



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 26, 2019 – 10:21 AM EDT

PDB ID : 4W2I  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with negamycin, mRNA and three deacylated tRNAs in the A, P and E sites  
Authors : Polikanov, Y.S.; Szal, T.; Jiang, F.; Gupta, P.; Matsuda, R.; Shiozuka, M.; Steitz, T.A.; Vazquez-Laslop, N.; Mankin, A.S.  
Deposited on : 2014-09-12  
Resolution : 2.70 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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.3.2  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

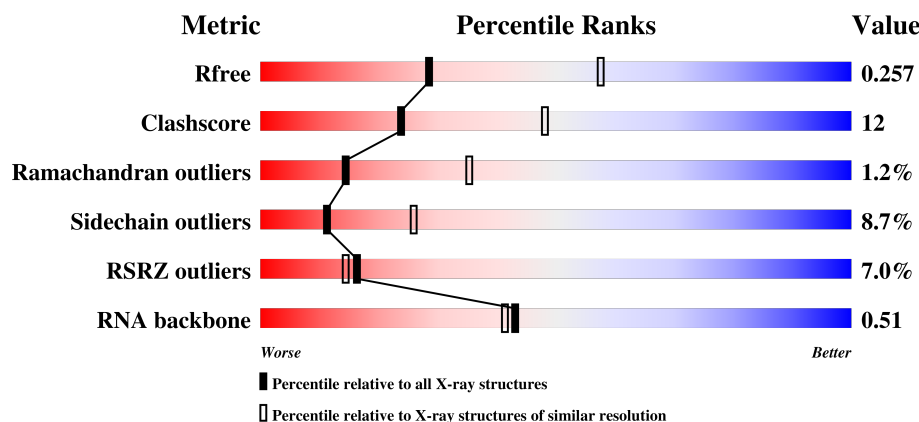
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (2.70-2.70)
RNA backbone	2636	1009 (3.00-2.40)

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

Mol	Chain	Length	Quality of chain
1	AA	1521	<div> <div>2%</div> <div>51% 36% 11% ..</div> </div>
1	CA	1521	<div> <div>2%</div> <div>46% 41% 11% .</div> </div>
2	AB	256	<div> <div>6%</div> <div>47% 36% 7% 10%</div> </div>
2	CB	256	<div> <div>17%</div> <div>44% 36% 10% 10%</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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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	AW	76	
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	77	
24	CX	77	
25	BA	2915	
25	DA	2915	
26	BB	121	
26	DB	121	

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Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
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	



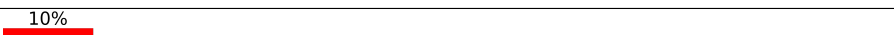
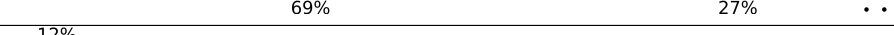


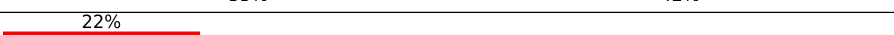

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Mol	Chain	Length	Quality of chain
39	DT	146	
40	BU	118	
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	

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Mol	Chain	Length	Quality of chain
52	B6	54	
52	D6	54	
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
56	MG	B5	103	-	-	-	X
56	MG	BA	3097	-	-	-	X
56	MG	BA	3195	-	-	-	X
56	MG	BA	3550	-	-	-	X
56	MG	BA	3646	-	-	-	X
56	MG	BA	3779	-	-	-	X
56	MG	BR	202	-	-	-	X
56	MG	DA	3577	-	-	-	X
57	NEG	AA	3216	-	-	X	-

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297376 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	1496	Total	C	N	O	P	0	0	0
			32163	14314	5963	10390	1496			
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	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	12	Total	C	N	O	P	0	0	0
			252	115	46	80	11			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0	0
			1588	713	285	515	73	2			
23	AY	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1541	688	278	502	72	1			
23	CY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

- Molecule 24 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2822	Total	C	N	O	P	0	0	0
			60792	27054	11380	19537	2821			
25	DA	2800	Total	C	N	O	P	0	0	0
			60311	26840	11284	19388	2799			

- 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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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		0	0	0
			877	553	175	149				
38	DS	110	Total	C	N	O		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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			558	352	102	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			532	339	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
			517	331	102	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	785	Total	Mg	0	0
			785	785		
56	CA	172	Total	Mg	0	0
			172	172		
56	DQ	4	Total	Mg	0	0
			4	4		
56	D3	1	Total	Mg	0	0
			1	1		
56	DF	6	Total	Mg	0	0
			6	6		
56	CV	1	Total	Mg	0	0
			1	1		
56	B8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BE	8	Total 8	Mg 8	0	0
56	AW	4	Total 4	Mg 4	0	0
56	DU	3	Total 3	Mg 3	0	0
56	B1	1	Total 1	Mg 1	0	0
56	AN	3	Total 3	Mg 3	0	0
56	BP	4	Total 4	Mg 4	0	0
56	AX	11	Total 11	Mg 11	0	0
56	CN	1	Total 1	Mg 1	0	0
56	DN	1	Total 1	Mg 1	0	0
56	CY	1	Total 1	Mg 1	0	0
56	DD	9	Total 9	Mg 9	0	0
56	B5	5	Total 5	Mg 5	0	0
56	BB	18	Total 18	Mg 18	0	0
56	BT	1	Total 1	Mg 1	0	0
56	D8	1	Total 1	Mg 1	0	0
56	AE	2	Total 2	Mg 2	0	0
56	DG	1	Total 1	Mg 1	0	0
56	B9	1	Total 1	Mg 1	0	0
56	BF	11	Total 11	Mg 11	0	0
56	AV	3	Total 3	Mg 3	0	0
56	BX	2	Total 2	Mg 2	0	0

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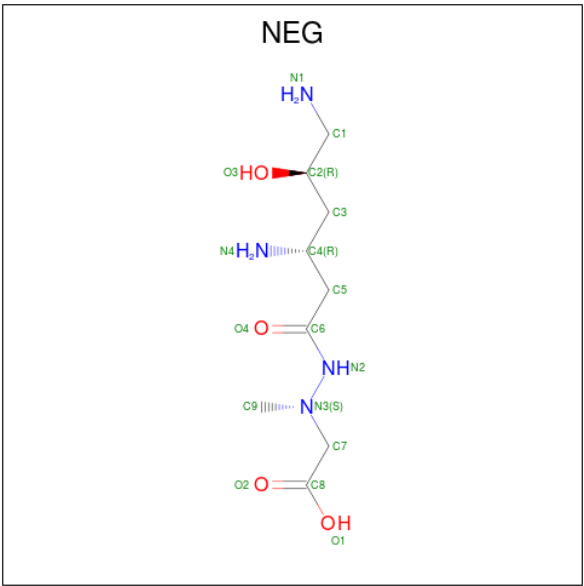
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B2	1	Total 1	Mg 1	0	0
56	AA	218	Total 218	Mg 218	0	0
56	BQ	5	Total 5	Mg 5	0	0
56	D7	1	Total 1	Mg 1	0	0
56	CX	2	Total 2	Mg 2	0	0
56	DV	3	Total 3	Mg 3	0	0
56	B6	1	Total 1	Mg 1	0	0
56	AM	1	Total 1	Mg 1	0	0
56	BU	9	Total 9	Mg 9	0	0
56	DR	2	Total 2	Mg 2	0	0
56	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	2	Total 2	Mg 2	0	0
56	BY	1	Total 1	Mg 1	0	0
56	DE	4	Total 4	Mg 4	0	0
56	B3	2	Total 2	Mg 2	0	0
56	CJ	1	Total 1	Mg 1	0	0
56	BR	3	Total 3	Mg 3	0	0
56	DA	623	Total 623	Mg 623	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CE	1	Total 1	Mg 1	0	0
56	DW	4	Total 4	Mg 4	0	0
56	D5	1	Total 1	Mg 1	0	0
56	B7	4	Total 4	Mg 4	0	0
56	CF	1	Total 1	Mg 1	0	0
56	BV	7	Total 7	Mg 7	0	0
56	DP	1	Total 1	Mg 1	0	0
56	DO	2	Total 2	Mg 2	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	CW	2	Total 2	Mg 2	0	0
56	CD	1	Total 1	Mg 1	0	0
56	BD	11	Total 11	Mg 11	0	0
56	B0	3	Total 3	Mg 3	0	0
56	AO	1	Total 1	Mg 1	0	0
56	BW	4	Total 4	Mg 4	0	0
56	AY	3	Total 3	Mg 3	0	0
56	CK	1	Total 1	Mg 1	0	0
56	AF	1	Total 1	Mg 1	0	0
56	DB	12	Total 12	Mg 12	0	0

- Molecule 57 is NEGAMYCIN (three-letter code: NEG) (formula: C<sub>9</sub>H<sub>20</sub>N<sub>4</sub>O<sub>4</sub>).



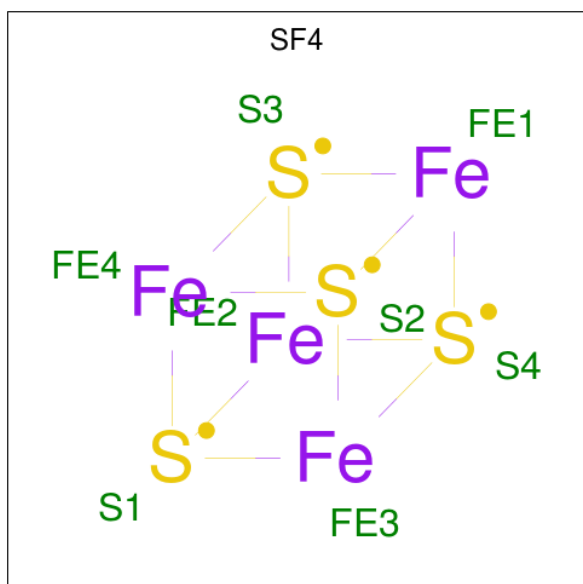
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AW	1	Total	C	N	O	0	0
			17	9	4	4		
57	AX	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CA	1	Total	C	N	O	0	0
			17	9	4	4		
57	CW	1	Total	C	N	O	0	0
			17	9	4	4		
57	CX	1	Total	C	N	O	0	0
			17	9	4	4		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula:  $\text{Zn}$ ).

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AX	1	Total 1	K 1	0	0
60	CX	1	Total 1	K 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	247	Total 247	O 247	0	0
61	AD	1	Total 1	O 1	0	0
61	AE	2	Total 2	O 2	0	0
61	AL	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AM	2	Total	O	0	0
			2	2		
61	AO	1	Total	O	0	0
			1	1		
61	AV	3	Total	O	0	0
			3	3		
61	AW	13	Total	O	0	0
			13	13		
61	AX	11	Total	O	0	0
			11	11		
61	AY	1	Total	O	0	0
			1	1		
61	BA	1396	Total	O	0	0
			1396	1396		
61	BB	34	Total	O	0	0
			34	34		
61	BD	12	Total	O	0	0
			12	12		
61	BE	11	Total	O	0	0
			11	11		
61	BF	5	Total	O	0	0
			5	5		
61	BG	3	Total	O	0	0
			3	3		
61	BI	1	Total	O	0	0
			1	1		
61	BN	1	Total	O	0	0
			1	1		
61	BO	2	Total	O	0	0
			2	2		
61	BP	23	Total	O	0	0
			23	23		
61	BQ	3	Total	O	0	0
			3	3		
61	BR	1	Total	O	0	0
			1	1		
61	BT	2	Total	O	0	0
			2	2		
61	BU	3	Total	O	0	0
			3	3		
61	BV	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BW	1	Total	O	0	0
			1	1		
61	BX	2	Total	O	0	0
			2	2		
61	BZ	1	Total	O	0	0
			1	1		
61	B0	8	Total	O	0	0
			8	8		
61	B3	1	Total	O	0	0
			1	1		
61	B5	6	Total	O	0	0
			6	6		
61	B6	1	Total	O	0	0
			1	1		
61	B7	2	Total	O	0	0
			2	2		
61	B8	7	Total	O	0	0
			7	7		
61	CA	184	Total	O	0	0
			184	184		
61	CJ	2	Total	O	0	0
			2	2		
61	CP	1	Total	O	0	0
			1	1		
61	CV	2	Total	O	0	0
			2	2		
61	CW	3	Total	O	0	0
			3	3		
61	CX	6	Total	O	0	0
			6	6		
61	DA	960	Total	O	0	0
			960	960		
61	DB	8	Total	O	0	0
			8	8		
61	DD	16	Total	O	0	0
			16	16		
61	DE	9	Total	O	0	0
			9	9		
61	DF	5	Total	O	0	0
			5	5		
61	DN	3	Total	O	0	0
			3	3		

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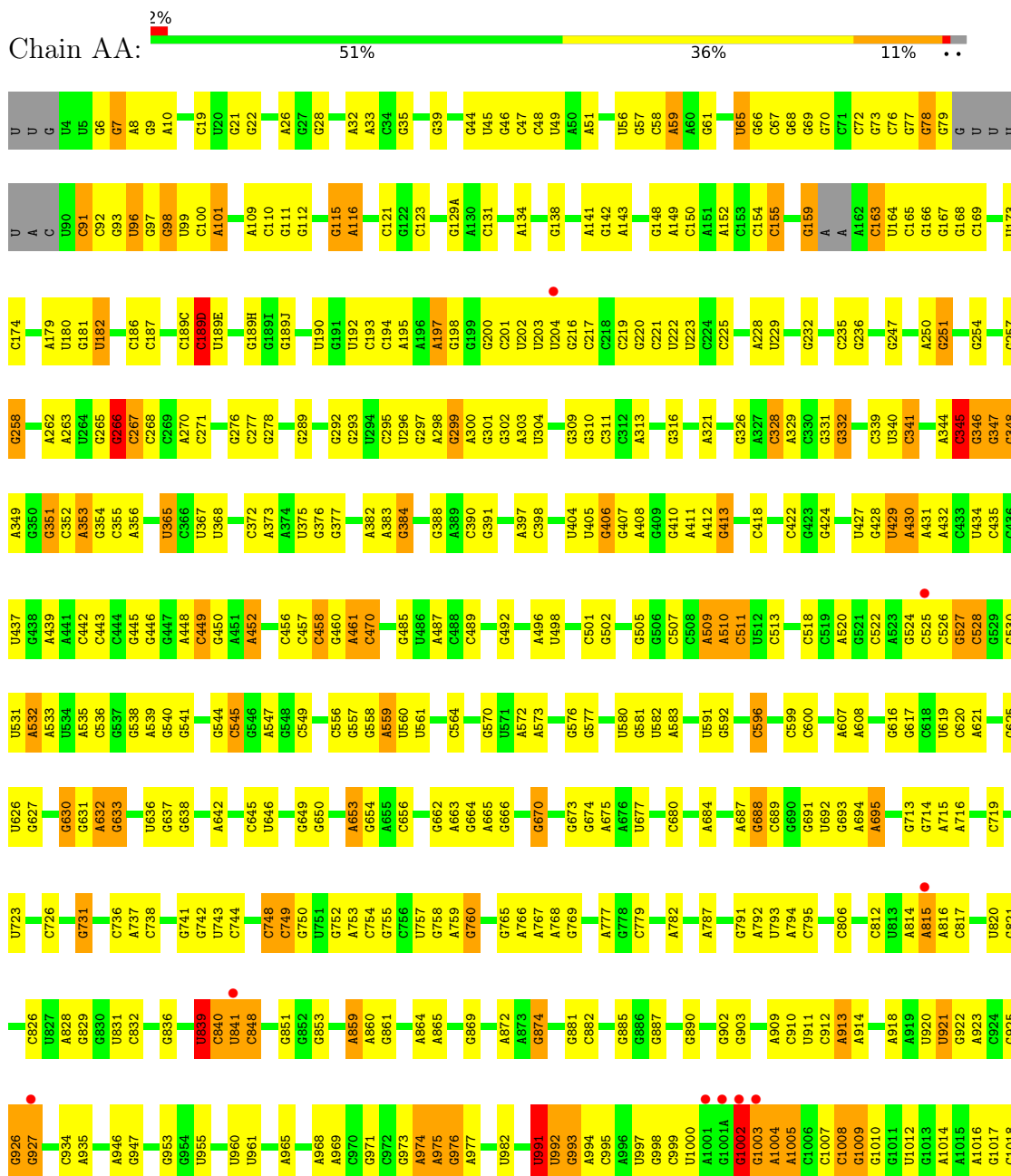
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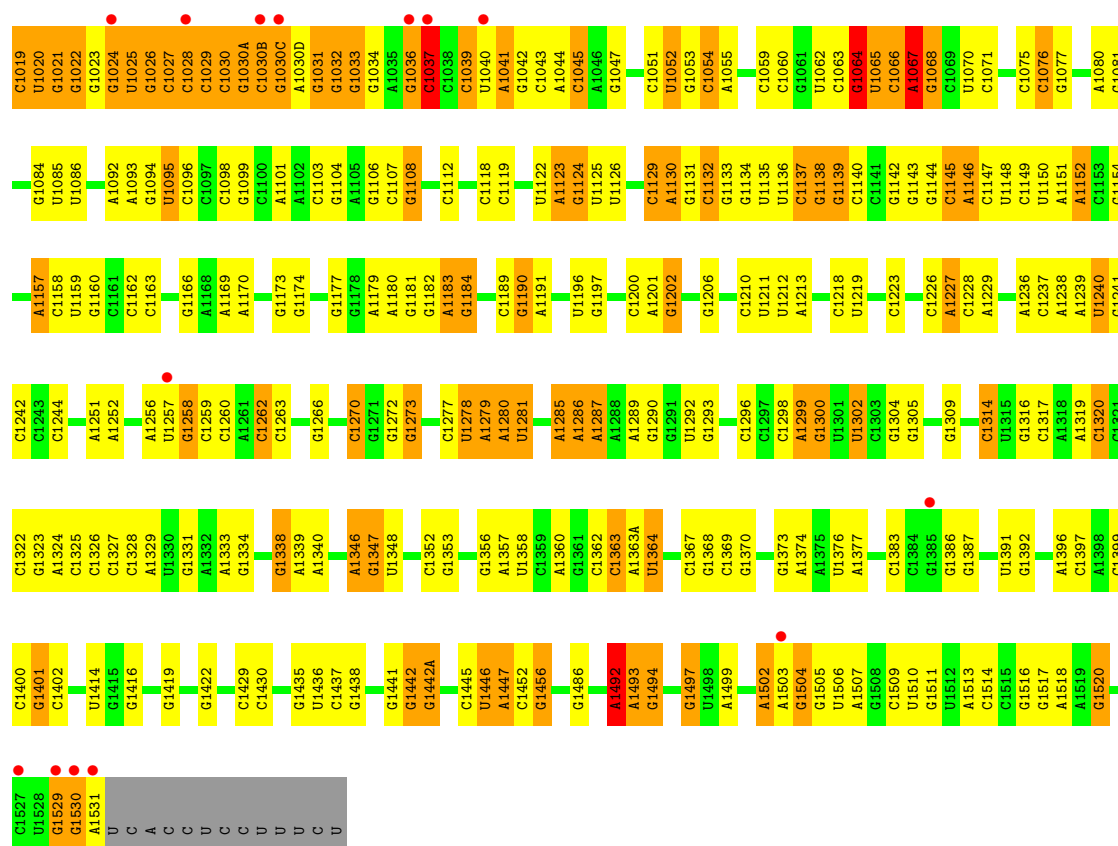
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DO	2	Total	O	0	0
			2	2		
61	DP	15	Total	O	0	0
			15	15		
61	DQ	1	Total	O	0	0
			1	1		
61	DR	1	Total	O	0	0
			1	1		
61	DU	1	Total	O	0	0
			1	1		
61	DW	1	Total	O	0	0
			1	1		
61	DX	1	Total	O	0	0
			1	1		
61	DY	2	Total	O	0	0
			2	2		
61	D0	8	Total	O	0	0
			8	8		
61	D1	4	Total	O	0	0
			4	4		
61	D7	2	Total	O	0	0
			2	2		
61	D8	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

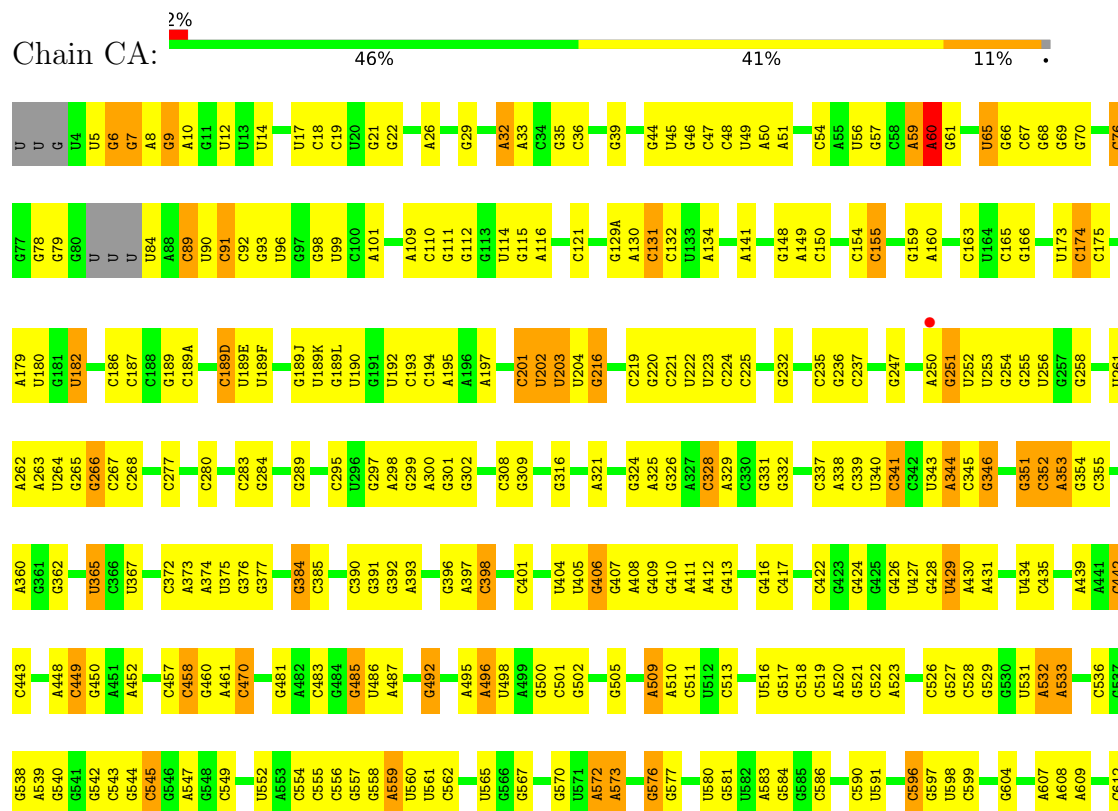
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

