	2Q	3002	1/1	0.92	0.21	-	41,41,41,41	0
56	MG	1A	3918	1/1	0.97	0.11	-	33,33,33,33	0
56	MG	1A	3831	1/1	0.92	0.13	-	68,68,68,68	0
56	MG	1A	3577	1/1	0.98	0.13	-	54,54,54,54	0
56	MG	1A	3647	1/1	0.95	0.16	-	16,16,16,16	0
56	MG	1B	231	1/1	0.90	0.23	-	59,59,59,59	0
56	MG	1A	4037	1/1	0.94	0.55	-	28,28,28,28	0
56	MG	1A	4001	1/1	0.94	0.11	-	45,45,45,45	0
56	MG	2A	3515	1/1	0.88	0.19	-	44,44,44,44	0
56	MG	2A	3265	1/1	0.94	0.17	-	46,46,46,46	0
56	MG	2a	1818	1/1	0.91	0.10	-	48,48,48,48	0
56	MG	1a	3118	1/1	0.95	0.09	-	65,65,65,65	0
56	MG	2x	102	1/1	0.96	0.19	-	57,57,57,57	0
56	MG	2a	1682	1/1	0.93	0.09	-	48,48,48,48	0
56	MG	1A	3798	1/1	0.93	0.26	-	45,45,45,45	0
56	MG	2a	1684	1/1	0.91	0.18	-	49,49,49,49	0
56	MG	2A	3389	1/1	0.81	0.20	-	35,35,35,35	0
56	MG	2B	3009	1/1	0.87	0.14	-	63,63,63,63	0
56	MG	10	105	1/1	0.89	0.10	-	50,50,50,50	0
56	MG	1A	3856	1/1	0.97	0.06	-	62,62,62,62	0
56	MG	1A	3414	1/1	0.66	0.28	-	55,55,55,55	0
56	MG	2A	3204	1/1	0.92	0.15	-	43,43,43,43	0
56	MG	2A	3056	1/1	0.94	0.09	-	52,52,52,52	0
56	MG	1A	3048	1/1	0.93	0.45	-	42,42,42,42	0
56	MG	2A	3285	1/1	0.79	0.13	-	58,58,58,58	0
56	MG	2A	3044	1/1	0.89	0.08	-	61,61,61,61	0
56	MG	2A	3070	1/1	0.94	0.15	-	33,33,33,33	0
56	MG	1A	3711	1/1	0.89	0.15	-	44,44,44,44	0
56	MG	1A	3336	1/1	0.93	0.25	-	35,35,35,35	0
56	MG	2v	3005	1/1	0.98	0.15	-	56,56,56,56	0
56	MG	2T	3003	1/1	0.93	0.11	-	41,41,41,41	0
56	MG	2a	1778	1/1	0.91	0.21	-	68,68,68,68	0
56	MG	1A	3630	1/1	0.96	0.24	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3101	1/1	0.93	0.44	-	28,28,28,28	0
56	MG	1A	3463	1/1	0.93	0.38	-	38,38,38,38	0
56	MG	1A	3803	1/1	0.90	0.34	-	41,41,41,41	0
56	MG	2A	3507	1/1	0.89	0.10	-	67,67,67,67	0
56	MG	2A	3221	1/1	0.91	0.16	-	54,54,54,54	0
56	MG	1A	3609	1/1	0.89	0.08	-	61,61,61,61	0
56	MG	1A	3353	1/1	0.98	0.43	-	35,35,35,35	0
56	MG	2A	3470	1/1	0.94	0.22	-	53,53,53,53	0
56	MG	2A	3703	1/1	0.93	0.14	-	50,50,50,50	0
56	MG	2B	3013	1/1	0.70	0.15	-	74,74,74,74	0
56	MG	2A	3283	1/1	0.92	0.14	-	42,42,42,42	0
56	MG	2a	1758	1/1	0.98	0.07	-	52,52,52,52	0
56	MG	1A	3237	1/1	0.91	0.16	-	49,49,49,49	0
56	MG	1T	201	1/1	0.91	0.18	-	42,42,42,42	0
56	MG	2A	3631	1/1	0.98	0.11	-	53,53,53,53	0
56	MG	2A	3348	1/1	0.95	0.13	-	47,47,47,47	0
56	MG	2A	3337	1/1	0.95	0.27	-	27,27,27,27	0
56	MG	1a	3069	1/1	0.82	0.15	-	59,59,59,59	0
56	MG	2a	1814	1/1	0.98	0.14	-	63,63,63,63	0
56	MG	1A	3298	1/1	0.92	0.16	-	40,40,40,40	0
56	MG	1A	3355	1/1	0.89	0.49	-	30,30,30,30	0
56	MG	1A	3383	1/1	0.93	0.18	-	42,42,42,42	0
56	MG	2A	3277	1/1	0.86	0.37	-	54,54,54,54	0
56	MG	1a	3112	1/1	0.92	0.09	-	48,48,48,48	0
56	MG	2A	3514	1/1	0.86	0.22	-	56,56,56,56	0
56	MG	1A	3381	1/1	0.95	0.08	-	46,46,46,46	0
56	MG	2A	3176	1/1	0.91	0.24	-	41,41,41,41	0
56	MG	2A	3728	1/1	0.91	0.17	-	56,56,56,56	0
56	MG	2A	3508	1/1	0.95	0.18	-	57,57,57,57	0
56	MG	2w	101	1/1	0.90	0.18	-	65,65,65,65	0
56	MG	2A	3592	1/1	0.89	0.12	-	43,43,43,43	0
56	MG	1a	3064	1/1	0.86	0.21	-	54,54,54,54	0
56	MG	1A	3724	1/1	0.95	0.10	-	44,44,44,44	0
56	MG	2a	1749	1/1	0.99	0.05	-	55,55,55,55	0
56	MG	1A	3734	1/1	0.97	0.08	-	42,42,42,42	0
56	MG	2A	3639	1/1	0.90	0.22	-	56,56,56,56	0
56	MG	1A	3014	1/1	0.90	0.32	-	27,27,27,27	0
56	MG	2A	3724	1/1	0.96	0.15	-	66,66,66,66	0
56	MG	2a	1752	1/1	0.86	0.16	-	62,62,62,62	0
56	MG	1a	3183	1/1	0.95	0.10	-	51,51,51,51	0
56	MG	2A	3425	1/1	0.84	0.11	-	59,59,59,59	0
56	MG	1A	3747	1/1	0.94	0.08	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3708	1/1	0.92	0.10	-	42,42,42,42	0
56	MG	2A	3612	1/1	0.87	0.20	-	65,65,65,65	0
56	MG	2A	3053	1/1	0.87	0.14	-	30,30,30,30	0
56	MG	2A	3530	1/1	0.89	0.16	-	64,64,64,64	0
56	MG	1A	3729	1/1	0.97	0.18	-	49,49,49,49	0
