



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 12:07 pm BST

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.;  
Gualerzi, C.O.; Steitz, T.A.  
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.

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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 : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11



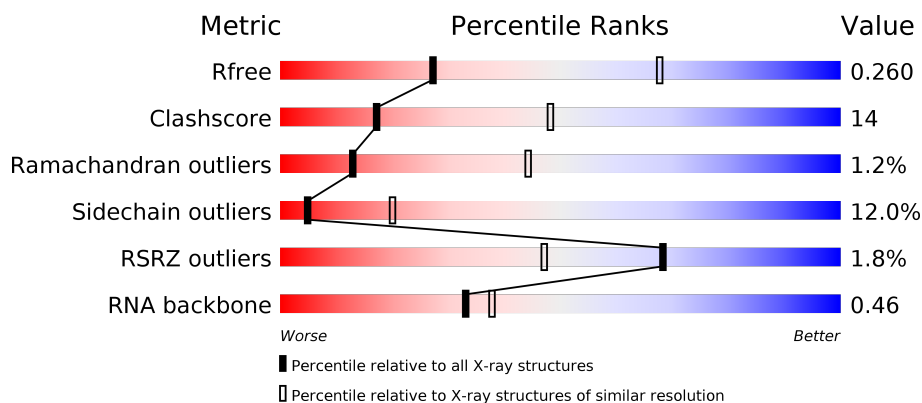
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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 on 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	<div> <div>2%</div> <div> <div>36%</div> <div>43%</div> <div>17%</div> <div>• •</div> </div> </div>
1	CA	1522	<div> <div>2%</div> <div> <div>34%</div> <div>43%</div> <div>18%</div> <div>• •</div> </div> </div>
2	AB	256	<div> <div>3%</div> <div> <div>38%</div> <div>39%</div> <div>11%</div> <div>• 10%</div> </div> </div>
2	CB	256	<div> <div>5%</div> <div> <div>36%</div> <div>44%</div> <div>10%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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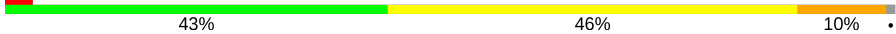



















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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AX	77	
23	CX	77	
24	AW	10	
24	CW	10	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	
27	BD	276	
27	DD	276	

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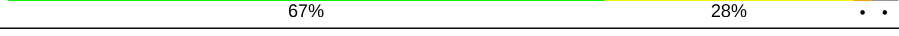


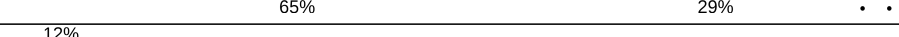

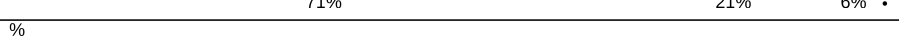


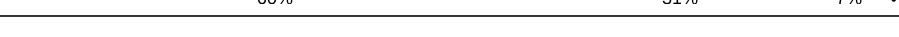

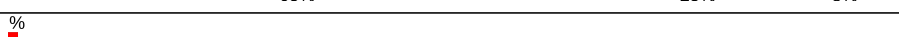
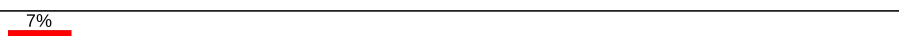

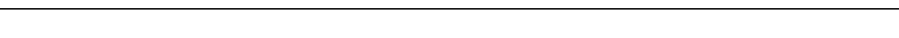
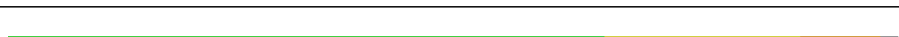


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Mol	Chain	Length	Quality of chain
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	118	
38	BS	112	
38	DS	112	
39	BT	146	
39	DT	146	
40	BU	118	

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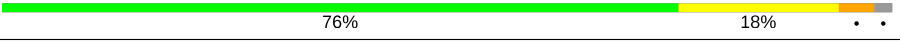


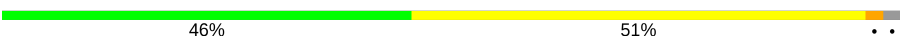


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Mol	Chain	Length	Quality of chain
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	
52	B6	54	
52	D6	54	

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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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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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

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
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
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
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
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
10	CJ	96	Total	C	N	O			
			714	445	138	131	0	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0
15	CO	88	Total	C	N	O	S		
			728	456	144	126	2	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
26	DB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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



- 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	B4	1	Total	Mg	0	0
			1	1		
56	BA	738	Total	Mg	0	0
			738	738		
56	AK	1	Total	Mg	0	0
			1	1		
56	DQ	5	Total	Mg	0	0
			5	5		
56	D3	1	Total	Mg	0	0
			1	1		
56	DF	6	Total	Mg	0	0
			6	6		
56	B8	3	Total	Mg	0	0
			3	3		
56	BE	10	Total	Mg	0	0
			10	10		
56	B1	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AN	2	Total 2	Mg 2	0	0
56	BP	4	Total 4	Mg 4	0	0
56	AX	9	Total 9	Mg 9	0	0
56	DN	1	Total 1	Mg 1	0	0
56	CA	172	Total 172	Mg 172	0	0
56	B5	1	Total 1	Mg 1	0	0
56	BB	18	Total 18	Mg 18	0	0
56	D8	1	Total 1	Mg 1	0	0
56	DG	1	Total 1	Mg 1	0	0
56	B9	1	Total 1	Mg 1	0	0
56	BF	8	Total 8	Mg 8	0	0
56	AV	1	Total 1	Mg 1	0	0
56	BX	1	Total 1	Mg 1	0	0
56	B2	1	Total 1	Mg 1	0	0
56	AA	221	Total 221	Mg 221	0	0
56	BQ	5	Total 5	Mg 5	0	0
56	CQ	1	Total 1	Mg 1	0	0
56	CX	3	Total 3	Mg 3	0	0
56	DV	4	Total 4	Mg 4	0	0
56	AM	1	Total 1	Mg 1	0	0
56	BU	8	Total 8	Mg 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DR	2	Total 2	Mg 2	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BN	6	Total 6	Mg 6	0	0
56	CT	1	Total 1	Mg 1	0	0
56	D0	1	Total 1	Mg 1	0	0
56	BG	4	Total 4	Mg 4	0	0
56	BY	1	Total 1	Mg 1	0	0
56	DE	6	Total 6	Mg 6	0	0
56	B3	3	Total 3	Mg 3	0	0
56	BR	4	Total 4	Mg 4	0	0
56	DA	653	Total 653	Mg 653	0	0
56	DW	2	Total 2	Mg 2	0	0
56	B7	4	Total 4	Mg 4	0	0
56	CF	1	Total 1	Mg 1	0	0
56	BV	4	Total 4	Mg 4	0	0
56	DO	1	Total 1	Mg 1	0	0
56	BO	1	Total 1	Mg 1	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	DY	1	Total 1	Mg 1	0	0
56	D5	2	Total 2	Mg 2	0	0
56	BD	12	Total 12	Mg 12	0	0

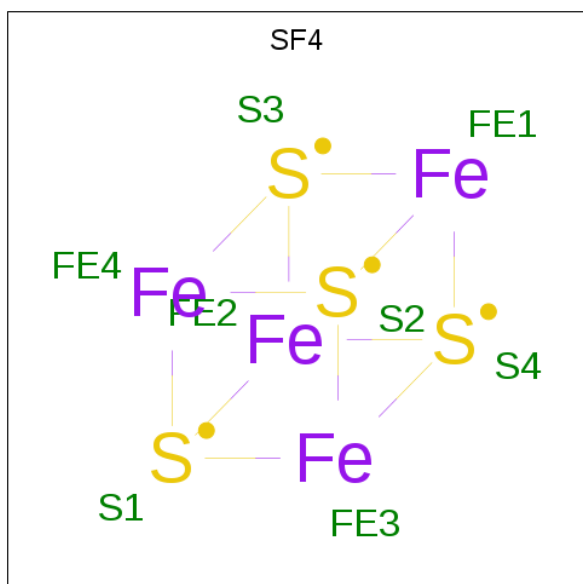
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B0	4	Total	Mg	0	0
			4	4		
56	CE	2	Total	Mg	0	0
			2	2		
56	BW	5	Total	Mg	0	0
			5	5		
56	DD	8	Total	Mg	0	0
			8	8		
56	AF	1	Total	Mg	0	0
			1	1		
56	DB	12	Total	Mg	0	0
			12	12		

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula:  $\text{Zn}$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	B5	1	Total	Zn	0	0
			1	1		

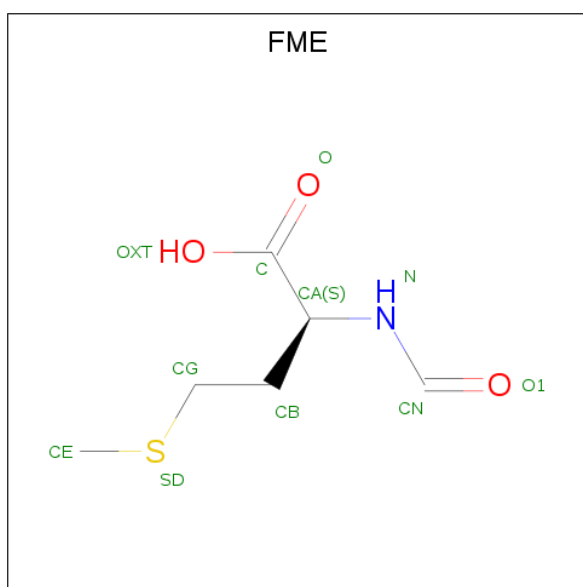
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	B4	1	Total	Zn	0	0
			1	1		
58	CN	1	Total	Zn	0	0
			1	1		
58	BY	1	Total	Zn	0	0
			1	1		
58	B9	1	Total	Zn	0	0
			1	1		
58	DY	1	Total	Zn	0	0
			1	1		
58	D5	1	Total	Zn	0	0
			1	1		
58	D4	1	Total	Zn	0	0
			1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

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula:  $C_6H_{11}NO_3S$ ).





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

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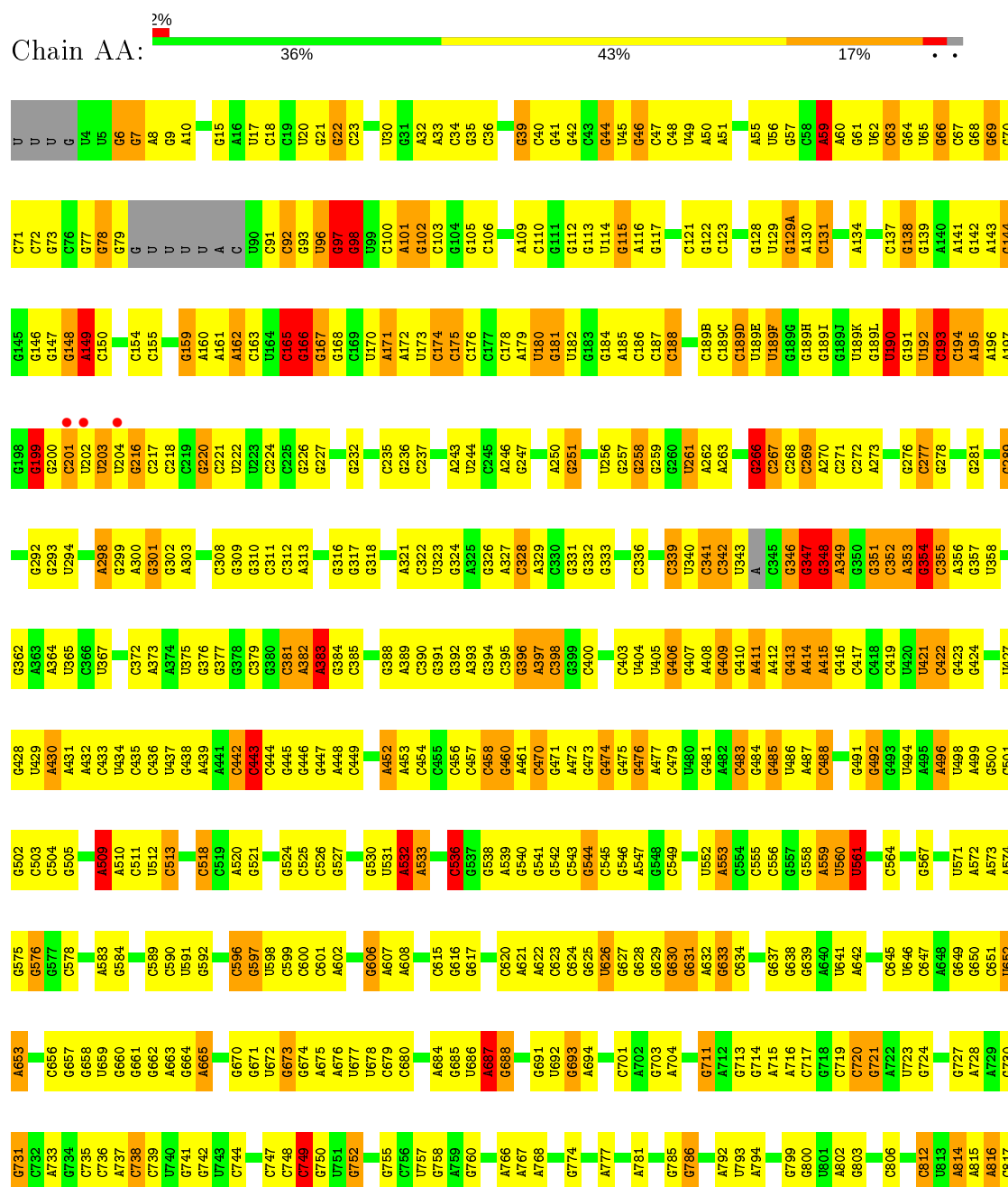
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DA	902	Total 902	O 902	0	0
61	DB	7	Total 7	O 7	0	0
61	DD	8	Total 8	O 8	0	0
61	DE	13	Total 13	O 13	0	0
61	DF	5	Total 5	O 5	0	0
61	DO	1	Total 1	O 1	0	0
61	DP	14	Total 14	O 14	0	0
61	DQ	3	Total 3	O 3	0	0
61	DU	4	Total 4	O 4	0	0
61	DV	1	Total 1	O 1	0	0
61	DX	2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



### 3 Residue-property plots

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

- Molecule 1: 16S Ribosomal RNA



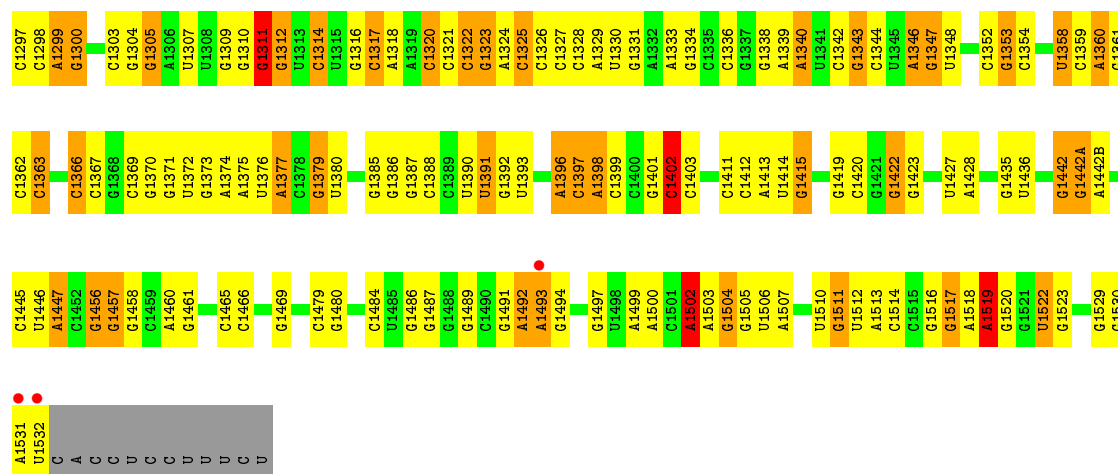




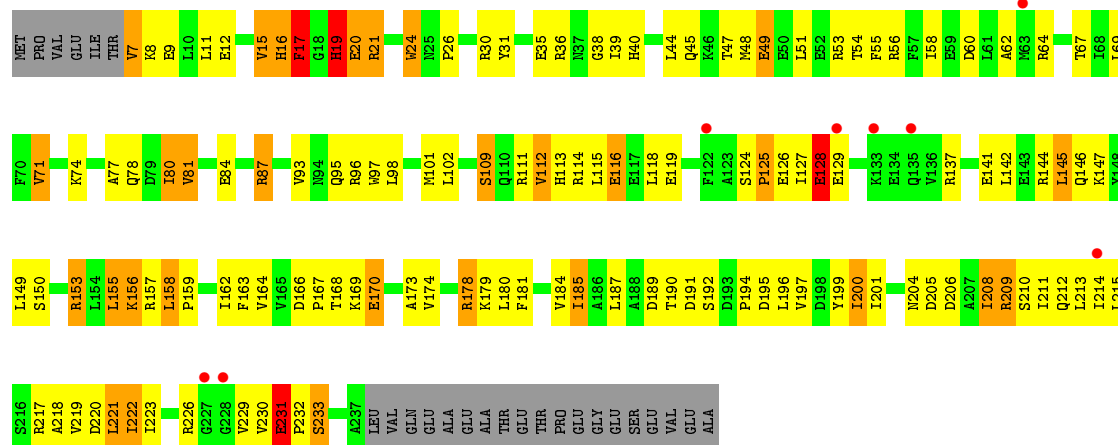


C1228	A1168	A1105	A1041	C985	A919	C834	G752	C680	A608	G538	C454	G388	C308	U223
A1169	A1168	G1106	G1042	A986	U920	U835	A753	G683	A609	A539	C455	A389	C308	
C1234	G1171	C1107	C1043	C989	U921	G836	G754	G684	G610	G540	C456	C390	G316	G226
U1235	C1172	C1109	A1044	C990	G922	G837	G755	A684	G615	G541	C457	G391	G316	G227
C1237	G1173	A1110	G1047	U991	A923	U838	G756	G686	G616	G542	C458	G392	A321	U228
A1238	G1174	A1111	G1048	U992	C924	U839	G757	U686	G616	C543	G460	A393	C322	A229
C1239	A1175	C1112	C1051	G993	G925	C840	G758	A687	A461	G544	C461	G396	C322	
A1240	G1176	C1113	U1052	U994	G926	U841	G759	G688	U619	C545	C470	U323	G232	G232
G1241	G1177	C1114	U1053	C995	G927	C848	A759	G689	C620	G546	C471	A397	C324	C233
C1242	A1178	C1115	U1054	A996	G928	C849	A760	G690	A621	C547	A472	C398	C234	C234
C1243	A1179	C1116	C1055	U997	C931	U850	A761	G691	A622	G399	G473	C399	C235	C235
C1244	A1180	C1117	U1055	G998	C932	G851	A768	U692	C623	U551	G474	C400	C327	G236
A1245	G1181	C1118	U1056	C999	C933	G855	G769	G693	C624	U552	C475	C401	C328	C237
C1246	G1182	G1120	G1057	U1000	G934	G858	G774	A694	G625	A553		G402	A329	
	A1183	U1121	G1058	A1001	C935	G859	G775	C701	U626	C554	G484	C403	C330	A243
C1249	G1184	U1122	C1059	G1001A	G936	A859	A776	A704	G627	C555	G485	U404	C331	U244
A1250	G1185	A1123	C1060	G1002	A937	A860	A777	U705	G628	C556	U486	U405	G332	C245
A1251	G1186	G1124	G1061	G1003	A938	G861		A706	G629	C557	A487	G406	G333	A246
A1252	G1187	U1125	U1062	A1004	G939	G861		G706	G630	G558	C488	G407		G247
	A1188	U1126	C1063	A1005	C940	A865		A707	G631	G559	A488	A408	C337	
C1253	G1189	C1127	U1064	C1006	G941	G868	G786	G708	A632	U560	C489	A409	A338	A250
G1254	C1190	G1128	U1065	C1007	G942	C868	G786	G709	G633	U561	G490	G410	C339	G251
U1257	A1191	C1129	C1066	G1008	G947	G869	A790	G710	G635	A563	G493	A411	C340	U252
G1258	C1192	A1130	A1067	C1009	C948	A872	G791	A712		C564	U494	A412	C341	U253
C1259	G1193	G1131	G1068	G1010		A873	G791	A713	G638	U565	A495	A414	C342	G254
A1261	U1194	C1132	C1069	G1011		A874	G792	G713	G639	A496		A415	U343	G255
C1262	U1196	G1133	U1070	G1012	G951	G874	U793	G714	G640	G568		C345	A344	
C1263	G1197	G1134	C1071	G1013	U952	C875	A794	A715	U641	G569		G346		G258
C1264	C1198	U1135	G1072	G953	U953	G876		A716	A642	U571	C501	C418	G347	U261
U1265	U1199	U1136	U1073	G954	G954	G877	G797	G719	U646	A572	G502	C422	G350	A262
G1266	C1200	C1137	G1074	U955	U955	G878	G798	G720	C647	A573	C503	C423	G351	A263
C1267	A1201	G1138	C1075	U956	U956	C879	G799	G721	G648	G576	C504	G424	C352	U264
A1268	G1202	C1139	U1076	U957	A958	C880	G800	A722	G649	G577	G505	G425	C353	G265
C1269	C1203	C1141	U1077	U959	C882	G881	U801	A723	G650	C578	G426	G426	G354	G266
U1270	A1204	G1142	U1078	A959	C882	G882	G802	G724	C651	A509	U427	G428	C355	C268
G1271	U1205	G1143	G1079	U960	G885	G885	U804	G725	U652	A510	G429	G428		C269
C1272	U1206	G1144	A1080	U961		G885	C805	C726	A653	C511	U429	U429	U358	A270
G1273	G1207	G1145	G1081	A964		G890	C806	G727	A654	C512	A430	A431	U359	C271
G1274	C1208	A1146	U1085	A965		U891			A655	C513	A432	A432		
U1278	C1209	C1147	U1086	G966		A892	C812	G731	C656	C518	C433	C433	A363	G276
A1279	C1210	U1149	U1087	A968		C893	U813	G732		C519	U434	U434	A364	C277
U1280	U1211	U1150	G1088	A969		G894	A814	A733	G660	C519	C435	C435	U365	G281
A1281	U1212	U1151	U1089	C970		C899	A815	A734	G661	C520	C436	U437	U367	A282
C1282	C1213	A1152	G1090	G971		A900	A816	G735	A662	G521	U437	C372	C372	C283
G1283	G1214	C1153	U1091	C972		A901	C817	C736	G664	C522	G438	C373	A373	G284
C1284	G1215	G1154	G1092	G973		G902	G818	A737	A665	U591	A439	A439	A374	U287
U1285	C1217	G1155	A1093	A974		G906		C738	G666	C525	A441	A441	A374	U287
A1286	C1218	G1156	U1094	A975		A907	G821	C739	G667	G527	C442	C442	U375	A288
A1287	U1219	A1157	U1095	G976		A908	C826	U740		C528	C443	C443	G376	G289
A1288	G1220	C1158	A978	A977		A908	U827	G741	G671	U531	G444	G444	G377	G292
A1289	C1221	U1159	G1034	A978		A908	U828	G742	U672	U598	G445	G445	G380	G293
G1290	C1160	G1160	A1035	C979		A913	A828		A532	C599	G446	G446	C381	
C1291	C1161	C1162	G1036	C980		A914	G829	C745	G673	C600	A533	G447	A382	G297
U1292	G1224	C1163	U1037	U981		A915	G830		G674	C601	U534	A448	G383	A298
C1293	A1225	A1102	C1038	U982		G916	U831	C749	U677	G606	A452		A384	G299
	A1227	C1103	G1103	A932		G917	U833	U751	U678	G332	A453		G384	A300
		G1104	A918	A918					C679	A607	G537			

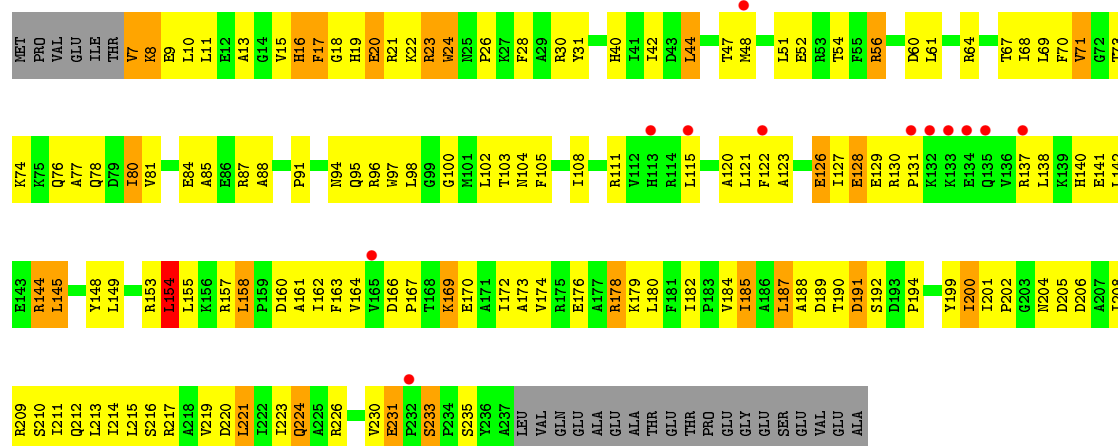




### • Molecule 2: 30S Ribosomal Protein S2

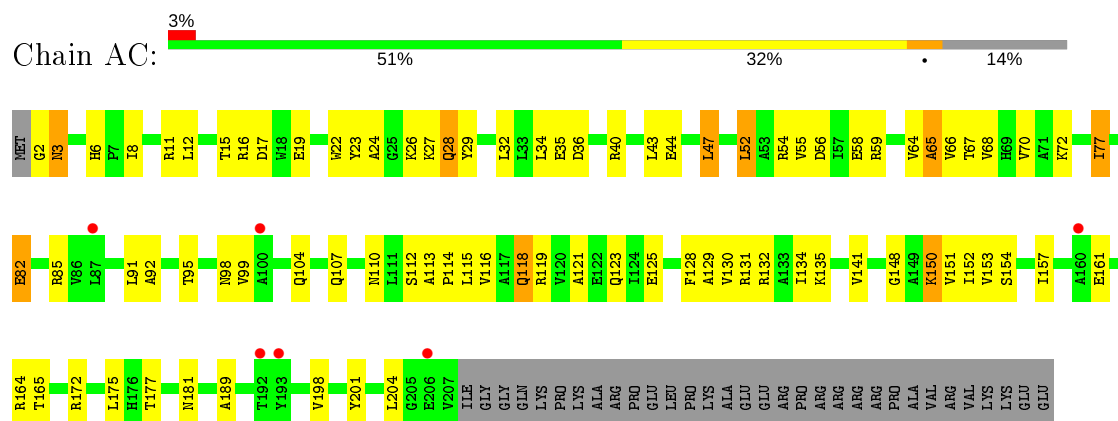


### • Molecule 2: 30S Ribosomal Protein S2

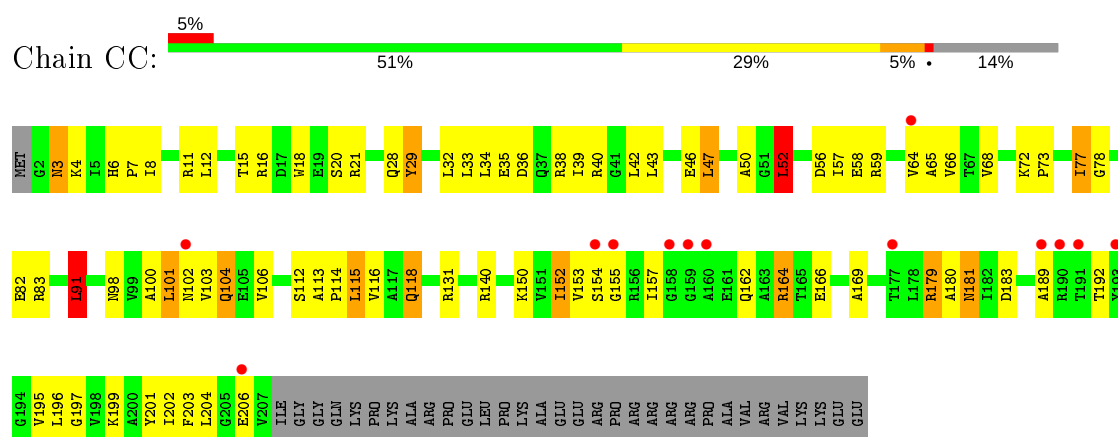




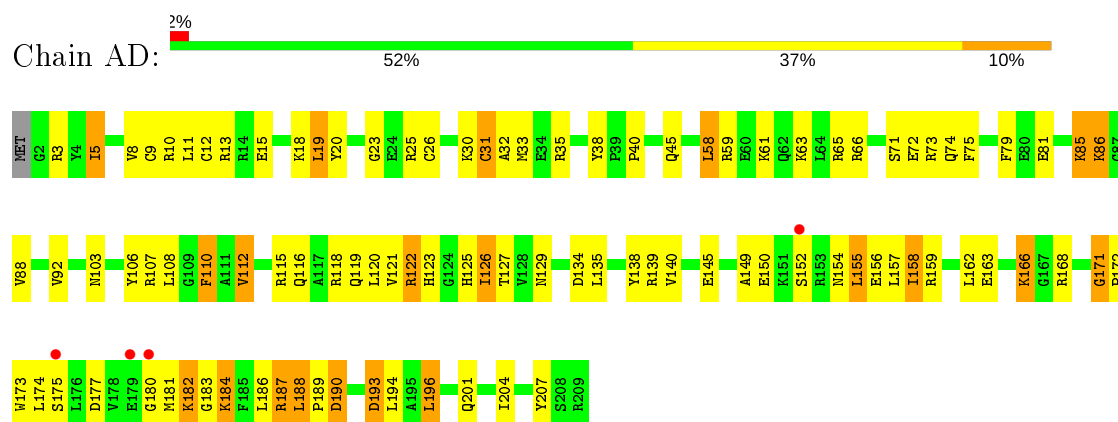
- Molecule 3: 30S Ribosomal Protein S3



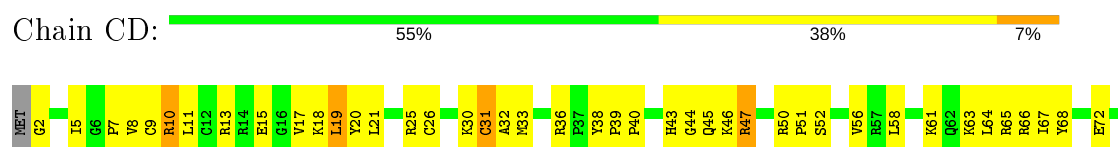
- Molecule 3: 30S Ribosomal Protein S3



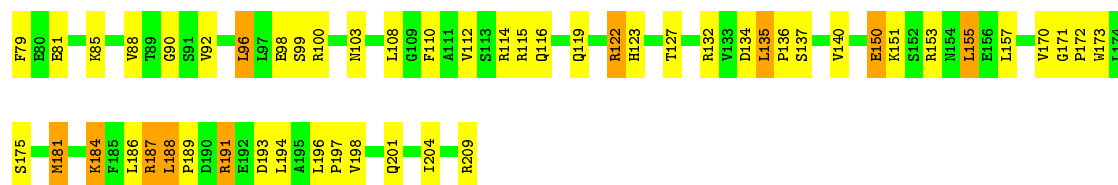
- Molecule 4: 30S Ribosomal Protein S4



- Molecule 4: 30S Ribosomal Protein S4

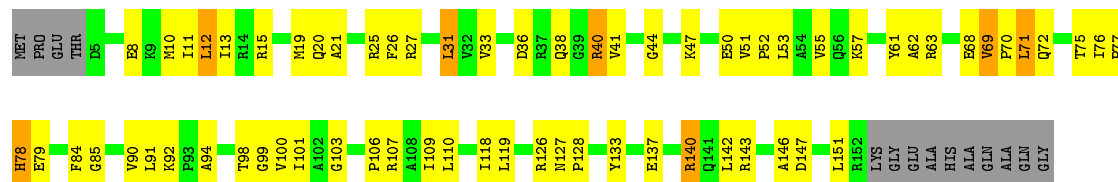






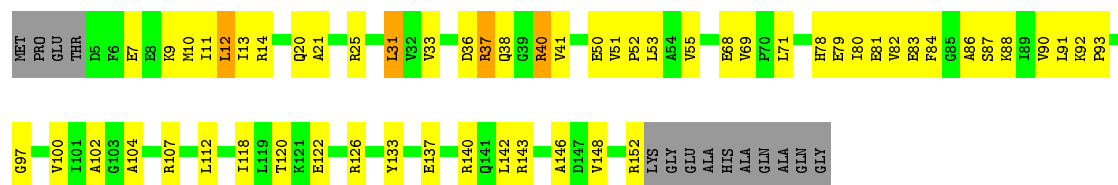
• Molecule 5: 30S Ribosomal Protein S5

Chain AE:



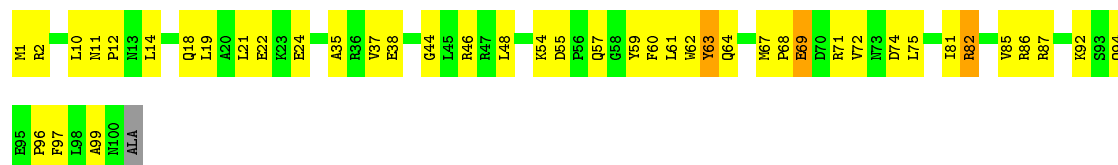
• Molecule 5: 30S Ribosomal Protein S5

Chain CE:



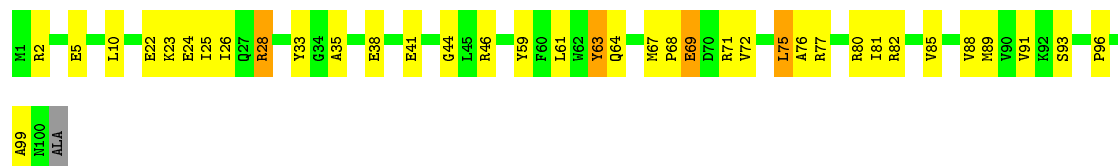
• Molecule 6: 30S Ribosomal Protein S6

Chain AF:



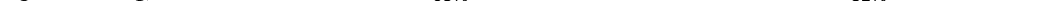
• Molecule 6: 30S Ribosomal Protein S6

Chain CF:

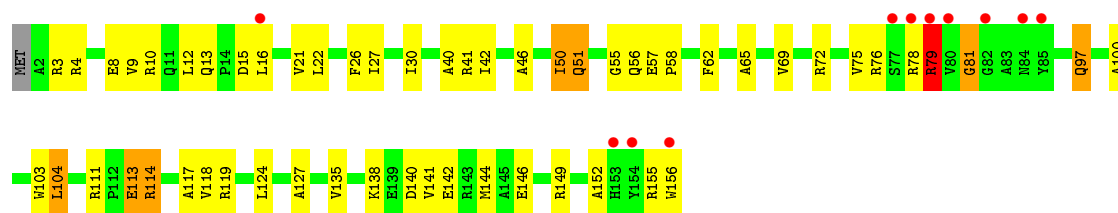


• Molecule 7: 30S Ribosomal Protein S7

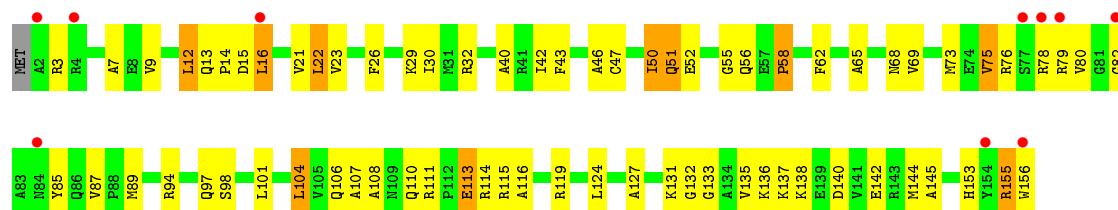
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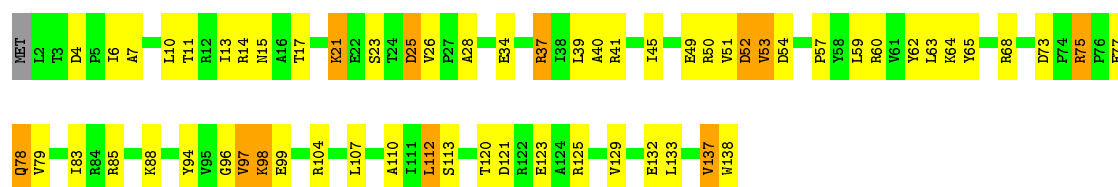




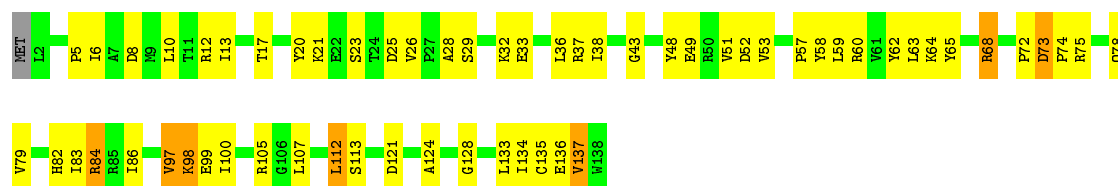
• Molecule 7: 30S Ribosomal Protein S7



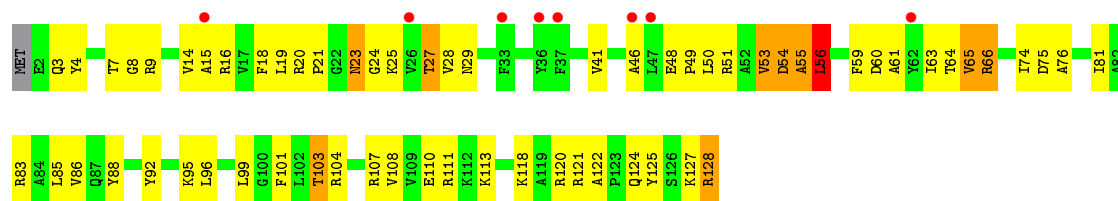
• Molecule 8: 30S Ribosomal Protein S8



• Molecule 8: 30S Ribosomal Protein S8

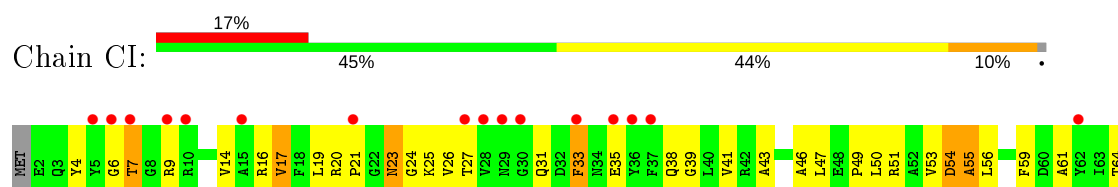


• Molecule 9: 30S Ribosomal Protein S9

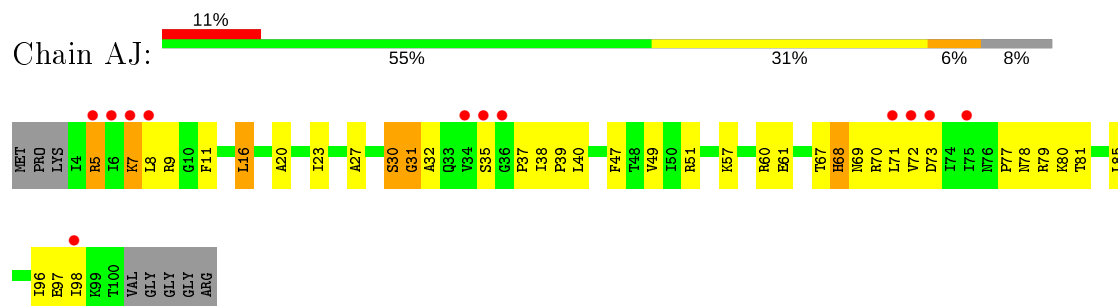


• Molecule 9: 30S Ribosomal Protein S9

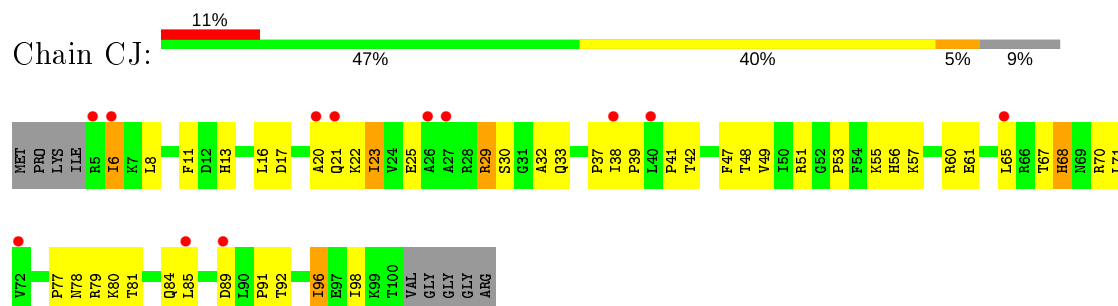




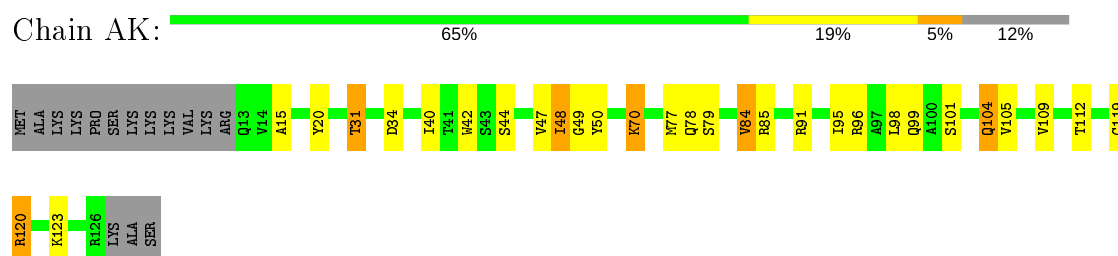
- Molecule 10: 30S Ribosomal Protein S10



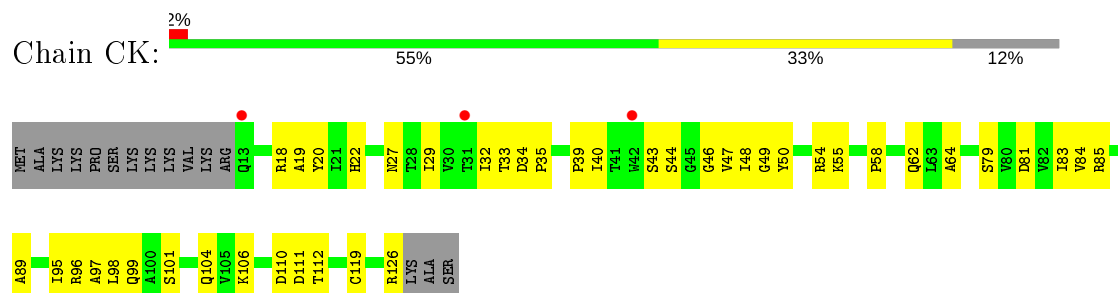
- Molecule 10: 30S Ribosomal Protein S10



- Molecule 11: 30S Ribosomal Protein S11

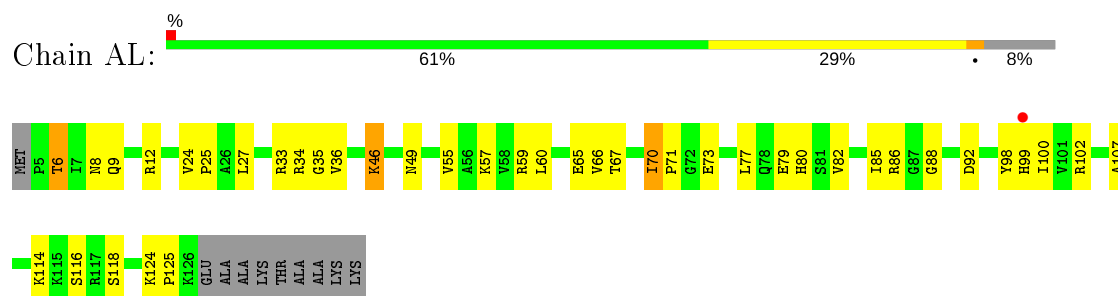


- Molecule 11: 30S Ribosomal Protein S11

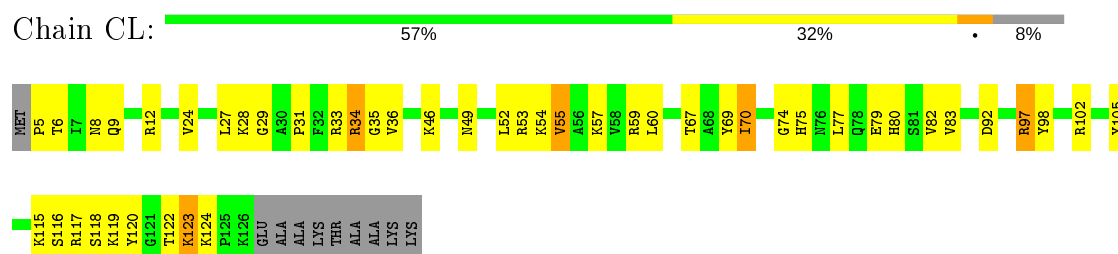




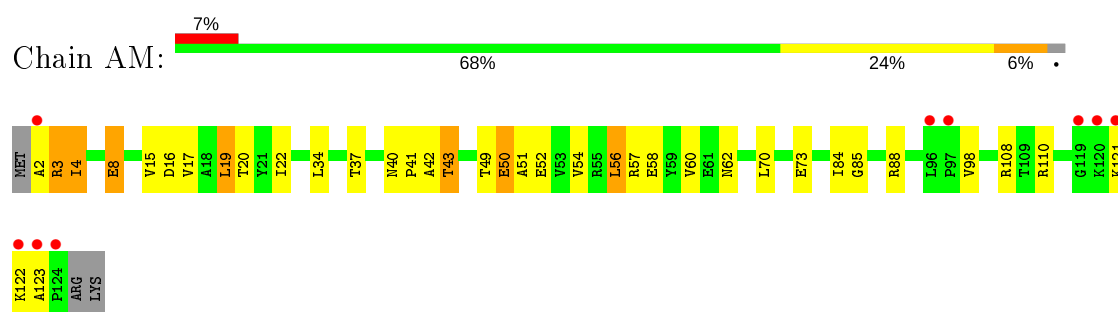
- Molecule 12: 30S Ribosomal Protein S12



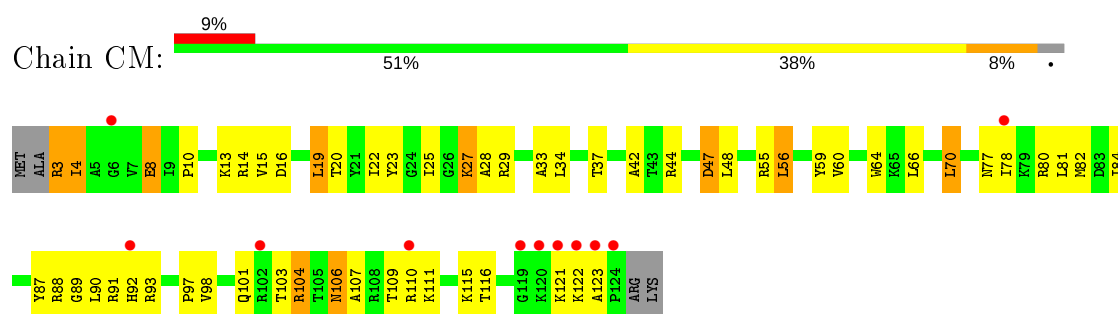
- Molecule 12: 30S Ribosomal Protein S12



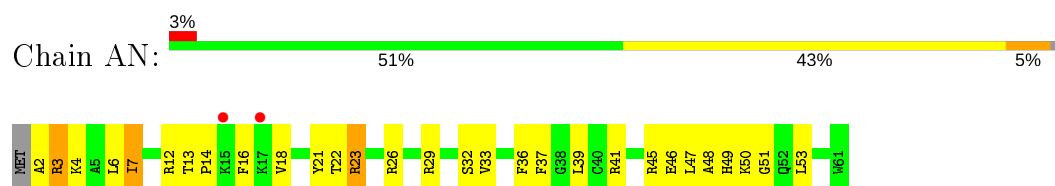
- Molecule 13: 30S Ribosomal Protein S13



- Molecule 13: 30S Ribosomal Protein S13

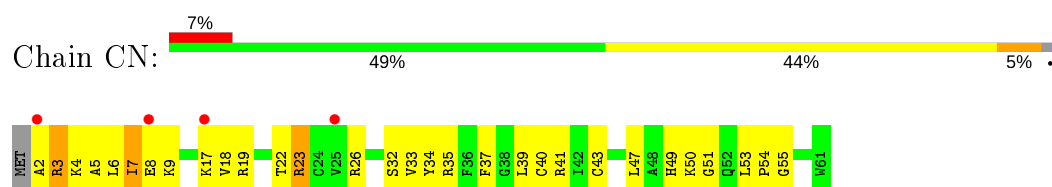


- Molecule 14: 30S Ribosomal Protein S14

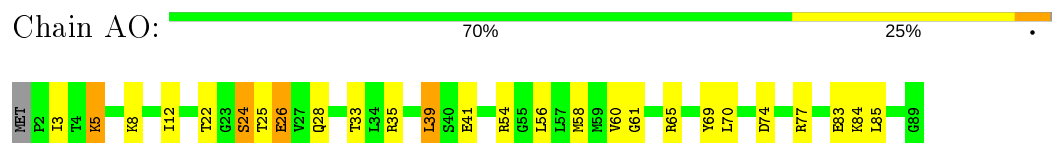


- Molecule 14: 30S Ribosomal Protein S14

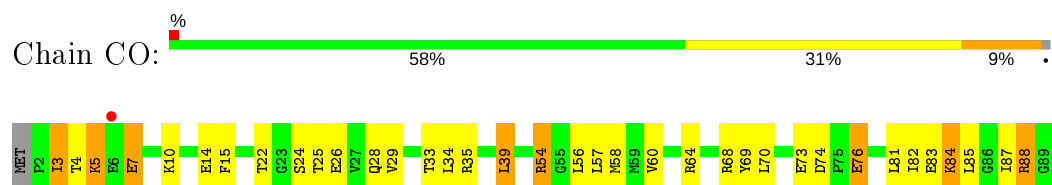




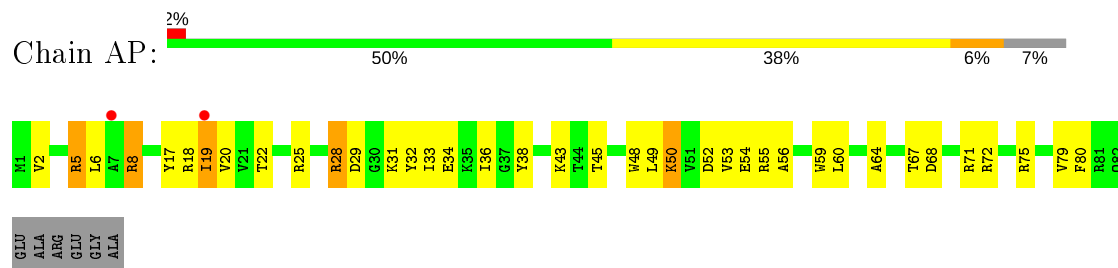
• Molecule 15: 30S Ribosomal Protein S15



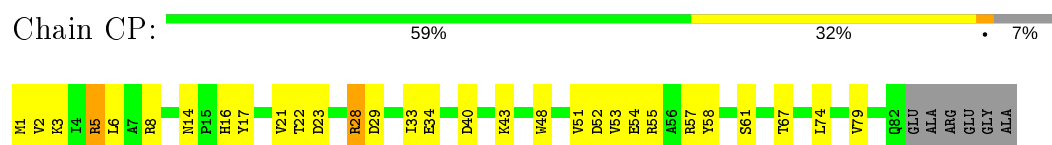
• Molecule 15: 30S Ribosomal Protein S15



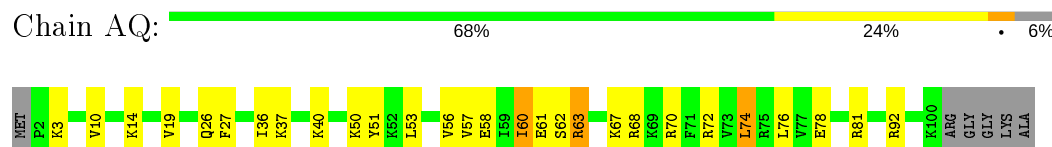
• Molecule 16: 30S Ribosomal Protein S16



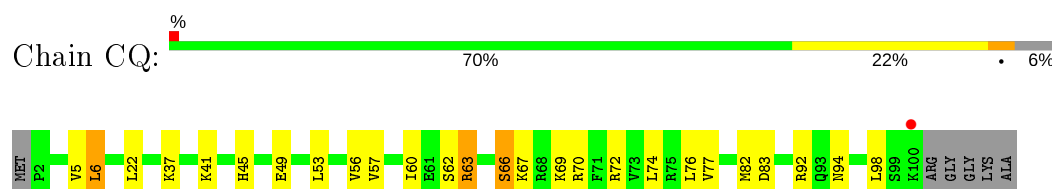
• Molecule 16: 30S Ribosomal Protein S16



• Molecule 17: 30S Ribosomal Protein S17



• Molecule 17: 30S Ribosomal Protein S17





MET	SER	THR	ASN	ALA	PRO	LYS	LYS	GLU	ALA	GLN	ARG	ARG	PRO	SER	ARG	LYS	A20	L26	G27	F28	D30	L31	R32	R35	L40	K41	R42	K49	L50	L51	P52	S59	K60	K61	E62	T69	I70	G77	L78	T82	R87	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

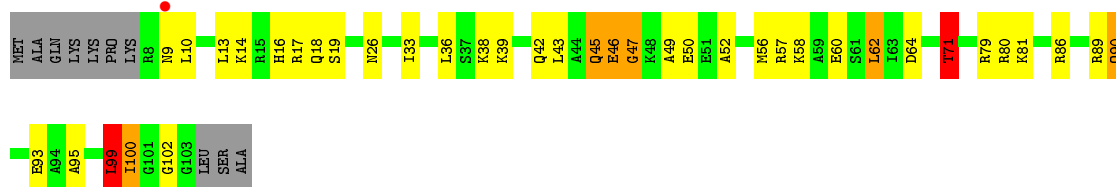
The diagram illustrates a network of protein interactions. A central column of proteins is flanked by two large groups of proteins. The proteins are color-coded: red for specific proteins (e.g., G72, E73, F74, R78, G84, LYS, GLU, ALA, LYS, THR, LYS, LYS, E27, K28, R29, L30, I31, R36, R37, S38, T39, I40, V41, V42, E43, E47, T48, I49, A50, V51, Y52, S53, G54, K55, Q56, S57, V58, P59, V60, Y61, T62, T63, E64, K65, V66, V67, K70, T71), green for others (e.g., P2, R3, S4, S5, L5, K6, R7, G8, V9, F10, V11, D12, L15, V19, L20, E21, L22, M23, R39, L40, V41, V42, E43, E47, T48, I49, A50, V51, Y52, S53, G54, K55, Q56, S57, V58, P59, V60, Y61, T62, T63, E64, K65, V66, V67, K70, T71), yellow for others (e.g., P2, R3, S4, S5, L5, K6, R7, G8, V9, F10, V11, D12, L15, V19, L20, E21, L22, M23, R39, L40, V41, V42, E43, E47, T48, I49, A50, V51, Y52, S53, G54, K55, Q56, S57, V58, P59, V60, Y61, T62, T63, E64, K65, V66, V67, K70, T71), and grey for others (e.g., P2, R3, S4, S5, L5, K6, R7, G8, V9, F10, V11, D12, L15, V19, L20, E21, L22, M23, R39, L40, V41, V42, E43, E47, T48, I49, A50, V51, Y52, S53, G54, K55, Q56, S57, V58, P59, V60, Y61, T62, T63, E64, K65, V66, V67, K70, T71).

The diagram illustrates a sequence of amino acids from H69 to V67. The sequence is as follows:

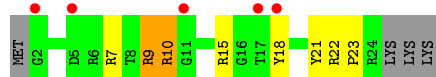
H69 (red dot), K70 (grey), L71 (orange), G72 (green), E73 (yellow), F74 (yellow), A75 (yellow, red dot), T79 (yellow, red dot), Y80 (yellow), H83 (yellow), G94 (green), LNS (yellow), GLU (yellow), ALA (yellow), LYS (grey), ALA (grey), THR (grey), LNS (grey), LNS (grey), E27 (yellow), K28 (orange, red dot), R29 (orange), L30 (orange), I31 (yellow), K32 (yellow), T33 (orange), Q34 (yellow, red dot), S35 (yellow), R36 (yellow), R37 (yellow), S38 (yellow, red dot), V41 (yellow), P42 (yellow), E43 (orange, red dot), M44 (green), H47 (yellow, red dot), T48 (yellow, red dot), I49 (green, red dot), A50 (yellow), Y51 (yellow), Y52 (yellow), N53 (yellow, red dot), G54 (yellow), A55 (yellow), Q56 (yellow), H57 (yellow), P59 (yellow), V60 (green), Y61 (yellow), T62 (yellow), T63 (orange), E64 (yellow), V67 (yellow, red dot).

[illegible]





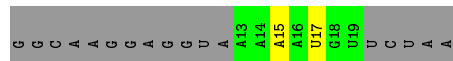
• Molecule 21: 30S Ribosomal Protein THX



