



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 11:20 AM EDT

PDB ID : 4V9S  
Title : Crystal structure of antibiotic GE82832 bound to 70S ribosome  
Authors : Bulkley, D.P.; Brandi, L.; Polikanov, Y.S.; Fabbretti, A.; O'Connor, M.;  
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Deposited on : 2013-12-05  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

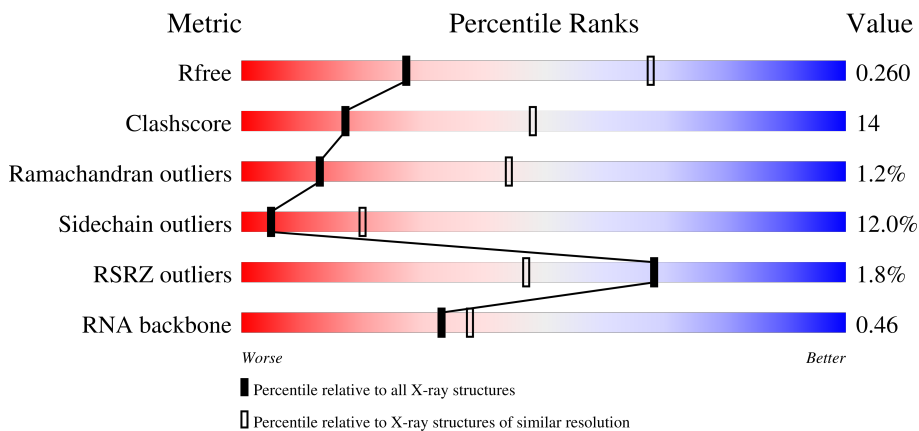
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	 2% 36% 43% 17% ••
1	CA	1522	 2% 34% 43% 18% ••
2	AB	256	 3% 38% 39% 11% • 10%
2	CB	256	 5% 36% 44% 10% 10%

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Mol	Chain	Length	Quality of chain
3	AC	239	3% 51% 32% 14%
3	CC	239	5% 51% 29% 14%
4	AD	209	2% 52% 37% 10%
4	CD	209	55% 38% 7%
5	AE	162	50% 37% 9%
5	CE	162	56% 33% 9%
6	AF	101	56% 40% 2%
6	CF	101	62% 33% 2%
7	AG	156	7% 63% 31% 2%
7	CG	156	6% 54% 39% 6%
8	AH	138	55% 36% 8%
8	CH	138	56% 38% 5%
9	AI	128	6% 50% 41% 7%
9	CI	128	17% 45% 44% 10%
10	AJ	105	11% 55% 31% 6% 8%
10	CJ	105	11% 47% 40% 5% 9%
11	AK	129	65% 19% 5% 12%
11	CK	129	2% 55% 33% 12%
12	AL	132	61% 29% 8%
12	CL	132	57% 32% 8%
13	AM	126	7% 68% 24% 6%
13	CM	126	9% 51% 38% 8%
14	AN	61	3% 51% 43% 5%
14	CN	61	7% 49% 44% 5%
15	AO	89	70% 25% 2%






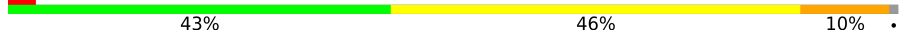



















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Mol	Chain	Length	Quality of chain
15	CO	89	% 58% 31% 9% 2% 2%
16	AP	88	2% 50% 38% 6% 7%
16	CP	88	59% 32% 7% 2% 2%
17	AQ	105	68% 24% 6% 2% 2%
17	CQ	105	70% 22% 6% 2% 2%
18	AR	88	55% 20% 23% 2% 2%
18	CR	88	41% 31% 5% 23%
19	AS	93	12% 45% 40% 11% 2%
19	CS	93	17% 38% 43% 9% 11%
20	AT	106	55% 27% 8% 9%
20	CT	106	% 54% 29% 6% 9%
21	AU	27	19% 56% 22% 7% 15%
21	CU	27	19% 48% 30% 7% 15%
22	AV	24	21% 8% 71%
22	CV	24	21% 75%
23	AX	77	58% 25% 13% 2% 2%
23	CX	77	40% 39% 17% 2% 2%
24	AW	10	10% 20% 60% 10%
24	CW	10	10% 10% 70% 10%
25	BA	2915	47% 34% 10% 6% 2%
25	DA	2915	% 38% 40% 13% 7% 2%
26	BB	122	51% 35% 12% 2% 2%
26	DB	122	36% 50% 10% 2% 2%
27	BD	276	72% 24% 2% 2% 2%
27	DD	276	66% 27% 7% 2% 2%

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Mol	Chain	Length	Quality of chain
28	BE	206	 71% 21% 7% .
28	DE	206	 62% 30% 6% ..
29	BF	210	 65% 28% . .
29	DF	210	 56% 36% . .
30	BG	182	 61% 32% 6% .
30	DG	182	 3% 43% 46% 10% .
31	BH	180	 64% 28% . .
31	DH	180	 9% 52% 39% 5% .
32	BI	148	 49% 39% 11% .
32	DI	148	 3% 58% 34% 6% .
33	BN	140	 78% 19% .
33	DN	140	 69% 27% .
34	BO	122	 72% 25% ..
34	DO	122	 61% 34% .
35	BP	150	 70% 25% . .
35	DP	150	 % 65% 28% 7% .
36	BQ	141	 62% 31% 6%
36	DQ	141	 55% 40% 5%
37	BR	118	 65% 25% 9%
37	DR	118	 60% 34% 6%
38	BS	112	 70% 22% 6% .
38	DS	112	 4% 46% 45% 8% .
39	BT	146	 62% 26% . 10%
39	DT	146	 60% 27% . 10%
40	BU	118	 69% 25% . .




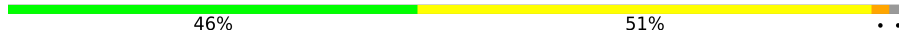


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Mol	Chain	Length	Quality of chain
40	DU	118	66% 27% 5% .
41	BV	101	81% 14% . .
41	DV	101	69% 27% . .
42	BW	113	79% 17% . .
42	DW	113	73% 23% . .
43	BX	96	73% 24% . .
43	DX	96	2% 61% 36% . .
44	BY	110	2% 65% 30% . .
44	DY	110	4% 67% 28% . .
45	BZ	206	48% 30% 5% 17%
45	DZ	206	50% 31% . 16%
46	B0	85	8% 65% 29% . .
46	D0	85	12% 68% 24% 6% .
47	B1	98	1% 71% 21% 6% .
47	D1	98	1% 63% 30% 6% .
48	B2	72	54% 39% . .
48	D2	72	60% 31% 7% .
49	B3	60	50% 43% 5% .
49	D3	60	2% 65% 25% 8% .
50	B4	71	1% 41% 41% 13% . .
50	D4	71	7% 48% 37% 11% . .
51	B5	60	72% 23% . .
51	D5	60	70% 23% 5% .
52	B6	54	67% 22% 9% .
52	D6	54	72% 22% . .

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Mol	Chain	Length	Quality of chain
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	D9	37	

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
24	2QY	CW	10	-	-	X	-
24	MVA	CW	9	-	-	X	-
56	MG	AA	3028	-	-	-	X
56	MG	AA	3035	-	-	-	X
56	MG	AA	3037	-	-	-	X
56	MG	AA	3043	-	-	-	X
56	MG	AA	3051	-	-	-	X
56	MG	AA	3079	-	-	-	X
56	MG	AA	3089	-	-	-	X
56	MG	AA	3093	-	-	-	X
56	MG	AA	3100	-	-	-	X
56	MG	AA	3114	-	-	-	X
56	MG	AA	3116	-	-	-	X
56	MG	AA	3120	-	-	-	X
56	MG	AA	3147	-	-	-	X
56	MG	B1	3001	-	-	-	X
56	MG	BA	3065	-	-	-	X
56	MG	BA	3069	-	-	-	X
56	MG	BA	3085	-	-	-	X
56	MG	BA	3087	-	-	-	X
56	MG	BA	3089	-	-	-	X
56	MG	BA	3094	-	-	-	X
56	MG	BA	3160	-	-	-	X
56	MG	BA	3231	-	-	-	X
56	MG	BA	3247	-	-	-	X
56	MG	BA	3295	-	-	-	X
56	MG	BA	3297	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
56	MG	BA	3622	-	-	-	X
56	MG	BA	3699	-	-	-	X
56	MG	CA	3016	-	-	-	X
56	MG	CA	3024	-	-	-	X
56	MG	CA	3030	-	-	-	X
56	MG	CA	3038	-	-	-	X
56	MG	CA	3041	-	-	-	X
56	MG	CA	3042	-	-	-	X
56	MG	CA	3053	-	-	-	X
56	MG	CA	3135	-	-	-	X
56	MG	DA	3064	-	-	-	X
56	MG	DA	3098	-	-	-	X
56	MG	DA	3103	-	-	-	X
56	MG	DA	3125	-	-	-	X
56	MG	DA	3186	-	-	-	X
56	MG	DA	3427	-	-	-	X
56	MG	DA	3438	-	-	-	X
56	MG	DA	3464	-	-	-	X
56	MG	DA	3545	-	-	-	X
56	MG	DA	3581	-	-	-	X
56	MG	DA	3615	-	-	-	X
56	MG	DW	202	-	-	-	X
59	FME	CX	101	-	-	-	X



## 2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 286321 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 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1498	Total	C	N	O	P	0	0	0
			32196	14328	5966	10404	1498			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

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

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
8	CH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			983	623	193	167			
9	CI	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AJ	97	Total	C	N	O	0	0	0
			709	440	138	131			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	CJ	96	714	445	138	131	0	0	0

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AK	114	829	516	155	155	3	0	0	0
11	CK	114	833	519	156	155	3	0	0	0

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AL	122	930	585	185	159	1	0	0	0
12	CL	122	930	585	185	159	1	0	0	0

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

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

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	AN	60	492	312	104	72	4	0	0	0
14	CN	60	492	312	104	72	4	0	0	0

- Molecule 15 is a protein called 30S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AO	88	728	456	144	126	2	0	0	0
15	CO	88	728	456	144	126	2	0	0	0

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
16	CP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	CR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
19	CS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
20	CT	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	7	Total	C	N	O	P	0	0	1
			114	49	22	37	6			
22	CV	6	Total	C	N	O	P	0	0	0
			113	49	22	36	6			

- Molecule 23 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	76	Total	C	N	O	P	0	0	0
			1623	723	294	530	76			
23	CX	76	Total	C	N	O	P	0	0	0
			1623	723	294	530	76			

- Molecule 24 is a protein called GE82832.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AW	10	Total	C	N	O	0	0	0
			93	67	10	16			
24	CW	10	Total	C	N	O	0	0	0
			93	67	10	16			

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2731	Total	C	N	O	P	0	0	0
			58834	26185	11020	18899	2730			
25	DA	2714	Total	C	N	O	P	0	0	0
			58458	26018	10942	18786	2712			

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
26	DB	120	2573	1146	476	832	119	0	0	0

- Molecule 27 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	BD	275	2136	1349	423	361	3	0	0	0
27	DD	275	2136	1349	423	361	3	0	0	0

- Molecule 28 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	BE	204	1559	985	298	270	6	0	0	0
28	DE	204	1559	985	298	270	6	0	0	0

- Molecule 29 is a protein called 50S Ribosomal Protein L4.

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

- Molecule 30 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	BG	181	1425	914	256	251	4	0	0	0
30	DG	181	1424	911	258	251	4	0	0	0

- Molecule 31 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	BH	174	1330	845	248	236	1	0	0	0
31	DH	174	1330	845	248	236	1	0	0	0

- Molecule 32 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	BI	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
32	DI	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	1			

- Molecule 33 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	BN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
33	DN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 34 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
34	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 35 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	BP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
35	DP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 36 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 37 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 38 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BS	110	Total	C	N	O	S	0	0	0
			877	553	175	149				
38	DS	110	Total	C	N	O	S	0	0	0
			870	549	173	148				

- Molecule 39 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
39	DT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 40 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
40	DU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 41 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
41	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 42 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	DW	112	886	557	174	153	2	0	0	0

- Molecule 43 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	BX	95	750	488	135	126	1	0	0	0
43	DX	95	750	488	135	126	1	0	0	0

- Molecule 44 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	BY	107	806	517	152	131	6	0	0	0
44	DY	107	806	517	152	131	6	0	0	0

- Molecule 45 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BZ	171	1349	862	243	242	2	0	0	0
45	DZ	174	1360	870	243	245	2	0	0	0

- Molecule 46 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	B0	83	653	404	139	109	1	0	0	0
46	D0	83	653	404	139	109	1	0	0	0

- Molecule 47 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	B1	97	755	475	148	131	1	0	0	0
47	D1	97	755	475	148	131	1	0	0	0

- Molecule 48 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
48	D2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 49 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B3	59	Total	C	N	O	0	0	0
			469	298	90	81			
49	D3	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 50 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	69	Total	C	N	O	S	0	0	0
			551	348	99	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			531	338	97	91	5			

- Molecule 51 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
51	D5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 52 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
52	D6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 53 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
53	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 54 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			
54	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 55 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
55	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	221	Total	Mg	0	0
			221	221		
56	AD	1	Total	Mg	0	0
			1	1		
56	AF	1	Total	Mg	0	0
			1	1		
56	AK	1	Total	Mg	0	0
			1	1		
56	AM	1	Total	Mg	0	0
			1	1		
56	AN	2	Total	Mg	0	0
			2	2		
56	AV	1	Total	Mg	0	0
			1	1		
56	AX	9	Total	Mg	0	0
			9	9		
56	BA	738	Total	Mg	0	0
			738	738		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BB	18	Total 18	Mg 18	0	0
56	BD	12	Total 12	Mg 12	0	0
56	BE	10	Total 10	Mg 10	0	0
56	BF	8	Total 8	Mg 8	0	0
56	BG	4	Total 4	Mg 4	0	0
56	BN	6	Total 6	Mg 6	0	0
56	BO	1	Total 1	Mg 1	0	0
56	BP	4	Total 4	Mg 4	0	0
56	BQ	5	Total 5	Mg 5	0	0
56	BR	4	Total 4	Mg 4	0	0
56	BU	8	Total 8	Mg 8	0	0
56	BV	4	Total 4	Mg 4	0	0
56	BW	5	Total 5	Mg 5	0	0
56	BX	1	Total 1	Mg 1	0	0
56	BY	1	Total 1	Mg 1	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	B0	4	Total 4	Mg 4	0	0
56	B1	1	Total 1	Mg 1	0	0
56	B2	1	Total 1	Mg 1	0	0
56	B3	3	Total 3	Mg 3	0	0
56	B4	1	Total 1	Mg 1	0	0

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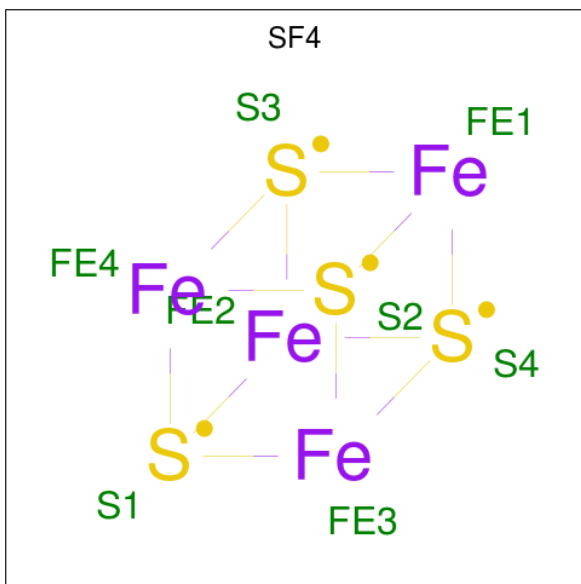
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B5	1	Total 1	Mg 1	0	0
56	B7	4	Total 4	Mg 4	0	0
56	B8	3	Total 3	Mg 3	0	0
56	B9	1	Total 1	Mg 1	0	0
56	CA	172	Total 172	Mg 172	0	0
56	CE	2	Total 2	Mg 2	0	0
56	CF	1	Total 1	Mg 1	0	0
56	CQ	1	Total 1	Mg 1	0	0
56	CT	1	Total 1	Mg 1	0	0
56	CX	3	Total 3	Mg 3	0	0
56	DA	653	Total 653	Mg 653	0	0
56	DB	12	Total 12	Mg 12	0	0
56	DD	8	Total 8	Mg 8	0	0
56	DE	6	Total 6	Mg 6	0	0
56	DF	6	Total 6	Mg 6	0	0
56	DG	1	Total 1	Mg 1	0	0
56	DN	1	Total 1	Mg 1	0	0
56	DO	1	Total 1	Mg 1	0	0
56	DQ	5	Total 5	Mg 5	0	0
56	DR	2	Total 2	Mg 2	0	0
56	DV	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DW	2	Total Mg 2 2	0	0
56	DY	1	Total Mg 1 1	0	0
56	D0	1	Total Mg 1 1	0	0
56	D3	1	Total Mg 1 1	0	0
56	D5	2	Total Mg 2 2	0	0
56	D8	1	Total Mg 1 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AD	1	Total Fe S 8 4 4	0	0
57	CD	1	Total Fe S 8 4 4	0	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

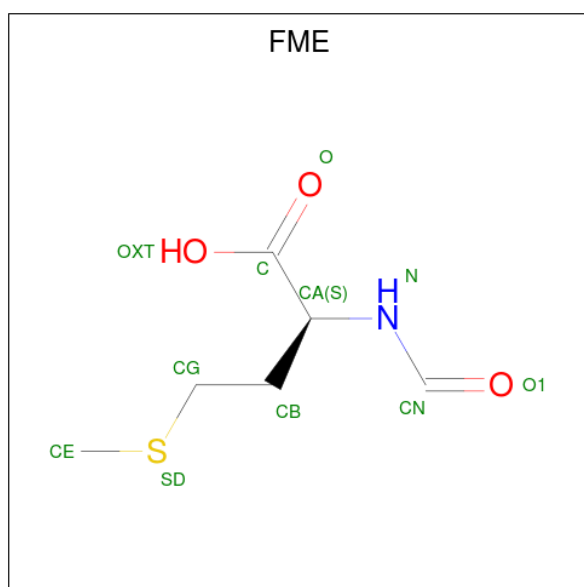
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AN	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	BY	1	Total Zn 1 1	0	0
58	B4	1	Total Zn 1 1	0	0
58	B5	1	Total Zn 1 1	0	0
58	B6	1	Total Zn 1 1	0	0
58	B9	1	Total Zn 1 1	0	0
58	CN	1	Total Zn 1 1	0	0
58	DY	1	Total Zn 1 1	0	0
58	D4	1	Total Zn 1 1	0	0
58	D5	1	Total Zn 1 1	0	0
58	D6	1	Total Zn 1 1	0	0
58	D9	1	Total Zn 1 1	0	0

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	AX	1	Total	C	N	O	S	0	0
			10	6	1	2	1		
59	CX	1	Total	C	N	O	S	0	0
			10	6	1	2	1		

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BA	1	Total	K	0	0
			1	1		
60	DA	1	Total	K	0	0
			1	1		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	148	Total	O	0	0
			148	148		
61	AD	1	Total	O	0	0
			1	1		
61	AE	3	Total	O	0	0
			3	3		
61	AJ	1	Total	O	0	0
			1	1		
61	AL	1	Total	O	0	0
			1	1		
61	AP	1	Total	O	0	0
			1	1		
61	AU	1	Total	O	0	0
			1	1		
61	AV	1	Total	O	0	0
			1	1		
61	AX	1	Total	O	0	0
			1	1		
61	BA	1092	Total	O	0	0
			1092	1092		
61	BB	26	Total	O	0	0
			26	26		
61	BD	8	Total	O	0	0
			8	8		
61	BE	9	Total	O	0	0
			9	9		
61	BF	4	Total	O	0	0
			4	4		

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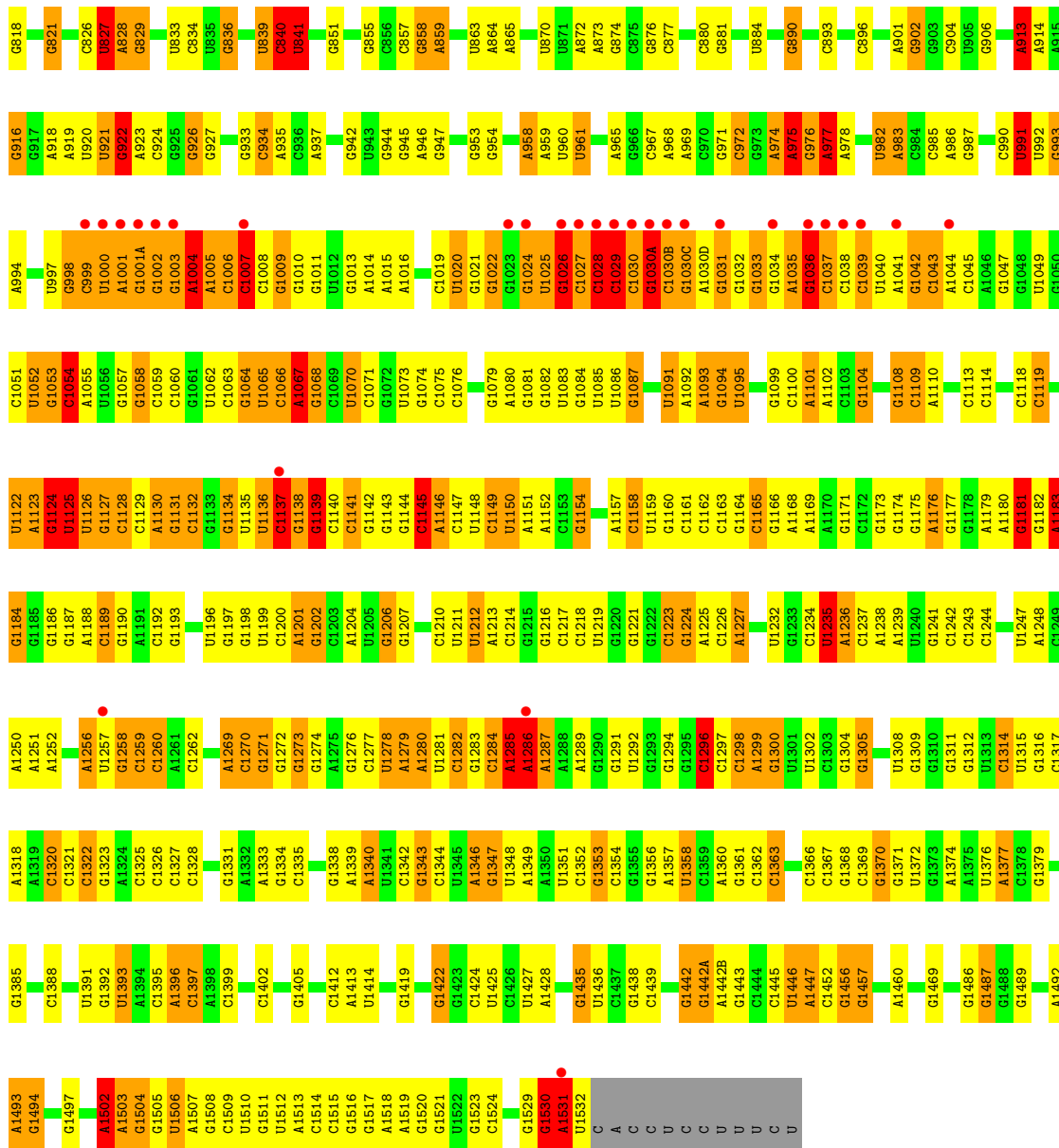
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	BG	1	Total O 1 1	0	0
61	BN	3	Total O 3 3	0	0
61	BO	2	Total O 2 2	0	0
61	BP	15	Total O 15 15	0	0
61	BQ	3	Total O 3 3	0	0
61	BR	1	Total O 1 1	0	0
61	BT	1	Total O 1 1	0	0
61	BU	4	Total O 4 4	0	0
61	BV	2	Total O 2 2	0	0
61	BW	2	Total O 2 2	0	0
61	BX	4	Total O 4 4	0	0
61	B0	4	Total O 4 4	0	0
61	B1	2	Total O 2 2	0	0
61	B5	3	Total O 3 3	0	0
61	B7	1	Total O 1 1	0	0
61	B8	8	Total O 8 8	0	0
61	CA	187	Total O 187 187	0	0
61	CE	2	Total O 2 2	0	0
61	CN	1	Total O 1 1	0	0
61	CT	1	Total O 1 1	0	0
61	CX	2	Total O 2 2	0	0

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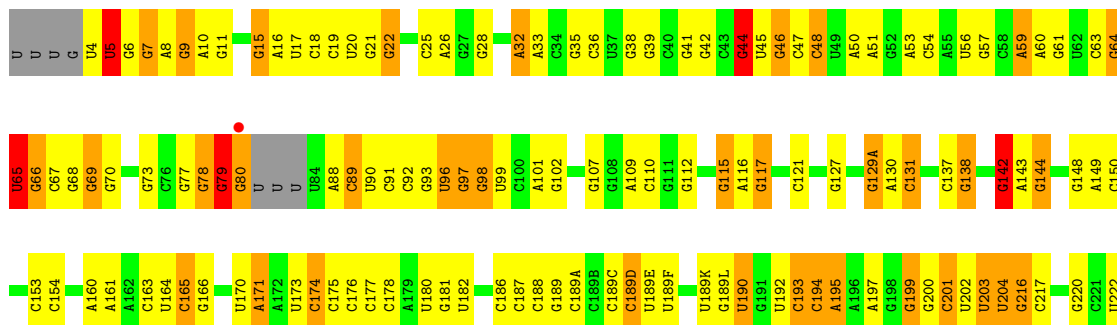
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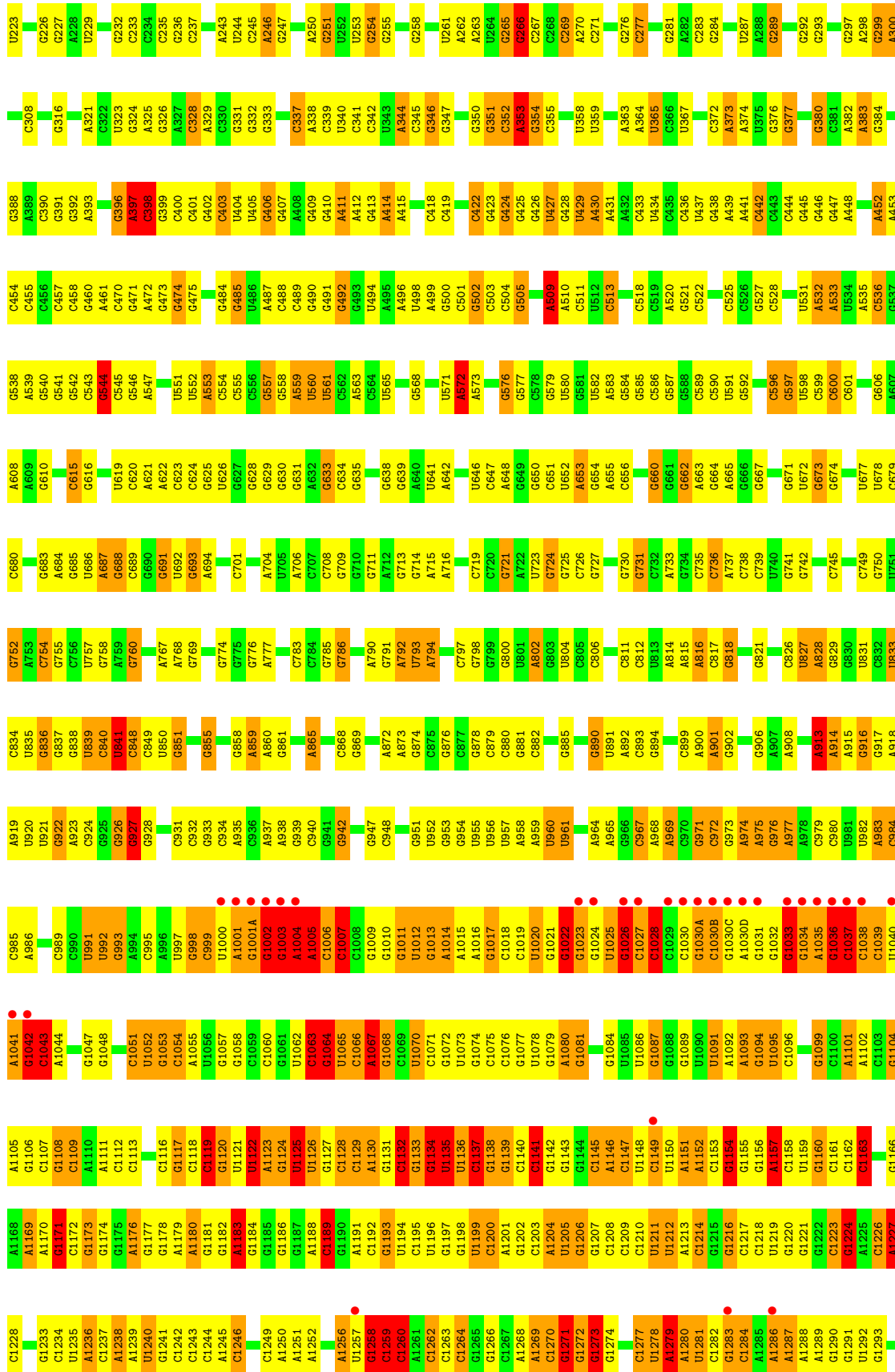
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DA	902	Total 902	O 902	0	0
61	DB	7	Total 7	O 7	0	0
61	DD	8	Total 8	O 8	0	0
61	DE	13	Total 13	O 13	0	0
61	DF	5	Total 5	O 5	0	0
61	DO	1	Total 1	O 1	0	0
61	DP	14	Total 14	O 14	0	0
61	DQ	3	Total 3	O 3	0	0
61	DU	4	Total 4	O 4	0	0
61	DV	1	Total 1	O 1	0	0
61	DX	2	Total 2	O 2	0	0
61	DY	2	Total 2	O 2	0	0
61	D0	5	Total 5	O 5	0	0
61	D1	1	Total 1	O 1	0	0
61	D7	2	Total 2	O 2	0	0
61	D8	4	Total 4	O 4	0	0