56	MG	1A	3018	1/1	0.89	0.14	-	43,43,43,43	0
56	MG	1B	205	1/1	0.99	0.30	-	45,45,45,45	0
56	MG	2a	1744	1/1	0.95	0.11	-	67,67,67,67	0
56	MG	1A	3479	1/1	0.90	0.13	-	30,30,30,30	0
56	MG	1a	3094	1/1	0.96	0.26	-	40,40,40,40	0
56	MG	1A	3435	1/1	0.91	0.13	-	56,56,56,56	0
56	MG	2A	3564	1/1	0.95	0.17	-	42,42,42,42	0
56	MG	1A	3857	1/1	0.94	0.16	-	32,32,32,32	0
56	MG	2A	3297	1/1	0.95	0.24	-	51,51,51,51	0
56	MG	1a	3096	1/1	0.88	0.18	-	47,47,47,47	0
56	MG	1v	3001	1/1	0.83	0.11	-	72,72,72,72	0
56	MG	2A	3482	1/1	0.99	0.17	-	38,38,38,38	0
56	MG	2A	3163	1/1	0.75	0.26	-	44,44,44,44	0
56	MG	1w	107	1/1	0.90	0.30	-	64,64,64,64	0
56	MG	2A	3645	1/1	0.95	0.15	-	33,33,33,33	0
56	MG	1A	3940	1/1	0.94	0.10	-	29,29,29,29	0
56	MG	1A	3775	1/1	0.91	0.13	-	41,41,41,41	0
56	MG	2A	3693	1/1	0.98	0.05	-	68,68,68,68	0
56	MG	1A	3356	1/1	0.89	0.19	-	48,48,48,48	0
56	MG	2A	3135	1/1	0.93	0.26	-	49,49,49,49	0
56	MG	1a	3142	1/1	0.91	0.10	-	64,64,64,64	0
56	MG	2A	3658	1/1	0.91	0.17	-	36,36,36,36	0
56	MG	2a	1700	1/1	0.90	0.29	-	62,62,62,62	0
56	MG	2B	3010	1/1	0.87	0.11	-	64,64,64,64	0
56	MG	1A	3312	1/1	0.94	0.24	-	42,42,42,42	0
56	MG	2A	3516	1/1	0.96	0.13	-	62,62,62,62	0
56	MG	1A	3892	1/1	0.98	0.20	-	33,33,33,33	0
56	MG	1A	3908	1/1	0.97	0.14	-	27,27,27,27	0
56	MG	1A	3763	1/1	0.95	0.14	-	22,22,22,22	0
56	MG	2A	3087	1/1	0.84	0.08	-	59,59,59,59	0
56	MG	1A	3967	1/1	0.88	0.27	-	53,53,53,53	0
56	MG	1x	113	1/1	0.98	0.12	-	58,58,58,58	0
56	MG	2A	3383	1/1	0.68	0.22	-	56,56,56,56	0
56	MG	1A	3361	1/1	0.78	0.37	-	57,57,57,57	0
56	MG	2A	3239	1/1	0.96	0.44	-	64,64,64,64	0
56	MG	1A	3488	1/1	0.94	0.12	-	23,23,23,23	0
56	MG	1A	3830	1/1	0.97	0.26	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2a	1772	1/1	0.81	0.17	-	54,54,54,54	0
56	MG	2A	3461	1/1	0.94	0.15	-	45,45,45,45	0
56	MG	1A	3986	1/1	0.60	0.24	-	67,67,67,67	0
56	MG	1A	3094	1/1	0.89	0.13	-	56,56,56,56	0
56	MG	2A	3731	1/1	0.89	0.11	-	37,37,37,37	0
56	MG	2A	3686	1/1	0.97	0.15	-	40,40,40,40	0
56	MG	1B	204	1/1	0.92	0.12	-	29,29,29,29	0
56	MG	2A	3353	1/1	0.74	0.16	-	35,35,35,35	0
56	MG	2A	3511	1/1	0.97	0.14	-	39,39,39,39	0
56	MG	1A	3382	1/1	0.94	0.12	-	41,41,41,41	0
56	MG	1A	3061	1/1	0.94	0.11	-	39,39,39,39	0
56	MG	1B	214	1/1	0.94	0.11	-	42,42,42,42	0
56	MG	2A	3254	1/1	0.93	0.17	-	34,34,34,34	0
56	MG	2a	1631	1/1	0.86	0.09	-	66,66,66,66	0
56	MG	2w	107	1/1	0.98	0.14	-	55,55,55,55	0
56	MG	1A	3845	1/1	0.94	0.30	-	42,42,42,42	0
56	MG	1A	3710	1/1	0.94	0.20	-	28,28,28,28	0
56	MG	1A	3215	1/1	0.92	0.18	-	54,54,54,54	0
56	MG	1B	222	1/1	0.97	0.22	-	48,48,48,48	0
56	MG	1B	234	1/1	0.98	0.06	-	41,41,41,41	0
56	MG	1A	3157	1/1	0.96	0.08	-	50,50,50,50	0
56	MG	2a	1619	1/1	0.96	0.34	-	53,53,53,53	0
56	MG	2A	3165	1/1	0.96	0.19	-	40,40,40,40	0
56	MG	1A	3728	1/1	0.97	0.12	-	39,39,39,39	0
56	MG	1A	3057	1/1	0.86	0.26	-	45,45,45,45	0
56	MG	1A	3005	1/1	0.94	0.13	-	36,36,36,36	0
56	MG	2a	1732	1/1	0.86	0.11	-	56,56,56,56	0
56	MG	1a	3152	1/1	0.96	0.10	-	60,60,60,60	0
56	MG	2A	3326	1/1	0.94	0.11	-	48,48,48,48	0
56	MG	2A	3710	1/1	0.76	0.07	-	76,76,76,76	0
56	MG	2a	1695	1/1	0.93	0.16	-	56,56,56,56	0
56	MG	1A	3965	1/1	0.87	0.16	-	63,63,63,63	0
56	MG	1A	3181	1/1	0.98	0.08	-	43,43,43,43	0
56	MG	2A	3518	1/1	0.89	0.13	-	45,45,45,45	0
56	MG	1a	3068	1/1	0.91	0.14	-	62,62,62,62	0
56	MG	2A	3296	1/1	0.83	0.40	-	54,54,54,54	0
56	MG	1A	3768	1/1	0.95	0.06	-	33,33,33,33	0
56	MG	2A	3619	1/1	0.91	0.09	-	60,60,60,60	0
56	MG	1a	3011	1/1	0.92	0.14	-	41,41,41,41	0
56	MG	1A	3539	1/1	0.96	0.07	-	20,20,20,20	0
56	MG	1A	3347	1/1	0.93	0.14	-	42,42,42,42	0
56	MG	2A	3245	1/1	0.90	0.11	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3680	1/1	0.95	0.08	-	62,62,62,62	0