• Molecule 21: 30S Ribosomal Protein THX



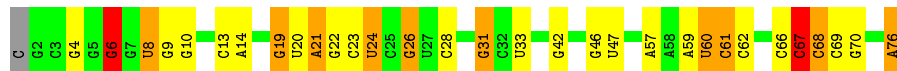
• Molecule 22: mRNA



• Molecule 22: mRNA



• Molecule 23: P-site tRNA



• Molecule 23: P-site tRNA



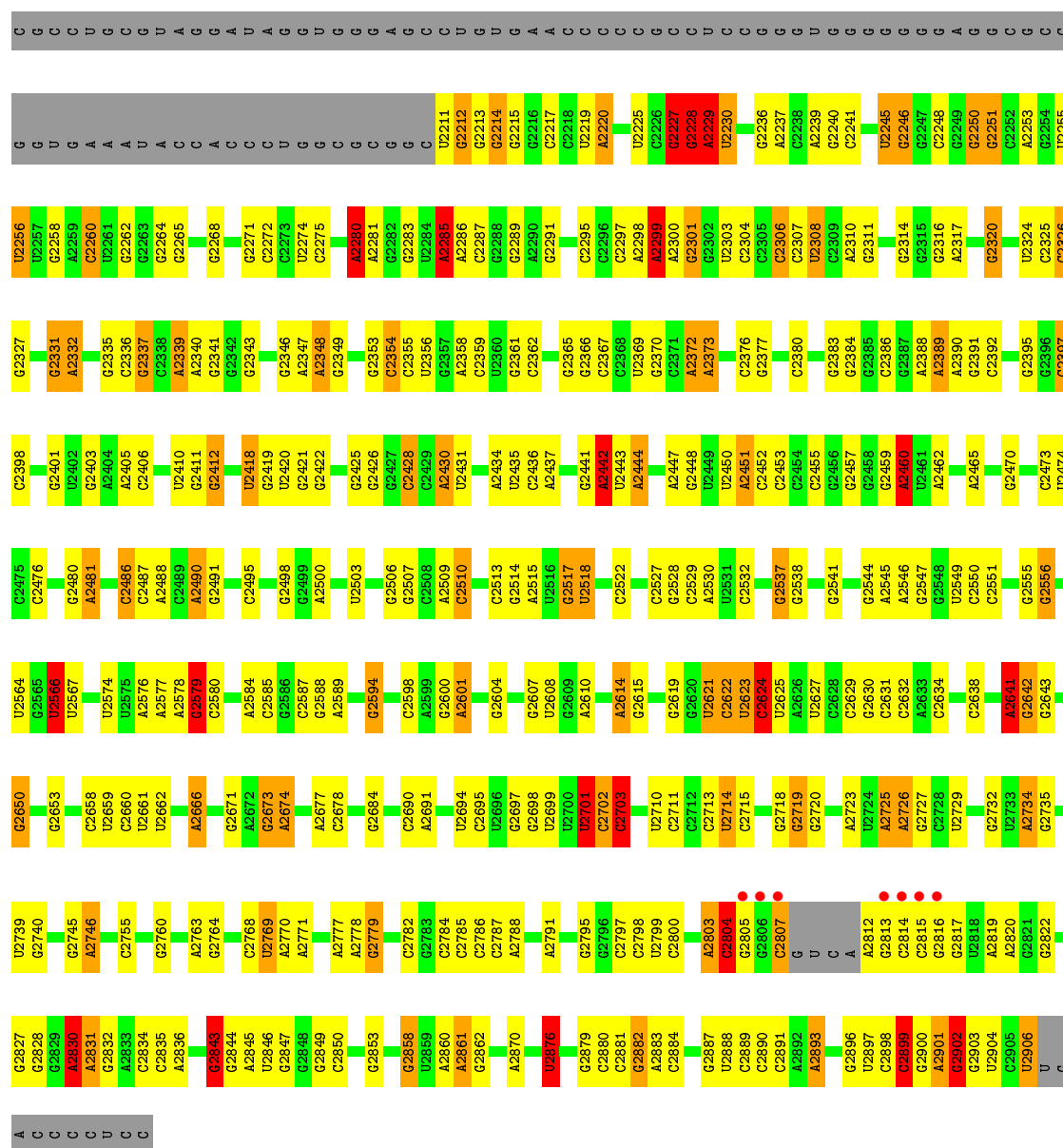




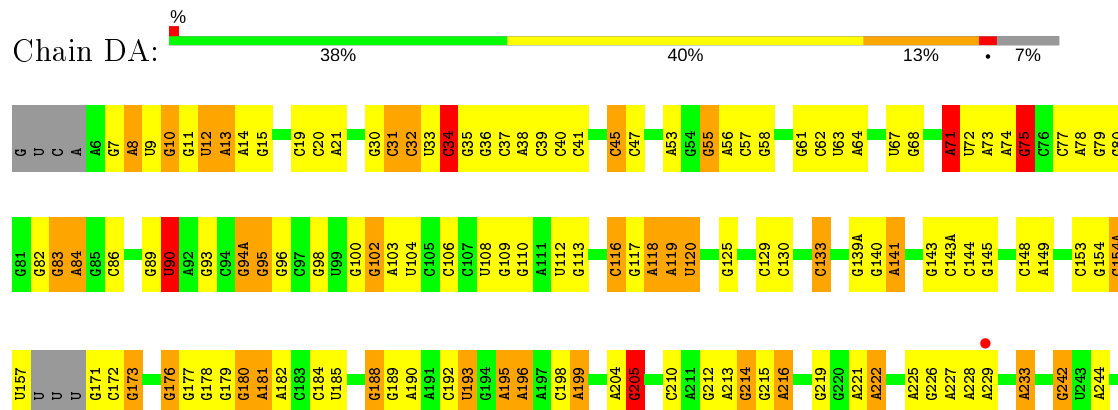


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G2059	G2060	A1959	C1858	G1787	C1707	A1614	G1529	A1430	A1347	G1248	G1156	A1096	G1019	A937	A851
G2061	G2062	A1960	A1860	G1708	G1709	G1615	G1530	C1432	G1356	A1249	G1158	C1098	C1020	C938	G852
C2063	C2064	C1963	G1870	A1791	G1710	A1617	A1536	U1440	U1359	C1252	G1168	C	G1024	C940	U857
A2065	U1977	U1977	G1871	G1792	A1711	A1618	G1537	A1441	C1360	A1255	G1171	G	A1029	U941	U858
C2066	C2067	U1985	C1874	A1793	A1712	U1625	A1539	U1442	C1361	U1256	A1174	G	A1030	A942	U859
C2067	C2067	A1986	A1878	G1795	A1715	G1628	A1540	C1444	A1363	C1263	A1175	G	C1032	C943	U860
G2070	G2071	C1987	A1879	G1800	A1716	G1629	A1541	G1454	C1366	A1265	U1176	U	A1034	A947	G864
G2074	G2074	A1988	U1882	A1804	A1717	A1630	A1542	G1459	A1367	C1266	G1177	G	G1035	C948	G865
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C2077	C2077	A1991	U1890	G1807	C1722	A1633	U1548	G1462	G1374	G1284	A1182	U	A1042	U951	U873
G2078	G2078	A1992	U1897	U1808	A1724	G1640	C1550	G1463	G1377	G1285	A1183	U	G1043	A956	U874
A2080	A2080	A1993	A1898	U1809	G1725	G1647	C1551	G1464	A1377	C1286	C1185	A	C1044	C945	U875
A2081	A2081	A1994	U1899	U1810	U1735	U1648	C1552	A1465	G1378	U1286	U1186	G	U1045	A946	A876
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C2087	C2087	U2013	C1908	A1816	U1740	A1654	A1556	C1472	G1384	C1297	G1195	G	C1054	G974	A882
C2088	C2088	U2014	C1908	A1817	G1742	A1655	A1557	A1473	G1385	G1297	G1195	C	A1055	C977	U886
G2091	G2091	U2015	A1911	A1818	G1743	A1656	C1559	G1475	U1387	A1299	C1199	C	A1055	A978	G892
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C2095	C2095	G1914	U1825	U1825	A1747	A1662	U1568	A1483	C1391	C1304	C1207	U	U1065	A986	A896
U2096	U2096	A1914	G1826	G1826	A1748	A1664	U1569	G1487	G1394	A1308	G1210	U	A1066	G987	G902
U2101	U2101	G1919	U1827	U1827	G1749	G1665	U1574	A1491	A1395	A1311	U1211	A	A1067	C903	G903
G2102	G2102	A1920	G1828	G1828	G1750	G1666	A1575	A1496	G1402	U1313	G1216	G	G1068	C904	C904
C2103	C2103	G1921	U1829	U1829	G1751	U1667	A1576	A1497	U1403	A1314	G1217	G	G1069	U905	U905
A2104	A2104	A1922	G1830	G1830	G1752	G1668	C1577	A1497	G1404	A1315	G1218	U	U1072	G992	A908
G2105	G2105	U1753	U1831	U1831	U1753	G1668	C1578	A1496	A1405	A1316	G1219	U	A1073	C994	G909
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C2107	C2107	G1758	G1833	G1833	G1758	G1680	G	A1496	G1410	A1320	G1221	G	G1075	C911	G911
U2108	U2108	C1759	A1834	A1834	C1759	A1681	U	A1500	A1412	A1321	A1222	U	G1076	A998	C912
G2109	G2109	U1760	U1835	U1835	U1760	C1682	A	U1501	A1412	A1321	C1223	A	A1077	G999	U918
C2110	C2110	U1765	U1836	U1836	U1765	C1683	C	G1502	A1416	A1324	C1224	U	U1079	G1001	U918
G2115	G2115	A1766	A1843	A1843	A1766	U1686	G1584	G1503	G1417	A1325	G1225	A	G1080	A1002	G922
G2116	G2116	A1767	G1844	G1844	A1767	C1687	G1588	G1504	U1418	G1326	G1229	G	G1085	U1003	G926
C2117	C2117	U1768	G1845	G1845	U1768	A1688	A1589	G1505	A1418	G1327	G1230	C	C1086	A1004	G927
U2118	U2118	G1769	A1846	A1846	G1769	G1689	C1590	G1506	G1417	U1338	G1231	U	C1087	C1006	G928
C2119	C2119	A1770	G1847	G1847	A1770	G1689	A1591	G1507	U1418	U1339	G1232	U	G1088	G1007	G929
U2121	U2121	C1775	A1849	A1849	C1775	G1695	A1592	G1513	C1421	U1340	G1233	A	C1089	U1008	G930
C2122	C2122	G1777	U1851	U1851	G1777	G1697	C1597	G1517	C1422	U1341	G1234	C	G1090	C1009	G931
G2123	G2123	A1778	A1852	A1852	A1778	G1698	U1597	G1518	C1423	C1342	A1234	U	A1091	C1010	G932
A2053	A2053	G1779	G1853	G1853	G1779	A1699	C1604	G1519	A1424	C1341	G1240	G	G1092	C1015	G1015
G2054	G2054	A1780	G1854	G1854	A1780	G1700	A1605	G1520	A1425	C1342	G1240	G	A1093	A994	A994
A2055	A2055	G1781	G1855	G1855	G1781	A1701	A1608	G1521	A1426	C1343	C1246	U	G1152	G1017	G935
U2056	U2056	C1782	A1702	A1702	C1782	A1702	G1608	G1522	G1426	C1343	C1246	U	U1154	G1017	G935





• Molecule 25: 23S Ribosomal RNA



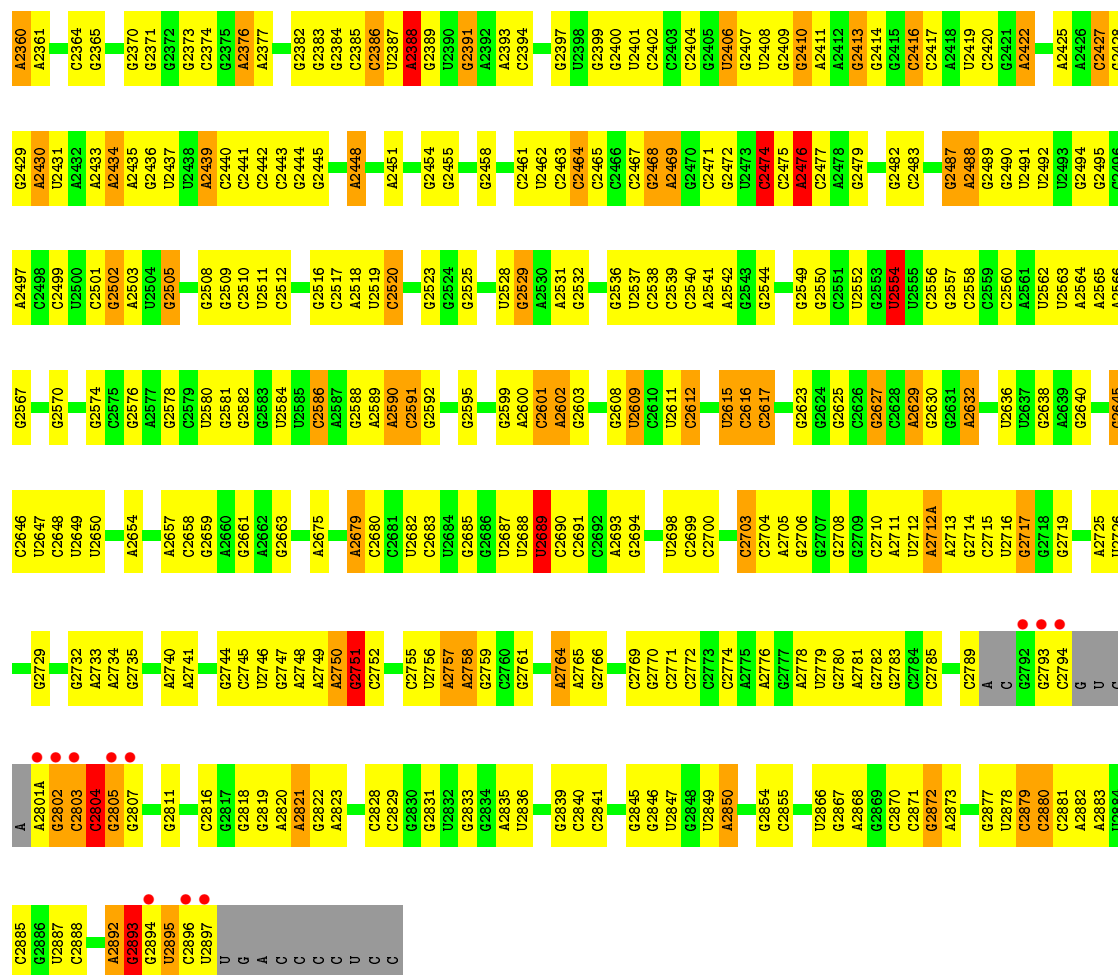






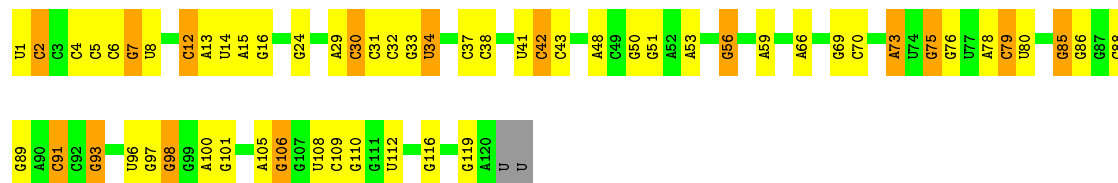






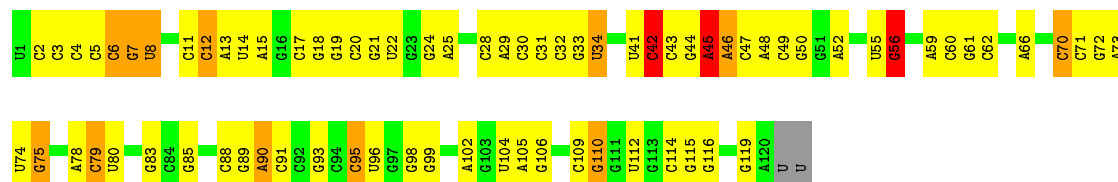
• Molecule 26: 5S Ribosomal RNA

Chain BB: 51% 35% 12%



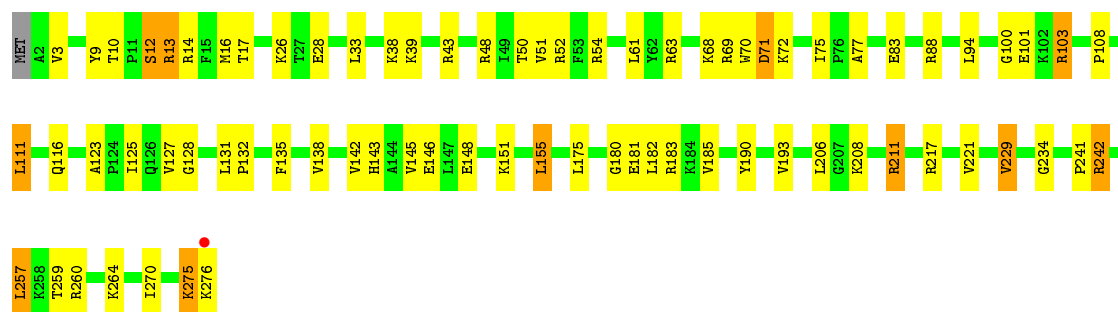
• Molecule 26: 5S Ribosomal RNA

Chain DB: 36% 50% 10%



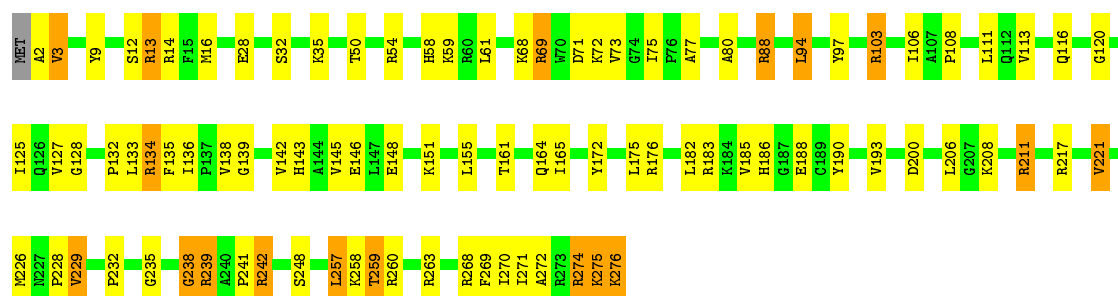


Chain BD: 



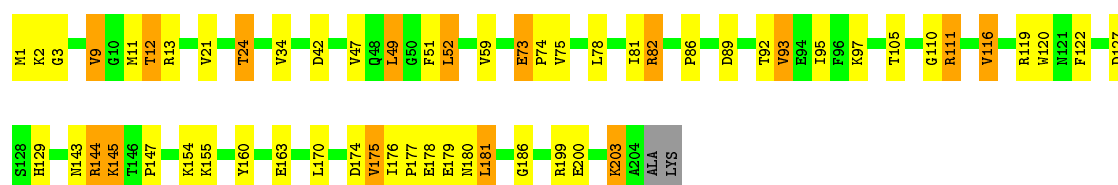
• Molecule 27: 50S Ribosomal Protein L2

Chain DD: 



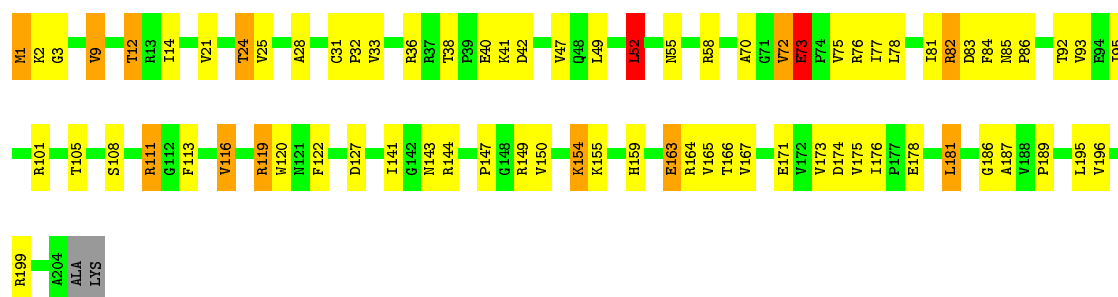
• Molecule 28: 50S Ribosomal Protein L3

Chain BE: 



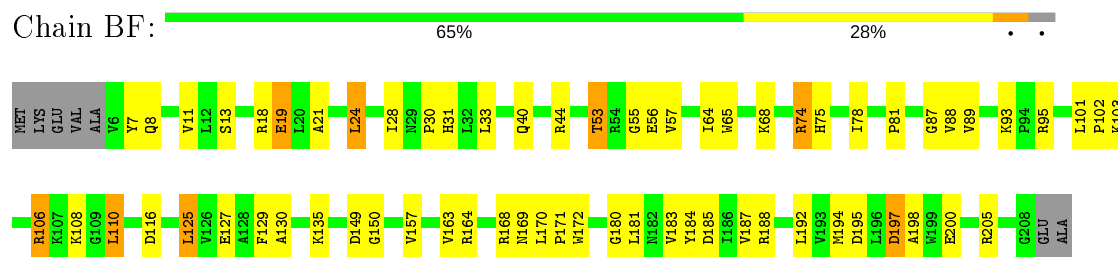
• Molecule 28: 50S Ribosomal Protein L3

Chain DE: 

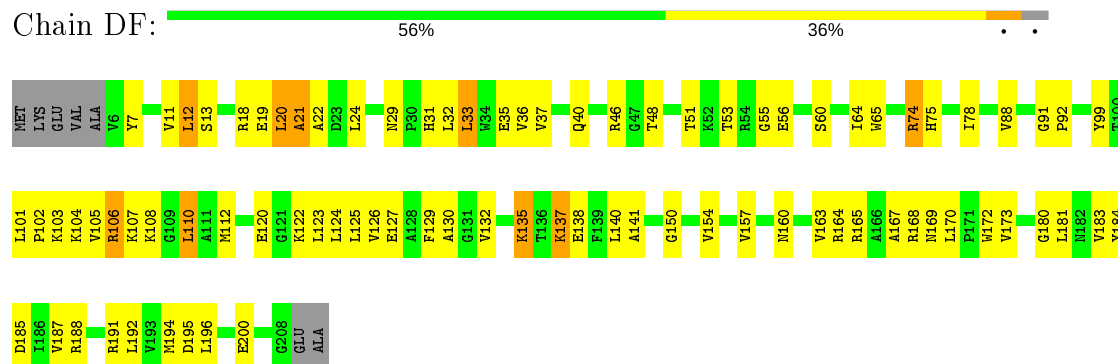


• Molecule 29: 50S Ribosomal Protein L4

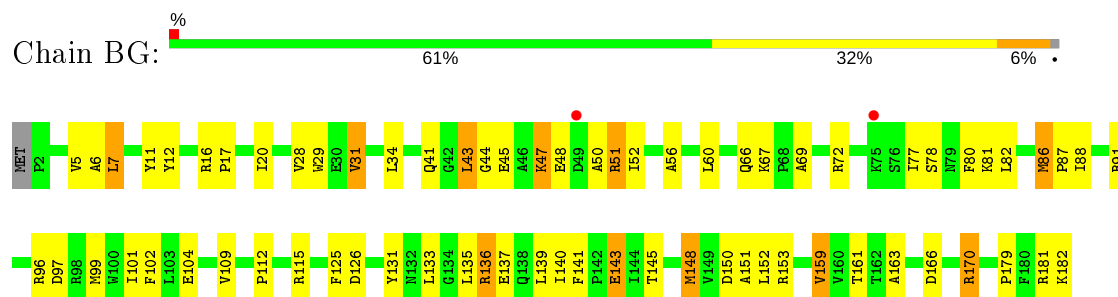




• Molecule 29: 50S Ribosomal Protein L4



• Molecule 30: 50S Ribosomal Protein L5



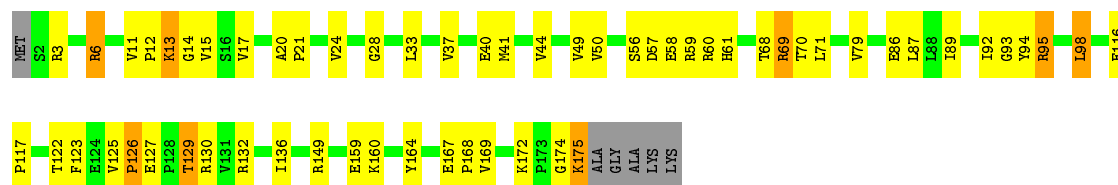
• Molecule 30: 50S Ribosomal Protein L5



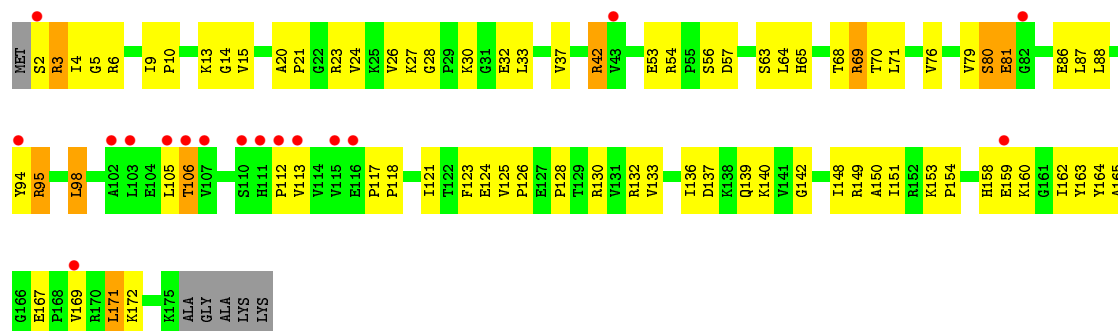
• Molecule 31: 50S Ribosomal Protein L6



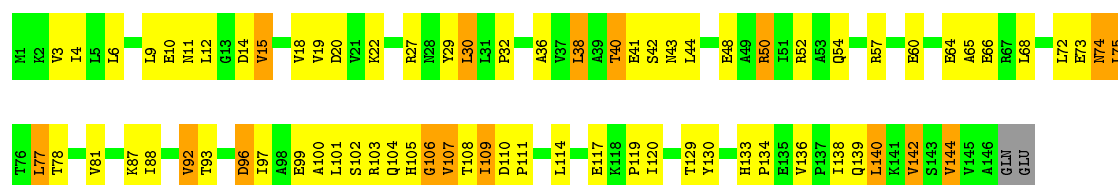




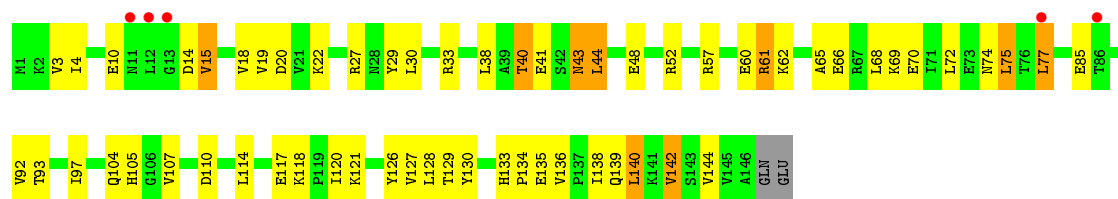
• Molecule 31: 50S Ribosomal Protein L6



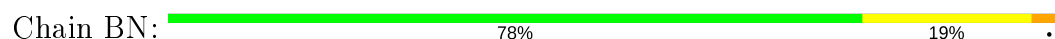
• Molecule 32: 50S Ribosomal Protein L9



• Molecule 32: 50S Ribosomal Protein L9



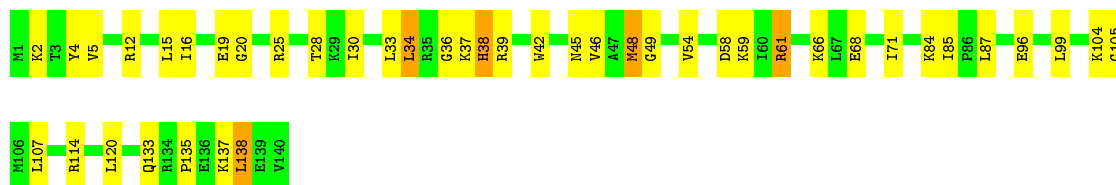
• Molecule 33: 50S Ribosomal Protein L13



• Molecule 33: 50S Ribosomal Protein L13



Chain DN:  69% 27% .



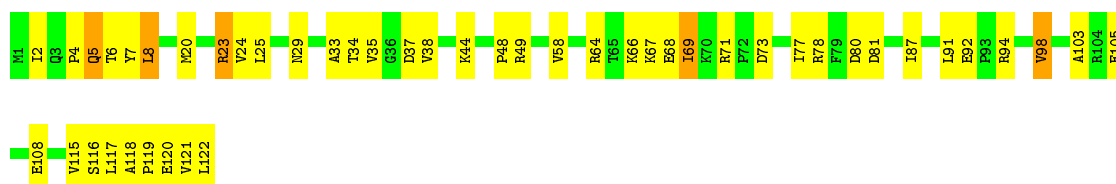
- Molecule 34: 50S Ribosomal Protein L14

Chain BO:  72% 25% ..



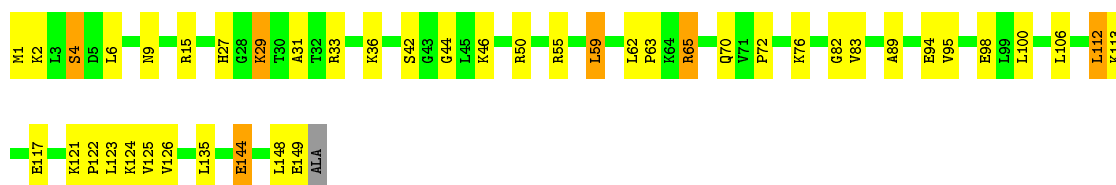
- Molecule 34: 50S Ribosomal Protein L14

Chain DO:  61% 34% .



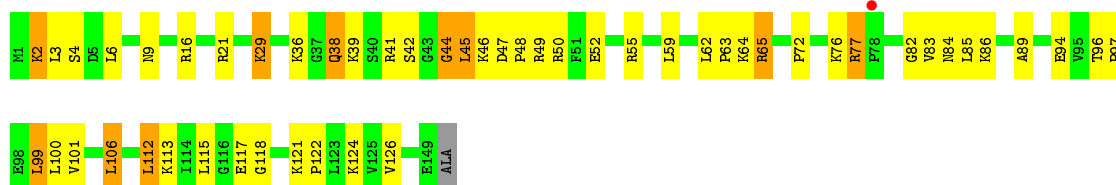
- Molecule 35: 50S Ribosomal Protein L15

Chain BP:  70% 25% ..



- Molecule 35: 50S Ribosomal Protein L15

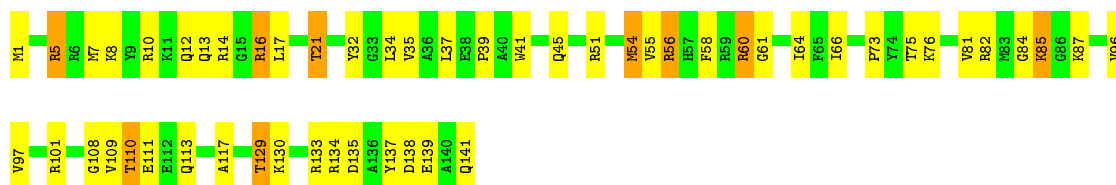
Chain DP:  65% 28% 7% .



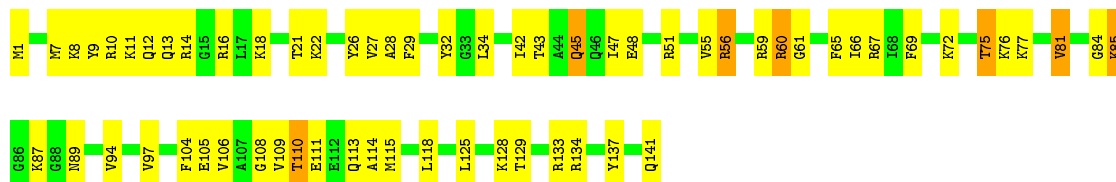
- Molecule 36: 50S Ribosomal Protein L16

Chain BQ:  62% 31% 6%





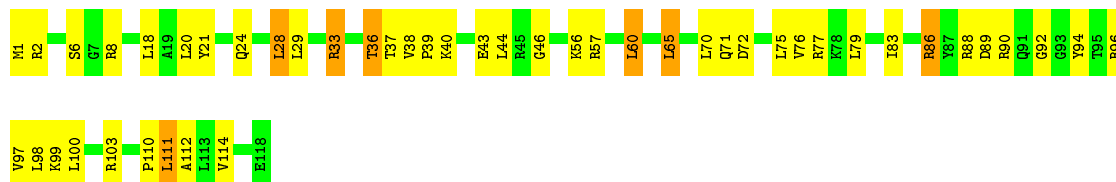
• Molecule 36: 50S Ribosomal Protein L16



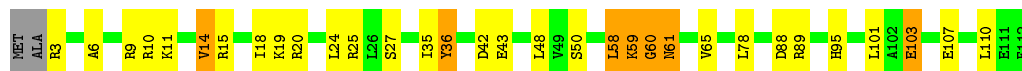
• Molecule 37: 50S Ribosomal Protein L17



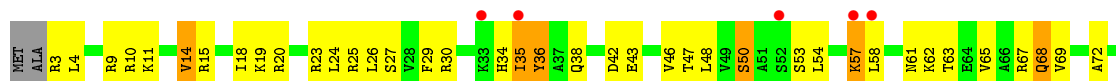
• Molecule 37: 50S Ribosomal Protein L17



• Molecule 38: 50S Ribosomal Protein L18



• Molecule 38: 50S Ribosomal Protein L18

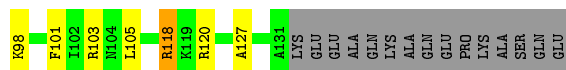
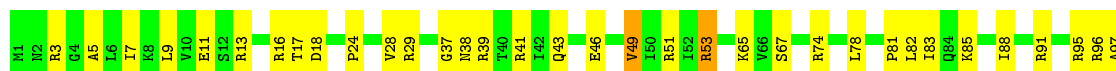






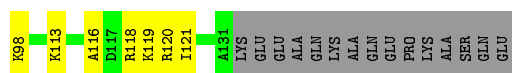
• Molecule 39: 50S Ribosomal Protein L19

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% 5%



• Molecule 40: 50S Ribosomal Protein L20

Chain DU: 66% 27% 5%



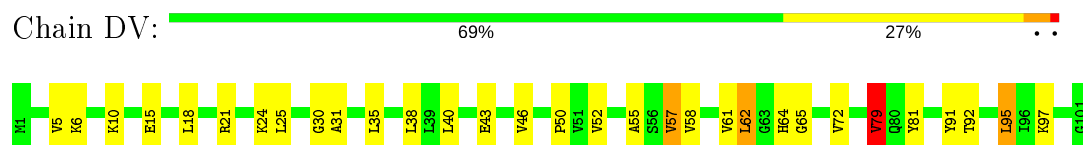
• Molecule 41: 50S Ribosomal Protein L21

Chain BV: 81% 14% 5%

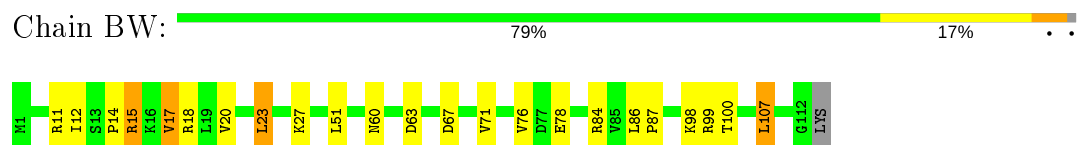




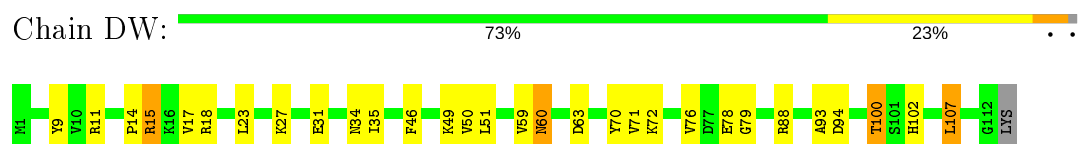
- Molecule 41: 50S Ribosomal Protein L21



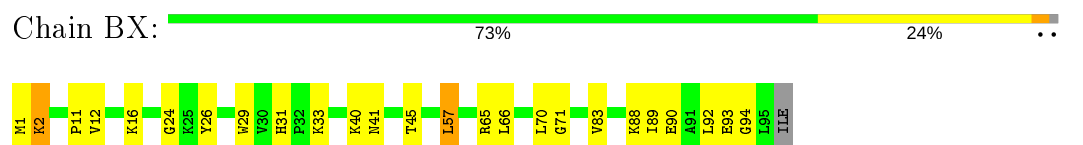
- Molecule 42: 50S Ribosomal Protein L22



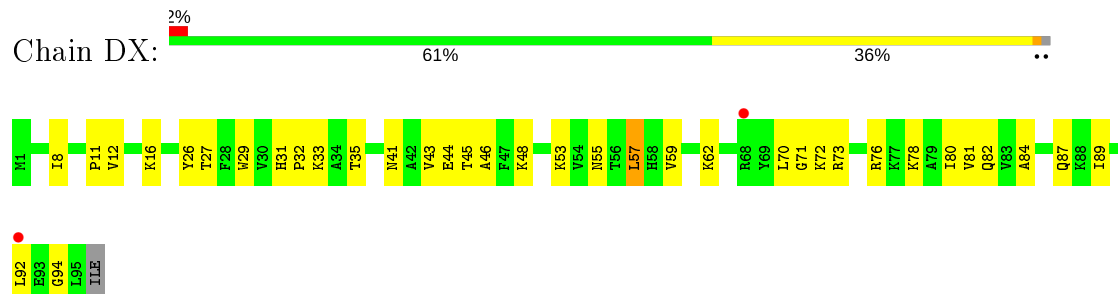
- Molecule 42: 50S Ribosomal Protein L22