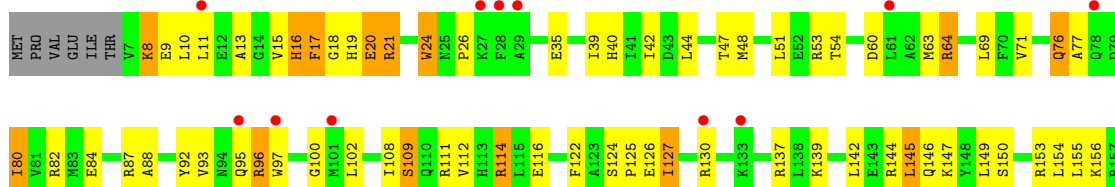
#### • Molecule 1: 16S Ribosomal RNA

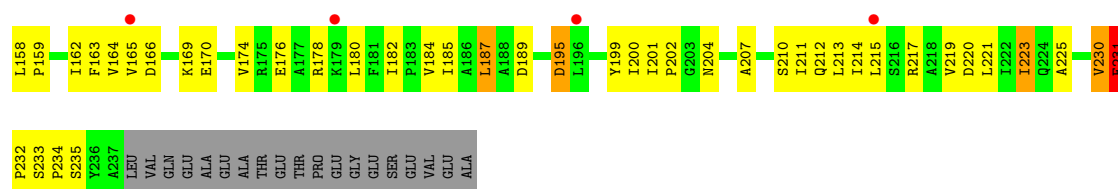




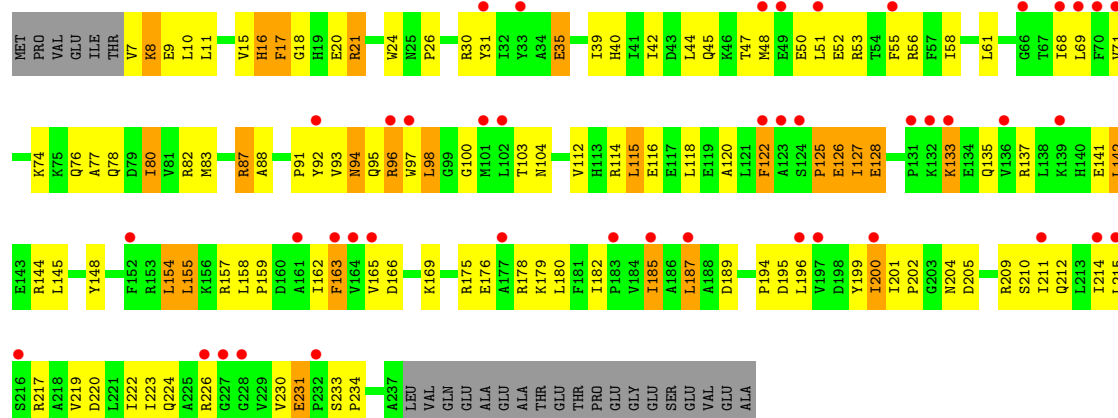
● Molecule 1: 16S Ribosomal RNA



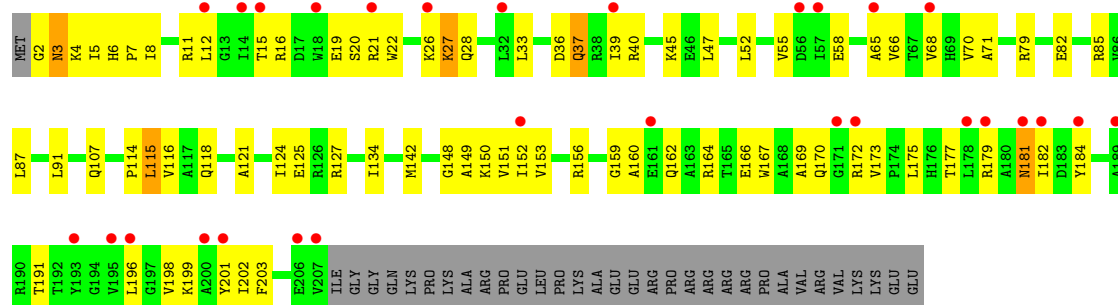




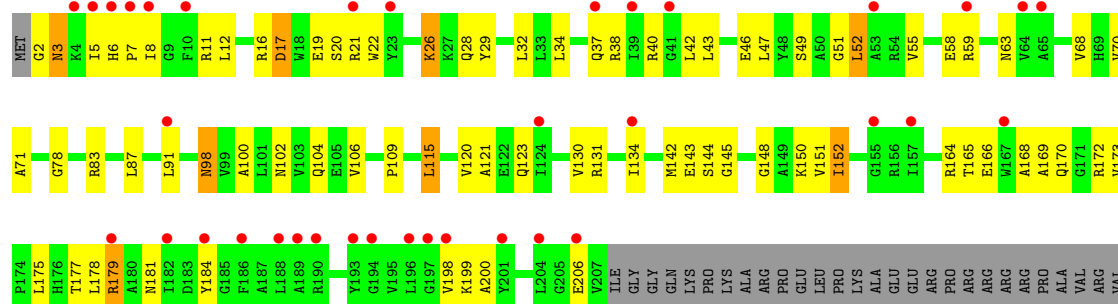
• Molecule 2: 30S Ribosomal Protein S2



• Molecule 3: 30S Ribosomal Protein S3

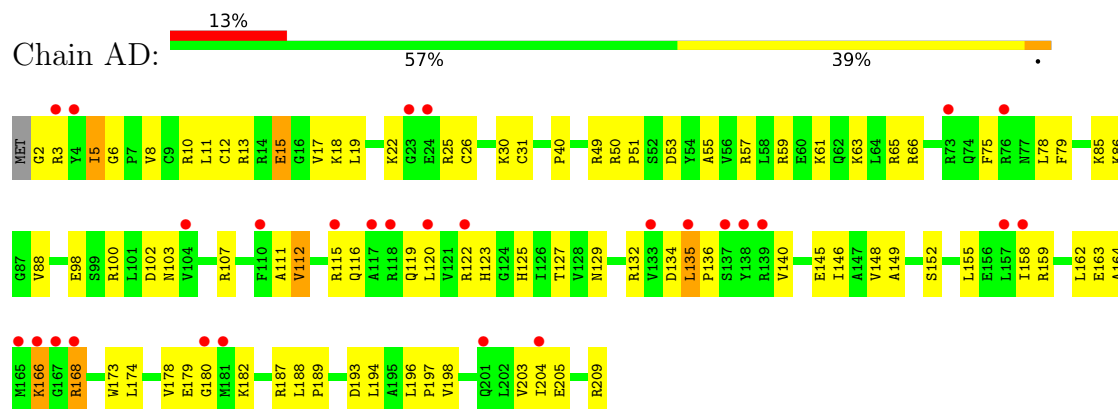


• Molecule 3: 30S Ribosomal Protein S3

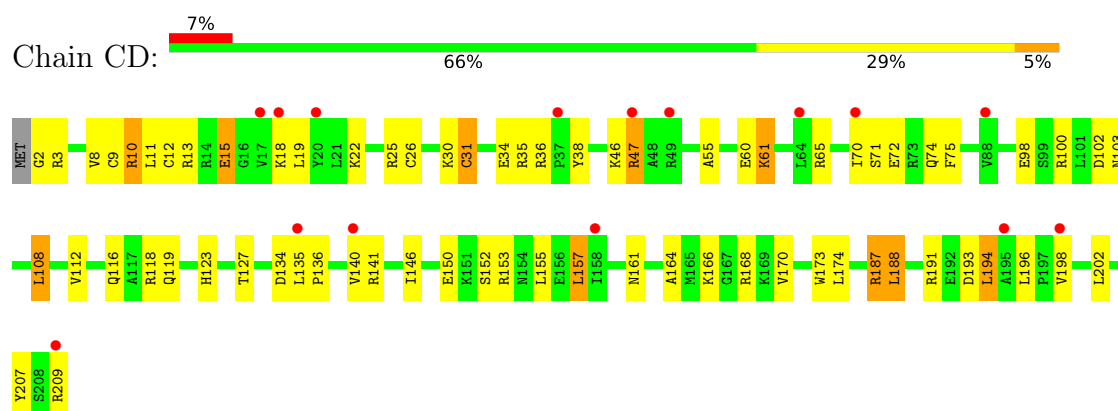


LYS  
LYS  
GLU  
GLU

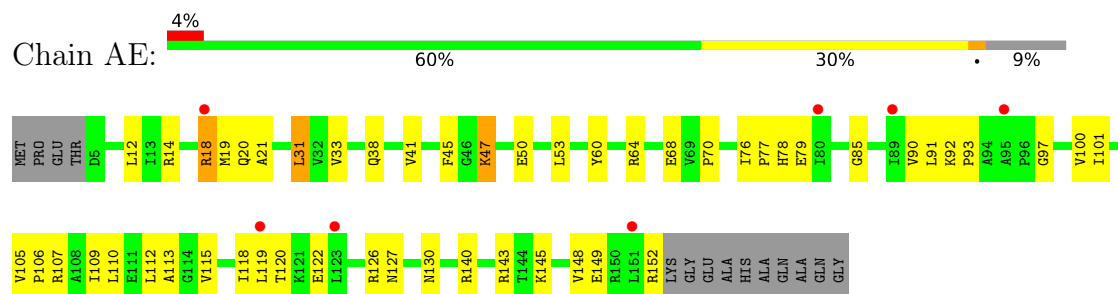
• Molecule 4: 30S Ribosomal Protein S4



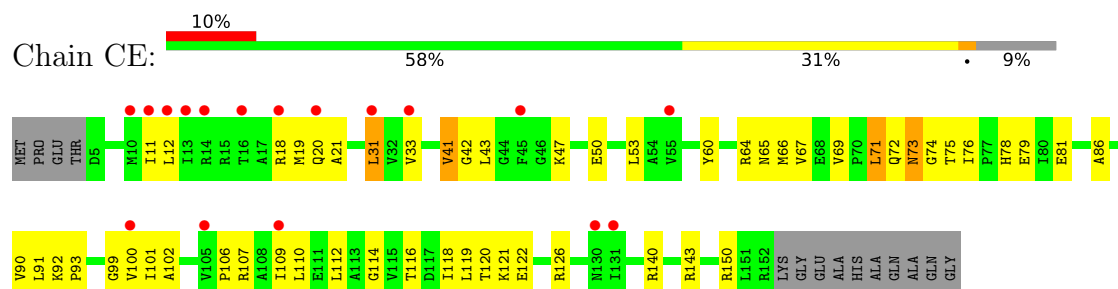
• Molecule 4: 30S Ribosomal Protein S4



• Molecule 5: 30S Ribosomal Protein S5


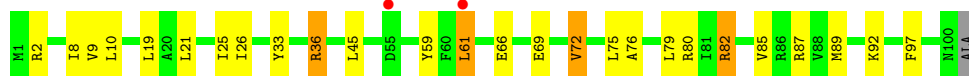


• Molecule 5: 30S Ribosomal Protein S5

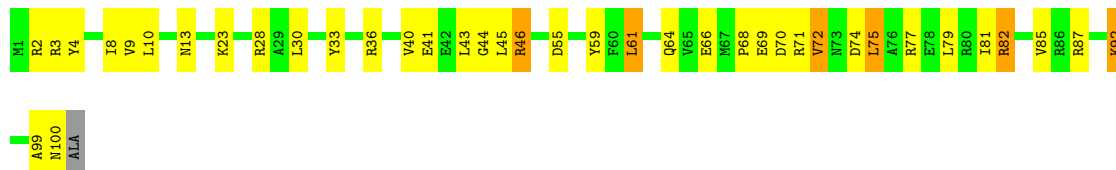





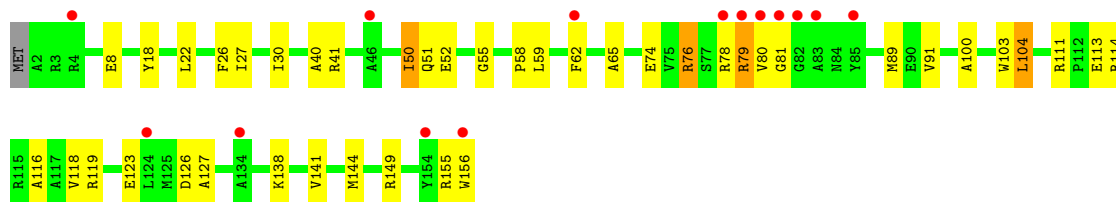
## ● Molecule 6: 30S Ribosomal Protein S6

Chain AF:  2% 73% 22% ..


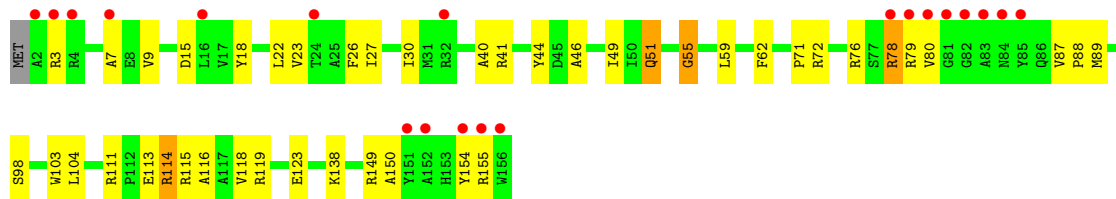
## ● Molecule 6: 30S Ribosomal Protein S6

Chain CF:  60% 33% 6% ..

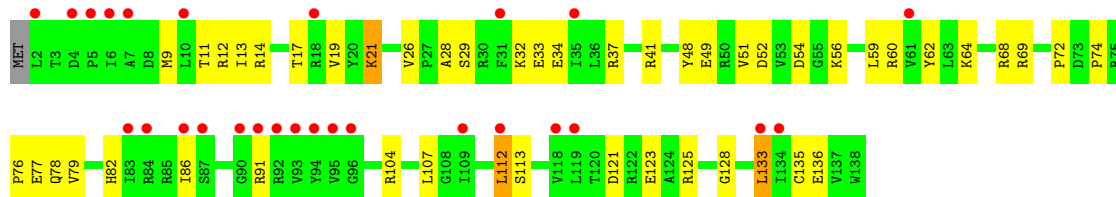
## ● Molecule 7: 30S Ribosomal Protein S7

Chain AG:  9% 72% 24% ..

## ● Molecule 7: 30S Ribosomal Protein S7

Chain CG:  13% 71% 26% ..

## ● Molecule 8: 30S Ribosomal Protein S8

Chain AH:  20% 64% 33% ..

## ● Molecule 8: 30S Ribosomal Protein S8

Chain CH:  17% 62% 36% ..

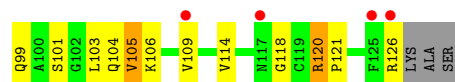


Chain AK: 



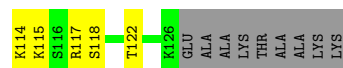
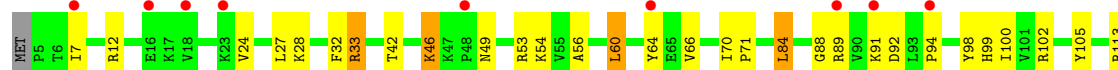
- Molecule 11: 30S Ribosomal Protein S11

Chain CK: 



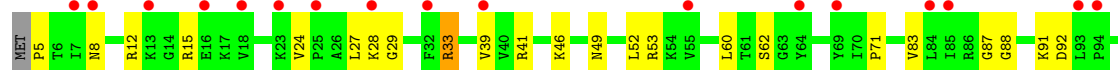
- Molecule 12: 30S Ribosomal Protein S12

Chain AL: 



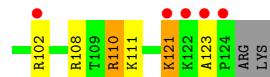
- Molecule 12: 30S Ribosomal Protein S12

Chain CL: 

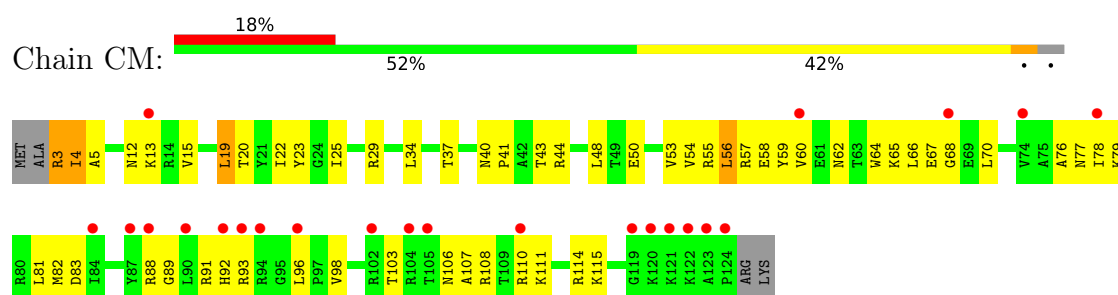


- Molecule 13: 30S Ribosomal Protein S13

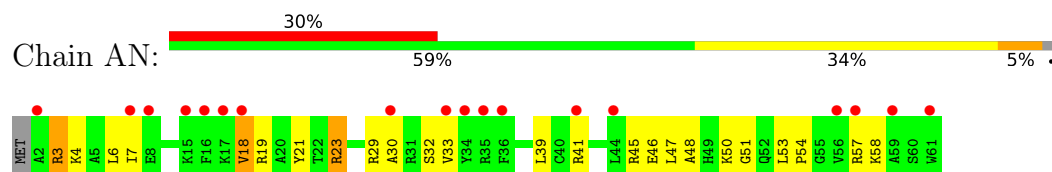
Chain AM: 



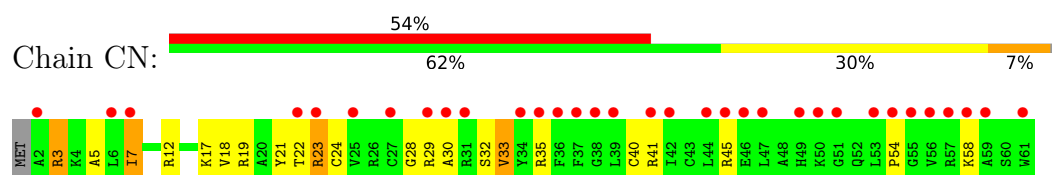
- Molecule 13: 30S Ribosomal Protein S13



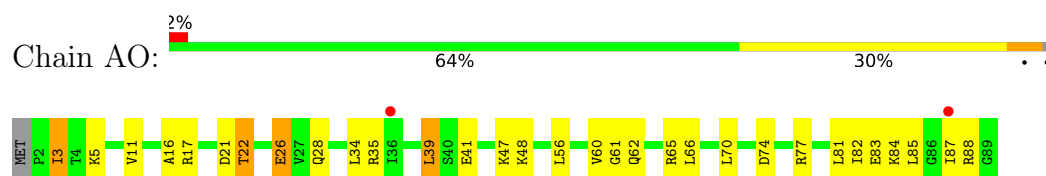
• Molecule 14: 30S Ribosomal Protein S14



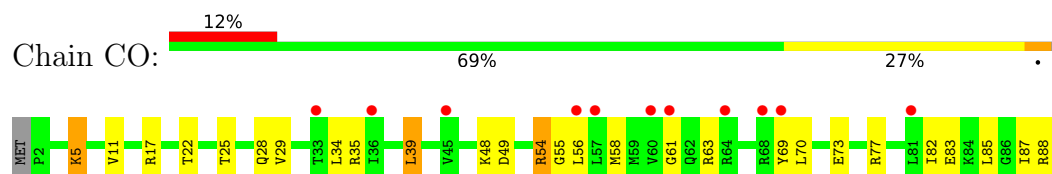
• Molecule 14: 30S Ribosomal Protein S14



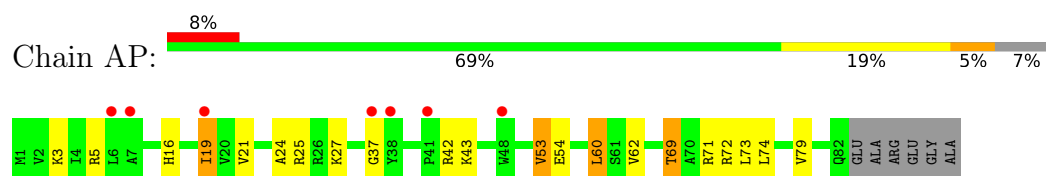
• Molecule 15: 30S Ribosomal Protein S15