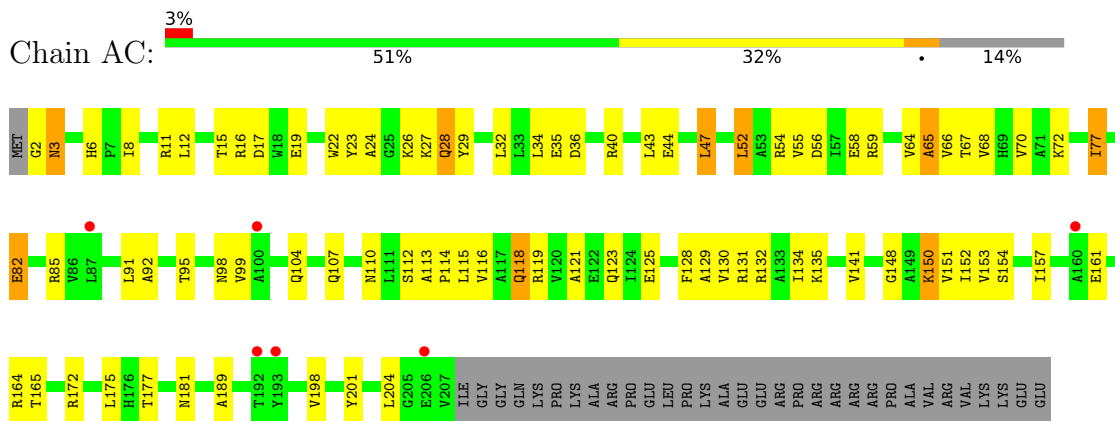
• Molecule 1: 16S Ribosomal RNA



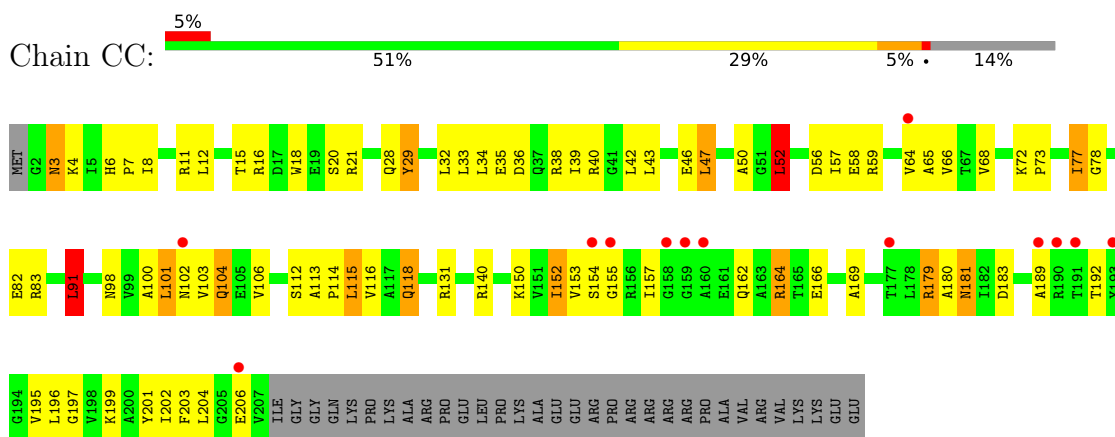




- Molecule 3: 30S Ribosomal Protein S3



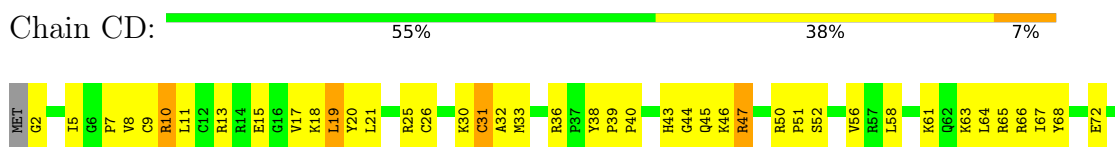
- Molecule 3: 30S Ribosomal Protein S3

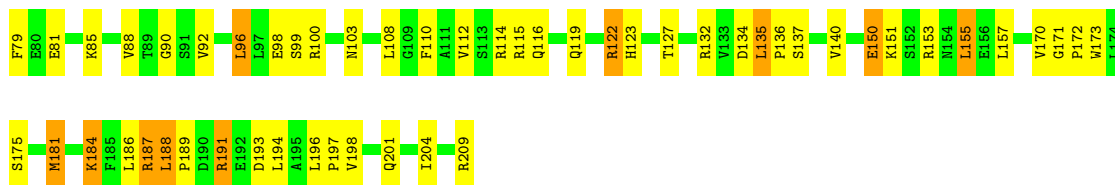


- Molecule 4: 30S Ribosomal Protein S4

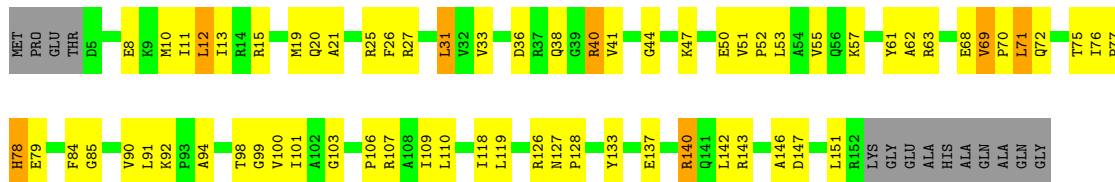


- Molecule 4: 30S Ribosomal Protein S4

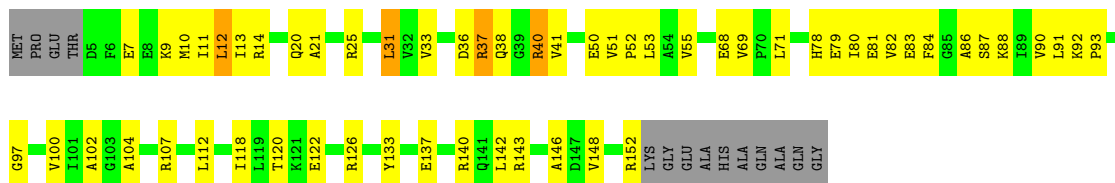




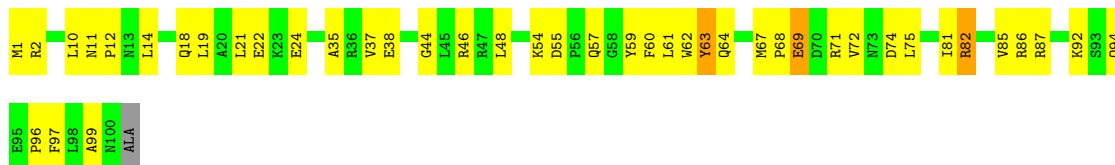
• Molecule 5: 30S Ribosomal Protein S5



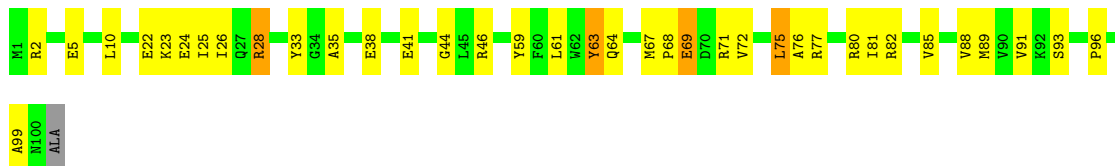
• Molecule 5: 30S Ribosomal Protein S5



• Molecule 6: 30S Ribosomal Protein S6



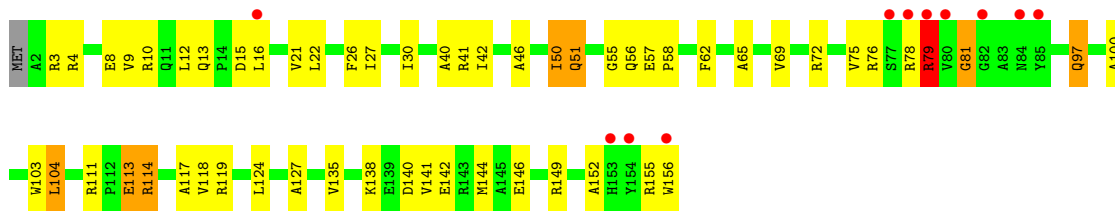
• Molecule 6: 30S Ribosomal Protein S6



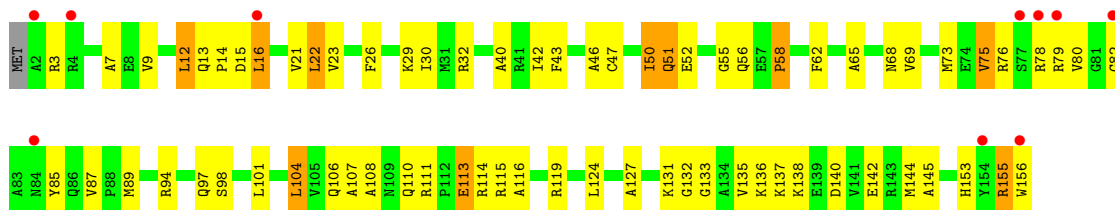
• Molecule 7: 30S Ribosomal Protein S7



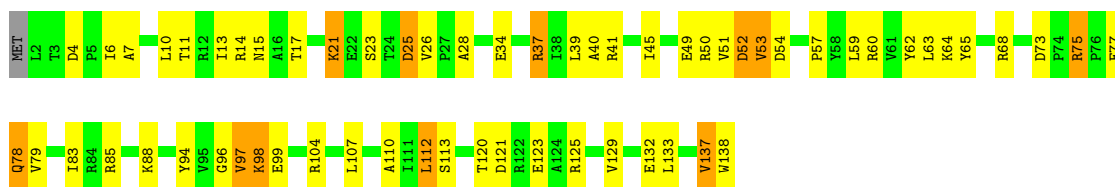




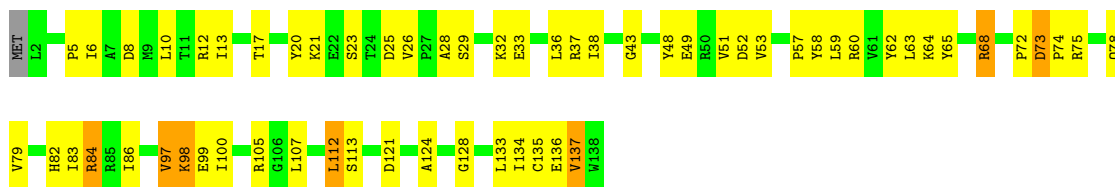
• Molecule 7: 30S Ribosomal Protein S7



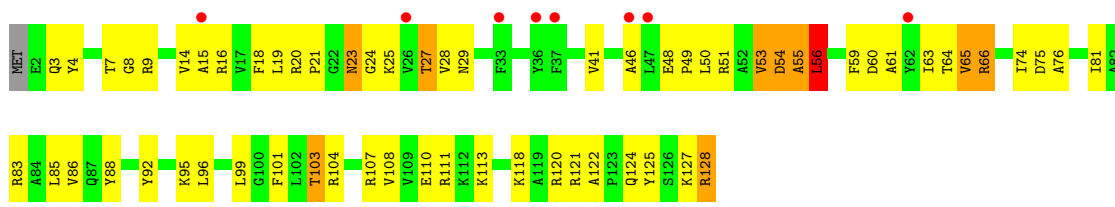
• Molecule 8: 30S Ribosomal Protein S8



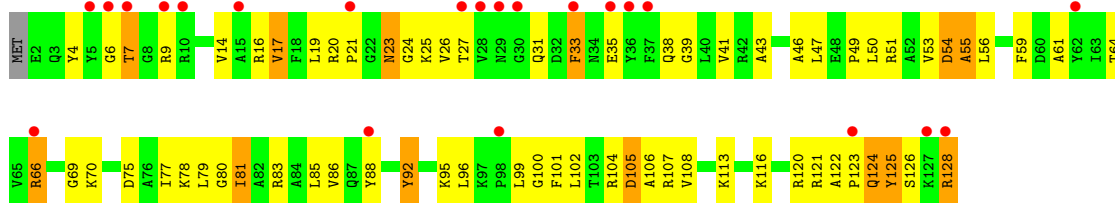
• Molecule 8: 30S Ribosomal Protein S8



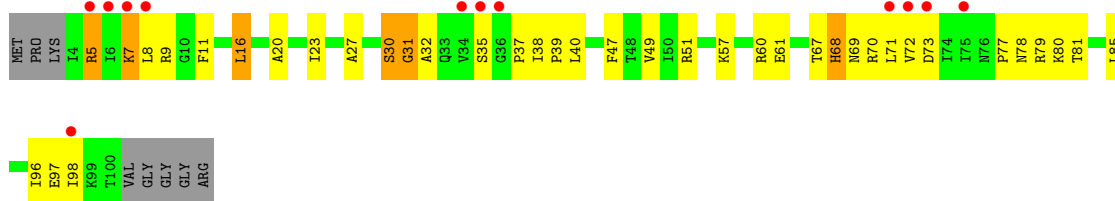
• Molecule 9: 30S Ribosomal Protein S9



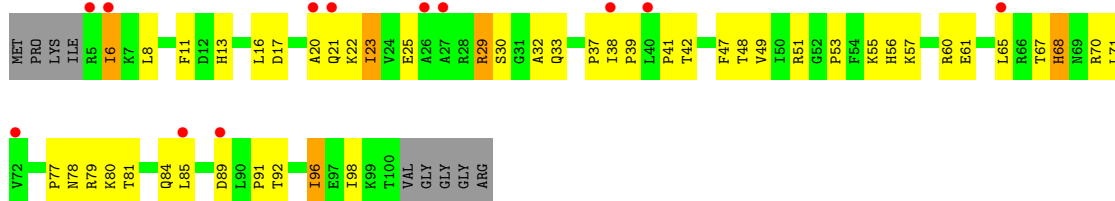
• Molecule 9: 30S Ribosomal Protein S9



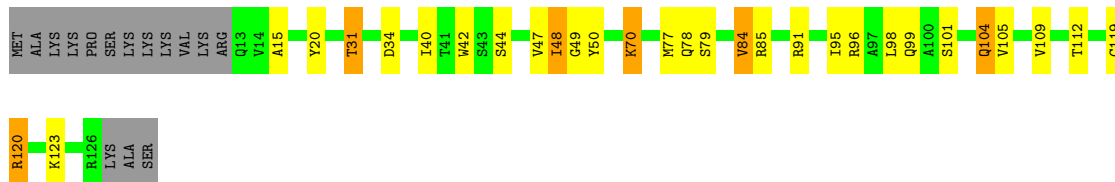
• Molecule 10: 30S Ribosomal Protein S10



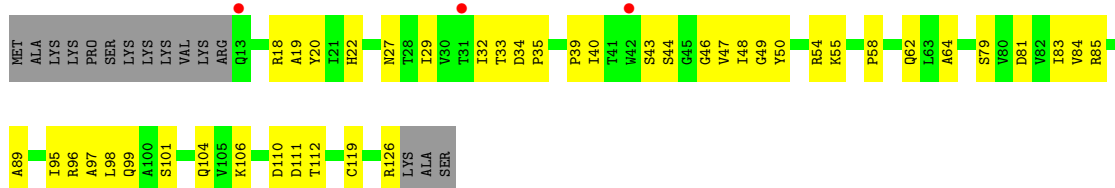
• Molecule 10: 30S Ribosomal Protein S10



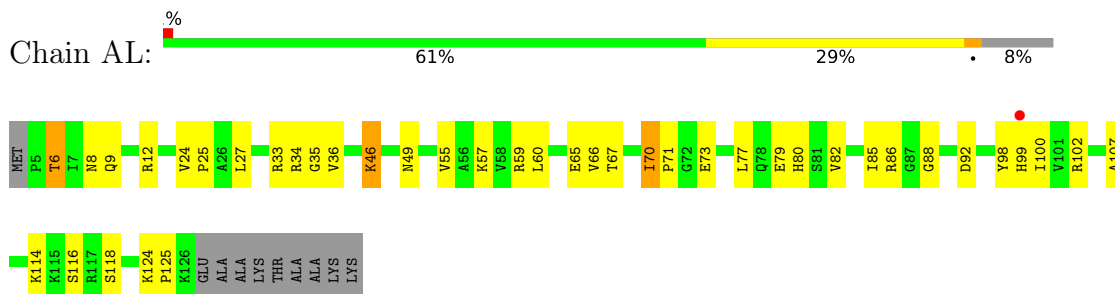
• Molecule 11: 30S Ribosomal Protein S11



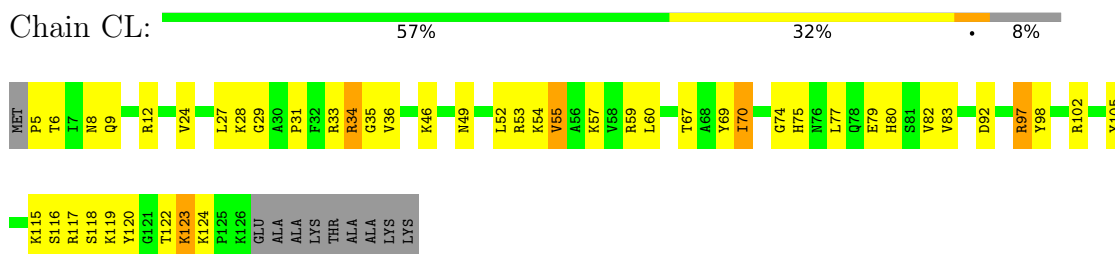
• Molecule 11: 30S Ribosomal Protein S11



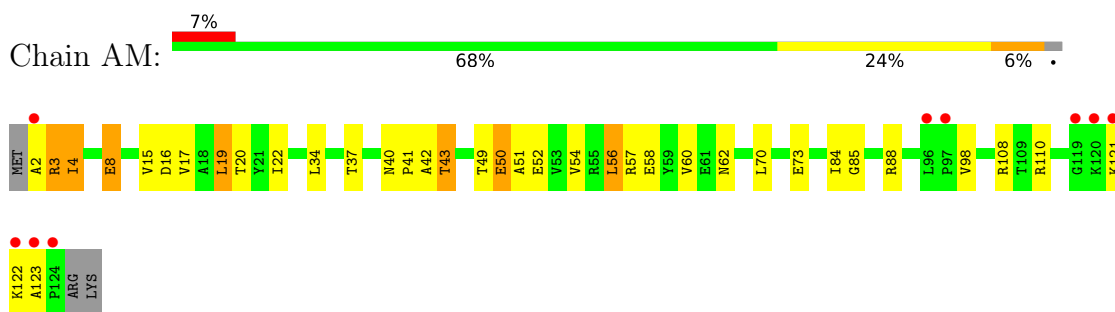
- Molecule 12: 30S Ribosomal Protein S12



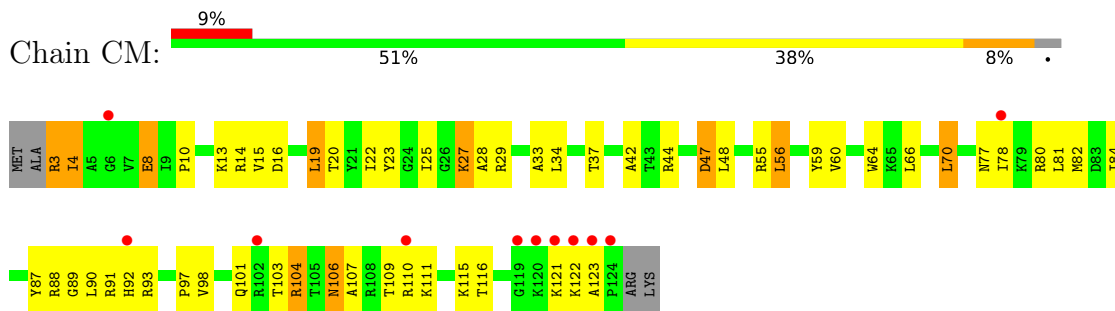
- Molecule 12: 30S Ribosomal Protein S12



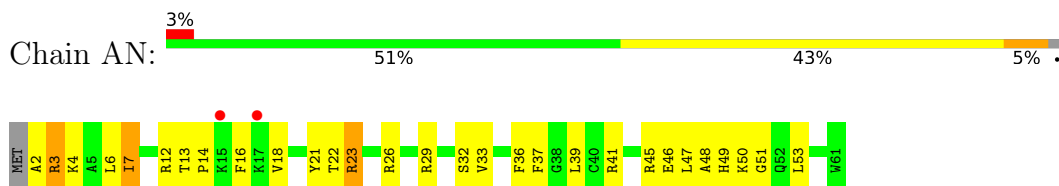
- Molecule 13: 30S Ribosomal Protein S13



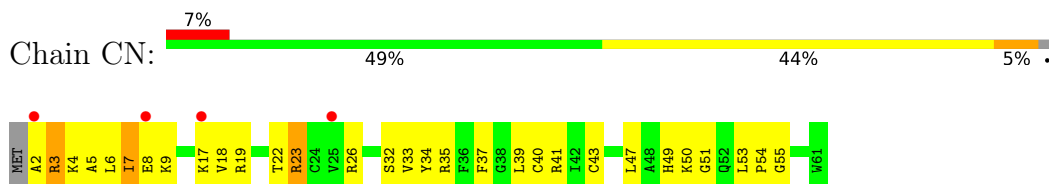
- Molecule 13: 30S Ribosomal Protein S13



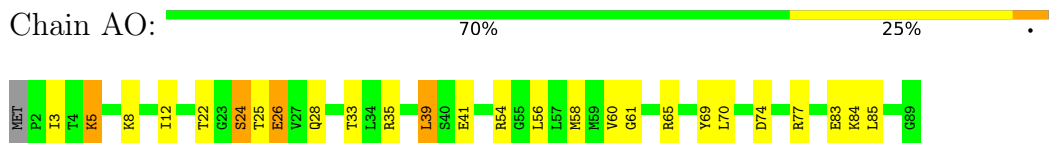
- Molecule 14: 30S Ribosomal Protein S14



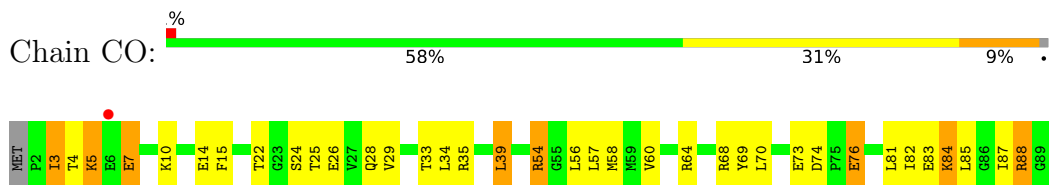
- Molecule 14: 30S Ribosomal Protein S14



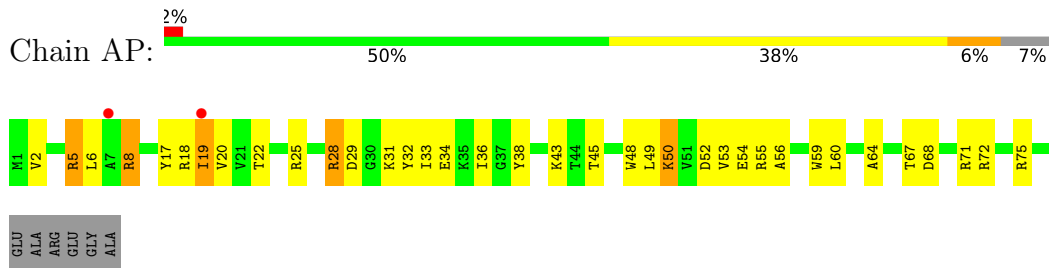
• Molecule 15: 30S Ribosomal Protein S15



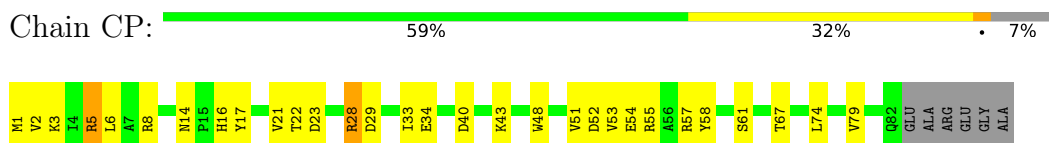
• Molecule 15: 30S Ribosomal Protein S15



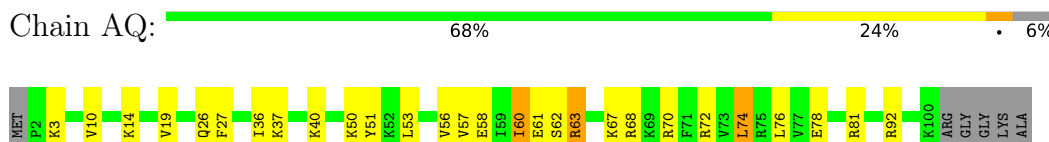
• Molecule 16: 30S Ribosomal Protein S16



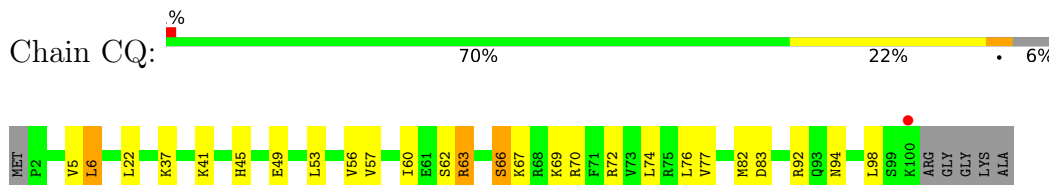
• Molecule 16: 30S Ribosomal Protein S16



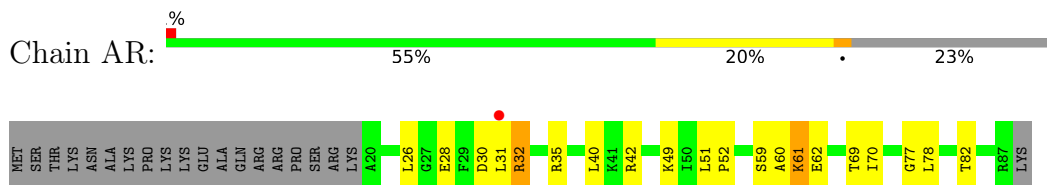
• Molecule 17: 30S Ribosomal Protein S17



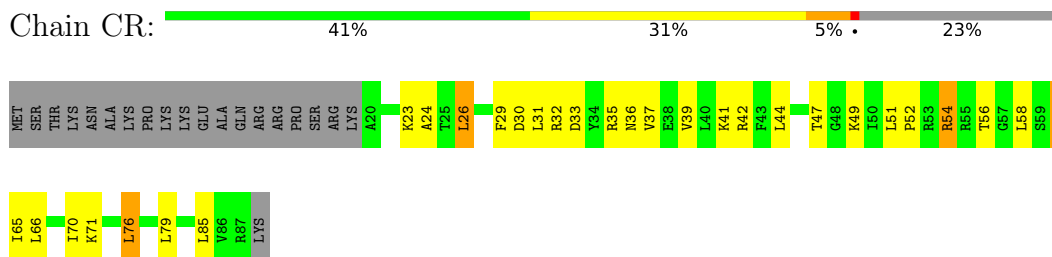
• Molecule 17: 30S Ribosomal Protein S17



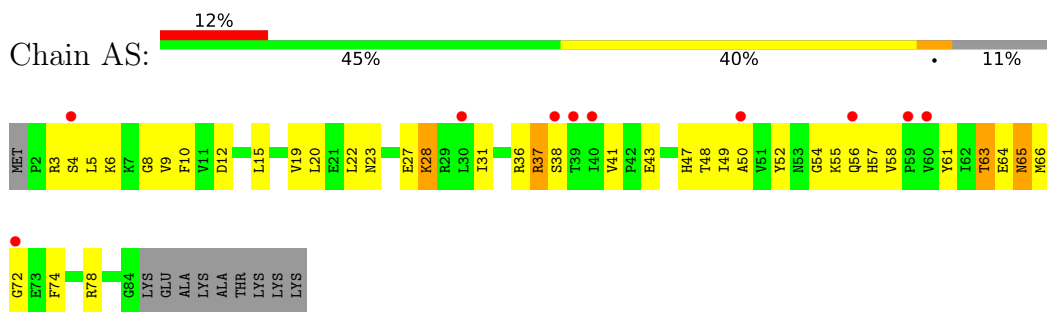
- Molecule 18: 30S Ribosomal Protein S18



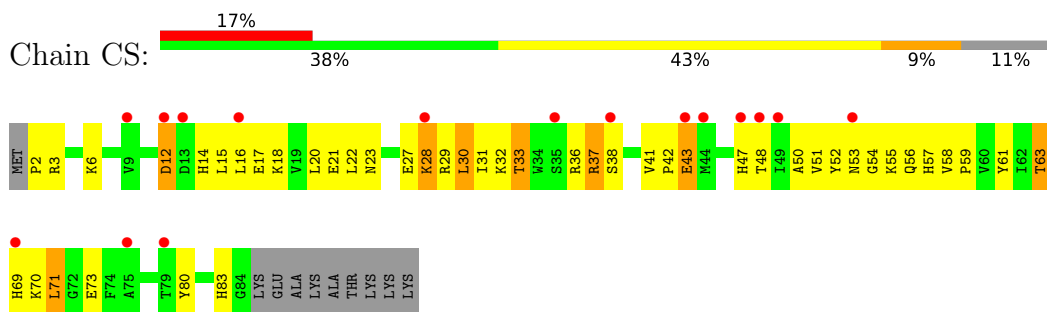
- Molecule 18: 30S Ribosomal Protein S18



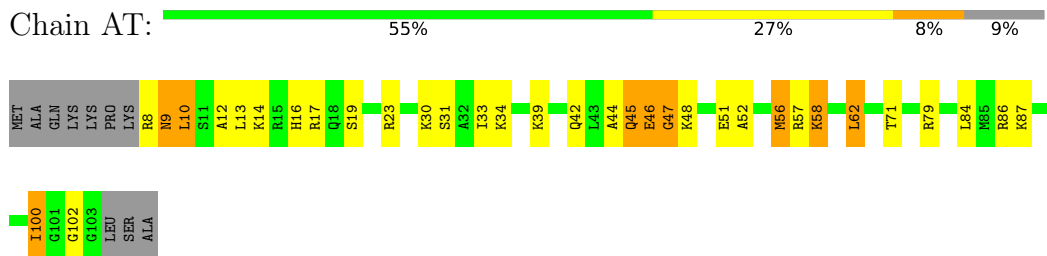
- Molecule 19: 30S Ribosomal Protein S19



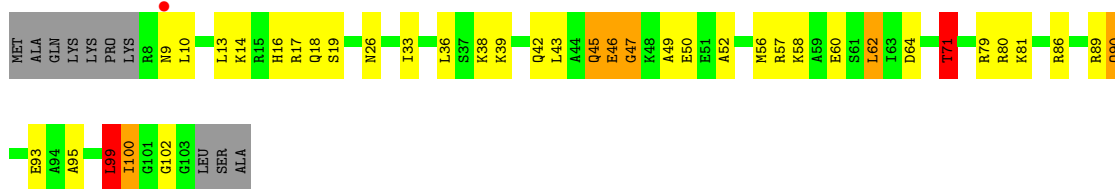
- Molecule 19: 30S Ribosomal Protein S19



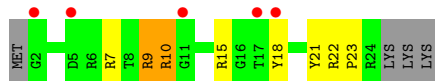
- Molecule 20: 30S Ribosomal Protein S20



- Molecule 20: 30S Ribosomal Protein S20



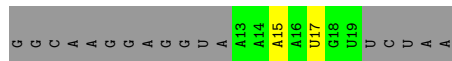
• Molecule 21: 30S Ribosomal Protein THX



• Molecule 21: 30S Ribosomal Protein THX



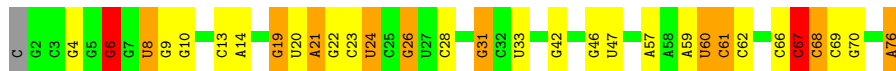
• Molecule 22: mRNA



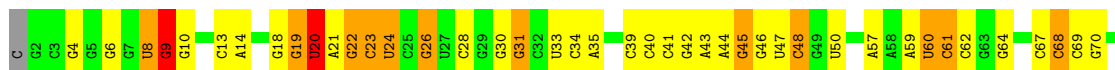
• Molecule 22: mRNA



• Molecule 23: P-site tRNA



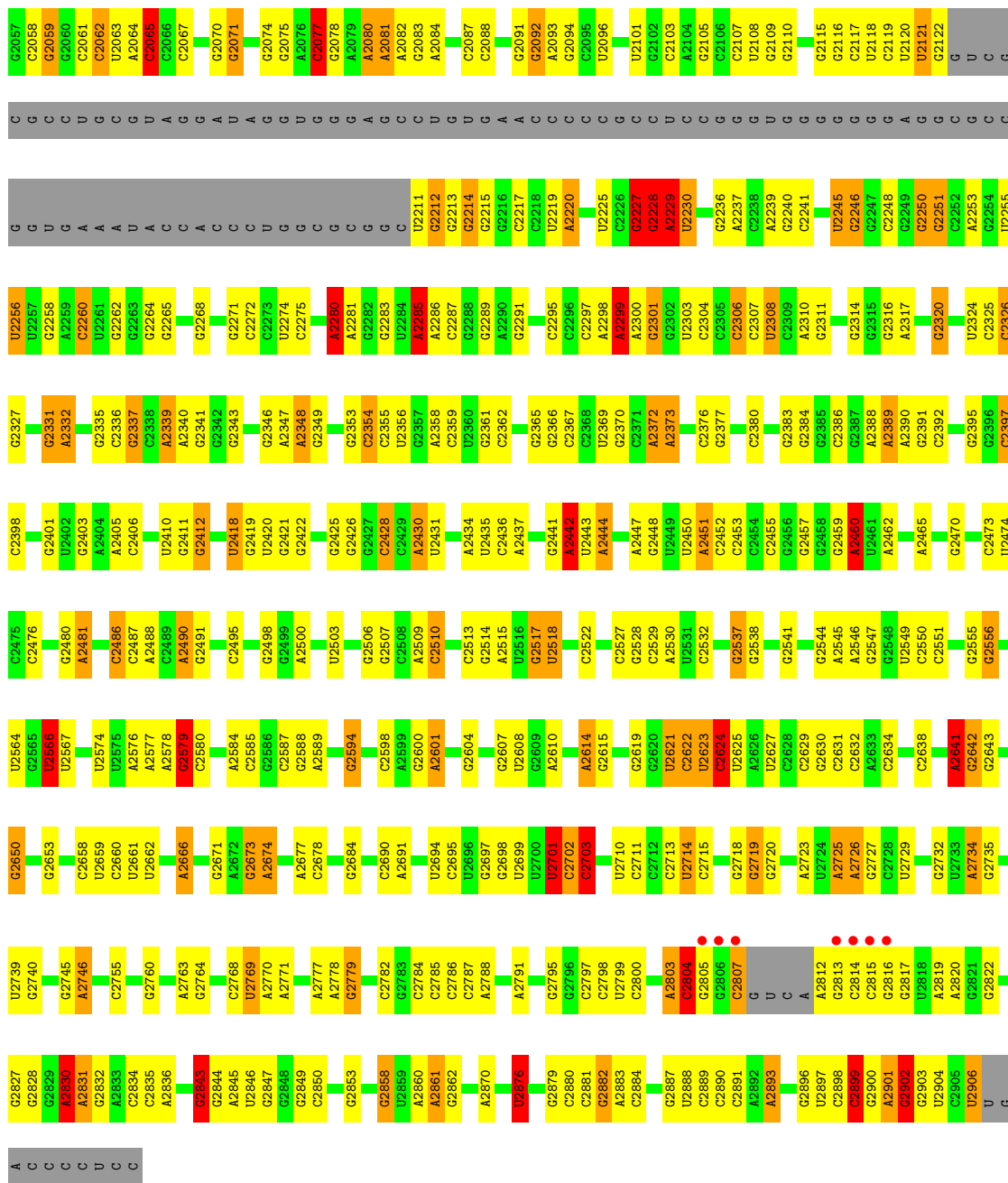
• Molecule 23: P-site tRNA



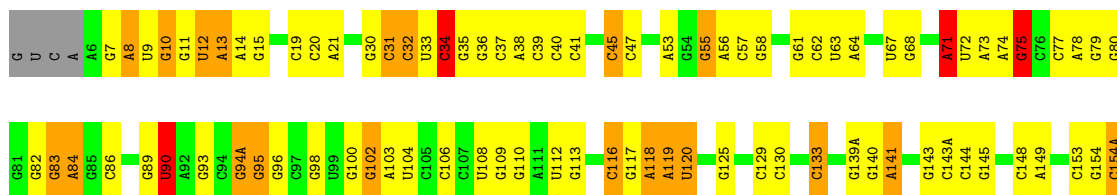


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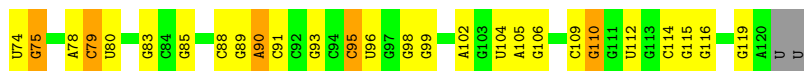
● Molecule 25: 23S Ribosomal RNA



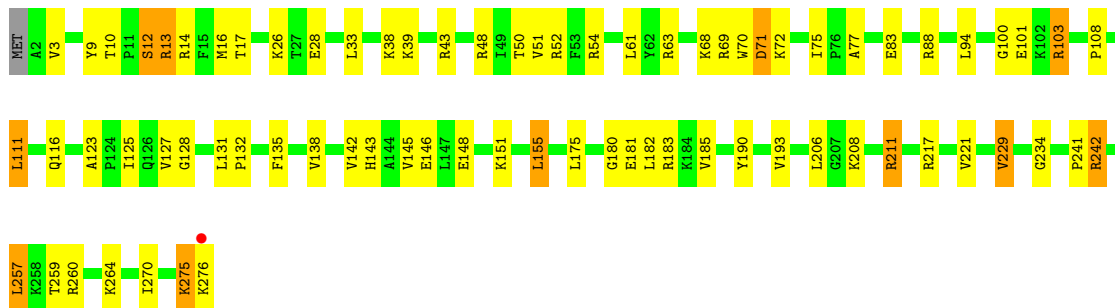




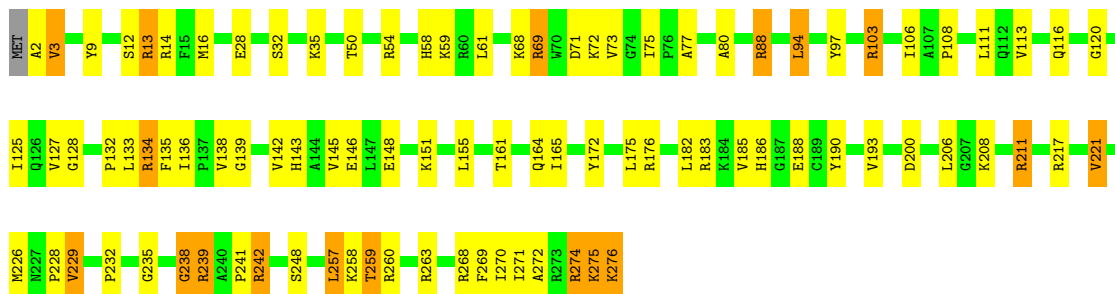




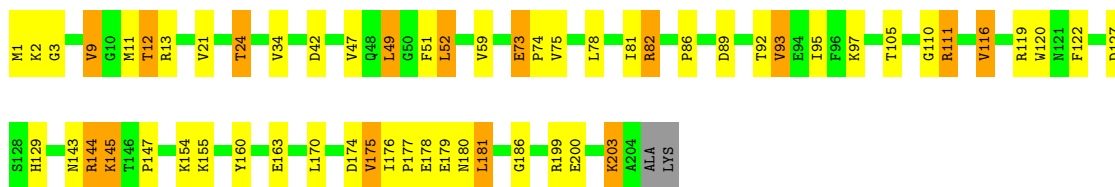
• Molecule 27: 50S Ribosomal Protein L2



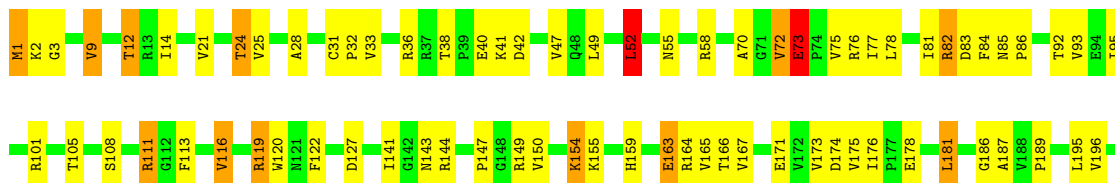
• Molecule 27: 50S Ribosomal Protein L2

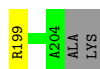


• Molecule 28: 50S Ribosomal Protein L3

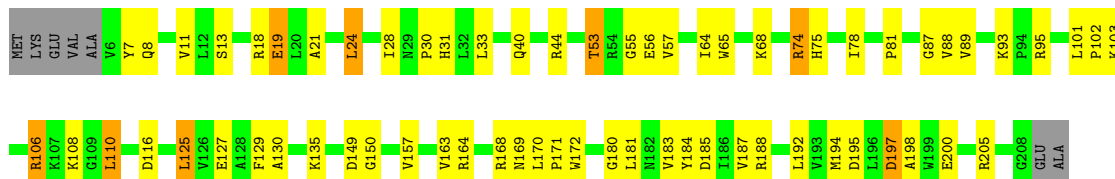


• Molecule 28: 50S Ribosomal Protein L3

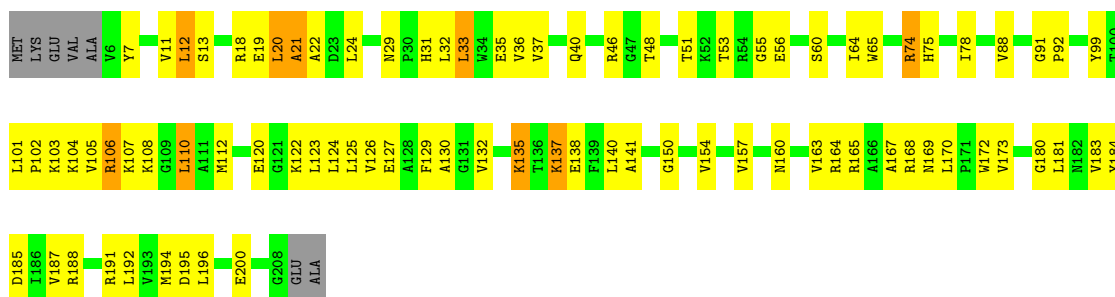




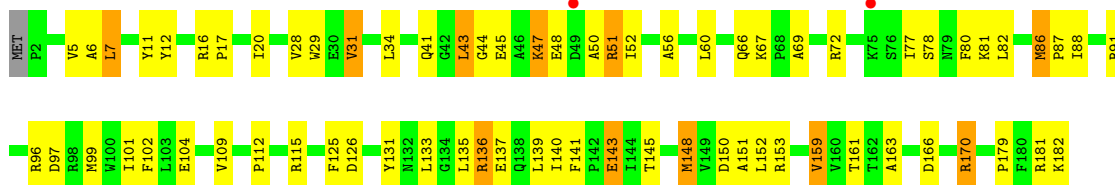
• Molecule 29: 50S Ribosomal Protein L4



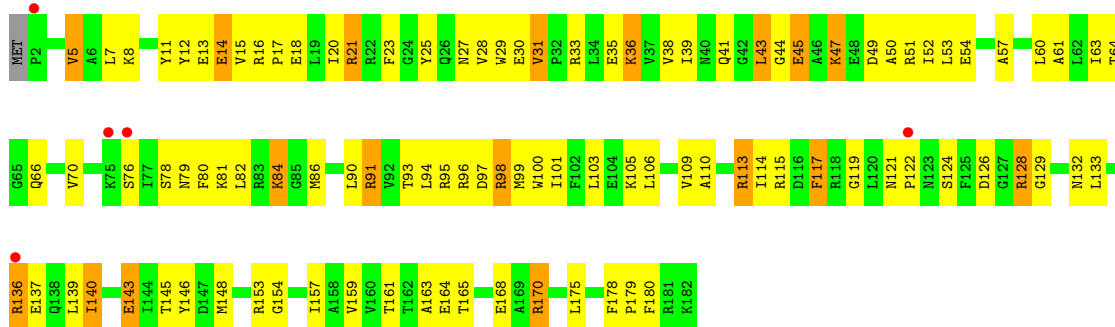
• Molecule 29: 50S Ribosomal Protein L4



• Molecule 30: 50S Ribosomal Protein L5

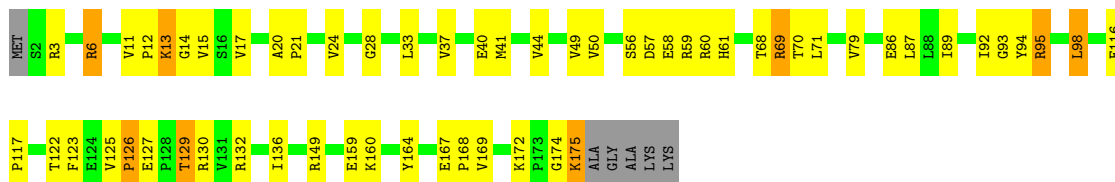


• Molecule 30: 50S Ribosomal Protein L5



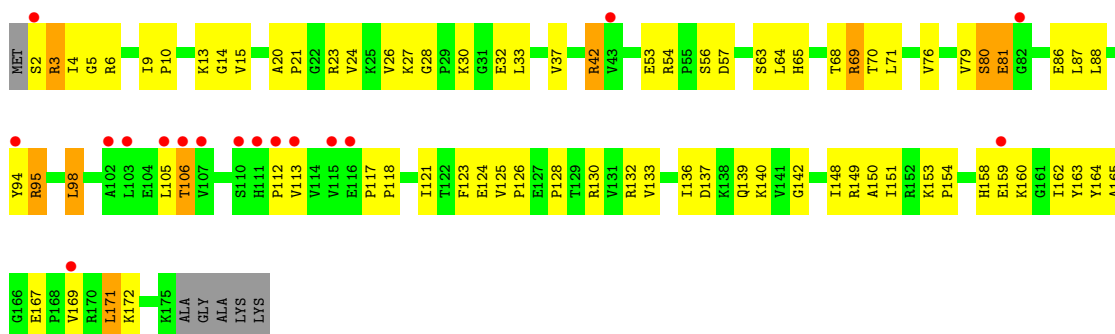
- Molecule 31: 50S Ribosomal Protein L6

Chain BH:  64% 28%



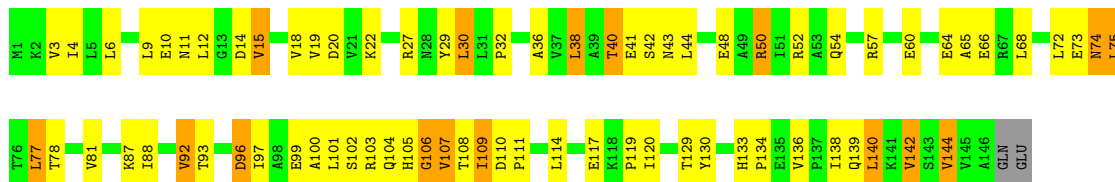
- Molecule 31: 50S Ribosomal Protein L6

Chain DH:  9% 52% 39% 5%



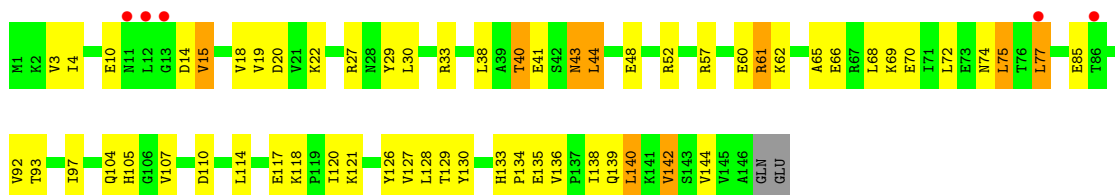
- Molecule 32: 50S Ribosomal Protein L9

Chain BI:  49% 39% 11%




- Molecule 32: 50S Ribosomal Protein L9

Chain DI:  3% 58% 34% 6%

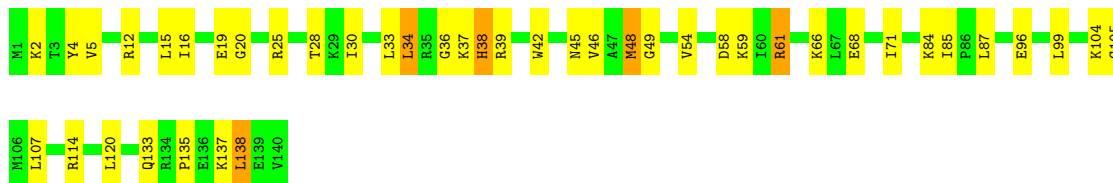


- Molecule 33: 50S Ribosomal Protein L13

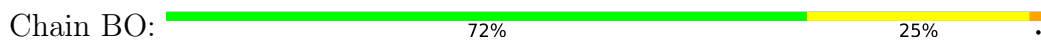
Chain BN:  78% 19%



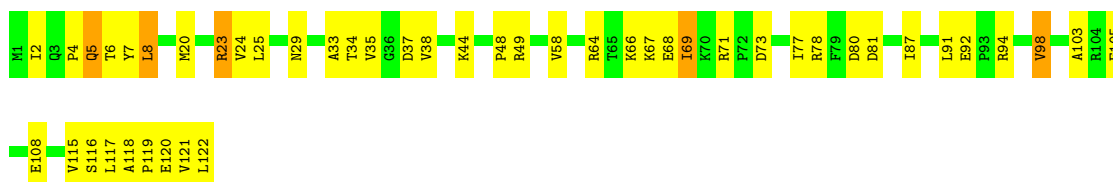
- Molecule 33: 50S Ribosomal Protein L13