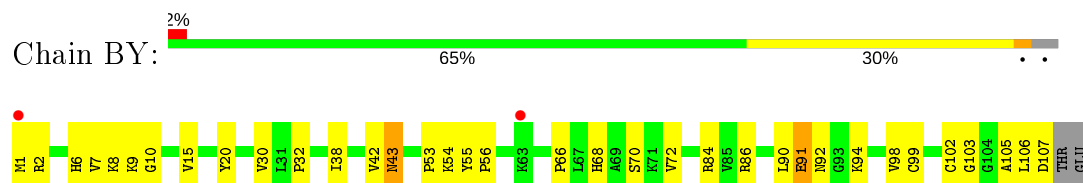
- Molecule 43: 50S Ribosomal Protein L23



- Molecule 43: 50S Ribosomal Protein L23



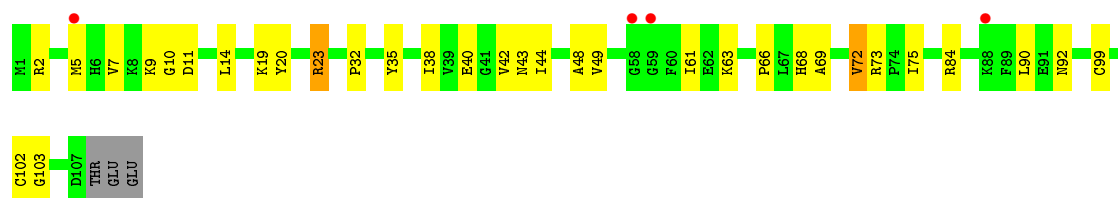
- Molecule 44: 50S Ribosomal Protein L24



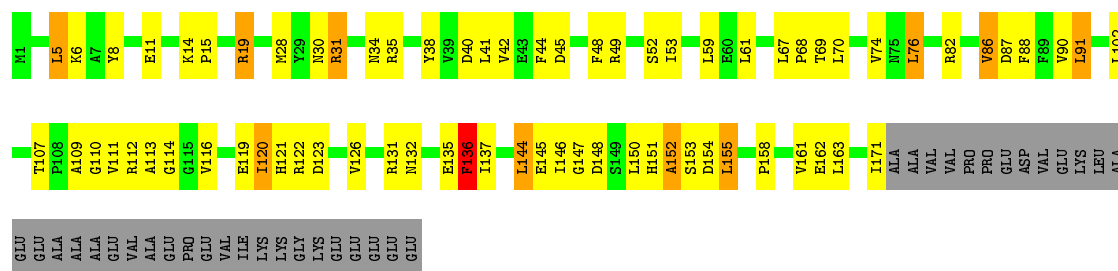
- Molecule 44: 50S Ribosomal Protein L24



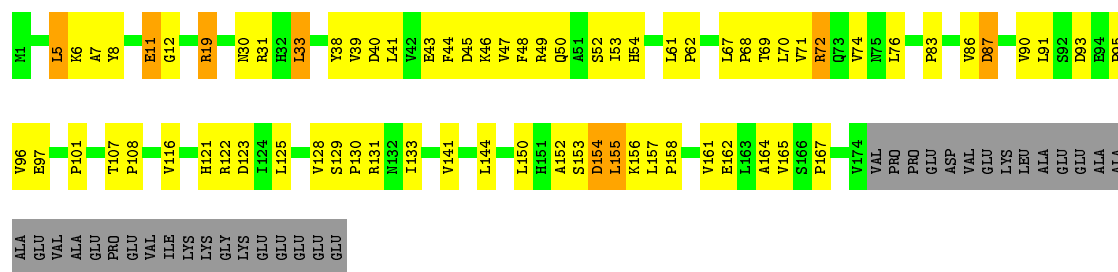




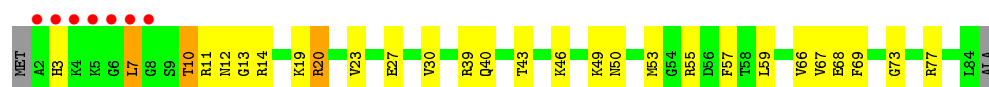
- Molecule 45: 50S Ribosomal Protein L25



- Molecule 45: 50S Ribosomal Protein L25



- Molecule 46: 50S Ribosomal Protein L27



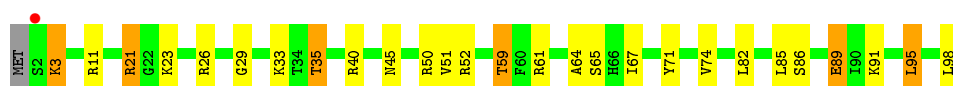
- Molecule 46: 50S Ribosomal Protein L27



- Molecule 47: 50S Ribosomal Protein L28



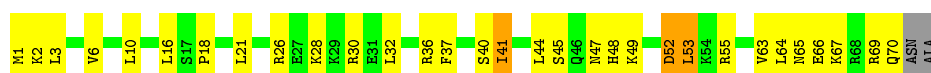




- Molecule 47: 50S Ribosomal Protein L28



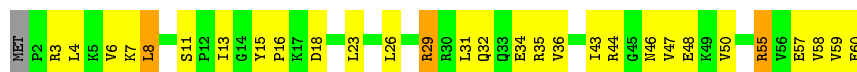
- Molecule 48: 50S Ribosomal Protein L29



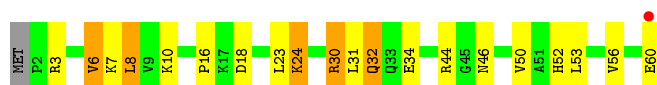
- Molecule 48: 50S Ribosomal Protein L29



- Molecule 49: 50S Ribosomal Protein L30



- Molecule 49: 50S Ribosomal Protein L30



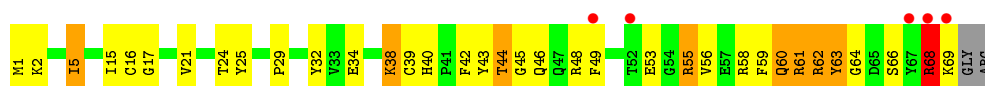
- Molecule 50: 50S Ribosomal Protein L31



- 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



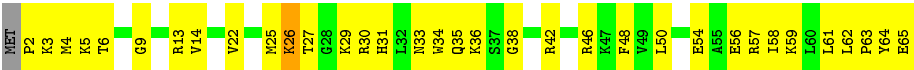
- Molecule 54: 50S Ribosomal Protein L35



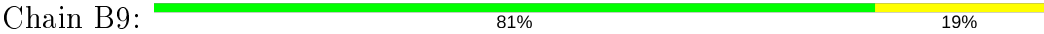




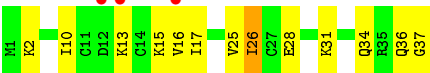
● Molecule 54: 50S Ribosomal Protein L35



● 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)	Xtriage
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	Xtriage
Anisotropy	0.077	Xtriage
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>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	286321	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage'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 ⓘ

### 5.1 Standard geometry ⓘ

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

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 ⓘ

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 ⓘ

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
45	BZ	87	ASP
3	CC	154	SER
42	DW	51	LEU
46	B0	55	ARG
53	B7	1	MET

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

Mol	Chain	Res	Type
44	BY	43	ASN
3	CC	28	GLN
37	DR	71	GLN
45	BZ	32	HIS
49	B3	32	GLN

### 5.3.3 RNA ⓘ

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	BA	2623	U
1	CA	560	U
25	DA	1790	C
25	BA	2763	A
1	CA	97	G

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

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	2R3	CW	8	24	-	7/11/12/14	0/1/1/1
24	MVA	CW	5	24	-	6/6/8/10	-
24	MVA	AW	9	24	-	5/6/8/10	-
24	2QZ	AW	1	24	-	3/6/10/12	-
24	MVA	CW	9	24	-	5/6/8/10	-
24	2QY	AW	10	24	-	3/4/8/10	0/1/1/1
24	2R1	AW	6	24	-	1/2/14/16	0/1/1/1
24	2R3	AW	8	24	-	4/11/12/14	0/1/1/1
24	MVA	AW	5	24	-	3/6/8/10	-
24	2QZ	CW	1	24	-	2/6/10/12	-
24	004	CW	3	24	-	0/4/6/8	0/1/1/1
24	2R1	CW	6	24	-	0/2/14/16	0/1/1/1
24	2QY	CW	10	24	-	2/4/8/10	0/1/1/1
24	004	AW	3	24	-	0/4/6/8	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	CW	8	2R3	N-CA-CB-OB
24	CW	8	2R3	N-CA-CB-CG
24	CW	8	2R3	C-CA-CB-OB
24	CW	8	2R3	C-CA-CB-CG
24	CW	5	MVA	N-CA-CB-CG1

There are no ring outliers.

13 monomers are involved in 23 short contacts:

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



## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z  > 2$
57	SF4	CD	501	4	0,12,12	0.00	-	-		
59	FME	CX	101	23	8,9,10	1.05	1 (12%)	7,9,11	1.32	2 (28%)
57	SF4	AD	501	4	0,12,12	0.00	-	-		
59	FME	AX	101	23	8,9,10	0.93	0	7,9,11	1.49	1 (14%)

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
57	SF4	CD	501	4	-	-	0/6/5/5
59	FME	CX	101	23	-	3/7/9/11	-
57	SF4	AD	501	4	-	-	0/6/5/5
59	FME	AX	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	CX	101	FME	O1-CN-N-CA
59	CX	101	FME	O-C-CA-CB
59	AX	101	FME	O1-CN-N-CA
59	AX	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
59	CX	101	FME	2	0
57	AD	501	SF4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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, 89, 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, 53, 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 ⓘ