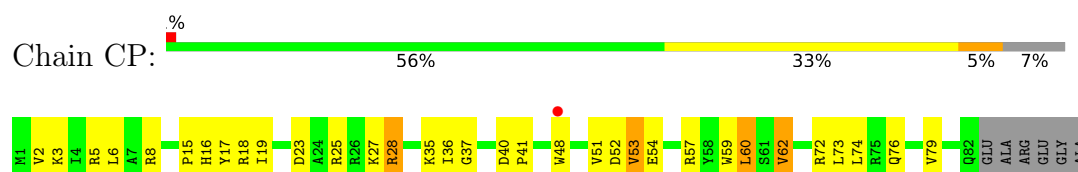
• Molecule 15: 30S Ribosomal Protein S15



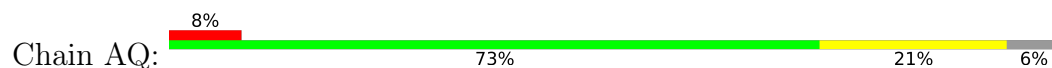
• Molecule 16: 30S Ribosomal Protein S16



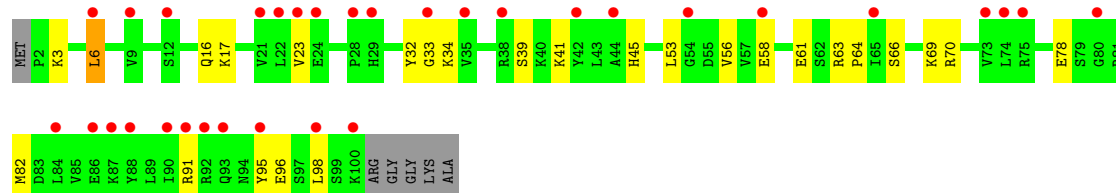
• Molecule 16: 30S Ribosomal Protein S16



- Molecule 17: 30S Ribosomal Protein S17



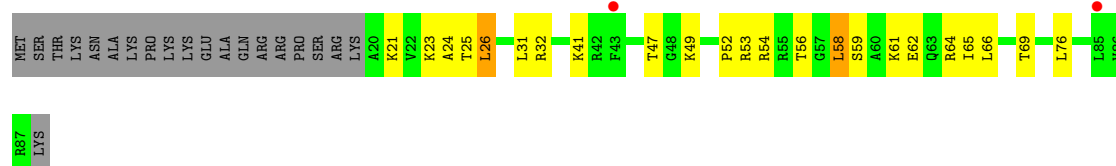
- Molecule 17: 30S Ribosomal Protein S17



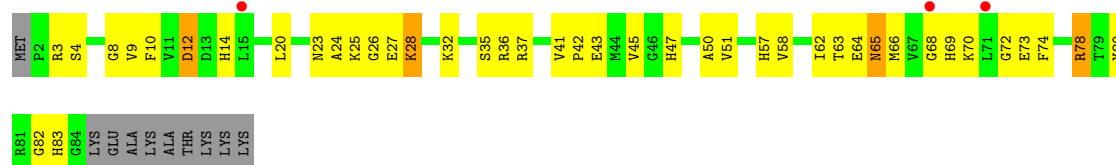
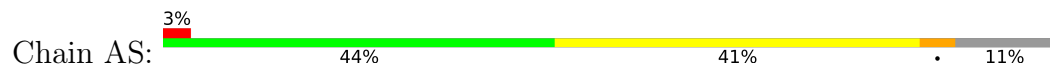
- Molecule 18: 30S Ribosomal Protein S18



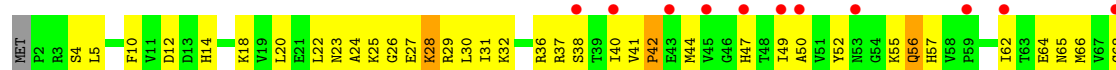
- Molecule 18: 30S Ribosomal Protein S18



- Molecule 19: 30S Ribosomal Protein S19

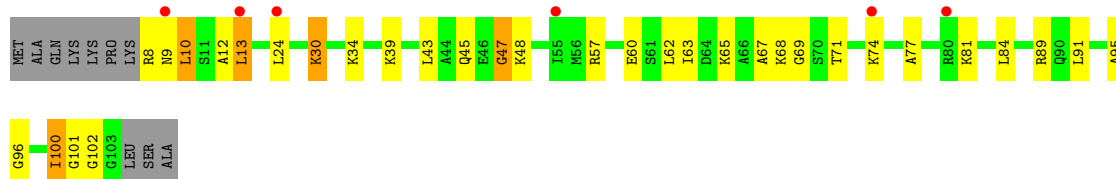


- Molecule 19: 30S Ribosomal Protein S19

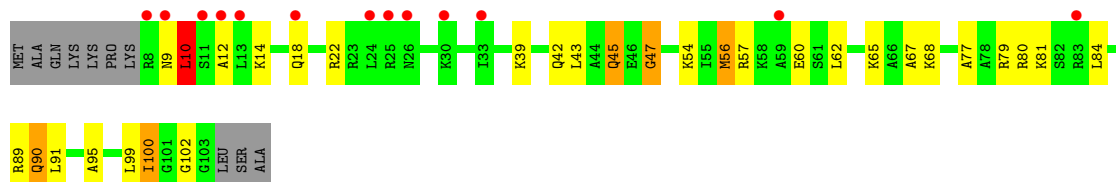




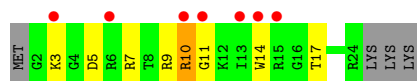
- Molecule 20: 30S Ribosomal Protein S20



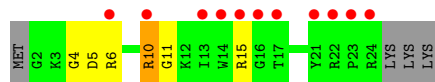
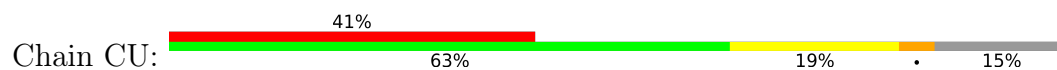
- Molecule 20: 30S Ribosomal Protein S20



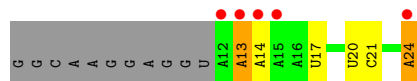
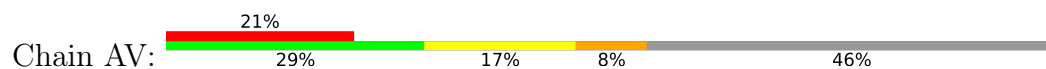
- Molecule 21: 30S Ribosomal Protein THX



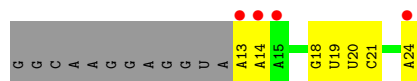
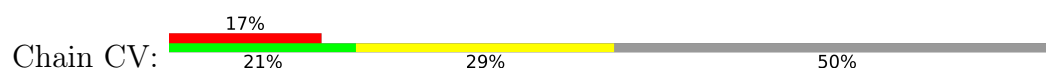
- Molecule 21: 30S Ribosomal Protein THX



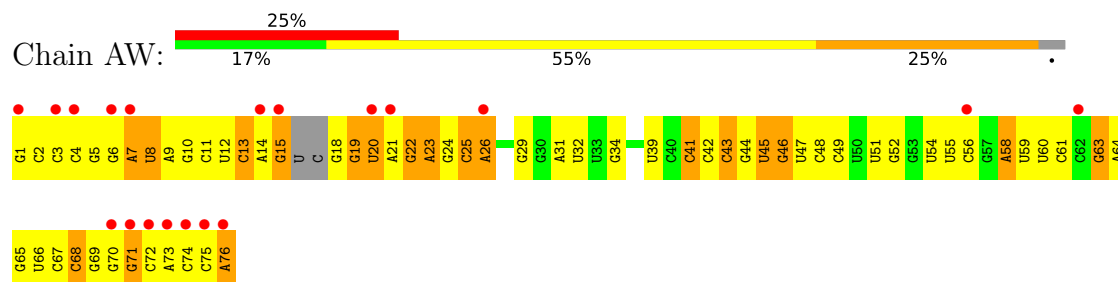
- Molecule 22: mRNA



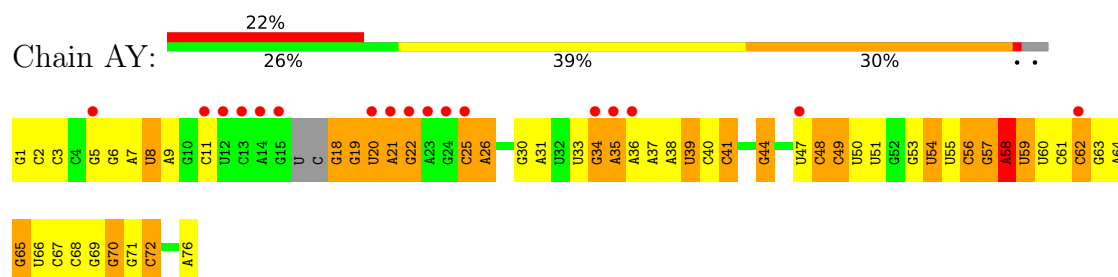
- Molecule 22: mRNA



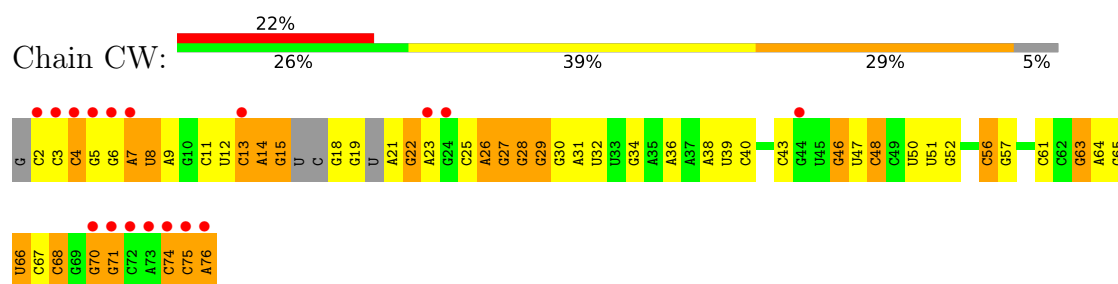
- Molecule 23: A/P-site tRNA



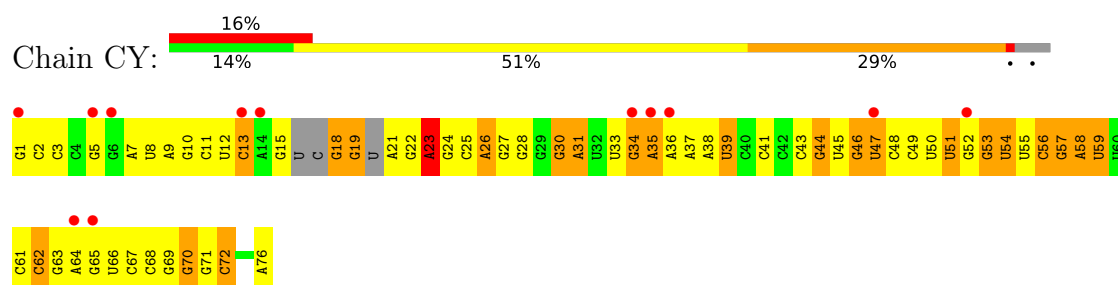
- Molecule 23: A/P-site tRNA



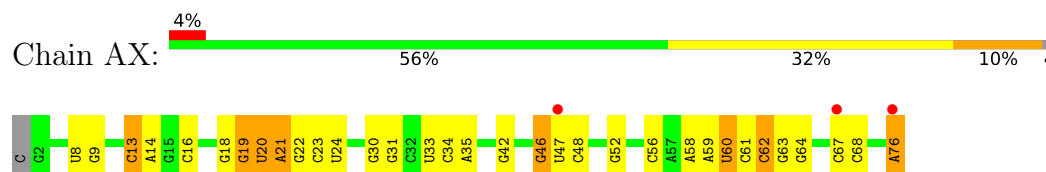
- Molecule 23: A/P-site tRNA



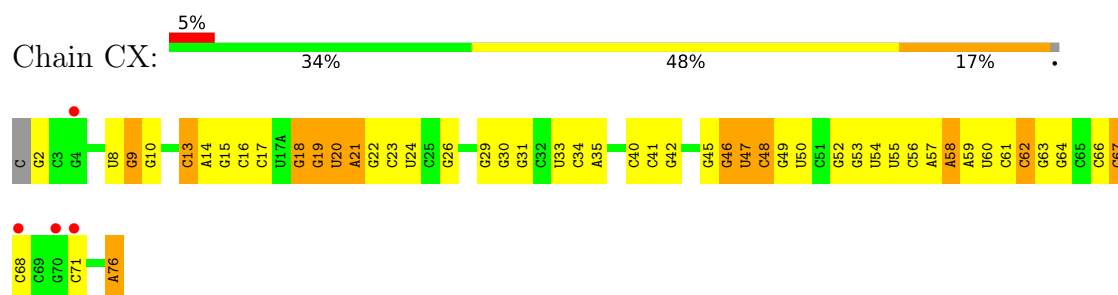
- Molecule 23: A/P-site tRNA



- Molecule 24: E-site tRNA



- Molecule 24: E-site tRNA

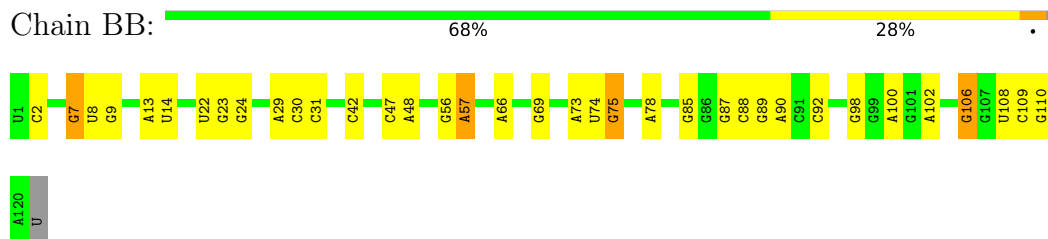
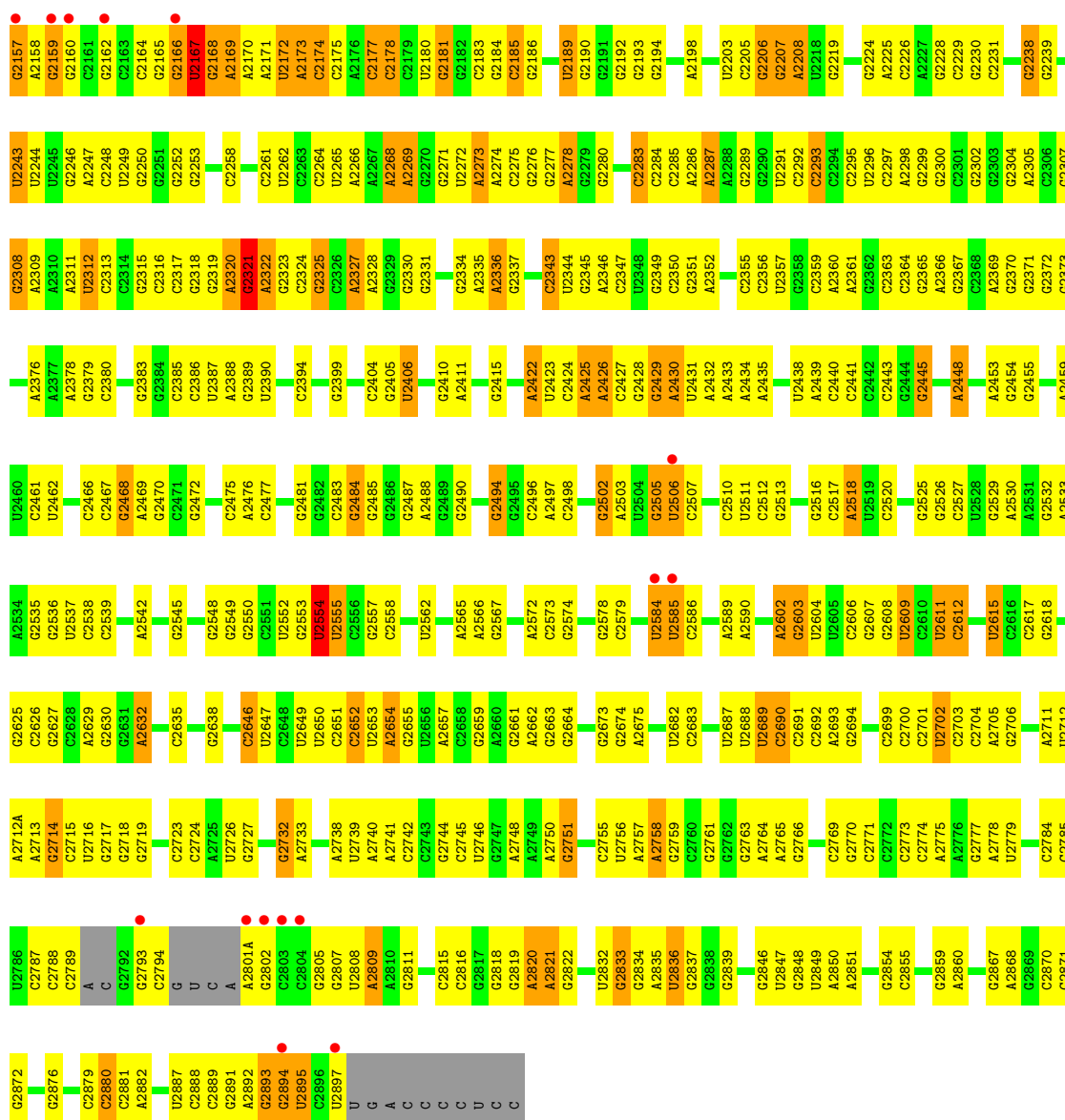