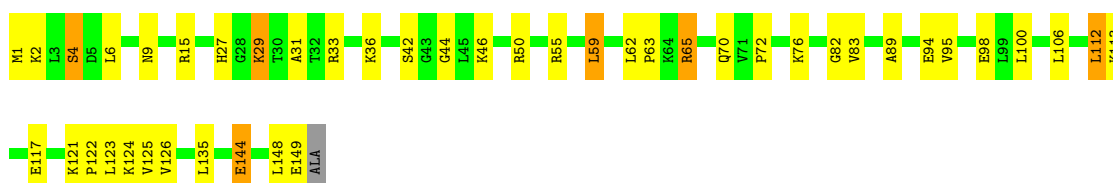
- Molecule 34: 50S Ribosomal Protein L14



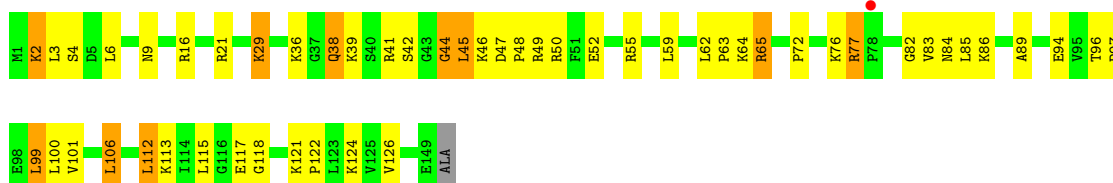
- Molecule 34: 50S Ribosomal Protein L14



- Molecule 35: 50S Ribosomal Protein L15



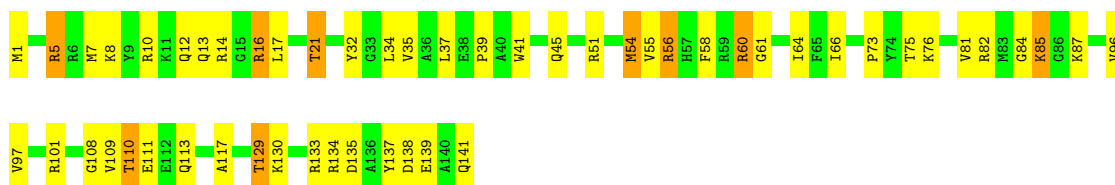
- Molecule 35: 50S Ribosomal Protein L15





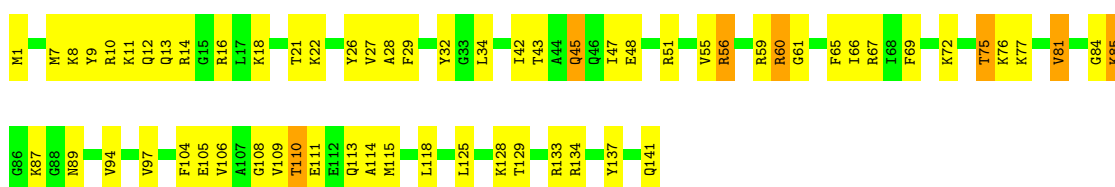
- Molecule 36: 50S Ribosomal Protein L16

Chain BQ: 62% 31% 6%



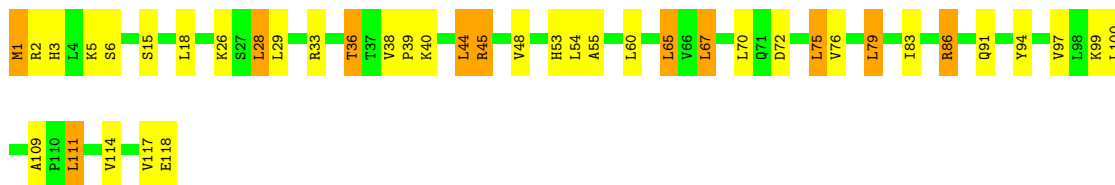
- Molecule 36: 50S Ribosomal Protein L16

Chain DQ: 55% 40% 5%



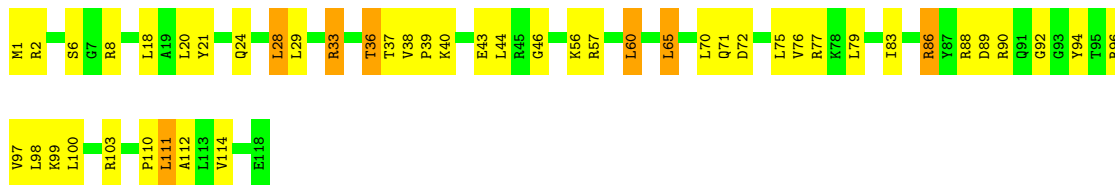
- Molecule 37: 50S Ribosomal Protein L17

Chain BR: 65% 25% 9%



- Molecule 37: 50S Ribosomal Protein L17

Chain DR: 60% 34% 6%



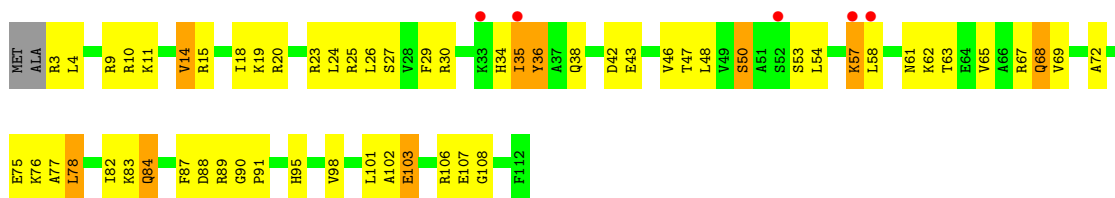
- Molecule 38: 50S Ribosomal Protein L18

Chain BS: 70% 22% 6%



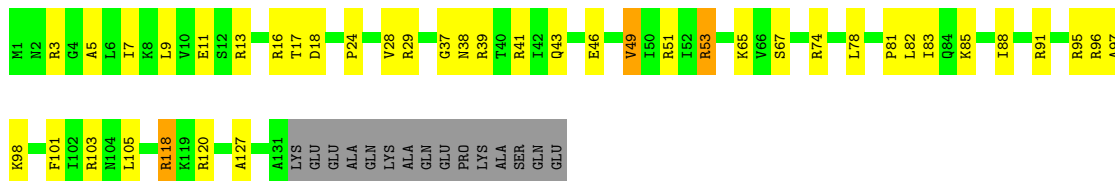
- Molecule 38: 50S Ribosomal Protein L18

Chain DS: 46% 45% 8% 4%



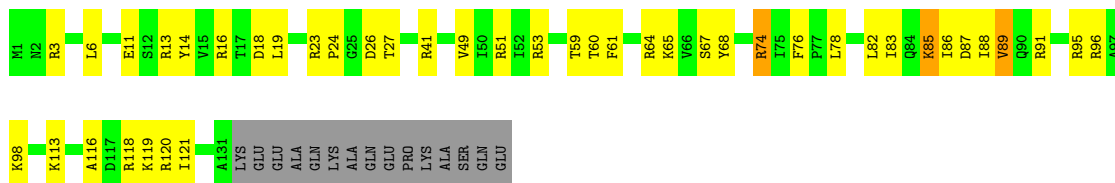
- Molecule 39: 50S Ribosomal Protein L19

Chain BT: 62% 26% 10%



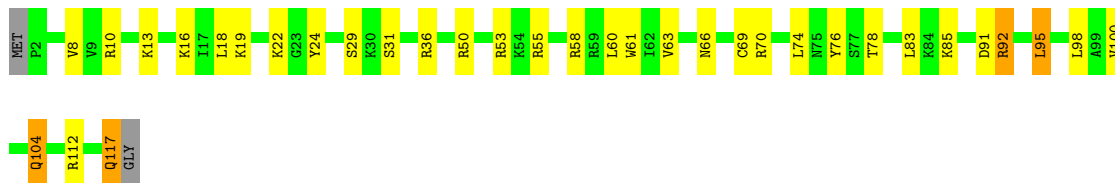
- Molecule 39: 50S Ribosomal Protein L19

Chain DT: 60% 27% 10%



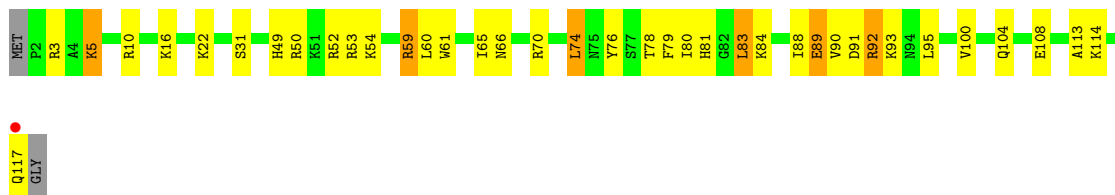
- Molecule 40: 50S Ribosomal Protein L20

Chain BU: 69% 25% 6%



- Molecule 40: 50S Ribosomal Protein L20

Chain DU: 66% 27% 5%



- Molecule 41: 50S Ribosomal Protein L21

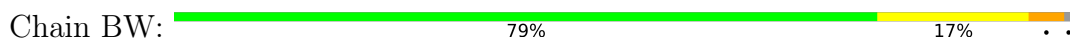
Chain BV: 81% 14% 5%



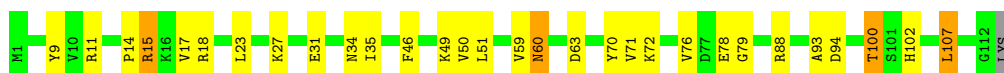
- Molecule 41: 50S Ribosomal Protein L21



- Molecule 42: 50S Ribosomal Protein L22



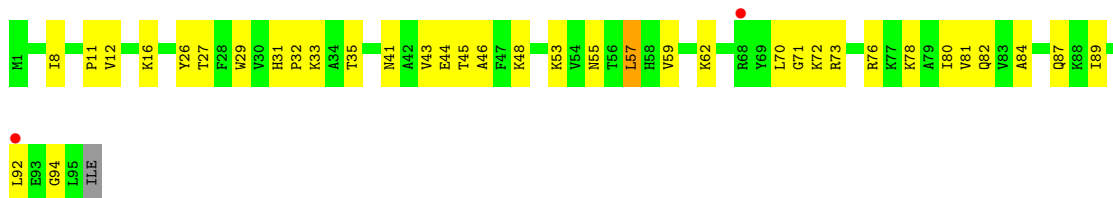
- Molecule 42: 50S Ribosomal Protein L22



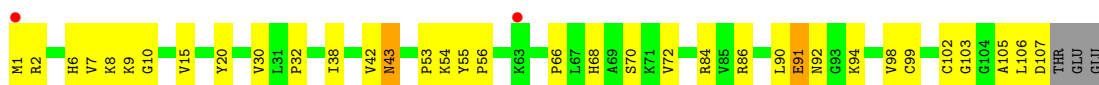
- Molecule 43: 50S Ribosomal Protein L23



- Molecule 43: 50S Ribosomal Protein L23

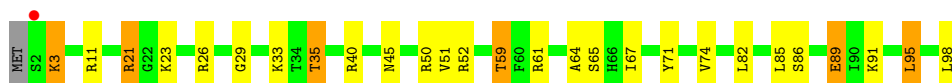
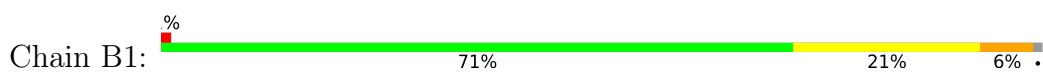


- Molecule 44: 50S Ribosomal Protein L24



- Molecule 44: 50S Ribosomal Protein L24

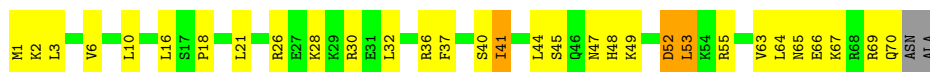




- Molecule 47: 50S Ribosomal Protein L28



- Molecule 48: 50S Ribosomal Protein L29



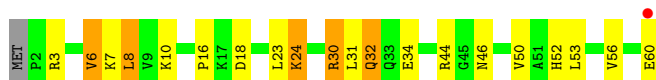
- Molecule 48: 50S Ribosomal Protein L29



- Molecule 49: 50S Ribosomal Protein L30



- Molecule 49: 50S Ribosomal Protein L30



- Molecule 50: 50S Ribosomal Protein L31



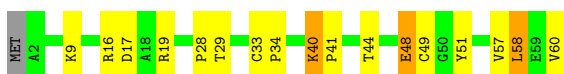
- Molecule 50: 50S Ribosomal Protein L31



- Molecule 51: 50S Ribosomal Protein L32



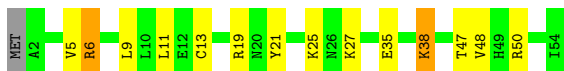
- Molecule 51: 50S Ribosomal Protein L32



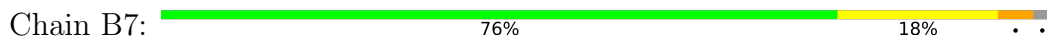
- Molecule 52: 50S Ribosomal Protein L33



- Molecule 52: 50S Ribosomal Protein L33



- Molecule 53: 50S Ribosomal Protein L34



- Molecule 53: 50S Ribosomal Protein L34

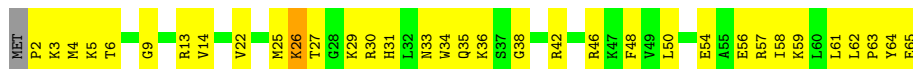


- Molecule 54: 50S Ribosomal Protein L35

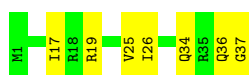
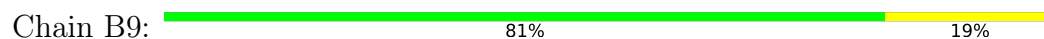




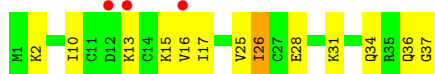
- Molecule 54: 50S Ribosomal Protein L35



- Molecule 55: 50S Ribosomal Protein L36



- Molecule 55: 50S Ribosomal Protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.68Å 450.64Å 622.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 3.10 49.68 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.68-3.10) 98.2 (49.68-3.10)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	0.25	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.203 , 0.260 0.203 , 0.260	Depositor DCC
$R_{free}$ test set	51894 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtrriage
Anisotropy	0.077	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 67.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	286321	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 004, 2QY, 2QZ, K, MVA, MG, ZN, 2R3, FME, 2R1, SF4

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	AA	0.75	2/36038 (0.0%)	1.31	240/56244 (0.4%)
1	CA	0.75	10/36170 (0.0%)	1.36	314/56452 (0.6%)
2	AB	0.49	0/1881	0.77	1/2542 (0.0%)
2	CB	0.54	0/1860	0.79	1/2518 (0.0%)
3	AC	0.47	0/1576	0.65	0/2130
3	CC	0.51	0/1566	0.71	2/2119 (0.1%)
4	AD	0.49	0/1689	0.73	0/2267
4	CD	0.49	0/1704	0.70	1/2284 (0.0%)
5	AE	0.47	0/1145	0.70	0/1543
5	CE	0.50	0/1149	0.71	0/1548
6	AF	0.47	0/819	0.69	0/1111
6	CF	0.52	0/829	0.74	1/1123 (0.1%)
7	AG	0.48	0/1250	0.67	1/1679 (0.1%)
7	CG	0.50	0/1254	0.71	1/1683 (0.1%)
8	AH	0.45	0/1108	0.66	0/1494
8	CH	0.48	0/1108	0.69	0/1494
9	AI	0.46	0/1002	0.72	0/1346
9	CI	0.56	0/997	0.75	1/1343 (0.1%)
10	AJ	0.47	0/722	0.68	0/982
10	CJ	0.51	0/727	0.68	0/988
11	AK	0.44	0/844	0.62	0/1145
11	CK	0.46	0/848	0.66	0/1149
12	AL	0.52	0/946	0.69	0/1274
12	CL	0.51	0/946	0.73	0/1274
13	AM	0.46	0/969	0.69	0/1302
13	CM	0.49	0/961	0.66	0/1291
14	AN	0.51	0/501	0.67	0/664
14	CN	0.54	0/501	0.68	0/664
15	AO	0.47	0/739	0.72	0/985
15	CO	0.46	0/739	0.73	0/985
16	AP	0.45	0/697	0.71	0/939
16	CP	0.47	0/693	0.65	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.48	0/836	0.66	0/1117
17	CQ	0.49	0/836	0.68	0/1117
18	AR	0.49	0/560	0.72	0/746
18	CR	0.51	0/560	0.75	1/746 (0.1%)
19	AS	0.47	0/667	0.68	0/900
19	CS	0.54	0/661	0.82	2/893 (0.2%)
20	AT	0.51	0/730	0.76	0/965
20	CT	0.44	0/729	0.68	0/965
21	AU	0.45	0/203	0.65	0/266
21	CU	0.51	0/203	0.68	0/266
22	AV	0.94	0/127	1.36	2/198 (1.0%)
22	CV	0.86	0/126	1.29	0/195
23	AX	0.85	5/1813 (0.3%)	1.59	36/2825 (1.3%)
23	CX	0.88	4/1813 (0.2%)	1.81	40/2825 (1.4%)
24	AW	0.50	0/20	0.80	0/23
24	CW	0.43	0/20	0.70	0/23
25	BA	1.06	33/65892 (0.1%)	1.42	649/102850 (0.6%)
25	DA	0.79	9/65466 (0.0%)	1.39	590/102184 (0.6%)
26	BB	0.82	0/2878	1.26	11/4490 (0.2%)
26	DB	0.89	0/2878	1.39	18/4490 (0.4%)
27	BD	0.67	1/2186 (0.0%)	0.78	1/2944 (0.0%)
27	DD	0.61	2/2186 (0.1%)	0.77	1/2944 (0.0%)
28	BE	0.69	0/1592	0.75	0/2149
28	DE	0.55	0/1592	0.77	1/2149 (0.0%)
29	BF	0.69	0/1619	0.76	0/2193
29	DF	0.53	0/1615	0.77	1/2188 (0.0%)
30	BG	0.46	0/1450	0.70	0/1959
30	DG	0.55	0/1449	0.74	0/1958
31	BH	0.60	0/1356	0.70	0/1834
31	DH	0.56	0/1356	0.70	0/1834
32	BI	0.49	0/1100	0.74	1/1501 (0.1%)
32	DI	0.48	0/1076	0.77	0/1471
33	BN	0.65	0/1144	0.73	0/1543
33	DN	0.50	0/1144	0.72	0/1543
34	BO	0.65	0/943	0.73	1/1269 (0.1%)
34	DO	0.54	0/943	0.73	1/1269 (0.1%)
35	BP	0.62	0/1152	0.77	0/1533
35	DP	0.53	0/1152	0.80	1/1533 (0.1%)
36	BQ	0.64	0/1143	0.76	0/1527
36	DQ	0.60	0/1143	0.79	0/1527
37	BR	0.59	0/982	0.78	0/1312
37	DR	0.49	0/982	0.71	0/1312
38	BS	0.54	0/887	0.77	0/1180

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DS	0.47	0/880	0.72	0/1172
39	BT	0.59	0/1105	0.79	1/1477 (0.1%)
39	DT	0.50	0/1097	0.72	0/1468
40	BU	0.71	1/977 (0.1%)	0.73	0/1301
40	DU	0.54	0/977	0.71	1/1301 (0.1%)
41	BV	0.68	0/782	0.74	1/1049 (0.1%)
41	DV	0.55	0/782	0.71	0/1049
42	BW	0.74	0/897	0.74	0/1205
42	DW	0.56	0/897	0.72	0/1205
43	BX	0.66	0/764	0.96	3/1025 (0.3%)
43	DX	0.55	0/764	0.75	1/1025 (0.1%)
44	BY	0.64	0/819	0.78	0/1095
44	DY	0.54	0/819	0.74	0/1095
45	BZ	0.56	0/1379	0.75	0/1873
45	DZ	0.53	0/1390	0.71	0/1890
46	B0	0.63	0/662	0.81	2/881 (0.2%)
46	D0	0.54	0/662	0.73	0/881
47	B1	0.61	0/762	0.74	0/1014
47	D1	0.51	0/762	0.75	1/1014 (0.1%)
48	B2	0.61	0/590	0.79	0/781
48	D2	0.48	0/590	0.66	0/781
49	B3	0.70	0/474	0.76	0/635
49	D3	0.45	0/469	0.67	0/630
50	B4	0.58	0/564	0.79	0/759
50	D4	0.59	0/544	0.86	1/735 (0.1%)
51	B5	0.66	0/469	0.78	0/635
51	D5	0.53	0/469	0.74	1/635 (0.2%)
52	B6	0.67	0/460	0.64	0/613
52	D6	0.53	0/456	0.70	0/608
53	B7	0.79	0/426	0.78	0/561
53	D7	0.62	0/426	0.76	1/561 (0.2%)
54	B8	0.70	0/519	0.71	0/684
54	D8	0.55	0/525	0.75	0/691
55	B9	0.69	0/310	0.76	0/407
55	D9	0.60	0/310	0.79	0/407
All	All	0.79	67/305966 (0.0%)	1.24	1933/457396 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	3
4	CD	0	1
7	AG	0	1
23	CX	1	0
24	AW	0	1
24	CW	0	1
27	DD	0	1
38	BS	0	1
45	BZ	0	1
50	B4	0	1
All	All	1	11

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AX	76	A	N7-C5	-11.16	1.32	1.39
1	CA	1154	G	C6-N1	-11.02	1.31	1.39
1	CA	1154	G	N1-C2	-10.69	1.29	1.37
25	BA	1188	A	N9-C4	-10.29	1.31	1.37
1	CA	1119	C	N3-C4	-10.20	1.26	1.33

The worst 5 of 1933 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CX	76	A	O4'-C1'-N9	38.71	139.17	108.20
1	CA	1119	C	N1-C2-O2	32.56	138.44	118.90
1	CA	1154	G	C5-C6-O6	28.63	145.78	128.60
1	CA	1154	G	N3-C2-N2	25.05	137.43	119.90
1	CA	1154	G	N1-C2-N2	-22.71	95.76	116.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	CX	76	A	C1'

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide
2	AB	8	LYS	Peptide
2	AB	9	GLU	Peptide
7	AG	79	ARG	Peptide
24	AW	4	PRO	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32196	0	16251	809	0
1	CA	32312	0	16307	915	0
2	AB	1846	0	1867	109	0
2	CB	1825	0	1828	119	0
3	AC	1552	0	1546	59	0
3	CC	1542	0	1517	66	0
4	AD	1659	0	1676	99	0
4	CD	1674	0	1714	78	0
5	AE	1129	0	1185	50	0
5	CE	1133	0	1191	45	0
6	AF	806	0	793	33	0
6	CF	816	0	808	27	0
7	AG	1231	0	1238	35	0
7	CG	1235	0	1249	56	0
8	AH	1088	0	1126	48	0
8	CH	1088	0	1126	46	0
9	AI	983	0	986	54	0
9	CI	978	0	966	57	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	47	0
11	AK	829	0	825	19	0
11	CK	833	0	836	29	0
12	AL	930	0	980	28	0
12	CL	930	0	980	34	0
13	AM	958	0	1002	25	0
13	CM	950	0	988	56	0
14	AN	492	0	529	26	0
14	CN	492	0	529	29	0
15	AO	728	0	760	16	0
15	CO	728	0	760	27	0
16	AP	681	0	697	29	0
16	CP	677	0	686	28	0
17	AQ	823	0	891	21	0
17	CQ	823	0	891	19	0
18	AR	555	0	618	17	0
18	CR	555	0	618	27	0
19	AS	652	0	662	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	646	0	644	56	0
20	AT	728	0	798	30	0
20	CT	727	0	796	28	0
21	AU	199	0	208	5	0
21	CU	199	0	208	7	0
22	AV	114	0	54	0	0
22	CV	113	0	54	0	0
23	AX	1623	0	823	18	0
23	CX	1623	0	824	24	0
24	AW	93	0	84	9	0
24	CW	93	0	84	14	0
25	BA	58834	0	29667	785	0
25	DA	58458	0	29482	1100	0
26	BB	2573	0	1306	38	0
26	DB	2573	0	1306	54	0
27	BD	2136	0	2218	64	0
27	DD	2136	0	2218	74	0
28	BE	1559	0	1618	38	0
28	DE	1559	0	1618	60	0
29	BF	1584	0	1625	46	0
29	DF	1580	0	1619	69	0
30	BG	1425	0	1443	45	0
30	DG	1424	0	1434	82	0
31	BH	1330	0	1407	33	0
31	DH	1330	0	1407	52	0
32	BI	1085	0	1114	42	0
32	DI	1061	0	1080	31	0
33	BN	1117	0	1183	17	0
33	DN	1117	0	1184	26	0
34	BO	933	0	996	24	0
34	DO	933	0	996	36	0
35	BP	1135	0	1212	37	0
35	DP	1135	0	1211	46	0
36	BQ	1122	0	1179	38	0
36	DQ	1122	0	1179	47	0
37	BR	968	0	1033	24	0
37	DR	968	0	1032	30	0
38	BS	877	0	938	25	0
38	DS	870	0	923	47	0
39	BT	1091	0	1151	28	0
39	DT	1083	0	1136	36	0
40	BU	959	0	1019	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DU	959	0	1019	37	0
41	BV	771	0	830	11	0
41	DV	771	0	830	23	0
42	BW	886	0	940	9	0
42	DW	886	0	940	17	0
43	BX	750	0	814	20	0
43	DX	750	0	814	25	0
44	BY	806	0	881	25	0
44	DY	806	0	881	21	0
45	BZ	1349	0	1355	47	0
45	DZ	1360	0	1363	48	0
46	B0	653	0	674	25	0
46	D0	653	0	674	23	0
47	B1	755	0	826	19	0
47	D1	755	0	826	26	0
48	B2	588	0	643	18	0
48	D2	588	0	643	20	0
49	B3	469	0	518	17	0
49	D3	464	0	514	12	0
50	B4	551	0	532	38	0
50	D4	531	0	502	32	0
51	B5	455	0	465	13	0
51	D5	455	0	465	11	0
52	B6	453	0	473	10	0
52	D6	449	0	469	10	0
53	B7	418	0	466	9	0
53	D7	418	0	467	9	0
54	B8	511	0	571	27	0
54	D8	517	0	582	27	0
55	B9	307	0	335	5	0
55	D9	307	0	335	10	0
56	AA	221	0	0	0	0
56	AD	1	0	0	0	0
56	AF	1	0	0	0	0
56	AK	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	2	0	0	0	0
56	AV	1	0	0	0	0
56	AX	9	0	0	0	0
56	B0	4	0	0	0	0
56	B1	1	0	0	0	0
56	B2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B3	3	0	0	0	0
56	B4	1	0	0	0	0
56	B5	1	0	0	0	0
56	B7	4	0	0	0	0
56	B8	3	0	0	0	0
56	B9	1	0	0	0	0
56	BA	738	0	0	0	0
56	BB	18	0	0	0	0
56	BD	12	0	0	0	0
56	BE	10	0	0	0	0
56	BF	8	0	0	0	0
56	BG	4	0	0	0	0
56	BN	6	0	0	0	0
56	BO	1	0	0	0	0
56	BP	4	0	0	0	0
56	BQ	5	0	0	0	0
56	BR	4	0	0	0	0
56	BU	8	0	0	0	0
56	BV	4	0	0	0	0
56	BW	5	0	0	0	0
56	BX	1	0	0	0	0
56	BY	1	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	172	0	0	0	0
56	CE	2	0	0	0	0
56	CF	1	0	0	0	0
56	CQ	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	3	0	0	0	0
56	D0	1	0	0	0	0
56	D3	1	0	0	0	0
56	D5	2	0	0	0	0
56	D8	1	0	0	0	0
56	DA	653	0	0	0	0
56	DB	12	0	0	0	0
56	DD	8	0	0	0	0
56	DE	6	0	0	0	0
56	DF	6	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	1	0	0	0	0
56	DQ	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DR	2	0	0	0	0
56	DV	4	0	0	0	0
56	DW	2	0	0	0	0
56	DY	1	0	0	0	0
57	AD	8	0	0	1	0
57	CD	8	0	0	1	0
58	AN	1	0	0	0	0
58	B4	1	0	0	0	0
58	B5	1	0	0	0	0
58	B6	1	0	0	0	0
58	B9	1	0	0	0	0
58	BY	1	0	0	0	0
58	CN	1	0	0	0	0
58	D4	1	0	0	0	0
58	D5	1	0	0	0	0
58	D6	1	0	0	0	0
58	D9	1	0	0	0	0
58	DY	1	0	0	0	0
59	AX	10	0	10	0	0
59	CX	10	0	10	2	0
60	BA	1	0	0	0	0
60	DA	1	0	0	0	0
61	AA	148	0	0	27	0
61	AD	1	0	0	0	0
61	AE	3	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	1	0	0	0	0
61	AP	1	0	0	0	0
61	AU	1	0	0	0	0
61	AV	1	0	0	0	0
61	AX	1	0	0	0	0
61	B0	4	0	0	0	0
61	B1	2	0	0	0	0
61	B5	3	0	0	1	0
61	B7	1	0	0	1	0
61	B8	8	0	0	1	0
61	BA	1092	0	0	113	0
61	BB	26	0	0	0	0
61	BD	8	0	0	1	0
61	BE	9	0	0	4	0
61	BF	4	0	0	0	0
61	BG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BN	3	0	0	0	0
61	BO	2	0	0	0	0
61	BP	15	0	0	3	0
61	BQ	3	0	0	1	0
61	BR	1	0	0	0	0
61	BT	1	0	0	0	0
61	BU	4	0	0	0	0
61	BV	2	0	0	0	0
61	BW	2	0	0	0	0
61	BX	4	0	0	1	0
61	CA	187	0	0	24	0
61	CE	2	0	0	0	0
61	CN	1	0	0	0	0
61	CT	1	0	0	0	0
61	CX	2	0	0	0	0
61	D0	5	0	0	1	0
61	D1	1	0	0	0	0
61	D7	2	0	0	0	0
61	D8	4	0	0	0	0
61	DA	902	0	0	120	0
61	DB	7	0	0	0	0
61	DD	8	0	0	0	0
61	DE	13	0	0	1	0
61	DF	5	0	0	0	0
61	DO	1	0	0	0	0
61	DP	14	0	0	0	0
61	DQ	3	0	0	1	0
61	DU	4	0	0	0	0
61	DV	1	0	0	0	0
61	DX	2	0	0	0	0
61	DY	2	0	0	0	0
All	All	286321	0	191126	6372	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 14.