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	9	8/9	0.93	0.24	65,78,87,91	0
24	MVA	AW	5	8/9	0.93	0.19	66,87,90,90	0
24	2R1	CW	6	10/11	0.94	0.11	79,86,90,94	0
24	MVA	CW	5	8/9	0.94	0.20	51,78,86,88	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	3295	1/1	0.40	0.57	75,75,75,75	0
56	MG	BA	3094	1/1	0.40	0.86	61,61,61,61	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	DA	3427	1/1	0.58	0.54	60,60,60,60	0
56	MG	CA	3042	1/1	0.58	0.56	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3464	1/1	0.60	0.56	50,50,50,50	0
56	MG	AA	3114	1/1	0.60	0.51	66,66,66,66	0
56	MG	AA	3079	1/1	0.60	1.07	74,74,74,74	0
56	MG	B4	3001	1/1	0.61	0.27	100,100,100,100	0
56	MG	AA	3116	1/1	0.61	0.53	52,52,52,52	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	BA	3622	1/1	0.65	0.52	77,77,77,77	0
56	MG	DA	3135	1/1	0.65	0.23	50,50,50,50	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	3545	1/1	0.67	0.62	75,75,75,75	0
56	MG	DA	3068	1/1	0.67	0.33	55,55,55,55	0
56	MG	DA	3131	1/1	0.68	0.23	54,54,54,54	0
56	MG	DA	3186	1/1	0.68	0.51	53,53,53,53	0
56	MG	CA	3025	1/1	0.69	0.18	94,94,94,94	0
56	MG	AA	3023	1/1	0.69	0.17	65,65,65,65	0
56	MG	DB	3003	1/1	0.69	0.12	63,63,63,63	0
56	MG	AX	102	1/1	0.69	0.25	74,74,74,74	0
56	MG	CA	3038	1/1	0.69	0.46	70,70,70,70	0
56	MG	DA	3125	1/1	0.69	0.55	48,48,48,48	0
56	MG	DA	3211	1/1	0.69	0.10	51,51,51,51	0
56	MG	CA	3135	1/1	0.70	0.56	76,76,76,76	0
56	MG	DA	3103	1/1	0.70	0.78	48,48,48,48	0
59	FME	CX	101	10/11	0.70	0.57	71,82,97,105	0
56	MG	BA	3579	1/1	0.70	0.24	63,63,63,63	0
56	MG	AA	3084	1/1	0.70	0.36	78,78,78,78	0
56	MG	BA	3235	1/1	0.71	0.28	47,47,47,47	0
56	MG	AA	3048	1/1	0.71	0.25	57,57,57,57	0
56	MG	BA	3270	1/1	0.71	0.31	50,50,50,50	0
56	MG	AA	3044	1/1	0.71	0.22	66,66,66,66	0
56	MG	DA	3581	1/1	0.71	0.86	73,73,73,73	0
56	MG	DA	3117	1/1	0.71	0.17	53,53,53,53	0
56	MG	AA	3128	1/1	0.71	0.20	68,68,68,68	0
56	MG	DA	3223	1/1	0.71	0.26	66,66,66,66	0
56	MG	CA	3030	1/1	0.71	0.45	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	CA	3024	1/1	0.72	0.44	65,65,65,65	0
58	ZN	B4	3002	1/1	0.72	0.07	165,165,165,165	0
56	MG	AA	3037	1/1	0.72	0.41	61,61,61,61	0
56	MG	BA	3703	1/1	0.72	0.22	31,31,31,31	0
56	MG	BA	3263	1/1	0.72	0.23	79,79,79,79	0
56	MG	CA	3067	1/1	0.73	0.30	80,80,80,80	0
56	MG	BF	307	1/1	0.73	0.40	47,47,47,47	0
56	MG	BA	3085	1/1	0.73	0.46	48,48,48,48	0
56	MG	BA	3297	1/1	0.73	1.46	53,53,53,53	0
56	MG	DW	202	1/1	0.73	0.42	58,58,58,58	0
56	MG	BA	3065	1/1	0.73	0.44	50,50,50,50	0
56	MG	CA	3055	1/1	0.73	0.28	62,62,62,62	0
56	MG	BA	3632	1/1	0.73	0.30	57,57,57,57	0
56	MG	AA	3065	1/1	0.73	0.27	60,60,60,60	0
56	MG	AA	3020	1/1	0.73	0.10	77,77,77,77	0
56	MG	BA	3289	1/1	0.73	0.34	60,60,60,60	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	DA	3438	1/1	0.74	0.51	70,70,70,70	0
56	MG	AA	3006	1/1	0.74	0.08	78,78,78,78	0
56	MG	BA	3089	1/1	0.74	0.57	61,61,61,61	0
56	MG	AA	3117	1/1	0.75	0.26	71,71,71,71	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	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	3064	1/1	0.76	0.41	50,50,50,50	0
56	MG	AA	3035	1/1	0.76	0.42	71,71,71,71	0
56	MG	DA	3410	1/1	0.76	0.22	69,69,69,69	0
56	MG	DA	3056	1/1	0.76	0.37	43,43,43,43	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	3228	1/1	0.76	0.25	45,45,45,45	0
56	MG	CA	3018	1/1	0.76	0.31	54,54,54,54	0
56	MG	BA	3075	1/1	0.76	0.26	45,45,45,45	0
56	MG	DA	3123	1/1	0.76	0.23	59,59,59,59	0
56	MG	BA	3206	1/1	0.76	0.35	57,57,57,57	0
56	MG	AA	3090	1/1	0.77	0.17	68,68,68,68	0
56	MG	DA	3587	1/1	0.77	0.14	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AX	108	1/1	0.77	0.21	61,61,61,61	0
56	MG	AA	3051	1/1	0.77	0.50	73,73,73,73	0
56	MG	AA	3120	1/1	0.77	0.63	71,71,71,71	0
56	MG	DA	3098	1/1	0.78	1.25	43,43,43,43	0
56	MG	BA	3087	1/1	0.78	0.45	61,61,61,61	0
56	MG	AA	3063	1/1	0.78	0.30	61,61,61,61	0
56	MG	BA	3241	1/1	0.78	0.38	63,63,63,63	0
56	MG	DA	3615	1/1	0.78	0.40	60,60,60,60	0
56	MG	AA	3100	1/1	0.78	0.67	40,40,40,40	0
56	MG	AA	3096	1/1	0.78	0.28	44,44,44,44	0
56	MG	AA	3127	1/1	0.78	0.18	62,62,62,62	0
56	MG	AA	3088	1/1	0.78	0.33	63,63,63,63	0
56	MG	BA	3160	1/1	0.78	0.65	53,53,53,53	0
56	MG	BA	3718	1/1	0.78	0.37	57,57,57,57	0
56	MG	BA	3275	1/1	0.78	0.20	46,46,46,46	0
56	MG	AA	3071	1/1	0.79	0.29	60,60,60,60	0
56	MG	BB	3005	1/1	0.79	0.28	61,61,61,61	0
56	MG	BA	3209	1/1	0.79	0.38	40,40,40,40	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	3352	1/1	0.79	0.38	47,47,47,47	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	CA	3021	1/1	0.79	0.22	53,53,53,53	0
56	MG	DG	3001	1/1	0.79	0.14	63,63,63,63	0
56	MG	AA	3089	1/1	0.80	0.43	78,78,78,78	0
56	MG	BA	3069	1/1	0.80	0.44	41,41,41,41	0
56	MG	DB	3007	1/1	0.80	0.27	45,45,45,45	0
56	MG	AA	3118	1/1	0.80	0.32	52,52,52,52	0
56	MG	AA	3061	1/1	0.80	0.19	82,82,82,82	0
56	MG	BA	3731	1/1	0.80	0.36	55,55,55,55	0
56	MG	DA	3454	1/1	0.80	0.31	55,55,55,55	0
56	MG	CA	3062	1/1	0.80	0.26	57,57,57,57	0
56	MG	BA	3658	1/1	0.80	0.27	79,79,79,79	0
56	MG	DA	3314	1/1	0.80	0.19	64,64,64,64	0
56	MG	B0	103	1/1	0.80	0.84	59,59,59,59	0
56	MG	CA	3147	1/1	0.80	0.26	66,66,66,66	0
56	MG	CA	3138	1/1	0.80	0.24	72,72,72,72	0
56	MG	BA	3158	1/1	0.80	0.54	64,64,64,64	0
56	MG	DA	3525	1/1	0.80	0.70	70,70,70,70	0
56	MG	DA	3293	1/1	0.80	0.27	53,53,53,53	0
56	MG	AA	3110	1/1	0.80	0.24	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	BA	3029	1/1	0.80	0.38	53,53,53,53	0
56	MG	DA	3113	1/1	0.80	0.57	43,43,43,43	0
56	MG	DA	3402	1/1	0.80	0.08	61,61,61,61	0
56	MG	DA	3499	1/1	0.80	0.13	46,46,46,46	0
56	MG	CA	3144	1/1	0.81	0.59	63,63,63,63	0
56	MG	DB	3001	1/1	0.81	0.25	68,68,68,68	0
56	MG	BA	3146	1/1	0.81	0.29	52,52,52,52	0
56	MG	AA	3012	1/1	0.81	0.14	56,56,56,56	0
56	MG	AX	103	1/1	0.81	0.08	66,66,66,66	0
56	MG	BB	3003	1/1	0.81	0.25	43,43,43,43	0
56	MG	BB	3004	1/1	0.81	0.26	54,54,54,54	0
56	MG	BA	3180	1/1	0.81	0.99	43,43,43,43	0
56	MG	BA	3155	1/1	0.81	0.38	57,57,57,57	0
56	MG	BW	201	1/1	0.81	0.88	53,53,53,53	0
56	MG	CA	3172	1/1	0.81	0.15	51,51,51,51	0
56	MG	DA	3003	1/1	0.81	0.35	56,56,56,56	0
56	MG	CA	3073	1/1	0.81	0.39	55,55,55,55	0
56	MG	BA	3370	1/1	0.81	0.19	54,54,54,54	0
56	MG	DE	302	1/1	0.81	0.38	44,44,44,44	0
56	MG	CA	3123	1/1	0.81	0.14	77,77,77,77	0
56	MG	AA	3085	1/1	0.81	0.32	69,69,69,69	0
56	MG	CE	3001	1/1	0.81	0.32	68,68,68,68	0
56	MG	AA	3030	1/1	0.81	0.32	69,69,69,69	0
56	MG	DA	3492	1/1	0.81	0.37	68,68,68,68	0
56	MG	DA	3647	1/1	0.81	0.37	66,66,66,66	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	DA	3187	1/1	0.82	0.44	59,59,59,59	0
56	MG	BA	3444	1/1	0.82	0.15	74,74,74,74	0
56	MG	BA	3677	1/1	0.82	0.27	67,67,67,67	0
56	MG	BA	3719	1/1	0.82	0.25	25,25,25,25	0
56	MG	BA	3739	1/1	0.82	0.76	50,50,50,50	0
56	MG	BA	3157	1/1	0.82	0.39	63,63,63,63	0
56	MG	CA	3007	1/1	0.82	0.56	68,68,68,68	0
56	MG	BA	3290	1/1	0.82	0.24	49,49,49,49	0
56	MG	AA	3038	1/1	0.82	0.35	66,66,66,66	0
56	MG	BA	3452	1/1	0.82	0.26	47,47,47,47	0
56	MG	DA	3497	1/1	0.82	0.23	60,60,60,60	0
56	MG	BA	3562	1/1	0.82	0.10	73,73,73,73	0
56	MG	DA	3024	1/1	0.82	0.36	65,65,65,65	0
56	MG	BD	311	1/1	0.82	0.54	45,45,45,45	0
56	MG	CA	3161	1/1	0.82	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3706	1/1	0.82	0.46	63,63,63,63	0
56	MG	BA	3244	1/1	0.82	0.47	65,65,65,65	0
56	MG	CA	3114	1/1	0.82	0.27	82,82,82,82	0
56	MG	BA	3611	1/1	0.82	0.28	52,52,52,52	0
56	MG	BA	3402	1/1	0.82	0.25	71,71,71,71	0
56	MG	B2	101	1/1	0.82	0.36	40,40,40,40	0
56	MG	CA	3015	1/1	0.82	0.34	51,51,51,51	0
56	MG	DA	3189	1/1	0.82	0.11	55,55,55,55	0
56	MG	BA	3083	1/1	0.82	0.23	63,63,63,63	0
56	MG	BA	3123	1/1	0.82	0.33	69,69,69,69	0
56	MG	BA	3736	1/1	0.82	0.24	48,48,48,48	0
56	MG	BA	3134	1/1	0.82	0.31	47,47,47,47	0
56	MG	DA	3279	1/1	0.82	0.31	63,63,63,63	0
56	MG	BA	3242	1/1	0.82	0.36	48,48,48,48	0
56	MG	DQ	205	1/1	0.82	0.40	55,55,55,55	0
56	MG	DA	3388	1/1	0.82	0.16	54,54,54,54	0
56	MG	DA	3367	1/1	0.83	0.26	42,42,42,42	0
56	MG	DA	3071	1/1	0.83	0.52	46,46,46,46	0
56	MG	DA	3087	1/1	0.83	0.16	49,49,49,49	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	BA	3166	1/1	0.83	0.53	59,59,59,59	0
56	MG	DA	3318	1/1	0.83	0.11	45,45,45,45	0
56	MG	BA	3071	1/1	0.83	0.30	55,55,55,55	0
56	MG	CA	3048	1/1	0.83	0.20	62,62,62,62	0
56	MG	BA	3279	1/1	0.83	0.22	48,48,48,48	0
56	MG	DA	3631	1/1	0.83	0.17	56,56,56,56	0
56	MG	BA	3068	1/1	0.83	0.45	54,54,54,54	0
56	MG	BZ	3001	1/1	0.83	0.28	61,61,61,61	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	BA	3496	1/1	0.83	0.40	57,57,57,57	0
56	MG	BA	3152	1/1	0.83	0.33	46,46,46,46	0
56	MG	CA	3003	1/1	0.83	0.11	66,66,66,66	0
56	MG	BA	3334	1/1	0.83	0.30	73,73,73,73	0
56	MG	CA	3032	1/1	0.83	0.20	42,42,42,42	0
56	MG	DA	3598	1/1	0.83	0.30	66,66,66,66	0
56	MG	CA	3139	1/1	0.83	0.27	75,75,75,75	0
56	MG	BA	3164	1/1	0.83	0.72	56,56,56,56	0
56	MG	CA	3035	1/1	0.83	0.23	52,52,52,52	0
56	MG	B0	102	1/1	0.83	0.61	40,40,40,40	0
56	MG	BA	3673	1/1	0.83	0.20	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3014	1/1	0.83	0.19	28,28,28,28	0
56	MG	DA	3256	1/1	0.84	0.18	63,63,63,63	0
56	MG	DA	3084	1/1	0.84	0.32	70,70,70,70	0
56	MG	CA	3031	1/1	0.84	0.39	53,53,53,53	0
56	MG	DA	3423	1/1	0.84	0.15	29,29,29,29	0
56	MG	CA	3023	1/1	0.84	0.14	37,37,37,37	0
56	MG	DA	3198	1/1	0.84	0.29	48,48,48,48	0
56	MG	BA	3598	1/1	0.84	0.12	56,56,56,56	0
56	MG	DA	3609	1/1	0.84	0.35	64,64,64,64	0
56	MG	AA	3077	1/1	0.84	0.41	65,65,65,65	0
56	MG	DA	3458	1/1	0.84	0.15	71,71,71,71	0
56	MG	CA	3070	1/1	0.84	0.34	55,55,55,55	0
56	MG	BA	3102	1/1	0.84	0.32	52,52,52,52	0
56	MG	AA	3029	1/1	0.84	0.69	52,52,52,52	0
56	MG	BA	3165	1/1	0.84	0.31	53,53,53,53	0
56	MG	DA	3483	1/1	0.84	0.19	49,49,49,49	0
56	MG	BA	3240	1/1	0.84	0.17	28,28,28,28	0
56	MG	AA	3059	1/1	0.84	1.19	54,54,54,54	0
56	MG	AA	3140	1/1	0.84	0.12	70,70,70,70	0
56	MG	DA	3104	1/1	0.84	0.28	62,62,62,62	0
56	MG	CA	3008	1/1	0.84	0.78	53,53,53,53	0
56	MG	BA	3288	1/1	0.84	0.22	61,61,61,61	0
56	MG	CA	3081	1/1	0.84	0.10	72,72,72,72	0
56	MG	BA	3285	1/1	0.85	0.14	32,32,32,32	0
56	MG	DD	307	1/1	0.85	0.61	38,38,38,38	0
56	MG	DA	3613	1/1	0.85	0.16	54,54,54,54	0
56	MG	DA	3357	1/1	0.85	0.20	56,56,56,56	0
56	MG	BA	3136	1/1	0.85	0.23	58,58,58,58	0
56	MG	CA	3109	1/1	0.85	0.11	83,83,83,83	0
56	MG	DA	3061	1/1	0.85	0.45	52,52,52,52	0
56	MG	DA	3099	1/1	0.85	0.27	44,44,44,44	0
56	MG	AA	3094	1/1	0.85	0.21	68,68,68,68	0
56	MG	DA	3157	1/1	0.85	0.99	62,62,62,62	0
56	MG	BA	3088	1/1	0.85	0.36	56,56,56,56	0
56	MG	BA	3111	1/1	0.85	0.40	53,53,53,53	0
56	MG	DA	3238	1/1	0.85	0.10	61,61,61,61	0
56	MG	DA	3222	1/1	0.85	0.13	71,71,71,71	0
56	MG	BA	3040	1/1	0.85	0.35	51,51,51,51	0
56	MG	BA	3140	1/1	0.85	0.19	64,64,64,64	0
56	MG	B7	104	1/1	0.85	0.13	51,51,51,51	0
58	ZN	D4	501	1/1	0.85	0.09	153,153,153,153	0
56	MG	DF	302	1/1	0.85	0.27	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	DA	3484	1/1	0.85	0.25	51,51,51,51	0
56	MG	CA	3005	1/1	0.85	0.32	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	DV	202	1/1	0.85	0.84	63,63,63,63	0
56	MG	BA	3135	1/1	0.85	0.17	42,42,42,42	0
56	MG	BB	3017	1/1	0.85	0.20	64,64,64,64	0
56	MG	DA	3065	1/1	0.85	0.19	38,38,38,38	0
56	MG	BA	3624	1/1	0.85	0.25	52,52,52,52	0
56	MG	BA	3669	1/1	0.85	0.24	75,75,75,75	0
56	MG	CA	3158	1/1	0.85	0.22	76,76,76,76	0
56	MG	DR	201	1/1	0.85	0.62	65,65,65,65	0
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	BA	3009	1/1	0.85	0.17	25,25,25,25	0
56	MG	CA	3103	1/1	0.85	0.19	83,83,83,83	0
56	MG	CA	3163	1/1	0.85	0.24	65,65,65,65	0
56	MG	DA	3456	1/1	0.85	0.13	47,47,47,47	0
56	MG	DA	3124	1/1	0.85	0.13	67,67,67,67	0
56	MG	BD	301	1/1	0.85	0.27	28,28,28,28	0
56	MG	AA	3218	1/1	0.85	0.54	65,65,65,65	0
56	MG	BU	205	1/1	0.85	0.33	42,42,42,42	0
56	MG	BA	3626	1/1	0.85	0.11	43,43,43,43	0
56	MG	AA	3015	1/1	0.85	0.16	73,73,73,73	0
56	MG	BA	3175	1/1	0.85	0.25	48,48,48,48	0
56	MG	BF	308	1/1	0.86	0.25	28,28,28,28	0
56	MG	BA	3590	1/1	0.86	0.13	64,64,64,64	0
56	MG	BA	3198	1/1	0.86	0.14	52,52,52,52	0
56	MG	B9	502	1/1	0.86	0.27	49,49,49,49	0
56	MG	DA	3632	1/1	0.86	0.19	71,71,71,71	0
56	MG	CA	3063	1/1	0.86	0.09	61,61,61,61	0
56	MG	BA	3282	1/1	0.86	0.37	49,49,49,49	0
56	MG	BA	3249	1/1	0.86	0.24	40,40,40,40	0
56	MG	AA	3004	1/1	0.86	0.15	55,55,55,55	0
56	MG	BA	3253	1/1	0.86	0.16	51,51,51,51	0
56	MG	DA	3168	1/1	0.86	0.39	48,48,48,48	0
56	MG	BA	3641	1/1	0.86	0.12	45,45,45,45	0
56	MG	DA	3070	1/1	0.86	0.27	44,44,44,44	0
56	MG	DA	3093	1/1	0.86	0.20	53,53,53,53	0
56	MG	CA	3131	1/1	0.86	0.10	55,55,55,55	0
56	MG	BA	3027	1/1	0.86	0.23	45,45,45,45	0
56	MG	BA	3277	1/1	0.86	0.37	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	BA	3712	1/1	0.86	0.09	58,58,58,58	0
56	MG	DA	3022	1/1	0.86	0.25	45,45,45,45	0
56	MG	DA	3112	1/1	0.86	0.43	54,54,54,54	0
56	MG	DA	3482	1/1	0.86	0.13	55,55,55,55	0
56	MG	BE	303	1/1	0.86	0.17	29,29,29,29	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	DA	3553	1/1	0.86	0.36	70,70,70,70	0
56	MG	AA	3013	1/1	0.86	0.23	78,78,78,78	0
56	MG	AX	106	1/1	0.86	0.17	73,73,73,73	0
56	MG	CQ	201	1/1	0.86	0.19	56,56,56,56	0
56	MG	BA	3110	1/1	0.86	0.34	55,55,55,55	0
56	MG	BA	3474	1/1	0.86	0.21	42,42,42,42	0
56	MG	DA	3592	1/1	0.86	0.15	65,65,65,65	0
56	MG	DV	203	1/1	0.86	0.74	54,54,54,54	0
56	MG	DA	3062	1/1	0.86	0.34	55,55,55,55	0
56	MG	CA	3054	1/1	0.86	0.39	48,48,48,48	0
56	MG	DA	3036	1/1	0.86	0.29	35,35,35,35	0
56	MG	CA	3110	1/1	0.86	0.21	97,97,97,97	0
59	FME	AX	101	10/11	0.86	0.44	48,75,97,113	0
56	MG	CA	3068	1/1	0.86	0.11	41,41,41,41	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	3495	1/1	0.87	0.34	84,84,84,84	0
56	MG	AA	3042	1/1	0.87	0.33	44,44,44,44	0
56	MG	DA	3079	1/1	0.87	0.27	37,37,37,37	0
56	MG	BA	3221	1/1	0.87	0.27	44,44,44,44	0
56	MG	DA	3081	1/1	0.87	0.20	48,48,48,48	0
56	MG	BA	3252	1/1	0.87	0.17	55,55,55,55	0
56	MG	BA	3268	1/1	0.87	0.17	46,46,46,46	0
56	MG	DA	3058	1/1	0.87	0.34	47,47,47,47	0
56	MG	DD	302	1/1	0.87	0.23	46,46,46,46	0
56	MG	DA	3260	1/1	0.87	0.10	40,40,40,40	0
56	MG	CA	3155	1/1	0.87	0.16	71,71,71,71	0
56	MG	AA	3074	1/1	0.87	0.44	47,47,47,47	0
56	MG	AA	3075	1/1	0.87	0.11	52,52,52,52	0
56	MG	DA	3053	1/1	0.87	0.15	42,42,42,42	0
56	MG	DA	3108	1/1	0.87	0.46	37,37,37,37	0
60	K	BA	3300	1/1	0.87	0.28	100,100,100,100	0
56	MG	BA	3156	1/1	0.87	0.40	56,56,56,56	0
56	MG	BB	3008	1/1	0.87	0.21	35,35,35,35	0
56	MG	DA	3171	1/1	0.87	0.25	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3236	1/1	0.87	0.17	36,36,36,36	0
56	MG	DA	3032	1/1	0.87	0.13	46,46,46,46	0
56	MG	AA	3137	1/1	0.87	0.21	42,42,42,42	0
56	MG	CA	3146	1/1	0.87	0.20	69,69,69,69	0
56	MG	DA	3115	1/1	0.87	0.09	63,63,63,63	0
56	MG	DA	3292	1/1	0.87	0.22	37,37,37,37	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	3166	1/1	0.87	0.18	48,48,48,48	0
56	MG	CA	3142	1/1	0.87	0.18	59,59,59,59	0
56	MG	BA	3727	1/1	0.87	0.66	68,68,68,68	0
56	MG	CA	3091	1/1	0.87	0.17	72,72,72,72	0
56	MG	AA	3067	1/1	0.87	0.37	87,87,87,87	0
56	MG	BW	203	1/1	0.87	0.32	45,45,45,45	0
56	MG	DA	3481	1/1	0.87	0.27	47,47,47,47	0
56	MG	DA	3060	1/1	0.87	0.25	55,55,55,55	0
56	MG	CA	3125	1/1	0.87	0.13	72,72,72,72	0
56	MG	DA	3080	1/1	0.87	0.14	44,44,44,44	0
56	MG	BA	3643	1/1	0.87	0.28	43,43,43,43	0
56	MG	DA	3009	1/1	0.87	0.12	31,31,31,31	0
56	MG	BA	3214	1/1	0.87	0.09	53,53,53,53	0
56	MG	DA	3161	1/1	0.87	0.30	60,60,60,60	0
56	MG	BA	3006	1/1	0.87	0.27	42,42,42,42	0
56	MG	DA	3500	1/1	0.87	0.17	50,50,50,50	0
56	MG	DA	3102	1/1	0.88	0.25	41,41,41,41	0
56	MG	DA	3208	1/1	0.88	0.94	43,43,43,43	0
56	MG	BN	3002	1/1	0.88	0.30	56,56,56,56	0
56	MG	DA	3240	1/1	0.88	0.26	51,51,51,51	0
56	MG	AA	3019	1/1	0.88	0.39	74,74,74,74	0
56	MG	BA	3100	1/1	0.88	0.25	48,48,48,48	0
56	MG	DA	3398	1/1	0.88	0.15	35,35,35,35	0
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	BA	3192	1/1	0.88	0.48	58,58,58,58	0
56	MG	DA	3185	1/1	0.88	0.58	52,52,52,52	0
56	MG	DA	3310	1/1	0.88	0.21	53,53,53,53	0
56	MG	AA	3050	1/1	0.88	0.50	63,63,63,63	0
56	MG	DA	3210	1/1	0.88	0.14	40,40,40,40	0
56	MG	AA	3138	1/1	0.88	0.54	37,37,37,37	0
56	MG	DA	3147	1/1	0.88	0.11	53,53,53,53	0
56	MG	BA	3514	1/1	0.88	0.14	37,37,37,37	0
56	MG	BA	3320	1/1	0.88	0.29	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3040	1/1	0.88	0.35	42,42,42,42	0
56	MG	DA	3343	1/1	0.88	0.21	41,41,41,41	0
56	MG	DA	3252	1/1	0.88	0.12	45,45,45,45	0
56	MG	AA	3131	1/1	0.88	0.50	56,56,56,56	0
56	MG	BA	3205	1/1	0.88	0.19	40,40,40,40	0
56	MG	CA	3034	1/1	0.88	0.26	65,65,65,65	0
56	MG	BA	3216	1/1	0.88	0.22	41,41,41,41	0
56	MG	DA	3134	1/1	0.88	0.23	46,46,46,46	0
56	MG	DA	3150	1/1	0.88	0.21	64,64,64,64	0
56	MG	BA	3168	1/1	0.88	0.28	42,42,42,42	0
56	MG	BA	3280	1/1	0.88	0.69	69,69,69,69	0
56	MG	DA	3599	1/1	0.88	0.23	72,72,72,72	0
56	MG	CA	3164	1/1	0.88	0.39	49,49,49,49	0
56	MG	AA	3033	1/1	0.88	0.38	64,64,64,64	0
56	MG	CA	3071	1/1	0.88	0.08	63,63,63,63	0
56	MG	BA	3062	1/1	0.88	0.34	42,42,42,42	0
56	MG	BA	3298	1/1	0.88	0.33	49,49,49,49	0
56	MG	DA	3092	1/1	0.88	0.60	39,39,39,39	0
56	MG	DA	3119	1/1	0.88	0.15	44,44,44,44	0
56	MG	BA	3354	1/1	0.88	0.15	74,74,74,74	0
56	MG	BG	3002	1/1	0.88	0.11	42,42,42,42	0
56	MG	DA	3122	1/1	0.88	0.15	62,62,62,62	0
56	MG	DA	3078	1/1	0.88	0.17	44,44,44,44	0
56	MG	DB	3011	1/1	0.88	0.34	55,55,55,55	0
56	MG	AN	103	1/1	0.88	0.38	60,60,60,60	0
56	MG	CA	3126	1/1	0.88	0.24	61,61,61,61	0
56	MG	BA	3163	1/1	0.88	0.17	50,50,50,50	0
56	MG	BA	3045	1/1	0.88	0.29	34,34,34,34	0
56	MG	BA	3373	1/1	0.88	0.28	36,36,36,36	0
56	MG	BA	3058	1/1	0.88	0.45	38,38,38,38	0
56	MG	CA	3027	1/1	0.88	0.17	57,57,57,57	0
56	MG	DA	3005	1/1	0.88	0.21	42,42,42,42	0
56	MG	AA	3046	1/1	0.88	0.12	73,73,73,73	0
56	MG	AA	3132	1/1	0.88	0.36	76,76,76,76	0
56	MG	BA	3346	1/1	0.88	0.23	37,37,37,37	0
56	MG	DA	3604	1/1	0.88	0.20	54,54,54,54	0
56	MG	DA	3224	1/1	0.88	0.15	47,47,47,47	0
56	MG	DA	3110	1/1	0.88	0.14	49,49,49,49	0
56	MG	DA	3086	1/1	0.88	0.30	43,43,43,43	0
56	MG	BA	3693	1/1	0.88	0.14	64,64,64,64	0
56	MG	DA	3067	1/1	0.88	0.54	43,43,43,43	0
56	MG	DQ	201	1/1	0.88	0.43	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	3009	1/1	0.88	0.23	79,79,79,79	0
56	MG	CA	3143	1/1	0.88	0.07	87,87,87,87	0
56	MG	DA	3524	1/1	0.88	0.12	28,28,28,28	0
56	MG	AA	3032	1/1	0.88	0.28	57,57,57,57	0
56	MG	CA	3157	1/1	0.88	0.11	54,54,54,54	0
56	MG	CA	3002	1/1	0.88	0.07	62,62,62,62	0
56	MG	BA	3023	1/1	0.88	0.13	66,66,66,66	0
56	MG	AA	3133	1/1	0.88	0.35	63,63,63,63	0
56	MG	BA	3092	1/1	0.88	0.27	51,51,51,51	0
56	MG	CA	3159	1/1	0.88	0.61	91,91,91,91	0
56	MG	DA	3460	1/1	0.89	0.36	50,50,50,50	0
56	MG	DA	3405	1/1	0.89	0.10	47,47,47,47	0
56	MG	BA	3336	1/1	0.89	0.21	54,54,54,54	0
56	MG	CA	3029	1/1	0.89	0.15	59,59,59,59	0
56	MG	BA	3509	1/1	0.89	0.16	27,27,27,27	0
56	MG	DA	3638	1/1	0.89	0.30	62,62,62,62	0
56	MG	DA	3487	1/1	0.89	0.19	57,57,57,57	0
56	MG	DA	3018	1/1	0.89	0.47	48,48,48,48	0
56	MG	DA	3132	1/1	0.89	0.71	54,54,54,54	0
56	MG	AA	3002	1/1	0.89	0.20	57,57,57,57	0
56	MG	DA	3191	1/1	0.89	0.44	47,47,47,47	0
56	MG	BA	3365	1/1	0.89	0.14	20,20,20,20	0
56	MG	BA	3218	1/1	0.89	0.20	62,62,62,62	0
56	MG	BA	3585	1/1	0.89	0.17	51,51,51,51	0
56	MG	DA	3145	1/1	0.89	0.46	65,65,65,65	0
56	MG	AA	3031	1/1	0.89	0.22	41,41,41,41	0
56	MG	DA	3590	1/1	0.89	0.17	80,80,80,80	0
56	MG	BA	3104	1/1	0.89	0.28	45,45,45,45	0
56	MG	DA	3167	1/1	0.89	0.23	48,48,48,48	0
56	MG	CA	3160	1/1	0.89	0.13	59,59,59,59	0
56	MG	BA	3523	1/1	0.89	0.12	48,48,48,48	0
56	MG	DA	3286	1/1	0.89	0.17	62,62,62,62	0
56	MG	BA	3237	1/1	0.89	0.55	51,51,51,51	0
56	MG	BA	3149	1/1	0.89	0.55	40,40,40,40	0
56	MG	BA	3005	1/1	0.89	0.18	36,36,36,36	0
56	MG	BA	3127	1/1	0.89	0.38	50,50,50,50	0
56	MG	BA	3355	1/1	0.89	0.23	64,64,64,64	0
56	MG	AA	3047	1/1	0.89	0.31	61,61,61,61	0
56	MG	AA	3039	1/1	0.89	0.24	60,60,60,60	0
56	MG	BN	3003	1/1	0.89	0.39	59,59,59,59	0
56	MG	DA	3195	1/1	0.89	0.10	50,50,50,50	0
56	MG	BA	3197	1/1	0.89	0.30	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3079	1/1	0.89	0.14	48,48,48,48	0
56	MG	DA	3200	1/1	0.89	0.21	42,42,42,42	0
56	MG	BA	3017	1/1	0.89	0.54	44,44,44,44	0
56	MG	BA	3103	1/1	0.89	0.12	53,53,53,53	0
56	MG	AA	3181	1/1	0.89	0.28	57,57,57,57	0
56	MG	BA	3292	1/1	0.89	0.21	63,63,63,63	0
56	MG	DA	3169	1/1	0.89	0.38	57,57,57,57	0
56	MG	DA	3253	1/1	0.89	0.14	42,42,42,42	0
56	MG	DA	3560	1/1	0.89	0.11	34,34,34,34	0
56	MG	CA	3037	1/1	0.89	0.31	67,67,67,67	0
56	MG	DV	204	1/1	0.89	0.21	41,41,41,41	0
56	MG	BA	3251	1/1	0.89	0.21	61,61,61,61	0
56	MG	DA	3623	1/1	0.89	0.17	53,53,53,53	0
56	MG	BA	3061	1/1	0.89	0.49	51,51,51,51	0
56	MG	CA	3086	1/1	0.89	0.20	80,80,80,80	0
56	MG	DA	3441	1/1	0.89	0.30	53,53,53,53	0
56	MG	DA	3243	1/1	0.89	0.21	67,67,67,67	0
56	MG	BA	3147	1/1	0.89	0.24	46,46,46,46	0
56	MG	DA	3048	1/1	0.89	0.37	37,37,37,37	0
56	MG	BA	3309	1/1	0.89	0.13	46,46,46,46	0
56	MG	DA	3194	1/1	0.89	0.13	48,48,48,48	0
56	MG	AA	3139	1/1	0.89	0.34	56,56,56,56	0
56	MG	BA	3356	1/1	0.89	0.27	56,56,56,56	0
56	MG	BA	3558	1/1	0.89	0.22	35,35,35,35	0
56	MG	DA	3159	1/1	0.89	0.24	51,51,51,51	0
56	MG	DA	3387	1/1	0.89	0.14	56,56,56,56	0
56	MG	AA	3134	1/1	0.89	0.43	70,70,70,70	0
56	MG	BA	3177	1/1	0.89	0.21	62,62,62,62	0
56	MG	BA	3664	1/1	0.89	0.26	68,68,68,68	0
56	MG	BA	3215	1/1	0.89	0.14	69,69,69,69	0
56	MG	DA	3361	1/1	0.89	0.11	61,61,61,61	0
56	MG	BA	3230	1/1	0.89	0.47	46,46,46,46	0
56	MG	CA	3036	1/1	0.89	0.52	68,68,68,68	0
56	MG	CA	3170	1/1	0.89	0.48	50,50,50,50	0
56	MG	DA	3503	1/1	0.90	0.17	71,71,71,71	0
56	MG	DA	3213	1/1	0.90	0.21	44,44,44,44	0
56	MG	BA	3463	1/1	0.90	0.20	55,55,55,55	0
56	MG	DA	3219	1/1	0.90	0.17	60,60,60,60	0
56	MG	B7	101	1/1	0.90	0.20	43,43,43,43	0
56	MG	BA	3596	1/1	0.90	0.12	51,51,51,51	0
56	MG	AA	3115	1/1	0.90	0.10	48,48,48,48	0