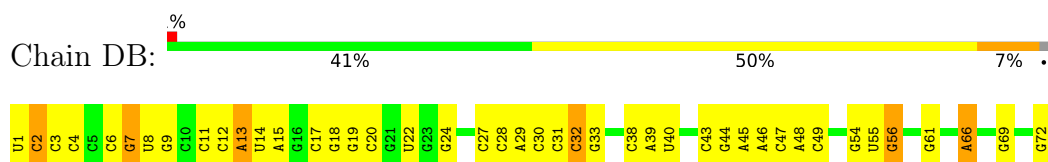






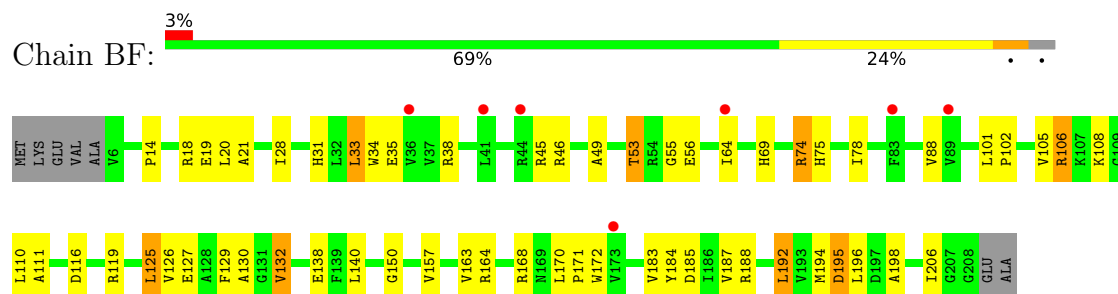


• Molecule 26: 5S Ribosomal RNA

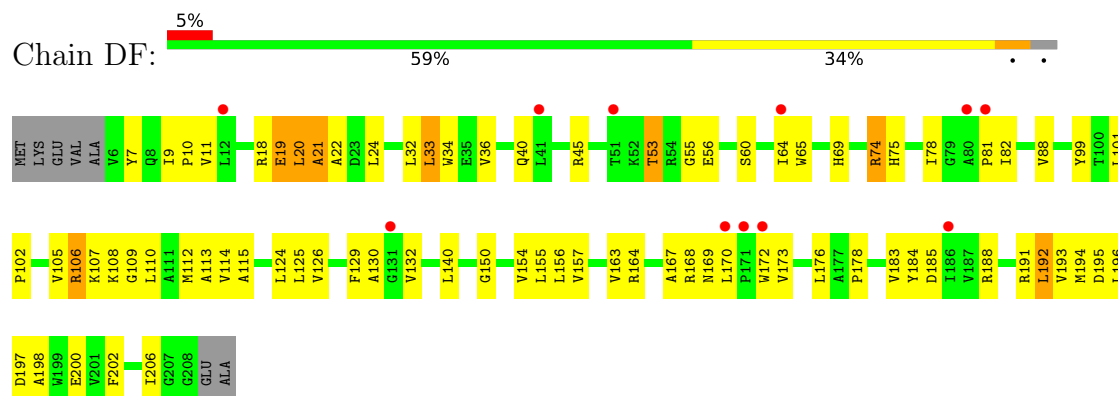




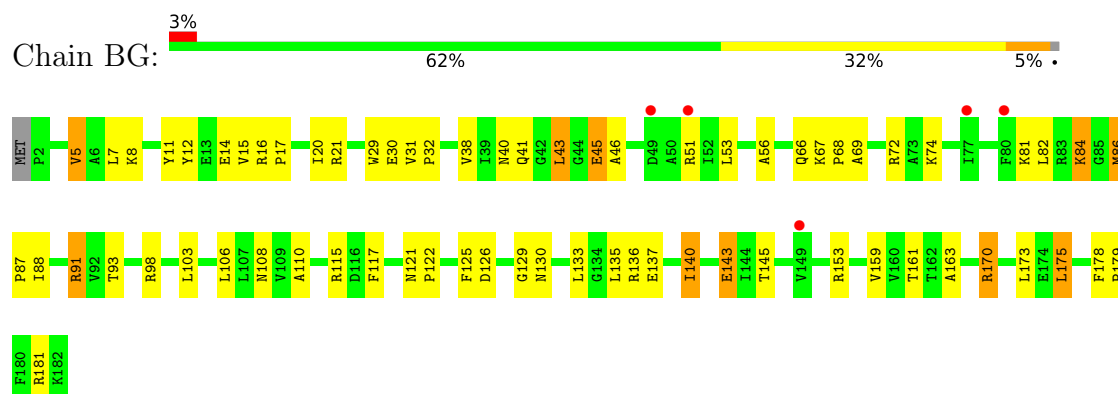
- Molecule 29: 50S Ribosomal Protein L4



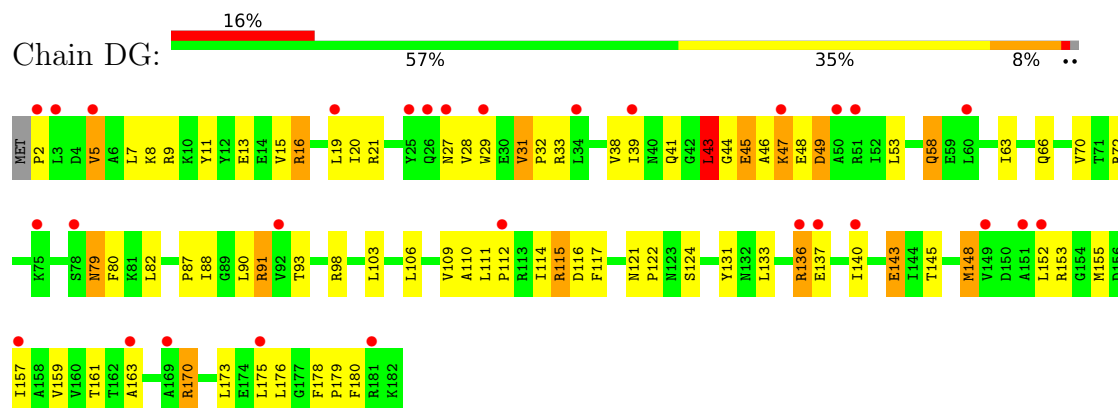
- Molecule 29: 50S Ribosomal Protein L4



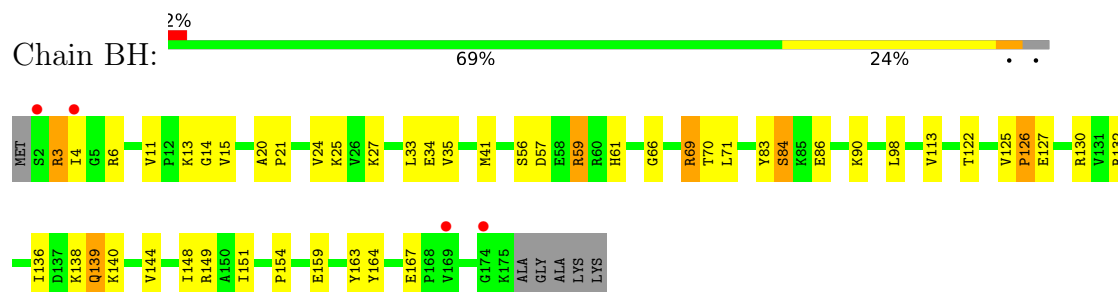
- Molecule 30: 50S Ribosomal Protein L5



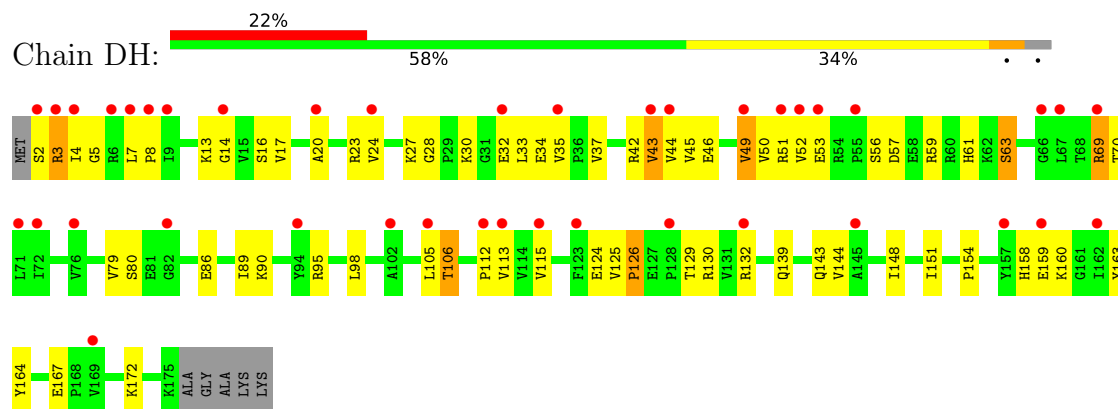
- Molecule 30: 50S Ribosomal Protein L5



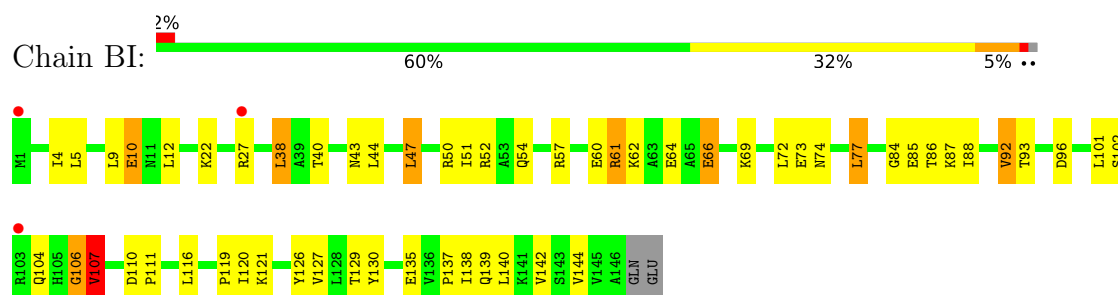
- Molecule 31: 50S Ribosomal Protein L6



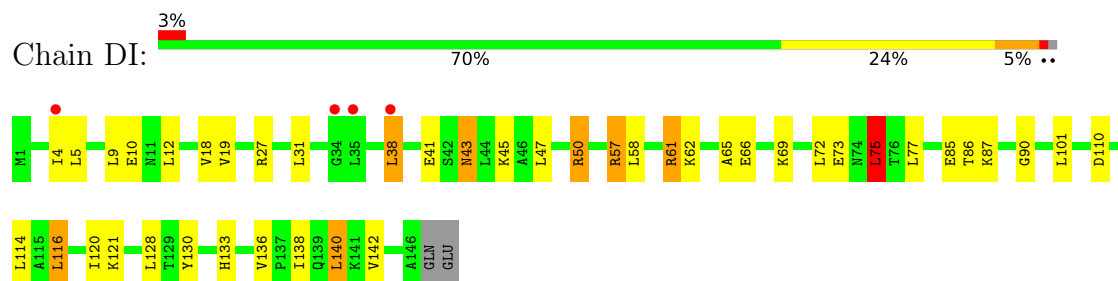
- Molecule 31: 50S Ribosomal Protein L6



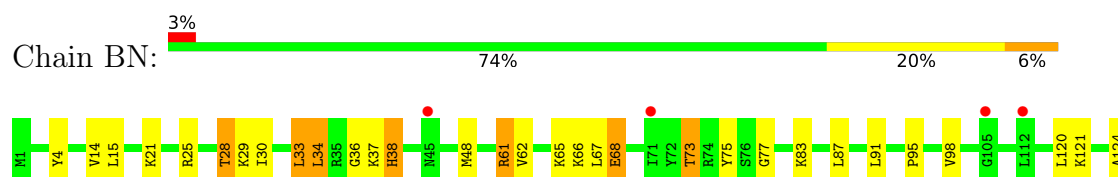
- Molecule 32: 50S Ribosomal Protein L9



- Molecule 32: 50S Ribosomal Protein L9

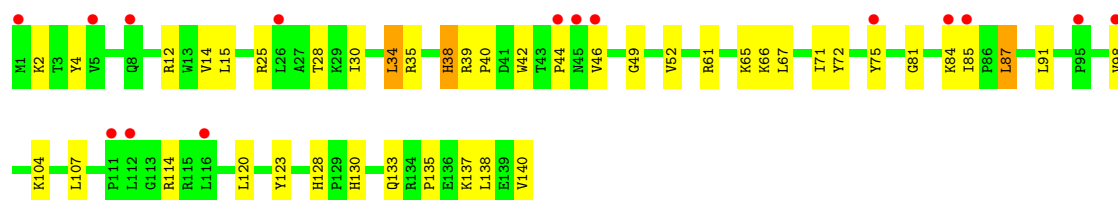


- Molecule 33: 50S Ribosomal Protein L13





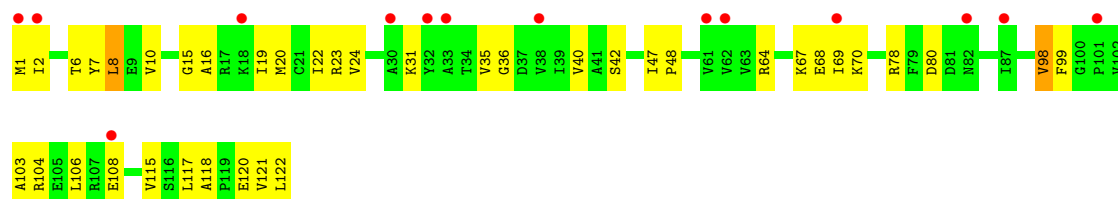
• Molecule 33: 50S Ribosomal Protein L13



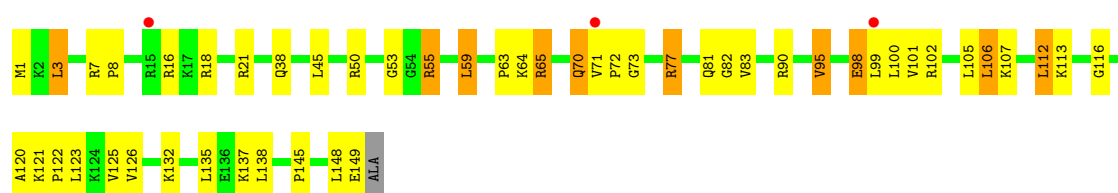
• Molecule 34: 50S Ribosomal Protein L14



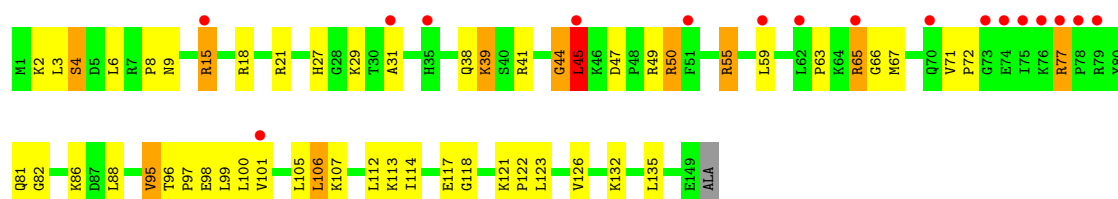
• Molecule 34: 50S Ribosomal Protein L14



• Molecule 35: 50S Ribosomal Protein L15



• Molecule 35: 50S Ribosomal Protein L15

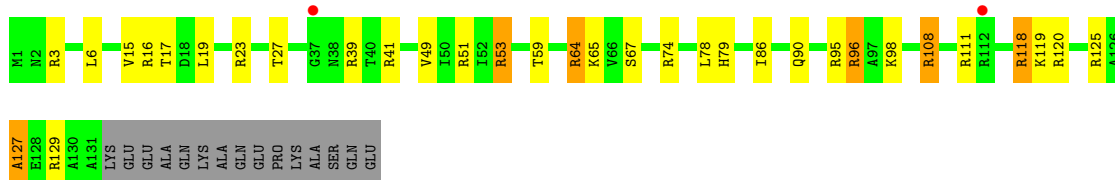




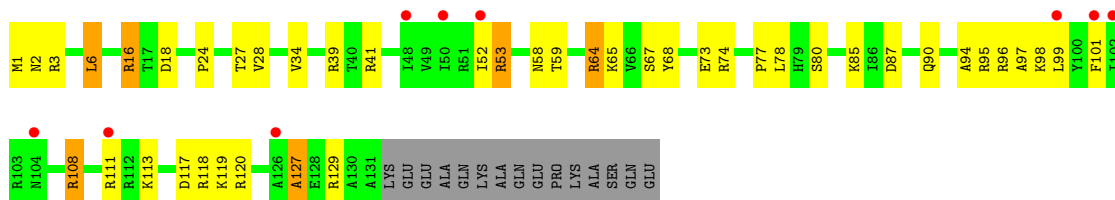
Chain DS:



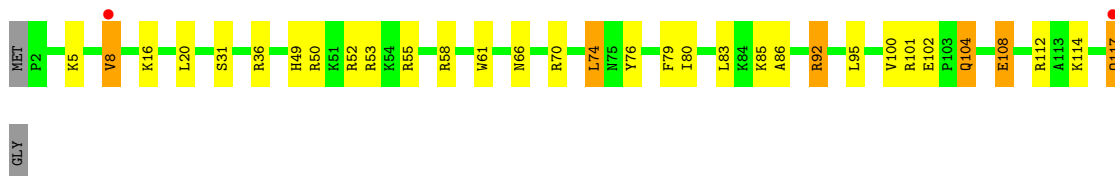
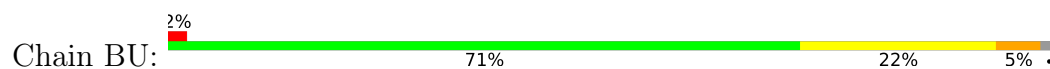
• Molecule 39: 50S Ribosomal Protein L19



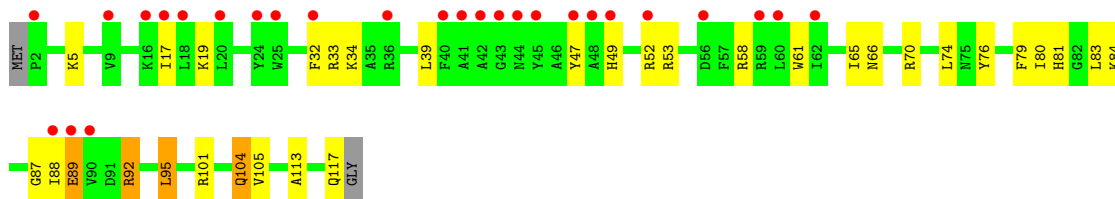
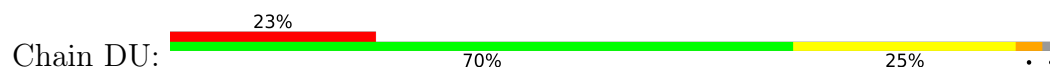
• Molecule 39: 50S Ribosomal Protein L19



• Molecule 40: 50S Ribosomal Protein L20



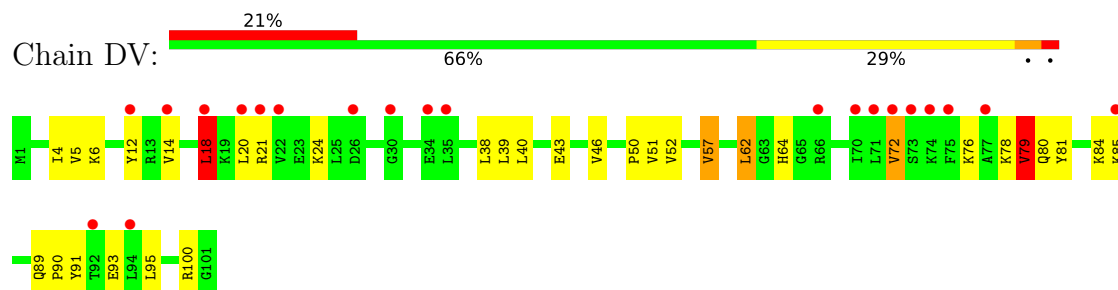
• Molecule 40: 50S Ribosomal Protein L20



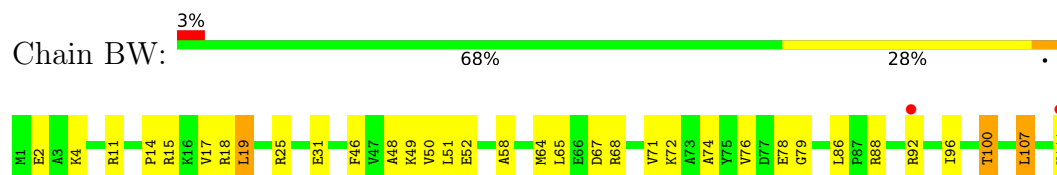
• Molecule 41: 50S Ribosomal Protein L21



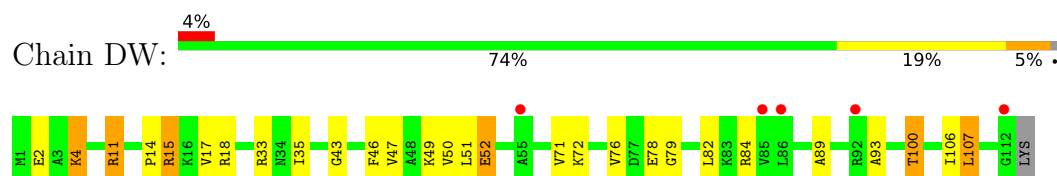
- Molecule 41: 50S Ribosomal Protein L21



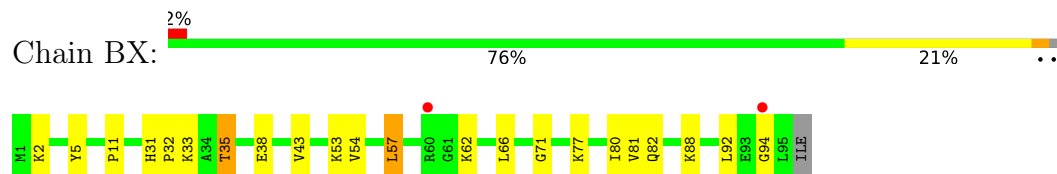
- Molecule 42: 50S Ribosomal Protein L22



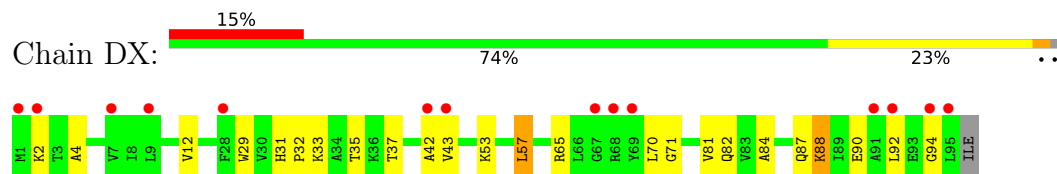
- Molecule 42: 50S Ribosomal Protein L22



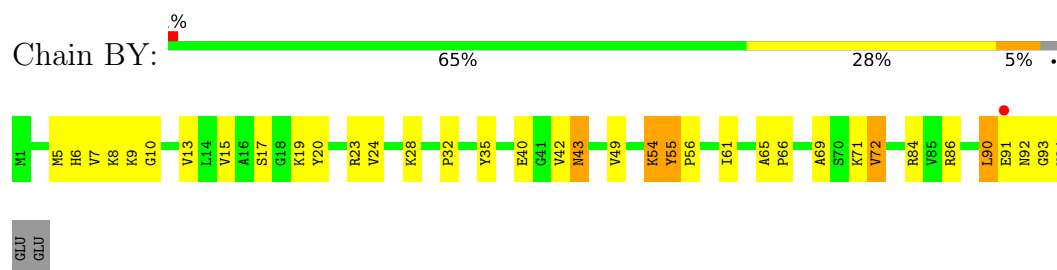
- Molecule 43: 50S Ribosomal Protein L23



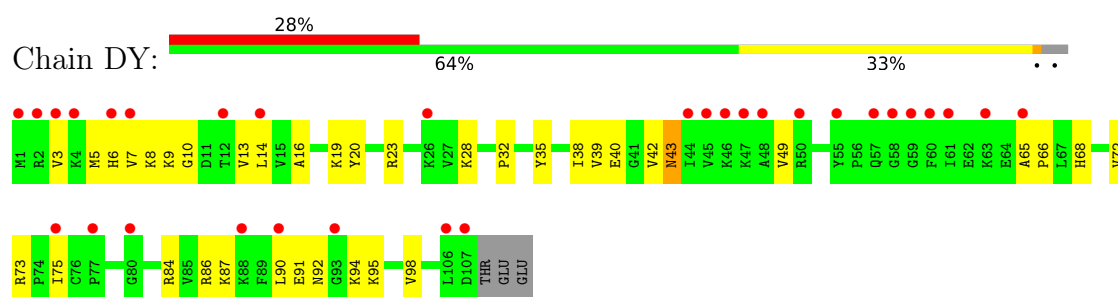
- Molecule 43: 50S Ribosomal Protein L23



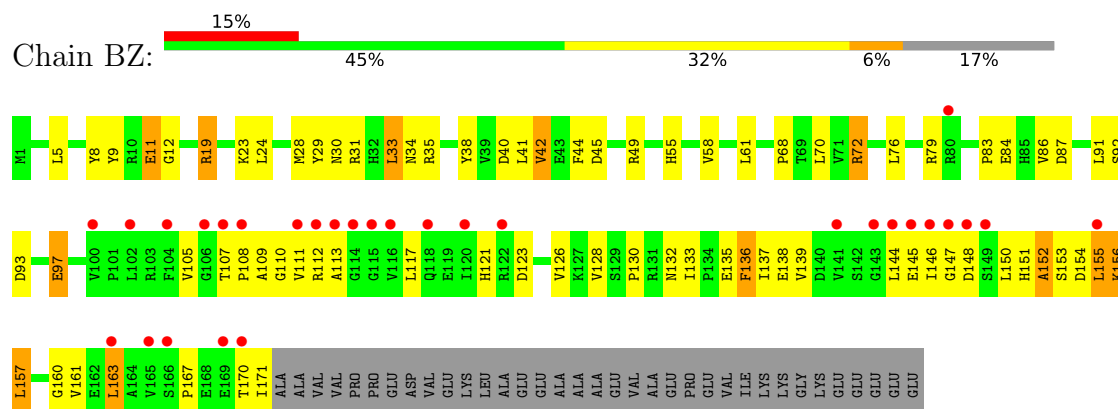
- Molecule 44: 50S Ribosomal Protein L24