The worst 5 of 6372 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:CA:1002:G:H1	1:CA:1038:C:N4	1.42	1.16
1:AA:348:G:H2'	1:AA:349:A:H5'	1.36	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1125:U:N3	1:AA:1127:G:N7	2.06	1.03
39:BT:16:ARG:NH2	39:BT:83:ILE:O	1.92	1.02
2:CB:185:ILE:HG22	2:CB:199:TYR:HB2	1.40	1.02

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	
2	AB	229/256 (90%)	200 (87%)	23 (10%)	6 (3%)	5	26
2	CB	229/256 (90%)	201 (88%)	18 (8%)	10 (4%)	2	15
3	AC	204/239 (85%)	179 (88%)	22 (11%)	3 (2%)	10	39
3	CC	204/239 (85%)	178 (87%)	24 (12%)	2 (1%)	15	49
4	AD	206/209 (99%)	182 (88%)	22 (11%)	2 (1%)	15	49
4	CD	206/209 (99%)	185 (90%)	18 (9%)	3 (2%)	10	39
5	AE	146/162 (90%)	127 (87%)	15 (10%)	4 (3%)	5	25
5	CE	146/162 (90%)	133 (91%)	10 (7%)	3 (2%)	7	30
6	AF	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
6	CF	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
7	AG	153/156 (98%)	137 (90%)	14 (9%)	2 (1%)	12	42
7	CG	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	22	57
8	AH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
8	CH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	22	57
9	AI	125/128 (98%)	111 (89%)	10 (8%)	4 (3%)	4	22
9	CI	125/128 (98%)	112 (90%)	11 (9%)	2 (2%)	9	37
10	AJ	95/105 (90%)	85 (90%)	7 (7%)	3 (3%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CJ	94/105 (90%)	86 (92%)	7 (7%)	1 (1%)	14	46
11	AK	112/129 (87%)	98 (88%)	13 (12%)	1 (1%)	17	52
11	CK	112/129 (87%)	99 (88%)	12 (11%)	1 (1%)	17	52
12	AL	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
12	CL	120/132 (91%)	112 (93%)	8 (7%)	0	100	100
13	AM	121/126 (96%)	106 (88%)	15 (12%)	0	100	100
13	CM	120/126 (95%)	104 (87%)	14 (12%)	2 (2%)	9	36
14	AN	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
14	CN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	CO	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	44
16	AP	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
16	CP	80/88 (91%)	70 (88%)	10 (12%)	0	100	100
17	AQ	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
18	AR	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	10	39
18	CR	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	10	39
19	AS	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
19	CS	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
20	AT	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	2	12
20	CT	94/106 (89%)	85 (90%)	3 (3%)	6 (6%)	1	8
21	AU	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
21	CU	21/27 (78%)	18 (86%)	1 (5%)	2 (10%)	0	3
24	AW	3/10 (30%)	1 (33%)	0	2 (67%)	0	0
24	CW	3/10 (30%)	1 (33%)	1 (33%)	1 (33%)	0	0
27	BD	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	34	69
27	DD	273/276 (99%)	257 (94%)	13 (5%)	3 (1%)	14	46
28	BE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	64
28	DE	202/206 (98%)	194 (96%)	6 (3%)	2 (1%)	15	49
29	BF	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	29	64
29	DF	201/210 (96%)	189 (94%)	10 (5%)	2 (1%)	15	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BG	179/182 (98%)	163 (91%)	13 (7%)	3 (2%)	9	36
30	DG	179/182 (98%)	160 (89%)	13 (7%)	6 (3%)	3	21
31	BH	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	25	59
31	DH	172/180 (96%)	159 (92%)	11 (6%)	2 (1%)	13	44
32	BI	144/148 (97%)	122 (85%)	17 (12%)	5 (4%)	3	20
32	DI	144/148 (97%)	123 (85%)	17 (12%)	4 (3%)	5	25
33	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
33	DN	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	22	57
34	BO	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	19	54
34	DO	120/122 (98%)	117 (98%)	2 (2%)	1 (1%)	19	54
35	BP	147/150 (98%)	132 (90%)	14 (10%)	1 (1%)	22	57
35	DP	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	11	40
36	BQ	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	22	57
36	DQ	139/141 (99%)	129 (93%)	8 (6%)	2 (1%)	11	40
37	BR	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	17	52
37	DR	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
38	BS	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	17	52
38	DS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	17	52
39	BT	129/146 (88%)	124 (96%)	4 (3%)	1 (1%)	19	54
39	DT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
40	BU	114/118 (97%)	114 (100%)	0	0	100	100
40	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
41	BV	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	49
41	DV	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	15	49
42	BW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
42	DW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
43	BX	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	46
43	DX	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
44	BY	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
44	DY	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
45	BZ	169/206 (82%)	150 (89%)	17 (10%)	2 (1%)	13	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	DZ	172/206 (84%)	157 (91%)	15 (9%)	0	100	100
46	B0	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	13	44
46	D0	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
47	B1	95/98 (97%)	93 (98%)	0	2 (2%)	7	30
47	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	46
48	B2	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
48	D2	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
49	B3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
49	D3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	B4	67/71 (94%)	50 (75%)	9 (13%)	8 (12%)	0	1
50	D4	67/71 (94%)	50 (75%)	8 (12%)	9 (13%)	0	1
51	B5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
51	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
52	B6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
52	D6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
53	B7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
53	D7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	6	29
54	B8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
54	D8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
55	B9	35/37 (95%)	35 (100%)	0	0	100	100
55	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11415/12148 (94%)	10525 (92%)	749 (7%)	141 (1%)	13	44

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	17	PHE
2	AB	125	PRO
3	AC	65	ALA
3	AC	107	GLN
4	AD	166	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	
2	AB	192/220 (87%)	147 (77%)	45 (23%)	1	3
2	CB	187/220 (85%)	152 (81%)	35 (19%)	1	7
3	AC	143/188 (76%)	125 (87%)	18 (13%)	4	18
3	CC	140/188 (74%)	122 (87%)	18 (13%)	4	18
4	AD	170/181 (94%)	145 (85%)	25 (15%)	3	13
4	CD	173/181 (96%)	152 (88%)	21 (12%)	5	20
5	AE	113/123 (92%)	104 (92%)	9 (8%)	12	40
5	CE	114/123 (93%)	107 (94%)	7 (6%)	18	49
6	AF	83/90 (92%)	76 (92%)	7 (8%)	11	38
6	CF	85/90 (94%)	79 (93%)	6 (7%)	14	44
7	AG	119/127 (94%)	100 (84%)	19 (16%)	2	11
7	CG	120/127 (94%)	102 (85%)	18 (15%)	3	12
8	AH	114/119 (96%)	98 (86%)	16 (14%)	3	15
8	CH	114/119 (96%)	102 (90%)	12 (10%)	7	26
9	AI	90/99 (91%)	76 (84%)	14 (16%)	2	11
9	CI	89/99 (90%)	75 (84%)	14 (16%)	2	11
10	AJ	66/92 (72%)	60 (91%)	6 (9%)	9	33
10	CJ	69/92 (75%)	64 (93%)	5 (7%)	14	44
11	AK	82/99 (83%)	73 (89%)	9 (11%)	6	25
11	CK	83/99 (84%)	77 (93%)	6 (7%)	14	44
12	AL	97/109 (89%)	90 (93%)	7 (7%)	14	44
12	CL	97/109 (89%)	87 (90%)	10 (10%)	7	27
13	AM	93/101 (92%)	82 (88%)	11 (12%)	5	21
13	CM	92/101 (91%)	80 (87%)	12 (13%)	4	18
14	AN	49/50 (98%)	41 (84%)	8 (16%)	2	10
14	CN	49/50 (98%)	42 (86%)	7 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	78/80 (98%)	69 (88%)	9 (12%)	5	22
15	CO	78/80 (98%)	66 (85%)	12 (15%)	2	11
16	AP	69/74 (93%)	60 (87%)	9 (13%)	4	18
16	CP	68/74 (92%)	63 (93%)	5 (7%)	13	42
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	22	54
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	13	42
18	AR	59/77 (77%)	55 (93%)	4 (7%)	16	45
18	CR	59/77 (77%)	52 (88%)	7 (12%)	5	20
19	AS	69/80 (86%)	63 (91%)	6 (9%)	10	36
19	CS	67/80 (84%)	57 (85%)	10 (15%)	3	13
20	AT	70/82 (85%)	61 (87%)	9 (13%)	4	18
20	CT	70/82 (85%)	60 (86%)	10 (14%)	3	14
21	AU	18/22 (82%)	14 (78%)	4 (22%)	1	4
21	CU	18/22 (82%)	16 (89%)	2 (11%)	6	24
24	AW	3/3 (100%)	2 (67%)	1 (33%)	0	0
24	CW	3/3 (100%)	2 (67%)	1 (33%)	0	0
27	BD	215/218 (99%)	198 (92%)	17 (8%)	12	40
27	DD	215/218 (99%)	190 (88%)	25 (12%)	5	22
28	BE	164/166 (99%)	142 (87%)	22 (13%)	4	16
28	DE	164/166 (99%)	144 (88%)	20 (12%)	5	19
29	BF	160/166 (96%)	143 (89%)	17 (11%)	6	26
29	DF	159/166 (96%)	145 (91%)	14 (9%)	10	36
30	BG	143/156 (92%)	123 (86%)	20 (14%)	3	15
30	DG	142/156 (91%)	116 (82%)	26 (18%)	1	7
31	BH	144/148 (97%)	129 (90%)	15 (10%)	7	27
31	DH	144/148 (97%)	131 (91%)	13 (9%)	9	34
32	BI	110/124 (89%)	82 (74%)	28 (26%)	0	1
32	DI	104/124 (84%)	86 (83%)	18 (17%)	2	9
33	BN	118/119 (99%)	103 (87%)	15 (13%)	4	18
33	DN	118/119 (99%)	102 (86%)	16 (14%)	3	16
34	BO	100/100 (100%)	94 (94%)	6 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DO	100/100 (100%)	91 (91%)	9 (9%)	9	34
35	BP	115/116 (99%)	102 (89%)	13 (11%)	6	23
35	DP	115/116 (99%)	104 (90%)	11 (10%)	8	31
36	BQ	111/111 (100%)	94 (85%)	17 (15%)	2	12
36	DQ	111/111 (100%)	96 (86%)	15 (14%)	4	16
37	BR	101/101 (100%)	83 (82%)	18 (18%)	2	8
37	DR	101/101 (100%)	85 (84%)	16 (16%)	2	11
38	BS	87/88 (99%)	77 (88%)	10 (12%)	5	22
38	DS	85/88 (97%)	70 (82%)	15 (18%)	2	8
39	BT	115/127 (91%)	104 (90%)	11 (10%)	8	31
39	DT	113/127 (89%)	105 (93%)	8 (7%)	14	44
40	BU	93/94 (99%)	83 (89%)	10 (11%)	6	25
40	DU	93/94 (99%)	82 (88%)	11 (12%)	5	21
41	BV	80/82 (98%)	69 (86%)	11 (14%)	3	16
41	DV	80/82 (98%)	71 (89%)	9 (11%)	6	23
42	BW	90/92 (98%)	79 (88%)	11 (12%)	5	19
42	DW	90/92 (98%)	80 (89%)	10 (11%)	6	24
43	BX	77/78 (99%)	73 (95%)	4 (5%)	23	55
43	DX	77/78 (99%)	74 (96%)	3 (4%)	32	65
44	BY	85/91 (93%)	79 (93%)	6 (7%)	14	44
44	DY	85/91 (93%)	79 (93%)	6 (7%)	14	44
45	BZ	145/179 (81%)	121 (83%)	24 (17%)	2	9
45	DZ	145/179 (81%)	126 (87%)	19 (13%)	4	17
46	B0	65/67 (97%)	61 (94%)	4 (6%)	18	49
46	D0	65/67 (97%)	59 (91%)	6 (9%)	9	33
47	B1	80/83 (96%)	72 (90%)	8 (10%)	7	28
47	D1	80/83 (96%)	73 (91%)	7 (9%)	10	36
48	B2	65/67 (97%)	56 (86%)	9 (14%)	3	16
48	D2	65/67 (97%)	57 (88%)	8 (12%)	4	19
49	B3	51/52 (98%)	44 (86%)	7 (14%)	3	16
49	D3	50/52 (96%)	43 (86%)	7 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B4	59/63 (94%)	48 (81%)	11 (19%)	1	7
50	D4	53/63 (84%)	45 (85%)	8 (15%)	3	12
51	B5	50/52 (96%)	45 (90%)	5 (10%)	7	28
51	D5	50/52 (96%)	45 (90%)	5 (10%)	7	28
52	B6	51/52 (98%)	45 (88%)	6 (12%)	5	21
52	D6	50/52 (96%)	46 (92%)	4 (8%)	12	40
53	B7	41/42 (98%)	37 (90%)	4 (10%)	8	29
53	D7	41/42 (98%)	39 (95%)	2 (5%)	25	57
54	B8	53/55 (96%)	49 (92%)	4 (8%)	13	42
54	D8	54/55 (98%)	50 (93%)	4 (7%)	13	42
55	B9	34/34 (100%)	33 (97%)	1 (3%)	42	72
55	D9	34/34 (100%)	33 (97%)	1 (3%)	42	72
All	All	9325/10072 (93%)	8209 (88%)	1116 (12%)	5	20

5 of 1116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	DN	87	LEU
36	DQ	7	MET
33	DN	85	ILE
44	DY	11	ASP
35	BP	98	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
49	B3	32	GLN
46	D0	3	HIS
4	CD	125	HIS
44	DY	43	ASN
31	DH	158	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1522 (98%)	393 (26%)	25 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	CA	1502/1522 (98%)	388 (25%)	31 (2%)
22	AV	4/24 (16%)	1 (25%)	0
22	CV	4/24 (16%)	1 (25%)	0
23	AX	75/77 (97%)	16 (21%)	0
23	CX	75/77 (97%)	16 (21%)	0
25	BA	2722/2915 (93%)	508 (18%)	40 (1%)
25	DA	2704/2915 (92%)	535 (19%)	37 (1%)
26	BB	119/122 (97%)	18 (15%)	0
26	DB	119/122 (97%)	24 (20%)	1 (0%)
All	All	8819/9320 (94%)	1900 (21%)	134 (1%)

5 of 1900 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	15	G
1	AA	22	G
1	AA	32	A

5 of 134 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	DA	1420	U
25	DA	1558	A
25	DA	2689	U
25	BA	1507	A
25	BA	1466	U

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

14 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
24	004	AW	3	24	9,10,11	0.97	1 (11%)	9,12,14	1.20	2 (22%)
24	004	CW	3	24	9,10,11	1.22	1 (11%)	9,12,14	0.97	0
24	2R1	AW	6	24	10,10,11	1.78	3 (30%)	6,13,15	5.49	2 (33%)
24	MVA	AW	9	24	6,7,8	0.46	0	7,8,10	0.95	1 (14%)
24	2R3	AW	8	24	12,14,15	0.80	0	16,18,20	1.73	5 (31%)
24	2QZ	CW	1	24	7,8,9	0.61	0	8,10,12	3.72	2 (25%)
24	MVA	CW	9	24	6,7,8	0.97	1 (16%)	7,8,10	1.53	1 (14%)
24	2R1	CW	6	24	10,10,11	1.86	2 (20%)	6,13,15	4.48	2 (33%)
24	2QY	AW	10	24	12,13,14	2.00	1 (8%)	13,16,18	3.53	4 (30%)
24	2QY	CW	10	24	12,13,14	2.25	2 (16%)	13,16,18	2.99	2 (15%)
24	2QZ	AW	1	24	7,8,9	0.38	0	8,10,12	4.18	1 (12%)
24	MVA	CW	5	24	6,7,8	0.70	0	7,8,10	1.42	1 (14%)
24	MVA	AW	5	24	6,7,8	0.37	0	7,8,10	1.11	0
24	2R3	CW	8	24	12,14,15	0.66	0	16,18,20	1.63	5 (31%)

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
24	004	AW	3	24	-	0/4/6/8	0/1/1/1
24	004	CW	3	24	-	0/4/6/8	0/1/1/1
24	2R1	AW	6	24	-	1/2/14/16	0/1/1/1
24	MVA	AW	9	24	-	5/6/8/10	-
24	2R3	AW	8	24	-	4/11/12/14	0/1/1/1
24	2QZ	CW	1	24	-	2/6/10/12	-
24	MVA	CW	9	24	-	5/6/8/10	-
24	2R1	CW	6	24	-	0/2/14/16	0/1/1/1
24	2QY	AW	10	24	-	3/4/8/10	0/1/1/1
24	2QY	CW	10	24	-	2/4/8/10	0/1/1/1
24	2QZ	AW	1	24	-	3/6/10/12	-
24	MVA	CW	5	24	-	6/6/8/10	-
24	MVA	AW	5	24	-	3/6/8/10	-
24	2R3	CW	8	24	-	7/11/12/14	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CW	10	2QY	C-CA	6.88	1.53	1.43
24	AW	10	2QY	C-CA	6.24	1.52	1.43
24	CW	6	2R1	CA-N	3.90	1.46	1.36
24	AW	6	2R1	CA-N	3.57	1.45	1.36
24	CW	6	2R1	C-CA	3.43	1.50	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AW	6	2R1	OD2-CG2-CB	-12.79	88.98	112.24
24	AW	1	2QZ	OG1-CB-CG2	11.22	142.97	109.74
24	CW	6	2R1	OD2-CG2-CB	-10.33	93.46	112.24
24	AW	10	2QY	CN-N-CA	-10.27	107.83	123.45
24	CW	1	2QZ	OG1-CB-CG2	9.77	138.68	109.74

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AW	1	2QZ	N-CA-CB-OG1
24	AW	1	2QZ	N-CA-CB-CG2
24	AW	1	2QZ	C-CA-CB-OG1
24	AW	5	MVA	CB-CA-N-CN
24	AW	5	MVA	C-CA-CB-CG1

There are no ring outliers.

13 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AW	3	004	1	0
24	CW	3	004	1	0
24	AW	6	2R1	1	0
24	AW	9	MVA	3	0
24	AW	8	2R3	1	0
24	CW	1	2QZ	2	0
24	CW	9	MVA	6	0
24	CW	6	2R1	1	0
24	AW	10	2QY	5	0
24	CW	10	2QY	9	0
24	AW	1	2QZ	2	0
24	CW	5	MVA	2	0
24	CW	8	2R3	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1991 ligands modelled in this entry, 1987 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
59	FME	AX	101	23	8,9,10	0.93	0	7,9,11	1.49	1 (14%)
57	SF4	CD	501	4	0,12,12	-	-	-		
57	SF4	AD	501	4	0,12,12	-	-	-		
59	FME	CX	101	23	8,9,10	1.05	1 (12%)	7,9,11	1.32	2 (28%)

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
59	FME	AX	101	23	-	3/7/9/11	-
57	SF4	CD	501	4	-	-	0/6/5/5
57	SF4	AD	501	4	-	-	0/6/5/5
59	FME	CX	101	23	-	3/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CX	101	FME	CA-N	2.14	1.49	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AX	101	FME	CA-N-CN	-2.85	118.44	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	CX	101	FME	CA-N-CN	-2.17	119.49	122.82
59	CX	101	FME	C-CA-N	2.10	113.52	109.73

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AX	101	FME	O1-CN-N-CA
59	AX	101	FME	O-C-CA-CB
59	CX	101	FME	O1-CN-N-CA
59	CX	101	FME	O-C-CA-CB
59	CX	101	FME	CA-CB-CG-SD

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	CD	501	SF4	1	0
57	AD	501	SF4	1	0
59	CX	101	FME	2	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	AA	1498/1522 (98%)	-0.17	32 (2%) 63 43	36, 80, 103, 123	0
1	CA	1503/1522 (98%)	-0.18	34 (2%) 60 39	38, 80, 103, 122	0
2	AB	231/256 (90%)	-0.07	8 (3%) 44 23	71, 88, 98, 107	0
2	CB	231/256 (90%)	0.20	12 (5%) 27 12	71, 89, 99, 108	0
3	AC	206/239 (86%)	0.18	6 (2%) 51 28	74, 87, 96, 108	0
3	CC	206/239 (86%)	0.33	13 (6%) 20 8	75, 89, 98, 106	0
4	AD	208/209 (99%)	0.06	4 (1%) 66 46	62, 80, 92, 99	0
4	CD	208/209 (99%)	-0.15	0 100 100	61, 79, 92, 99	0
5	AE	148/162 (91%)	-0.25	0 100 100	53, 73, 83, 96	0
5	CE	148/162 (91%)	-0.22	0 100 100	54, 74, 85, 98	0
6	AF	100/101 (99%)	-0.22	0 100 100	60, 78, 89, 92	0
6	CF	100/101 (99%)	-0.32	0 100 100	62, 79, 89, 94	0
7	AG	155/156 (99%)	0.29	11 (7%) 16 6	74, 85, 97, 104	0
7	CG	155/156 (99%)	0.36	10 (6%) 18 8	76, 86, 99, 105	0
8	AH	137/138 (99%)	-0.08	0 100 100	60, 75, 83, 90	0
8	CH	137/138 (99%)	-0.15	0 100 100	61, 76, 83, 90	0
9	AI	127/128 (99%)	0.44	8 (6%) 20 8	70, 92, 99, 103	0
9	CI	127/128 (99%)	0.98	22 (17%) 1 0	69, 93, 100, 105	0
10	AJ	97/105 (92%)	0.66	12 (12%) 4 1	71, 93, 101, 106	0
10	CJ	96/105 (91%)	0.68	12 (12%) 3 1	75, 95, 102, 107	0
11	AK	114/129 (88%)	-0.24	0 100 100	53, 74, 88, 93	0
11	CK	114/129 (88%)	-0.02	3 (2%) 56 33	54, 76, 88, 93	0
12	AL	122/132 (92%)	-0.18	1 (0%) 86 72	56, 68, 80, 86	0
12	CL	122/132 (92%)	-0.19	0 100 100	55, 68, 79, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	123/126 (97%)	0.29	9 (7%) 15 6	67, 83, 95, 104	0
13	CM	122/126 (96%)	0.58	11 (9%) 9 3	77, 91, 101, 105	0
14	AN	60/61 (98%)	0.17	2 (3%) 46 24	74, 85, 95, 97	0
14	CN	60/61 (98%)	0.56	4 (6%) 17 7	77, 88, 95, 100	0
15	AO	88/89 (98%)	-0.23	0 100 100	59, 73, 87, 94	0
15	CO	88/89 (98%)	0.04	1 (1%) 80 64	58, 73, 87, 95	0
16	AP	82/88 (93%)	0.41	2 (2%) 59 37	66, 77, 88, 95	0
16	CP	82/88 (93%)	-0.01	0 100 100	66, 76, 88, 93	0
17	AQ	99/105 (94%)	0.02	0 100 100	59, 73, 84, 87	0
17	CQ	99/105 (94%)	-0.07	1 (1%) 82 67	60, 73, 84, 85	0
18	AR	68/88 (77%)	0.16	1 (1%) 73 54	66, 76, 86, 90	0
18	CR	68/88 (77%)	0.39	0 100 100	67, 77, 87, 89	0
19	AS	83/93 (89%)	0.79	11 (13%) 3 1	79, 91, 100, 105	0
19	CS	83/93 (89%)	1.23	16 (19%) 1 0	82, 92, 102, 106	0
20	AT	96/106 (90%)	0.07	0 100 100	62, 75, 88, 91	0
20	CT	96/106 (90%)	0.09	1 (1%) 82 67	62, 75, 86, 94	0
21	AU	23/27 (85%)	1.22	5 (21%) 0 0	76, 87, 90, 91	0
21	CU	23/27 (85%)	1.16	5 (21%) 0 0	77, 87, 91, 92	0
22	AV	7/24 (29%)	0.02	0 100 100	61, 73, 97, 100	0
22	CV	6/24 (25%)	0.36	0 100 100	64, 75, 94, 103	0
23	AX	76/77 (98%)	0.02	0 100 100	48, 79, 96, 101	0
23	CX	76/77 (98%)	0.02	0 100 100	47, 81, 98, 101	0
24	AW	3/10 (30%)	-0.00	0 100 100	78, 78, 93, 96	0
24	CW	3/10 (30%)	0.56	1 (33%) 0 0	67, 67, 87, 96	0
25	BA	2731/2915 (93%)	-0.28	11 (0%) 92 84	24, 44, 86, 114	0
25	DA	2714/2915 (93%)	-0.49	18 (0%) 87 75	27, 48, 87, 118	0
26	BB	120/122 (98%)	-0.40	0 100 100	41, 68, 81, 96	0
26	DB	120/122 (98%)	-0.33	0 100 100	47, 73, 86, 98	0
27	BD	275/276 (99%)	-0.47	1 (0%) 92 84	24, 41, 62, 85	0
27	DD	275/276 (99%)	-0.47	0 100 100	25, 44, 63, 86	0
28	BE	204/206 (99%)	-0.35	0 100 100	22, 45, 68, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DE	204/206 (99%)	-0.45	0 100 100	24, 47, 70, 90	0
29	BF	203/210 (96%)	-0.33	0 100 100	24, 52, 77, 97	0
29	DF	203/210 (96%)	-0.45	0 100 100	25, 56, 79, 96	0
30	BG	181/182 (99%)	-0.30	2 (1%) 80 64	61, 76, 89, 100	0
30	DG	181/182 (99%)	0.09	5 (2%) 53 30	65, 79, 91, 100	0
31	BH	174/180 (96%)	-0.32	0 100 100	49, 67, 81, 85	0
31	DH	174/180 (96%)	0.52	17 (9%) 7 2	54, 72, 85, 89	0
32	BI	146/148 (98%)	-0.16	0 100 100	49, 77, 88, 94	0
32	DI	146/148 (98%)	0.14	5 (3%) 45 24	49, 78, 88, 94	0
33	BN	140/140 (100%)	-0.37	0 100 100	33, 48, 71, 78	0
33	DN	140/140 (100%)	-0.42	0 100 100	35, 52, 73, 81	0
34	BO	122/122 (100%)	-0.50	0 100 100	23, 40, 61, 76	0
34	DO	122/122 (100%)	-0.47	0 100 100	37, 53, 71, 80	0
35	BP	149/150 (99%)	-0.32	0 100 100	25, 54, 77, 83	0
35	DP	149/150 (99%)	-0.07	1 (0%) 87 75	27, 57, 81, 87	0
36	BQ	141/141 (100%)	-0.33	0 100 100	36, 52, 68, 79	0
36	DQ	141/141 (100%)	-0.45	0 100 100	38, 55, 71, 81	0
37	BR	118/118 (100%)	-0.50	0 100 100	20, 35, 52, 64	0
37	DR	118/118 (100%)	-0.40	0 100 100	36, 52, 68, 84	0
38	BS	110/112 (98%)	-0.43	0 100 100	35, 54, 71, 85	0
38	DS	110/112 (98%)	0.27	5 (4%) 33 16	65, 81, 92, 95	0
39	BT	131/146 (89%)	-0.48	0 100 100	31, 45, 75, 92	0
39	DT	131/146 (89%)	-0.45	0 100 100	45, 59, 80, 90	0
40	BU	116/118 (98%)	-0.64	0 100 100	21, 31, 52, 63	0
40	DU	116/118 (98%)	-0.34	1 (0%) 84 69	36, 61, 78, 92	0
41	BV	101/101 (100%)	-0.42	0 100 100	27, 53, 73, 80	0
41	DV	101/101 (100%)	-0.19	0 100 100	29, 58, 78, 80	0
42	BW	112/113 (99%)	-0.43	0 100 100	27, 38, 62, 92	0
42	DW	112/113 (99%)	-0.25	0 100 100	30, 42, 64, 94	0
43	BX	95/96 (98%)	-0.37	0 100 100	29, 47, 72, 81	0
43	DX	95/96 (98%)	-0.29	2 (2%) 63 43	33, 51, 73, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BY	107/110 (97%)	-0.19	2 (1%) 66 46	39, 61, 80, 89	0
44	DY	107/110 (97%)	0.29	4 (3%) 41 21	43, 65, 82, 92	0
45	BZ	171/206 (83%)	-0.39	0 100 100	53, 71, 85, 96	0
45	DZ	174/206 (84%)	-0.07	0 100 100	58, 74, 87, 95	0
46	B0	83/85 (97%)	-0.08	7 (8%) 11 4	25, 39, 80, 108	0
46	D0	83/85 (97%)	0.42	10 (12%) 4 2	42, 66, 86, 104	0
47	B1	97/98 (98%)	-0.27	1 (1%) 82 67	27, 44, 74, 83	0
47	D1	97/98 (98%)	-0.23	1 (1%) 82 67	35, 58, 79, 86	0
48	B2	70/72 (97%)	-0.54	0 100 100	35, 48, 64, 90	0
48	D2	70/72 (97%)	-0.26	0 100 100	59, 74, 83, 92	0
49	B3	59/60 (98%)	-0.36	0 100 100	24, 38, 63, 85	0
49	D3	59/60 (98%)	0.19	1 (1%) 70 49	45, 62, 80, 90	0
50	B4	69/71 (97%)	-0.18	1 (1%) 75 56	60, 85, 103, 105	0
50	D4	69/71 (97%)	0.38	5 (7%) 15 6	82, 96, 106, 112	0
51	B5	59/60 (98%)	-0.61	0 100 100	14, 36, 59, 74	0
51	D5	59/60 (98%)	-0.54	0 100 100	31, 50, 72, 82	0
52	B6	53/54 (98%)	-0.27	0 100 100	43, 53, 68, 75	0
52	D6	53/54 (98%)	-0.25	0 100 100	45, 56, 69, 73	0
53	B7	48/49 (97%)	-0.30	0 100 100	24, 32, 62, 84	0
53	D7	48/49 (97%)	-0.15	1 (2%) 63 43	26, 35, 63, 86	0
54	B8	64/65 (98%)	-0.30	0 100 100	31, 42, 51, 64	0
54	D8	64/65 (98%)	-0.30	0 100 100	34, 46, 56, 66	0
55	B9	37/37 (100%)	0.06	0 100 100	43, 53, 71, 77	0
55	D9	37/37 (100%)	0.62	3 (8%) 12 5	46, 58, 73, 78	0
All	All	20462/21468 (95%)	-0.18	362 (1%) 68 47	14, 65, 95, 123	0

The worst 5 of 362 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	15.2
13	CM	123	ALA	12.7
13	AM	124	PRO	9.7
13	AM	123	ALA	9.5
46	B0	3	HIS	8.1