56	MG	AA	3119	1/1	0.90	0.37	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3075	1/1	0.90	0.33	44,44,44,44	0
56	MG	BA	3457	1/1	0.90	0.12	57,57,57,57	0
56	MG	BA	3181	1/1	0.90	0.34	38,38,38,38	0
56	MG	AA	3184	1/1	0.90	0.10	72,72,72,72	0
56	MG	BQ	203	1/1	0.90	0.22	58,58,58,58	0
56	MG	DA	3391	1/1	0.90	0.14	41,41,41,41	0
56	MG	DA	3066	1/1	0.90	0.37	53,53,53,53	0
56	MG	DA	3548	1/1	0.90	0.13	37,37,37,37	0
56	MG	BA	3255	1/1	0.90	0.18	41,41,41,41	0
56	MG	DA	3042	1/1	0.90	0.25	36,36,36,36	0
56	MG	BA	3144	1/1	0.90	0.27	74,74,74,74	0
56	MG	CT	3001	1/1	0.90	0.43	57,57,57,57	0
56	MG	BA	3105	1/1	0.90	0.44	34,34,34,34	0
56	MG	AA	3123	1/1	0.90	0.43	39,39,39,39	0
56	MG	BE	305	1/1	0.90	0.70	42,42,42,42	0
56	MG	DA	3096	1/1	0.90	0.17	60,60,60,60	0
56	MG	BA	3159	1/1	0.90	0.30	48,48,48,48	0
56	MG	DA	3602	1/1	0.90	0.19	52,52,52,52	0
56	MG	BA	3671	1/1	0.90	0.33	57,57,57,57	0
56	MG	AA	3052	1/1	0.90	0.25	60,60,60,60	0
56	MG	BA	3125	1/1	0.90	0.20	39,39,39,39	0
56	MG	BA	3708	1/1	0.90	0.23	40,40,40,40	0
56	MG	DA	3359	1/1	0.90	0.23	46,46,46,46	0
56	MG	BA	3011	1/1	0.90	0.09	37,37,37,37	0
56	MG	BA	3350	1/1	0.90	0.24	47,47,47,47	0
56	MG	DA	3620	1/1	0.90	0.19	71,71,71,71	0
56	MG	DA	3126	1/1	0.90	0.34	43,43,43,43	0
56	MG	DA	3284	1/1	0.90	0.14	68,68,68,68	0
56	MG	DA	3440	1/1	0.90	0.32	33,33,33,33	0
56	MG	BA	3139	1/1	0.90	0.25	51,51,51,51	0
56	MG	AA	3080	1/1	0.90	0.17	53,53,53,53	0
56	MG	DA	3517	1/1	0.90	0.19	50,50,50,50	0
56	MG	BA	3194	1/1	0.90	0.18	55,55,55,55	0
56	MG	CA	3150	1/1	0.90	0.12	59,59,59,59	0
56	MG	DA	3369	1/1	0.90	0.13	47,47,47,47	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	DA	3640	1/1	0.90	0.68	56,56,56,56	0
56	MG	DA	3128	1/1	0.90	0.19	52,52,52,52	0
56	MG	BA	3007	1/1	0.90	0.23	35,35,35,35	0
56	MG	DA	3593	1/1	0.90	0.23	73,73,73,73	0
56	MG	CA	3046	1/1	0.90	0.38	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3183	1/1	0.90	0.24	48,48,48,48	0
56	MG	BA	3047	1/1	0.90	0.42	47,47,47,47	0
56	MG	DA	3129	1/1	0.90	0.14	43,43,43,43	0
56	MG	DA	3582	1/1	0.90	0.11	52,52,52,52	0
56	MG	DA	3077	1/1	0.90	0.28	50,50,50,50	0
56	MG	AA	3092	1/1	0.90	0.51	50,50,50,50	0
56	MG	DA	3538	1/1	0.90	0.18	44,44,44,44	0
56	MG	BA	3683	1/1	0.90	0.22	60,60,60,60	0
56	MG	BA	3730	1/1	0.90	0.64	45,45,45,45	0
56	MG	DA	3461	1/1	0.90	0.21	41,41,41,41	0
56	MG	BA	3609	1/1	0.90	0.12	46,46,46,46	0
56	MG	BA	3578	1/1	0.90	0.32	54,54,54,54	0
56	MG	BA	3243	1/1	0.90	0.15	48,48,48,48	0
56	MG	DA	3624	1/1	0.90	0.40	51,51,51,51	0
56	MG	DA	3264	1/1	0.90	0.32	49,49,49,49	0
56	MG	BA	3714	1/1	0.90	0.21	58,58,58,58	0
56	MG	DA	3218	1/1	0.90	0.25	62,62,62,62	0
56	MG	DA	3465	1/1	0.90	0.16	49,49,49,49	0
56	MG	BA	3174	1/1	0.90	0.09	48,48,48,48	0
56	MG	B7	103	1/1	0.90	0.85	48,48,48,48	0
56	MG	BA	3019	1/1	0.90	0.18	39,39,39,39	0
56	MG	AA	3005	1/1	0.90	0.20	66,66,66,66	0
56	MG	BA	3560	1/1	0.90	0.20	61,61,61,61	0
56	MG	DA	3462	1/1	0.90	0.11	55,55,55,55	0
56	MG	DA	3610	1/1	0.90	0.28	54,54,54,54	0
56	MG	AA	3003	1/1	0.90	0.24	63,63,63,63	0
56	MG	BA	3577	1/1	0.90	0.10	52,52,52,52	0
56	MG	BA	3048	1/1	0.90	0.23	31,31,31,31	0
56	MG	DA	3363	1/1	0.90	0.09	57,57,57,57	0
56	MG	DA	3044	1/1	0.90	0.13	46,46,46,46	0
56	MG	DF	303	1/1	0.90	0.33	43,43,43,43	0
56	MG	DB	3005	1/1	0.90	0.26	43,43,43,43	0
56	MG	AA	3124	1/1	0.90	0.10	57,57,57,57	0
56	MG	BA	3738	1/1	0.90	0.35	59,59,59,59	0
56	MG	DA	3254	1/1	0.90	0.22	30,30,30,30	0
56	MG	DA	3046	1/1	0.90	0.18	56,56,56,56	0
56	MG	AA	3217	1/1	0.90	0.65	67,67,67,67	0
56	MG	AA	3215	1/1	0.90	0.10	53,53,53,53	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	AA	3180	1/1	0.90	0.38	66,66,66,66	0
56	MG	BA	3114	1/1	0.90	0.36	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3162	1/1	0.91	0.21	46,46,46,46	0
56	MG	DA	3653	1/1	0.91	0.35	60,60,60,60	0
56	MG	CA	3119	1/1	0.91	0.24	64,64,64,64	0
56	MG	AN	101	1/1	0.91	0.19	63,63,63,63	0
56	MG	BA	3049	1/1	0.91	0.38	35,35,35,35	0
56	MG	BA	3248	1/1	0.91	0.24	43,43,43,43	0
56	MG	BF	302	1/1	0.91	0.31	46,46,46,46	0
56	MG	BA	3568	1/1	0.91	0.23	47,47,47,47	0
56	MG	CA	3151	1/1	0.91	0.25	80,80,80,80	0
56	MG	AA	3142	1/1	0.91	0.26	38,38,38,38	0
56	MG	DA	3419	1/1	0.91	0.17	31,31,31,31	0
56	MG	DA	3172	1/1	0.91	0.43	51,51,51,51	0
56	MG	DA	3594	1/1	0.91	0.30	47,47,47,47	0
56	MG	BA	3666	1/1	0.91	0.32	61,61,61,61	0
56	MG	BA	3507	1/1	0.91	0.10	68,68,68,68	0
56	MG	BA	3055	1/1	0.91	0.23	44,44,44,44	0
56	MG	DA	3226	1/1	0.91	0.21	50,50,50,50	0
56	MG	DA	3621	1/1	0.91	0.14	54,54,54,54	0
56	MG	BA	3262	1/1	0.91	0.20	56,56,56,56	0
56	MG	BA	3335	1/1	0.91	0.17	35,35,35,35	0
56	MG	DA	3567	1/1	0.91	0.15	62,62,62,62	0
56	MG	BB	3009	1/1	0.91	0.16	48,48,48,48	0
56	MG	DA	3051	1/1	0.91	0.12	46,46,46,46	0
56	MG	BA	3464	1/1	0.91	0.10	43,43,43,43	0
56	MG	DA	3342	1/1	0.91	0.12	52,52,52,52	0
56	MG	BA	3466	1/1	0.91	0.14	61,61,61,61	0
56	MG	DA	3496	1/1	0.91	0.15	53,53,53,53	0
56	MG	BA	3187	1/1	0.91	0.64	50,50,50,50	0
56	MG	BA	3689	1/1	0.91	0.23	39,39,39,39	0
56	MG	BA	3481	1/1	0.91	0.23	38,38,38,38	0
56	MG	AX	105	1/1	0.91	0.69	56,56,56,56	0
56	MG	BA	3391	1/1	0.91	0.14	48,48,48,48	0
56	MG	BA	3020	1/1	0.91	0.11	45,45,45,45	0
56	MG	BA	3638	1/1	0.91	0.21	37,37,37,37	0
56	MG	BA	3505	1/1	0.91	0.19	59,59,59,59	0
56	MG	BN	3001	1/1	0.91	0.76	54,54,54,54	0
56	MG	DF	301	1/1	0.91	0.51	32,32,32,32	0
56	MG	BA	3132	1/1	0.91	0.25	35,35,35,35	0
56	MG	DA	3526	1/1	0.91	0.19	54,54,54,54	0
56	MG	DA	3512	1/1	0.91	0.25	61,61,61,61	0
56	MG	BA	3372	1/1	0.91	0.17	38,38,38,38	0
56	MG	AA	3219	1/1	0.91	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3619	1/1	0.91	0.27	40,40,40,40	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	DA	3635	1/1	0.91	0.32	58,58,58,58	0
56	MG	DA	3401	1/1	0.91	0.29	58,58,58,58	0
56	MG	BA	3303	1/1	0.91	0.16	35,35,35,35	0
56	MG	BA	3443	1/1	0.91	0.17	26,26,26,26	0
56	MG	DA	3360	1/1	0.91	0.25	41,41,41,41	0
56	MG	BA	3106	1/1	0.91	0.12	48,48,48,48	0
56	MG	BA	3226	1/1	0.91	0.30	32,32,32,32	0
56	MG	BD	312	1/1	0.91	0.85	80,80,80,80	0
56	MG	CA	3106	1/1	0.91	0.34	64,64,64,64	0
56	MG	AA	3011	1/1	0.91	1.19	55,55,55,55	0
56	MG	CA	3056	1/1	0.91	0.11	64,64,64,64	0
56	MG	BA	3269	1/1	0.91	0.65	34,34,34,34	0
56	MG	DA	3041	1/1	0.91	0.45	57,57,57,57	0
56	MG	DF	304	1/1	0.91	0.28	44,44,44,44	0
56	MG	AA	3121	1/1	0.91	0.53	51,51,51,51	0
56	MG	BA	3024	1/1	0.91	0.40	35,35,35,35	0
56	MG	BA	3056	1/1	0.91	0.42	44,44,44,44	0
56	MG	BA	3676	1/1	0.91	0.22	51,51,51,51	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	DA	3315	1/1	0.91	0.09	31,31,31,31	0
56	MG	CA	3010	1/1	0.91	0.11	32,32,32,32	0
56	MG	DA	3376	1/1	0.91	0.08	31,31,31,31	0
56	MG	BA	3653	1/1	0.91	0.15	69,69,69,69	0
56	MG	DA	3149	1/1	0.91	0.06	47,47,47,47	0
56	MG	BA	3143	1/1	0.91	0.31	40,40,40,40	0
56	MG	AA	3169	1/1	0.91	0.16	76,76,76,76	0
56	MG	DA	3430	1/1	0.91	0.28	55,55,55,55	0
56	MG	DA	3339	1/1	0.91	0.10	37,37,37,37	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	3331	1/1	0.91	0.19	47,47,47,47	0
56	MG	AA	3081	1/1	0.91	0.23	41,41,41,41	0
56	MG	DA	3069	1/1	0.91	0.12	51,51,51,51	0
56	MG	DA	3148	1/1	0.91	0.23	47,47,47,47	0
56	MG	DA	3033	1/1	0.91	0.25	39,39,39,39	0
56	MG	CA	3006	1/1	0.91	0.17	77,77,77,77	0
56	MG	AA	3101	1/1	0.91	0.15	56,56,56,56	0
56	MG	DA	3143	1/1	0.91	0.22	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	AA	3125	1/1	0.91	0.16	47,47,47,47	0
56	MG	AA	3136	1/1	0.91	0.08	62,62,62,62	0
56	MG	D8	5001	1/1	0.91	0.41	47,47,47,47	0
56	MG	DA	3073	1/1	0.91	0.18	44,44,44,44	0
56	MG	CA	3047	1/1	0.91	0.16	63,63,63,63	0
56	MG	CA	3152	1/1	0.92	0.38	55,55,55,55	0
56	MG	DA	3040	1/1	0.92	0.10	42,42,42,42	0
56	MG	DA	3221	1/1	0.92	0.18	49,49,49,49	0
56	MG	BA	3617	1/1	0.92	0.24	62,62,62,62	0
56	MG	DA	3170	1/1	0.92	0.80	57,57,57,57	0
56	MG	AA	3105	1/1	0.92	0.22	46,46,46,46	0
56	MG	DA	3179	1/1	0.92	0.22	46,46,46,46	0
56	MG	AA	3190	1/1	0.92	0.32	67,67,67,67	0
56	MG	DA	3295	1/1	0.92	0.24	39,39,39,39	0
56	MG	DA	3536	1/1	0.92	0.16	80,80,80,80	0
56	MG	DA	3029	1/1	0.92	0.10	61,61,61,61	0
56	MG	DA	3505	1/1	0.92	0.06	65,65,65,65	0
56	MG	BA	3258	1/1	0.92	0.23	40,40,40,40	0
56	MG	BA	3016	1/1	0.92	0.24	33,33,33,33	0
56	MG	DA	3151	1/1	0.92	0.29	60,60,60,60	0
56	MG	AA	3211	1/1	0.92	0.20	36,36,36,36	0
56	MG	AA	3162	1/1	0.92	0.23	74,74,74,74	0
56	MG	DA	3532	1/1	0.92	0.10	57,57,57,57	0
56	MG	AA	3194	1/1	0.92	0.19	54,54,54,54	0
56	MG	BA	3225	1/1	0.92	0.33	62,62,62,62	0
56	MG	DA	3502	1/1	0.92	0.12	65,65,65,65	0
56	MG	DA	3246	1/1	0.92	0.17	24,24,24,24	0
56	MG	CA	3111	1/1	0.92	0.12	64,64,64,64	0
56	MG	CA	3104	1/1	0.92	0.19	62,62,62,62	0
56	MG	CA	3140	1/1	0.92	0.16	73,73,73,73	0
56	MG	BA	3502	1/1	0.92	0.20	43,43,43,43	0
56	MG	BA	3698	1/1	0.92	0.20	41,41,41,41	0
56	MG	BA	3188	1/1	0.92	0.15	37,37,37,37	0
56	MG	DA	3097	1/1	0.92	0.22	61,61,61,61	0
56	MG	DA	3459	1/1	0.92	0.11	33,33,33,33	0
56	MG	DA	3651	1/1	0.92	0.60	52,52,52,52	0
56	MG	DA	3111	1/1	0.92	0.23	53,53,53,53	0
56	MG	BA	3735	1/1	0.92	0.20	45,45,45,45	0
56	MG	BA	3325	1/1	0.92	0.19	58,58,58,58	0
56	MG	DA	3453	1/1	0.92	0.36	61,61,61,61	0
56	MG	BA	3254	1/1	0.92	0.19	59,59,59,59	0
56	MG	CA	3136	1/1	0.92	0.18	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3109	1/1	0.92	0.55	66,66,66,66	0
56	MG	DA	3139	1/1	0.92	0.18	40,40,40,40	0
56	MG	DA	3014	1/1	0.92	0.21	34,34,34,34	0
56	MG	DA	3597	1/1	0.92	0.23	47,47,47,47	0
56	MG	DA	3006	1/1	0.92	0.16	42,42,42,42	0
56	MG	BU	201	1/1	0.92	0.75	39,39,39,39	0
56	MG	BA	3141	1/1	0.92	0.30	43,43,43,43	0
56	MG	DA	3636	1/1	0.92	0.14	61,61,61,61	0
56	MG	DA	3050	1/1	0.92	0.57	31,31,31,31	0
56	MG	AA	3191	1/1	0.92	0.13	71,71,71,71	0
56	MG	BA	3401	1/1	0.92	0.12	42,42,42,42	0
56	MG	DA	3562	1/1	0.92	0.10	61,61,61,61	0
56	MG	BA	3468	1/1	0.92	0.17	30,30,30,30	0
56	MG	AA	3082	1/1	0.92	0.24	39,39,39,39	0
56	MG	BA	3196	1/1	0.92	0.76	56,56,56,56	0
56	MG	DA	3296	1/1	0.92	0.09	31,31,31,31	0
56	MG	BA	3633	1/1	0.92	0.13	58,58,58,58	0
56	MG	BA	3099	1/1	0.92	0.17	44,44,44,44	0
56	MG	DA	3074	1/1	0.92	0.21	54,54,54,54	0
56	MG	DA	3543	1/1	0.92	0.15	42,42,42,42	0
56	MG	DA	3188	1/1	0.92	0.33	47,47,47,47	0
56	MG	DA	3225	1/1	0.92	0.16	45,45,45,45	0
56	MG	AA	3041	1/1	0.92	0.15	49,49,49,49	0
56	MG	DA	3340	1/1	0.92	0.14	47,47,47,47	0
56	MG	BA	3406	1/1	0.92	0.14	28,28,28,28	0
56	MG	BR	204	1/1	0.92	0.61	43,43,43,43	0
56	MG	DA	3489	1/1	0.92	0.16	36,36,36,36	0
56	MG	AA	3072	1/1	0.92	0.26	79,79,79,79	0
56	MG	BA	3256	1/1	0.92	0.17	58,58,58,58	0
56	MG	BA	3652	1/1	0.92	0.20	64,64,64,64	0
56	MG	BA	3328	1/1	0.92	0.21	42,42,42,42	0
56	MG	BA	3108	1/1	0.92	0.14	55,55,55,55	0
56	MG	DA	3554	1/1	0.92	0.18	70,70,70,70	0
56	MG	DA	3478	1/1	0.92	0.25	46,46,46,46	0
56	MG	BB	3014	1/1	0.92	0.13	69,69,69,69	0
56	MG	BG	3001	1/1	0.92	0.13	64,64,64,64	0
56	MG	BA	3090	1/1	0.92	0.20	46,46,46,46	0
56	MG	BA	3122	1/1	0.92	0.27	52,52,52,52	0
56	MG	AA	3200	1/1	0.92	0.24	68,68,68,68	0
56	MG	AA	3069	1/1	0.92	0.14	84,84,84,84	0
56	MG	BD	304	1/1	0.92	0.51	58,58,58,58	0
56	MG	DA	3202	1/1	0.92	0.33	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	3432	1/1	0.92	0.17	60,60,60,60	0
56	MG	BA	3601	1/1	0.92	0.28	64,64,64,64	0
56	MG	DA	3509	1/1	0.92	0.13	55,55,55,55	0
56	MG	DA	3611	1/1	0.92	0.09	42,42,42,42	0
56	MG	AA	3034	1/1	0.92	0.18	48,48,48,48	0
56	MG	CA	3105	1/1	0.92	0.09	79,79,79,79	0
56	MG	DA	3116	1/1	0.92	0.31	39,39,39,39	0
56	MG	BA	3039	1/1	0.92	0.14	42,42,42,42	0
56	MG	AA	3024	1/1	0.92	0.18	53,53,53,53	0
56	MG	DA	3107	1/1	0.92	0.30	55,55,55,55	0
56	MG	CA	3117	1/1	0.92	0.15	68,68,68,68	0
56	MG	AA	3098	1/1	0.92	0.35	72,72,72,72	0
56	MG	DA	3013	1/1	0.92	0.09	47,47,47,47	0
56	MG	BA	3052	1/1	0.92	0.25	29,29,29,29	0
56	MG	AA	3154	1/1	0.92	0.08	63,63,63,63	0
56	MG	AA	3025	1/1	0.92	0.14	69,69,69,69	0
56	MG	CA	3065	1/1	0.92	0.23	75,75,75,75	0
56	MG	BA	3374	1/1	0.92	0.19	44,44,44,44	0
56	MG	BA	3245	1/1	0.92	0.30	47,47,47,47	0
56	MG	BF	304	1/1	0.92	0.09	35,35,35,35	0
56	MG	AA	3036	1/1	0.92	0.23	71,71,71,71	0
56	MG	AA	3198	1/1	0.92	0.11	87,87,87,87	0
56	MG	BA	3430	1/1	0.92	0.32	49,49,49,49	0
56	MG	DA	3537	1/1	0.93	0.22	65,65,65,65	0
56	MG	DA	3470	1/1	0.93	0.28	52,52,52,52	0
56	MG	DA	3326	1/1	0.93	0.20	33,33,33,33	0
56	MG	BA	3515	1/1	0.93	0.05	56,56,56,56	0
56	MG	BA	3133	1/1	0.93	0.27	32,32,32,32	0
56	MG	BA	3072	1/1	0.93	0.28	45,45,45,45	0
56	MG	DA	3366	1/1	0.93	0.35	36,36,36,36	0
56	MG	BA	3246	1/1	0.93	0.24	46,46,46,46	0
56	MG	BA	3599	1/1	0.93	0.31	46,46,46,46	0
56	MG	AA	3135	1/1	0.93	0.23	41,41,41,41	0
56	MG	CA	3134	1/1	0.93	0.17	82,82,82,82	0
56	MG	BA	3549	1/1	0.93	0.22	27,27,27,27	0
56	MG	DA	3414	1/1	0.93	0.17	49,49,49,49	0
56	MG	BA	3597	1/1	0.93	0.35	60,60,60,60	0
56	MG	DA	3603	1/1	0.93	0.16	55,55,55,55	0
56	MG	DA	3054	1/1	0.93	0.11	51,51,51,51	0
56	MG	BA	3387	1/1	0.93	0.07	48,48,48,48	0
56	MG	AA	3066	1/1	0.93	0.31	38,38,38,38	0
56	MG	BA	3273	1/1	0.93	0.39	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	DA	3336	1/1	0.93	0.12	27,27,27,27	0
56	MG	B0	101	1/1	0.93	0.20	36,36,36,36	0
56	MG	BA	3690	1/1	0.93	0.17	53,53,53,53	0
58	ZN	AN	102	1/1	0.93	0.12	90,90,90,90	0
56	MG	BD	306	1/1	0.93	0.45	46,46,46,46	0
56	MG	BA	3687	1/1	0.93	0.22	38,38,38,38	0
56	MG	DA	3424	1/1	0.93	0.20	30,30,30,30	0
56	MG	DB	3012	1/1	0.93	0.27	59,59,59,59	0
56	MG	BA	3238	1/1	0.93	0.16	51,51,51,51	0
56	MG	BA	3403	1/1	0.93	0.21	41,41,41,41	0
56	MG	DA	3008	1/1	0.93	0.23	51,51,51,51	0
56	MG	DW	201	1/1	0.93	0.31	46,46,46,46	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	CA	3107	1/1	0.93	0.12	60,60,60,60	0
56	MG	DA	3273	1/1	0.93	0.13	30,30,30,30	0
56	MG	DA	3521	1/1	0.93	0.12	62,62,62,62	0
56	MG	BA	3098	1/1	0.93	0.15	35,35,35,35	0
56	MG	BA	3394	1/1	0.93	0.12	49,49,49,49	0
56	MG	CA	3019	1/1	0.93	0.07	49,49,49,49	0
56	MG	DA	3199	1/1	0.93	0.13	42,42,42,42	0
56	MG	B8	101	1/1	0.93	0.47	49,49,49,49	0
56	MG	DA	3020	1/1	0.93	0.30	52,52,52,52	0
56	MG	AA	3058	1/1	0.93	0.16	50,50,50,50	0
56	MG	BA	3589	1/1	0.93	0.15	51,51,51,51	0
56	MG	BA	3257	1/1	0.93	0.30	38,38,38,38	0
56	MG	BA	3182	1/1	0.93	0.31	51,51,51,51	0
60	K	DA	3231	1/1	0.93	0.22	96,96,96,96	0
56	MG	DA	3305	1/1	0.93	0.09	33,33,33,33	0
56	MG	DA	3400	1/1	0.93	0.19	42,42,42,42	0
56	MG	BA	3067	1/1	0.93	0.33	53,53,53,53	0
56	MG	DA	3072	1/1	0.93	0.14	41,41,41,41	0
56	MG	DA	3579	1/1	0.93	0.17	23,23,23,23	0
56	MG	DA	3233	1/1	0.93	0.19	42,42,42,42	0
56	MG	DA	3281	1/1	0.93	0.21	42,42,42,42	0
56	MG	CA	3074	1/1	0.93	0.18	54,54,54,54	0
56	MG	AA	3008	1/1	0.93	0.41	54,54,54,54	0
56	MG	DA	3280	1/1	0.93	0.20	57,57,57,57	0
56	MG	DA	3474	1/1	0.93	0.08	61,61,61,61	0
56	MG	DA	3144	1/1	0.93	0.39	36,36,36,36	0
56	MG	BA	3684	1/1	0.93	0.17	58,58,58,58	0
56	MG	DA	3415	1/1	0.93	0.25	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	CA	3099	1/1	0.93	0.33	65,65,65,65	0
56	MG	CA	3087	1/1	0.93	0.19	41,41,41,41	0
56	MG	BA	3050	1/1	0.93	0.15	21,21,21,21	0
56	MG	AA	3026	1/1	0.93	0.17	41,41,41,41	0
56	MG	DA	3556	1/1	0.93	0.08	56,56,56,56	0
56	MG	BA	3446	1/1	0.93	0.13	49,49,49,49	0
56	MG	DA	3303	1/1	0.93	0.17	47,47,47,47	0
56	MG	BX	3001	1/1	0.93	0.29	55,55,55,55	0
56	MG	CA	3141	1/1	0.93	0.25	70,70,70,70	0
56	MG	AA	3189	1/1	0.93	0.10	77,77,77,77	0
56	MG	AA	3202	1/1	0.93	0.23	76,76,76,76	0
56	MG	DA	3443	1/1	0.93	0.17	53,53,53,53	0
56	MG	BA	3640	1/1	0.93	0.25	60,60,60,60	0
56	MG	DA	3212	1/1	0.93	0.09	48,48,48,48	0
56	MG	BA	3728	1/1	0.93	0.52	32,32,32,32	0
56	MG	DA	3373	1/1	0.93	0.23	29,29,29,29	0
56	MG	BA	3408	1/1	0.93	0.15	24,24,24,24	0
56	MG	AA	3146	1/1	0.93	0.20	48,48,48,48	0
56	MG	DA	3002	1/1	0.93	0.19	55,55,55,55	0
56	MG	DA	3643	1/1	0.93	0.72	53,53,53,53	0
56	MG	AA	3173	1/1	0.93	0.24	32,32,32,32	0
56	MG	BW	205	1/1	0.93	0.46	41,41,41,41	0
56	MG	BA	3028	1/1	0.93	0.21	48,48,48,48	0
56	MG	BA	3030	1/1	0.93	0.43	51,51,51,51	0
56	MG	DA	3527	1/1	0.93	0.10	46,46,46,46	0
56	MG	DA	3437	1/1	0.93	0.14	49,49,49,49	0
56	MG	AV	101	1/1	0.93	0.17	36,36,36,36	0
56	MG	BA	3722	1/1	0.93	0.17	32,32,32,32	0
56	MG	BA	3060	1/1	0.93	0.40	40,40,40,40	0
56	MG	BA	3153	1/1	0.93	0.32	35,35,35,35	0
56	MG	AA	3049	1/1	0.93	0.50	51,51,51,51	0
58	ZN	CN	501	1/1	0.93	0.12	108,108,108,108	0
56	MG	DA	3155	1/1	0.93	0.17	50,50,50,50	0
56	MG	DA	3559	1/1	0.93	0.19	46,46,46,46	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	3152	1/1	0.93	0.09	19,19,19,19	0
56	MG	DA	3580	1/1	0.93	0.14	46,46,46,46	0
56	MG	BA	3555	1/1	0.93	0.18	53,53,53,53	0
56	MG	BA	3704	1/1	0.93	0.19	85,85,85,85	0
56	MG	DD	308	1/1	0.93	0.15	55,55,55,55	0
56	MG	BA	3608	1/1	0.93	0.13	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	AA	3201	1/1	0.93	0.12	67,67,67,67	0
56	MG	DA	3015	1/1	0.93	0.26	49,49,49,49	0
56	MG	B3	103	1/1	0.93	0.62	41,41,41,41	0
56	MG	DA	3450	1/1	0.93	0.16	43,43,43,43	0
56	MG	AA	3167	1/1	0.93	0.19	67,67,67,67	0
56	MG	DA	3278	1/1	0.93	0.17	47,47,47,47	0
56	MG	BA	3724	1/1	0.93	0.19	58,58,58,58	0
56	MG	DA	3012	1/1	0.93	0.18	57,57,57,57	0
56	MG	AA	3177	1/1	0.93	0.14	80,80,80,80	0
56	MG	BB	3006	1/1	0.93	0.24	39,39,39,39	0
56	MG	AA	3068	1/1	0.93	0.08	66,66,66,66	0
56	MG	BA	3012	1/1	0.93	0.16	40,40,40,40	0
56	MG	CA	3089	1/1	0.93	0.15	52,52,52,52	0
56	MG	BA	3647	1/1	0.93	0.10	34,34,34,34	0
56	MG	BA	3250	1/1	0.93	0.21	45,45,45,45	0
56	MG	BA	3711	1/1	0.93	0.17	86,86,86,86	0
56	MG	BA	3716	1/1	0.93	0.11	27,27,27,27	0
56	MG	AA	3199	1/1	0.93	0.17	88,88,88,88	0
56	MG	BU	204	1/1	0.93	0.39	44,44,44,44	0
56	MG	DA	3255	1/1	0.93	0.20	40,40,40,40	0
56	MG	BA	3299	1/1	0.93	0.23	9,9,9,9	0
56	MG	BA	3592	1/1	0.93	0.17	28,28,28,28	0
56	MG	DA	3447	1/1	0.93	0.05	56,56,56,56	0
56	MG	BA	3193	1/1	0.93	0.57	52,52,52,52	0
56	MG	BA	3357	1/1	0.93	0.13	49,49,49,49	0
56	MG	BA	3190	1/1	0.93	0.20	42,42,42,42	0
56	MG	CA	3097	1/1	0.93	0.15	48,48,48,48	0
56	MG	DA	3472	1/1	0.93	0.17	36,36,36,36	0
56	MG	DA	3334	1/1	0.93	0.16	49,49,49,49	0
56	MG	DA	3076	1/1	0.93	0.56	44,44,44,44	0
56	MG	AA	3060	1/1	0.93	0.53	60,60,60,60	0
56	MG	DA	3627	1/1	0.93	0.21	43,43,43,43	0
56	MG	AA	3018	1/1	0.94	0.27	38,38,38,38	0
56	MG	BA	3535	1/1	0.94	0.19	37,37,37,37	0
56	MG	DA	3052	1/1	0.94	0.20	23,23,23,23	0
56	MG	DA	3207	1/1	0.94	0.13	58,58,58,58	0
56	MG	AA	3210	1/1	0.94	0.06	40,40,40,40	0
56	MG	DA	3646	1/1	0.94	0.07	38,38,38,38	0
56	MG	AA	3016	1/1	0.94	0.07	63,63,63,63	0
56	MG	BA	3091	1/1	0.94	0.60	45,45,45,45	0
56	MG	BA	3211	1/1	0.94	0.29	38,38,38,38	0
56	MG	AA	3112	1/1	0.94	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3074	1/1	0.94	0.08	42,42,42,42	0
56	MG	DA	3237	1/1	0.94	0.15	45,45,45,45	0
56	MG	DA	3362	1/1	0.94	0.13	41,41,41,41	0
56	MG	DA	3101	1/1	0.94	0.33	48,48,48,48	0
56	MG	BA	3293	1/1	0.94	0.18	45,45,45,45	0
56	MG	BD	305	1/1	0.94	0.23	48,48,48,48	0
56	MG	DA	3364	1/1	0.94	0.19	32,32,32,32	0
56	MG	DA	3196	1/1	0.94	0.34	44,44,44,44	0
56	MG	DF	305	1/1	0.94	0.73	39,39,39,39	0
56	MG	BA	3661	1/1	0.94	0.15	68,68,68,68	0
56	MG	BQ	202	1/1	0.94	0.30	28,28,28,28	0
56	MG	DY	502	1/1	0.94	0.10	60,60,60,60	0
56	MG	CA	3014	1/1	0.94	0.17	50,50,50,50	0
56	MG	BA	3635	1/1	0.94	0.10	78,78,78,78	0
56	MG	CA	3061	1/1	0.94	0.30	46,46,46,46	0
56	MG	AA	3053	1/1	0.94	0.33	49,49,49,49	0
56	MG	BA	3631	1/1	0.94	0.14	78,78,78,78	0
56	MG	DA	3574	1/1	0.94	0.17	56,56,56,56	0
56	MG	DE	305	1/1	0.94	0.64	65,65,65,65	0
56	MG	DA	3578	1/1	0.94	0.38	49,49,49,49	0
56	MG	BA	3185	1/1	0.94	0.20	47,47,47,47	0
56	MG	DQ	202	1/1	0.94	0.22	34,34,34,34	0
56	MG	DA	3393	1/1	0.94	0.19	41,41,41,41	0
56	MG	BA	3650	1/1	0.94	0.15	45,45,45,45	0
56	MG	BA	3344	1/1	0.94	0.09	30,30,30,30	0
56	MG	BA	3148	1/1	0.94	0.35	52,52,52,52	0
56	MG	BA	3419	1/1	0.94	0.14	24,24,24,24	0
56	MG	BA	3082	1/1	0.94	0.29	41,41,41,41	0
56	MG	DA	3137	1/1	0.94	0.27	56,56,56,56	0
56	MG	CA	3076	1/1	0.94	0.33	40,40,40,40	0
56	MG	BA	3057	1/1	0.94	0.27	35,35,35,35	0
56	MG	BA	3386	1/1	0.94	0.14	58,58,58,58	0
56	MG	DA	3285	1/1	0.94	0.26	55,55,55,55	0
56	MG	DA	3027	1/1	0.94	0.43	39,39,39,39	0
56	MG	BA	3377	1/1	0.94	0.14	32,32,32,32	0
56	MG	DA	3209	1/1	0.94	0.17	41,41,41,41	0
56	MG	BA	3086	1/1	0.94	0.33	49,49,49,49	0
56	MG	DA	3433	1/1	0.94	0.17	48,48,48,48	0
56	MG	BA	3546	1/1	0.94	0.31	48,48,48,48	0
56	MG	AA	3095	1/1	0.94	0.24	58,58,58,58	0
56	MG	CA	3058	1/1	0.94	0.10	40,40,40,40	0
56	MG	AM	3001	1/1	0.94	0.06	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3476	1/1	0.94	0.13	40,40,40,40	0
56	MG	BA	3511	1/1	0.94	0.16	39,39,39,39	0
56	MG	DA	3358	1/1	0.94	0.18	46,46,46,46	0
56	MG	CA	3116	1/1	0.94	0.17	76,76,76,76	0
56	MG	DD	305	1/1	0.94	0.64	49,49,49,49	0
56	MG	CA	3149	1/1	0.94	0.18	74,74,74,74	0
56	MG	BA	3573	1/1	0.94	0.16	56,56,56,56	0
56	MG	AA	3145	1/1	0.94	0.25	63,63,63,63	0
56	MG	BA	3161	1/1	0.94	0.65	49,49,49,49	0
56	MG	BA	3439	1/1	0.94	0.16	34,34,34,34	0
56	MG	DA	3229	1/1	0.94	0.11	40,40,40,40	0
56	MG	BA	3124	1/1	0.94	0.23	39,39,39,39	0
56	MG	BA	3304	1/1	0.94	0.19	49,49,49,49	0
56	MG	BA	3499	1/1	0.94	0.17	55,55,55,55	0
56	MG	BA	3084	1/1	0.94	0.14	33,33,33,33	0
56	MG	BA	3659	1/1	0.94	0.21	46,46,46,46	0
56	MG	AF	3001	1/1	0.94	0.17	61,61,61,61	0
56	MG	DA	3288	1/1	0.94	0.17	47,47,47,47	0
56	MG	DA	3539	1/1	0.94	0.17	53,53,53,53	0
56	MG	BA	3686	1/1	0.94	0.14	25,25,25,25	0
56	MG	DA	3100	1/1	0.94	0.50	56,56,56,56	0
56	MG	AA	3017	1/1	0.94	0.27	55,55,55,55	0
56	MG	BA	3079	1/1	0.94	0.28	42,42,42,42	0
56	MG	DB	3009	1/1	0.94	0.37	40,40,40,40	0
56	MG	DA	3038	1/1	0.94	0.15	39,39,39,39	0
56	MG	BA	3692	1/1	0.94	0.40	36,36,36,36	0
56	MG	DA	3435	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	DA	3378	1/1	0.94	0.15	45,45,45,45	0
56	MG	CA	3137	1/1	0.94	0.13	48,48,48,48	0
56	MG	DA	3510	1/1	0.94	0.23	63,63,63,63	0
56	MG	DA	3634	1/1	0.94	0.14	51,51,51,51	0
56	MG	DA	3164	1/1	0.94	0.26	48,48,48,48	0