56	MG	1A	3431	1/1	0.90	0.41	-	34,34,34,34	0
56	MG	1A	3413	1/1	0.91	0.28	-	55,55,55,55	0
56	MG	2D	304	1/1	0.85	0.14	-	53,53,53,53	0
56	MG	2A	3573	1/1	0.94	0.30	-	37,37,37,37	0
56	MG	2A	3233	1/1	0.93	0.26	-	42,42,42,42	0
56	MG	1A	3385	1/1	0.97	0.30	-	29,29,29,29	0
56	MG	2E	305	1/1	0.81	0.14	-	51,51,51,51	0
56	MG	1A	3002	1/1	0.87	0.18	-	46,46,46,46	0
56	MG	2A	3295	1/1	0.95	0.26	-	43,43,43,43	0
56	MG	1A	3276	1/1	0.94	0.17	-	40,40,40,40	0
56	MG	1N	203	1/1	0.90	0.13	-	51,51,51,51	0
56	MG	1A	3922	1/1	0.92	0.09	-	49,49,49,49	0
56	MG	1A	3054	1/1	0.89	0.12	-	26,26,26,26	0
56	MG	1A	3957	1/1	0.93	0.12	-	55,55,55,55	0
56	MG	1A	3638	1/1	0.94	0.15	-	56,56,56,56	0
56	MG	1A	3555	1/1	0.93	0.09	-	29,29,29,29	0
56	MG	2a	1722	1/1	0.84	0.18	-	79,79,79,79	0
56	MG	1A	3822	1/1	0.96	0.10	-	45,45,45,45	0
56	MG	2B	3016	1/1	0.79	0.10	-	54,54,54,54	0
56	MG	1A	3950	1/1	0.95	0.13	-	54,54,54,54	0
56	MG	2a	1623	1/1	0.94	0.14	-	46,46,46,46	0
56	MG	2A	3172	1/1	0.97	0.32	-	48,48,48,48	0
56	MG	2A	3560	1/1	0.80	0.08	-	50,50,50,50	0
56	MG	1A	3063	1/1	0.96	0.31	-	23,23,23,23	0
56	MG	2W	202	1/1	0.77	0.54	-	46,46,46,46	0
56	MG	1A	3910	1/1	0.96	0.10	-	32,32,32,32	0
56	MG	1A	3930	1/1	0.96	0.23	-	33,33,33,33	0
56	MG	2A	3284	1/1	0.96	0.08	-	37,37,37,37	0
56	MG	1A	3019	1/1	0.93	0.16	-	32,32,32,32	0
56	MG	1A	3869	1/1	0.93	0.19	-	19,19,19,19	0
56	MG	2A	3255	1/1	0.93	0.22	-	54,54,54,54	0
56	MG	1A	3853	1/1	0.96	0.07	-	38,38,38,38	0
56	MG	2a	1751	1/1	0.84	0.12	-	87,87,87,87	0
56	MG	2A	3081	1/1	0.95	0.09	-	53,53,53,53	0
56	MG	2A	3039	1/1	0.96	0.15	-	25,25,25,25	0
56	MG	2a	1820	1/1	0.91	0.21	-	60,60,60,60	0
56	MG	1A	3999	1/1	0.96	0.17	-	25,25,25,25	0
56	MG	2A	3321	1/1	0.88	0.21	-	44,44,44,44	0
56	MG	1A	3990	1/1	0.90	0.08	-	38,38,38,38	0
56	MG	2a	1741	1/1	0.97	0.09	-	57,57,57,57	0
56	MG	1A	3100	1/1	0.91	0.20	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3588	1/1	0.96	0.16	-	32,32,32,32	0
56	MG	2A	3150	1/1	0.96	0.21	-	49,49,49,49	0
56	MG	1a	3045	1/1	0.98	0.11	-	52,52,52,52	0
56	MG	2A	3720	1/1	0.47	0.17	-	97,97,97,97	0
56	MG	1A	3458	1/1	0.73	0.15	-	68,68,68,68	0
56	MG	1A	3976	1/1	0.95	0.09	-	50,50,50,50	0
56	MG	1A	3273	1/1	0.94	0.09	-	38,38,38,38	0
56	MG	2A	3604	1/1	0.86	0.10	-	58,58,58,58	0
56	MG	1A	3134	1/1	0.94	0.46	-	30,30,30,30	0
56	MG	2A	3533	1/1	0.95	0.34	-	52,52,52,52	0
56	MG	2A	3333	1/1	0.95	0.12	-	25,25,25,25	0
56	MG	1A	3374	1/1	0.92	0.41	-	40,40,40,40	0
56	MG	1a	3095	1/1	0.98	0.12	-	55,55,55,55	0
56	MG	23	101	1/1	0.92	0.61	-	54,54,54,54	0
56	MG	2a	1633	1/1	0.89	0.11	-	63,63,63,63	0
56	MG	2a	1647	1/1	0.84	0.13	-	80,80,80,80	0
56	MG	2A	3595	1/1	0.93	0.09	-	59,59,59,59	0
56	MG	1A	3008	1/1	0.96	0.16	-	18,18,18,18	0
56	MG	1a	3131	1/1	0.98	0.10	-	38,38,38,38	0
56	MG	2A	3051	1/1	0.99	0.05	-	46,46,46,46	0
56	MG	2A	3611	1/1	0.97	0.14	-	47,47,47,47	0
56	MG	2a	1656	1/1	0.77	0.14	-	68,68,68,68	0
56	MG	1A	3568	1/1	0.89	0.10	-	30,30,30,30	0
56	MG	2A	3251	1/1	0.93	0.20	-	49,49,49,49	0
56	MG	2A	3102	1/1	0.87	0.38	-	44,44,44,44	0
56	MG	2A	3503	1/1	0.93	0.16	-	54,54,54,54	0
56	MG	1A	3532	1/1	0.95	0.16	-	29,29,29,29	0
56	MG	1a	3082	1/1	0.96	0.48	-	41,41,41,41	0
56	MG	1A	3041	1/1	0.98	0.11	-	32,32,32,32	0
56	MG	2A	3093	1/1	0.80	0.13	-	58,58,58,58	0
56	MG	1A	3243	1/1	0.91	0.29	-	25,25,25,25	0
56	MG	1A	3204	1/1	0.95	0.29	-	39,39,39,39	0
56	MG	2A	3164	1/1	0.97	0.37	-	53,53,53,53	0
56	MG	1A	3760	1/1	0.81	0.13	-	44,44,44,44	0
56	MG	1A	3394	1/1	0.96	0.23	-	37,37,37,37	0
56	MG	1B	232	1/1	0.82	0.14	-	66,66,66,66	0
56	MG	2A	3475	1/1	0.98	0.20	-	37,37,37,37	0
56	MG	2a	1687	1/1	0.98	0.05	-	40,40,40,40	0