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	004	AW	3	10/11	0.83	0.13	71,89,99,106	0
24	2R1	AW	6	10/11	0.90	0.12	68,82,98,104	0
24	2QY	CW	10	13/14	0.91	0.14	55,69,84,94	0
24	MVA	CW	9	8/9	0.92	0.21	61,72,80,84	0
24	MVA	AW	5	8/9	0.93	0.19	66,87,90,90	0
24	MVA	AW	9	8/9	0.93	0.24	65,78,87,91	0
24	MVA	CW	5	8/9	0.94	0.20	51,78,86,88	0
24	2R1	CW	6	10/11	0.94	0.11	79,86,90,94	0
24	004	CW	3	10/11	0.94	0.15	60,76,84,86	0
24	2QZ	AW	1	9/10	0.95	0.22	58,64,81,82	0
24	2QZ	CW	1	9/10	0.95	0.24	57,72,81,93	0
24	2R3	AW	8	14/15	0.95	0.15	54,79,87,90	0
24	2R3	CW	8	14/15	0.96	0.11	47,70,74,79	0
24	2QY	AW	10	13/14	0.97	0.14	55,67,75,79	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	AA	3093	1/1	0.37	0.58	88,88,88,88	0
56	MG	BA	3094	1/1	0.40	0.86	61,61,61,61	0
56	MG	BA	3295	1/1	0.40	0.57	75,75,75,75	0
56	MG	AA	3043	1/1	0.50	0.50	74,74,74,74	0
56	MG	CA	3041	1/1	0.50	0.69	75,75,75,75	0
56	MG	BA	3247	1/1	0.51	0.96	68,68,68,68	0
56	MG	CA	3042	1/1	0.58	0.56	85,85,85,85	0
56	MG	DA	3427	1/1	0.58	0.54	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3079	1/1	0.60	1.07	74,74,74,74	0
56	MG	AA	3114	1/1	0.60	0.51	66,66,66,66	0
56	MG	DA	3464	1/1	0.60	0.56	50,50,50,50	0
56	MG	AA	3116	1/1	0.61	0.53	52,52,52,52	0
56	MG	B4	3001	1/1	0.61	0.27	100,100,100,100	0
56	MG	CA	3053	1/1	0.62	1.19	73,73,73,73	0
56	MG	AA	3147	1/1	0.63	0.49	61,61,61,61	0
56	MG	BA	3613	1/1	0.64	0.29	76,76,76,76	0
56	MG	AA	3087	1/1	0.64	0.36	72,72,72,72	0
56	MG	CA	3016	1/1	0.64	0.48	76,76,76,76	0
56	MG	AA	3045	1/1	0.64	0.31	61,61,61,61	0
56	MG	AA	3028	1/1	0.65	0.46	60,60,60,60	0
56	MG	DA	3135	1/1	0.65	0.23	50,50,50,50	0
56	MG	BA	3622	1/1	0.65	0.52	77,77,77,77	0
56	MG	AA	3129	1/1	0.65	0.30	77,77,77,77	0
56	MG	DA	3162	1/1	0.66	0.13	71,71,71,71	0
56	MG	BA	3691	1/1	0.67	0.38	49,49,49,49	0
56	MG	DA	3068	1/1	0.67	0.33	55,55,55,55	0
56	MG	DA	3545	1/1	0.67	0.62	75,75,75,75	0
56	MG	DA	3186	1/1	0.68	0.51	53,53,53,53	0
56	MG	DA	3131	1/1	0.68	0.23	54,54,54,54	0
56	MG	CA	3025	1/1	0.69	0.18	94,94,94,94	0
56	MG	CA	3038	1/1	0.69	0.46	70,70,70,70	0
56	MG	DA	3211	1/1	0.69	0.10	51,51,51,51	0
56	MG	DA	3125	1/1	0.69	0.55	48,48,48,48	0
56	MG	AA	3023	1/1	0.69	0.17	65,65,65,65	0
56	MG	AX	102	1/1	0.69	0.25	74,74,74,74	0
56	MG	DB	3003	1/1	0.69	0.12	63,63,63,63	0
56	MG	AA	3084	1/1	0.70	0.36	78,78,78,78	0
56	MG	DA	3103	1/1	0.70	0.78	48,48,48,48	0
56	MG	BA	3579	1/1	0.70	0.24	63,63,63,63	0
56	MG	CA	3135	1/1	0.70	0.56	76,76,76,76	0
59	FME	CX	101	10/11	0.70	0.57	71,82,97,105	0
56	MG	CA	3030	1/1	0.71	0.45	73,73,73,73	0
56	MG	AA	3048	1/1	0.71	0.25	57,57,57,57	0
56	MG	DA	3223	1/1	0.71	0.26	66,66,66,66	0
56	MG	DA	3117	1/1	0.71	0.17	53,53,53,53	0
56	MG	BA	3270	1/1	0.71	0.31	50,50,50,50	0
56	MG	AA	3128	1/1	0.71	0.20	68,68,68,68	0
56	MG	DA	3581	1/1	0.71	0.86	73,73,73,73	0
56	MG	AA	3044	1/1	0.71	0.22	66,66,66,66	0
56	MG	BA	3235	1/1	0.71	0.28	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3024	1/1	0.72	0.44	65,65,65,65	0
56	MG	BA	3703	1/1	0.72	0.22	31,31,31,31	0
56	MG	AA	3037	1/1	0.72	0.41	61,61,61,61	0
58	ZN	B4	3002	1/1	0.72	0.07	165,165,165,165	0
56	MG	BA	3263	1/1	0.72	0.23	79,79,79,79	0
56	MG	CA	3055	1/1	0.73	0.28	62,62,62,62	0
56	MG	CA	3067	1/1	0.73	0.30	80,80,80,80	0
56	MG	BA	3065	1/1	0.73	0.44	50,50,50,50	0
56	MG	BA	3085	1/1	0.73	0.46	48,48,48,48	0
56	MG	AA	3020	1/1	0.73	0.10	77,77,77,77	0
56	MG	BA	3632	1/1	0.73	0.30	57,57,57,57	0
56	MG	BA	3289	1/1	0.73	0.34	60,60,60,60	0
56	MG	AA	3065	1/1	0.73	0.27	60,60,60,60	0
56	MG	DW	202	1/1	0.73	0.42	58,58,58,58	0
56	MG	BF	307	1/1	0.73	0.40	47,47,47,47	0
56	MG	BA	3297	1/1	0.73	1.46	53,53,53,53	0
56	MG	B1	3001	1/1	0.74	0.86	54,54,54,54	0
56	MG	AA	3086	1/1	0.74	0.30	51,51,51,51	0
56	MG	BA	3287	1/1	0.74	0.17	53,53,53,53	0
56	MG	BA	3699	1/1	0.74	0.52	56,56,56,56	0
56	MG	BA	3089	1/1	0.74	0.57	61,61,61,61	0
56	MG	AA	3006	1/1	0.74	0.08	78,78,78,78	0
56	MG	DA	3438	1/1	0.74	0.51	70,70,70,70	0
56	MG	DA	3011	1/1	0.75	0.38	45,45,45,45	0
56	MG	DA	3049	1/1	0.75	0.30	58,58,58,58	0
56	MG	AA	3117	1/1	0.75	0.26	71,71,71,71	0
56	MG	AA	3035	1/1	0.76	0.42	71,71,71,71	0
56	MG	BA	3206	1/1	0.76	0.35	57,57,57,57	0
56	MG	DA	3056	1/1	0.76	0.37	43,43,43,43	0
56	MG	DA	3228	1/1	0.76	0.25	45,45,45,45	0
56	MG	DA	3410	1/1	0.76	0.22	69,69,69,69	0
56	MG	DA	3064	1/1	0.76	0.41	50,50,50,50	0
56	MG	CA	3018	1/1	0.76	0.31	54,54,54,54	0
56	MG	BA	3231	1/1	0.76	0.55	38,38,38,38	0
56	MG	BU	206	1/1	0.76	0.38	60,60,60,60	0
56	MG	DA	3123	1/1	0.76	0.23	59,59,59,59	0
56	MG	BA	3075	1/1	0.76	0.26	45,45,45,45	0
56	MG	CA	3127	1/1	0.76	0.25	79,79,79,79	0
56	MG	CA	3033	1/1	0.76	0.19	68,68,68,68	0
56	MG	CX	103	1/1	0.76	0.25	60,60,60,60	0
56	MG	DA	3587	1/1	0.77	0.14	64,64,64,64	0
56	MG	AX	108	1/1	0.77	0.21	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3090	1/1	0.77	0.17	68,68,68,68	0
56	MG	AA	3120	1/1	0.77	0.63	71,71,71,71	0
56	MG	AA	3051	1/1	0.77	0.50	73,73,73,73	0
56	MG	AA	3100	1/1	0.78	0.67	40,40,40,40	0
56	MG	AA	3127	1/1	0.78	0.18	62,62,62,62	0
56	MG	BA	3275	1/1	0.78	0.20	46,46,46,46	0
56	MG	BA	3160	1/1	0.78	0.65	53,53,53,53	0
56	MG	AA	3063	1/1	0.78	0.30	61,61,61,61	0
56	MG	BA	3718	1/1	0.78	0.37	57,57,57,57	0
56	MG	AA	3088	1/1	0.78	0.33	63,63,63,63	0
56	MG	DA	3615	1/1	0.78	0.40	60,60,60,60	0
56	MG	AA	3096	1/1	0.78	0.28	44,44,44,44	0
56	MG	BA	3241	1/1	0.78	0.38	63,63,63,63	0
56	MG	BA	3087	1/1	0.78	0.45	61,61,61,61	0
56	MG	DA	3098	1/1	0.78	1.25	43,43,43,43	0
56	MG	DA	3089	1/1	0.79	0.39	57,57,57,57	0
56	MG	BA	3022	1/1	0.79	0.34	52,52,52,52	0
56	MG	BB	3005	1/1	0.79	0.28	61,61,61,61	0
56	MG	CA	3021	1/1	0.79	0.22	53,53,53,53	0
56	MG	BA	3209	1/1	0.79	0.38	40,40,40,40	0
56	MG	DA	3352	1/1	0.79	0.38	47,47,47,47	0
56	MG	DG	3001	1/1	0.79	0.14	63,63,63,63	0
56	MG	AA	3071	1/1	0.79	0.29	60,60,60,60	0
56	MG	AA	3113	1/1	0.79	0.28	68,68,68,68	0
56	MG	AA	3076	1/1	0.79	0.29	66,66,66,66	0
56	MG	DA	3293	1/1	0.80	0.27	53,53,53,53	0
56	MG	DA	3314	1/1	0.80	0.19	64,64,64,64	0
56	MG	BA	3158	1/1	0.80	0.54	64,64,64,64	0
56	MG	DA	3402	1/1	0.80	0.08	61,61,61,61	0
56	MG	CA	3062	1/1	0.80	0.26	57,57,57,57	0
56	MG	BA	3069	1/1	0.80	0.44	41,41,41,41	0
56	MG	DA	3113	1/1	0.80	0.57	43,43,43,43	0
56	MG	DA	3454	1/1	0.80	0.31	55,55,55,55	0
56	MG	BA	3731	1/1	0.80	0.36	55,55,55,55	0
56	MG	DA	3499	1/1	0.80	0.13	46,46,46,46	0
56	MG	DA	3525	1/1	0.80	0.70	70,70,70,70	0
56	MG	AA	3110	1/1	0.80	0.24	48,48,48,48	0
56	MG	CA	3138	1/1	0.80	0.24	72,72,72,72	0
56	MG	CA	3147	1/1	0.80	0.26	66,66,66,66	0
56	MG	AA	3061	1/1	0.80	0.19	82,82,82,82	0
56	MG	AA	3118	1/1	0.80	0.32	52,52,52,52	0
56	MG	DB	3007	1/1	0.80	0.27	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	B0	103	1/1	0.80	0.84	59,59,59,59	0
56	MG	BA	3658	1/1	0.80	0.27	79,79,79,79	0
56	MG	BA	3029	1/1	0.80	0.38	53,53,53,53	0
56	MG	AA	3089	1/1	0.80	0.43	78,78,78,78	0
56	MG	BA	3370	1/1	0.81	0.19	54,54,54,54	0
56	MG	BA	3180	1/1	0.81	0.99	43,43,43,43	0
56	MG	CA	3057	1/1	0.81	0.26	49,49,49,49	0
56	MG	CA	3060	1/1	0.81	0.37	43,43,43,43	0
56	MG	AA	3085	1/1	0.81	0.32	69,69,69,69	0
56	MG	BB	3003	1/1	0.81	0.25	43,43,43,43	0
56	MG	CA	3073	1/1	0.81	0.39	55,55,55,55	0
56	MG	DA	3492	1/1	0.81	0.37	68,68,68,68	0
56	MG	CA	3123	1/1	0.81	0.14	77,77,77,77	0
56	MG	BB	3004	1/1	0.81	0.26	54,54,54,54	0
56	MG	AA	3012	1/1	0.81	0.14	56,56,56,56	0
56	MG	BA	3146	1/1	0.81	0.29	52,52,52,52	0
56	MG	CA	3144	1/1	0.81	0.59	63,63,63,63	0
56	MG	BA	3155	1/1	0.81	0.38	57,57,57,57	0
56	MG	DA	3647	1/1	0.81	0.37	66,66,66,66	0
56	MG	DB	3001	1/1	0.81	0.25	68,68,68,68	0
56	MG	CA	3172	1/1	0.81	0.15	51,51,51,51	0
56	MG	CE	3001	1/1	0.81	0.32	68,68,68,68	0
56	MG	DE	302	1/1	0.81	0.38	44,44,44,44	0
56	MG	BW	201	1/1	0.81	0.88	53,53,53,53	0
56	MG	DA	3003	1/1	0.81	0.35	56,56,56,56	0
56	MG	AA	3030	1/1	0.81	0.32	69,69,69,69	0
56	MG	AX	103	1/1	0.81	0.08	66,66,66,66	0
56	MG	CA	3015	1/1	0.82	0.34	51,51,51,51	0
56	MG	BA	3244	1/1	0.82	0.47	65,65,65,65	0
56	MG	DA	3279	1/1	0.82	0.31	63,63,63,63	0
56	MG	CA	3161	1/1	0.82	0.12	54,54,54,54	0
56	MG	BA	3083	1/1	0.82	0.23	63,63,63,63	0
56	MG	BA	3157	1/1	0.82	0.39	63,63,63,63	0
56	MG	DA	3388	1/1	0.82	0.16	54,54,54,54	0
56	MG	BA	3706	1/1	0.82	0.46	63,63,63,63	0
56	MG	BA	3402	1/1	0.82	0.25	71,71,71,71	0
56	MG	BA	3719	1/1	0.82	0.25	25,25,25,25	0
56	MG	DA	3024	1/1	0.82	0.36	65,65,65,65	0
56	MG	BA	3444	1/1	0.82	0.15	74,74,74,74	0
56	MG	BA	3736	1/1	0.82	0.24	48,48,48,48	0
56	MG	BA	3739	1/1	0.82	0.76	50,50,50,50	0
56	MG	DA	3497	1/1	0.82	0.23	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3452	1/1	0.82	0.26	47,47,47,47	0
56	MG	BA	3562	1/1	0.82	0.10	73,73,73,73	0
56	MG	BA	3123	1/1	0.82	0.33	69,69,69,69	0
56	MG	BD	311	1/1	0.82	0.54	45,45,45,45	0
56	MG	BA	3611	1/1	0.82	0.28	52,52,52,52	0
56	MG	BA	3134	1/1	0.82	0.31	47,47,47,47	0
56	MG	AA	3038	1/1	0.82	0.35	66,66,66,66	0
56	MG	BA	3242	1/1	0.82	0.36	48,48,48,48	0
56	MG	CA	3114	1/1	0.82	0.27	82,82,82,82	0
56	MG	BA	3290	1/1	0.82	0.24	49,49,49,49	0
56	MG	B2	101	1/1	0.82	0.36	40,40,40,40	0
56	MG	BA	3677	1/1	0.82	0.27	67,67,67,67	0
56	MG	DQ	205	1/1	0.82	0.40	55,55,55,55	0
56	MG	DA	3187	1/1	0.82	0.44	59,59,59,59	0
56	MG	DA	3189	1/1	0.82	0.11	55,55,55,55	0
56	MG	CA	3007	1/1	0.82	0.56	68,68,68,68	0
56	MG	BZ	3001	1/1	0.83	0.28	61,61,61,61	0
56	MG	CA	3032	1/1	0.83	0.20	42,42,42,42	0
56	MG	B0	102	1/1	0.83	0.61	40,40,40,40	0
56	MG	CA	3139	1/1	0.83	0.27	75,75,75,75	0
56	MG	CA	3035	1/1	0.83	0.23	52,52,52,52	0
56	MG	AA	3014	1/1	0.83	0.19	28,28,28,28	0
56	MG	BA	3334	1/1	0.83	0.30	73,73,73,73	0
56	MG	BA	3071	1/1	0.83	0.30	55,55,55,55	0
56	MG	DA	3140	1/1	0.83	0.34	54,54,54,54	0
56	MG	DA	3515	1/1	0.83	0.21	48,48,48,48	0
56	MG	CA	3048	1/1	0.83	0.20	62,62,62,62	0
56	MG	DA	3163	1/1	0.83	0.18	39,39,39,39	0
56	MG	AA	3022	1/1	0.83	0.27	48,48,48,48	0
56	MG	CA	3003	1/1	0.83	0.11	66,66,66,66	0
56	MG	DA	3598	1/1	0.83	0.30	66,66,66,66	0
56	MG	BA	3673	1/1	0.83	0.20	53,53,53,53	0
56	MG	DA	3631	1/1	0.83	0.17	56,56,56,56	0
56	MG	BA	3279	1/1	0.83	0.22	48,48,48,48	0
56	MG	BA	3164	1/1	0.83	0.72	56,56,56,56	0
56	MG	BA	3496	1/1	0.83	0.40	57,57,57,57	0
56	MG	BA	3166	1/1	0.83	0.53	59,59,59,59	0
56	MG	BA	3152	1/1	0.83	0.33	46,46,46,46	0
56	MG	DA	3071	1/1	0.83	0.52	46,46,46,46	0
56	MG	DA	3318	1/1	0.83	0.11	45,45,45,45	0
56	MG	DA	3087	1/1	0.83	0.16	49,49,49,49	0
56	MG	DA	3367	1/1	0.83	0.26	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3068	1/1	0.83	0.45	54,54,54,54	0
56	MG	DA	3198	1/1	0.84	0.29	48,48,48,48	0
56	MG	BA	3240	1/1	0.84	0.17	28,28,28,28	0
56	MG	BA	3102	1/1	0.84	0.32	52,52,52,52	0
56	MG	CA	3031	1/1	0.84	0.39	53,53,53,53	0
56	MG	DA	3256	1/1	0.84	0.18	63,63,63,63	0
56	MG	DA	3104	1/1	0.84	0.28	62,62,62,62	0
56	MG	AA	3059	1/1	0.84	1.19	54,54,54,54	0
56	MG	CA	3070	1/1	0.84	0.34	55,55,55,55	0
56	MG	BA	3288	1/1	0.84	0.22	61,61,61,61	0
56	MG	DA	3609	1/1	0.84	0.35	64,64,64,64	0
56	MG	CA	3081	1/1	0.84	0.10	72,72,72,72	0
56	MG	CA	3008	1/1	0.84	0.78	53,53,53,53	0
56	MG	AA	3029	1/1	0.84	0.69	52,52,52,52	0
56	MG	AA	3077	1/1	0.84	0.41	65,65,65,65	0
56	MG	AA	3140	1/1	0.84	0.12	70,70,70,70	0
56	MG	DA	3423	1/1	0.84	0.15	29,29,29,29	0
56	MG	BA	3165	1/1	0.84	0.31	53,53,53,53	0
56	MG	CA	3023	1/1	0.84	0.14	37,37,37,37	0
56	MG	DA	3084	1/1	0.84	0.32	70,70,70,70	0
56	MG	DA	3458	1/1	0.84	0.15	71,71,71,71	0
56	MG	BA	3598	1/1	0.84	0.12	56,56,56,56	0
56	MG	DA	3483	1/1	0.84	0.19	49,49,49,49	0
56	MG	BA	3136	1/1	0.85	0.23	58,58,58,58	0
56	MG	DA	3357	1/1	0.85	0.20	56,56,56,56	0
56	MG	BA	3140	1/1	0.85	0.19	64,64,64,64	0
56	MG	BA	3040	1/1	0.85	0.35	51,51,51,51	0
56	MG	AA	3015	1/1	0.85	0.16	73,73,73,73	0
56	MG	BA	3624	1/1	0.85	0.25	52,52,52,52	0
56	MG	CA	3103	1/1	0.85	0.19	83,83,83,83	0
56	MG	DA	3099	1/1	0.85	0.27	44,44,44,44	0
56	MG	CA	3109	1/1	0.85	0.11	83,83,83,83	0
56	MG	BA	3626	1/1	0.85	0.11	43,43,43,43	0
56	MG	DA	3456	1/1	0.85	0.13	47,47,47,47	0
56	MG	BB	3017	1/1	0.85	0.20	64,64,64,64	0
56	MG	BD	301	1/1	0.85	0.27	28,28,28,28	0
56	MG	BA	3088	1/1	0.85	0.36	56,56,56,56	0
56	MG	DA	3484	1/1	0.85	0.25	51,51,51,51	0
56	MG	DA	3124	1/1	0.85	0.13	67,67,67,67	0
56	MG	AA	3094	1/1	0.85	0.21	68,68,68,68	0
56	MG	BU	205	1/1	0.85	0.33	42,42,42,42	0
56	MG	BA	3669	1/1	0.85	0.24	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3164	1/1	0.85	0.38	69,69,69,69	0
56	MG	DA	3531	1/1	0.85	0.09	57,57,57,57	0
56	MG	DA	3157	1/1	0.85	0.99	62,62,62,62	0
56	MG	CA	3158	1/1	0.85	0.22	76,76,76,76	0
56	MG	BA	3009	1/1	0.85	0.17	25,25,25,25	0
56	MG	CA	3163	1/1	0.85	0.24	65,65,65,65	0
56	MG	BA	3111	1/1	0.85	0.40	53,53,53,53	0
56	MG	DA	3613	1/1	0.85	0.16	54,54,54,54	0
56	MG	CA	3039	1/1	0.85	0.36	72,72,72,72	0
56	MG	AA	3212	1/1	0.85	0.15	79,79,79,79	0
56	MG	AA	3218	1/1	0.85	0.54	65,65,65,65	0
56	MG	DA	3222	1/1	0.85	0.13	71,71,71,71	0
56	MG	BA	3175	1/1	0.85	0.25	48,48,48,48	0
56	MG	BA	3135	1/1	0.85	0.17	42,42,42,42	0
56	MG	DD	307	1/1	0.85	0.61	38,38,38,38	0
56	MG	DA	3238	1/1	0.85	0.10	61,61,61,61	0
56	MG	DF	302	1/1	0.85	0.27	43,43,43,43	0
56	MG	B7	104	1/1	0.85	0.13	51,51,51,51	0
56	MG	BA	3285	1/1	0.85	0.14	32,32,32,32	0
56	MG	DR	201	1/1	0.85	0.62	65,65,65,65	0
56	MG	DV	202	1/1	0.85	0.84	63,63,63,63	0
56	MG	DA	3061	1/1	0.85	0.45	52,52,52,52	0
56	MG	CA	3005	1/1	0.85	0.32	54,54,54,54	0
58	ZN	D4	501	1/1	0.85	0.09	153,153,153,153	0
56	MG	DA	3065	1/1	0.85	0.19	38,38,38,38	0
56	MG	BA	3110	1/1	0.86	0.34	55,55,55,55	0
56	MG	BE	303	1/1	0.86	0.17	29,29,29,29	0
56	MG	DA	3482	1/1	0.86	0.13	55,55,55,55	0
56	MG	CQ	201	1/1	0.86	0.19	56,56,56,56	0
56	MG	BA	3027	1/1	0.86	0.23	45,45,45,45	0
56	MG	CA	3063	1/1	0.86	0.09	61,61,61,61	0
56	MG	BF	308	1/1	0.86	0.25	28,28,28,28	0
56	MG	DA	3022	1/1	0.86	0.25	45,45,45,45	0
56	MG	DA	3168	1/1	0.86	0.39	48,48,48,48	0
56	MG	CA	3068	1/1	0.86	0.11	41,41,41,41	0
56	MG	DA	3036	1/1	0.86	0.29	35,35,35,35	0
56	MG	BA	3249	1/1	0.86	0.24	40,40,40,40	0
56	MG	DA	3553	1/1	0.86	0.36	70,70,70,70	0
56	MG	BA	3590	1/1	0.86	0.13	64,64,64,64	0
56	MG	BA	3253	1/1	0.86	0.16	51,51,51,51	0
56	MG	DA	3592	1/1	0.86	0.15	65,65,65,65	0
56	MG	DA	3062	1/1	0.86	0.34	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3712	1/1	0.86	0.09	58,58,58,58	0
56	MG	AX	106	1/1	0.86	0.17	73,73,73,73	0
56	MG	CA	3110	1/1	0.86	0.21	97,97,97,97	0
56	MG	DA	3070	1/1	0.86	0.27	44,44,44,44	0
56	MG	DA	3632	1/1	0.86	0.19	71,71,71,71	0
56	MG	AA	3004	1/1	0.86	0.15	55,55,55,55	0
56	MG	AA	3013	1/1	0.86	0.23	78,78,78,78	0
56	MG	BA	3277	1/1	0.86	0.37	45,45,45,45	0
56	MG	CA	3131	1/1	0.86	0.10	55,55,55,55	0
56	MG	DA	3093	1/1	0.86	0.20	53,53,53,53	0
56	MG	DA	3095	1/1	0.86	0.23	61,61,61,61	0
56	MG	AA	3001	1/1	0.86	0.18	68,68,68,68	0
56	MG	BA	3282	1/1	0.86	0.37	49,49,49,49	0
56	MG	B9	502	1/1	0.86	0.27	49,49,49,49	0
56	MG	BA	3641	1/1	0.86	0.12	45,45,45,45	0
56	MG	DA	3112	1/1	0.86	0.43	54,54,54,54	0
56	MG	DV	203	1/1	0.86	0.74	54,54,54,54	0
56	MG	BA	3198	1/1	0.86	0.14	52,52,52,52	0
56	MG	D5	101	1/1	0.86	0.48	53,53,53,53	0
56	MG	BA	3462	1/1	0.86	0.12	52,52,52,52	0
56	MG	CA	3054	1/1	0.86	0.39	48,48,48,48	0
59	FME	AX	101	10/11	0.86	0.44	48,75,97,113	0
56	MG	BA	3474	1/1	0.86	0.21	42,42,42,42	0
56	MG	DA	3481	1/1	0.87	0.27	47,47,47,47	0
56	MG	DA	3032	1/1	0.87	0.13	46,46,46,46	0
56	MG	BA	3643	1/1	0.87	0.28	43,43,43,43	0
56	MG	BA	3156	1/1	0.87	0.40	56,56,56,56	0
56	MG	DA	3053	1/1	0.87	0.15	42,42,42,42	0
56	MG	DA	3161	1/1	0.87	0.30	60,60,60,60	0
56	MG	CA	3125	1/1	0.87	0.13	72,72,72,72	0
56	MG	DA	3500	1/1	0.87	0.17	50,50,50,50	0
56	MG	DA	3058	1/1	0.87	0.34	47,47,47,47	0
56	MG	DA	3060	1/1	0.87	0.25	55,55,55,55	0
56	MG	DA	3171	1/1	0.87	0.25	39,39,39,39	0
56	MG	BB	3008	1/1	0.87	0.21	35,35,35,35	0
56	MG	BA	3495	1/1	0.87	0.34	84,84,84,84	0
56	MG	BA	3006	1/1	0.87	0.27	42,42,42,42	0
56	MG	BA	3501	1/1	0.87	0.25	59,59,59,59	0
56	MG	DA	3591	1/1	0.87	0.26	58,58,58,58	0
56	MG	AA	3075	1/1	0.87	0.11	52,52,52,52	0
56	MG	CA	3142	1/1	0.87	0.18	59,59,59,59	0
56	MG	AA	3137	1/1	0.87	0.21	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	DA	3079	1/1	0.87	0.27	37,37,37,37	0
56	MG	DA	3080	1/1	0.87	0.14	44,44,44,44	0
56	MG	DA	3081	1/1	0.87	0.20	48,48,48,48	0
56	MG	DA	3260	1/1	0.87	0.10	40,40,40,40	0
56	MG	CA	3146	1/1	0.87	0.20	69,69,69,69	0
56	MG	DA	3292	1/1	0.87	0.22	37,37,37,37	0
56	MG	BA	3252	1/1	0.87	0.17	55,55,55,55	0
56	MG	CA	3155	1/1	0.87	0.16	71,71,71,71	0
56	MG	DD	302	1/1	0.87	0.23	46,46,46,46	0
56	MG	BA	3214	1/1	0.87	0.09	53,53,53,53	0
56	MG	BA	3221	1/1	0.87	0.27	44,44,44,44	0
56	MG	BA	3268	1/1	0.87	0.17	46,46,46,46	0
56	MG	BW	203	1/1	0.87	0.32	45,45,45,45	0
56	MG	AA	3067	1/1	0.87	0.37	87,87,87,87	0
56	MG	BA	3727	1/1	0.87	0.66	68,68,68,68	0
56	MG	DA	3108	1/1	0.87	0.46	37,37,37,37	0
56	MG	AA	3042	1/1	0.87	0.33	44,44,44,44	0
56	MG	CA	3091	1/1	0.87	0.17	72,72,72,72	0
56	MG	DA	3115	1/1	0.87	0.09	63,63,63,63	0
56	MG	DA	3009	1/1	0.87	0.12	31,31,31,31	0
56	MG	BA	3236	1/1	0.87	0.17	36,36,36,36	0
56	MG	AA	3074	1/1	0.87	0.44	47,47,47,47	0
56	MG	AA	3166	1/1	0.87	0.18	48,48,48,48	0
60	K	BA	3300	1/1	0.87	0.28	100,100,100,100	0
56	MG	BA	3092	1/1	0.88	0.27	51,51,51,51	0
56	MG	DA	3067	1/1	0.88	0.54	43,43,43,43	0
56	MG	BA	3163	1/1	0.88	0.17	50,50,50,50	0
56	MG	AA	3032	1/1	0.88	0.28	57,57,57,57	0
56	MG	DA	3310	1/1	0.88	0.21	53,53,53,53	0
56	MG	BA	3100	1/1	0.88	0.25	48,48,48,48	0
56	MG	DA	3078	1/1	0.88	0.17	44,44,44,44	0
56	MG	DA	3343	1/1	0.88	0.21	41,41,41,41	0
56	MG	AA	3131	1/1	0.88	0.50	56,56,56,56	0
56	MG	CA	3126	1/1	0.88	0.24	61,61,61,61	0
56	MG	BA	3168	1/1	0.88	0.28	42,42,42,42	0
56	MG	BA	3045	1/1	0.88	0.29	34,34,34,34	0
56	MG	DA	3398	1/1	0.88	0.15	35,35,35,35	0
56	MG	DA	3086	1/1	0.88	0.30	43,43,43,43	0
56	MG	BA	3514	1/1	0.88	0.14	37,37,37,37	0
56	MG	BA	3058	1/1	0.88	0.45	38,38,38,38	0
56	MG	DA	3092	1/1	0.88	0.60	39,39,39,39	0
56	MG	CA	3027	1/1	0.88	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	BA	3192	1/1	0.88	0.48	58,58,58,58	0
56	MG	CA	3143	1/1	0.88	0.07	87,87,87,87	0
56	MG	BA	3062	1/1	0.88	0.34	42,42,42,42	0
56	MG	DA	3102	1/1	0.88	0.25	41,41,41,41	0
56	MG	BA	3205	1/1	0.88	0.19	40,40,40,40	0
56	MG	BA	3280	1/1	0.88	0.69	69,69,69,69	0
56	MG	CA	3034	1/1	0.88	0.26	65,65,65,65	0
56	MG	DA	3110	1/1	0.88	0.14	49,49,49,49	0
56	MG	CA	3157	1/1	0.88	0.11	54,54,54,54	0
56	MG	AN	103	1/1	0.88	0.38	60,60,60,60	0
56	MG	CA	3159	1/1	0.88	0.61	91,91,91,91	0
56	MG	AA	3132	1/1	0.88	0.36	76,76,76,76	0
56	MG	DA	3119	1/1	0.88	0.15	44,44,44,44	0
56	MG	DA	3524	1/1	0.88	0.12	28,28,28,28	0
56	MG	DA	3122	1/1	0.88	0.15	62,62,62,62	0
56	MG	AA	3133	1/1	0.88	0.35	63,63,63,63	0
56	MG	CA	3164	1/1	0.88	0.39	49,49,49,49	0
56	MG	CA	3040	1/1	0.88	0.35	42,42,42,42	0
56	MG	BG	3002	1/1	0.88	0.11	42,42,42,42	0
56	MG	DA	3134	1/1	0.88	0.23	46,46,46,46	0
56	MG	BN	3002	1/1	0.88	0.30	56,56,56,56	0
56	MG	BA	3216	1/1	0.88	0.22	41,41,41,41	0
56	MG	DA	3147	1/1	0.88	0.11	53,53,53,53	0
56	MG	DA	3599	1/1	0.88	0.23	72,72,72,72	0
56	MG	DA	3604	1/1	0.88	0.20	54,54,54,54	0
56	MG	DA	3150	1/1	0.88	0.21	64,64,64,64	0
56	MG	AA	3046	1/1	0.88	0.12	73,73,73,73	0
56	MG	DA	3005	1/1	0.88	0.21	42,42,42,42	0
56	MG	AA	3138	1/1	0.88	0.54	37,37,37,37	0
56	MG	AA	3033	1/1	0.88	0.38	64,64,64,64	0
56	MG	AA	3050	1/1	0.88	0.50	63,63,63,63	0
56	MG	BA	3298	1/1	0.88	0.33	49,49,49,49	0
56	MG	DA	3185	1/1	0.88	0.58	52,52,52,52	0
56	MG	BA	3320	1/1	0.88	0.29	57,57,57,57	0
56	MG	DB	3011	1/1	0.88	0.34	55,55,55,55	0
56	MG	AA	3009	1/1	0.88	0.23	79,79,79,79	0
56	MG	BA	3346	1/1	0.88	0.23	37,37,37,37	0
56	MG	BA	3693	1/1	0.88	0.14	64,64,64,64	0
56	MG	DA	3208	1/1	0.88	0.94	43,43,43,43	0
56	MG	DA	3210	1/1	0.88	0.14	40,40,40,40	0
56	MG	DQ	201	1/1	0.88	0.43	48,48,48,48	0
56	MG	BA	3354	1/1	0.88	0.15	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3214	1/1	0.88	0.27	64,64,64,64	0
56	MG	DA	3217	1/1	0.88	0.57	54,54,54,54	0
56	MG	CA	3071	1/1	0.88	0.08	63,63,63,63	0
56	MG	BA	3023	1/1	0.88	0.13	66,66,66,66	0
56	MG	DA	3224	1/1	0.88	0.15	47,47,47,47	0
56	MG	CA	3002	1/1	0.88	0.07	62,62,62,62	0
56	MG	BA	3373	1/1	0.88	0.28	36,36,36,36	0
56	MG	DA	3240	1/1	0.88	0.26	51,51,51,51	0
56	MG	DA	3252	1/1	0.88	0.12	45,45,45,45	0
56	MG	AA	3019	1/1	0.88	0.39	74,74,74,74	0
56	MG	BA	3103	1/1	0.89	0.12	53,53,53,53	0
56	MG	DA	3405	1/1	0.89	0.10	47,47,47,47	0
56	MG	DA	3132	1/1	0.89	0.71	54,54,54,54	0
56	MG	CA	3079	1/1	0.89	0.14	48,48,48,48	0
56	MG	DA	3048	1/1	0.89	0.37	37,37,37,37	0
56	MG	BA	3104	1/1	0.89	0.28	45,45,45,45	0
56	MG	DA	3441	1/1	0.89	0.30	53,53,53,53	0
56	MG	DA	3145	1/1	0.89	0.46	65,65,65,65	0
56	MG	CA	3086	1/1	0.89	0.20	80,80,80,80	0
56	MG	BA	3215	1/1	0.89	0.14	69,69,69,69	0
56	MG	DA	3460	1/1	0.89	0.36	50,50,50,50	0
56	MG	AA	3002	1/1	0.89	0.20	57,57,57,57	0
56	MG	DA	3159	1/1	0.89	0.24	51,51,51,51	0
56	MG	BA	3218	1/1	0.89	0.20	62,62,62,62	0
56	MG	AA	3181	1/1	0.89	0.28	57,57,57,57	0
56	MG	BA	3509	1/1	0.89	0.16	27,27,27,27	0
56	MG	DA	3487	1/1	0.89	0.19	57,57,57,57	0
56	MG	DA	3167	1/1	0.89	0.23	48,48,48,48	0
56	MG	BA	3230	1/1	0.89	0.47	46,46,46,46	0
56	MG	DA	3169	1/1	0.89	0.38	57,57,57,57	0
56	MG	BA	3523	1/1	0.89	0.12	48,48,48,48	0
56	MG	BA	3558	1/1	0.89	0.22	35,35,35,35	0
56	MG	BA	3005	1/1	0.89	0.18	36,36,36,36	0
56	MG	CA	3029	1/1	0.89	0.15	59,59,59,59	0
56	MG	BA	3127	1/1	0.89	0.38	50,50,50,50	0
56	MG	DA	3191	1/1	0.89	0.44	47,47,47,47	0
56	MG	DA	3194	1/1	0.89	0.13	48,48,48,48	0
56	MG	DA	3560	1/1	0.89	0.11	34,34,34,34	0
56	MG	DA	3195	1/1	0.89	0.10	50,50,50,50	0
56	MG	BA	3585	1/1	0.89	0.17	51,51,51,51	0
56	MG	DA	3590	1/1	0.89	0.17	80,80,80,80	0
56	MG	DA	3200	1/1	0.89	0.21	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3047	1/1	0.89	0.31	61,61,61,61	0
56	MG	BA	3237	1/1	0.89	0.55	51,51,51,51	0
56	MG	BA	3292	1/1	0.89	0.21	63,63,63,63	0
56	MG	BA	3061	1/1	0.89	0.49	51,51,51,51	0
56	MG	CA	3036	1/1	0.89	0.52	68,68,68,68	0
56	MG	CA	3037	1/1	0.89	0.31	67,67,67,67	0
56	MG	AA	3139	1/1	0.89	0.34	56,56,56,56	0
56	MG	DA	3623	1/1	0.89	0.17	53,53,53,53	0
56	MG	BA	3017	1/1	0.89	0.54	44,44,44,44	0
56	MG	BN	3003	1/1	0.89	0.39	59,59,59,59	0
56	MG	DA	3638	1/1	0.89	0.30	62,62,62,62	0
56	MG	BA	3309	1/1	0.89	0.13	46,46,46,46	0
56	MG	CA	3160	1/1	0.89	0.13	59,59,59,59	0
56	MG	DA	3243	1/1	0.89	0.21	67,67,67,67	0
56	MG	BA	3177	1/1	0.89	0.21	62,62,62,62	0