56	MG	BA	3570	1/1	0.94	0.12	61,61,61,61	0
56	MG	DA	3063	1/1	0.94	0.12	52,52,52,52	0
56	MG	DA	3469	1/1	0.94	0.21	47,47,47,47	0
56	MG	DA	3106	1/1	0.94	0.21	41,41,41,41	0
56	MG	BA	3107	1/1	0.94	0.23	40,40,40,40	0
56	MG	DA	3392	1/1	0.94	0.17	35,35,35,35	0
56	MG	CA	3167	1/1	0.94	0.09	78,78,78,78	0
56	MG	BA	3610	1/1	0.94	0.21	40,40,40,40	0
56	MG	DA	3528	1/1	0.94	0.09	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	3449	1/1	0.94	0.12	21,21,21,21	0
56	MG	DR	202	1/1	0.94	0.18	37,37,37,37	0
56	MG	BA	3453	1/1	0.94	0.19	18,18,18,18	0
56	MG	DA	3442	1/1	0.94	0.19	40,40,40,40	0
56	MG	AA	3197	1/1	0.94	0.30	69,69,69,69	0
56	MG	DA	3127	1/1	0.94	0.09	48,48,48,48	0
56	MG	BA	3142	1/1	0.94	0.71	46,46,46,46	0
56	MG	DA	3090	1/1	0.94	0.34	47,47,47,47	0
56	MG	DA	3452	1/1	0.94	0.17	56,56,56,56	0
56	MG	AA	3010	1/1	0.94	0.37	70,70,70,70	0
56	MG	DA	3057	1/1	0.94	0.16	52,52,52,52	0
56	MG	DA	3114	1/1	0.94	0.19	37,37,37,37	0
56	MG	BA	3066	1/1	0.94	0.26	44,44,44,44	0
56	MG	DA	3156	1/1	0.94	0.56	29,29,29,29	0
56	MG	B0	104	1/1	0.94	0.10	43,43,43,43	0
56	MG	BB	3018	1/1	0.94	0.19	60,60,60,60	0
56	MG	DA	3175	1/1	0.94	0.17	40,40,40,40	0
56	MG	CA	3124	1/1	0.94	0.17	61,61,61,61	0
56	MG	BQ	205	1/1	0.94	0.42	49,49,49,49	0
56	MG	CA	3044	1/1	0.94	0.20	63,63,63,63	0
56	MG	BA	3178	1/1	0.94	0.28	48,48,48,48	0
56	MG	BA	3261	1/1	0.94	0.26	34,34,34,34	0
56	MG	BA	3306	1/1	0.94	0.14	48,48,48,48	0
56	MG	BA	3565	1/1	0.94	0.11	55,55,55,55	0
56	MG	DA	3572	1/1	0.94	0.11	53,53,53,53	0
56	MG	BA	3465	1/1	0.94	0.12	40,40,40,40	0
56	MG	DA	3146	1/1	0.94	0.18	34,34,34,34	0
56	MG	BD	307	1/1	0.94	0.20	43,43,43,43	0
56	MG	BA	3417	1/1	0.94	0.18	18,18,18,18	0
56	MG	BA	3412	1/1	0.94	0.18	26,26,26,26	0
56	MG	DA	3383	1/1	0.94	0.09	56,56,56,56	0
56	MG	BA	3278	1/1	0.94	0.17	34,34,34,34	0
56	MG	DA	3552	1/1	0.94	0.12	34,34,34,34	0
56	MG	DA	3564	1/1	0.94	0.77	61,61,61,61	0
56	MG	BR	202	1/1	0.94	0.29	27,27,27,27	0
56	MG	DA	3347	1/1	0.94	0.19	62,62,62,62	0
56	MG	DA	3501	1/1	0.94	0.20	23,23,23,23	0
56	MG	BA	3259	1/1	0.94	0.49	27,27,27,27	0
56	MG	DA	3016	1/1	0.94	0.27	37,37,37,37	0
56	MG	BY	201	1/1	0.94	0.43	58,58,58,58	0
56	MG	BA	3431	1/1	0.94	0.23	17,17,17,17	0
56	MG	AA	3109	1/1	0.94	0.33	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3018	1/1	0.94	0.34	40,40,40,40	0
56	MG	AA	3209	1/1	0.94	0.40	70,70,70,70	0
56	MG	BA	3482	1/1	0.94	0.17	72,72,72,72	0
56	MG	BA	3717	1/1	0.94	0.22	57,57,57,57	0
56	MG	DA	3204	1/1	0.94	0.41	34,34,34,34	0
56	MG	BA	3044	1/1	0.94	0.30	42,42,42,42	0
56	MG	BA	3688	1/1	0.94	0.11	54,54,54,54	0
56	MG	DB	3008	1/1	0.94	0.09	45,45,45,45	0
56	MG	DA	3617	1/1	0.94	0.19	58,58,58,58	0
56	MG	AA	3054	1/1	0.94	0.20	45,45,45,45	0
56	MG	CA	3084	1/1	0.94	0.11	64,64,64,64	0
56	MG	BA	3301	1/1	0.94	0.13	56,56,56,56	0
56	MG	CF	3001	1/1	0.94	0.22	55,55,55,55	0
56	MG	DA	3494	1/1	0.95	0.09	78,78,78,78	0
56	MG	CA	3013	1/1	0.95	0.12	51,51,51,51	0
56	MG	DA	3325	1/1	0.95	0.17	36,36,36,36	0
56	MG	BA	3014	1/1	0.95	0.77	34,34,34,34	0
56	MG	BA	3358	1/1	0.95	0.09	33,33,33,33	0
56	MG	DA	3534	1/1	0.95	0.19	45,45,45,45	0
56	MG	BA	3138	1/1	0.95	0.17	46,46,46,46	0
56	MG	DA	3220	1/1	0.95	0.12	37,37,37,37	0
56	MG	BA	3145	1/1	0.95	0.40	38,38,38,38	0
56	MG	BA	3422	1/1	0.95	0.23	42,42,42,42	0
56	MG	BA	3639	1/1	0.95	0.16	50,50,50,50	0
56	MG	BA	3421	1/1	0.95	0.12	36,36,36,36	0
56	MG	DB	3010	1/1	0.95	0.18	73,73,73,73	0
56	MG	CA	3102	1/1	0.95	0.09	41,41,41,41	0
56	MG	DD	301	1/1	0.95	0.32	46,46,46,46	0
56	MG	DA	3507	1/1	0.95	0.15	54,54,54,54	0
56	MG	DA	3297	1/1	0.95	0.14	57,57,57,57	0
56	MG	DA	3017	1/1	0.95	0.16	46,46,46,46	0
56	MG	DA	3511	1/1	0.95	0.08	65,65,65,65	0
56	MG	DA	3490	1/1	0.95	0.10	39,39,39,39	0
56	MG	BA	3353	1/1	0.95	0.24	57,57,57,57	0
56	MG	DA	3353	1/1	0.95	0.10	62,62,62,62	0
56	MG	DA	3319	1/1	0.95	0.18	53,53,53,53	0
56	MG	AA	3196	1/1	0.95	0.31	65,65,65,65	0
56	MG	BA	3053	1/1	0.95	0.35	39,39,39,39	0
56	MG	DA	3382	1/1	0.95	0.14	25,25,25,25	0
56	MG	BA	3645	1/1	0.95	0.09	56,56,56,56	0
56	MG	DA	3329	1/1	0.95	0.16	53,53,53,53	0
56	MG	DA	3047	1/1	0.95	0.08	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	BG	3004	1/1	0.95	0.04	62,62,62,62	0
56	MG	AA	3130	1/1	0.95	0.23	46,46,46,46	0
56	MG	DA	3197	1/1	0.95	0.45	36,36,36,36	0
56	MG	BA	3510	1/1	0.95	0.24	40,40,40,40	0
56	MG	BA	3594	1/1	0.95	0.31	42,42,42,42	0
56	MG	BA	3326	1/1	0.95	0.08	41,41,41,41	0
56	MG	AA	3155	1/1	0.95	0.16	70,70,70,70	0
56	MG	BA	3595	1/1	0.95	0.16	41,41,41,41	0
56	MG	BA	3498	1/1	0.95	0.15	39,39,39,39	0
56	MG	DA	3516	1/1	0.95	0.17	40,40,40,40	0
56	MG	DA	3055	1/1	0.95	0.21	48,48,48,48	0
56	MG	DA	3520	1/1	0.95	0.20	51,51,51,51	0
56	MG	BA	3672	1/1	0.95	0.30	48,48,48,48	0
56	MG	B5	502	1/1	0.95	0.10	54,54,54,54	0
56	MG	BA	3397	1/1	0.95	0.19	28,28,28,28	0
56	MG	BA	3233	1/1	0.95	0.18	47,47,47,47	0
56	MG	DA	3479	1/1	0.95	0.19	57,57,57,57	0
56	MG	DA	3121	1/1	0.95	0.19	48,48,48,48	0
56	MG	BA	3461	1/1	0.95	0.24	36,36,36,36	0
56	MG	BA	3312	1/1	0.95	0.10	58,58,58,58	0
56	MG	DA	3283	1/1	0.95	0.21	33,33,33,33	0
56	MG	BA	3330	1/1	0.95	0.16	39,39,39,39	0
56	MG	AA	3007	1/1	0.95	0.19	82,82,82,82	0
56	MG	AA	3187	1/1	0.95	0.04	62,62,62,62	0
56	MG	BA	3078	1/1	0.95	0.26	17,17,17,17	0
56	MG	BA	3545	1/1	0.95	0.24	47,47,47,47	0
56	MG	DA	3267	1/1	0.95	0.17	61,61,61,61	0
56	MG	DA	3001	1/1	0.95	0.30	78,78,78,78	0
56	MG	DA	3004	1/1	0.95	0.19	29,29,29,29	0
56	MG	BA	3348	1/1	0.95	0.20	64,64,64,64	0
56	MG	BA	3605	1/1	0.95	0.30	59,59,59,59	0
56	MG	BA	3580	1/1	0.95	0.12	58,58,58,58	0
56	MG	BA	3588	1/1	0.95	0.21	48,48,48,48	0
56	MG	BA	3576	1/1	0.95	0.26	23,23,23,23	0
56	MG	CA	3082	1/1	0.95	0.08	47,47,47,47	0
56	MG	BA	3697	1/1	0.95	0.14	78,78,78,78	0
56	MG	BV	202	1/1	0.95	0.44	56,56,56,56	0
56	MG	DA	3245	1/1	0.95	0.15	37,37,37,37	0
56	MG	DA	3261	1/1	0.95	0.22	35,35,35,35	0
56	MG	DA	3406	1/1	0.95	0.12	40,40,40,40	0
56	MG	DA	3138	1/1	0.95	0.22	42,42,42,42	0
56	MG	BA	3563	1/1	0.95	0.21	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3042	1/1	0.95	0.76	47,47,47,47	0
56	MG	BA	3548	1/1	0.95	0.22	50,50,50,50	0
56	MG	BA	3547	1/1	0.95	0.18	31,31,31,31	0
56	MG	BU	208	1/1	0.95	0.88	56,56,56,56	0
56	MG	DA	3550	1/1	0.95	0.17	53,53,53,53	0
56	MG	DA	3407	1/1	0.95	0.24	21,21,21,21	0
56	MG	CA	3156	1/1	0.95	0.15	70,70,70,70	0
56	MG	DA	3216	1/1	0.95	0.17	31,31,31,31	0
56	MG	BA	3700	1/1	0.95	0.12	67,67,67,67	0
56	MG	BA	3470	1/1	0.95	0.24	54,54,54,54	0
56	MG	DA	3306	1/1	0.95	0.21	33,33,33,33	0
56	MG	BA	3202	1/1	0.95	0.24	41,41,41,41	0
56	MG	DD	306	1/1	0.95	1.14	44,44,44,44	0
56	MG	AX	104	1/1	0.95	0.14	76,76,76,76	0
56	MG	BA	3627	1/1	0.95	0.20	50,50,50,50	0
56	MG	BA	3271	1/1	0.95	0.12	36,36,36,36	0
56	MG	DA	3614	1/1	0.95	0.20	48,48,48,48	0
56	MG	DA	3010	1/1	0.95	0.14	39,39,39,39	0
56	MG	AA	3070	1/1	0.95	0.10	75,75,75,75	0
56	MG	BA	3484	1/1	0.95	0.17	54,54,54,54	0
56	MG	BA	3628	1/1	0.95	0.21	41,41,41,41	0
56	MG	DA	3141	1/1	0.95	0.13	62,62,62,62	0
56	MG	DA	3451	1/1	0.95	0.07	49,49,49,49	0
56	MG	AA	3195	1/1	0.95	0.16	71,71,71,71	0
56	MG	BA	3339	1/1	0.95	0.22	43,43,43,43	0
56	MG	DA	3118	1/1	0.95	0.10	39,39,39,39	0
56	MG	AA	3056	1/1	0.95	0.19	39,39,39,39	0
56	MG	CA	3020	1/1	0.95	0.18	47,47,47,47	0
56	MG	BA	3201	1/1	0.95	0.29	36,36,36,36	0
56	MG	AA	3168	1/1	0.95	0.31	68,68,68,68	0
56	MG	AA	3083	1/1	0.95	0.09	65,65,65,65	0
56	MG	DA	3555	1/1	0.95	0.12	41,41,41,41	0
56	MG	DB	3006	1/1	0.95	0.13	42,42,42,42	0
56	MG	BA	3286	1/1	0.95	0.26	32,32,32,32	0
56	MG	BA	3129	1/1	0.95	0.25	36,36,36,36	0
56	MG	DA	3648	1/1	0.95	0.17	52,52,52,52	0
56	MG	BA	3284	1/1	0.95	0.10	54,54,54,54	0
56	MG	BV	203	1/1	0.95	1.03	46,46,46,46	0
56	MG	BA	3037	1/1	0.95	0.20	31,31,31,31	0
56	MG	DE	306	1/1	0.95	0.14	32,32,32,32	0
56	MG	AA	3213	1/1	0.95	0.16	29,29,29,29	0
56	MG	CA	3011	1/1	0.95	0.28	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	3040	1/1	0.95	0.12	55,55,55,55	0
56	MG	BA	3332	1/1	0.95	0.19	39,39,39,39	0
56	MG	AA	3078	1/1	0.95	0.27	42,42,42,42	0
56	MG	BA	3229	1/1	0.95	0.15	22,22,22,22	0
56	MG	DA	3030	1/1	0.95	0.28	51,51,51,51	0
56	MG	DA	3322	1/1	0.95	0.13	55,55,55,55	0
56	MG	BA	3506	1/1	0.95	0.14	30,30,30,30	0
56	MG	CA	3090	1/1	0.95	0.18	73,73,73,73	0
56	MG	DA	3298	1/1	0.95	0.32	37,37,37,37	0
56	MG	D5	102	1/1	0.95	0.58	55,55,55,55	0
56	MG	AA	3064	1/1	0.95	0.30	79,79,79,79	0
56	MG	BA	3441	1/1	0.95	0.25	25,25,25,25	0
56	MG	BA	3620	1/1	0.95	0.12	47,47,47,47	0
56	MG	AA	3111	1/1	0.95	0.17	95,95,95,95	0
56	MG	DA	3396	1/1	0.95	0.19	35,35,35,35	0
56	MG	CA	3108	1/1	0.95	0.21	52,52,52,52	0
56	MG	DA	3506	1/1	0.95	0.07	59,59,59,59	0
56	MG	DA	3154	1/1	0.95	0.61	45,45,45,45	0
56	MG	AA	3126	1/1	0.95	0.16	54,54,54,54	0
56	MG	BA	3169	1/1	0.95	0.70	46,46,46,46	0
56	MG	BA	3224	1/1	0.95	0.73	64,64,64,64	0
56	MG	DA	3535	1/1	0.95	0.19	33,33,33,33	0
56	MG	DA	3601	1/1	0.95	0.12	77,77,77,77	0
56	MG	AA	3216	1/1	0.95	0.14	58,58,58,58	0
56	MG	BA	3189	1/1	0.95	0.16	54,54,54,54	0
56	MG	BA	3540	1/1	0.95	0.27	34,34,34,34	0
56	MG	BA	3097	1/1	0.95	0.19	33,33,33,33	0
56	MG	DA	3619	1/1	0.95	0.22	48,48,48,48	0
56	MG	DA	3522	1/1	0.95	0.17	61,61,61,61	0
56	MG	BA	3041	1/1	0.95	0.38	32,32,32,32	0
56	MG	DA	3083	1/1	0.95	0.25	41,41,41,41	0
56	MG	DA	3350	1/1	0.95	0.04	32,32,32,32	0
56	MG	DA	3232	1/1	0.95	0.25	50,50,50,50	0
56	MG	BA	3260	1/1	0.95	0.17	22,22,22,22	0
56	MG	BA	3541	1/1	0.95	0.23	30,30,30,30	0
56	MG	DA	3384	1/1	0.95	0.11	23,23,23,23	0
56	MG	DA	3654	1/1	0.95	0.17	52,52,52,52	0
56	MG	CA	3094	1/1	0.95	0.18	43,43,43,43	0
56	MG	BA	3276	1/1	0.95	0.32	40,40,40,40	0
56	MG	DA	3034	1/1	0.95	0.15	40,40,40,40	0
56	MG	DB	3002	1/1	0.95	0.25	56,56,56,56	0
56	MG	DA	3120	1/1	0.95	0.76	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3299	1/1	0.95	0.22	40,40,40,40	0
56	MG	DA	3444	1/1	0.95	0.13	43,43,43,43	0
56	MG	BA	3004	1/1	0.95	0.12	24,24,24,24	0
56	MG	DA	3558	1/1	0.95	0.18	37,37,37,37	0
56	MG	DA	3570	1/1	0.95	0.22	28,28,28,28	0
56	MG	DA	3566	1/1	0.95	0.14	71,71,71,71	0
56	MG	BA	3616	1/1	0.95	0.10	33,33,33,33	0
56	MG	DA	3263	1/1	0.95	0.19	31,31,31,31	0
56	MG	CA	3075	1/1	0.95	0.17	76,76,76,76	0
56	MG	BE	307	1/1	0.95	0.24	39,39,39,39	0
56	MG	BA	3618	1/1	0.95	0.27	46,46,46,46	0
56	MG	DA	3585	1/1	0.95	0.15	62,62,62,62	0
56	MG	DA	3589	1/1	0.95	0.18	59,59,59,59	0
56	MG	AA	3170	1/1	0.95	0.16	101,101,101,101	0
56	MG	DA	3130	1/1	0.95	0.12	32,32,32,32	0
56	MG	BN	3005	1/1	0.95	0.85	52,52,52,52	0
56	MG	DA	3434	1/1	0.95	0.26	49,49,49,49	0
56	MG	DA	3565	1/1	0.95	0.07	57,57,57,57	0
56	MG	BA	3500	1/1	0.95	0.15	37,37,37,37	0
56	MG	BA	3603	1/1	0.95	0.08	39,39,39,39	0
56	MG	BA	3059	1/1	0.95	0.60	45,45,45,45	0
56	MG	DA	3626	1/1	0.95	0.07	68,68,68,68	0
56	MG	DA	3411	1/1	0.95	0.17	21,21,21,21	0
56	MG	BA	3043	1/1	0.95	0.17	52,52,52,52	0
56	MG	BA	3101	1/1	0.95	0.17	35,35,35,35	0
56	MG	DA	3031	1/1	0.95	0.29	55,55,55,55	0
56	MG	AA	3148	1/1	0.95	0.21	66,66,66,66	0
56	MG	DA	3307	1/1	0.95	0.30	37,37,37,37	0
56	MG	BU	202	1/1	0.95	0.36	32,32,32,32	0
56	MG	BP	201	1/1	0.95	0.66	40,40,40,40	0
56	MG	DA	3576	1/1	0.95	0.15	38,38,38,38	0
56	MG	CA	3066	1/1	0.95	0.10	55,55,55,55	0
56	MG	DA	3595	1/1	0.95	0.18	72,72,72,72	0
56	MG	AA	3122	1/1	0.95	0.54	44,44,44,44	0
56	MG	BA	3073	1/1	0.95	0.85	41,41,41,41	0
56	MG	CA	3009	1/1	0.95	0.14	47,47,47,47	0
56	MG	BA	3674	1/1	0.95	0.18	55,55,55,55	0
56	MG	BA	3654	1/1	0.95	0.16	25,25,25,25	0
56	MG	DA	3021	1/1	0.95	0.15	35,35,35,35	0
56	MG	BA	3426	1/1	0.96	0.27	51,51,51,51	0
56	MG	BA	3709	1/1	0.96	0.12	86,86,86,86	0
56	MG	BA	3324	1/1	0.96	0.18	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	3422	1/1	0.96	0.11	38,38,38,38	0
56	MG	DA	3007	1/1	0.96	0.23	30,30,30,30	0
56	MG	D3	101	1/1	0.96	0.45	63,63,63,63	0
56	MG	DA	3276	1/1	0.96	0.22	36,36,36,36	0
56	MG	BA	3630	1/1	0.96	0.25	52,52,52,52	0
56	MG	DA	3417	1/1	0.96	0.15	34,34,34,34	0
56	MG	BA	3385	1/1	0.96	0.24	26,26,26,26	0
56	MG	DA	3270	1/1	0.96	0.20	36,36,36,36	0
56	MG	BA	3199	1/1	0.96	0.46	36,36,36,36	0
56	MG	DA	3259	1/1	0.96	0.15	47,47,47,47	0
56	MG	CA	3028	1/1	0.96	0.44	43,43,43,43	0
56	MG	BA	3413	1/1	0.96	0.14	20,20,20,20	0
56	MG	BA	3405	1/1	0.96	0.14	34,34,34,34	0
56	MG	AA	3178	1/1	0.96	0.18	65,65,65,65	0
56	MG	AA	3157	1/1	0.96	0.08	35,35,35,35	0
56	MG	CA	3132	1/1	0.96	0.11	70,70,70,70	0
56	MG	DA	3082	1/1	0.96	0.10	19,19,19,19	0
56	MG	DA	3606	1/1	0.96	0.10	58,58,58,58	0
56	MG	DA	3182	1/1	0.96	0.16	32,32,32,32	0
56	MG	BA	3440	1/1	0.96	0.40	38,38,38,38	0
56	MG	BA	3512	1/1	0.96	0.23	40,40,40,40	0
56	MG	DA	3348	1/1	0.96	0.32	37,37,37,37	0
56	MG	BA	3395	1/1	0.96	0.20	25,25,25,25	0
56	MG	BA	3366	1/1	0.96	0.09	63,63,63,63	0
56	MG	DA	3416	1/1	0.96	0.07	44,44,44,44	0
56	MG	BA	3524	1/1	0.96	0.25	55,55,55,55	0
56	MG	BA	3223	1/1	0.96	0.68	47,47,47,47	0
56	MG	CA	3113	1/1	0.96	0.23	77,77,77,77	0
56	MG	BA	3367	1/1	0.96	0.15	50,50,50,50	0
56	MG	BA	3615	1/1	0.96	0.17	36,36,36,36	0
56	MG	BA	3537	1/1	0.96	0.38	31,31,31,31	0
56	MG	BA	3217	1/1	0.96	0.09	28,28,28,28	0
56	MG	DA	3486	1/1	0.96	0.12	38,38,38,38	0
56	MG	DA	3321	1/1	0.96	0.23	41,41,41,41	0
56	MG	DA	3409	1/1	0.96	0.15	32,32,32,32	0
56	MG	BA	3035	1/1	0.96	0.09	37,37,37,37	0
56	MG	BA	3651	1/1	0.96	0.13	45,45,45,45	0
56	MG	DE	301	1/1	0.96	0.61	51,51,51,51	0
56	MG	BV	204	1/1	0.96	0.20	20,20,20,20	0
56	MG	DA	3607	1/1	0.96	0.10	45,45,45,45	0
56	MG	DA	3463	1/1	0.96	0.37	43,43,43,43	0
56	MG	BA	3538	1/1	0.96	0.15	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	BA	3368	1/1	0.96	0.20	35,35,35,35	0
56	MG	DA	3568	1/1	0.96	0.10	42,42,42,42	0
56	MG	DB	3004	1/1	0.96	0.14	68,68,68,68	0
56	MG	BA	3380	1/1	0.96	0.13	53,53,53,53	0
56	MG	CA	3145	1/1	0.96	0.08	43,43,43,43	0
56	MG	BA	3191	1/1	0.96	0.19	52,52,52,52	0
56	MG	BA	3076	1/1	0.96	0.23	41,41,41,41	0
56	MG	BA	3584	1/1	0.96	0.18	22,22,22,22	0
56	MG	BA	3649	1/1	0.96	0.17	66,66,66,66	0
56	MG	BA	3121	1/1	0.96	0.27	57,57,57,57	0
56	MG	BA	3118	1/1	0.96	0.19	39,39,39,39	0
56	MG	AA	3175	1/1	0.96	0.14	76,76,76,76	0
56	MG	CA	3026	1/1	0.96	0.07	52,52,52,52	0
56	MG	DA	3420	1/1	0.96	0.13	51,51,51,51	0
56	MG	BA	3234	1/1	0.96	0.30	55,55,55,55	0
56	MG	BB	3002	1/1	0.96	0.19	59,59,59,59	0
56	MG	BA	3130	1/1	0.96	0.58	43,43,43,43	0
56	MG	BA	3176	1/1	0.96	0.19	38,38,38,38	0
56	MG	BA	3117	1/1	0.96	0.24	25,25,25,25	0
56	MG	DA	3403	1/1	0.96	0.14	28,28,28,28	0
56	MG	CA	3096	1/1	0.96	0.10	60,60,60,60	0
56	MG	DA	3485	1/1	0.96	0.09	38,38,38,38	0
56	MG	BA	3266	1/1	0.96	0.33	46,46,46,46	0
56	MG	DA	3341	1/1	0.96	0.19	23,23,23,23	0
56	MG	BA	3151	1/1	0.96	0.06	52,52,52,52	0
56	MG	BA	3665	1/1	0.96	0.21	39,39,39,39	0
56	MG	BA	3021	1/1	0.96	0.27	42,42,42,42	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	BA	3542	1/1	0.96	0.23	19,19,19,19	0
56	MG	DA	3429	1/1	0.96	0.18	44,44,44,44	0
56	MG	DA	3203	1/1	0.96	0.13	41,41,41,41	0
56	MG	DA	3247	1/1	0.96	0.08	31,31,31,31	0
56	MG	DA	3642	1/1	0.96	0.13	35,35,35,35	0
56	MG	BA	3477	1/1	0.96	0.11	25,25,25,25	0
56	MG	BA	3340	1/1	0.96	0.13	57,57,57,57	0
56	MG	AA	3055	1/1	0.96	0.20	50,50,50,50	0
56	MG	BA	3551	1/1	0.96	0.22	25,25,25,25	0
56	MG	BE	301	1/1	0.96	0.56	43,43,43,43	0
56	MG	BA	3488	1/1	0.96	0.35	35,35,35,35	0
56	MG	DA	3637	1/1	0.96	0.28	48,48,48,48	0
56	MG	BA	3685	1/1	0.96	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3108	1/1	0.96	0.47	67,67,67,67	0
56	MG	BA	3054	1/1	0.96	0.29	46,46,46,46	0
56	MG	BA	3606	1/1	0.96	0.23	25,25,25,25	0
56	MG	DA	3622	1/1	0.96	0.08	55,55,55,55	0
56	MG	DA	3153	1/1	0.96	0.20	38,38,38,38	0
56	MG	DA	3201	1/1	0.96	0.12	48,48,48,48	0
56	MG	BA	3472	1/1	0.96	0.08	30,30,30,30	0
56	MG	DA	3641	1/1	0.96	0.43	61,61,61,61	0
56	MG	BA	3737	1/1	0.96	0.25	60,60,60,60	0
56	MG	DV	201	1/1	0.96	0.38	55,55,55,55	0
56	MG	DA	3248	1/1	0.96	0.29	51,51,51,51	0
56	MG	BA	3715	1/1	0.96	0.13	47,47,47,47	0
56	MG	DN	5001	1/1	0.96	0.12	75,75,75,75	0
56	MG	DA	3289	1/1	0.96	0.13	26,26,26,26	0
56	MG	DA	3491	1/1	0.96	0.15	56,56,56,56	0
56	MG	BD	309	1/1	0.96	0.14	42,42,42,42	0
56	MG	DA	3605	1/1	0.96	0.15	44,44,44,44	0
56	MG	DA	3166	1/1	0.96	0.08	32,32,32,32	0
56	MG	BA	3361	1/1	0.96	0.26	34,34,34,34	0
56	MG	DA	3381	1/1	0.96	0.27	47,47,47,47	0
56	MG	BA	3571	1/1	0.96	0.08	65,65,65,65	0
56	MG	DF	306	1/1	0.96	0.23	50,50,50,50	0
56	MG	BA	3013	1/1	0.96	0.14	40,40,40,40	0
56	MG	DA	3158	1/1	0.96	0.34	57,57,57,57	0
56	MG	DA	3386	1/1	0.96	0.18	56,56,56,56	0
56	MG	DA	3439	1/1	0.96	0.19	28,28,28,28	0
56	MG	DA	3629	1/1	0.96	0.17	19,19,19,19	0
56	MG	DA	3399	1/1	0.96	0.19	41,41,41,41	0
56	MG	BG	3003	1/1	0.96	0.15	42,42,42,42	0
56	MG	BA	3503	1/1	0.96	0.28	31,31,31,31	0
56	MG	BA	3213	1/1	0.96	0.05	41,41,41,41	0
56	MG	BA	3109	1/1	0.96	0.09	36,36,36,36	0
56	MG	DA	3557	1/1	0.96	0.12	45,45,45,45	0
56	MG	BA	3485	1/1	0.96	0.29	44,44,44,44	0
56	MG	DA	3257	1/1	0.96	0.10	48,48,48,48	0
56	MG	BA	3513	1/1	0.96	0.11	45,45,45,45	0
56	MG	DA	3432	1/1	0.96	0.27	66,66,66,66	0
56	MG	DE	304	1/1	0.96	0.20	41,41,41,41	0
56	MG	DA	3091	1/1	0.96	0.38	44,44,44,44	0
56	MG	DA	3311	1/1	0.96	0.09	32,32,32,32	0
56	MG	BA	3219	1/1	0.96	0.22	65,65,65,65	0
56	MG	DA	3397	1/1	0.96	0.18	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	3291	1/1	0.96	0.17	41,41,41,41	0
56	MG	BA	3001	1/1	0.96	0.15	69,69,69,69	0
56	MG	BA	3642	1/1	0.96	0.24	51,51,51,51	0
56	MG	AD	502	1/1	0.96	0.46	43,43,43,43	0
56	MG	AA	3104	1/1	0.96	0.16	37,37,37,37	0
56	MG	BA	3015	1/1	0.96	0.34	44,44,44,44	0
56	MG	BA	3384	1/1	0.96	0.39	60,60,60,60	0
56	MG	CA	3095	1/1	0.96	0.11	39,39,39,39	0
56	MG	BA	3112	1/1	0.96	0.09	38,38,38,38	0
56	MG	BA	3561	1/1	0.96	0.19	24,24,24,24	0
56	MG	BA	3648	1/1	0.96	0.30	49,49,49,49	0
56	MG	AA	3099	1/1	0.96	0.42	60,60,60,60	0
56	MG	DA	3457	1/1	0.96	0.12	37,37,37,37	0
56	MG	DA	3333	1/1	0.96	0.24	58,58,58,58	0
56	MG	BD	302	1/1	0.96	0.36	58,58,58,58	0
56	MG	BA	3726	1/1	0.96	0.55	47,47,47,47	0
56	MG	AA	3021	1/1	0.96	0.20	76,76,76,76	0
56	MG	DA	3530	1/1	0.96	0.15	49,49,49,49	0
56	MG	AA	3183	1/1	0.96	0.10	42,42,42,42	0
56	MG	BA	3497	1/1	0.96	0.14	62,62,62,62	0
56	MG	CA	3115	1/1	0.96	0.09	55,55,55,55	0
56	MG	AA	3107	1/1	0.96	0.31	44,44,44,44	0
56	MG	BA	3707	1/1	0.96	0.20	36,36,36,36	0
56	MG	DA	3639	1/1	0.96	0.30	15,15,15,15	0
56	MG	DA	3513	1/1	0.96	0.22	49,49,49,49	0
56	MG	BB	3007	1/1	0.96	0.09	47,47,47,47	0
56	MG	AA	3161	1/1	0.96	0.12	72,72,72,72	0
56	MG	BA	3265	1/1	0.96	0.11	20,20,20,20	0
56	MG	DA	3468	1/1	0.96	0.14	48,48,48,48	0
56	MG	DA	3389	1/1	0.96	0.28	27,27,27,27	0
56	MG	BP	204	1/1	0.96	0.17	55,55,55,55	0
56	MG	DA	3039	1/1	0.96	0.40	59,59,59,59	0
56	MG	DA	3094	1/1	0.96	0.18	26,26,26,26	0
56	MG	BA	3625	1/1	0.96	0.13	51,51,51,51	0
56	MG	BA	3543	1/1	0.96	0.29	52,52,52,52	0
56	MG	AA	3174	1/1	0.96	0.22	33,33,33,33	0
56	MG	DA	3152	1/1	0.96	0.23	50,50,50,50	0
56	MG	BA	3607	1/1	0.96	0.43	53,53,53,53	0
56	MG	DA	3266	1/1	0.96	0.23	43,43,43,43	0
56	MG	CA	3072	1/1	0.96	0.22	38,38,38,38	0
56	MG	BW	202	1/1	0.96	0.18	34,34,34,34	0
56	MG	DA	3249	1/1	0.96	0.21	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3575	1/1	0.96	0.19	43,43,43,43	0
56	MG	BA	3663	1/1	0.96	0.23	56,56,56,56	0
56	MG	DA	3178	1/1	0.96	0.37	43,43,43,43	0
56	MG	DA	3235	1/1	0.96	0.19	50,50,50,50	0
56	MG	DA	3206	1/1	0.96	0.26	42,42,42,42	0
56	MG	DA	3498	1/1	0.96	0.18	56,56,56,56	0
56	MG	DA	3577	1/1	0.96	0.25	44,44,44,44	0
56	MG	BA	3343	1/1	0.96	0.19	40,40,40,40	0
56	MG	AA	3153	1/1	0.96	0.13	45,45,45,45	0
58	ZN	D9	501	1/1	0.96	0.05	66,66,66,66	0
56	MG	DA	3633	1/1	0.96	0.20	54,54,54,54	0
56	MG	BA	3025	1/1	0.96	0.25	28,28,28,28	0
56	MG	BA	3483	1/1	0.96	0.26	53,53,53,53	0
56	MG	BW	204	1/1	0.96	0.35	35,35,35,35	0
56	MG	BA	3575	1/1	0.96	0.19	51,51,51,51	0
56	MG	DA	3425	1/1	0.96	0.11	27,27,27,27	0
56	MG	BA	3566	1/1	0.96	0.09	53,53,53,53	0
56	MG	DA	3518	1/1	0.96	0.20	40,40,40,40	0
56	MG	DA	3426	1/1	0.96	0.15	74,74,74,74	0
56	MG	DA	3287	1/1	0.96	0.27	53,53,53,53	0
56	MG	CA	3012	1/1	0.96	0.12	49,49,49,49	0
56	MG	BA	3345	1/1	0.96	0.21	33,33,33,33	0
56	MG	BA	3458	1/1	0.96	0.12	29,29,29,29	0
56	MG	BA	3425	1/1	0.96	0.36	36,36,36,36	0
56	MG	DA	3265	1/1	0.96	0.27	51,51,51,51	0
56	MG	BA	3657	1/1	0.96	0.16	56,56,56,56	0
56	MG	BA	3536	1/1	0.96	0.14	27,27,27,27	0
56	MG	BA	3504	1/1	0.96	0.29	41,41,41,41	0
56	MG	DA	3628	1/1	0.96	0.22	63,63,63,63	0
56	MG	BA	3362	1/1	0.96	0.09	43,43,43,43	0
56	MG	DA	3133	1/1	0.96	0.15	33,33,33,33	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	3142	1/1	0.96	0.24	33,33,33,33	0
56	MG	BD	303	1/1	0.96	0.19	42,42,42,42	0
56	MG	BA	3427	1/1	0.96	0.12	48,48,48,48	0
56	MG	BV	201	1/1	0.96	0.40	53,53,53,53	0
56	MG	BA	3667	1/1	0.96	0.09	63,63,63,63	0
56	MG	BA	3434	1/1	0.96	0.12	32,32,32,32	0
56	MG	DA	3294	1/1	0.96	0.10	47,47,47,47	0
56	MG	BA	3376	1/1	0.96	0.10	48,48,48,48	0
56	MG	AA	3106	1/1	0.96	0.25	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	AA	3149	1/1	0.96	0.09	50,50,50,50	0
56	MG	BA	3093	1/1	0.96	0.22	25,25,25,25	0
56	MG	BA	3319	1/1	0.96	0.17	25,25,25,25	0
56	MG	DA	3544	1/1	0.96	0.11	51,51,51,51	0
56	MG	BA	3604	1/1	0.96	0.11	72,72,72,72	0
56	MG	CA	3004	1/1	0.96	0.21	96,96,96,96	0
56	MG	CA	3078	1/1	0.96	0.29	46,46,46,46	0
56	MG	BA	3220	1/1	0.97	0.10	57,57,57,57	0
56	MG	DA	3374	1/1	0.97	0.05	37,37,37,37	0
56	MG	BA	3317	1/1	0.97	0.15	40,40,40,40	0
56	MG	AA	3057	1/1	0.97	0.09	37,37,37,37	0
56	MG	DA	3563	1/1	0.97	0.15	64,64,64,64	0
56	MG	BA	3587	1/1	0.97	0.18	23,23,23,23	0
56	MG	BD	308	1/1	0.97	0.33	23,23,23,23	0
56	MG	BA	3701	1/1	0.97	0.13	32,32,32,32	0
56	MG	BA	3077	1/1	0.97	0.20	39,39,39,39	0
56	MG	DA	3445	1/1	0.97	0.23	39,39,39,39	0
56	MG	BA	3119	1/1	0.97	0.25	58,58,58,58	0
56	MG	BA	3323	1/1	0.97	0.15	23,23,23,23	0
56	MG	BA	3456	1/1	0.97	0.10	52,52,52,52	0
56	MG	DA	3309	1/1	0.97	0.17	33,33,33,33	0