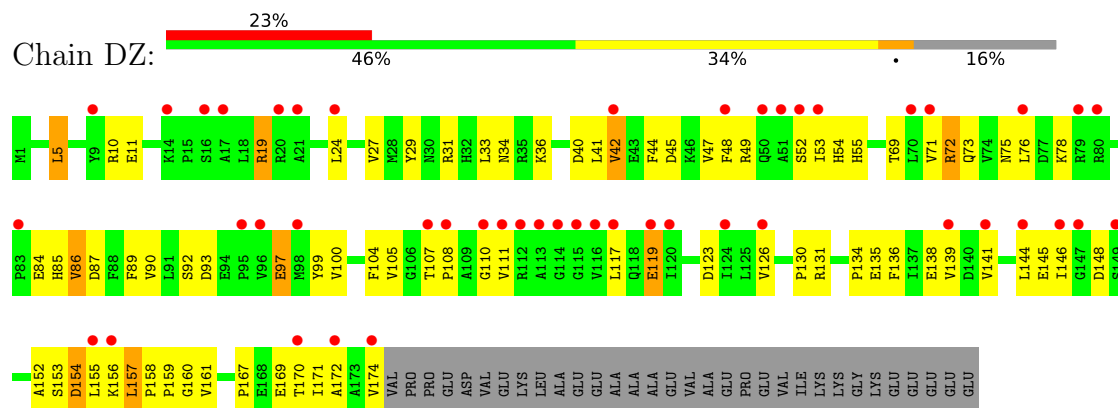
- Molecule 44: 50S Ribosomal Protein L24



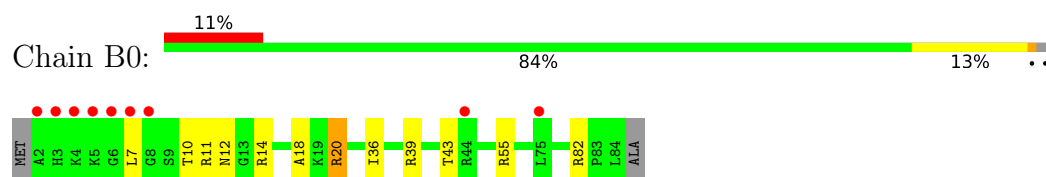
• Molecule 45: 50S Ribosomal Protein L25



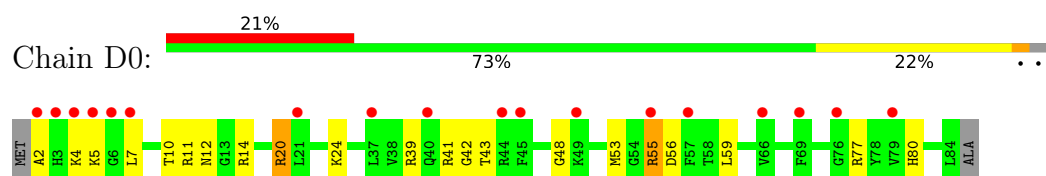
• Molecule 45: 50S Ribosomal Protein L25



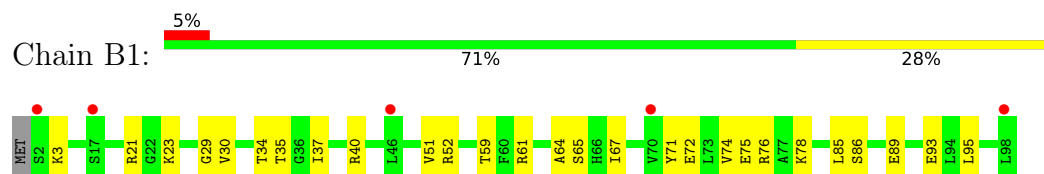
• Molecule 46: 50S Ribosomal Protein L27



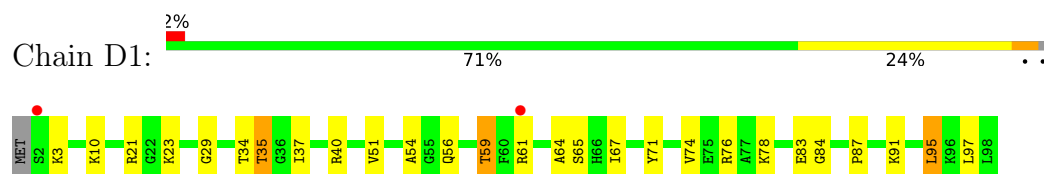
• Molecule 46: 50S Ribosomal Protein L27



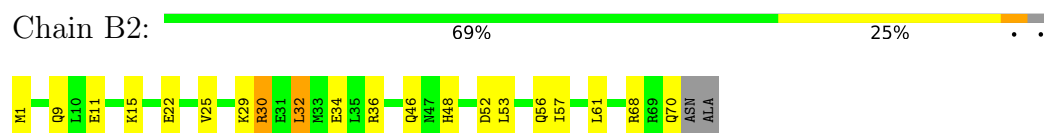
- Molecule 47: 50S Ribosomal Protein L28



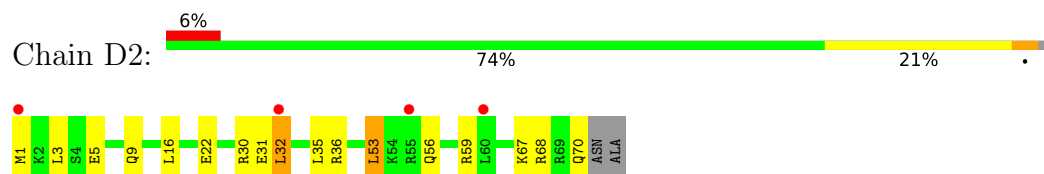
- Molecule 47: 50S Ribosomal Protein L28



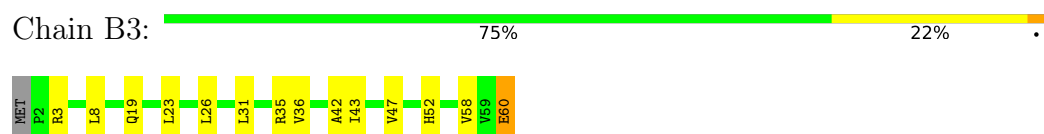
- Molecule 48: 50S Ribosomal Protein L29



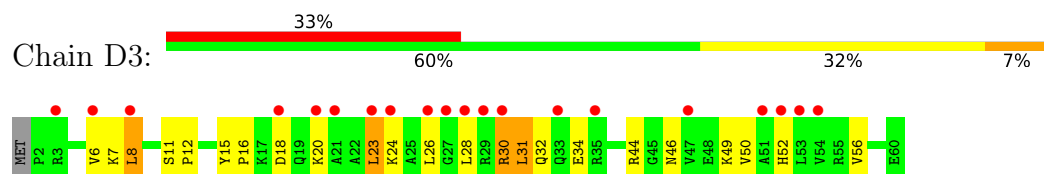
- Molecule 48: 50S Ribosomal Protein L29



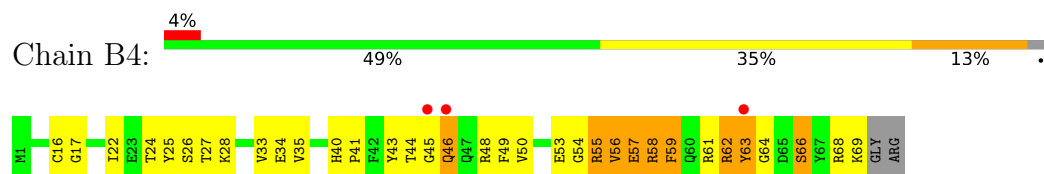
- Molecule 49: 50S Ribosomal Protein L30



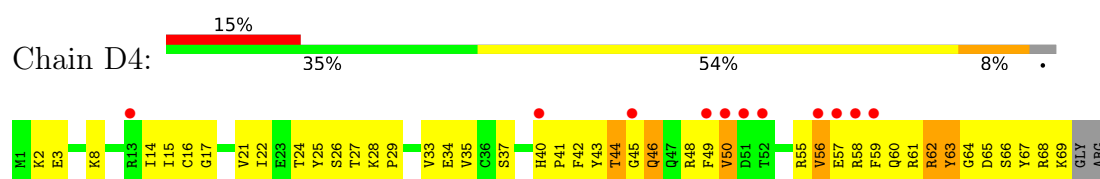
- Molecule 49: 50S Ribosomal Protein L30



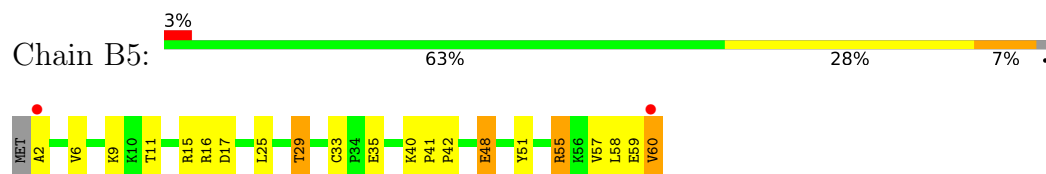
- Molecule 50: 50S Ribosomal Protein L31



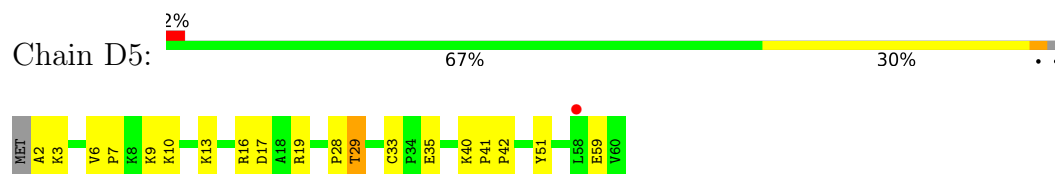
- Molecule 50: 50S Ribosomal Protein L31



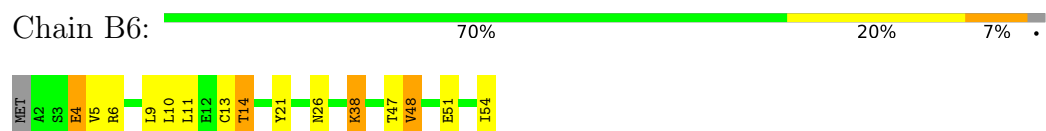
• Molecule 51: 50S Ribosomal Protein L32



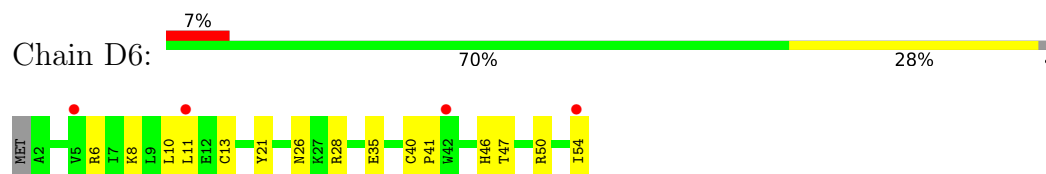
• Molecule 51: 50S Ribosomal Protein L32



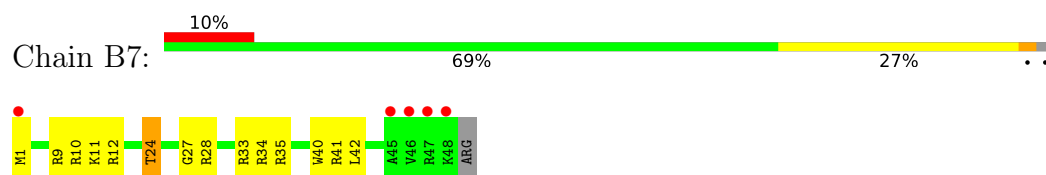
• Molecule 52: 50S Ribosomal Protein L33



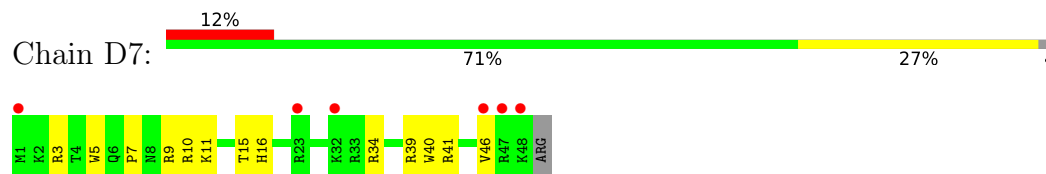
• Molecule 52: 50S Ribosomal Protein L33



• Molecule 53: 50S Ribosomal Protein L34



• Molecule 53: 50S Ribosomal Protein L34

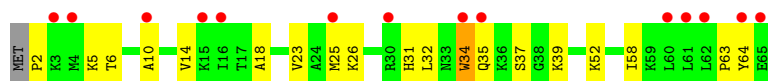


• Molecule 54: 50S Ribosomal Protein L35

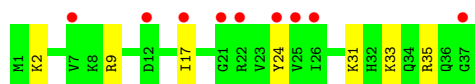
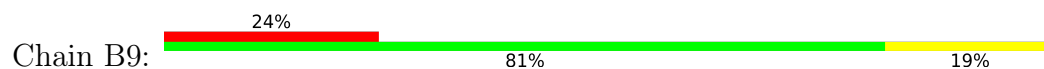




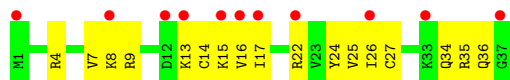
• Molecule 54: 50S Ribosomal Protein L35



• 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, $\alpha$ , $\beta$ , $\gamma$	208.25Å 443.61Å 619.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.25 – 2.70 360.63 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (124.25-2.70) 97.2 (360.63-2.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.210 , 0.257 0.209 , 0.257	Depositor DCC
$R_{free}$ test set	75600 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.2	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	297376	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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: 5MU, ZN, MIA, NEG, SF4, MG, 5MC, 4SU, 7MG, K, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AA	0.44	0/36002	0.92	46/56188 (0.1%)
1	CA	0.42	0/36170	0.94	42/56452 (0.1%)
2	AB	0.32	0/1881	0.59	0/2542
2	CB	0.32	0/1860	0.62	1/2518 (0.0%)
3	AC	0.30	0/1576	0.50	0/2130
3	CC	0.30	0/1566	0.53	0/2119
4	AD	0.31	0/1689	0.53	0/2267
4	CD	0.31	0/1704	0.55	1/2284 (0.0%)
5	AE	0.33	0/1145	0.53	0/1543
5	CE	0.33	0/1149	0.57	0/1548
6	AF	0.32	0/819	0.54	0/1111
6	CF	0.31	0/829	0.51	1/1123 (0.1%)
7	AG	0.30	0/1250	0.49	0/1679
7	CG	0.29	0/1254	0.52	0/1683
8	AH	0.29	0/1108	0.51	0/1494
8	CH	0.30	0/1108	0.52	0/1494
9	AI	0.30	0/1002	0.55	0/1346
9	CI	0.32	0/997	0.56	0/1343
10	AJ	0.29	0/722	0.56	0/982
10	CJ	0.31	0/727	0.58	0/988
11	AK	0.30	0/844	0.51	0/1145
11	CK	0.31	0/848	0.51	0/1149
12	AL	0.34	0/946	0.55	1/1274 (0.1%)
12	CL	0.33	0/946	0.58	0/1274
13	AM	0.32	0/969	0.59	0/1302
13	CM	0.29	0/961	0.54	0/1291
14	AN	0.30	0/501	0.50	0/664
14	CN	0.34	0/501	0.54	0/664
15	AO	0.34	0/739	0.53	0/985
15	CO	0.31	0/739	0.49	0/985
16	AP	0.32	0/697	0.57	0/939
16	CP	0.31	0/693	0.51	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.31	0/836	0.52	0/1117
17	CQ	0.31	0/836	0.50	0/1117
18	AR	0.33	0/560	0.49	0/746
18	CR	0.28	0/560	0.51	0/746
19	AS	0.29	0/667	0.50	0/900
19	CS	0.32	0/661	0.63	0/893
20	AT	0.29	0/730	0.56	0/965
20	CT	0.29	0/729	0.52	0/965
21	AU	0.29	0/203	0.53	0/266
21	CU	0.34	0/203	0.52	0/266
22	AV	0.51	0/310	0.97	1/480 (0.2%)
22	CV	0.44	0/282	1.00	2/437 (0.5%)
23	AW	0.54	0/1602	1.16	6/2493 (0.2%)
23	AY	0.50	0/1602	1.09	2/2493 (0.1%)
23	CW	0.50	0/1556	1.10	2/2418 (0.1%)
23	CY	0.53	0/1579	1.15	2/2455 (0.1%)
24	AX	0.58	1/1725 (0.1%)	1.16	14/2689 (0.5%)
24	CX	0.52	0/1725	1.12	11/2689 (0.4%)
25	BA	0.65	6/68083 (0.0%)	1.00	128/106274 (0.1%)
25	DA	0.49	1/67542 (0.0%)	0.97	74/105428 (0.1%)
26	BB	0.51	0/2878	0.92	0/4490
26	DB	0.48	0/2878	0.91	2/4490 (0.0%)
27	BD	0.43	0/2186	0.62	0/2944
27	DD	0.39	0/2186	0.59	0/2944
28	BE	0.45	0/1592	0.58	0/2149
28	DE	0.37	0/1592	0.61	1/2149 (0.0%)
29	BF	0.39	0/1619	0.57	0/2193
29	DF	0.35	0/1615	0.58	0/2188
30	BG	0.32	0/1450	0.52	0/1959
30	DG	0.32	0/1449	0.55	0/1958
31	BH	0.36	0/1356	0.54	0/1834
31	DH	0.33	0/1356	0.53	0/1834
32	BI	0.32	0/1100	0.58	0/1501
32	DI	0.30	0/1076	0.56	1/1471 (0.1%)
33	BN	0.39	0/1144	0.53	0/1543
33	DN	0.33	0/1144	0.55	0/1543
34	BO	0.41	0/943	0.59	0/1269
34	DO	0.35	0/943	0.55	1/1269 (0.1%)
35	BP	0.39	0/1152	0.59	0/1533
35	DP	0.34	0/1152	0.64	1/1533 (0.1%)
36	BQ	0.41	0/1143	0.53	0/1527
36	DQ	0.35	0/1143	0.56	0/1527
37	BR	0.42	0/982	0.62	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	DR	0.33	0/982	0.57	0/1312
38	BS	0.36	0/887	0.55	0/1180
38	DS	0.30	0/880	0.55	0/1172
39	BT	0.38	0/1105	0.58	0/1477
39	DT	0.32	0/1097	0.54	0/1468
40	BU	0.44	0/977	0.59	0/1301
40	DU	0.30	0/977	0.48	0/1301
41	BV	0.42	0/782	0.60	0/1049
41	DV	0.32	0/782	0.54	1/1049 (0.1%)
42	BW	0.44	0/897	0.57	0/1205
42	DW	0.34	0/897	0.52	0/1205
43	BX	0.43	0/764	0.61	1/1025 (0.1%)
43	DX	0.35	0/764	0.55	1/1025 (0.1%)
44	BY	0.40	0/819	0.59	0/1095
44	DY	0.33	0/819	0.53	0/1095
45	BZ	0.34	0/1379	0.59	0/1873
45	DZ	0.32	0/1390	0.56	0/1890
46	B0	0.42	0/662	0.63	0/881
46	D0	0.33	0/662	0.53	0/881
47	B1	0.41	0/762	0.56	0/1014
47	D1	0.35	0/762	0.54	0/1014
48	B2	0.38	0/590	0.58	0/781
48	D2	0.28	0/590	0.48	0/781
49	B3	0.37	0/474	0.58	0/635
49	D3	0.30	0/469	0.52	0/630
50	B4	0.37	0/571	0.71	0/768
50	D4	0.35	0/545	0.57	0/737
51	B5	0.43	0/469	0.64	0/635
51	D5	0.34	0/469	0.54	0/635
52	B6	0.41	0/460	0.57	0/613
52	D6	0.35	0/456	0.45	0/608
53	B7	0.44	0/426	0.60	0/561
53	D7	0.36	0/426	0.55	0/561
54	B8	0.43	0/525	0.61	0/691
54	D8	0.36	0/525	0.54	0/691
55	B9	0.42	0/310	0.50	0/407
55	D9	0.36	0/310	0.56	0/407
All	All	0.48	8/316673 (0.0%)	0.89	343/474091 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	1
7	AG	0	1
7	CG	0	1
38	BS	0	1
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	553	A	N9-C4	-8.54	1.32	1.37
25	BA	354	A	N9-C4	-8.21	1.32	1.37
25	BA	1188	A	N9-C4	-7.54	1.33	1.37
25	BA	990	A	N9-C4	-6.34	1.34	1.37
25	BA	2299	A	N9-C4	-6.34	1.34	1.37