56	MG	DA	3253	1/1	0.89	0.14	42,42,42,42	0
56	MG	AA	3039	1/1	0.89	0.24	60,60,60,60	0
56	MG	BA	3336	1/1	0.89	0.21	54,54,54,54	0
56	MG	CA	3170	1/1	0.89	0.48	50,50,50,50	0
56	MG	DA	3286	1/1	0.89	0.17	62,62,62,62	0
56	MG	BA	3147	1/1	0.89	0.24	46,46,46,46	0
56	MG	BA	3664	1/1	0.89	0.26	68,68,68,68	0
56	MG	BA	3251	1/1	0.89	0.21	61,61,61,61	0
56	MG	BA	3355	1/1	0.89	0.23	64,64,64,64	0
56	MG	BA	3356	1/1	0.89	0.27	56,56,56,56	0
56	MG	BA	3365	1/1	0.89	0.14	20,20,20,20	0
56	MG	DV	204	1/1	0.89	0.21	41,41,41,41	0
56	MG	BA	3197	1/1	0.89	0.30	39,39,39,39	0
56	MG	BA	3149	1/1	0.89	0.55	40,40,40,40	0
56	MG	DA	3361	1/1	0.89	0.11	61,61,61,61	0
56	MG	DA	3018	1/1	0.89	0.47	48,48,48,48	0
56	MG	DA	3387	1/1	0.89	0.14	56,56,56,56	0
56	MG	AA	3031	1/1	0.89	0.22	41,41,41,41	0
56	MG	AA	3134	1/1	0.89	0.43	70,70,70,70	0
56	MG	DA	3359	1/1	0.90	0.23	46,46,46,46	0
56	MG	BA	3181	1/1	0.90	0.34	38,38,38,38	0
56	MG	DA	3363	1/1	0.90	0.09	57,57,57,57	0
56	MG	BA	3730	1/1	0.90	0.64	45,45,45,45	0
56	MG	DA	3369	1/1	0.90	0.13	47,47,47,47	0
56	MG	BA	3183	1/1	0.90	0.24	48,48,48,48	0
56	MG	AA	3003	1/1	0.90	0.24	63,63,63,63	0
56	MG	DA	3391	1/1	0.90	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3738	1/1	0.90	0.35	59,59,59,59	0
56	MG	BA	3194	1/1	0.90	0.18	55,55,55,55	0
56	MG	AA	3092	1/1	0.90	0.51	50,50,50,50	0
56	MG	AA	3180	1/1	0.90	0.38	66,66,66,66	0
56	MG	BA	3007	1/1	0.90	0.23	35,35,35,35	0
56	MG	DA	3126	1/1	0.90	0.34	43,43,43,43	0
56	MG	DA	3128	1/1	0.90	0.19	52,52,52,52	0
56	MG	DA	3440	1/1	0.90	0.32	33,33,33,33	0
56	MG	DA	3129	1/1	0.90	0.14	43,43,43,43	0
56	MG	BA	3139	1/1	0.90	0.25	51,51,51,51	0
56	MG	CT	3001	1/1	0.90	0.43	57,57,57,57	0
56	MG	BA	3560	1/1	0.90	0.20	61,61,61,61	0
56	MG	AA	3119	1/1	0.90	0.37	63,63,63,63	0
56	MG	DA	3461	1/1	0.90	0.21	41,41,41,41	0
56	MG	DA	3462	1/1	0.90	0.11	55,55,55,55	0
56	MG	BA	3577	1/1	0.90	0.10	52,52,52,52	0
56	MG	DA	3465	1/1	0.90	0.16	49,49,49,49	0
56	MG	CA	3046	1/1	0.90	0.38	53,53,53,53	0
56	MG	BA	3578	1/1	0.90	0.32	54,54,54,54	0
56	MG	BE	305	1/1	0.90	0.70	42,42,42,42	0
56	MG	BA	3144	1/1	0.90	0.27	74,74,74,74	0
56	MG	BA	3011	1/1	0.90	0.09	37,37,37,37	0
56	MG	AA	3184	1/1	0.90	0.10	72,72,72,72	0
56	MG	BA	3596	1/1	0.90	0.12	51,51,51,51	0
56	MG	DA	3042	1/1	0.90	0.25	36,36,36,36	0
56	MG	DA	3044	1/1	0.90	0.13	46,46,46,46	0
56	MG	DA	3503	1/1	0.90	0.17	71,71,71,71	0
56	MG	DA	3046	1/1	0.90	0.18	56,56,56,56	0
56	MG	DA	3517	1/1	0.90	0.19	50,50,50,50	0
56	MG	BA	3019	1/1	0.90	0.18	39,39,39,39	0
56	MG	BQ	203	1/1	0.90	0.22	58,58,58,58	0
56	MG	BA	3609	1/1	0.90	0.12	46,46,46,46	0
56	MG	DA	3538	1/1	0.90	0.18	44,44,44,44	0
56	MG	AA	3080	1/1	0.90	0.17	53,53,53,53	0
56	MG	DA	3548	1/1	0.90	0.13	37,37,37,37	0
56	MG	AA	3215	1/1	0.90	0.10	53,53,53,53	0
56	MG	AA	3217	1/1	0.90	0.65	67,67,67,67	0
56	MG	AA	3123	1/1	0.90	0.43	39,39,39,39	0
56	MG	DA	3582	1/1	0.90	0.11	52,52,52,52	0
56	MG	DA	3193	1/1	0.90	0.22	65,65,65,65	0
56	MG	AK	3001	1/1	0.90	0.18	45,45,45,45	0
56	MG	BA	3159	1/1	0.90	0.30	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3124	1/1	0.90	0.10	57,57,57,57	0
56	MG	DA	3593	1/1	0.90	0.23	73,73,73,73	0
56	MG	DA	3066	1/1	0.90	0.37	53,53,53,53	0
56	MG	BA	3047	1/1	0.90	0.42	47,47,47,47	0
56	MG	DA	3602	1/1	0.90	0.19	52,52,52,52	0
56	MG	BA	3350	1/1	0.90	0.24	47,47,47,47	0
56	MG	B7	101	1/1	0.90	0.20	43,43,43,43	0
56	MG	DA	3610	1/1	0.90	0.28	54,54,54,54	0
56	MG	DA	3213	1/1	0.90	0.21	44,44,44,44	0
56	MG	B7	103	1/1	0.90	0.85	48,48,48,48	0
56	MG	DA	3620	1/1	0.90	0.19	71,71,71,71	0
56	MG	DA	3075	1/1	0.90	0.33	44,44,44,44	0
56	MG	DA	3624	1/1	0.90	0.40	51,51,51,51	0
56	MG	DA	3218	1/1	0.90	0.25	62,62,62,62	0
56	MG	DA	3219	1/1	0.90	0.17	60,60,60,60	0
56	MG	DA	3077	1/1	0.90	0.28	50,50,50,50	0
56	MG	DA	3640	1/1	0.90	0.68	56,56,56,56	0
56	MG	BA	3048	1/1	0.90	0.23	31,31,31,31	0
56	MG	BA	3243	1/1	0.90	0.15	48,48,48,48	0
56	MG	BA	3671	1/1	0.90	0.33	57,57,57,57	0
56	MG	DB	3005	1/1	0.90	0.26	43,43,43,43	0
56	MG	BA	3105	1/1	0.90	0.44	34,34,34,34	0
56	MG	AA	3052	1/1	0.90	0.25	60,60,60,60	0
56	MG	BA	3683	1/1	0.90	0.22	60,60,60,60	0
56	MG	AA	3115	1/1	0.90	0.10	48,48,48,48	0
56	MG	BA	3174	1/1	0.90	0.09	48,48,48,48	0
56	MG	DA	3254	1/1	0.90	0.22	30,30,30,30	0
56	MG	DF	303	1/1	0.90	0.33	43,43,43,43	0
56	MG	BA	3114	1/1	0.90	0.36	51,51,51,51	0
56	MG	AA	3005	1/1	0.90	0.20	66,66,66,66	0
56	MG	DA	3264	1/1	0.90	0.32	49,49,49,49	0
56	MG	BA	3255	1/1	0.90	0.18	41,41,41,41	0
56	MG	DA	3284	1/1	0.90	0.14	68,68,68,68	0
56	MG	DA	3096	1/1	0.90	0.17	60,60,60,60	0
56	MG	BA	3708	1/1	0.90	0.23	40,40,40,40	0
56	MG	BA	3457	1/1	0.90	0.12	57,57,57,57	0
56	MG	BA	3714	1/1	0.90	0.21	58,58,58,58	0
56	MG	CA	3150	1/1	0.90	0.12	59,59,59,59	0
56	MG	CA	3153	1/1	0.90	0.10	83,83,83,83	0
56	MG	DA	3105	1/1	0.90	0.38	48,48,48,48	0
56	MG	BA	3125	1/1	0.90	0.20	39,39,39,39	0
56	MG	BA	3463	1/1	0.90	0.20	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3049	1/1	0.91	0.38	35,35,35,35	0
56	MG	BA	3055	1/1	0.91	0.23	44,44,44,44	0
56	MG	BA	3262	1/1	0.91	0.20	56,56,56,56	0
56	MG	BA	3056	1/1	0.91	0.42	44,44,44,44	0
56	MG	BA	3638	1/1	0.91	0.21	37,37,37,37	0
56	MG	DA	3051	1/1	0.91	0.12	46,46,46,46	0
56	MG	BA	3372	1/1	0.91	0.17	38,38,38,38	0
56	MG	AA	3169	1/1	0.91	0.16	76,76,76,76	0
56	MG	BA	3653	1/1	0.91	0.15	69,69,69,69	0
56	MG	DA	3172	1/1	0.91	0.43	51,51,51,51	0
56	MG	DA	3466	1/1	0.91	0.14	56,56,56,56	0
56	MG	DA	3183	1/1	0.91	0.11	54,54,54,54	0
56	MG	BA	3391	1/1	0.91	0.14	48,48,48,48	0
56	MG	BA	3269	1/1	0.91	0.65	34,34,34,34	0
56	MG	BA	3666	1/1	0.91	0.32	61,61,61,61	0
56	MG	BA	3443	1/1	0.91	0.17	26,26,26,26	0
56	MG	AN	101	1/1	0.91	0.19	63,63,63,63	0
56	MG	DA	3496	1/1	0.91	0.15	53,53,53,53	0
56	MG	CA	3106	1/1	0.91	0.34	64,64,64,64	0
56	MG	BA	3106	1/1	0.91	0.12	48,48,48,48	0
56	MG	BA	3676	1/1	0.91	0.22	51,51,51,51	0
56	MG	DA	3069	1/1	0.91	0.12	51,51,51,51	0
56	MG	DA	3512	1/1	0.91	0.25	61,61,61,61	0
56	MG	AA	3081	1/1	0.91	0.23	41,41,41,41	0
56	MG	CA	3119	1/1	0.91	0.24	64,64,64,64	0
56	MG	DA	3073	1/1	0.91	0.18	44,44,44,44	0
56	MG	AA	3125	1/1	0.91	0.16	47,47,47,47	0
56	MG	DA	3526	1/1	0.91	0.19	54,54,54,54	0
56	MG	BA	3689	1/1	0.91	0.23	39,39,39,39	0
56	MG	BA	3020	1/1	0.91	0.11	45,45,45,45	0
56	MG	BA	3464	1/1	0.91	0.10	43,43,43,43	0
56	MG	CA	3006	1/1	0.91	0.17	77,77,77,77	0
56	MG	BA	3466	1/1	0.91	0.14	61,61,61,61	0
56	MG	AA	3101	1/1	0.91	0.15	56,56,56,56	0
56	MG	DA	3567	1/1	0.91	0.15	62,62,62,62	0
56	MG	CA	3010	1/1	0.91	0.11	32,32,32,32	0
56	MG	BA	3481	1/1	0.91	0.23	38,38,38,38	0
56	MG	DA	3226	1/1	0.91	0.21	50,50,50,50	0
56	MG	BA	3226	1/1	0.91	0.30	32,32,32,32	0
56	MG	AX	105	1/1	0.91	0.69	56,56,56,56	0
56	MG	BA	3024	1/1	0.91	0.40	35,35,35,35	0
56	MG	BA	3505	1/1	0.91	0.19	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3594	1/1	0.91	0.30	47,47,47,47	0
56	MG	BA	3507	1/1	0.91	0.10	68,68,68,68	0
56	MG	CA	3151	1/1	0.91	0.25	80,80,80,80	0
56	MG	BA	3132	1/1	0.91	0.25	35,35,35,35	0
56	MG	AA	3142	1/1	0.91	0.26	38,38,38,38	0
56	MG	BA	3172	1/1	0.91	0.98	48,48,48,48	0
56	MG	AX	107	1/1	0.91	0.25	66,66,66,66	0
56	MG	BA	3038	1/1	0.91	0.60	51,51,51,51	0
56	MG	BA	3137	1/1	0.91	0.29	42,42,42,42	0
56	MG	BA	3568	1/1	0.91	0.23	47,47,47,47	0
56	MG	DA	3621	1/1	0.91	0.14	54,54,54,54	0
56	MG	CA	3162	1/1	0.91	0.21	46,46,46,46	0
56	MG	BA	3303	1/1	0.91	0.16	35,35,35,35	0
56	MG	AA	3121	1/1	0.91	0.53	51,51,51,51	0
56	MG	AA	3136	1/1	0.91	0.08	62,62,62,62	0
56	MG	DA	3635	1/1	0.91	0.32	58,58,58,58	0
56	MG	DA	3315	1/1	0.91	0.09	31,31,31,31	0
56	MG	BB	3009	1/1	0.91	0.16	48,48,48,48	0
56	MG	DA	3339	1/1	0.91	0.10	37,37,37,37	0
56	MG	DA	3653	1/1	0.91	0.35	60,60,60,60	0
56	MG	DA	3342	1/1	0.91	0.12	52,52,52,52	0
56	MG	BA	3331	1/1	0.91	0.19	47,47,47,47	0
56	MG	BA	3143	1/1	0.91	0.31	40,40,40,40	0
56	MG	BA	3335	1/1	0.91	0.17	35,35,35,35	0
56	MG	BD	312	1/1	0.91	0.85	80,80,80,80	0
56	MG	DA	3360	1/1	0.91	0.25	41,41,41,41	0
56	MG	BA	3248	1/1	0.91	0.24	43,43,43,43	0
56	MG	BA	3187	1/1	0.91	0.64	50,50,50,50	0
56	MG	DF	301	1/1	0.91	0.51	32,32,32,32	0
56	MG	CA	3047	1/1	0.91	0.16	63,63,63,63	0
56	MG	BF	302	1/1	0.91	0.31	46,46,46,46	0
56	MG	DF	304	1/1	0.91	0.28	44,44,44,44	0
56	MG	DA	3376	1/1	0.91	0.08	31,31,31,31	0
56	MG	AA	3011	1/1	0.91	1.19	55,55,55,55	0
56	MG	AA	3219	1/1	0.91	0.20	57,57,57,57	0
56	MG	BA	3619	1/1	0.91	0.27	40,40,40,40	0
56	MG	CA	3056	1/1	0.91	0.11	64,64,64,64	0
56	MG	DA	3401	1/1	0.91	0.29	58,58,58,58	0
56	MG	DA	3143	1/1	0.91	0.22	46,46,46,46	0
56	MG	DA	3033	1/1	0.91	0.25	39,39,39,39	0
56	MG	BN	3001	1/1	0.91	0.76	54,54,54,54	0
56	MG	D8	5001	1/1	0.91	0.41	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	DA	3419	1/1	0.91	0.17	31,31,31,31	0
56	MG	DA	3148	1/1	0.91	0.23	47,47,47,47	0
56	MG	DA	3149	1/1	0.91	0.06	47,47,47,47	0
56	MG	DA	3430	1/1	0.91	0.28	55,55,55,55	0
56	MG	DA	3041	1/1	0.91	0.45	57,57,57,57	0
56	MG	AA	3200	1/1	0.92	0.24	68,68,68,68	0
56	MG	BA	3108	1/1	0.92	0.14	55,55,55,55	0
56	MG	BA	3225	1/1	0.92	0.33	62,62,62,62	0
56	MG	DA	3459	1/1	0.92	0.11	33,33,33,33	0
56	MG	DA	3050	1/1	0.92	0.57	31,31,31,31	0
56	MG	AA	3211	1/1	0.92	0.20	36,36,36,36	0
56	MG	DA	3170	1/1	0.92	0.80	57,57,57,57	0
56	MG	BA	3468	1/1	0.92	0.17	30,30,30,30	0
56	MG	AA	3025	1/1	0.92	0.14	69,69,69,69	0
56	MG	DA	3179	1/1	0.92	0.22	46,46,46,46	0
56	MG	DA	3478	1/1	0.92	0.25	46,46,46,46	0
56	MG	CA	3104	1/1	0.92	0.19	62,62,62,62	0
56	MG	CA	3105	1/1	0.92	0.09	79,79,79,79	0
56	MG	BA	3016	1/1	0.92	0.24	33,33,33,33	0
56	MG	BA	3122	1/1	0.92	0.27	52,52,52,52	0
56	MG	DA	3188	1/1	0.92	0.33	47,47,47,47	0
56	MG	DA	3489	1/1	0.92	0.16	36,36,36,36	0
56	MG	AA	3034	1/1	0.92	0.18	48,48,48,48	0
56	MG	CA	3111	1/1	0.92	0.12	64,64,64,64	0
56	MG	BA	3698	1/1	0.92	0.20	41,41,41,41	0
56	MG	CA	3117	1/1	0.92	0.15	68,68,68,68	0
56	MG	AA	3024	1/1	0.92	0.18	53,53,53,53	0
56	MG	DA	3502	1/1	0.92	0.12	65,65,65,65	0
56	MG	BA	3502	1/1	0.92	0.20	43,43,43,43	0
56	MG	DA	3505	1/1	0.92	0.06	65,65,65,65	0
56	MG	DA	3509	1/1	0.92	0.13	55,55,55,55	0
56	MG	AA	3098	1/1	0.92	0.35	72,72,72,72	0
56	MG	DA	3202	1/1	0.92	0.33	42,42,42,42	0
56	MG	AA	3154	1/1	0.92	0.08	63,63,63,63	0
56	MG	AA	3162	1/1	0.92	0.23	74,74,74,74	0
56	MG	DA	3074	1/1	0.92	0.21	54,54,54,54	0
56	MG	AA	3041	1/1	0.92	0.15	49,49,49,49	0
56	MG	AA	3069	1/1	0.92	0.14	84,84,84,84	0
56	MG	DA	3532	1/1	0.92	0.10	57,57,57,57	0
56	MG	DA	3536	1/1	0.92	0.16	80,80,80,80	0
56	MG	CA	3136	1/1	0.92	0.18	45,45,45,45	0
56	MG	DA	3543	1/1	0.92	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3325	1/1	0.92	0.19	58,58,58,58	0
56	MG	BA	3328	1/1	0.92	0.21	42,42,42,42	0
56	MG	DA	3221	1/1	0.92	0.18	49,49,49,49	0
56	MG	DA	3554	1/1	0.92	0.18	70,70,70,70	0
56	MG	CA	3140	1/1	0.92	0.16	73,73,73,73	0
56	MG	DA	3562	1/1	0.92	0.10	61,61,61,61	0
56	MG	BA	3245	1/1	0.92	0.30	47,47,47,47	0
56	MG	AA	3105	1/1	0.92	0.22	46,46,46,46	0
56	MG	DA	3225	1/1	0.92	0.16	45,45,45,45	0
56	MG	BA	3735	1/1	0.92	0.20	45,45,45,45	0
56	MG	AA	3036	1/1	0.92	0.23	71,71,71,71	0
56	MG	BA	3039	1/1	0.92	0.14	42,42,42,42	0
56	MG	BA	3188	1/1	0.92	0.15	37,37,37,37	0
56	MG	BA	3141	1/1	0.92	0.30	43,43,43,43	0
56	MG	DA	3246	1/1	0.92	0.17	24,24,24,24	0
56	MG	DA	3597	1/1	0.92	0.23	47,47,47,47	0
56	MG	CA	3152	1/1	0.92	0.38	55,55,55,55	0
56	MG	DA	3097	1/1	0.92	0.22	61,61,61,61	0
56	MG	BA	3090	1/1	0.92	0.20	46,46,46,46	0
56	MG	BA	3254	1/1	0.92	0.19	59,59,59,59	0
56	MG	BA	3196	1/1	0.92	0.76	56,56,56,56	0
56	MG	BA	3601	1/1	0.92	0.28	64,64,64,64	0
56	MG	DA	3611	1/1	0.92	0.09	42,42,42,42	0
56	MG	BB	3014	1/1	0.92	0.13	69,69,69,69	0
56	MG	BA	3256	1/1	0.92	0.17	58,58,58,58	0
56	MG	DA	3107	1/1	0.92	0.30	55,55,55,55	0
56	MG	BA	3258	1/1	0.92	0.23	40,40,40,40	0
56	MG	DA	3109	1/1	0.92	0.55	66,66,66,66	0
56	MG	DA	3295	1/1	0.92	0.24	39,39,39,39	0
56	MG	DA	3296	1/1	0.92	0.09	31,31,31,31	0
56	MG	BD	304	1/1	0.92	0.51	58,58,58,58	0
56	MG	DA	3111	1/1	0.92	0.23	53,53,53,53	0
56	MG	DA	3636	1/1	0.92	0.14	61,61,61,61	0
56	MG	AA	3072	1/1	0.92	0.26	79,79,79,79	0
56	MG	BA	3617	1/1	0.92	0.24	62,62,62,62	0
56	MG	AA	3082	1/1	0.92	0.24	39,39,39,39	0
56	MG	DA	3651	1/1	0.92	0.60	52,52,52,52	0
56	MG	DA	3340	1/1	0.92	0.14	47,47,47,47	0
56	MG	DA	3116	1/1	0.92	0.31	39,39,39,39	0
56	MG	BA	3374	1/1	0.92	0.19	44,44,44,44	0
56	MG	BA	3099	1/1	0.92	0.17	44,44,44,44	0
56	MG	BF	304	1/1	0.92	0.09	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	BA	3401	1/1	0.92	0.12	42,42,42,42	0
56	MG	AA	3190	1/1	0.92	0.32	67,67,67,67	0
56	MG	BG	3001	1/1	0.92	0.13	64,64,64,64	0
56	MG	BA	3633	1/1	0.92	0.13	58,58,58,58	0
56	MG	DA	3006	1/1	0.92	0.16	42,42,42,42	0
56	MG	BA	3406	1/1	0.92	0.14	28,28,28,28	0
56	MG	BA	3430	1/1	0.92	0.32	49,49,49,49	0
56	MG	DA	3013	1/1	0.92	0.09	47,47,47,47	0
56	MG	DA	3014	1/1	0.92	0.21	34,34,34,34	0
56	MG	BA	3432	1/1	0.92	0.17	60,60,60,60	0
56	MG	DA	3139	1/1	0.92	0.18	40,40,40,40	0
56	MG	BA	3652	1/1	0.92	0.20	64,64,64,64	0
56	MG	BR	204	1/1	0.92	0.61	43,43,43,43	0
56	MG	DA	3029	1/1	0.92	0.10	61,61,61,61	0
56	MG	BU	201	1/1	0.92	0.75	39,39,39,39	0
56	MG	CA	3065	1/1	0.92	0.23	75,75,75,75	0
56	MG	AA	3191	1/1	0.92	0.13	71,71,71,71	0
56	MG	DA	3040	1/1	0.92	0.10	42,42,42,42	0
56	MG	DA	3151	1/1	0.92	0.29	60,60,60,60	0
56	MG	AA	3194	1/1	0.92	0.19	54,54,54,54	0
56	MG	BA	3052	1/1	0.92	0.25	29,29,29,29	0
56	MG	AA	3198	1/1	0.92	0.11	87,87,87,87	0
56	MG	DA	3453	1/1	0.92	0.36	61,61,61,61	0
56	MG	AA	3152	1/1	0.93	0.09	19,19,19,19	0
56	MG	BA	3357	1/1	0.93	0.13	49,49,49,49	0
56	MG	DA	3424	1/1	0.93	0.20	30,30,30,30	0
56	MG	DA	3144	1/1	0.93	0.39	36,36,36,36	0
56	MG	DA	3008	1/1	0.93	0.23	51,51,51,51	0
56	MG	DA	3437	1/1	0.93	0.14	49,49,49,49	0
56	MG	BA	3589	1/1	0.93	0.15	51,51,51,51	0
56	MG	AA	3135	1/1	0.93	0.23	41,41,41,41	0
56	MG	DA	3012	1/1	0.93	0.18	57,57,57,57	0
56	MG	DA	3443	1/1	0.93	0.17	53,53,53,53	0
56	MG	DA	3447	1/1	0.93	0.05	56,56,56,56	0
56	MG	DA	3450	1/1	0.93	0.16	43,43,43,43	0
56	MG	BA	3592	1/1	0.93	0.17	28,28,28,28	0
56	MG	BB	3006	1/1	0.93	0.24	39,39,39,39	0
56	MG	DA	3155	1/1	0.93	0.17	50,50,50,50	0
56	MG	DA	3015	1/1	0.93	0.26	49,49,49,49	0
56	MG	BA	3257	1/1	0.93	0.30	38,38,38,38	0
56	MG	DA	3020	1/1	0.93	0.30	52,52,52,52	0
56	MG	BA	3597	1/1	0.93	0.35	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3066	1/1	0.93	0.31	38,38,38,38	0
56	MG	BA	3599	1/1	0.93	0.31	46,46,46,46	0
56	MG	AA	3199	1/1	0.93	0.17	88,88,88,88	0
56	MG	BA	3608	1/1	0.93	0.13	68,68,68,68	0
56	MG	DA	3470	1/1	0.93	0.28	52,52,52,52	0
56	MG	DA	3472	1/1	0.93	0.17	36,36,36,36	0
56	MG	DA	3474	1/1	0.93	0.08	61,61,61,61	0
56	MG	BD	306	1/1	0.93	0.45	46,46,46,46	0
56	MG	BA	3098	1/1	0.93	0.15	35,35,35,35	0
56	MG	BA	3387	1/1	0.93	0.07	48,48,48,48	0
56	MG	AA	3008	1/1	0.93	0.41	54,54,54,54	0
56	MG	BA	3394	1/1	0.93	0.12	49,49,49,49	0
56	MG	DA	3045	1/1	0.93	0.37	41,41,41,41	0
56	MG	BE	306	1/1	0.93	0.44	46,46,46,46	0
56	MG	AA	3201	1/1	0.93	0.12	67,67,67,67	0
56	MG	BA	3153	1/1	0.93	0.32	35,35,35,35	0
56	MG	BA	3403	1/1	0.93	0.21	41,41,41,41	0
56	MG	BA	3273	1/1	0.93	0.39	42,42,42,42	0
56	MG	BA	3408	1/1	0.93	0.15	24,24,24,24	0
56	MG	DA	3054	1/1	0.93	0.11	51,51,51,51	0
56	MG	AA	3202	1/1	0.93	0.23	76,76,76,76	0
56	MG	CA	3074	1/1	0.93	0.18	54,54,54,54	0
56	MG	DA	3199	1/1	0.93	0.13	42,42,42,42	0
56	MG	BA	3050	1/1	0.93	0.15	21,21,21,21	0
56	MG	BA	3640	1/1	0.93	0.25	60,60,60,60	0
56	MG	AA	3206	1/1	0.93	0.07	70,70,70,70	0
56	MG	DA	3519	1/1	0.93	0.14	44,44,44,44	0
56	MG	DA	3521	1/1	0.93	0.12	62,62,62,62	0
56	MG	CA	3087	1/1	0.93	0.19	41,41,41,41	0
56	MG	CA	3089	1/1	0.93	0.15	52,52,52,52	0
56	MG	DA	3212	1/1	0.93	0.09	48,48,48,48	0
56	MG	DA	3527	1/1	0.93	0.10	46,46,46,46	0
56	MG	AA	3068	1/1	0.93	0.08	66,66,66,66	0
56	MG	CA	3097	1/1	0.93	0.15	48,48,48,48	0
56	MG	CA	3099	1/1	0.93	0.33	65,65,65,65	0
56	MG	DA	3537	1/1	0.93	0.22	65,65,65,65	0
56	MG	BA	3647	1/1	0.93	0.10	34,34,34,34	0
56	MG	BA	3446	1/1	0.93	0.13	49,49,49,49	0
56	MG	BU	204	1/1	0.93	0.39	44,44,44,44	0
56	MG	DA	3072	1/1	0.93	0.14	41,41,41,41	0
56	MG	AA	3167	1/1	0.93	0.19	67,67,67,67	0
56	MG	CA	3107	1/1	0.93	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3556	1/1	0.93	0.08	56,56,56,56	0
56	MG	DA	3559	1/1	0.93	0.19	46,46,46,46	0
56	MG	BA	3012	1/1	0.93	0.16	40,40,40,40	0
56	MG	DA	3076	1/1	0.93	0.56	44,44,44,44	0
56	MG	BA	3060	1/1	0.93	0.40	40,40,40,40	0
56	MG	DA	3579	1/1	0.93	0.17	23,23,23,23	0
56	MG	DA	3580	1/1	0.93	0.14	46,46,46,46	0
56	MG	DA	3233	1/1	0.93	0.19	42,42,42,42	0
56	MG	AA	3060	1/1	0.93	0.53	60,60,60,60	0
56	MG	BW	205	1/1	0.93	0.46	41,41,41,41	0
56	MG	BX	3001	1/1	0.93	0.29	55,55,55,55	0
56	MG	AA	3173	1/1	0.93	0.24	32,32,32,32	0
56	MG	B0	101	1/1	0.93	0.20	36,36,36,36	0
56	MG	AA	3177	1/1	0.93	0.14	80,80,80,80	0
56	MG	BA	3067	1/1	0.93	0.33	53,53,53,53	0
56	MG	DA	3255	1/1	0.93	0.20	40,40,40,40	0
56	MG	BA	3238	1/1	0.93	0.16	51,51,51,51	0
56	MG	AA	3026	1/1	0.93	0.17	41,41,41,41	0
56	MG	CA	3134	1/1	0.93	0.17	82,82,82,82	0
56	MG	DA	3603	1/1	0.93	0.16	55,55,55,55	0
56	MG	DA	3273	1/1	0.93	0.13	30,30,30,30	0
56	MG	DA	3278	1/1	0.93	0.17	47,47,47,47	0
56	MG	B3	103	1/1	0.93	0.62	41,41,41,41	0
56	MG	DA	3280	1/1	0.93	0.20	57,57,57,57	0
56	MG	DA	3281	1/1	0.93	0.21	42,42,42,42	0
56	MG	AA	3049	1/1	0.93	0.50	51,51,51,51	0
56	MG	BA	3684	1/1	0.93	0.17	58,58,58,58	0
56	MG	BA	3687	1/1	0.93	0.22	38,38,38,38	0
56	MG	BA	3299	1/1	0.93	0.23	9,9,9,9	0
56	MG	CA	3141	1/1	0.93	0.25	70,70,70,70	0
56	MG	DA	3627	1/1	0.93	0.21	43,43,43,43	0
56	MG	B8	101	1/1	0.93	0.47	49,49,49,49	0
56	MG	DA	3303	1/1	0.93	0.17	47,47,47,47	0
56	MG	DA	3305	1/1	0.93	0.09	33,33,33,33	0
56	MG	BA	3690	1/1	0.93	0.17	53,53,53,53	0
56	MG	AA	3146	1/1	0.93	0.20	48,48,48,48	0
56	MG	BA	3133	1/1	0.93	0.27	32,32,32,32	0
56	MG	DA	3643	1/1	0.93	0.72	53,53,53,53	0
56	MG	BA	3072	1/1	0.93	0.28	45,45,45,45	0
56	MG	DA	3326	1/1	0.93	0.20	33,33,33,33	0
56	MG	DA	3334	1/1	0.93	0.16	49,49,49,49	0
56	MG	DA	3336	1/1	0.93	0.12	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3189	1/1	0.93	0.10	77,77,77,77	0
56	MG	BA	3246	1/1	0.93	0.24	46,46,46,46	0
56	MG	BA	3704	1/1	0.93	0.19	85,85,85,85	0
56	MG	BA	3182	1/1	0.93	0.31	51,51,51,51	0
56	MG	DB	3012	1/1	0.93	0.27	59,59,59,59	0
56	MG	BA	3515	1/1	0.93	0.05	56,56,56,56	0
56	MG	BA	3711	1/1	0.93	0.17	86,86,86,86	0
56	MG	DD	308	1/1	0.93	0.15	55,55,55,55	0
56	MG	AV	101	1/1	0.93	0.17	36,36,36,36	0
56	MG	CA	3019	1/1	0.93	0.07	49,49,49,49	0
56	MG	BA	3549	1/1	0.93	0.22	27,27,27,27	0
56	MG	BA	3716	1/1	0.93	0.11	27,27,27,27	0
56	MG	DA	3366	1/1	0.93	0.35	36,36,36,36	0
56	MG	BA	3555	1/1	0.93	0.18	53,53,53,53	0
56	MG	BA	3028	1/1	0.93	0.21	48,48,48,48	0
56	MG	DA	3373	1/1	0.93	0.23	29,29,29,29	0
56	MG	BA	3722	1/1	0.93	0.17	32,32,32,32	0
56	MG	BA	3724	1/1	0.93	0.19	58,58,58,58	0
56	MG	BA	3250	1/1	0.93	0.21	45,45,45,45	0
56	MG	BA	3728	1/1	0.93	0.52	32,32,32,32	0
56	MG	DW	201	1/1	0.93	0.31	46,46,46,46	0
56	MG	AA	3058	1/1	0.93	0.16	50,50,50,50	0
56	MG	DA	3400	1/1	0.93	0.19	42,42,42,42	0
56	MG	BA	3190	1/1	0.93	0.20	42,42,42,42	0
58	ZN	AN	102	1/1	0.93	0.12	90,90,90,90	0
56	MG	BA	3030	1/1	0.93	0.43	51,51,51,51	0
58	ZN	CN	501	1/1	0.93	0.12	108,108,108,108	0
56	MG	DA	3002	1/1	0.93	0.19	55,55,55,55	0
56	MG	BA	3193	1/1	0.93	0.57	52,52,52,52	0
56	MG	DA	3414	1/1	0.93	0.17	49,49,49,49	0
56	MG	DA	3415	1/1	0.93	0.25	56,56,56,56	0
60	K	DA	3231	1/1	0.93	0.22	96,96,96,96	0
56	MG	DA	3442	1/1	0.94	0.19	40,40,40,40	0
56	MG	AA	3018	1/1	0.94	0.27	38,38,38,38	0
56	MG	BD	307	1/1	0.94	0.20	43,43,43,43	0
56	MG	DA	3164	1/1	0.94	0.26	48,48,48,48	0
56	MG	DA	3452	1/1	0.94	0.17	56,56,56,56	0
56	MG	DA	3027	1/1	0.94	0.43	39,39,39,39	0
56	MG	BA	3431	1/1	0.94	0.23	17,17,17,17	0
56	MG	CA	3058	1/1	0.94	0.10	40,40,40,40	0
56	MG	AA	3010	1/1	0.94	0.37	70,70,70,70	0
56	MG	CA	3061	1/1	0.94	0.30	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3038	1/1	0.94	0.15	39,39,39,39	0
56	MG	DA	3175	1/1	0.94	0.17	40,40,40,40	0
56	MG	BA	3439	1/1	0.94	0.16	34,34,34,34	0
56	MG	BA	3178	1/1	0.94	0.28	48,48,48,48	0
56	MG	BA	3631	1/1	0.94	0.14	78,78,78,78	0
56	MG	AA	3209	1/1	0.94	0.40	70,70,70,70	0
56	MG	DA	3469	1/1	0.94	0.21	47,47,47,47	0
56	MG	BA	3293	1/1	0.94	0.18	45,45,45,45	0
56	MG	BA	3635	1/1	0.94	0.10	78,78,78,78	0
56	MG	BA	3449	1/1	0.94	0.12	21,21,21,21	0
56	MG	AA	3210	1/1	0.94	0.06	40,40,40,40	0
56	MG	BA	3453	1/1	0.94	0.19	18,18,18,18	0
56	MG	CA	3076	1/1	0.94	0.33	40,40,40,40	0
56	MG	DA	3052	1/1	0.94	0.20	23,23,23,23	0
56	MG	DA	3196	1/1	0.94	0.34	44,44,44,44	0
56	MG	BA	3091	1/1	0.94	0.60	45,45,45,45	0
56	MG	BA	3057	1/1	0.94	0.27	35,35,35,35	0
56	MG	CA	3084	1/1	0.94	0.11	64,64,64,64	0
56	MG	DA	3057	1/1	0.94	0.16	52,52,52,52	0
56	MG	DA	3204	1/1	0.94	0.41	34,34,34,34	0
56	MG	DA	3207	1/1	0.94	0.13	58,58,58,58	0
56	MG	BA	3650	1/1	0.94	0.15	45,45,45,45	0
56	MG	DA	3501	1/1	0.94	0.20	23,23,23,23	0
56	MG	DA	3209	1/1	0.94	0.17	41,41,41,41	0
56	MG	BQ	202	1/1	0.94	0.30	28,28,28,28	0
56	MG	BA	3185	1/1	0.94	0.20	47,47,47,47	0
56	MG	BQ	205	1/1	0.94	0.42	49,49,49,49	0
56	MG	DA	3510	1/1	0.94	0.23	63,63,63,63	0
56	MG	DA	3063	1/1	0.94	0.12	52,52,52,52	0
56	MG	BR	202	1/1	0.94	0.29	27,27,27,27	0
56	MG	BA	3301	1/1	0.94	0.13	56,56,56,56	0
56	MG	BA	3465	1/1	0.94	0.12	40,40,40,40	0
56	MG	BA	3659	1/1	0.94	0.21	46,46,46,46	0
56	MG	BA	3660	1/1	0.94	0.27	71,71,71,71	0
56	MG	BA	3661	1/1	0.94	0.15	68,68,68,68	0
56	MG	AA	3016	1/1	0.94	0.07	63,63,63,63	0
56	MG	BA	3304	1/1	0.94	0.19	49,49,49,49	0
56	MG	DA	3528	1/1	0.94	0.09	56,56,56,56	0
56	MG	BA	3306	1/1	0.94	0.14	48,48,48,48	0
56	MG	BA	3476	1/1	0.94	0.13	40,40,40,40	0
56	MG	BY	201	1/1	0.94	0.43	58,58,58,58	0
56	MG	DA	3229	1/1	0.94	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3116	1/1	0.94	0.17	76,76,76,76	0
56	MG	DA	3539	1/1	0.94	0.17	53,53,53,53	0
56	MG	DA	3237	1/1	0.94	0.15	45,45,45,45	0
56	MG	BA	3142	1/1	0.94	0.71	46,46,46,46	0
56	MG	BA	3482	1/1	0.94	0.17	72,72,72,72	0
56	MG	DA	3552	1/1	0.94	0.12	34,34,34,34	0
56	MG	AA	3017	1/1	0.94	0.27	55,55,55,55	0
56	MG	CA	3124	1/1	0.94	0.17	61,61,61,61	0
56	MG	AA	3053	1/1	0.94	0.33	49,49,49,49	0
56	MG	B0	104	1/1	0.94	0.10	43,43,43,43	0
56	MG	BA	3499	1/1	0.94	0.17	55,55,55,55	0
56	MG	BA	3686	1/1	0.94	0.14	25,25,25,25	0
56	MG	DA	3564	1/1	0.94	0.77	61,61,61,61	0
56	MG	AA	3109	1/1	0.94	0.33	65,65,65,65	0