56	MG	BA	3296	1/1	0.97	0.25	46,46,46,46	0
56	MG	D0	101	1/1	0.97	0.12	63,63,63,63	0
56	MG	BA	3115	1/1	0.97	0.26	36,36,36,36	0
56	MG	DD	304	1/1	0.97	0.23	35,35,35,35	0
56	MG	BA	3450	1/1	0.97	0.27	46,46,46,46	0
56	MG	BA	3360	1/1	0.97	0.19	38,38,38,38	0
56	MG	BA	3349	1/1	0.97	0.26	43,43,43,43	0
56	MG	BA	3437	1/1	0.97	0.15	42,42,42,42	0
56	MG	BA	3184	1/1	0.97	0.38	49,49,49,49	0
56	MG	BA	3032	1/1	0.97	0.19	49,49,49,49	0
56	MG	BF	301	1/1	0.97	0.52	45,45,45,45	0
56	MG	CX	104	1/1	0.97	0.14	40,40,40,40	0
56	MG	BA	3621	1/1	0.97	0.36	74,74,74,74	0
56	MG	BB	3015	1/1	0.97	0.10	37,37,37,37	0
56	MG	CA	3121	1/1	0.97	0.27	53,53,53,53	0
56	MG	DA	3242	1/1	0.97	0.23	35,35,35,35	0
56	MG	BQ	204	1/1	0.97	0.18	12,12,12,12	0
56	MG	CA	3118	1/1	0.97	0.08	37,37,37,37	0
56	MG	BA	3564	1/1	0.97	0.07	52,52,52,52	0
56	MG	DA	3037	1/1	0.97	0.30	35,35,35,35	0
56	MG	CA	3120	1/1	0.97	0.19	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3251	1/1	0.97	0.15	54,54,54,54	0
56	MG	DA	3596	1/1	0.97	0.10	67,67,67,67	0
56	MG	BA	3063	1/1	0.97	0.28	43,43,43,43	0
56	MG	BA	3530	1/1	0.97	0.28	31,31,31,31	0
56	MG	BA	3034	1/1	0.97	0.41	52,52,52,52	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	3272	1/1	0.97	0.34	7,7,7,7	0
56	MG	BA	3171	1/1	0.97	0.41	40,40,40,40	0
56	MG	BA	3232	1/1	0.97	0.15	29,29,29,29	0
56	MG	AA	3221	1/1	0.97	0.10	64,64,64,64	0
56	MG	BA	3455	1/1	0.97	0.14	47,47,47,47	0
56	MG	CA	3130	1/1	0.97	0.08	65,65,65,65	0
56	MG	BA	3636	1/1	0.97	0.11	36,36,36,36	0
56	MG	AA	3186	1/1	0.97	0.07	49,49,49,49	0
56	MG	DA	3446	1/1	0.97	0.11	52,52,52,52	0
56	MG	DA	3085	1/1	0.97	0.12	36,36,36,36	0
56	MG	AA	3156	1/1	0.97	0.17	62,62,62,62	0
56	MG	CX	102	1/1	0.97	0.06	61,61,61,61	0
56	MG	DA	3495	1/1	0.97	0.22	39,39,39,39	0
56	MG	BA	3539	1/1	0.97	0.16	35,35,35,35	0
56	MG	DA	3335	1/1	0.97	0.26	38,38,38,38	0
56	MG	DA	3176	1/1	0.97	0.27	39,39,39,39	0
56	MG	DA	3436	1/1	0.97	0.07	62,62,62,62	0
58	ZN	D6	501	1/1	0.97	0.12	61,61,61,61	0
56	MG	DA	3586	1/1	0.97	0.09	29,29,29,29	0
56	MG	BA	3267	1/1	0.97	0.16	41,41,41,41	0
56	MG	BA	3338	1/1	0.97	0.21	50,50,50,50	0
56	MG	DA	3344	1/1	0.97	0.11	26,26,26,26	0
56	MG	DA	3258	1/1	0.97	0.18	32,32,32,32	0
56	MG	AA	3158	1/1	0.97	0.20	44,44,44,44	0
56	MG	BA	3490	1/1	0.97	0.26	38,38,38,38	0
58	ZN	DY	501	1/1	0.97	0.05	83,83,83,83	0
56	MG	DA	3431	1/1	0.97	0.12	41,41,41,41	0
56	MG	BA	3486	1/1	0.97	0.06	38,38,38,38	0
56	MG	DA	3584	1/1	0.97	0.16	61,61,61,61	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	DA	3239	1/1	0.97	0.21	39,39,39,39	0
56	MG	DA	3274	1/1	0.97	0.09	52,52,52,52	0
56	MG	BA	3720	1/1	0.97	0.20	33,33,33,33	0
56	MG	BA	3521	1/1	0.97	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3518	1/1	0.97	0.10	41,41,41,41	0
56	MG	DA	3573	1/1	0.97	0.19	40,40,40,40	0
56	MG	DA	3160	1/1	0.97	0.15	44,44,44,44	0
56	MG	BA	3162	1/1	0.97	0.19	23,23,23,23	0
56	MG	DA	3428	1/1	0.97	0.27	51,51,51,51	0
56	MG	DA	3302	1/1	0.97	0.18	22,22,22,22	0
56	MG	BA	3327	1/1	0.97	0.15	38,38,38,38	0
56	MG	BE	304	1/1	0.97	0.09	49,49,49,49	0
56	MG	CA	3043	1/1	0.97	0.34	49,49,49,49	0
56	MG	CA	3083	1/1	0.97	0.08	39,39,39,39	0
56	MG	BA	3369	1/1	0.97	0.22	45,45,45,45	0
56	MG	AA	3208	1/1	0.97	0.34	46,46,46,46	0
56	MG	CA	3050	1/1	0.97	0.13	43,43,43,43	0
56	MG	DA	3449	1/1	0.97	0.09	43,43,43,43	0
56	MG	DA	3173	1/1	0.97	0.41	39,39,39,39	0
56	MG	DA	3583	1/1	0.97	0.28	48,48,48,48	0
56	MG	BA	3170	1/1	0.97	0.66	48,48,48,48	0
56	MG	DQ	203	1/1	0.97	0.32	57,57,57,57	0
56	MG	DA	3630	1/1	0.97	0.20	40,40,40,40	0
56	MG	BA	3710	1/1	0.97	0.21	48,48,48,48	0
56	MG	AA	3176	1/1	0.97	0.09	63,63,63,63	0
56	MG	BA	3600	1/1	0.97	0.15	47,47,47,47	0
56	MG	BA	3210	1/1	0.97	0.11	34,34,34,34	0
56	MG	DA	3282	1/1	0.97	0.14	36,36,36,36	0
56	MG	BA	3302	1/1	0.97	0.13	27,27,27,27	0
56	MG	DA	3547	1/1	0.97	0.10	41,41,41,41	0
56	MG	BA	3002	1/1	0.97	0.20	54,54,54,54	0
56	MG	BA	3694	1/1	0.97	0.37	56,56,56,56	0
56	MG	AX	110	1/1	0.97	0.20	42,42,42,42	0
56	MG	BA	3623	1/1	0.97	0.21	47,47,47,47	0
56	MG	BA	3489	1/1	0.97	0.14	43,43,43,43	0
56	MG	DA	3241	1/1	0.97	0.21	15,15,15,15	0
56	MG	DA	3023	1/1	0.97	0.28	52,52,52,52	0
56	MG	BA	3212	1/1	0.97	0.28	43,43,43,43	0
56	MG	DA	3088	1/1	0.97	0.15	46,46,46,46	0
56	MG	DA	3300	1/1	0.97	0.15	37,37,37,37	0
56	MG	BA	3682	1/1	0.97	0.22	38,38,38,38	0
56	MG	DA	3180	1/1	0.97	0.21	46,46,46,46	0
56	MG	BA	3559	1/1	0.97	0.14	48,48,48,48	0
56	MG	AA	3182	1/1	0.97	0.12	49,49,49,49	0
56	MG	BA	3493	1/1	0.97	0.37	15,15,15,15	0
56	MG	DA	3421	1/1	0.97	0.19	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	DO	5001	1/1	0.97	0.12	35,35,35,35	0
56	MG	DA	3412	1/1	0.97	0.28	30,30,30,30	0
56	MG	AA	3204	1/1	0.97	0.14	54,54,54,54	0
56	MG	CA	3166	1/1	0.97	0.23	59,59,59,59	0
56	MG	AA	3102	1/1	0.97	0.06	64,64,64,64	0
56	MG	BP	202	1/1	0.97	0.11	40,40,40,40	0
56	MG	BA	3552	1/1	0.97	0.23	29,29,29,29	0
56	MG	BA	3120	1/1	0.97	0.09	51,51,51,51	0
56	MG	BA	3364	1/1	0.97	0.24	29,29,29,29	0
56	MG	AA	3185	1/1	0.97	0.28	46,46,46,46	0
56	MG	DQ	204	1/1	0.97	0.13	43,43,43,43	0
56	MG	BA	3644	1/1	0.97	0.16	43,43,43,43	0
56	MG	DD	303	1/1	0.97	0.20	19,19,19,19	0
56	MG	BA	3680	1/1	0.97	0.35	37,37,37,37	0
56	MG	DA	3508	1/1	0.97	0.19	38,38,38,38	0
56	MG	BA	3116	1/1	0.97	0.20	31,31,31,31	0
56	MG	BA	3311	1/1	0.97	0.23	42,42,42,42	0
56	MG	DA	3371	1/1	0.97	0.07	44,44,44,44	0
56	MG	BA	3554	1/1	0.97	0.20	31,31,31,31	0
56	MG	BA	3096	1/1	0.97	0.35	62,62,62,62	0
56	MG	DA	3275	1/1	0.97	0.07	38,38,38,38	0
56	MG	DA	3455	1/1	0.97	0.17	60,60,60,60	0
56	MG	BA	3572	1/1	0.97	0.20	36,36,36,36	0
56	MG	DA	3616	1/1	0.97	0.23	62,62,62,62	0
56	MG	BF	305	1/1	0.97	0.32	35,35,35,35	0
56	MG	BA	3550	1/1	0.97	0.24	45,45,45,45	0
56	MG	BA	3404	1/1	0.97	0.15	35,35,35,35	0
56	MG	BA	3428	1/1	0.97	0.11	45,45,45,45	0
56	MG	BA	3294	1/1	0.97	0.28	37,37,37,37	0
56	MG	BA	3167	1/1	0.97	0.39	39,39,39,39	0
56	MG	BA	3734	1/1	0.97	0.26	45,45,45,45	0
56	MG	DA	3514	1/1	0.97	0.12	39,39,39,39	0
56	MG	BA	3479	1/1	0.97	0.10	56,56,56,56	0
56	MG	BA	3351	1/1	0.97	0.07	30,30,30,30	0
56	MG	DA	3291	1/1	0.97	0.24	35,35,35,35	0
56	MG	BA	3396	1/1	0.97	0.18	22,22,22,22	0
56	MG	DA	3504	1/1	0.97	0.08	44,44,44,44	0
56	MG	BA	3593	1/1	0.97	0.14	74,74,74,74	0
56	MG	BA	3438	1/1	0.97	0.18	30,30,30,30	0
56	MG	BA	3315	1/1	0.97	0.11	37,37,37,37	0
56	MG	DA	3571	1/1	0.97	0.14	46,46,46,46	0
56	MG	BE	310	1/1	0.97	0.24	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3705	1/1	0.97	0.05	39,39,39,39	0
56	MG	CA	3088	1/1	0.97	0.26	43,43,43,43	0
56	MG	BA	3026	1/1	0.97	0.47	36,36,36,36	0
56	MG	CA	3171	1/1	0.97	0.32	67,67,67,67	0
56	MG	CA	3049	1/1	0.97	0.24	53,53,53,53	0
56	MG	DA	3375	1/1	0.97	0.14	60,60,60,60	0
56	MG	BA	3582	1/1	0.97	0.22	25,25,25,25	0
56	MG	BB	3001	1/1	0.97	0.17	54,54,54,54	0
56	MG	BF	306	1/1	0.97	0.18	37,37,37,37	0
56	MG	BA	3517	1/1	0.97	0.08	49,49,49,49	0
56	MG	DA	3262	1/1	0.97	0.22	44,44,44,44	0
56	MG	AA	3207	1/1	0.97	0.28	45,45,45,45	0
56	MG	BA	3064	1/1	0.97	0.19	39,39,39,39	0
56	MG	DA	3349	1/1	0.97	0.17	54,54,54,54	0
56	MG	BA	3379	1/1	0.97	0.22	22,22,22,22	0
56	MG	BO	201	1/1	0.97	0.14	70,70,70,70	0
56	MG	DA	3136	1/1	0.97	0.11	49,49,49,49	0
56	MG	BA	3329	1/1	0.97	0.13	29,29,29,29	0
56	MG	CA	3169	1/1	0.97	0.16	57,57,57,57	0
56	MG	BA	3695	1/1	0.97	0.17	15,15,15,15	0
56	MG	DA	3184	1/1	0.97	0.32	45,45,45,45	0
56	MG	BA	3003	1/1	0.97	0.16	43,43,43,43	0
56	MG	DA	3269	1/1	0.97	0.12	48,48,48,48	0
56	MG	BA	3473	1/1	0.97	0.11	51,51,51,51	0
56	MG	AA	3150	1/1	0.97	0.27	46,46,46,46	0
56	MG	AA	3203	1/1	0.97	0.12	63,63,63,63	0
56	MG	DA	3650	1/1	0.97	0.58	48,48,48,48	0
56	MG	BA	3721	1/1	0.97	0.08	25,25,25,25	0
56	MG	BA	3646	1/1	0.97	0.23	52,52,52,52	0
56	MG	BA	3204	1/1	0.97	0.40	25,25,25,25	0
56	MG	B8	103	1/1	0.97	0.19	24,24,24,24	0
56	MG	BA	3392	1/1	0.97	0.26	56,56,56,56	0
56	MG	BA	3363	1/1	0.97	0.15	39,39,39,39	0
56	MG	BA	3031	1/1	0.97	0.79	41,41,41,41	0
56	MG	BA	3527	1/1	0.97	0.18	64,64,64,64	0
56	MG	BA	3274	1/1	0.97	0.16	52,52,52,52	0
56	MG	BA	3475	1/1	0.97	0.21	36,36,36,36	0
56	MG	BA	3696	1/1	0.97	0.26	39,39,39,39	0
56	MG	BA	3729	1/1	0.97	0.40	46,46,46,46	0
56	MG	BA	3451	1/1	0.97	0.30	28,28,28,28	0
56	MG	DA	3493	1/1	0.97	0.15	29,29,29,29	0
56	MG	AA	3171	1/1	0.97	0.25	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3629	1/1	0.97	0.13	47,47,47,47	0
56	MG	BA	3239	1/1	0.97	0.10	33,33,33,33	0
56	MG	BA	3314	1/1	0.97	0.17	24,24,24,24	0
56	MG	BA	3534	1/1	0.97	0.12	41,41,41,41	0
56	MG	DA	3368	1/1	0.97	0.12	39,39,39,39	0
56	MG	BA	3400	1/1	0.97	0.19	24,24,24,24	0
56	MG	BP	203	1/1	0.97	0.69	29,29,29,29	0
56	MG	BA	3668	1/1	0.97	0.13	38,38,38,38	0
56	MG	DA	3546	1/1	0.97	0.12	44,44,44,44	0
56	MG	BA	3333	1/1	0.97	0.12	49,49,49,49	0
56	MG	BA	3033	1/1	0.97	0.37	35,35,35,35	0
56	MG	CA	3101	1/1	0.97	0.18	70,70,70,70	0
56	MG	BA	3713	1/1	0.97	0.10	66,66,66,66	0
56	MG	CA	3052	1/1	0.97	0.12	39,39,39,39	0
56	MG	BA	3469	1/1	0.97	0.09	38,38,38,38	0
56	MG	DA	3043	1/1	0.97	0.45	54,54,54,54	0
56	MG	BA	3435	1/1	0.97	0.23	24,24,24,24	0
56	MG	DA	3192	1/1	0.97	0.12	47,47,47,47	0
56	MG	BA	3173	1/1	0.97	0.58	37,37,37,37	0
56	MG	DA	3488	1/1	0.97	0.04	46,46,46,46	0
56	MG	BR	203	1/1	0.97	0.18	15,15,15,15	0
56	MG	BA	3532	1/1	0.97	0.18	34,34,34,34	0
56	MG	BA	3352	1/1	0.97	0.12	34,34,34,34	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	BA	3447	1/1	0.97	0.13	37,37,37,37	0
56	MG	CA	3112	1/1	0.97	0.23	59,59,59,59	0
56	MG	CA	3059	1/1	0.97	0.27	51,51,51,51	0
56	MG	CA	3045	1/1	0.97	0.09	54,54,54,54	0
56	MG	DA	3356	1/1	0.97	0.11	27,27,27,27	0
56	MG	BA	3556	1/1	0.98	0.31	27,27,27,27	0
56	MG	AA	3193	1/1	0.98	0.10	60,60,60,60	0
56	MG	BA	3602	1/1	0.98	0.09	35,35,35,35	0
56	MG	BA	3433	1/1	0.98	0.24	39,39,39,39	0
58	ZN	BY	202	1/1	0.98	0.09	71,71,71,71	0
56	MG	DA	3215	1/1	0.98	0.30	29,29,29,29	0
56	MG	DA	3475	1/1	0.98	0.11	36,36,36,36	0
56	MG	BA	3436	1/1	0.98	0.09	37,37,37,37	0
56	MG	BA	3411	1/1	0.98	0.15	38,38,38,38	0
56	MG	CA	3051	1/1	0.98	0.10	63,63,63,63	0
56	MG	BA	3393	1/1	0.98	0.18	38,38,38,38	0
56	MG	DA	3551	1/1	0.98	0.08	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	BA	3723	1/1	0.98	0.14	49,49,49,49	0
56	MG	BA	3150	1/1	0.98	0.45	34,34,34,34	0
56	MG	DA	3177	1/1	0.98	0.08	33,33,33,33	0
56	MG	DA	3313	1/1	0.98	0.17	52,52,52,52	0
56	MG	BA	3445	1/1	0.98	0.20	25,25,25,25	0
56	MG	BB	3016	1/1	0.98	0.12	21,21,21,21	0
56	MG	BA	3491	1/1	0.98	0.19	23,23,23,23	0
56	MG	DA	3404	1/1	0.98	0.16	47,47,47,47	0
56	MG	AA	3179	1/1	0.98	0.26	34,34,34,34	0
56	MG	DA	3290	1/1	0.98	0.07	42,42,42,42	0
56	MG	BA	3347	1/1	0.98	0.27	25,25,25,25	0
56	MG	BA	3733	1/1	0.98	0.11	27,27,27,27	0
56	MG	BA	3310	1/1	0.98	0.17	13,13,13,13	0
56	MG	DA	3308	1/1	0.98	0.32	30,30,30,30	0
56	MG	BA	3591	1/1	0.98	0.32	48,48,48,48	0
56	MG	BA	3424	1/1	0.98	0.17	15,15,15,15	0
56	MG	BA	3569	1/1	0.98	0.18	19,19,19,19	0
56	MG	CE	3002	1/1	0.98	0.07	55,55,55,55	0
56	MG	BA	3337	1/1	0.98	0.17	23,23,23,23	0
56	MG	DA	3480	1/1	0.98	0.09	52,52,52,52	0
56	MG	BA	3341	1/1	0.98	0.09	33,33,33,33	0
56	MG	DA	3268	1/1	0.98	0.17	40,40,40,40	0
56	MG	BA	3679	1/1	0.98	0.40	27,27,27,27	0
56	MG	BA	3448	1/1	0.98	0.09	29,29,29,29	0
56	MG	BA	3207	1/1	0.98	0.23	35,35,35,35	0
56	MG	BA	3681	1/1	0.98	0.14	40,40,40,40	0
56	MG	AA	3165	1/1	0.98	0.15	23,23,23,23	0
56	MG	CA	3128	1/1	0.98	0.26	41,41,41,41	0
56	MG	AA	3220	1/1	0.98	0.12	40,40,40,40	0
56	MG	BA	3010	1/1	0.98	0.17	32,32,32,32	0
56	MG	BA	3586	1/1	0.98	0.19	29,29,29,29	0
56	MG	DA	3354	1/1	0.98	0.15	27,27,27,27	0
56	MG	CA	3098	1/1	0.98	0.23	46,46,46,46	0
56	MG	BN	3004	1/1	0.98	0.40	66,66,66,66	0
56	MG	BA	3081	1/1	0.98	0.08	14,14,14,14	0
56	MG	DA	3380	1/1	0.98	0.16	26,26,26,26	0
56	MG	BA	3525	1/1	0.98	0.23	43,43,43,43	0
56	MG	CA	3064	1/1	0.98	0.12	58,58,58,58	0
56	MG	DA	3569	1/1	0.98	0.19	37,37,37,37	0
56	MG	BA	3487	1/1	0.98	0.12	31,31,31,31	0
56	MG	DA	3236	1/1	0.98	0.17	46,46,46,46	0
56	MG	BA	3283	1/1	0.98	0.15	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3372	1/1	0.98	0.12	45,45,45,45	0
56	MG	BA	3420	1/1	0.98	0.30	33,33,33,33	0
56	MG	BA	3418	1/1	0.98	0.15	27,27,27,27	0
56	MG	DA	3035	1/1	0.98	0.23	56,56,56,56	0
56	MG	BB	3013	1/1	0.98	0.10	39,39,39,39	0
56	MG	DA	3059	1/1	0.98	0.08	46,46,46,46	0
56	MG	B8	102	1/1	0.98	0.10	60,60,60,60	0
56	MG	DA	3174	1/1	0.98	0.26	41,41,41,41	0
56	MG	DA	3523	1/1	0.98	0.06	55,55,55,55	0
56	MG	DA	3370	1/1	0.98	0.15	38,38,38,38	0
56	MG	DA	3418	1/1	0.98	0.17	29,29,29,29	0
56	MG	DA	3026	1/1	0.98	0.21	37,37,37,37	0
56	MG	BU	207	1/1	0.98	0.21	40,40,40,40	0
56	MG	BA	3316	1/1	0.98	0.16	28,28,28,28	0
56	MG	BA	3264	1/1	0.98	0.17	30,30,30,30	0
56	MG	BA	3454	1/1	0.98	0.09	22,22,22,22	0
56	MG	DA	3561	1/1	0.98	0.19	45,45,45,45	0
56	MG	DA	3448	1/1	0.98	0.08	57,57,57,57	0
56	MG	DA	3600	1/1	0.98	0.07	45,45,45,45	0
56	MG	BA	3228	1/1	0.98	0.27	63,63,63,63	0
56	MG	BB	3012	1/1	0.98	0.15	56,56,56,56	0
56	MG	BA	3557	1/1	0.98	0.23	31,31,31,31	0
56	MG	BA	3522	1/1	0.98	0.14	49,49,49,49	0
56	MG	DA	3477	1/1	0.98	0.09	49,49,49,49	0
56	MG	B3	101	1/1	0.98	0.15	28,28,28,28	0
56	MG	DA	3394	1/1	0.98	0.14	47,47,47,47	0
56	MG	BA	3113	1/1	0.98	0.09	32,32,32,32	0
56	MG	CA	3022	1/1	0.98	0.04	70,70,70,70	0
56	MG	DA	3588	1/1	0.98	0.18	40,40,40,40	0
56	MG	BA	3389	1/1	0.98	0.12	48,48,48,48	0
56	MG	DA	3277	1/1	0.98	0.25	49,49,49,49	0
56	MG	DA	3244	1/1	0.98	0.31	29,29,29,29	0
56	MG	DA	3337	1/1	0.98	0.09	27,27,27,27	0
56	MG	CA	3168	1/1	0.98	0.39	77,77,77,77	0
56	MG	BA	3670	1/1	0.98	0.08	59,59,59,59	0
56	MG	CA	3148	1/1	0.98	0.19	68,68,68,68	0
56	MG	DA	3408	1/1	0.98	0.22	37,37,37,37	0
56	MG	BA	3544	1/1	0.98	0.23	27,27,27,27	0
56	MG	BA	3036	1/1	0.98	0.18	38,38,38,38	0
56	MG	BU	203	1/1	0.98	0.35	33,33,33,33	0
56	MG	DA	3317	1/1	0.98	0.12	32,32,32,32	0
56	MG	BE	308	1/1	0.98	0.18	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	BA	3008	1/1	0.98	0.13	50,50,50,50	0
56	MG	DA	3316	1/1	0.98	0.17	58,58,58,58	0
56	MG	DA	3165	1/1	0.98	0.24	44,44,44,44	0
56	MG	BA	3222	1/1	0.98	0.29	25,25,25,25	0
56	MG	DA	3649	1/1	0.98	0.24	24,24,24,24	0
56	MG	DA	3529	1/1	0.98	0.10	63,63,63,63	0
56	MG	BA	3574	1/1	0.98	0.08	54,54,54,54	0
56	MG	BA	3467	1/1	0.98	0.06	40,40,40,40	0
56	MG	AA	3027	1/1	0.98	0.06	55,55,55,55	0
56	MG	BA	3305	1/1	0.98	0.13	44,44,44,44	0
56	MG	DA	3205	1/1	0.98	0.09	38,38,38,38	0
56	MG	DA	3541	1/1	0.98	0.28	35,35,35,35	0
56	MG	BA	3581	1/1	0.98	0.10	51,51,51,51	0
56	MG	BA	3382	1/1	0.98	0.13	51,51,51,51	0
56	MG	DA	3365	1/1	0.98	0.06	40,40,40,40	0
56	MG	BD	310	1/1	0.98	0.31	48,48,48,48	0
56	MG	BA	3533	1/1	0.98	0.18	32,32,32,32	0
56	MG	AA	3062	1/1	0.98	0.08	32,32,32,32	0
56	MG	DA	3250	1/1	0.98	0.14	31,31,31,31	0
56	MG	DA	3377	1/1	0.98	0.24	59,59,59,59	0
56	MG	AA	3091	1/1	0.98	0.15	75,75,75,75	0
56	MG	CA	3133	1/1	0.98	0.05	49,49,49,49	0
56	MG	BA	3702	1/1	0.98	0.12	56,56,56,56	0
56	MG	BR	201	1/1	0.98	0.60	51,51,51,51	0
56	MG	BA	3046	1/1	0.98	0.14	29,29,29,29	0
56	MG	CA	3129	1/1	0.98	0.14	45,45,45,45	0
56	MG	BA	3095	1/1	0.98	0.47	55,55,55,55	0
56	MG	BA	3131	1/1	0.98	0.72	54,54,54,54	0
56	MG	BA	3208	1/1	0.98	0.28	41,41,41,41	0
56	MG	DA	3473	1/1	0.98	0.31	32,32,32,32	0
56	MG	DA	3227	1/1	0.98	0.14	53,53,53,53	0
56	MG	BA	3308	1/1	0.98	0.08	44,44,44,44	0
56	MG	BE	302	1/1	0.98	0.22	33,33,33,33	0
56	MG	DA	3330	1/1	0.98	0.14	37,37,37,37	0
56	MG	BA	3070	1/1	0.98	0.13	35,35,35,35	0
56	MG	CA	3165	1/1	0.98	0.08	40,40,40,40	0
56	MG	DA	3644	1/1	0.98	0.08	42,42,42,42	0
56	MG	BA	3678	1/1	0.98	0.16	53,53,53,53	0
56	MG	DA	3327	1/1	0.98	0.18	29,29,29,29	0
56	MG	DA	3025	1/1	0.98	0.38	44,44,44,44	0
56	MG	BA	3478	1/1	0.98	0.15	29,29,29,29	0
56	MG	BA	3381	1/1	0.98	0.10	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3675	1/1	0.98	0.12	49,49,49,49	0
56	MG	AA	3097	1/1	0.98	0.25	43,43,43,43	0
56	MG	CA	3100	1/1	0.98	0.11	60,60,60,60	0
56	MG	DA	3385	1/1	0.98	0.15	35,35,35,35	0
56	MG	BA	3655	1/1	0.98	0.21	52,52,52,52	0
56	MG	DA	3019	1/1	0.98	0.13	30,30,30,30	0
56	MG	BA	3519	1/1	0.98	0.12	39,39,39,39	0
56	MG	BA	3281	1/1	0.98	0.18	52,52,52,52	0
56	MG	BA	3526	1/1	0.98	0.19	19,19,19,19	0
56	MG	DA	3476	1/1	0.98	0.20	45,45,45,45	0
56	MG	AA	3143	1/1	0.98	0.15	45,45,45,45	0
56	MG	BA	3227	1/1	0.98	0.30	32,32,32,32	0
56	MG	BA	3725	1/1	0.98	0.12	49,49,49,49	0
56	MG	BA	3612	1/1	0.98	0.15	37,37,37,37	0
56	MG	BA	3480	1/1	0.98	0.20	17,17,17,17	0
56	MG	AA	3205	1/1	0.98	0.19	61,61,61,61	0
56	MG	DA	3652	1/1	0.98	0.60	60,60,60,60	0
56	MG	DE	303	1/1	0.98	0.11	41,41,41,41	0
56	MG	BA	3179	1/1	0.98	0.20	43,43,43,43	0
56	MG	AA	3192	1/1	0.98	0.08	57,57,57,57	0
56	MG	BA	3388	1/1	0.98	0.15	34,34,34,34	0
56	MG	DA	3390	1/1	0.98	0.09	42,42,42,42	0
56	MG	BA	3313	1/1	0.98	0.27	36,36,36,36	0
56	MG	BA	3375	1/1	0.98	0.24	31,31,31,31	0
56	MG	CA	3092	1/1	0.98	0.12	47,47,47,47	0
56	MG	DA	3395	1/1	0.98	0.21	34,34,34,34	0
56	MG	DA	3533	1/1	0.98	0.08	68,68,68,68	0
56	MG	BA	3429	1/1	0.98	0.14	20,20,20,20	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
56	MG	AA	3103	1/1	0.98	0.19	38,38,38,38	0
56	MG	CA	3085	1/1	0.98	0.30	43,43,43,43	0
56	MG	BE	309	1/1	0.98	0.27	25,25,25,25	0
56	MG	BA	3398	1/1	0.98	0.11	41,41,41,41	0
56	MG	BA	3656	1/1	0.98	0.11	33,33,33,33	0
56	MG	BA	3634	1/1	0.98	0.70	63,63,63,63	0
56	MG	BA	3567	1/1	0.98	0.22	37,37,37,37	0
56	MG	BA	3583	1/1	0.98	0.20	27,27,27,27	0
56	MG	AA	3163	1/1	0.98	0.17	28,28,28,28	0
56	MG	AA	3172	1/1	0.98	0.05	53,53,53,53	0
56	MG	DA	3320	1/1	0.98	0.17	30,30,30,30	0
56	MG	DA	3351	1/1	0.98	0.38	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	3323	1/1	0.98	0.18	30,30,30,30	0
56	MG	CA	3093	1/1	0.98	0.06	53,53,53,53	0
56	MG	DA	3645	1/1	0.98	0.09	30,30,30,30	0
56	MG	BA	3186	1/1	0.98	0.14	53,53,53,53	0
56	MG	BA	3459	1/1	0.98	0.22	31,31,31,31	0
56	MG	B3	102	1/1	0.98	0.13	59,59,59,59	0
56	MG	BA	3195	1/1	0.98	0.33	47,47,47,47	0
56	MG	BQ	201	1/1	0.98	0.43	61,61,61,61	0
56	MG	AA	3141	1/1	0.98	0.21	48,48,48,48	0
56	MG	BA	3529	1/1	0.98	0.21	35,35,35,35	0
56	MG	DA	3234	1/1	0.98	0.23	33,33,33,33	0
56	MG	DA	3608	1/1	0.98	0.27	57,57,57,57	0
56	MG	CA	3017	1/1	0.98	0.24	42,42,42,42	0
56	MG	BA	3528	1/1	0.99	0.22	33,33,33,33	0
56	MG	BA	3154	1/1	0.99	0.17	61,61,61,61	0
56	MG	DA	3332	1/1	0.99	0.13	33,33,33,33	0
56	MG	DA	3324	1/1	0.99	0.23	40,40,40,40	0
56	MG	BA	3460	1/1	0.99	0.13	33,33,33,33	0
56	MG	CA	3122	1/1	0.99	0.07	47,47,47,47	0
56	MG	BA	3051	1/1	0.99	0.15	20,20,20,20	0
56	MG	B7	102	1/1	0.99	0.25	40,40,40,40	0
56	MG	BA	3128	1/1	0.99	0.27	40,40,40,40	0
56	MG	BA	3423	1/1	0.99	0.07	26,26,26,26	0
56	MG	BA	3416	1/1	0.99	0.25	42,42,42,42	0
56	MG	BF	303	1/1	0.99	0.27	36,36,36,36	0
56	MG	DA	3028	1/1	0.99	0.06	35,35,35,35	0
56	MG	DA	3230	1/1	0.99	0.16	62,62,62,62	0
56	MG	DA	3181	1/1	0.99	0.30	36,36,36,36	0
56	MG	BA	3516	1/1	0.99	0.09	47,47,47,47	0
56	MG	DA	3355	1/1	0.99	0.26	18,18,18,18	0
56	MG	CA	3069	1/1	0.99	0.11	69,69,69,69	0
56	MG	CA	3001	1/1	0.99	0.21	55,55,55,55	0
56	MG	DA	3540	1/1	0.99	0.23	54,54,54,54	0
56	MG	BA	3383	1/1	0.99	0.18	38,38,38,38	0
56	MG	CA	3080	1/1	0.99	0.14	55,55,55,55	0
56	MG	DA	3338	1/1	0.99	0.14	29,29,29,29	0
56	MG	BA	3531	1/1	0.99	0.29	38,38,38,38	0
56	MG	BA	3508	1/1	0.99	0.14	34,34,34,34	0
56	MG	AX	109	1/1	0.99	0.09	43,43,43,43	0
56	MG	BA	3399	1/1	0.99	0.19	18,18,18,18	0
56	MG	AA	3188	1/1	0.99	0.24	53,53,53,53	0
56	MG	BA	3407	1/1	0.99	0.19	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3410	1/1	0.99	0.15	27,27,27,27	0
56	MG	BA	3520	1/1	0.99	0.14	34,34,34,34	0
56	MG	DA	3346	1/1	0.99	0.23	29,29,29,29	0
58	ZN	D5	103	1/1	0.99	0.07	70,70,70,70	0
56	MG	DA	3312	1/1	0.99	0.27	43,43,43,43	0
56	MG	BA	3494	1/1	0.99	0.34	18,18,18,18	0
56	MG	DA	3612	1/1	0.99	0.15	39,39,39,39	0
56	MG	BA	3342	1/1	0.99	0.19	31,31,31,31	0
57	SF4	AD	501	8/8	0.99	0.14	59,72,92,96	0
56	MG	DA	3190	1/1	0.99	0.13	37,37,37,37	0
56	MG	BB	3011	1/1	0.99	0.15	37,37,37,37	0
56	MG	BA	3318	1/1	0.99	0.13	33,33,33,33	0
56	MG	BA	3471	1/1	0.99	0.17	51,51,51,51	0
56	MG	BA	3442	1/1	0.99	0.15	12,12,12,12	0
56	MG	AA	3151	1/1	0.99	0.08	41,41,41,41	0
56	MG	BA	3200	1/1	0.99	0.27	25,25,25,25	0
56	MG	CA	3154	1/1	0.99	0.13	49,49,49,49	0
56	MG	DA	3272	1/1	0.99	0.28	27,27,27,27	0
56	MG	BA	3492	1/1	0.99	0.25	23,23,23,23	0
56	MG	DA	3301	1/1	0.99	0.14	45,45,45,45	0
56	MG	BA	3415	1/1	0.99	0.24	27,27,27,27	0
56	MG	BA	3126	1/1	0.99	0.22	24,24,24,24	0
56	MG	BA	3553	1/1	0.99	0.13	31,31,31,31	0
56	MG	BA	3371	1/1	0.99	0.18	15,15,15,15	0
56	MG	DA	3379	1/1	0.99	0.22	28,28,28,28	0
56	MG	AA	3214	1/1	0.99	0.27	75,75,75,75	0
56	MG	DA	3549	1/1	0.99	0.24	52,52,52,52	0
56	MG	BA	3378	1/1	0.99	0.12	20,20,20,20	0
56	MG	DA	3618	1/1	0.99	0.12	39,39,39,39	0
56	MG	BB	3010	1/1	0.99	0.26	40,40,40,40	0
56	MG	DA	3542	1/1	0.99	0.18	32,32,32,32	0
56	MG	CA	3077	1/1	0.99	0.22	53,53,53,53	0
56	MG	BA	3409	1/1	0.99	0.23	27,27,27,27	0
56	MG	DA	3271	1/1	0.99	0.20	37,37,37,37	0
57	SF4	CD	501	8/8	0.99	0.14	64,75,91,95	0
56	MG	BA	3732	1/1	0.99	0.52	61,61,61,61	0
56	MG	BA	3414	1/1	0.99	0.21	19,19,19,19	0
56	MG	AA	3159	1/1	0.99	0.32	57,57,57,57	0
56	MG	BA	3614	1/1	0.99	0.42	30,30,30,30	0
56	MG	AA	3073	1/1	0.99	0.07	46,46,46,46	0
56	MG	BN	3006	1/1	0.99	0.12	24,24,24,24	0
56	MG	BA	3662	1/1	0.99	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3413	1/1	0.99	0.20	53,53,53,53	0
56	MG	DA	3331	1/1	0.99	0.09	34,34,34,34	0
56	MG	BA	3321	1/1	0.99	0.16	29,29,29,29	0
56	MG	AA	3144	1/1	0.99	0.08	48,48,48,48	0
58	ZN	B5	501	1/1	0.99	0.11	54,54,54,54	0
56	MG	DA	3625	1/1	0.99	0.10	35,35,35,35	0
58	ZN	B6	501	1/1	1.00	0.13	49,49,49,49	0
56	MG	DA	3304	1/1	1.00	0.11	35,35,35,35	0
58	ZN	B9	501	1/1	1.00	0.12	48,48,48,48	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.