The worst 5 of 343 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	553	A	C2-N3-C4	-12.04	104.58	110.60
25	BA	354	A	C2-N3-C4	-11.68	104.76	110.60
1	AA	345	C	N1-C2-O2	11.09	125.55	118.90
25	BA	1686	U	O5'-P-OP2	-10.46	96.29	105.70
1	CA	1154	G	C5-C6-O6	10.31	134.78	128.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	8	LYS	Peptide
7	AG	79	ARG	Peptide
38	BS	58	LEU	Peptide
7	CG	78	ARG	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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32163	0	16234	552	0
1	CA	32312	0	16308	628	0
2	AB	1846	0	1867	78	0
2	CB	1825	0	1828	97	0
3	AC	1552	0	1546	55	0
3	CC	1542	0	1517	57	0
4	AD	1659	0	1676	64	0
4	CD	1674	0	1714	46	0
5	AE	1129	0	1185	36	0
5	CE	1133	0	1191	38	0
6	AF	806	0	793	20	0
6	CF	816	0	808	29	0
7	AG	1231	0	1238	27	0
7	CG	1235	0	1249	37	0
8	AH	1088	0	1126	35	0
8	CH	1088	0	1126	39	0
9	AI	983	0	986	41	0
9	CI	978	0	966	45	0
10	AJ	709	0	650	32	0
10	CJ	714	0	672	46	0
11	AK	829	0	825	14	0
11	CK	833	0	836	20	0
12	AL	930	0	980	28	0
12	CL	930	0	980	31	0
13	AM	958	0	1002	41	0
13	CM	950	0	988	43	0
14	AN	492	0	529	22	0
14	CN	492	0	529	24	0
15	AO	728	0	760	20	0
15	CO	728	0	760	23	0
16	AP	681	0	697	21	0
16	CP	677	0	686	22	0
17	AQ	823	0	891	17	0
17	CQ	823	0	891	20	0
18	AR	555	0	618	16	0
18	CR	555	0	618	17	0
19	AS	652	0	662	38	0
19	CS	646	0	644	35	0
20	AT	728	0	798	21	0
20	CT	727	0	796	18	0
21	AU	199	0	208	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	CU	199	0	208	4	0
22	AV	277	0	140	7	0
22	CV	252	0	130	6	0
23	AW	1588	0	820	66	0
23	AY	1581	0	805	62	0
23	CW	1541	0	784	47	0
23	CY	1561	0	796	65	0
24	AX	1625	0	828	13	0
24	CX	1625	0	828	31	0
25	BA	60792	0	30654	800	0
25	DA	60311	0	30412	1121	0
26	BB	2573	0	1306	23	0
26	DB	2573	0	1306	63	0
27	BD	2136	0	2218	67	0
27	DD	2136	0	2218	69	0
28	BE	1559	0	1618	35	0
28	DE	1559	0	1618	52	0
29	BF	1584	0	1625	41	0
29	DF	1580	0	1619	61	0
30	BG	1425	0	1443	41	0
30	DG	1424	0	1434	57	0
31	BH	1330	0	1407	30	0
31	DH	1330	0	1407	42	0
32	BI	1085	0	1114	38	0
32	DI	1061	0	1080	20	0
33	BN	1117	0	1184	24	0
33	DN	1117	0	1184	29	0
34	BO	933	0	996	22	0
34	DO	933	0	996	27	0
35	BP	1135	0	1212	44	0
35	DP	1135	0	1212	48	0
36	BQ	1122	0	1179	37	0
36	DQ	1122	0	1179	62	0
37	BR	968	0	1033	20	0
37	DR	968	0	1033	27	0
38	BS	877	0	938	20	0
38	DS	870	0	923	28	0
39	BT	1091	0	1151	22	0
39	DT	1083	0	1136	32	0
40	BU	959	0	1019	27	0
40	DU	959	0	1019	29	0
41	BV	771	0	830	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	DV	771	0	830	20	0
42	BW	886	0	940	21	0
42	DW	886	0	939	17	0
43	BX	750	0	814	18	0
43	DX	750	0	814	17	0
44	BY	806	0	881	26	0
44	DY	806	0	881	29	0
45	BZ	1349	0	1355	51	0
45	DZ	1360	0	1363	64	0
46	B0	653	0	674	13	0
46	D0	653	0	674	22	0
47	B1	755	0	826	17	0
47	D1	755	0	826	18	0
48	B2	588	0	643	11	0
48	D2	588	0	643	10	0
49	B3	469	0	518	6	0
49	D3	464	0	514	17	0
50	B4	558	0	544	27	0
50	D4	532	0	503	30	0
51	B5	455	0	465	15	0
51	D5	455	0	465	13	0
52	B6	453	0	473	10	0
52	D6	449	0	469	10	0
53	B7	418	0	467	18	0
53	D7	418	0	467	13	0
54	B8	517	0	582	25	0
54	D8	517	0	582	15	0
55	B9	307	0	335	4	0
55	D9	307	0	335	13	0
56	AA	218	0	0	0	0
56	AD	1	0	0	0	0
56	AE	2	0	0	0	0
56	AF	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	3	0	0	0	0
56	AO	1	0	0	0	0
56	AV	3	0	0	0	0
56	AW	4	0	0	0	0
56	AX	11	0	0	0	0
56	AY	3	0	0	0	0
56	B0	3	0	0	0	0
56	B1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B2	1	0	0	0	0
56	B3	2	0	0	0	0
56	B4	1	0	0	0	0
56	B5	5	0	0	0	0
56	B6	1	0	0	0	0
56	B7	4	0	0	0	0
56	B8	1	0	0	0	0
56	B9	1	0	0	0	0
56	BA	785	0	0	0	0
56	BB	18	0	0	0	0
56	BD	11	0	0	0	0
56	BE	8	0	0	0	0
56	BF	11	0	0	0	0
56	BG	2	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	3	0	0	0	0
56	BT	1	0	0	0	0
56	BU	9	0	0	0	0
56	BV	7	0	0	0	0
56	BW	4	0	0	0	0
56	BX	2	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	CD	1	0	0	0	0
56	CE	1	0	0	0	0
56	CF	1	0	0	0	0
56	CJ	1	0	0	0	0
56	CK	1	0	0	0	0
56	CN	1	0	0	0	0
56	CT	1	0	0	0	0
56	CV	1	0	0	0	0
56	CW	2	0	0	0	0
56	CX	2	0	0	0	0
56	CY	1	0	0	0	0
56	D0	1	0	0	0	0
56	D3	1	0	0	0	0
56	D5	1	0	0	0	0
56	D7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	D8	1	0	0	0	0
56	DA	623	0	0	0	0
56	DB	12	0	0	0	0
56	DD	9	0	0	0	0
56	DE	4	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	2	0	0	0	0
56	DP	1	0	0	0	0
56	DQ	4	0	0	0	0
56	DR	2	0	0	0	0
56	DU	3	0	0	0	0
56	DV	3	0	0	0	0
56	DW	4	0	0	0	0
56	DY	1	0	0	0	0
57	AA	119	0	133	18	0
57	AW	17	0	19	2	0
57	AX	17	0	19	3	0
57	CA	136	0	152	13	0
57	CW	17	0	19	1	0
57	CX	17	0	19	5	0
58	AD	8	0	0	0	0
58	CD	8	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	247	0	0	9	0
61	AD	1	0	0	0	0
61	AE	2	0	0	0	0
61	AL	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	AM	2	0	0	0	0
61	AO	1	0	0	0	0
61	AV	3	0	0	0	0
61	AW	13	0	0	2	0
61	AX	11	0	0	2	0
61	AY	1	0	0	0	0
61	B0	8	0	0	0	0
61	B3	1	0	0	0	0
61	B5	6	0	0	1	0
61	B6	1	0	0	0	0
61	B7	2	0	0	1	0
61	B8	7	0	0	1	0
61	BA	1396	0	0	65	0
61	BB	34	0	0	1	0
61	BD	12	0	0	2	0
61	BE	11	0	0	3	0
61	BF	5	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BN	1	0	0	0	0
61	BO	2	0	0	0	0
61	BP	23	0	0	1	0
61	BQ	3	0	0	0	0
61	BR	1	0	0	0	0
61	BT	2	0	0	0	0
61	BU	3	0	0	0	0
61	BV	2	0	0	0	0
61	BW	1	0	0	1	0
61	BX	2	0	0	0	0
61	BZ	1	0	0	1	0
61	CA	184	0	0	14	0
61	CJ	2	0	0	2	0
61	CP	1	0	0	0	0
61	CV	2	0	0	0	0
61	CW	3	0	0	1	0
61	CX	6	0	0	0	0
61	D0	8	0	0	1	0
61	D1	4	0	0	0	0
61	D7	2	0	0	0	0
61	D8	1	0	0	0	0
61	DA	960	0	0	63	0
61	DB	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DD	16	0	0	2	0
61	DE	9	0	0	0	0
61	DF	5	0	0	0	0
61	DN	3	0	0	0	0
61	DO	2	0	0	0	0
61	DP	15	0	0	0	0
61	DQ	1	0	0	1	0
61	DR	1	0	0	0	0
61	DU	1	0	0	0	0
61	DW	1	0	0	0	0
61	DX	1	0	0	0	0
61	DY	2	0	0	1	0
All	All	297376	0	196603	5587	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 12.

The worst 5 of 5587 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)
23:CW:27:G:H1	23:CW:43:C:N4	1.53	1.07
23:CY:7:A:N6	23:CY:66:U:H3	1.50	1.07
23:AY:49:C:N4	23:AY:65:G:H1	1.56	1.03
23:CY:15:G:N2	23:CY:48:C:H42	1.55	1.03
53:B7:24:THR:HG22	53:B7:27:GLY:H	1.24	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%)	196 (86%)	24 (10%)	9 (4%)	3	7
2	CB	229/256 (90%)	195 (85%)	24 (10%)	10 (4%)	3	6
3	AC	204/239 (85%)	182 (89%)	18 (9%)	4 (2%)	8	21
3	CC	204/239 (85%)	182 (89%)	19 (9%)	3 (2%)	11	29
4	AD	206/209 (99%)	193 (94%)	12 (6%)	1 (0%)	31	58
4	CD	206/209 (99%)	196 (95%)	8 (4%)	2 (1%)	17	41
5	AE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	24	50
5	CE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	24	50
6	AF	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
6	CF	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	17	41
7	AG	153/156 (98%)	141 (92%)	9 (6%)	3 (2%)	8	21
7	CG	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	8	21
8	AH	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	24	50
8	CH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	24	50
9	AI	125/128 (98%)	113 (90%)	10 (8%)	2 (2%)	11	27
9	CI	125/128 (98%)	112 (90%)	10 (8%)	3 (2%)	6	16
10	AJ	95/105 (90%)	82 (86%)	7 (7%)	6 (6%)	1	2
10	CJ	94/105 (90%)	81 (86%)	7 (7%)	6 (6%)	1	2
11	AK	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	9	24
11	CK	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	9	24
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
13	AM	121/126 (96%)	109 (90%)	11 (9%)	1 (1%)	21	47
13	CM	120/126 (95%)	107 (89%)	11 (9%)	2 (2%)	10	25
14	AN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
14	CN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	CO	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	14	35
16	AP	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	13	33
16	CP	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	13	33
17	AQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	17	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	66/88 (75%)	65 (98%)	0	1 (2%)	11	29
18	CR	66/88 (75%)	65 (98%)	0	1 (2%)	11	29
19	AS	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	6	16
19	CS	81/93 (87%)	69 (85%)	10 (12%)	2 (2%)	6	16
20	AT	94/106 (89%)	86 (92%)	2 (2%)	6 (6%)	1	2
20	CT	94/106 (89%)	87 (93%)	1 (1%)	6 (6%)	1	2
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
21	CU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
27	BD	273/276 (99%)	257 (94%)	15 (6%)	1 (0%)	36	64
27	DD	273/276 (99%)	255 (93%)	16 (6%)	2 (1%)	24	50
28	BE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	31	58
28	DE	202/206 (98%)	195 (96%)	5 (2%)	2 (1%)	17	41
29	BF	201/210 (96%)	199 (99%)	1 (0%)	1 (0%)	31	58
29	DF	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	17	41
30	BG	179/182 (98%)	167 (93%)	10 (6%)	2 (1%)	16	38
30	DG	179/182 (98%)	166 (93%)	10 (6%)	3 (2%)	10	25
31	BH	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	27	54
31	DH	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	27	54
32	BI	144/148 (97%)	128 (89%)	12 (8%)	4 (3%)	5	13
32	DI	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	12	31
33	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
33	DN	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	24	50
34	BO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	21	47
34	DO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
35	BP	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	24	50
35	DP	147/150 (98%)	137 (93%)	7 (5%)	3 (2%)	8	21
36	BQ	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
36	DQ	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	24	50
37	BR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
37	DR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
38	BS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	19	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	19	44
39	BT	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	21	47
39	DT	129/146 (88%)	124 (96%)	4 (3%)	1 (1%)	21	47
40	BU	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
40	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
41	BV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	17	41
41	DV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	17	41
42	BW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
42	DW	110/113 (97%)	110 (100%)	0	0	100	100
43	BX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
43	DX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	BY	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	17	41
44	DY	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
45	BZ	169/206 (82%)	145 (86%)	21 (12%)	3 (2%)	9	24
45	DZ	172/206 (84%)	153 (89%)	18 (10%)	1 (1%)	27	54
46	B0	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
46	D0	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	14	35
47	B1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
47	D1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
48	B2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
48	D2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
49	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
49	D3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	B4	67/71 (94%)	50 (75%)	12 (18%)	5 (8%)	1	1
50	D4	67/71 (94%)	51 (76%)	8 (12%)	8 (12%)	0	0
51	B5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
51	D5	57/60 (95%)	57 (100%)	0	0	100	100
52	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
52	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	B7	46/49 (94%)	46 (100%)	0	0	100	100
53	D7	46/49 (94%)	45 (98%)	0	1 (2%)	7	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	B8	62/65 (95%)	62 (100%)	0	0	100	100
54	D8	62/65 (95%)	62 (100%)	0	0	100	100
55	B9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
55	D9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
All	All	11409/12128 (94%)	10706 (94%)	562 (5%)	141 (1%)	14	35

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	HIS
2	AB	17	PHE
2	AB	231	GLU
7	AG	80	VAL
9	AI	44	VAL

### 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%)	162 (84%)	30 (16%)	3	7
2	CB	187/220 (85%)	163 (87%)	24 (13%)	5	11
3	AC	143/188 (76%)	132 (92%)	11 (8%)	14	33
3	CC	140/188 (74%)	130 (93%)	10 (7%)	16	38
4	AD	170/181 (94%)	161 (95%)	9 (5%)	25	52
4	CD	173/181 (96%)	159 (92%)	14 (8%)	13	29
5	AE	113/123 (92%)	106 (94%)	7 (6%)	20	44
5	CE	114/123 (93%)	103 (90%)	11 (10%)	9	21
6	AF	83/90 (92%)	79 (95%)	4 (5%)	28	57
6	CF	85/90 (94%)	77 (91%)	8 (9%)	9	22
7	AG	119/127 (94%)	112 (94%)	7 (6%)	21	47
7	CG	120/127 (94%)	114 (95%)	6 (5%)	27	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AH	114/119 (96%)	108 (95%)	6 (5%)	25	52
8	CH	114/119 (96%)	109 (96%)	5 (4%)	31	60
9	AI	90/99 (91%)	80 (89%)	10 (11%)	7	16
9	CI	89/99 (90%)	77 (86%)	12 (14%)	4	10
10	AJ	66/92 (72%)	62 (94%)	4 (6%)	20	45
10	CJ	69/92 (75%)	67 (97%)	2 (3%)	45	75
11	AK	82/99 (83%)	74 (90%)	8 (10%)	9	20
11	CK	83/99 (84%)	73 (88%)	10 (12%)	5	13
12	AL	97/109 (89%)	94 (97%)	3 (3%)	43	73
12	CL	97/109 (89%)	94 (97%)	3 (3%)	43	73
13	AM	93/101 (92%)	83 (89%)	10 (11%)	7	16
13	CM	92/101 (91%)	84 (91%)	8 (9%)	11	26
14	AN	49/50 (98%)	42 (86%)	7 (14%)	3	9
14	CN	49/50 (98%)	43 (88%)	6 (12%)	5	12
15	AO	78/80 (98%)	69 (88%)	9 (12%)	6	14
15	CO	78/80 (98%)	74 (95%)	4 (5%)	26	54
16	AP	69/74 (93%)	63 (91%)	6 (9%)	11	26
16	CP	68/74 (92%)	63 (93%)	5 (7%)	15	35
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	42	73
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	56	83
18	AR	59/77 (77%)	54 (92%)	5 (8%)	12	27
18	CR	59/77 (77%)	56 (95%)	3 (5%)	26	54
19	AS	69/80 (86%)	65 (94%)	4 (6%)	22	47
19	CS	67/80 (84%)	60 (90%)	7 (10%)	8	17
20	AT	70/82 (85%)	63 (90%)	7 (10%)	8	20
20	CT	70/82 (85%)	63 (90%)	7 (10%)	8	20
21	AU	18/22 (82%)	16 (89%)	2 (11%)	7	16
21	CU	18/22 (82%)	17 (94%)	1 (6%)	23	49
27	BD	215/218 (99%)	200 (93%)	15 (7%)	16	38
27	DD	215/218 (99%)	197 (92%)	18 (8%)	12	27
28	BE	164/166 (99%)	147 (90%)	17 (10%)	8	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	DE	164/166 (99%)	146 (89%)	18 (11%)	7	16
29	BF	160/166 (96%)	147 (92%)	13 (8%)	13	29
29	DF	159/166 (96%)	148 (93%)	11 (7%)	17	39
30	BG	143/156 (92%)	125 (87%)	18 (13%)	5	11
30	DG	142/156 (91%)	123 (87%)	19 (13%)	4	10
31	BH	144/148 (97%)	135 (94%)	9 (6%)	20	44
31	DH	144/148 (97%)	130 (90%)	14 (10%)	9	21
32	BI	110/124 (89%)	92 (84%)	18 (16%)	2	6
32	DI	104/124 (84%)	88 (85%)	16 (15%)	3	7
33	BN	118/119 (99%)	101 (86%)	17 (14%)	3	9
33	DN	118/119 (99%)	109 (92%)	9 (8%)	14	33
34	BO	100/100 (100%)	94 (94%)	6 (6%)	21	46
34	DO	100/100 (100%)	96 (96%)	4 (4%)	34	64
35	BP	115/116 (99%)	102 (89%)	13 (11%)	6	15
35	DP	115/116 (99%)	102 (89%)	13 (11%)	6	15
36	BQ	111/111 (100%)	101 (91%)	10 (9%)	10	24
36	DQ	111/111 (100%)	100 (90%)	11 (10%)	8	20
37	BR	101/101 (100%)	88 (87%)	13 (13%)	5	11
37	DR	101/101 (100%)	87 (86%)	14 (14%)	4	9
38	BS	87/88 (99%)	80 (92%)	7 (8%)	13	30
38	DS	85/88 (97%)	75 (88%)	10 (12%)	6	13
39	BT	115/127 (91%)	106 (92%)	9 (8%)	14	32
39	DT	113/127 (89%)	102 (90%)	11 (10%)	9	21
40	BU	93/94 (99%)	84 (90%)	9 (10%)	9	21
40	DU	93/94 (99%)	88 (95%)	5 (5%)	24	51
41	BV	80/82 (98%)	72 (90%)	8 (10%)	8	20
41	DV	80/82 (98%)	71 (89%)	9 (11%)	6	15
42	BW	90/92 (98%)	82 (91%)	8 (9%)	11	25
42	DW	90/92 (98%)	82 (91%)	8 (9%)	11	25
43	BX	77/78 (99%)	73 (95%)	4 (5%)	25	53
43	DX	77/78 (99%)	75 (97%)	2 (3%)	49	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	BY	85/91 (93%)	78 (92%)	7 (8%)	12	29
44	DY	85/91 (93%)	82 (96%)	3 (4%)	39	69
45	BZ	145/179 (81%)	132 (91%)	13 (9%)	10	24
45	DZ	145/179 (81%)	130 (90%)	15 (10%)	8	18
46	B0	65/67 (97%)	61 (94%)	4 (6%)	20	44
46	D0	65/67 (97%)	62 (95%)	3 (5%)	29	59
47	B1	80/83 (96%)	73 (91%)	7 (9%)	11	25
47	D1	80/83 (96%)	74 (92%)	6 (8%)	15	34
48	B2	65/67 (97%)	61 (94%)	4 (6%)	20	44
48	D2	65/67 (97%)	61 (94%)	4 (6%)	20	44
49	B3	51/52 (98%)	46 (90%)	5 (10%)	9	20
49	D3	50/52 (96%)	43 (86%)	7 (14%)	4	9
50	B4	60/63 (95%)	50 (83%)	10 (17%)	2	6
50	D4	53/63 (84%)	44 (83%)	9 (17%)	2	5
51	B5	50/52 (96%)	43 (86%)	7 (14%)	4	9
51	D5	50/52 (96%)	45 (90%)	5 (10%)	8	20
52	B6	51/52 (98%)	47 (92%)	4 (8%)	14	32
52	D6	50/52 (96%)	49 (98%)	1 (2%)	58	84
53	B7	41/42 (98%)	39 (95%)	2 (5%)	27	56
53	D7	41/42 (98%)	41 (100%)	0	100	100
54	B8	54/55 (98%)	50 (93%)	4 (7%)	15	35
54	D8	54/55 (98%)	48 (89%)	6 (11%)	7	16
55	B9	34/34 (100%)	33 (97%)	1 (3%)	45	75
55	D9	34/34 (100%)	32 (94%)	2 (6%)	21	47
All	All	9321/10066 (93%)	8506 (91%)	815 (9%)	11	26