56	MG	1A	3203	1/1	0.90	0.16	-	27,27,27,27	0
56	MG	1A	3357	1/1	0.82	0.23	-	43,43,43,43	0
56	MG	2A	3554	1/1	0.93	0.14	-	24,24,24,24	0
56	MG	1A	3791	1/1	0.98	0.34	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3260	1/1	0.97	0.15	-	18,18,18,18	0
56	MG	2A	3492	1/1	0.88	0.22	-	49,49,49,49	0
56	MG	2A	3459	1/1	0.98	0.08	-	50,50,50,50	0
56	MG	2A	3315	1/1	0.98	0.21	-	42,42,42,42	0
56	MG	2A	3685	1/1	0.92	0.14	-	41,41,41,41	0
56	MG	2A	3412	1/1	0.96	0.14	-	47,47,47,47	0
56	MG	1a	3043	1/1	0.91	0.12	-	50,50,50,50	0
56	MG	1E	304	1/1	0.97	0.33	-	22,22,22,22	0
56	MG	2w	106	1/1	0.73	0.33	-	59,59,59,59	0
56	MG	1A	3349	1/1	0.91	0.13	-	39,39,39,39	0
56	MG	2A	3367	1/1	0.97	0.13	-	28,28,28,28	0
56	MG	1A	3135	1/1	0.88	0.27	-	23,23,23,23	0
56	MG	1A	3369	1/1	0.94	0.11	-	38,38,38,38	0
56	MG	1A	3226	1/1	0.76	0.82	-	49,49,49,49	0
56	MG	2A	3238	1/1	0.91	0.14	-	60,60,60,60	0
56	MG	1A	3800	1/1	0.99	0.20	-	54,54,54,54	0
56	MG	1A	3125	1/1	0.95	0.28	-	19,19,19,19	0
56	MG	2Q	3003	1/1	0.87	0.64	-	52,52,52,52	0
56	MG	1A	3373	1/1	0.88	0.12	-	41,41,41,41	0
56	MG	2A	3023	1/1	0.95	0.12	-	41,41,41,41	0
56	MG	1A	3543	1/1	0.96	0.14	-	20,20,20,20	0
56	MG	2A	3258	1/1	0.64	0.17	-	58,58,58,58	0
56	MG	1a	3144	1/1	0.94	0.19	-	66,66,66,66	0
56	MG	1A	3446	1/1	0.96	0.11	-	43,43,43,43	0
56	MG	1a	3153	1/1	0.96	0.10	-	52,52,52,52	0
56	MG	1a	3123	1/1	0.91	0.13	-	60,60,60,60	0
56	MG	2A	3183	1/1	0.90	0.21	-	38,38,38,38	0
56	MG	1A	3056	1/1	0.95	0.15	-	50,50,50,50	0
56	MG	1A	4016	1/1	0.86	0.11	-	55,55,55,55	0
56	MG	1A	3597	1/1	0.95	0.09	-	50,50,50,50	0
56	MG	1A	3398	1/1	0.88	0.12	-	37,37,37,37	0
56	MG	1A	3759	1/1	0.89	0.13	-	32,32,32,32	0
56	MG	1A	3403	1/1	0.96	0.23	-	33,33,33,33	0
56	MG	1A	3657	1/1	0.97	0.13	-	23,23,23,23	0
56	MG	2a	1605	1/1	0.85	0.13	-	61,61,61,61	0
56	MG	1A	3082	1/1	0.95	0.15	-	40,40,40,40	0
56	MG	1a	3180	1/1	0.87	0.10	-	62,62,62,62	0
56	MG	1A	3234	1/1	0.95	0.11	-	43,43,43,43	0
56	MG	2A	3694	1/1	0.97	0.09	-	54,54,54,54	0
56	MG	2A	3146	1/1	0.94	0.15	-	50,50,50,50	0
56	MG	2A	3059	1/1	0.98	0.16	-	35,35,35,35	0
56	MG	1U	202	1/1	0.96	0.11	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3085	1/1	0.88	0.14	-	13,13,13,13	0
56	MG	2a	1615	1/1	0.85	0.22	-	54,54,54,54	0
56	MG	1A	3091	1/1	0.98	0.18	-	31,31,31,31	0
56	MG	1A	3137	1/1	0.85	0.42	-	40,40,40,40	0
56	MG	2A	3159	1/1	0.92	0.14	-	50,50,50,50	0
56	MG	1A	3291	1/1	0.91	0.21	-	38,38,38,38	0
56	MG	1A	3868	1/1	0.97	0.14	-	24,24,24,24	0
56	MG	1A	3023	1/1	0.97	0.16	-	43,43,43,43	0
56	MG	1A	3527	1/1	0.88	0.24	-	66,66,66,66	0
56	MG	13	102	1/1	0.89	0.13	-	46,46,46,46	0
56	MG	1w	109	1/1	0.99	0.41	-	37,37,37,37	0
56	MG	2A	3637	1/1	0.97	0.10	-	53,53,53,53	0
56	MG	2A	3324	1/1	0.97	0.06	-	40,40,40,40	0
56	MG	2a	1723	1/1	0.91	0.14	-	57,57,57,57	0
56	MG	1a	3189	1/1	0.92	0.12	-	53,53,53,53	0
56	MG	2a	1696	1/1	0.91	0.15	-	48,48,48,48	0
56	MG	2a	1692	1/1	0.95	0.32	-	60,60,60,60	0
56	MG	2A	3122	1/1	0.97	0.15	-	26,26,26,26	0
56	MG	2a	1624	1/1	0.92	0.11	-	78,78,78,78	0
56	MG	1a	3200	1/1	0.95	0.15	-	41,41,41,41	0
56	MG	1A	3513	1/1	0.87	0.16	-	29,29,29,29	0
56	MG	2a	1654	1/1	0.94	0.27	-	58,58,58,58	0
56	MG	2A	3372	1/1	0.95	0.23	-	42,42,42,42	0
56	MG	1a	3029	1/1	0.93	0.10	-	49,49,49,49	0
56	MG	2a	1793	1/1	0.92	0.14	-	53,53,53,53	0
56	MG	1a	3136	1/1	0.97	0.12	-	49,49,49,49	0
56	MG	1A	3287	1/1	0.93	0.13	-	30,30,30,30	0
56	MG	2a	1792	1/1	0.85	0.09	-	61,61,61,61	0
56	MG	1A	3805	1/1	0.94	0.20	-	60,60,60,60	0
56	MG	1A	3079	1/1	0.95	0.16	-	32,32,32,32	0
56	MG	2A	3108	1/1	0.93	0.30	-	49,49,49,49	0
56	MG	1A	3205	1/1	0.94	0.59	-	28,28,28,28	0
56	MG	2A	3226	1/1	0.91	0.32	-	42,42,42,42	0
56	MG	1A	3280	1/1	0.92	0.51	-	26,26,26,26	0