56	MG	DA	3572	1/1	0.94	0.11	53,53,53,53	0
56	MG	DA	3574	1/1	0.94	0.17	56,56,56,56	0
56	MG	DA	3578	1/1	0.94	0.38	49,49,49,49	0
56	MG	BA	3688	1/1	0.94	0.11	54,54,54,54	0
56	MG	DA	3090	1/1	0.94	0.34	47,47,47,47	0
56	MG	AA	3197	1/1	0.94	0.30	69,69,69,69	0
56	MG	CA	3137	1/1	0.94	0.13	48,48,48,48	0
56	MG	BA	3148	1/1	0.94	0.35	52,52,52,52	0
56	MG	BA	3066	1/1	0.94	0.26	44,44,44,44	0
56	MG	BA	3692	1/1	0.94	0.40	36,36,36,36	0
56	MG	AA	3054	1/1	0.94	0.20	45,45,45,45	0
56	MG	DA	3285	1/1	0.94	0.26	55,55,55,55	0
56	MG	BA	3511	1/1	0.94	0.16	39,39,39,39	0
56	MG	DA	3288	1/1	0.94	0.17	47,47,47,47	0
56	MG	DA	3100	1/1	0.94	0.50	56,56,56,56	0
56	MG	DA	3101	1/1	0.94	0.33	48,48,48,48	0
56	MG	BA	3344	1/1	0.94	0.09	30,30,30,30	0
56	MG	AF	3001	1/1	0.94	0.17	61,61,61,61	0
56	MG	AA	3145	1/1	0.94	0.25	63,63,63,63	0
56	MG	BA	3535	1/1	0.94	0.19	37,37,37,37	0
56	MG	DA	3106	1/1	0.94	0.21	41,41,41,41	0
56	MG	CA	3149	1/1	0.94	0.18	74,74,74,74	0
56	MG	BA	3546	1/1	0.94	0.31	48,48,48,48	0
56	MG	BA	3107	1/1	0.94	0.23	40,40,40,40	0
56	MG	DA	3617	1/1	0.94	0.19	58,58,58,58	0
56	MG	CA	3014	1/1	0.94	0.17	50,50,50,50	0
56	MG	BA	3259	1/1	0.94	0.49	27,27,27,27	0
56	MG	BA	3261	1/1	0.94	0.26	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3211	1/1	0.94	0.29	38,38,38,38	0
56	MG	DA	3114	1/1	0.94	0.19	37,37,37,37	0
56	MG	BA	3717	1/1	0.94	0.22	57,57,57,57	0
56	MG	BA	3044	1/1	0.94	0.30	42,42,42,42	0
56	MG	DA	3634	1/1	0.94	0.14	51,51,51,51	0
56	MG	DA	3347	1/1	0.94	0.19	62,62,62,62	0
56	MG	BA	3565	1/1	0.94	0.11	55,55,55,55	0
56	MG	AM	3001	1/1	0.94	0.06	65,65,65,65	0
56	MG	DA	3358	1/1	0.94	0.18	46,46,46,46	0
56	MG	BA	3570	1/1	0.94	0.12	61,61,61,61	0
56	MG	DA	3646	1/1	0.94	0.07	38,38,38,38	0
56	MG	BA	3573	1/1	0.94	0.16	56,56,56,56	0
56	MG	BA	3074	1/1	0.94	0.08	42,42,42,42	0
56	MG	DA	3362	1/1	0.94	0.13	41,41,41,41	0
56	MG	CA	3167	1/1	0.94	0.09	78,78,78,78	0
56	MG	DA	3364	1/1	0.94	0.19	32,32,32,32	0
56	MG	AA	3112	1/1	0.94	0.12	51,51,51,51	0
56	MG	DA	3127	1/1	0.94	0.09	48,48,48,48	0
56	MG	DB	3008	1/1	0.94	0.09	45,45,45,45	0
56	MG	DB	3009	1/1	0.94	0.37	40,40,40,40	0
56	MG	BA	3161	1/1	0.94	0.65	49,49,49,49	0
56	MG	BA	3377	1/1	0.94	0.14	32,32,32,32	0
56	MG	CF	3001	1/1	0.94	0.22	55,55,55,55	0
56	MG	DD	305	1/1	0.94	0.64	49,49,49,49	0
56	MG	DA	3378	1/1	0.94	0.15	45,45,45,45	0
56	MG	DA	3383	1/1	0.94	0.09	56,56,56,56	0
56	MG	BA	3386	1/1	0.94	0.14	58,58,58,58	0
56	MG	DE	305	1/1	0.94	0.64	65,65,65,65	0
56	MG	BA	3079	1/1	0.94	0.28	42,42,42,42	0
56	MG	BA	3082	1/1	0.94	0.29	41,41,41,41	0
56	MG	DA	3392	1/1	0.94	0.17	35,35,35,35	0
56	MG	DA	3393	1/1	0.94	0.19	41,41,41,41	0
56	MG	DF	305	1/1	0.94	0.73	39,39,39,39	0
56	MG	DA	3137	1/1	0.94	0.27	56,56,56,56	0
56	MG	BA	3278	1/1	0.94	0.17	34,34,34,34	0
56	MG	DQ	202	1/1	0.94	0.22	34,34,34,34	0
56	MG	BA	3124	1/1	0.94	0.23	39,39,39,39	0
56	MG	AA	3095	1/1	0.94	0.24	58,58,58,58	0
56	MG	DR	202	1/1	0.94	0.18	37,37,37,37	0
56	MG	BA	3084	1/1	0.94	0.14	33,33,33,33	0
56	MG	BA	3018	1/1	0.94	0.34	40,40,40,40	0
56	MG	DA	3146	1/1	0.94	0.18	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3086	1/1	0.94	0.33	49,49,49,49	0
56	MG	BA	3412	1/1	0.94	0.18	26,26,26,26	0
56	MG	DY	502	1/1	0.94	0.10	60,60,60,60	0
56	MG	CA	3044	1/1	0.94	0.20	63,63,63,63	0
56	MG	BA	3610	1/1	0.94	0.21	40,40,40,40	0
56	MG	BB	3018	1/1	0.94	0.19	60,60,60,60	0
56	MG	BA	3417	1/1	0.94	0.18	18,18,18,18	0
56	MG	DA	3433	1/1	0.94	0.17	48,48,48,48	0
56	MG	DA	3435	1/1	0.94	0.21	46,46,46,46	0
56	MG	DA	3156	1/1	0.94	0.56	29,29,29,29	0
56	MG	DA	3016	1/1	0.94	0.27	37,37,37,37	0
56	MG	BA	3419	1/1	0.94	0.14	24,24,24,24	0
56	MG	BD	305	1/1	0.94	0.23	48,48,48,48	0
56	MG	CA	3013	1/1	0.95	0.12	51,51,51,51	0
56	MG	BA	3510	1/1	0.95	0.24	40,40,40,40	0
56	MG	AA	3213	1/1	0.95	0.16	29,29,29,29	0
56	MG	DA	3434	1/1	0.95	0.26	49,49,49,49	0
56	MG	BA	3348	1/1	0.95	0.20	64,64,64,64	0
56	MG	AA	3187	1/1	0.95	0.04	62,62,62,62	0
56	MG	DA	3001	1/1	0.95	0.30	78,78,78,78	0
56	MG	BA	3697	1/1	0.95	0.14	78,78,78,78	0
56	MG	DA	3154	1/1	0.95	0.61	45,45,45,45	0
56	MG	CA	3020	1/1	0.95	0.18	47,47,47,47	0
56	MG	DA	3004	1/1	0.95	0.19	29,29,29,29	0
56	MG	DA	3444	1/1	0.95	0.13	43,43,43,43	0
56	MG	BA	3353	1/1	0.95	0.24	57,57,57,57	0
56	MG	AA	3216	1/1	0.95	0.14	58,58,58,58	0
56	MG	DA	3451	1/1	0.95	0.07	49,49,49,49	0
56	MG	BA	3700	1/1	0.95	0.12	67,67,67,67	0
56	MG	BA	3540	1/1	0.95	0.27	34,34,34,34	0
56	MG	DA	3010	1/1	0.95	0.14	39,39,39,39	0
56	MG	BA	3541	1/1	0.95	0.23	30,30,30,30	0
56	MG	BA	3545	1/1	0.95	0.24	47,47,47,47	0
56	MG	AA	3083	1/1	0.95	0.09	65,65,65,65	0
56	MG	BA	3547	1/1	0.95	0.18	31,31,31,31	0
56	MG	BA	3548	1/1	0.95	0.22	50,50,50,50	0
56	MG	BA	3053	1/1	0.95	0.35	39,39,39,39	0
56	MG	DA	3017	1/1	0.95	0.16	46,46,46,46	0
56	MG	BA	3145	1/1	0.95	0.40	38,38,38,38	0
56	MG	BA	3358	1/1	0.95	0.09	33,33,33,33	0
56	MG	DA	3021	1/1	0.95	0.15	35,35,35,35	0
56	MG	BA	3260	1/1	0.95	0.17	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3014	1/1	0.95	0.77	34,34,34,34	0
56	MG	BA	3563	1/1	0.95	0.21	37,37,37,37	0
56	MG	BA	3201	1/1	0.95	0.29	36,36,36,36	0
56	MG	DA	3479	1/1	0.95	0.19	57,57,57,57	0
56	MG	DA	3030	1/1	0.95	0.28	51,51,51,51	0
56	MG	DA	3031	1/1	0.95	0.29	55,55,55,55	0
56	MG	BA	3202	1/1	0.95	0.24	41,41,41,41	0
56	MG	BA	3097	1/1	0.95	0.19	33,33,33,33	0
56	MG	DA	3034	1/1	0.95	0.15	40,40,40,40	0
56	MG	AA	3007	1/1	0.95	0.19	82,82,82,82	0
56	MG	DA	3490	1/1	0.95	0.10	39,39,39,39	0
56	MG	DA	3197	1/1	0.95	0.45	36,36,36,36	0
56	MG	DA	3494	1/1	0.95	0.09	78,78,78,78	0
56	MG	BA	3576	1/1	0.95	0.26	23,23,23,23	0
56	MG	AA	3155	1/1	0.95	0.16	70,70,70,70	0
56	MG	BA	3271	1/1	0.95	0.12	36,36,36,36	0
56	MG	AA	3078	1/1	0.95	0.27	42,42,42,42	0
56	MG	BA	3580	1/1	0.95	0.12	58,58,58,58	0
56	MG	BA	3101	1/1	0.95	0.17	35,35,35,35	0
56	MG	BA	3588	1/1	0.95	0.21	48,48,48,48	0
56	MG	DA	3047	1/1	0.95	0.08	34,34,34,34	0
56	MG	DA	3506	1/1	0.95	0.07	59,59,59,59	0
56	MG	DA	3507	1/1	0.95	0.15	54,54,54,54	0
56	MG	BA	3397	1/1	0.95	0.19	28,28,28,28	0
56	MG	BA	3276	1/1	0.95	0.32	40,40,40,40	0
56	MG	DA	3511	1/1	0.95	0.08	65,65,65,65	0
56	MG	BA	3059	1/1	0.95	0.60	45,45,45,45	0
56	MG	BA	3594	1/1	0.95	0.31	42,42,42,42	0
56	MG	DA	3516	1/1	0.95	0.17	40,40,40,40	0
56	MG	BA	3595	1/1	0.95	0.16	41,41,41,41	0
56	MG	DA	3216	1/1	0.95	0.17	31,31,31,31	0
56	MG	DA	3520	1/1	0.95	0.20	51,51,51,51	0
56	MG	AA	3195	1/1	0.95	0.16	71,71,71,71	0
56	MG	DA	3522	1/1	0.95	0.17	61,61,61,61	0
56	MG	AA	3196	1/1	0.95	0.31	65,65,65,65	0
56	MG	DA	3055	1/1	0.95	0.21	48,48,48,48	0
56	MG	DA	3220	1/1	0.95	0.12	37,37,37,37	0
56	MG	AA	3126	1/1	0.95	0.16	54,54,54,54	0
56	MG	CA	3066	1/1	0.95	0.10	55,55,55,55	0
56	MG	BA	3224	1/1	0.95	0.73	64,64,64,64	0
56	MG	BA	3284	1/1	0.95	0.10	54,54,54,54	0
56	MG	DA	3534	1/1	0.95	0.19	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3535	1/1	0.95	0.19	33,33,33,33	0
56	MG	BA	3603	1/1	0.95	0.08	39,39,39,39	0
56	MG	BA	3605	1/1	0.95	0.30	59,59,59,59	0
56	MG	AA	3040	1/1	0.95	0.12	55,55,55,55	0
56	MG	BA	3421	1/1	0.95	0.12	36,36,36,36	0
56	MG	DA	3232	1/1	0.95	0.25	50,50,50,50	0
56	MG	CA	3075	1/1	0.95	0.17	76,76,76,76	0
56	MG	BA	3422	1/1	0.95	0.23	42,42,42,42	0
56	MG	DA	3550	1/1	0.95	0.17	53,53,53,53	0
56	MG	BA	3286	1/1	0.95	0.26	32,32,32,32	0
56	MG	AA	3064	1/1	0.95	0.30	79,79,79,79	0
56	MG	CA	3082	1/1	0.95	0.08	47,47,47,47	0
56	MG	DA	3555	1/1	0.95	0.12	41,41,41,41	0
56	MG	DA	3245	1/1	0.95	0.15	37,37,37,37	0
56	MG	DA	3558	1/1	0.95	0.18	37,37,37,37	0
56	MG	BE	307	1/1	0.95	0.24	39,39,39,39	0
56	MG	BA	3616	1/1	0.95	0.10	33,33,33,33	0
56	MG	BA	3229	1/1	0.95	0.15	22,22,22,22	0
56	MG	BA	3618	1/1	0.95	0.27	46,46,46,46	0
56	MG	DA	3565	1/1	0.95	0.07	57,57,57,57	0
56	MG	DA	3566	1/1	0.95	0.14	71,71,71,71	0
56	MG	CA	3090	1/1	0.95	0.18	73,73,73,73	0
56	MG	DA	3570	1/1	0.95	0.22	28,28,28,28	0
56	MG	AA	3168	1/1	0.95	0.31	68,68,68,68	0
56	MG	CA	3094	1/1	0.95	0.18	43,43,43,43	0
56	MG	DA	3576	1/1	0.95	0.15	38,38,38,38	0
56	MG	DA	3261	1/1	0.95	0.22	35,35,35,35	0
56	MG	DA	3263	1/1	0.95	0.19	31,31,31,31	0
56	MG	BA	3620	1/1	0.95	0.12	47,47,47,47	0
56	MG	DA	3267	1/1	0.95	0.17	61,61,61,61	0
56	MG	BA	3441	1/1	0.95	0.25	25,25,25,25	0
56	MG	DA	3585	1/1	0.95	0.15	62,62,62,62	0
56	MG	CA	3102	1/1	0.95	0.09	41,41,41,41	0
56	MG	DA	3589	1/1	0.95	0.18	59,59,59,59	0
56	MG	BG	3004	1/1	0.95	0.04	62,62,62,62	0
56	MG	AA	3111	1/1	0.95	0.17	95,95,95,95	0
56	MG	DA	3083	1/1	0.95	0.25	41,41,41,41	0
56	MG	DA	3283	1/1	0.95	0.21	33,33,33,33	0
56	MG	BA	3233	1/1	0.95	0.18	47,47,47,47	0
56	MG	DA	3595	1/1	0.95	0.18	72,72,72,72	0
56	MG	BA	3627	1/1	0.95	0.20	50,50,50,50	0
56	MG	BN	3005	1/1	0.95	0.85	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3108	1/1	0.95	0.21	52,52,52,52	0
56	MG	DA	3601	1/1	0.95	0.12	77,77,77,77	0
56	MG	BP	201	1/1	0.95	0.66	40,40,40,40	0
56	MG	BA	3628	1/1	0.95	0.21	41,41,41,41	0
56	MG	AX	104	1/1	0.95	0.14	76,76,76,76	0
56	MG	AA	3170	1/1	0.95	0.16	101,101,101,101	0
56	MG	DA	3297	1/1	0.95	0.14	57,57,57,57	0
56	MG	DA	3298	1/1	0.95	0.32	37,37,37,37	0
56	MG	DA	3299	1/1	0.95	0.22	40,40,40,40	0
56	MG	DA	3614	1/1	0.95	0.20	48,48,48,48	0
56	MG	BA	3037	1/1	0.95	0.20	31,31,31,31	0
56	MG	BA	3073	1/1	0.95	0.85	41,41,41,41	0
56	MG	DA	3619	1/1	0.95	0.22	48,48,48,48	0
56	MG	DA	3306	1/1	0.95	0.21	33,33,33,33	0
56	MG	DA	3307	1/1	0.95	0.30	37,37,37,37	0
56	MG	BA	3169	1/1	0.95	0.70	46,46,46,46	0
56	MG	BU	202	1/1	0.95	0.36	32,32,32,32	0
56	MG	DA	3626	1/1	0.95	0.07	68,68,68,68	0
56	MG	BA	3639	1/1	0.95	0.16	50,50,50,50	0
56	MG	BA	3461	1/1	0.95	0.24	36,36,36,36	0
56	MG	DA	3319	1/1	0.95	0.18	53,53,53,53	0
56	MG	DA	3322	1/1	0.95	0.13	55,55,55,55	0
56	MG	DA	3325	1/1	0.95	0.17	36,36,36,36	0
56	MG	AA	3130	1/1	0.95	0.23	46,46,46,46	0
56	MG	DA	3329	1/1	0.95	0.16	53,53,53,53	0
56	MG	BU	208	1/1	0.95	0.88	56,56,56,56	0
56	MG	BV	202	1/1	0.95	0.44	56,56,56,56	0
56	MG	BV	203	1/1	0.95	1.03	46,46,46,46	0
56	MG	AA	3056	1/1	0.95	0.19	39,39,39,39	0
56	MG	DA	3648	1/1	0.95	0.17	52,52,52,52	0
56	MG	BA	3645	1/1	0.95	0.09	56,56,56,56	0
56	MG	BA	3078	1/1	0.95	0.26	17,17,17,17	0
56	MG	DA	3654	1/1	0.95	0.17	52,52,52,52	0
56	MG	BA	3129	1/1	0.95	0.25	36,36,36,36	0
56	MG	DB	3002	1/1	0.95	0.25	56,56,56,56	0
56	MG	DA	3350	1/1	0.95	0.04	32,32,32,32	0
56	MG	AA	3070	1/1	0.95	0.10	75,75,75,75	0
56	MG	DB	3006	1/1	0.95	0.13	42,42,42,42	0
56	MG	DA	3353	1/1	0.95	0.10	62,62,62,62	0
56	MG	BA	3312	1/1	0.95	0.10	58,58,58,58	0
56	MG	BA	3654	1/1	0.95	0.16	25,25,25,25	0
56	MG	DB	3010	1/1	0.95	0.18	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3470	1/1	0.95	0.24	54,54,54,54	0
56	MG	BA	3041	1/1	0.95	0.38	32,32,32,32	0
56	MG	DD	301	1/1	0.95	0.32	46,46,46,46	0
56	MG	BA	3042	1/1	0.95	0.76	47,47,47,47	0
56	MG	BA	3326	1/1	0.95	0.08	41,41,41,41	0
56	MG	DD	306	1/1	0.95	1.14	44,44,44,44	0
56	MG	BA	3043	1/1	0.95	0.17	52,52,52,52	0
56	MG	DA	3118	1/1	0.95	0.10	39,39,39,39	0
56	MG	BA	3484	1/1	0.95	0.17	54,54,54,54	0
56	MG	DA	3120	1/1	0.95	0.76	51,51,51,51	0
56	MG	DE	306	1/1	0.95	0.14	32,32,32,32	0
56	MG	DA	3121	1/1	0.95	0.19	48,48,48,48	0
56	MG	BA	3330	1/1	0.95	0.16	39,39,39,39	0
56	MG	B5	502	1/1	0.95	0.10	54,54,54,54	0
56	MG	BA	3004	1/1	0.95	0.12	24,24,24,24	0
56	MG	DA	3382	1/1	0.95	0.14	25,25,25,25	0
56	MG	BA	3672	1/1	0.95	0.30	48,48,48,48	0
56	MG	DA	3384	1/1	0.95	0.11	23,23,23,23	0
56	MG	BA	3498	1/1	0.95	0.15	39,39,39,39	0
56	MG	CA	3156	1/1	0.95	0.15	70,70,70,70	0
56	MG	BA	3674	1/1	0.95	0.18	55,55,55,55	0
56	MG	BA	3332	1/1	0.95	0.19	39,39,39,39	0
56	MG	DA	3130	1/1	0.95	0.12	32,32,32,32	0
56	MG	DA	3396	1/1	0.95	0.19	35,35,35,35	0
56	MG	BA	3500	1/1	0.95	0.15	37,37,37,37	0
56	MG	AA	3122	1/1	0.95	0.54	44,44,44,44	0
56	MG	BA	3138	1/1	0.95	0.17	46,46,46,46	0
56	MG	AA	3148	1/1	0.95	0.21	66,66,66,66	0
56	MG	BA	3506	1/1	0.95	0.14	30,30,30,30	0
56	MG	D5	102	1/1	0.95	0.58	55,55,55,55	0
56	MG	DA	3406	1/1	0.95	0.12	40,40,40,40	0
56	MG	DA	3407	1/1	0.95	0.24	21,21,21,21	0
56	MG	DA	3138	1/1	0.95	0.22	42,42,42,42	0
56	MG	DA	3411	1/1	0.95	0.17	21,21,21,21	0
56	MG	BA	3339	1/1	0.95	0.22	43,43,43,43	0
56	MG	CA	3009	1/1	0.95	0.14	47,47,47,47	0
56	MG	DA	3141	1/1	0.95	0.13	62,62,62,62	0
56	MG	BA	3189	1/1	0.95	0.16	54,54,54,54	0
56	MG	CA	3011	1/1	0.95	0.28	42,42,42,42	0
56	MG	BA	3076	1/1	0.96	0.23	41,41,41,41	0
56	MG	BA	3291	1/1	0.96	0.17	41,41,41,41	0
56	MG	BA	3395	1/1	0.96	0.20	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3178	1/1	0.96	0.37	43,43,43,43	0
56	MG	AA	3149	1/1	0.96	0.09	50,50,50,50	0
56	MG	DA	3182	1/1	0.96	0.16	32,32,32,32	0
56	MG	BA	3551	1/1	0.96	0.22	25,25,25,25	0
56	MG	BA	3021	1/1	0.96	0.27	42,42,42,42	0
56	MG	BA	3191	1/1	0.96	0.19	52,52,52,52	0
56	MG	CA	3026	1/1	0.96	0.07	52,52,52,52	0
56	MG	BA	3109	1/1	0.96	0.09	36,36,36,36	0
56	MG	DA	3457	1/1	0.96	0.12	37,37,37,37	0
56	MG	CA	3028	1/1	0.96	0.44	43,43,43,43	0
56	MG	BA	3561	1/1	0.96	0.19	24,24,24,24	0
56	MG	BA	3707	1/1	0.96	0.20	36,36,36,36	0
56	MG	BA	3405	1/1	0.96	0.14	34,34,34,34	0
56	MG	BA	3709	1/1	0.96	0.12	86,86,86,86	0
56	MG	DA	3463	1/1	0.96	0.37	43,43,43,43	0
56	MG	AA	3104	1/1	0.96	0.16	37,37,37,37	0
56	MG	BA	3151	1/1	0.96	0.06	52,52,52,52	0
56	MG	BA	3566	1/1	0.96	0.09	53,53,53,53	0
56	MG	DA	3468	1/1	0.96	0.14	48,48,48,48	0
56	MG	BA	3715	1/1	0.96	0.13	47,47,47,47	0
56	MG	AA	3153	1/1	0.96	0.13	45,45,45,45	0
56	MG	DA	3201	1/1	0.96	0.12	48,48,48,48	0
56	MG	BA	3413	1/1	0.96	0.14	20,20,20,20	0
56	MG	DA	3203	1/1	0.96	0.13	41,41,41,41	0
56	MG	DA	3039	1/1	0.96	0.40	59,59,59,59	0
56	MG	DA	3206	1/1	0.96	0.26	42,42,42,42	0
56	MG	BA	3571	1/1	0.96	0.08	65,65,65,65	0
56	MG	BA	3112	1/1	0.96	0.09	38,38,38,38	0
56	MG	BA	3575	1/1	0.96	0.19	51,51,51,51	0
56	MG	DA	3485	1/1	0.96	0.09	38,38,38,38	0
56	MG	DA	3486	1/1	0.96	0.12	38,38,38,38	0
56	MG	BA	3054	1/1	0.96	0.29	46,46,46,46	0
56	MG	BA	3726	1/1	0.96	0.55	47,47,47,47	0
56	MG	BA	3199	1/1	0.96	0.46	36,36,36,36	0
56	MG	DA	3491	1/1	0.96	0.15	56,56,56,56	0
56	MG	BA	3117	1/1	0.96	0.24	25,25,25,25	0
56	MG	BA	3425	1/1	0.96	0.36	36,36,36,36	0
56	MG	BA	3426	1/1	0.96	0.27	51,51,51,51	0
56	MG	BA	3584	1/1	0.96	0.18	22,22,22,22	0
56	MG	DA	3498	1/1	0.96	0.18	56,56,56,56	0
56	MG	BA	3427	1/1	0.96	0.12	48,48,48,48	0
56	MG	BA	3737	1/1	0.96	0.25	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3118	1/1	0.96	0.19	39,39,39,39	0
56	MG	BA	3319	1/1	0.96	0.17	25,25,25,25	0
56	MG	BB	3002	1/1	0.96	0.19	59,59,59,59	0
56	MG	BA	3121	1/1	0.96	0.27	57,57,57,57	0
56	MG	BA	3434	1/1	0.96	0.12	32,32,32,32	0
56	MG	BA	3324	1/1	0.96	0.18	36,36,36,36	0
56	MG	BA	3440	1/1	0.96	0.40	38,38,38,38	0
56	MG	BB	3007	1/1	0.96	0.09	47,47,47,47	0
56	MG	AA	3099	1/1	0.96	0.42	60,60,60,60	0
56	MG	BA	3025	1/1	0.96	0.25	28,28,28,28	0
56	MG	DA	3513	1/1	0.96	0.22	49,49,49,49	0
56	MG	BA	3001	1/1	0.96	0.15	69,69,69,69	0
56	MG	DA	3235	1/1	0.96	0.19	50,50,50,50	0
56	MG	BA	3213	1/1	0.96	0.05	41,41,41,41	0
56	MG	DA	3518	1/1	0.96	0.20	40,40,40,40	0
56	MG	CA	3072	1/1	0.96	0.22	38,38,38,38	0
56	MG	AA	3174	1/1	0.96	0.22	33,33,33,33	0
56	MG	AA	3175	1/1	0.96	0.14	76,76,76,76	0
56	MG	BD	302	1/1	0.96	0.36	58,58,58,58	0
56	MG	BD	303	1/1	0.96	0.19	42,42,42,42	0
56	MG	DA	3247	1/1	0.96	0.08	31,31,31,31	0
56	MG	DA	3248	1/1	0.96	0.29	51,51,51,51	0
56	MG	DA	3249	1/1	0.96	0.21	28,28,28,28	0
56	MG	CA	3078	1/1	0.96	0.29	46,46,46,46	0
56	MG	DA	3530	1/1	0.96	0.15	49,49,49,49	0
56	MG	BA	3604	1/1	0.96	0.11	72,72,72,72	0
56	MG	AD	502	1/1	0.96	0.46	43,43,43,43	0
56	MG	BA	3606	1/1	0.96	0.23	25,25,25,25	0
56	MG	BA	3607	1/1	0.96	0.43	53,53,53,53	0
56	MG	DA	3257	1/1	0.96	0.10	48,48,48,48	0
56	MG	DA	3259	1/1	0.96	0.15	47,47,47,47	0
56	MG	BD	309	1/1	0.96	0.14	42,42,42,42	0
56	MG	BA	3217	1/1	0.96	0.09	28,28,28,28	0
56	MG	BA	3458	1/1	0.96	0.12	29,29,29,29	0
56	MG	DA	3544	1/1	0.96	0.11	51,51,51,51	0
56	MG	BE	301	1/1	0.96	0.56	43,43,43,43	0
56	MG	DA	3265	1/1	0.96	0.27	51,51,51,51	0
56	MG	DA	3266	1/1	0.96	0.23	43,43,43,43	0
56	MG	BA	3265	1/1	0.96	0.11	20,20,20,20	0
56	MG	DA	3270	1/1	0.96	0.20	36,36,36,36	0
56	MG	BA	3266	1/1	0.96	0.33	46,46,46,46	0
56	MG	DA	3276	1/1	0.96	0.22	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3082	1/1	0.96	0.10	19,19,19,19	0
56	MG	DA	3557	1/1	0.96	0.12	45,45,45,45	0
56	MG	CA	3095	1/1	0.96	0.11	39,39,39,39	0
56	MG	CA	3096	1/1	0.96	0.10	60,60,60,60	0
56	MG	BA	3340	1/1	0.96	0.13	57,57,57,57	0
56	MG	BA	3615	1/1	0.96	0.17	36,36,36,36	0
56	MG	BA	3343	1/1	0.96	0.19	40,40,40,40	0
56	MG	BA	3130	1/1	0.96	0.58	43,43,43,43	0
56	MG	DA	3091	1/1	0.96	0.38	44,44,44,44	0
56	MG	DA	3287	1/1	0.96	0.27	53,53,53,53	0
56	MG	DA	3568	1/1	0.96	0.10	42,42,42,42	0
56	MG	BA	3345	1/1	0.96	0.21	33,33,33,33	0
56	MG	DA	3289	1/1	0.96	0.13	26,26,26,26	0
56	MG	BA	3219	1/1	0.96	0.22	65,65,65,65	0
56	MG	DA	3575	1/1	0.96	0.19	43,43,43,43	0
56	MG	DA	3094	1/1	0.96	0.18	26,26,26,26	0
56	MG	DA	3577	1/1	0.96	0.25	44,44,44,44	0
56	MG	DA	3294	1/1	0.96	0.10	47,47,47,47	0
56	MG	BA	3035	1/1	0.96	0.09	37,37,37,37	0
56	MG	BA	3472	1/1	0.96	0.08	30,30,30,30	0
56	MG	BG	3003	1/1	0.96	0.15	42,42,42,42	0
56	MG	BA	3223	1/1	0.96	0.68	47,47,47,47	0
56	MG	BA	3625	1/1	0.96	0.13	51,51,51,51	0
56	MG	AA	3106	1/1	0.96	0.25	56,56,56,56	0
56	MG	CA	3113	1/1	0.96	0.23	77,77,77,77	0
56	MG	BA	3477	1/1	0.96	0.11	25,25,25,25	0
56	MG	CA	3115	1/1	0.96	0.09	55,55,55,55	0
56	MG	BA	3093	1/1	0.96	0.22	25,25,25,25	0
56	MG	DA	3311	1/1	0.96	0.09	32,32,32,32	0
56	MG	BA	3630	1/1	0.96	0.25	52,52,52,52	0
56	MG	BP	204	1/1	0.96	0.17	55,55,55,55	0
56	MG	AA	3178	1/1	0.96	0.18	65,65,65,65	0
56	MG	BA	3483	1/1	0.96	0.26	53,53,53,53	0
56	MG	DA	3321	1/1	0.96	0.23	41,41,41,41	0
56	MG	AA	3157	1/1	0.96	0.08	35,35,35,35	0
56	MG	BA	3485	1/1	0.96	0.29	44,44,44,44	0
56	MG	BA	3637	1/1	0.96	0.35	33,33,33,33	0
56	MG	DA	3328	1/1	0.96	0.15	28,28,28,28	0
56	MG	DA	3605	1/1	0.96	0.15	44,44,44,44	0
56	MG	DA	3606	1/1	0.96	0.10	58,58,58,58	0
56	MG	DA	3607	1/1	0.96	0.10	45,45,45,45	0
56	MG	BA	3488	1/1	0.96	0.35	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	DA	3333	1/1	0.96	0.24	58,58,58,58	0
56	MG	CA	3132	1/1	0.96	0.11	70,70,70,70	0
56	MG	BA	3176	1/1	0.96	0.19	38,38,38,38	0
56	MG	AA	3161	1/1	0.96	0.12	72,72,72,72	0
56	MG	BA	3497	1/1	0.96	0.14	62,62,62,62	0
56	MG	DA	3341	1/1	0.96	0.19	23,23,23,23	0
56	MG	BA	3642	1/1	0.96	0.24	51,51,51,51	0
56	MG	BA	3359	1/1	0.96	0.20	23,23,23,23	0
56	MG	DA	3345	1/1	0.96	0.09	31,31,31,31	0
56	MG	DA	3622	1/1	0.96	0.08	55,55,55,55	0
56	MG	BV	201	1/1	0.96	0.40	53,53,53,53	0
56	MG	DA	3348	1/1	0.96	0.32	37,37,37,37	0
56	MG	BA	3361	1/1	0.96	0.26	34,34,34,34	0
56	MG	BA	3362	1/1	0.96	0.09	43,43,43,43	0
56	MG	DA	3628	1/1	0.96	0.22	63,63,63,63	0
56	MG	DA	3629	1/1	0.96	0.17	19,19,19,19	0
56	MG	BV	204	1/1	0.96	0.20	20,20,20,20	0
56	MG	BA	3648	1/1	0.96	0.30	49,49,49,49	0
56	MG	DA	3633	1/1	0.96	0.20	54,54,54,54	0
56	MG	BW	202	1/1	0.96	0.18	34,34,34,34	0
56	MG	CA	3145	1/1	0.96	0.08	43,43,43,43	0
56	MG	BA	3649	1/1	0.96	0.17	66,66,66,66	0
56	MG	DA	3637	1/1	0.96	0.28	48,48,48,48	0
56	MG	BW	204	1/1	0.96	0.35	35,35,35,35	0
56	MG	DA	3639	1/1	0.96	0.30	15,15,15,15	0
56	MG	BA	3013	1/1	0.96	0.14	40,40,40,40	0
56	MG	DA	3641	1/1	0.96	0.43	61,61,61,61	0
56	MG	DA	3642	1/1	0.96	0.13	35,35,35,35	0
56	MG	BA	3651	1/1	0.96	0.13	45,45,45,45	0
56	MG	BA	3366	1/1	0.96	0.09	63,63,63,63	0
56	MG	BA	3503	1/1	0.96	0.28	31,31,31,31	0
56	MG	BA	3504	1/1	0.96	0.29	41,41,41,41	0
56	MG	DA	3133	1/1	0.96	0.15	33,33,33,33	0
56	MG	BA	3657	1/1	0.96	0.16	56,56,56,56	0
56	MG	BA	3367	1/1	0.96	0.15	50,50,50,50	0
56	MG	BA	3368	1/1	0.96	0.20	35,35,35,35	0
56	MG	DA	3381	1/1	0.96	0.27	47,47,47,47	0
56	MG	BA	3234	1/1	0.96	0.30	55,55,55,55	0
56	MG	DB	3004	1/1	0.96	0.14	68,68,68,68	0
56	MG	AA	3183	1/1	0.96	0.10	42,42,42,42	0
56	MG	BA	3663	1/1	0.96	0.23	56,56,56,56	0
56	MG	DA	3386	1/1	0.96	0.18	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3015	1/1	0.96	0.34	44,44,44,44	0
56	MG	DA	3142	1/1	0.96	0.24	33,33,33,33	0
56	MG	DA	3389	1/1	0.96	0.28	27,27,27,27	0
56	MG	BA	3665	1/1	0.96	0.21	39,39,39,39	0
56	MG	AA	3107	1/1	0.96	0.31	44,44,44,44	0
56	MG	BA	3667	1/1	0.96	0.09	63,63,63,63	0
56	MG	BA	3512	1/1	0.96	0.23	40,40,40,40	0
56	MG	DA	3397	1/1	0.96	0.18	41,41,41,41	0
56	MG	BA	3513	1/1	0.96	0.11	45,45,45,45	0
56	MG	DA	3399	1/1	0.96	0.19	41,41,41,41	0
56	MG	BA	3376	1/1	0.96	0.10	48,48,48,48	0
56	MG	DE	301	1/1	0.96	0.61	51,51,51,51	0
56	MG	AA	3108	1/1	0.96	0.47	67,67,67,67	0
56	MG	DE	304	1/1	0.96	0.20	41,41,41,41	0
56	MG	BA	3380	1/1	0.96	0.13	53,53,53,53	0
56	MG	DA	3403	1/1	0.96	0.14	28,28,28,28	0
56	MG	CA	3004	1/1	0.96	0.21	96,96,96,96	0
56	MG	DA	3152	1/1	0.96	0.23	50,50,50,50	0
56	MG	DA	3153	1/1	0.96	0.20	38,38,38,38	0
56	MG	DA	3409	1/1	0.96	0.15	32,32,32,32	0
56	MG	BA	3524	1/1	0.96	0.25	55,55,55,55	0
56	MG	DF	306	1/1	0.96	0.23	50,50,50,50	0
56	MG	BA	3384	1/1	0.96	0.39	60,60,60,60	0
56	MG	DN	5001	1/1	0.96	0.12	75,75,75,75	0
56	MG	BA	3536	1/1	0.96	0.14	27,27,27,27	0
56	MG	BA	3537	1/1	0.96	0.38	31,31,31,31	0
56	MG	DA	3416	1/1	0.96	0.07	44,44,44,44	0
56	MG	DA	3417	1/1	0.96	0.15	34,34,34,34	0
56	MG	DA	3158	1/1	0.96	0.34	57,57,57,57	0
56	MG	DV	201	1/1	0.96	0.38	55,55,55,55	0
56	MG	DA	3420	1/1	0.96	0.13	51,51,51,51	0
56	MG	DA	3422	1/1	0.96	0.11	38,38,38,38	0
56	MG	BA	3685	1/1	0.96	0.09	67,67,67,67	0
56	MG	BA	3538	1/1	0.96	0.15	36,36,36,36	0
56	MG	DA	3425	1/1	0.96	0.11	27,27,27,27	0
56	MG	DA	3426	1/1	0.96	0.15	74,74,74,74	0
56	MG	D3	101	1/1	0.96	0.45	63,63,63,63	0
56	MG	BA	3385	1/1	0.96	0.24	26,26,26,26	0
56	MG	DA	3429	1/1	0.96	0.18	44,44,44,44	0
56	MG	CA	3012	1/1	0.96	0.12	49,49,49,49	0
56	MG	DA	3432	1/1	0.96	0.27	66,66,66,66	0
56	MG	DA	3007	1/1	0.96	0.23	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	DA	3166	1/1	0.96	0.08	32,32,32,32	0
56	MG	AA	3021	1/1	0.96	0.20	76,76,76,76	0
58	ZN	D9	501	1/1	0.96	0.05	66,66,66,66	0
56	MG	BA	3542	1/1	0.96	0.23	19,19,19,19	0
56	MG	BA	3543	1/1	0.96	0.29	52,52,52,52	0
56	MG	DA	3439	1/1	0.96	0.19	28,28,28,28	0
56	MG	AA	3055	1/1	0.96	0.20	50,50,50,50	0
56	MG	BA	3695	1/1	0.97	0.17	15,15,15,15	0
56	MG	BA	3696	1/1	0.97	0.26	39,39,39,39	0
56	MG	BA	3554	1/1	0.97	0.20	31,31,31,31	0
56	MG	DA	3023	1/1	0.97	0.28	52,52,52,52	0
56	MG	AA	3160	1/1	0.97	0.30	52,52,52,52	0