5 of 815 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	B0	55	ARG
4	CD	135	LEU
43	DX	88	LYS
48	B2	53	LEU
55	B9	33	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
40	BU	117	GLN
3	CC	104	GLN
39	DT	123	GLN
43	BX	82	GLN
48	B2	70	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1493/1521 (98%)	280 (18%)	27 (1%)
1	CA	1501/1521 (98%)	280 (18%)	24 (1%)
22	AV	12/24 (50%)	2 (16%)	0
22	CV	11/24 (45%)	2 (18%)	0
23	AW	71/76 (93%)	31 (43%)	1 (1%)
23	AY	72/76 (94%)	33 (45%)	4 (5%)
23	CW	68/76 (89%)	30 (44%)	2 (2%)
23	CY	70/76 (92%)	31 (44%)	1 (1%)
24	AX	75/77 (97%)	21 (28%)	2 (2%)
24	CX	75/77 (97%)	21 (28%)	1 (1%)
25	BA	2814/2915 (96%)	455 (16%)	28 (0%)
25	DA	2791/2915 (95%)	518 (18%)	29 (1%)
26	BB	119/121 (98%)	13 (10%)	2 (1%)
26	DB	119/121 (98%)	14 (11%)	0
All	All	9291/9620 (96%)	1731 (18%)	121 (1%)

5 of 1731 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	32	A
1	AA	39	G

5 of 121 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2170	G
1	CA	266	G
25	DA	1992	G

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Mol	Chain	Res	Type
25	BA	2347	A
25	BA	2902	G

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

36 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$
23	PSU	AW	32	23	16,21,22	1.37	1 (6%)	20,30,33	3.29	6 (30%)
23	MIA	AW	37	23	22,31,32	2.37	4 (18%)	26,44,47	2.76	10 (38%)
23	PSU	AW	39	23	16,21,22	1.52	2 (12%)	20,30,33	3.55	6 (30%)
23	7MG	AW	46	23	20,26,27	2.08	3 (15%)	24,39,42	2.48	6 (25%)
23	5MU	AW	54	23	13,22,23	0.75	0	14,32,35	2.13	2 (14%)
23	PSU	AW	55	23	16,21,22	1.24	1 (6%)	20,30,33	3.55	7 (35%)
23	4SU	AW	8	23	13,21,22	1.28	1 (7%)	14,30,33	1.80	2 (14%)
24	5MC	AX	32	24	14,22,23	1.46	1 (7%)	17,32,35	1.63	4 (23%)
24	5MU	AX	54	24	13,22,23	0.81	0	14,32,35	2.08	2 (14%)
24	PSU	AX	55	24	16,21,22	1.59	2 (12%)	20,30,33	3.17	6 (30%)
24	4SU	AX	8	24	13,21,22	1.59	2 (15%)	14,30,33	2.97	2 (14%)
23	PSU	AY	32	23	16,21,22	1.44	1 (6%)	20,30,33	3.04	6 (30%)
23	MIA	AY	37	23	17,24,32	1.31	2 (11%)	16,35,47	1.36	2 (12%)
23	PSU	AY	39	23	16,21,22	1.44	4 (25%)	20,30,33	3.35	6 (30%)
23	7MG	AY	46	23	20,26,27	2.06	3 (15%)	24,39,42	2.70	7 (29%)
23	5MU	AY	54	23	13,22,23	0.88	1 (7%)	14,32,35	2.64	2 (14%)
23	PSU	AY	55	23	16,21,22	1.29	1 (6%)	20,30,33	3.03	7 (35%)
23	4SU	AY	8	23	13,21,22	1.27	1 (7%)	14,30,33	1.77	2 (14%)
23	PSU	CW	32	23	16,21,22	1.37	1 (6%)	20,30,33	3.13	6 (30%)
23	MIA	CW	37	23	17,24,32	1.25	2 (11%)	16,35,47	1.39	2 (12%)
23	PSU	CW	39	23	16,21,22	1.43	2 (12%)	20,30,33	3.07	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	7MG	CW	46	23	20,26,27	2.12	3 (15%)	24,39,42	2.60	6 (25%)
23	5MU	CW	54	23	13,22,23	0.75	0	14,32,35	2.51	1 (7%)
23	PSU	CW	55	23	16,21,22	1.18	1 (6%)	20,30,33	3.42	6 (30%)
23	4SU	CW	8	23	13,21,22	1.29	1 (7%)	14,30,33	1.46	2 (14%)
24	5MC	CX	32	24	14,22,23	1.51	1 (7%)	17,32,35	1.48	3 (17%)
24	5MU	CX	54	24	13,22,23	0.77	0	14,32,35	1.75	2 (14%)
24	PSU	CX	55	24	16,21,22	1.33	1 (6%)	20,30,33	3.17	6 (30%)
24	4SU	CX	8	24	13,21,22	1.52	2 (15%)	14,30,33	2.58	2 (14%)
23	PSU	CY	32	23	16,21,22	1.14	1 (6%)	20,30,33	3.18	5 (25%)
23	MIA	CY	37	23	17,24,32	1.33	2 (11%)	16,35,47	1.36	2 (12%)
23	PSU	CY	39	23	16,21,22	1.48	2 (12%)	20,30,33	2.87	6 (30%)
23	7MG	CY	46	23	20,26,27	2.08	3 (15%)	24,39,42	2.50	5 (20%)
23	5MU	CY	54	23	13,22,23	0.74	0	14,32,35	1.91	2 (14%)
23	PSU	CY	55	23	16,21,22	1.11	2 (12%)	20,30,33	3.63	7 (35%)
23	4SU	CY	8	23	13,21,22	1.30	1 (7%)	14,30,33	1.67	2 (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
23	PSU	AW	32	23	-	0/7/25/26	0/2/2/2
23	MIA	AW	37	23	-	1/11/33/34	0/3/3/3
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	AW	46	23	-	3/7/37/38	0/3/3/3
23	5MU	AW	54	23	-	0/3/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/3/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	AX	54	24	-	0/3/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/3/25/26	0/2/2/2
23	PSU	AY	32	23	-	0/7/25/26	0/2/2/2
23	MIA	AY	37	23	-	0/3/25/34	0/3/3/3
23	PSU	AY	39	23	-	2/7/25/26	0/2/2/2
23	7MG	AY	46	23	-	4/7/37/38	0/3/3/3
23	5MU	AY	54	23	-	2/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	AY	55	23	-	1/7/25/26	0/2/2/2
23	4SU	AY	8	23	-	2/3/25/26	0/2/2/2
23	PSU	CW	32	23	-	0/7/25/26	0/2/2/2
23	MIA	CW	37	23	-	0/3/25/34	0/3/3/3
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	3/7/37/38	0/3/3/3
23	5MU	CW	54	23	-	0/3/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
23	4SU	CW	8	23	-	0/3/25/26	0/2/2/2
24	5MC	CX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/3/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/3/25/26	0/2/2/2
23	PSU	CY	32	23	-	0/7/25/26	0/2/2/2
23	MIA	CY	37	23	-	3/3/25/34	0/3/3/3
23	PSU	CY	39	23	-	2/7/25/26	0/2/2/2
23	7MG	CY	46	23	-	2/7/37/38	0/3/3/3
23	5MU	CY	54	23	-	2/3/25/26	0/2/2/2
23	PSU	CY	55	23	-	0/7/25/26	0/2/2/2
23	4SU	CY	8	23	-	2/3/25/26	0/2/2/2

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	CW	46	7MG	C6-C5	7.04	1.49	1.41
23	AW	37	MIA	C2-S10	-6.93	1.70	1.75
23	AW	37	MIA	C13-C14	6.93	1.52	1.32
23	AW	46	7MG	C6-C5	6.35	1.48	1.41
23	AY	46	7MG	C6-C5	6.24	1.48	1.41

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	55	PSU	N1-C2-N3	-10.03	120.46	128.43
23	AW	39	PSU	N1-C2-N3	-9.75	120.68	128.43
24	AX	8	4SU	C2-N3-C4	9.70	129.21	115.15
23	AW	37	MIA	C12-C13-C14	-9.54	108.30	127.10
23	AY	54	5MU	C4-N3-C2	9.32	123.01	115.14

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	CY	54	5MU	C3'-C4'-C5'-O5'
23	CY	54	5MU	O4'-C4'-C5'-O5'
23	CY	37	MIA	C3'-C4'-C5'-O5'
23	AY	46	7MG	C2'-C1'-N9-C8
23	AW	37	MIA	C12-C13-C14-C16

There are no ring outliers.

24 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	32	PSU	1	0
23	AW	39	PSU	1	0
23	AW	46	7MG	1	0
23	AW	54	5MU	2	0
23	AW	55	PSU	3	0
23	AW	8	4SU	1	0
24	AX	8	4SU	1	0
23	AY	37	MIA	2	0
23	AY	39	PSU	1	0
23	AY	54	5MU	3	0
23	AY	55	PSU	3	0
23	AY	8	4SU	4	0
23	CW	32	PSU	1	0
23	CW	39	PSU	3	0
23	CW	46	7MG	3	0
23	CW	8	4SU	2	0
24	CX	54	5MU	2	0
24	CX	55	PSU	1	0
24	CX	8	4SU	1	0
23	CY	37	MIA	1	0
23	CY	39	PSU	1	0
23	CY	46	7MG	5	0
23	CY	54	5MU	1	0
23	CY	55	PSU	5	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2048 ligands modelled in this entry, 2027 are monoatomic - leaving 21 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	NEG	AA	3216	56	9,16,16	0.57	0	9,20,20	2.49	2 (22%)
57	NEG	AA	3217	-	9,16,16	0.55	0	9,20,20	2.43	2 (22%)
57	NEG	AA	3218	56	9,16,16	0.68	0	9,20,20	2.13	2 (22%)
57	NEG	AA	3219	-	9,16,16	0.59	0	9,20,20	2.54	3 (33%)
57	NEG	AA	3220	-	9,16,16	0.71	0	9,20,20	2.27	3 (33%)
57	NEG	AA	3221	-	9,16,16	0.59	0	9,20,20	1.67	1 (11%)
57	NEG	AA	3222	-	9,16,16	0.44	0	9,20,20	1.79	1 (11%)
58	SF4	AD	501	4	0,12,12	0.00	-	-		
57	NEG	AW	3004	-	9,16,16	0.44	0	9,20,20	1.36	1 (11%)
57	NEG	AX	3013	-	9,16,16	0.77	0	9,20,20	2.78	3 (33%)
57	NEG	CA	3170	56	9,16,16	0.54	0	9,20,20	1.11	1 (11%)
57	NEG	CA	3171	-	9,16,16	0.43	0	9,20,20	2.79	3 (33%)
57	NEG	CA	3172	-	9,16,16	0.53	0	9,20,20	2.38	2 (22%)
57	NEG	CA	3173	-	9,16,16	0.65	0	9,20,20	2.35	2 (22%)
57	NEG	CA	3174	-	9,16,16	0.69	0	9,20,20	4.77	3 (33%)
57	NEG	CA	3175	-	9,16,16	0.65	0	9,20,20	2.65	4 (44%)
57	NEG	CA	3176	-	9,16,16	0.56	0	9,20,20	1.61	2 (22%)
57	NEG	CA	3177	-	9,16,16	0.78	0	9,20,20	4.28	5 (55%)
58	SF4	CD	302	4	0,12,12	0.00	-	-		
57	NEG	CW	3002	-	9,16,16	0.57	0	9,20,20	1.45	3 (33%)
57	NEG	CX	3004	-	9,16,16	0.36	0	9,20,20	2.31	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
57	NEG	AA	3216	56	-	0/15/18/18	-
57	NEG	AA	3217	-	-	2/15/18/18	-
57	NEG	AA	3218	56	-	1/15/18/18	-
57	NEG	AA	3219	-	-	2/15/18/18	-
57	NEG	AA	3220	-	-	3/15/18/18	-
57	NEG	AA	3221	-	-	4/15/18/18	-
57	NEG	AA	3222	-	-	2/15/18/18	-
58	SF4	AD	501	4	-	-	0/6/5/5
57	NEG	AW	3004	-	-	0/15/18/18	-
57	NEG	AX	3013	-	-	5/15/18/18	-
57	NEG	CA	3170	56	-	2/15/18/18	-
57	NEG	CA	3171	-	-	2/15/18/18	-
57	NEG	CA	3172	-	-	2/15/18/18	-
57	NEG	CA	3173	-	-	2/15/18/18	-
57	NEG	CA	3174	-	-	1/15/18/18	-
57	NEG	CA	3175	-	-	7/15/18/18	-
57	NEG	CA	3176	-	-	0/15/18/18	-
57	NEG	CA	3177	-	-	2/15/18/18	-
58	SF4	CD	302	4	-	-	0/6/5/5
57	NEG	CW	3002	-	-	0/15/18/18	-
57	NEG	CX	3004	-	-	2/15/18/18	-

There are no bond length outliers.

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	CA	3174	NEG	C9-N3-N2	10.54	119.34	109.17
57	CA	3177	NEG	C9-N3-N2	9.45	118.29	109.17
57	CA	3174	NEG	C6-N2-N3	8.14	128.42	120.29
57	CA	3177	NEG	C6-N2-N3	6.92	127.21	120.29
57	AA	3216	NEG	C9-N3-N2	6.67	115.60	109.17

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	AA	3222	NEG	C6-N2-N3-C9
57	AA	3220	NEG	C6-N2-N3-C7
57	CA	3175	NEG	C6-N2-N3-C7

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Mol	Chain	Res	Type	Atoms
57	CA	3177	NEG	C6-N2-N3-C9
57	CA	3174	NEG	C6-N2-N3-C9

There are no ring outliers.

15 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	3216	NEG	7	0
57	AA	3217	NEG	1	0
57	AA	3218	NEG	1	0
57	AA	3219	NEG	1	0
57	AA	3220	NEG	4	0
57	AA	3221	NEG	4	0
57	AW	3004	NEG	2	0
57	AX	3013	NEG	3	0
57	CA	3171	NEG	1	0
57	CA	3173	NEG	2	0
57	CA	3174	NEG	5	0
57	CA	3175	NEG	3	0
57	CA	3177	NEG	2	0
57	CW	3002	NEG	1	0
57	CX	3004	NEG	5	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	1496/1521 (98%)	0.46	23 (1%) 73 75	36, 68, 97, 112	0
1	CA	1503/1521 (98%)	0.32	26 (1%) 70 71	38, 71, 97, 111	0
2	AB	231/256 (90%)	0.55	15 (6%) 19 17	67, 83, 93, 99	0
2	CB	231/256 (90%)	1.02	44 (19%) 1 1	69, 85, 94, 100	0
3	AC	206/239 (86%)	0.83	29 (14%) 2 1	65, 78, 88, 96	0
3	CC	206/239 (86%)	1.09	36 (17%) 1 1	68, 80, 90, 96	0
4	AD	208/209 (99%)	0.87	28 (13%) 3 2	53, 68, 80, 87	0
4	CD	208/209 (99%)	0.85	15 (7%) 15 13	54, 67, 80, 90	0
5	AE	148/162 (91%)	0.78	7 (4%) 31 29	54, 70, 81, 86	0
5	CE	148/162 (91%)	0.91	17 (11%) 5 4	57, 72, 82, 88	0
6	AF	100/101 (99%)	0.51	2 (2%) 65 66	53, 67, 78, 87	0
6	CF	100/101 (99%)	0.16	0 100 100	54, 68, 80, 87	0
7	AG	155/156 (99%)	0.65	14 (9%) 9 7	62, 75, 86, 95	0
7	CG	155/156 (99%)	0.88	20 (12%) 3 2	63, 77, 86, 99	0
8	AH	137/138 (99%)	1.11	27 (19%) 1 0	57, 70, 78, 85	0
8	CH	137/138 (99%)	1.00	24 (17%) 1 1	60, 72, 81, 85	0
9	AI	127/128 (99%)	0.99	22 (17%) 1 1	57, 82, 90, 94	0
9	CI	127/128 (99%)	1.96	59 (46%) 0 0	65, 84, 91, 95	0
10	AJ	97/105 (92%)	1.26	33 (34%) 0 0	63, 85, 94, 98	0
10	CJ	96/105 (91%)	1.33	29 (30%) 0 0	65, 86, 94, 99	0
11	AK	114/129 (88%)	0.84	3 (2%) 56 56	47, 66, 78, 84	0
11	CK	114/129 (88%)	0.70	11 (9%) 8 6	49, 68, 79, 85	0
12	AL	122/132 (92%)	0.85	9 (7%) 14 12	48, 57, 69, 79	0
12	CL	122/132 (92%)	0.95	18 (14%) 2 1	50, 60, 71, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	123/126 (97%)	0.55	5 (4%) 37 35	52, 70, 84, 96	0
13	CM	122/126 (96%)	1.14	23 (18%) 1 1	70, 83, 93, 99	0
14	AN	60/61 (98%)	1.46	18 (30%) 0 0	64, 77, 83, 89	0
14	CN	60/61 (98%)	2.67	33 (55%) 0 0	67, 80, 87, 90	0
15	AO	88/89 (98%)	0.56	2 (2%) 60 61	49, 66, 77, 84	0
15	CO	88/89 (98%)	0.75	11 (12%) 4 3	51, 67, 79, 85	0
16	AP	82/88 (93%)	1.04	7 (8%) 11 8	53, 67, 78, 82	0
16	CP	82/88 (93%)	0.81	1 (1%) 79 80	54, 66, 77, 82	0
17	AQ	99/105 (94%)	0.80	8 (8%) 12 9	53, 69, 81, 83	0
17	CQ	99/105 (94%)	1.64	32 (32%) 0 0	55, 70, 81, 85	0
18	AR	68/88 (77%)	0.58	3 (4%) 34 32	54, 67, 80, 82	0
18	CR	68/88 (77%)	0.37	2 (2%) 51 51	54, 69, 81, 85	0
19	AS	83/93 (89%)	0.61	3 (3%) 42 42	68, 80, 88, 97	0
19	CS	83/93 (89%)	1.19	19 (22%) 0 0	71, 82, 91, 97	0
20	AT	96/106 (90%)	0.68	6 (6%) 20 19	57, 69, 85, 90	0
20	CT	96/106 (90%)	0.94	13 (13%) 3 2	56, 69, 85, 90	0
21	AU	23/27 (85%)	1.33	7 (30%) 0 0	62, 71, 78, 81	0
21	CU	23/27 (85%)	1.98	11 (47%) 0 0	65, 74, 80, 83	0
22	AV	13/24 (54%)	1.74	5 (38%) 0 0	51, 61, 91, 97	0
22	CV	12/24 (50%)	1.53	4 (33%) 0 0	55, 65, 91, 92	0
23	AW	67/76 (88%)	1.31	19 (28%) 0 0	50, 93, 102, 108	0
23	AY	67/76 (88%)	1.21	17 (25%) 0 0	37, 101, 106, 107	0
23	CW	65/76 (85%)	1.13	17 (26%) 0 0	69, 100, 108, 110	0
23	CY	66/76 (86%)	1.16	12 (18%) 1 1	40, 101, 106, 107	0
24	AX	72/77 (93%)	0.66	3 (4%) 36 34	45, 69, 85, 96	0
24	CX	72/77 (93%)	0.51	4 (5%) 24 23	46, 72, 87, 98	0
25	BA	2822/2915 (96%)	0.86	53 (1%) 66 68	22, 42, 94, 110	0
25	DA	2800/2915 (96%)	0.36	68 (2%) 59 59	25, 47, 96, 113	0
26	BB	120/121 (99%)	0.53	0 100 100	41, 61, 72, 92	0
26	DB	120/121 (99%)	-0.04	1 (0%) 86 87	48, 67, 78, 93	0
27	BD	275/276 (99%)	0.96	12 (4%) 34 32	21, 38, 55, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	DD	275/276 (99%)	0.72	7 (2%) 57 58	23, 41, 57, 85	0
28	BE	204/206 (99%)	0.82	4 (1%) 65 66	19, 45, 67, 84	0
28	DE	204/206 (99%)	0.54	5 (2%) 57 58	22, 49, 69, 84	0
29	BF	203/210 (96%)	0.74	7 (3%) 45 44	23, 50, 74, 95	0
29	DF	203/210 (96%)	0.64	11 (5%) 26 24	25, 55, 77, 95	0
30	BG	181/182 (99%)	0.55	5 (2%) 53 53	52, 68, 82, 94	0
30	DG	181/182 (99%)	0.97	29 (16%) 1 1	57, 72, 84, 92	0
31	BH	174/180 (96%)	0.78	4 (2%) 60 61	51, 69, 80, 87	0
31	DH	174/180 (96%)	1.31	40 (22%) 0 0	57, 74, 84, 88	0
32	BI	146/148 (98%)	0.29	3 (2%) 63 64	45, 71, 84, 88	0
32	DI	146/148 (98%)	0.26	4 (2%) 54 54	46, 72, 84, 89	0
33	BN	140/140 (100%)	0.86	4 (2%) 51 51	32, 48, 69, 78	0
33	DN	140/140 (100%)	0.83	15 (10%) 6 4	37, 53, 72, 79	0
34	BO	122/122 (100%)	0.55	0 100 100	23, 39, 59, 65	0
34	DO	122/122 (100%)	1.01	14 (11%) 5 4	43, 58, 72, 84	0
35	BP	149/150 (99%)	0.78	3 (2%) 65 66	23, 53, 76, 82	0
35	DP	149/150 (99%)	0.90	17 (11%) 5 4	28, 57, 78, 83	0
36	BQ	141/141 (100%)	1.13	16 (11%) 5 4	32, 53, 69, 81	0
36	DQ	141/141 (100%)	1.08	23 (16%) 1 1	36, 58, 73, 82	0
37	BR	118/118 (100%)	0.74	1 (0%) 86 87	19, 33, 48, 59	0
37	DR	118/118 (100%)	0.69	2 (1%) 70 71	32, 51, 65, 78	0
38	BS	110/112 (98%)	0.69	1 (0%) 84 85	36, 50, 67, 72	0
38	DS	110/112 (98%)	0.49	7 (6%) 19 17	64, 77, 88, 94	0
39	BT	131/146 (89%)	0.45	2 (1%) 73 75	28, 41, 69, 88	0
39	DT	131/146 (89%)	0.78	9 (6%) 17 15	45, 60, 78, 88	0
40	BU	116/118 (98%)	0.79	2 (1%) 70 71	17, 29, 43, 67	0
40	DU	116/118 (98%)	1.18	27 (23%) 0 0	36, 64, 80, 89	0
41	BV	101/101 (100%)	0.42	0 100 100	18, 36, 55, 73	0
41	DV	101/101 (100%)	1.21	21 (20%) 1 0	42, 77, 87, 93	0
42	BW	112/113 (99%)	0.78	3 (2%) 54 54	17, 29, 52, 89	0
42	DW	112/113 (99%)	0.83	5 (4%) 33 31	35, 49, 71, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BX	95/96 (98%)	0.53	2 (2%) 63 64	15, 33, 65, 84	0
43	DX	95/96 (98%)	1.12	14 (14%) 2 1	38, 57, 76, 84	0
44	BY	107/110 (97%)	0.43	1 (0%) 84 85	33, 48, 75, 84	0
44	DY	107/110 (97%)	1.51	31 (28%) 0 0	54, 70, 86, 93	0
45	BZ	171/206 (83%)	1.27	30 (17%) 1 1	38, 69, 102, 108	0
45	DZ	174/206 (84%)	1.50	47 (27%) 0 0	71, 88, 101, 108	0
46	B0	83/85 (97%)	1.05	9 (10%) 6 4	25, 37, 67, 83	0
46	D0	83/85 (97%)	1.63	18 (21%) 0 0	46, 69, 81, 91	0
47	B1	97/98 (98%)	0.91	5 (5%) 27 25	19, 40, 69, 76	0
47	D1	97/98 (98%)	0.67	2 (2%) 63 64	33, 53, 77, 79	0
48	B2	70/72 (97%)	0.60	0 100 100	32, 42, 62, 80	0
48	D2	70/72 (97%)	0.80	4 (5%) 24 22	54, 70, 81, 84	0
49	B3	59/60 (98%)	0.55	0 100 100	22, 36, 55, 80	0
49	D3	59/60 (98%)	1.91	20 (33%) 0 0	52, 67, 82, 85	0
50	B4	69/71 (97%)	0.33	3 (4%) 35 33	53, 73, 93, 94	0
50	D4	69/71 (97%)	0.82	11 (15%) 2 1	76, 87, 99, 107	0
51	B5	59/60 (98%)	0.79	2 (3%) 45 44	18, 31, 46, 68	0
51	D5	59/60 (98%)	0.62	1 (1%) 70 71	28, 50, 68, 77	0
52	B6	53/54 (98%)	0.58	0 100 100	29, 40, 59, 67	0
52	D6	53/54 (98%)	0.84	4 (7%) 14 12	47, 61, 75, 79	0
53	B7	48/49 (97%)	1.04	5 (10%) 6 4	16, 25, 55, 66	0
53	D7	48/49 (97%)	1.25	6 (12%) 4 3	28, 37, 62, 71	0
54	B8	64/65 (98%)	0.72	2 (3%) 49 49	23, 32, 43, 58	0
54	D8	64/65 (98%)	1.40	14 (21%) 0 0	43, 57, 65, 71	0
55	B9	37/37 (100%)	1.40	9 (24%) 0 0	31, 50, 69, 75	0
55	D9	37/37 (100%)	1.48	11 (29%) 0 0	49, 60, 73, 77	0
All	All	20900/21748 (96%)	0.73	1472 (7%) 16 14	15, 62, 92, 113	0