56	MG	21	3001	1/1	0.88	0.54	-	36,36,36,36	0
56	MG	1a	3091	1/1	0.93	0.22	-	46,46,46,46	0
56	MG	2A	3050	1/1	0.93	0.14	-	38,38,38,38	0
56	MG	1V	201	1/1	0.93	0.10	-	40,40,40,40	0
56	MG	1A	3787	1/1	0.94	0.14	-	36,36,36,36	0
56	MG	1a	3032	1/1	0.93	0.19	-	54,54,54,54	0
56	MG	2x	105	1/1	0.98	0.14	-	47,47,47,47	0
56	MG	1A	3059	1/1	0.95	0.20	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3566	1/1	0.89	0.17	-	62,62,62,62	0
56	MG	1A	3207	1/1	0.85	0.28	-	52,52,52,52	0
56	MG	1a	3199	1/1	0.98	0.19	-	47,47,47,47	0
56	MG	1A	3767	1/1	0.95	0.10	-	41,41,41,41	0
56	MG	1A	3811	1/1	0.93	0.08	-	32,32,32,32	0
56	MG	2a	1764	1/1	0.92	0.17	-	51,51,51,51	0
56	MG	1A	3092	1/1	0.94	0.17	-	44,44,44,44	0
56	MG	1A	3765	1/1	0.96	0.20	-	19,19,19,19	0
56	MG	2A	3002	1/1	0.86	0.13	-	61,61,61,61	0
56	MG	2A	3049	1/1	0.89	0.12	-	53,53,53,53	0
56	MG	2B	3007	1/1	0.94	0.10	-	56,56,56,56	0
56	MG	1A	3709	1/1	0.94	0.17	-	30,30,30,30	0
56	MG	1A	3659	1/1	0.95	0.20	-	40,40,40,40	0
56	MG	1A	3104	1/1	0.89	0.22	-	45,45,45,45	0
56	MG	2A	3476	1/1	0.93	0.12	-	44,44,44,44	0
56	MG	1a	3079	1/1	0.97	0.14	-	47,47,47,47	0
56	MG	1A	3320	1/1	0.96	0.07	-	48,48,48,48	0
56	MG	1A	3876	1/1	0.92	0.21	-	34,34,34,34	0
56	MG	1A	3462	1/1	0.94	0.31	-	22,22,22,22	0
56	MG	1a	3081	1/1	0.96	0.09	-	67,67,67,67	0
56	MG	2A	3336	1/1	0.97	0.14	-	58,58,58,58	0
56	MG	1A	3322	1/1	0.95	0.36	-	38,38,38,38	0
56	MG	1A	3120	1/1	0.98	0.33	-	29,29,29,29	0
56	MG	2a	1720	1/1	0.94	0.18	-	66,66,66,66	0
56	MG	2A	3688	1/1	0.90	0.14	-	57,57,57,57	0
56	MG	2A	3599	1/1	0.95	0.09	-	61,61,61,61	0
56	MG	2A	3730	1/1	0.87	0.35	-	32,32,32,32	0
56	MG	1D	301	1/1	0.79	0.28	-	44,44,44,44	0
56	MG	2A	3484	1/1	0.90	0.11	-	70,70,70,70	0
56	MG	2A	3202	1/1	0.88	0.14	-	56,56,56,56	0
56	MG	2A	3526	1/1	0.95	0.11	-	49,49,49,49	0
56	MG	1A	3238	1/1	0.92	0.16	-	33,33,33,33	0
56	MG	2a	1776	1/1	0.98	0.11	-	47,47,47,47	0
56	MG	1A	3580	1/1	0.98	0.07	-	18,18,18,18	0
56	MG	2a	1804	1/1	0.91	0.11	-	48,48,48,48	0
56	MG	1A	4054	1/1	0.94	0.48	-	37,37,37,37	0
56	MG	2A	3524	1/1	0.82	0.12	-	61,61,61,61	0
56	MG	2A	3306	1/1	0.97	0.22	-	47,47,47,47	0
56	MG	2A	3227	1/1	0.96	0.09	-	40,40,40,40	0
56	MG	2A	3105	1/1	0.96	0.22	-	34,34,34,34	0
56	MG	1A	3395	1/1	0.98	0.14	-	33,33,33,33	0
56	MG	1a	3075	1/1	0.96	0.11	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3903	1/1	0.86	0.12	-	23,23,23,23	0
56	MG	1A	3053	1/1	0.98	0.06	-	43,43,43,43	0
56	MG	1a	3049	1/1	0.81	0.16	-	60,60,60,60	0
56	MG	1q	201	1/1	0.92	0.08	-	50,50,50,50	0
56	MG	2A	3182	1/1	0.94	0.64	-	43,43,43,43	0
56	MG	1A	3692	1/1	0.91	0.12	-	29,29,29,29	0
56	MG	2A	3469	1/1	0.98	0.29	-	39,39,39,39	0
56	MG	1A	3136	1/1	0.98	0.08	-	21,21,21,21	0
56	MG	1A	4029	1/1	0.94	0.33	-	36,36,36,36	0
56	MG	2A	3397	1/1	0.98	0.12	-	37,37,37,37	0
56	MG	1A	3719	1/1	0.96	0.08	-	47,47,47,47	0
56	MG	2A	3047	1/1	0.97	0.14	-	60,60,60,60	0
56	MG	1A	3411	1/1	0.90	0.12	-	45,45,45,45	0
56	MG	1w	101	1/1	0.87	0.30	-	74,74,74,74	0
56	MG	2a	1651	1/1	0.82	0.08	-	60,60,60,60	0
56	MG	2A	3655	1/1	0.94	0.15	-	53,53,53,53	0
56	MG	2A	3246	1/1	0.96	0.24	-	48,48,48,48	0
56	MG	2A	3294	1/1	0.94	0.28	-	45,45,45,45	0
56	MG	1A	3919	1/1	0.94	0.15	-	42,42,42,42	0
56	MG	1A	3581	1/1	0.94	0.19	-	19,19,19,19	0
56	MG	1A	3313	1/1	0.87	0.39	-	35,35,35,35	0
56	MG	2a	1787	1/1	0.97	0.06	-	53,53,53,53	0
56	MG	1a	3161	1/1	0.86	0.08	-	53,53,53,53	0
56	MG	1A	3258	1/1	0.99	0.20	-	33,33,33,33	0
56	MG	2a	1773	1/1	0.79	0.20	-	70,70,70,70	0
56	MG	1a	3016	1/1	0.97	0.12	-	38,38,38,38	0
56	MG	2a	1626	1/1	0.89	0.08	-	50,50,50,50	0
56	MG	2A	3718	1/1	0.94	0.10	-	56,56,56,56	0
56	MG	2A	3094	1/1	0.85	0.16	-	47,47,47,47	0