56	MG	BA	3322	1/1	0.97	0.23	22,22,22,22	0
56	MG	BA	3559	1/1	0.97	0.14	48,48,48,48	0
56	MG	BA	3701	1/1	0.97	0.13	32,32,32,32	0
56	MG	BA	3323	1/1	0.97	0.15	23,23,23,23	0
56	MG	BA	3203	1/1	0.97	0.26	32,32,32,32	0
56	MG	DA	3471	1/1	0.97	0.14	37,37,37,37	0
56	MG	BA	3705	1/1	0.97	0.05	39,39,39,39	0
56	MG	BA	3204	1/1	0.97	0.40	25,25,25,25	0
56	MG	AA	3207	1/1	0.97	0.28	45,45,45,45	0
56	MG	DA	3037	1/1	0.97	0.30	35,35,35,35	0
56	MG	BA	3564	1/1	0.97	0.07	52,52,52,52	0
56	MG	BA	3428	1/1	0.97	0.11	45,45,45,45	0
56	MG	BA	3710	1/1	0.97	0.21	48,48,48,48	0
56	MG	BA	3327	1/1	0.97	0.15	38,38,38,38	0
56	MG	BA	3031	1/1	0.97	0.79	41,41,41,41	0
56	MG	DA	3043	1/1	0.97	0.45	54,54,54,54	0
56	MG	BA	3713	1/1	0.97	0.10	66,66,66,66	0
56	MG	DA	3488	1/1	0.97	0.04	46,46,46,46	0
56	MG	BA	3329	1/1	0.97	0.13	29,29,29,29	0
56	MG	BA	3162	1/1	0.97	0.19	23,23,23,23	0
56	MG	BA	3572	1/1	0.97	0.20	36,36,36,36	0
56	MG	BA	3435	1/1	0.97	0.23	24,24,24,24	0
56	MG	DA	3493	1/1	0.97	0.15	29,29,29,29	0
56	MG	BA	3437	1/1	0.97	0.15	42,42,42,42	0
56	MG	DA	3495	1/1	0.97	0.22	39,39,39,39	0
56	MG	BA	3438	1/1	0.97	0.18	30,30,30,30	0
56	MG	DA	3239	1/1	0.97	0.21	39,39,39,39	0
56	MG	BA	3720	1/1	0.97	0.20	33,33,33,33	0
56	MG	DA	3241	1/1	0.97	0.21	15,15,15,15	0
56	MG	DA	3242	1/1	0.97	0.23	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3721	1/1	0.97	0.08	25,25,25,25	0
56	MG	CA	3043	1/1	0.97	0.34	49,49,49,49	0
56	MG	BA	3210	1/1	0.97	0.11	34,34,34,34	0
56	MG	DA	3504	1/1	0.97	0.08	44,44,44,44	0
56	MG	CA	3045	1/1	0.97	0.09	54,54,54,54	0
56	MG	BA	3032	1/1	0.97	0.19	49,49,49,49	0
56	MG	BA	3333	1/1	0.97	0.12	49,49,49,49	0
56	MG	DA	3508	1/1	0.97	0.19	38,38,38,38	0
56	MG	DA	3251	1/1	0.97	0.15	54,54,54,54	0
56	MG	BA	3212	1/1	0.97	0.28	43,43,43,43	0
56	MG	CA	3049	1/1	0.97	0.24	53,53,53,53	0
56	MG	CA	3050	1/1	0.97	0.13	43,43,43,43	0
56	MG	CA	3052	1/1	0.97	0.12	39,39,39,39	0
56	MG	DA	3514	1/1	0.97	0.12	39,39,39,39	0
56	MG	BA	3582	1/1	0.97	0.22	25,25,25,25	0
56	MG	BA	3729	1/1	0.97	0.40	46,46,46,46	0
56	MG	DA	3258	1/1	0.97	0.18	32,32,32,32	0
56	MG	BA	3033	1/1	0.97	0.37	35,35,35,35	0
56	MG	BA	3034	1/1	0.97	0.41	52,52,52,52	0
56	MG	BA	3734	1/1	0.97	0.26	45,45,45,45	0
56	MG	DA	3262	1/1	0.97	0.22	44,44,44,44	0
56	MG	BA	3587	1/1	0.97	0.18	23,23,23,23	0
56	MG	CA	3059	1/1	0.97	0.27	51,51,51,51	0
56	MG	BA	3447	1/1	0.97	0.13	37,37,37,37	0
56	MG	BA	3338	1/1	0.97	0.21	50,50,50,50	0
56	MG	BA	3450	1/1	0.97	0.27	46,46,46,46	0
56	MG	DA	3269	1/1	0.97	0.12	48,48,48,48	0
56	MG	BA	3451	1/1	0.97	0.30	28,28,28,28	0
56	MG	BB	3001	1/1	0.97	0.17	54,54,54,54	0
56	MG	DA	3274	1/1	0.97	0.09	52,52,52,52	0
56	MG	DA	3275	1/1	0.97	0.07	38,38,38,38	0
56	MG	BA	3593	1/1	0.97	0.14	74,74,74,74	0
56	MG	AA	3208	1/1	0.97	0.34	46,46,46,46	0
56	MG	BA	3167	1/1	0.97	0.39	39,39,39,39	0
56	MG	BA	3455	1/1	0.97	0.14	47,47,47,47	0
56	MG	BA	3456	1/1	0.97	0.10	52,52,52,52	0
56	MG	DA	3282	1/1	0.97	0.14	36,36,36,36	0
56	MG	BA	3267	1/1	0.97	0.16	41,41,41,41	0
56	MG	BA	3063	1/1	0.97	0.28	43,43,43,43	0
56	MG	DA	3546	1/1	0.97	0.12	44,44,44,44	0
56	MG	DA	3547	1/1	0.97	0.10	41,41,41,41	0
56	MG	BA	3600	1/1	0.97	0.15	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3064	1/1	0.97	0.19	39,39,39,39	0
56	MG	BB	3015	1/1	0.97	0.10	37,37,37,37	0
56	MG	DA	3085	1/1	0.97	0.12	36,36,36,36	0
56	MG	BA	3170	1/1	0.97	0.66	48,48,48,48	0
56	MG	DA	3291	1/1	0.97	0.24	35,35,35,35	0
56	MG	BA	3220	1/1	0.97	0.10	57,57,57,57	0
56	MG	DA	3088	1/1	0.97	0.15	46,46,46,46	0
56	MG	BA	3349	1/1	0.97	0.26	43,43,43,43	0
56	MG	BA	3272	1/1	0.97	0.34	7,7,7,7	0
56	MG	CA	3083	1/1	0.97	0.08	39,39,39,39	0
56	MG	BA	3351	1/1	0.97	0.07	30,30,30,30	0
56	MG	DA	3563	1/1	0.97	0.15	64,64,64,64	0
56	MG	BA	3352	1/1	0.97	0.12	34,34,34,34	0
56	MG	BA	3469	1/1	0.97	0.09	38,38,38,38	0
56	MG	DA	3300	1/1	0.97	0.15	37,37,37,37	0
56	MG	DA	3302	1/1	0.97	0.18	22,22,22,22	0
56	MG	CA	3088	1/1	0.97	0.26	43,43,43,43	0
56	MG	BA	3171	1/1	0.97	0.41	40,40,40,40	0
56	MG	DA	3571	1/1	0.97	0.14	46,46,46,46	0
56	MG	BA	3274	1/1	0.97	0.16	52,52,52,52	0
56	MG	DA	3573	1/1	0.97	0.19	40,40,40,40	0
56	MG	BD	308	1/1	0.97	0.33	23,23,23,23	0
56	MG	DA	3309	1/1	0.97	0.17	33,33,33,33	0
56	MG	BA	3473	1/1	0.97	0.11	51,51,51,51	0
56	MG	BA	3096	1/1	0.97	0.35	62,62,62,62	0
56	MG	BA	3475	1/1	0.97	0.21	36,36,36,36	0
56	MG	BA	3173	1/1	0.97	0.58	37,37,37,37	0
56	MG	AA	3150	1/1	0.97	0.27	46,46,46,46	0
56	MG	CA	3101	1/1	0.97	0.18	70,70,70,70	0
56	MG	BE	304	1/1	0.97	0.09	49,49,49,49	0
56	MG	DA	3583	1/1	0.97	0.28	48,48,48,48	0
56	MG	DA	3584	1/1	0.97	0.16	61,61,61,61	0
56	MG	BA	3479	1/1	0.97	0.10	56,56,56,56	0
56	MG	DA	3586	1/1	0.97	0.09	29,29,29,29	0
56	MG	AA	3102	1/1	0.97	0.06	64,64,64,64	0
56	MG	BA	3621	1/1	0.97	0.36	74,74,74,74	0
56	MG	BE	310	1/1	0.97	0.24	50,50,50,50	0
56	MG	BF	301	1/1	0.97	0.52	45,45,45,45	0
56	MG	AA	3171	1/1	0.97	0.25	72,72,72,72	0
56	MG	BA	3623	1/1	0.97	0.21	47,47,47,47	0
56	MG	DA	3335	1/1	0.97	0.26	38,38,38,38	0
56	MG	BF	305	1/1	0.97	0.32	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3596	1/1	0.97	0.10	67,67,67,67	0
56	MG	BF	306	1/1	0.97	0.18	37,37,37,37	0
56	MG	CA	3112	1/1	0.97	0.23	59,59,59,59	0
56	MG	BA	3360	1/1	0.97	0.19	38,38,38,38	0
56	MG	AA	3182	1/1	0.97	0.12	49,49,49,49	0
56	MG	AA	3156	1/1	0.97	0.17	62,62,62,62	0
56	MG	DA	3344	1/1	0.97	0.11	26,26,26,26	0
56	MG	BA	3486	1/1	0.97	0.06	38,38,38,38	0
56	MG	BA	3363	1/1	0.97	0.15	39,39,39,39	0
56	MG	CA	3118	1/1	0.97	0.08	37,37,37,37	0
56	MG	DA	3349	1/1	0.97	0.17	54,54,54,54	0
56	MG	BA	3629	1/1	0.97	0.13	47,47,47,47	0
56	MG	CA	3120	1/1	0.97	0.19	58,58,58,58	0
56	MG	CA	3121	1/1	0.97	0.27	53,53,53,53	0
56	MG	DA	3356	1/1	0.97	0.11	27,27,27,27	0
56	MG	BA	3489	1/1	0.97	0.14	43,43,43,43	0
56	MG	BA	3490	1/1	0.97	0.26	38,38,38,38	0
56	MG	DA	3616	1/1	0.97	0.23	62,62,62,62	0
56	MG	BA	3493	1/1	0.97	0.37	15,15,15,15	0
56	MG	BA	3364	1/1	0.97	0.24	29,29,29,29	0
56	MG	BO	201	1/1	0.97	0.14	70,70,70,70	0
56	MG	CA	3130	1/1	0.97	0.08	65,65,65,65	0
56	MG	BA	3232	1/1	0.97	0.15	29,29,29,29	0
56	MG	BP	202	1/1	0.97	0.11	40,40,40,40	0
56	MG	BP	203	1/1	0.97	0.69	29,29,29,29	0
56	MG	BA	3636	1/1	0.97	0.11	36,36,36,36	0
56	MG	DA	3368	1/1	0.97	0.12	39,39,39,39	0
56	MG	AA	3057	1/1	0.97	0.09	37,37,37,37	0
56	MG	DA	3371	1/1	0.97	0.07	44,44,44,44	0
56	MG	DA	3630	1/1	0.97	0.20	40,40,40,40	0
56	MG	DA	3136	1/1	0.97	0.11	49,49,49,49	0
56	MG	DA	3374	1/1	0.97	0.05	37,37,37,37	0
56	MG	DA	3375	1/1	0.97	0.14	60,60,60,60	0
56	MG	AA	3185	1/1	0.97	0.28	46,46,46,46	0
56	MG	BQ	204	1/1	0.97	0.18	12,12,12,12	0
56	MG	AA	3186	1/1	0.97	0.07	49,49,49,49	0
56	MG	BA	3369	1/1	0.97	0.22	45,45,45,45	0
56	MG	BR	203	1/1	0.97	0.18	15,15,15,15	0
56	MG	AA	3158	1/1	0.97	0.20	44,44,44,44	0
56	MG	BA	3184	1/1	0.97	0.38	49,49,49,49	0
56	MG	AX	110	1/1	0.97	0.20	42,42,42,42	0
56	MG	BA	3644	1/1	0.97	0.16	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3239	1/1	0.97	0.10	33,33,33,33	0
56	MG	BA	3646	1/1	0.97	0.23	52,52,52,52	0
56	MG	AA	3176	1/1	0.97	0.09	63,63,63,63	0
56	MG	BA	3077	1/1	0.97	0.20	39,39,39,39	0
56	MG	DA	3650	1/1	0.97	0.58	48,48,48,48	0
56	MG	BA	3379	1/1	0.97	0.22	22,22,22,22	0
56	MG	BA	3294	1/1	0.97	0.28	37,37,37,37	0
56	MG	BA	3002	1/1	0.97	0.20	54,54,54,54	0
56	MG	BA	3296	1/1	0.97	0.25	46,46,46,46	0
56	MG	BA	3003	1/1	0.97	0.16	43,43,43,43	0
56	MG	BA	3080	1/1	0.97	0.52	45,45,45,45	0
56	MG	BA	3390	1/1	0.97	0.25	30,30,30,30	0
56	MG	AA	3221	1/1	0.97	0.10	64,64,64,64	0
56	MG	BA	3517	1/1	0.97	0.08	49,49,49,49	0
56	MG	BA	3518	1/1	0.97	0.10	41,41,41,41	0
56	MG	DA	3160	1/1	0.97	0.15	44,44,44,44	0
56	MG	BA	3521	1/1	0.97	0.12	49,49,49,49	0
56	MG	BA	3392	1/1	0.97	0.26	56,56,56,56	0
56	MG	BA	3026	1/1	0.97	0.47	36,36,36,36	0
56	MG	DA	3412	1/1	0.97	0.28	30,30,30,30	0
56	MG	CA	3166	1/1	0.97	0.23	59,59,59,59	0
56	MG	BA	3527	1/1	0.97	0.18	64,64,64,64	0
56	MG	DD	303	1/1	0.97	0.20	19,19,19,19	0
56	MG	DD	304	1/1	0.97	0.23	35,35,35,35	0
56	MG	CA	3169	1/1	0.97	0.16	57,57,57,57	0
56	MG	BA	3530	1/1	0.97	0.28	31,31,31,31	0
56	MG	CA	3171	1/1	0.97	0.32	67,67,67,67	0
56	MG	BA	3532	1/1	0.97	0.18	34,34,34,34	0
56	MG	DA	3421	1/1	0.97	0.19	34,34,34,34	0
56	MG	BA	3668	1/1	0.97	0.13	38,38,38,38	0
56	MG	BA	3534	1/1	0.97	0.12	41,41,41,41	0
56	MG	DA	3173	1/1	0.97	0.41	39,39,39,39	0
56	MG	BA	3302	1/1	0.97	0.13	27,27,27,27	0
56	MG	DA	3176	1/1	0.97	0.27	39,39,39,39	0
56	MG	BA	3396	1/1	0.97	0.18	22,22,22,22	0
56	MG	DA	3428	1/1	0.97	0.27	51,51,51,51	0
56	MG	CX	102	1/1	0.97	0.06	61,61,61,61	0
56	MG	DA	3180	1/1	0.97	0.21	46,46,46,46	0
56	MG	DA	3431	1/1	0.97	0.12	41,41,41,41	0
56	MG	BA	3115	1/1	0.97	0.26	36,36,36,36	0
56	MG	CX	104	1/1	0.97	0.14	40,40,40,40	0
56	MG	DO	5001	1/1	0.97	0.12	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3184	1/1	0.97	0.32	45,45,45,45	0
56	MG	BA	3400	1/1	0.97	0.19	24,24,24,24	0
56	MG	DQ	203	1/1	0.97	0.32	57,57,57,57	0
56	MG	DQ	204	1/1	0.97	0.13	43,43,43,43	0
56	MG	DA	3436	1/1	0.97	0.07	62,62,62,62	0
56	MG	BA	3539	1/1	0.97	0.16	35,35,35,35	0
56	MG	BA	3116	1/1	0.97	0.20	31,31,31,31	0
56	MG	B8	103	1/1	0.97	0.19	24,24,24,24	0
56	MG	BA	3680	1/1	0.97	0.35	37,37,37,37	0
56	MG	BA	3682	1/1	0.97	0.22	38,38,38,38	0
56	MG	DA	3192	1/1	0.97	0.12	47,47,47,47	0
56	MG	AA	3203	1/1	0.97	0.12	63,63,63,63	0
56	MG	AA	3204	1/1	0.97	0.14	54,54,54,54	0
56	MG	DA	3445	1/1	0.97	0.23	39,39,39,39	0
56	MG	D0	101	1/1	0.97	0.12	63,63,63,63	0
56	MG	DA	3446	1/1	0.97	0.11	52,52,52,52	0
56	MG	BA	3404	1/1	0.97	0.15	35,35,35,35	0
56	MG	DA	3449	1/1	0.97	0.09	43,43,43,43	0
56	MG	BA	3311	1/1	0.97	0.23	42,42,42,42	0
56	MG	BA	3119	1/1	0.97	0.25	58,58,58,58	0
56	MG	BA	3314	1/1	0.97	0.17	24,24,24,24	0
56	MG	BA	3315	1/1	0.97	0.11	37,37,37,37	0
58	ZN	DY	501	1/1	0.97	0.05	83,83,83,83	0
56	MG	BA	3317	1/1	0.97	0.15	40,40,40,40	0
58	ZN	D6	501	1/1	0.97	0.12	61,61,61,61	0
56	MG	DA	3455	1/1	0.97	0.17	60,60,60,60	0
56	MG	BA	3550	1/1	0.97	0.24	45,45,45,45	0
56	MG	BA	3120	1/1	0.97	0.09	51,51,51,51	0
56	MG	BA	3552	1/1	0.97	0.23	29,29,29,29	0
56	MG	BA	3694	1/1	0.97	0.37	56,56,56,56	0
56	MG	AA	3103	1/1	0.98	0.19	38,38,38,38	0
56	MG	DA	3523	1/1	0.98	0.06	55,55,55,55	0
56	MG	BA	3179	1/1	0.98	0.20	43,43,43,43	0
56	MG	DA	3174	1/1	0.98	0.26	41,41,41,41	0
56	MG	BA	3602	1/1	0.98	0.09	35,35,35,35	0
56	MG	BA	3081	1/1	0.98	0.08	14,14,14,14	0
56	MG	DA	3177	1/1	0.98	0.08	33,33,33,33	0
56	MG	DA	3529	1/1	0.98	0.10	63,63,63,63	0
56	MG	CA	3085	1/1	0.98	0.30	43,43,43,43	0
56	MG	AA	3172	1/1	0.98	0.05	53,53,53,53	0
56	MG	BU	203	1/1	0.98	0.35	33,33,33,33	0
56	MG	DA	3533	1/1	0.98	0.08	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3351	1/1	0.98	0.38	35,35,35,35	0
56	MG	AA	3163	1/1	0.98	0.17	28,28,28,28	0
56	MG	BA	3702	1/1	0.98	0.12	56,56,56,56	0
56	MG	DA	3354	1/1	0.98	0.15	27,27,27,27	0
56	MG	BA	3281	1/1	0.98	0.18	52,52,52,52	0
56	MG	BU	207	1/1	0.98	0.21	40,40,40,40	0
56	MG	DA	3541	1/1	0.98	0.28	35,35,35,35	0
56	MG	CA	3092	1/1	0.98	0.12	47,47,47,47	0
56	MG	CA	3093	1/1	0.98	0.06	53,53,53,53	0
56	MG	BA	3131	1/1	0.98	0.72	54,54,54,54	0
56	MG	BA	3519	1/1	0.98	0.12	39,39,39,39	0
56	MG	BA	3445	1/1	0.98	0.20	25,25,25,25	0
56	MG	BA	3522	1/1	0.98	0.14	49,49,49,49	0
56	MG	CA	3098	1/1	0.98	0.23	46,46,46,46	0
56	MG	DA	3551	1/1	0.98	0.08	52,52,52,52	0
56	MG	DA	3365	1/1	0.98	0.06	40,40,40,40	0
56	MG	BA	3375	1/1	0.98	0.24	31,31,31,31	0
56	MG	CA	3100	1/1	0.98	0.11	60,60,60,60	0
56	MG	BA	3612	1/1	0.98	0.15	37,37,37,37	0
56	MG	BA	3283	1/1	0.98	0.15	17,17,17,17	0
56	MG	DA	3370	1/1	0.98	0.15	38,38,38,38	0
56	MG	DA	3059	1/1	0.98	0.08	46,46,46,46	0
56	MG	DA	3372	1/1	0.98	0.12	45,45,45,45	0
56	MG	BA	3525	1/1	0.98	0.23	43,43,43,43	0
56	MG	DA	3561	1/1	0.98	0.19	45,45,45,45	0
56	MG	BA	3526	1/1	0.98	0.19	19,19,19,19	0
56	MG	BA	3448	1/1	0.98	0.09	29,29,29,29	0
56	MG	BA	3529	1/1	0.98	0.21	35,35,35,35	0
56	MG	DA	3377	1/1	0.98	0.24	59,59,59,59	0
56	MG	BA	3008	1/1	0.98	0.13	50,50,50,50	0
56	MG	DA	3380	1/1	0.98	0.16	26,26,26,26	0
56	MG	AA	3062	1/1	0.98	0.08	32,32,32,32	0
56	MG	DA	3569	1/1	0.98	0.19	37,37,37,37	0
56	MG	DA	3205	1/1	0.98	0.09	38,38,38,38	0
56	MG	BA	3533	1/1	0.98	0.18	32,32,32,32	0
56	MG	BA	3186	1/1	0.98	0.14	53,53,53,53	0
56	MG	DA	3385	1/1	0.98	0.15	35,35,35,35	0
56	MG	BA	3381	1/1	0.98	0.10	37,37,37,37	0
56	MG	BA	3382	1/1	0.98	0.13	51,51,51,51	0
56	MG	BA	3454	1/1	0.98	0.09	22,22,22,22	0
56	MG	BA	3010	1/1	0.98	0.17	32,32,32,32	0
56	MG	DA	3390	1/1	0.98	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	B3	101	1/1	0.98	0.15	28,28,28,28	0
56	MG	B3	102	1/1	0.98	0.13	59,59,59,59	0
56	MG	BA	3723	1/1	0.98	0.14	49,49,49,49	0
56	MG	DA	3394	1/1	0.98	0.14	47,47,47,47	0
56	MG	DA	3395	1/1	0.98	0.21	34,34,34,34	0
56	MG	DA	3215	1/1	0.98	0.30	29,29,29,29	0
56	MG	BA	3046	1/1	0.98	0.14	29,29,29,29	0
56	MG	BA	3725	1/1	0.98	0.12	49,49,49,49	0
56	MG	AA	3165	1/1	0.98	0.15	23,23,23,23	0
56	MG	DA	3588	1/1	0.98	0.18	40,40,40,40	0
56	MG	AA	3027	1/1	0.98	0.06	55,55,55,55	0
56	MG	BA	3459	1/1	0.98	0.22	31,31,31,31	0
56	MG	BA	3388	1/1	0.98	0.15	34,34,34,34	0
56	MG	B8	102	1/1	0.98	0.10	60,60,60,60	0
56	MG	DA	3404	1/1	0.98	0.16	47,47,47,47	0
56	MG	BA	3544	1/1	0.98	0.23	27,27,27,27	0
56	MG	BA	3389	1/1	0.98	0.12	48,48,48,48	0
56	MG	CA	3128	1/1	0.98	0.26	41,41,41,41	0
56	MG	DA	3408	1/1	0.98	0.22	37,37,37,37	0
56	MG	CA	3129	1/1	0.98	0.14	45,45,45,45	0
56	MG	DA	3227	1/1	0.98	0.14	53,53,53,53	0
56	MG	DA	3600	1/1	0.98	0.07	45,45,45,45	0
56	MG	BA	3733	1/1	0.98	0.11	27,27,27,27	0
56	MG	BA	3634	1/1	0.98	0.70	63,63,63,63	0
56	MG	BA	3222	1/1	0.98	0.29	25,25,25,25	0
56	MG	CA	3133	1/1	0.98	0.05	49,49,49,49	0
56	MG	DA	3234	1/1	0.98	0.23	33,33,33,33	0
56	MG	BA	3337	1/1	0.98	0.17	23,23,23,23	0
56	MG	DA	3418	1/1	0.98	0.17	29,29,29,29	0
56	MG	DA	3608	1/1	0.98	0.27	57,57,57,57	0
56	MG	DA	3236	1/1	0.98	0.17	46,46,46,46	0
56	MG	AA	3141	1/1	0.98	0.21	48,48,48,48	0
56	MG	BA	3393	1/1	0.98	0.18	38,38,38,38	0
56	MG	BA	3467	1/1	0.98	0.06	40,40,40,40	0
56	MG	BA	3113	1/1	0.98	0.09	32,32,32,32	0
56	MG	BA	3070	1/1	0.98	0.13	35,35,35,35	0
56	MG	BA	3341	1/1	0.98	0.09	33,33,33,33	0
56	MG	AA	3097	1/1	0.98	0.25	43,43,43,43	0
56	MG	DA	3244	1/1	0.98	0.31	29,29,29,29	0
56	MG	BA	3556	1/1	0.98	0.31	27,27,27,27	0
56	MG	BA	3557	1/1	0.98	0.23	31,31,31,31	0
56	MG	BA	3398	1/1	0.98	0.11	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3227	1/1	0.98	0.30	32,32,32,32	0
56	MG	CA	3017	1/1	0.98	0.24	42,42,42,42	0
56	MG	DA	3250	1/1	0.98	0.14	31,31,31,31	0
56	MG	BA	3228	1/1	0.98	0.27	63,63,63,63	0
56	MG	CA	3148	1/1	0.98	0.19	68,68,68,68	0
56	MG	BB	3012	1/1	0.98	0.15	56,56,56,56	0
56	MG	BB	3013	1/1	0.98	0.10	39,39,39,39	0
56	MG	BA	3195	1/1	0.98	0.33	47,47,47,47	0
56	MG	CA	3022	1/1	0.98	0.04	70,70,70,70	0
56	MG	BA	3347	1/1	0.98	0.27	25,25,25,25	0
56	MG	BB	3016	1/1	0.98	0.12	21,21,21,21	0
56	MG	BA	3478	1/1	0.98	0.15	29,29,29,29	0
56	MG	AA	3179	1/1	0.98	0.26	34,34,34,34	0
56	MG	BA	3480	1/1	0.98	0.20	17,17,17,17	0
56	MG	BA	3264	1/1	0.98	0.17	30,30,30,30	0
56	MG	BA	3655	1/1	0.98	0.21	52,52,52,52	0
56	MG	BA	3656	1/1	0.98	0.11	33,33,33,33	0
56	MG	DA	3448	1/1	0.98	0.08	57,57,57,57	0
56	MG	BA	3567	1/1	0.98	0.22	37,37,37,37	0
56	MG	AA	3220	1/1	0.98	0.12	40,40,40,40	0
56	MG	DA	3644	1/1	0.98	0.08	42,42,42,42	0
56	MG	DA	3645	1/1	0.98	0.09	30,30,30,30	0
56	MG	BA	3569	1/1	0.98	0.18	19,19,19,19	0
56	MG	DA	3268	1/1	0.98	0.17	40,40,40,40	0
56	MG	CA	3165	1/1	0.98	0.08	40,40,40,40	0
56	MG	DA	3649	1/1	0.98	0.24	24,24,24,24	0
56	MG	BA	3095	1/1	0.98	0.47	55,55,55,55	0
56	MG	BA	3411	1/1	0.98	0.15	38,38,38,38	0
56	MG	DA	3652	1/1	0.98	0.60	60,60,60,60	0
56	MG	CA	3168	1/1	0.98	0.39	77,77,77,77	0
56	MG	BD	310	1/1	0.98	0.31	48,48,48,48	0
56	MG	AA	3205	1/1	0.98	0.19	61,61,61,61	0
56	MG	DA	3277	1/1	0.98	0.25	49,49,49,49	0
56	MG	BA	3305	1/1	0.98	0.13	44,44,44,44	0
56	MG	BA	3574	1/1	0.98	0.08	54,54,54,54	0
56	MG	BE	302	1/1	0.98	0.22	33,33,33,33	0
56	MG	CE	3002	1/1	0.98	0.07	55,55,55,55	0
56	MG	BA	3487	1/1	0.98	0.12	31,31,31,31	0
56	MG	AA	3192	1/1	0.98	0.08	57,57,57,57	0
56	MG	BA	3418	1/1	0.98	0.15	27,27,27,27	0
56	MG	DA	3467	1/1	0.98	0.09	35,35,35,35	0
56	MG	BA	3307	1/1	0.98	0.20	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3670	1/1	0.98	0.08	59,59,59,59	0
56	MG	BE	308	1/1	0.98	0.18	52,52,52,52	0
56	MG	BE	309	1/1	0.98	0.27	25,25,25,25	0
56	MG	BA	3491	1/1	0.98	0.19	23,23,23,23	0
56	MG	DA	3473	1/1	0.98	0.31	32,32,32,32	0
56	MG	DA	3290	1/1	0.98	0.07	42,42,42,42	0
56	MG	DA	3475	1/1	0.98	0.11	36,36,36,36	0
56	MG	DA	3476	1/1	0.98	0.20	45,45,45,45	0
56	MG	DA	3477	1/1	0.98	0.09	49,49,49,49	0
56	MG	BA	3420	1/1	0.98	0.30	33,33,33,33	0
56	MG	BA	3581	1/1	0.98	0.10	51,51,51,51	0
56	MG	DE	303	1/1	0.98	0.11	41,41,41,41	0
56	MG	DA	3480	1/1	0.98	0.09	52,52,52,52	0
56	MG	CA	3051	1/1	0.98	0.10	63,63,63,63	0
56	MG	BA	3308	1/1	0.98	0.08	44,44,44,44	0
56	MG	BA	3675	1/1	0.98	0.12	49,49,49,49	0
56	MG	BA	3583	1/1	0.98	0.20	27,27,27,27	0
56	MG	BA	3036	1/1	0.98	0.18	38,38,38,38	0
56	MG	BA	3678	1/1	0.98	0.16	53,53,53,53	0
56	MG	BA	3679	1/1	0.98	0.40	27,27,27,27	0
56	MG	BA	3424	1/1	0.98	0.17	15,15,15,15	0
56	MG	BA	3681	1/1	0.98	0.14	40,40,40,40	0
56	MG	BA	3586	1/1	0.98	0.19	29,29,29,29	0
56	MG	BA	3310	1/1	0.98	0.17	13,13,13,13	0
56	MG	AA	3193	1/1	0.98	0.10	60,60,60,60	0
56	MG	AA	3143	1/1	0.98	0.15	45,45,45,45	0
56	MG	DA	3308	1/1	0.98	0.32	30,30,30,30	0
56	MG	CA	3064	1/1	0.98	0.12	58,58,58,58	0
56	MG	DA	3019	1/1	0.98	0.13	30,30,30,30	0
56	MG	BN	3004	1/1	0.98	0.40	66,66,66,66	0
56	MG	DA	3313	1/1	0.98	0.17	52,52,52,52	0
56	MG	BA	3313	1/1	0.98	0.27	36,36,36,36	0
56	MG	BA	3591	1/1	0.98	0.32	48,48,48,48	0
56	MG	DA	3316	1/1	0.98	0.17	58,58,58,58	0
56	MG	DA	3317	1/1	0.98	0.12	32,32,32,32	0
56	MG	BA	3429	1/1	0.98	0.14	20,20,20,20	0
56	MG	BA	3150	1/1	0.98	0.45	34,34,34,34	0
56	MG	DA	3320	1/1	0.98	0.17	30,30,30,30	0
56	MG	DA	3025	1/1	0.98	0.38	44,44,44,44	0
56	MG	DA	3026	1/1	0.98	0.21	37,37,37,37	0
56	MG	DA	3323	1/1	0.98	0.18	30,30,30,30	0
56	MG	AA	3091	1/1	0.98	0.15	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3316	1/1	0.98	0.16	28,28,28,28	0
56	MG	DA	3327	1/1	0.98	0.18	29,29,29,29	0
58	ZN	BY	202	1/1	0.98	0.09	71,71,71,71	0
56	MG	BQ	201	1/1	0.98	0.43	61,61,61,61	0
56	MG	DA	3165	1/1	0.98	0.24	44,44,44,44	0
56	MG	DA	3330	1/1	0.98	0.14	37,37,37,37	0
56	MG	BA	3433	1/1	0.98	0.24	39,39,39,39	0
56	MG	BA	3207	1/1	0.98	0.23	35,35,35,35	0
56	MG	BA	3208	1/1	0.98	0.28	41,41,41,41	0
56	MG	BA	3436	1/1	0.98	0.09	37,37,37,37	0
56	MG	DA	3337	1/1	0.98	0.09	27,27,27,27	0
56	MG	DA	3035	1/1	0.98	0.23	56,56,56,56	0
56	MG	BR	201	1/1	0.98	0.60	51,51,51,51	0
56	MG	AX	109	1/1	0.99	0.09	43,43,43,43	0
56	MG	AA	3159	1/1	0.99	0.32	57,57,57,57	0
56	MG	AA	3188	1/1	0.99	0.24	53,53,53,53	0
56	MG	BA	3508	1/1	0.99	0.14	34,34,34,34	0
56	MG	BA	3378	1/1	0.99	0.12	20,20,20,20	0
56	MG	BA	3318	1/1	0.99	0.13	33,33,33,33	0
56	MG	DA	3312	1/1	0.99	0.27	43,43,43,43	0
56	MG	BA	3423	1/1	0.99	0.07	26,26,26,26	0
56	MG	DA	3379	1/1	0.99	0.22	28,28,28,28	0
56	MG	BF	303	1/1	0.99	0.27	36,36,36,36	0
56	MG	CA	3069	1/1	0.99	0.11	69,69,69,69	0
56	MG	BA	3051	1/1	0.99	0.15	20,20,20,20	0
56	MG	BA	3662	1/1	0.99	0.12	39,39,39,39	0
56	MG	BA	3399	1/1	0.99	0.19	18,18,18,18	0
56	MG	CA	3122	1/1	0.99	0.07	47,47,47,47	0
56	MG	BA	3154	1/1	0.99	0.17	61,61,61,61	0
56	MG	BA	3321	1/1	0.99	0.16	29,29,29,29	0
56	MG	BA	3516	1/1	0.99	0.09	47,47,47,47	0
56	MG	BA	3553	1/1	0.99	0.13	31,31,31,31	0
56	MG	DA	3324	1/1	0.99	0.23	40,40,40,40	0
56	MG	CA	3077	1/1	0.99	0.22	53,53,53,53	0
56	MG	BA	3383	1/1	0.99	0.18	38,38,38,38	0
56	MG	AA	3214	1/1	0.99	0.27	75,75,75,75	0
56	MG	CA	3080	1/1	0.99	0.14	55,55,55,55	0
56	MG	BB	3010	1/1	0.99	0.26	40,40,40,40	0
56	MG	BB	3011	1/1	0.99	0.15	37,37,37,37	0
56	MG	DA	3331	1/1	0.99	0.09	34,34,34,34	0
56	MG	DA	3332	1/1	0.99	0.13	33,33,33,33	0
56	MG	BA	3200	1/1	0.99	0.27	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3271	1/1	0.99	0.20	37,37,37,37	0
56	MG	DA	3272	1/1	0.99	0.28	27,27,27,27	0
56	MG	BA	3520	1/1	0.99	0.14	34,34,34,34	0
56	MG	AA	3144	1/1	0.99	0.08	48,48,48,48	0
56	MG	DA	3338	1/1	0.99	0.14	29,29,29,29	0
56	MG	BN	3006	1/1	0.99	0.12	24,24,24,24	0
56	MG	DA	3540	1/1	0.99	0.23	54,54,54,54	0
56	MG	BA	3126	1/1	0.99	0.22	24,24,24,24	0
56	MG	DA	3612	1/1	0.99	0.15	39,39,39,39	0
56	MG	DA	3542	1/1	0.99	0.18	32,32,32,32	0
56	MG	BA	3460	1/1	0.99	0.13	33,33,33,33	0
56	MG	B7	102	1/1	0.99	0.25	40,40,40,40	0
56	MG	BA	3407	1/1	0.99	0.19	15,15,15,15	0
56	MG	AA	3151	1/1	0.99	0.08	41,41,41,41	0
56	MG	DA	3618	1/1	0.99	0.12	39,39,39,39	0
56	MG	BA	3492	1/1	0.99	0.25	23,23,23,23	0
56	MG	DA	3346	1/1	0.99	0.23	29,29,29,29	0
56	MG	DA	3549	1/1	0.99	0.24	52,52,52,52	0
56	MG	DA	3413	1/1	0.99	0.20	53,53,53,53	0
56	MG	BA	3409	1/1	0.99	0.23	27,27,27,27	0
56	MG	BA	3528	1/1	0.99	0.22	33,33,33,33	0
56	MG	DA	3625	1/1	0.99	0.10	35,35,35,35	0
56	MG	BA	3494	1/1	0.99	0.34	18,18,18,18	0
56	MG	CA	3001	1/1	0.99	0.21	55,55,55,55	0
56	MG	BA	3410	1/1	0.99	0.15	27,27,27,27	0
56	MG	BA	3531	1/1	0.99	0.29	38,38,38,38	0
56	MG	DA	3230	1/1	0.99	0.16	62,62,62,62	0
56	MG	BA	3371	1/1	0.99	0.18	15,15,15,15	0
56	MG	DA	3355	1/1	0.99	0.26	18,18,18,18	0
56	MG	BA	3128	1/1	0.99	0.27	40,40,40,40	0
56	MG	BA	3342	1/1	0.99	0.19	31,31,31,31	0
56	MG	BA	3414	1/1	0.99	0.21	19,19,19,19	0
57	SF4	AD	501	8/8	0.99	0.14	59,72,92,96	0
57	SF4	CD	501	8/8	0.99	0.14	64,75,91,95	0
56	MG	BA	3415	1/1	0.99	0.24	27,27,27,27	0
56	MG	DA	3181	1/1	0.99	0.30	36,36,36,36	0
56	MG	CA	3154	1/1	0.99	0.13	49,49,49,49	0
58	ZN	B5	501	1/1	0.99	0.11	54,54,54,54	0
56	MG	BA	3442	1/1	0.99	0.15	12,12,12,12	0
56	MG	BA	3471	1/1	0.99	0.17	51,51,51,51	0
56	MG	DA	3028	1/1	0.99	0.06	35,35,35,35	0
58	ZN	D5	103	1/1	0.99	0.07	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3416	1/1	0.99	0.25	42,42,42,42	0
56	MG	BA	3614	1/1	0.99	0.42	30,30,30,30	0
56	MG	DA	3301	1/1	0.99	0.14	45,45,45,45	0
56	MG	AA	3073	1/1	0.99	0.07	46,46,46,46	0
56	MG	BA	3732	1/1	0.99	0.52	61,61,61,61	0
56	MG	DA	3190	1/1	0.99	0.13	37,37,37,37	0
58	ZN	B6	501	1/1	1.00	0.13	49,49,49,49	0
58	ZN	B9	501	1/1	1.00	0.12	48,48,48,48	0
56	MG	DA	3304	1/1	1.00	0.11	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.