56	MG	1A	3440	1/1	0.96	0.33	-	28,28,28,28	0
56	MG	1a	3062	1/1	0.94	0.08	-	36,36,36,36	0
56	MG	2A	3629	1/1	0.98	0.18	-	62,62,62,62	0
56	MG	2a	1768	1/1	0.96	0.05	-	55,55,55,55	0
56	MG	1Z	3003	1/1	0.73	0.17	-	52,52,52,52	0
56	MG	2A	3187	1/1	0.92	0.26	-	54,54,54,54	0
56	MG	1A	3988	1/1	0.94	0.09	-	34,34,34,34	0
56	MG	1a	3137	1/1	0.96	0.15	-	51,51,51,51	0
56	MG	1A	3881	1/1	0.88	0.11	-	44,44,44,44	0
56	MG	1B	212	1/1	0.81	0.29	-	46,46,46,46	0
56	MG	1A	3124	1/1	0.96	0.07	-	33,33,33,33	0
56	MG	2A	3280	1/1	0.87	0.47	-	50,50,50,50	0
56	MG	1a	3103	1/1	0.93	0.07	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3340	1/1	0.93	0.13	-	47,47,47,47	0
56	MG	2A	3005	1/1	0.95	0.11	-	42,42,42,42	0
56	MG	2A	3232	1/1	0.91	0.12	-	54,54,54,54	0
56	MG	2A	3666	1/1	0.89	0.14	-	46,46,46,46	0
56	MG	2A	3632	1/1	0.94	0.32	-	62,62,62,62	0
56	MG	2A	3169	1/1	0.96	0.07	-	45,45,45,45	0
56	MG	2A	3288	1/1	0.99	0.25	-	30,30,30,30	0
56	MG	2a	1677	1/1	0.94	0.15	-	55,55,55,55	0
56	MG	1A	3898	1/1	0.56	0.15	-	71,71,71,71	0
56	MG	1a	3167	1/1	0.94	0.07	-	42,42,42,42	0
56	MG	2A	3220	1/1	0.86	0.12	-	49,49,49,49	0
56	MG	2a	1757	1/1	0.93	0.12	-	48,48,48,48	0
56	MG	1A	3420	1/1	0.92	0.13	-	49,49,49,49	0
56	MG	1A	3779	1/1	0.88	0.10	-	50,50,50,50	0
56	MG	1A	3086	1/1	0.81	0.15	-	55,55,55,55	0
56	MG	2A	3318	1/1	0.90	0.34	-	42,42,42,42	0
56	MG	1A	3501	1/1	0.96	0.21	-	30,30,30,30	0
56	MG	1A	3785	1/1	0.95	0.20	-	35,35,35,35	0
56	MG	1a	3204	1/1	0.98	0.10	-	44,44,44,44	0
56	MG	1A	3293	1/1	0.78	0.23	-	51,51,51,51	0
56	MG	2a	1699	1/1	0.97	0.05	-	58,58,58,58	0
56	MG	1A	3793	1/1	0.99	0.25	-	26,26,26,26	0
56	MG	1a	3024	1/1	0.80	0.16	-	52,52,52,52	0
56	MG	2B	3012	1/1	0.79	0.16	-	75,75,75,75	0
56	MG	1a	3023	1/1	0.94	0.15	-	44,44,44,44	0
56	MG	2B	3011	1/1	0.95	0.14	-	69,69,69,69	0
56	MG	2A	3338	1/1	0.90	0.26	-	42,42,42,42	0
56	MG	1A	4018	1/1	0.91	0.34	-	24,24,24,24	0
56	MG	1A	3265	1/1	0.92	0.18	-	26,26,26,26	0
56	MG	2a	1771	1/1	0.95	0.11	-	62,62,62,62	0
56	MG	1B	237	1/1	0.95	0.16	-	46,46,46,46	0
56	MG	2A	3311	1/1	0.85	0.23	-	50,50,50,50	0
56	MG	1A	3523	1/1	0.82	0.12	-	46,46,46,46	0
56	MG	2A	3259	1/1	0.75	0.20	-	53,53,53,53	0
56	MG	2a	1686	1/1	0.90	0.23	-	67,67,67,67	0
56	MG	2A	3222	1/1	0.93	0.16	-	44,44,44,44	0
56	MG	2A	3721	1/1	0.98	0.07	-	50,50,50,50	0
56	MG	1A	3047	1/1	0.86	0.14	-	50,50,50,50	0
56	MG	1A	3911	1/1	0.97	0.10	-	29,29,29,29	0
56	MG	2A	3007	1/1	0.94	0.10	-	32,32,32,32	0
56	MG	2a	1685	1/1	0.93	0.10	-	53,53,53,53	0
56	MG	1a	3005	1/1	0.95	0.11	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3426	1/1	0.87	0.18	-	48,48,48,48	0
56	MG	1A	3679	1/1	0.79	0.23	-	14,14,14,14	0
56	MG	2A	3139	1/1	0.91	0.13	-	41,41,41,41	0
56	MG	2A	3471	1/1	0.93	0.20	-	37,37,37,37	0
56	MG	2A	3276	1/1	0.92	0.21	-	58,58,58,58	0
56	MG	1A	3784	1/1	0.97	0.12	-	57,57,57,57	0
56	MG	1A	3781	1/1	0.84	0.19	-	51,51,51,51	0
56	MG	1A	3867	1/1	0.93	0.14	-	19,19,19,19	0
56	MG	1A	3338	1/1	0.99	0.22	-	19,19,19,19	0
56	MG	2P	201	1/1	0.97	0.13	-	54,54,54,54	0
56	MG	2a	1829	1/1	0.82	0.30	-	68,68,68,68	0
56	MG	1A	3697	1/1	0.89	0.20	-	27,27,27,27	0
56	MG	1a	3184	1/1	0.97	0.08	-	49,49,49,49	0
56	MG	2a	1782	1/1	0.95	0.14	-	58,58,58,58	0
56	MG	1A	3633	1/1	0.97	0.10	-	52,52,52,52	0
56	MG	2A	3219	1/1	0.91	0.32	-	54,54,54,54	0
56	MG	2a	1662	1/1	0.81	0.11	-	59,59,59,59	0
56	MG	2A	3558	1/1	0.82	0.28	-	50,50,50,50	0
56	MG	2a	1805	1/1	0.96	0.05	-	53,53,53,53	0
56	MG	2A	3498	1/1	0.95	0.06	-	46,46,46,46	0
56	MG	1a	3093	1/1	0.91	0.16	-	49,49,49,49	0
56	MG	1A	3459	1/1	0.80	0.20	-	53,53,53,53	0
56	MG	2A	3502	1/1	0.92	0.16	-	42,42,42,42	0
56	MG	2w	109	1/1	0.74	0.13	-	63,63,63,63	0
56	MG	2A	3620	1/1	0.92	0.09	-	34,34,34,34	0
57	K	2A	3745	1/1	0.97	0.08	-	53,53,53,53	0
56	MG	1A	3478	1/1	0.94	0.20	-	47,47,47,47	0
56	MG	2A	3179	1/1	0.93	0.17	-	45,45,45,45	0
56	MG	1y	103	1/1	0.84	0.26	-	82,82,82,82	0
56	MG	2A	3098	1/1	0.90	0.35	-	68,68,68,68	0
56	MG	1A	3564	1/1	0.94	0.21	-	36,36,36,36	0
56	MG	2A	3479	1/1	0.95	0.15	-	34,34,34,34	0
56	MG	1A	3107	1/1	0.91	0.26	-	24,24,24,24	0
56	MG	2A	3439	1/1	0.81	0.11	-	49,49,49,49	0
56	MG	2B	3014	1/1	0.83	0.31	-	71,71,71,71	0
56	MG	1A	3151	1/1	0.95	0.21	-	36,36,36,36	0
56	MG	2a	1638	1/1	0.91	0.23	-	49,49,49,49	0
56	MG	2a	1650	1/1	0.89	0.16	-	68,68,68,68	0
56	MG	1A	3517	1/1	0.97	0.15	-	28,28,28,28	0
56	MG	1A	3735	1/1	0.89	0.14	-	22,22,22,22	0
56	MG	2j	8002	1/1	0.94	0.05	-	62,62,62,62	0
56	MG	1A	3282	1/1	0.88	0.21	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	2A	3260	1/1	0.96	0.16	-	48,48,48,48	0
56	MG	2A	3640	1/1	0.92	0.23	-	47,47,47,47	0
56	MG	1O	201	1/1	0.90	0.15	-	45,45,45,45	0
56	MG	1B	216	1/1	0.98	0.16	-	42,42,42,42	0
56	MG	1a	3191	1/1	0.94	0.08	-	53,53,53,53	0
56	MG	2A	3738	1/1	0.86	0.17	-	63,63,63,63	0
56	MG	1A	3343	1/1	0.97	0.24	-	30,30,30,30	0
56	MG	1A	3973	1/1	0.95	0.13	-	47,47,47,47	0
56	MG	1A	3325	1/1	0.98	0.13	-	33,33,33,33	0
56	MG	2A	3201	1/1	0.76	0.20	-	55,55,55,55	0
56	MG	2a	1642	1/1	0.89	0.21	-	55,55,55,55	0
56	MG	1A	3801	1/1	0.83	0.25	-	71,71,71,71	0
56	MG	1A	3342	1/1	0.95	0.32	-	21,21,21,21	0
56	MG	1a	3086	1/1	0.97	0.07	-	60,60,60,60	0
56	MG	2A	3322	1/1	0.87	0.36	-	55,55,55,55	0
56	MG	2A	3539	1/1	0.86	0.10	-	59,59,59,59	0
56	MG	1B	211	1/1	0.70	0.75	-	45,45,45,45	0
56	MG	1A	3861	1/1	0.90	0.12	-	58,58,58,58	0
56	MG	2A	3577	1/1	0.95	0.21	-	45,45,45,45	0
56	MG	1A	3493	1/1	0.93	0.32	-	23,23,23,23	0
56	MG	2a	1606	1/1	0.96	0.07	-	43,43,43,43	0
56	MG	1A	3363	1/1	0.82	0.17	-	32,32,32,32	0
56	MG	2a	1621	1/1	0.89	0.55	-	65,65,65,65	0
56	MG	2A	3481	1/1	0.92	0.25	-	58,58,58,58	0
56	MG	2a	1635	1/1	0.95	0.15	-	39,39,39,39	0
56	MG	1A	3261	1/1	0.92	0.10	-	35,35,35,35	0
56	MG	1Z	3001	1/1	0.93	0.26	-	42,42,42,42	0
56	MG	1a	3067	1/1	0.95	0.16	-	46,46,46,46	0
56	MG	1A	3109	1/1	0.93	0.41	-	50,50,50,50	0
56	MG	1A	4009	1/1	0.89	0.22	-	41,41,41,41	0
56	MG	1O	204	1/1	0.97	0.10	-	45,45,45,45	0
56	MG	2a	1794	1/1	0.95	0.15	-	58,58,58,58	0
56	MG	2A	3519	1/1	0.97	0.14	-	35,35,35,35	0
56	MG	2A	3404	1/1	0.98	0.18	-	39,39,39,39	0
56	MG	2A	3281	1/1	0.86	0.09	-	60,60,60,60	0
56	MG	1A	3351	1/1	0.95	0.11	-	34,34,34,34	0
56	MG	2A	3711	1/1	0.96	0.07	-	37,37,37,37	0
56	MG	1a	3092	1/1	0.90	0.11	-	55,55,55,55	0
56	MG	1A	3121	1/1	0.90	0.39	-	33,33,33,33	0
56	MG	2A	3699	1/1	0.95	0.11	-	39,39,39,39	0
56	MG	1a	3078	1/1	0.97	0.11	-	48,48,48,48	0
56	MG	1A	3875	1/1	0.96	0.17	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
56	MG	2A	3635	1/1	0.91	0.14	-	57,57,57,57	0
56	MG	2a	1636	1/1	0.83	0.09	-	66,66,66,66	0
56	MG	2A	3451	1/1	0.96	0.09	-	44,44,44,44	0
56	MG	1A	3698	1/1	0.92	0.12	-	41,41,41,41	0
56	MG	1A	4004	1/1	0.94	0.27	-	55,55,55,55	0
56	MG	1B	225	1/1	0.94	0.17	-	57,57,57,57	0
56	MG	1A	3814	1/1	0.97	0.14	-	8,8,8,8	0
56	MG	1w	108	1/1	0.85	0.16	-	66,66,66,66	0
56	MG	2j	8001	1/1	0.83	0.11	-	66,66,66,66	0
56	MG	1A	3366	1/1	0.69	0.29	-	50,50,50,50	0
56	MG	1A	3330	1/1	0.93	0.17	-	28,28,28,28	0
56	MG	1A	3419	1/1	0.96	0.14	-	42,42,42,42	0
56	MG	1A	3145	1/1	0.92	0.62	-	34,34,34,34	0
56	MG	2a	1707	1/1	0.93	0.22	-	68,68,68,68	0
56	MG	1G	3004	1/1	0.94	0.11	-	38,38,38,38	0
56	MG	1A	3122	1/1	0.96	0.13	-	32,32,32,32	0
56	MG	1A	3897	1/1	0.93	0.14	-	44,44,44,44	0
56	MG	2a	1721	1/1	0.95	0.04	-	73,73,73,73	0
56	MG	1A	4017	1/1	0.97	0.41	-	37,37,37,37	0
56	MG	1s	101	1/1	0.93	0.20	-	62,62,62,62	0
56	MG	2A	3653	1/1	0.83	0.22	-	37,37,37,37	0
56	MG	1A	3388	1/1	0.95	0.18	-	30,30,30,30	0
56	MG	1a	3055	1/1	0.92	0.14	-	49,49,49,49	0
56	MG	1a	3196	1/1	0.94	0.06	-	46,46,46,46	0
56	MG	2A	3118	1/1	0.93	0.19	-	42,42,42,42	0
56	MG	2A	3474	1/1	0.95	0.15	-	35,35,35,35	0
56	MG	1a	3201	1/1	0.98	0.06	-	44,44,44,44	0
56	MG	1Q	205	1/1	0.92	0.11	-	28,28,28,28	0
56	MG	2A	3161	1/1	0.93	0.37	-	46,46,46,46	0
56	MG	2A	3676	1/1	0.86	0.13	-	79,79,79,79	0
56	MG	1A	3259	1/1	0.95	0.16	-	45,45,45,45	0
56	MG	1A	3036	1/1	0.90	0.21	-	26,26,26,26	0
56	MG	1A	3447	1/1	0.92	0.32	-	47,47,47,47	0
56	MG	2a	1713	1/1	0.89	0.13	-	48,48,48,48	0
56	MG	2E	302	1/1	0.97	0.09	-	44,44,44,44	0
56	MG	1A	3598	1/1	0.96	0.34	-	48,48,48,48	0
56	MG	2a	1808	1/1	0.87	0.19	-	58,58,58,58	0
56	MG	1A	3948	1/1	0.98	0.09	-	14,14,14,14	0
56	MG	1A	3264	1/1	0.91	0.09	-	39,39,39,39	0
56	MG	2A	3075	1/1	0.92	0.16	-	51,51,51,51	0
56	MG	2A	3250	1/1	0.92	0.15	-	51,51,51,51	0
56	MG	1A	3379	1/1	0.92	0.39	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1a	3089	1/1	0.85	0.15	-	40,40,40,40	0
56	MG	1A	3717	1/1	0.96	0.10	-	45,45,45,45	0
56	MG	2A	3151	1/1	0.97	0.09	-	47,47,47,47	0
56	MG	1A	3604	1/1	0.97	0.11	-	28,28,28,28	0
56	MG	1A	3624	1/1	0.94	0.13	-	26,26,26,26	0
56	MG	2A	3598	1/1	0.95	0.14	-	39,39,39,39	0
56	MG	2A	3591	1/1	0.92	0.12	-	34,34,34,34	0
56	MG	1A	3152	1/1	0.92	0.17	-	43,43,43,43	0
56	MG	1A	3248	1/1	0.82	0.14	-	49,49,49,49	0
56	MG	2O	8002	1/1	0.94	0.12	-	52,52,52,52	0
56	MG	2A	3178	1/1	0.93	0.17	-	44,44,44,44	0
56	MG	2A	3647	1/1	0.97	0.11	-	51,51,51,51	0
56	MG	2A	3188	1/1	0.87	0.12	-	57,57,57,57	0
56	MG	2A	3234	1/1	0.91	0.34	-	47,47,47,47	0
56	MG	1a	3026	1/1	0.84	0.11	-	72,72,72,72	0
56	MG	2E	309	1/1	0.99	0.06	-	41,41,41,41	0
56	MG	1E	301	1/1	0.90	0.59	-	26,26,26,26	0
56	MG	1A	3968	1/1	0.90	0.20	-	55,55,55,55	0
56	MG	1A	3944	1/1	0.88	0.13	-	39,39,39,39	0
56	MG	2A	3436	1/1	0.83	0.14	-	62,62,62,62	0
56	MG	1a	3186	1/1	0.87	0.19	-	48,48,48,48	0
56	MG	1A	3389	1/1	0.94	0.21	-	34,34,34,34	0
56	MG	2a	1767	1/1	0.91	0.08	-	39,39,39,39	0
56	MG	1A	3114	1/1	0.97	0.32	-	22,22,22,22	0
56	MG	2A	3018	1/1	0.91	0.37	-	51,51,51,51	0
56	MG	2A	3104	1/1	0.94	0.12	-	51,51,51,51	0
56	MG	1a	3146	1/1	0.93	0.16	-	64,64,64,64	0
56	MG	1A	3938	1/1	0.92	0.26	-	40,40,40,40	0
56	MG	1a	3066	1/1	0.95	0.10	-	58,58,58,58	0
56	MG	2a	1618	1/1	0.95	0.42	-	51,51,51,51	0
56	MG	2A	3435	1/1	0.94	0.11	-	47,47,47,47	0
56	MG	2A	3200	1/1	0.95	0.24	-	50,50,50,50	0
56	MG	1Y	502	1/1	0.91	0.10	-	67,67,67,67	0
56	MG	1a	3179	1/1	0.99	0.13	-	39,39,39,39	0
56	MG	1A	3622	1/1	0.90	0.08	-	56,56,56,56	0
56	MG	2a	1668	1/1	0.96	0.17	-	55,55,55,55	0
56	MG	2A	3567	1/1	0.95	0.10	-	44,44,44,44	0
56	MG	2a	1701	1/1	0.89	0.10	-	72,72,72,72	0
56	MG	2a	1745	1/1	0.87	0.13	-	64,64,64,64	0
56	MG	1A	3323	1/1	0.94	0.22	-	19,19,19,19	0
56	MG	1A	3195	1/1	0.92	0.49	-	27,27,27,27	0
56	MG	2A	3689	1/1	0.87	0.13	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3500	1/1	0.97	0.13	-	49,49,49,49	0
56	MG	2a	1783	1/1	0.92	0.11	-	62,62,62,62	0
56	MG	1A	3774	1/1	0.96	0.11	-	56,56,56,56	0
56	MG	1A	3052	1/1	0.87	0.14	-	31,31,31,31	0
56	MG	1A	3448	1/1	0.97	0.18	-	37,37,37,37	0
56	MG	1A	3946	1/1	0.96	0.11	-	46,46,46,46	0
56	MG	2A	3270	1/1	0.96	0.33	-	34,34,34,34	0
56	MG	1A	3818	1/1	0.95	0.05	-	21,21,21,21	0
56	MG	2A	3593	1/1	0.93	0.16	-	47,47,47,47	0
56	MG	2A	3058	1/1	0.81	0.20	-	65,65,65,65	0
56	MG	2A	3408	1/1	0.92	0.10	-	53,53,53,53	0
56	MG	1A	3871	1/1	0.97	0.05	-	59,59,59,59	0
56	MG	2A	3174	1/1	0.88	0.24	-	47,47,47,47	0

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

There are no such residues in this entry.