The worst 5 of 1472 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	CG	82	GLY	17.5
13	CM	124	PRO	15.4

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Mol	Chain	Res	Type	RSRZ
13	AM	123	ALA	13.5
45	BZ	111	VAL	12.9
45	BZ	115	GLY	12.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
23	4SU	CY	8	20/21	0.69	0.24	95,103,122,140	0
23	PSU	AY	55	20/21	0.70	0.25	88,103,115,132	0
23	4SU	CW	8	20/21	0.72	0.22	85,105,116,130	0
23	7MG	CY	46	24/25	0.72	0.24	91,105,113,139	0
23	PSU	CY	55	20/21	0.73	0.36	91,104,118,129	0
23	5MU	AY	54	21/22	0.76	0.29	85,97,115,141	0
23	4SU	AY	8	20/21	0.77	0.20	99,105,115,127	0
23	PSU	CW	55	20/21	0.79	0.20	76,95,105,108	0
23	5MU	CY	54	21/22	0.80	0.29	88,99,111,135	0
23	PSU	AW	55	20/21	0.81	0.26	57,85,93,93	0
23	7MG	AY	46	24/25	0.81	0.28	92,100,111,135	0
23	7MG	CW	46	24/25	0.82	0.24	93,104,114,127	0
23	7MG	AW	46	24/25	0.82	0.15	74,94,116,138	0
23	MIA	AY	37	22/30	0.83	0.22	82,91,103,118	0
23	PSU	CY	39	20/21	0.84	0.22	79,92,100,112	0
23	PSU	CY	32	20/21	0.85	0.20	83,95,100,107	0
23	MIA	CY	37	22/30	0.86	0.27	75,93,102,117	0
23	4SU	AW	8	20/21	0.89	0.16	81,89,100,121	0
24	PSU	CX	55	20/21	0.91	0.14	62,70,83,92	0
24	4SU	CX	8	20/21	0.92	0.20	73,82,90,90	0
23	PSU	AY	32	20/21	0.92	0.17	83,93,99,105	0
23	5MU	CW	54	21/22	0.92	0.14	72,81,90,93	0
23	PSU	AY	39	20/21	0.92	0.22	76,89,100,102	0
23	5MU	AW	54	21/22	0.93	0.23	57,76,85,89	0
24	5MU	CX	54	21/22	0.94	0.24	69,80,89,95	0
23	MIA	CW	37	22/30	0.94	0.19	53,72,83,85	0
24	PSU	AX	55	20/21	0.94	0.17	60,68,83,92	0
24	4SU	AX	8	20/21	0.95	0.20	47,62,81,87	0
24	5MU	AX	54	21/22	0.95	0.17	60,70,77,80	0
24	5MC	CX	32	21/22	0.95	0.22	63,72,77,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	PSU	CW	32	20/21	0.95	0.23	62,82,97,97	0
23	PSU	CW	39	20/21	0.95	0.26	62,79,88,94	0
23	PSU	AW	32	20/21	0.96	0.21	39,59,64,65	0
23	PSU	AW	39	20/21	0.96	0.21	37,57,68,72	0
23	MIA	AW	37	29/30	0.96	0.27	36,49,67,72	0
24	5MC	AX	32	21/22	0.97	0.24	38,56,66,77	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3495	1/1	0.36	0.10	57,57,57,57	0
56	MG	AY	3001	1/1	0.39	0.25	92,92,92,92	0
56	MG	DA	3122	1/1	0.42	0.30	71,71,71,71	0
56	MG	DA	3417	1/1	0.53	0.18	71,71,71,71	0
56	MG	CA	3124	1/1	0.56	0.19	90,90,90,90	0
56	MG	CA	3134	1/1	0.57	0.14	78,78,78,78	0
56	MG	AY	3003	1/1	0.57	0.26	78,78,78,78	0
56	MG	DA	3491	1/1	0.57	0.12	69,69,69,69	0
56	MG	AA	3015	1/1	0.59	0.16	56,56,56,56	0
56	MG	CA	3126	1/1	0.60	0.23	76,76,76,76	0
56	MG	CA	3004	1/1	0.60	0.18	69,69,69,69	0
56	MG	CA	3007	1/1	0.60	0.16	69,69,69,69	0
56	MG	BA	3327	1/1	0.61	0.37	74,74,74,74	0
56	MG	DA	3054	1/1	0.62	0.32	59,59,59,59	0
56	MG	BA	3733	1/1	0.62	0.07	78,78,78,78	0
56	MG	DA	3437	1/1	0.62	0.14	47,47,47,47	0
56	MG	BA	3099	1/1	0.62	0.37	58,58,58,58	0
56	MG	DA	3463	1/1	0.63	0.20	53,53,53,53	0
56	MG	AA	3068	1/1	0.63	0.18	70,70,70,70	0
56	MG	BA	3550	1/1	0.63	0.49	74,74,74,74	0
56	MG	BA	3134	1/1	0.64	0.18	57,57,57,57	0
56	MG	DA	3526	1/1	0.65	0.21	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	BA	3639	1/1	0.65	0.26	55,55,55,55	0
56	MG	DA	3340	1/1	0.65	0.18	60,60,60,60	0
56	MG	BA	3199	1/1	0.66	0.28	55,55,55,55	0
56	MG	BN	3002	1/1	0.67	0.31	53,53,53,53	0
56	MG	BA	3637	1/1	0.67	0.27	34,34,34,34	0
56	MG	DA	3575	1/1	0.67	0.19	58,58,58,58	0
56	MG	BA	3519	1/1	0.67	0.14	56,56,56,56	0
56	MG	AA	3183	1/1	0.68	0.16	63,63,63,63	0
56	MG	DA	3087	1/1	0.68	0.10	49,49,49,49	0
56	MG	CA	3068	1/1	0.68	0.15	77,77,77,77	0
56	MG	CA	3036	1/1	0.68	0.15	69,69,69,69	0
56	MG	AA	3188	1/1	0.69	0.12	69,69,69,69	0
56	MG	AA	3206	1/1	0.69	0.24	62,62,62,62	0
59	ZN	D4	501	1/1	0.69	0.12	137,137,137,137	0
56	MG	BA	3322	1/1	0.69	0.23	58,58,58,58	0
56	MG	AA	3035	1/1	0.69	0.16	69,69,69,69	0
56	MG	CA	3031	1/1	0.69	0.22	71,71,71,71	0
56	MG	BA	3480	1/1	0.69	0.20	29,29,29,29	0
56	MG	BA	3508	1/1	0.69	0.31	61,61,61,61	0
56	MG	CA	3145	1/1	0.70	0.14	62,62,62,62	0
56	MG	DA	3306	1/1	0.70	0.14	57,57,57,57	0
56	MG	BA	3761	1/1	0.70	0.17	65,65,65,65	0
56	MG	DA	3601	1/1	0.70	0.16	75,75,75,75	0
56	MG	DA	3114	1/1	0.70	0.21	53,53,53,53	0
56	MG	AA	3075	1/1	0.71	0.24	81,81,81,81	0
56	MG	BA	3214	1/1	0.71	0.26	64,64,64,64	0
56	MG	BA	3195	1/1	0.71	0.50	53,53,53,53	0
56	MG	DA	3470	1/1	0.71	0.13	65,65,65,65	0
56	MG	AA	3168	1/1	0.71	0.18	76,76,76,76	0
56	MG	BA	3656	1/1	0.71	0.19	34,34,34,34	0
56	MG	DA	3513	1/1	0.71	0.09	58,58,58,58	0
56	MG	AA	3192	1/1	0.71	0.20	71,71,71,71	0
56	MG	DP	201	1/1	0.72	0.26	50,50,50,50	0
56	MG	BA	3217	1/1	0.72	0.28	66,66,66,66	0
56	MG	CA	3005	1/1	0.72	0.12	62,62,62,62	0
56	MG	AA	3014	1/1	0.72	0.10	64,64,64,64	0
56	MG	BA	3610	1/1	0.72	0.20	64,64,64,64	0
56	MG	BA	3741	1/1	0.72	0.15	68,68,68,68	0
56	MG	BA	3307	1/1	0.72	0.13	57,57,57,57	0
56	MG	CA	3090	1/1	0.72	0.14	70,70,70,70	0
56	MG	BA	3633	1/1	0.72	0.09	58,58,58,58	0
56	MG	DA	3573	1/1	0.72	0.11	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3736	1/1	0.73	0.09	73,73,73,73	0
56	MG	DO	201	1/1	0.73	0.38	59,59,59,59	0
56	MG	BA	3097	1/1	0.73	0.41	33,33,33,33	0
56	MG	BA	3779	1/1	0.73	0.40	52,52,52,52	0
56	MG	DA	3583	1/1	0.73	0.13	44,44,44,44	0
56	MG	DA	3226	1/1	0.73	0.26	70,70,70,70	0
56	MG	BB	3001	1/1	0.73	0.21	56,56,56,56	0
56	MG	AA	3032	1/1	0.74	0.18	62,62,62,62	0
56	MG	BA	3544	1/1	0.74	0.26	57,57,57,57	0
56	MG	DA	3148	1/1	0.74	0.14	53,53,53,53	0
56	MG	CA	3002	1/1	0.74	0.12	65,65,65,65	0
56	MG	DA	3179	1/1	0.74	0.19	61,61,61,61	0
56	MG	AA	3179	1/1	0.74	0.12	85,85,85,85	0
56	MG	DA	3195	1/1	0.74	0.15	56,56,56,56	0
56	MG	DA	3472	1/1	0.74	0.16	40,40,40,40	0
56	MG	BA	3074	1/1	0.74	0.17	58,58,58,58	0
56	MG	CA	3001	1/1	0.74	0.15	59,59,59,59	0
56	MG	DA	3540	1/1	0.75	0.11	65,65,65,65	0
56	MG	CJ	5001	1/1	0.75	0.10	75,75,75,75	0
56	MG	BA	3599	1/1	0.75	0.10	59,59,59,59	0
56	MG	BA	3078	1/1	0.75	0.13	48,48,48,48	0
56	MG	BA	3726	1/1	0.75	0.18	61,61,61,61	0
56	MG	BA	3618	1/1	0.75	0.19	64,64,64,64	0
56	MG	DA	3079	1/1	0.75	0.16	60,60,60,60	0
56	MG	BA	3247	1/1	0.75	0.20	49,49,49,49	0
56	MG	BA	3532	1/1	0.75	0.14	73,73,73,73	0
56	MG	BA	3329	1/1	0.75	0.30	57,57,57,57	0
56	MG	BA	3002	1/1	0.75	0.17	36,36,36,36	0
56	MG	DA	3453	1/1	0.75	0.31	77,77,77,77	0
56	MG	AA	3082	1/1	0.75	0.16	70,70,70,70	0
56	MG	AA	3044	1/1	0.76	0.17	67,67,67,67	0
56	MG	AA	3041	1/1	0.76	0.14	64,64,64,64	0
56	MG	DA	3614	1/1	0.76	0.14	34,34,34,34	0
56	MG	DA	3192	1/1	0.76	0.16	49,49,49,49	0
56	MG	BA	3730	1/1	0.76	0.28	45,45,45,45	0
56	MG	DA	3224	1/1	0.76	0.22	27,27,27,27	0
56	MG	BA	3077	1/1	0.76	0.17	59,59,59,59	0
56	MG	BA	3176	1/1	0.76	0.19	41,41,41,41	0
56	MG	AF	3001	1/1	0.76	0.14	48,48,48,48	0
56	MG	DA	3276	1/1	0.77	0.15	57,57,57,57	0
56	MG	AA	3105	1/1	0.77	0.10	66,66,66,66	0
56	MG	CA	3051	1/1	0.77	0.15	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3242	1/1	0.77	0.13	56,56,56,56	0
56	MG	BA	3751	1/1	0.77	0.14	51,51,51,51	0
56	MG	DA	3322	1/1	0.77	0.09	46,46,46,46	0
56	MG	BR	202	1/1	0.77	0.49	51,51,51,51	0
56	MG	B2	3001	1/1	0.77	0.29	54,54,54,54	0
56	MG	DA	3061	1/1	0.77	0.14	63,63,63,63	0
56	MG	DA	3180	1/1	0.77	0.12	50,50,50,50	0
56	MG	B5	103	1/1	0.77	0.67	51,51,51,51	0
56	MG	AA	3106	1/1	0.77	0.14	62,62,62,62	0
56	MG	AA	3111	1/1	0.77	0.15	65,65,65,65	0
56	MG	DA	3147	1/1	0.78	0.12	49,49,49,49	0
56	MG	AA	3087	1/1	0.78	0.17	59,59,59,59	0
56	MG	AA	3099	1/1	0.78	0.11	59,59,59,59	0
56	MG	DA	3073	1/1	0.78	0.24	50,50,50,50	0
56	MG	DA	3048	1/1	0.78	0.12	58,58,58,58	0
56	MG	AA	3045	1/1	0.78	0.29	68,68,68,68	0
56	MG	AA	3159	1/1	0.78	0.11	70,70,70,70	0
56	MG	BA	3227	1/1	0.78	0.19	38,38,38,38	0
56	MG	BA	3646	1/1	0.78	0.42	48,48,48,48	0
56	MG	CA	3003	1/1	0.78	0.20	65,65,65,65	0
56	MG	DA	3287	1/1	0.78	0.21	50,50,50,50	0
56	MG	BA	3069	1/1	0.78	0.19	46,46,46,46	0
56	MG	CA	3136	1/1	0.78	0.20	73,73,73,73	0
56	MG	BA	3154	1/1	0.78	0.29	58,58,58,58	0
56	MG	DA	3036	1/1	0.79	0.34	48,48,48,48	0
56	MG	DA	3398	1/1	0.79	0.17	73,73,73,73	0
56	MG	AX	3009	1/1	0.79	0.19	72,72,72,72	0
56	MG	DA	3085	1/1	0.79	0.12	65,65,65,65	0
56	MG	CA	3058	1/1	0.79	0.20	64,64,64,64	0
56	MG	BA	3729	1/1	0.79	0.18	55,55,55,55	0
56	MG	DA	3103	1/1	0.79	0.12	60,60,60,60	0
56	MG	DA	3183	1/1	0.79	0.18	57,57,57,57	0
56	MG	DA	3081	1/1	0.79	0.20	53,53,53,53	0
56	MG	BA	3737	1/1	0.79	0.12	68,68,68,68	0
56	MG	BA	3616	1/1	0.79	0.11	43,43,43,43	0
56	MG	BB	3016	1/1	0.79	0.14	63,63,63,63	0
56	MG	DA	3577	1/1	0.79	0.46	72,72,72,72	0
56	MG	AA	3128	1/1	0.79	0.14	60,60,60,60	0
56	MG	DB	3005	1/1	0.80	0.34	77,77,77,77	0
56	MG	BE	303	1/1	0.80	0.26	61,61,61,61	0
56	MG	BA	3731	1/1	0.80	0.13	57,57,57,57	0
56	MG	DA	3199	1/1	0.80	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	BA	3580	1/1	0.80	0.15	61,61,61,61	0
56	MG	AX	3002	1/1	0.80	0.24	71,71,71,71	0
56	MG	DA	3515	1/1	0.80	0.12	56,56,56,56	0
56	MG	AX	3003	1/1	0.80	0.13	74,74,74,74	0
56	MG	DA	3138	1/1	0.80	0.20	46,46,46,46	0
56	MG	DA	3605	1/1	0.80	0.12	53,53,53,53	0
56	MG	BA	3235	1/1	0.80	0.16	65,65,65,65	0
56	MG	DA	3311	1/1	0.80	0.13	54,54,54,54	0
56	MG	BA	3638	1/1	0.80	0.22	47,47,47,47	0
56	MG	DA	3039	1/1	0.80	0.21	50,50,50,50	0
56	MG	DA	3490	1/1	0.80	0.08	49,49,49,49	0
56	MG	BA	3031	1/1	0.80	0.21	49,49,49,49	0
56	MG	DA	3029	1/1	0.80	0.16	52,52,52,52	0
56	MG	DA	3091	1/1	0.80	0.15	57,57,57,57	0
56	MG	DA	3010	1/1	0.80	0.20	55,55,55,55	0
56	MG	CA	3055	1/1	0.80	0.19	63,63,63,63	0
56	MG	DA	3131	1/1	0.80	0.16	63,63,63,63	0
56	MG	DA	3426	1/1	0.80	0.11	53,53,53,53	0
56	MG	BA	3030	1/1	0.80	0.12	50,50,50,50	0
56	MG	DA	3514	1/1	0.80	0.13	67,67,67,67	0
56	MG	DA	3030	1/1	0.80	0.13	54,54,54,54	0
56	MG	DA	3218	1/1	0.80	0.11	53,53,53,53	0
56	MG	AA	3225	1/1	0.81	0.16	55,55,55,55	0
56	MG	AA	3049	1/1	0.81	0.13	59,59,59,59	0
56	MG	AA	3003	1/1	0.81	0.23	79,79,79,79	0
56	MG	DA	3163	1/1	0.81	0.68	63,63,63,63	0
56	MG	BA	3548	1/1	0.81	0.15	50,50,50,50	0
56	MG	AA	3004	1/1	0.81	0.10	67,67,67,67	0
56	MG	DA	3213	1/1	0.81	0.22	58,58,58,58	0
56	MG	DA	3365	1/1	0.81	0.21	54,54,54,54	0
56	MG	BA	3208	1/1	0.81	0.21	47,47,47,47	0
56	MG	BA	3582	1/1	0.81	0.13	63,63,63,63	0
56	MG	CA	3021	1/1	0.81	0.12	66,66,66,66	0
56	MG	BA	3059	1/1	0.81	0.15	40,40,40,40	0
56	MG	BA	3186	1/1	0.81	0.24	59,59,59,59	0
56	MG	CA	3061	1/1	0.81	0.19	61,61,61,61	0
56	MG	BP	204	1/1	0.81	0.13	54,54,54,54	0
56	MG	BA	3665	1/1	0.81	0.18	45,45,45,45	0
56	MG	DA	3314	1/1	0.81	0.09	46,46,46,46	0
56	MG	DA	3042	1/1	0.81	0.14	71,71,71,71	0
56	MG	BA	3555	1/1	0.81	0.19	49,49,49,49	0
56	MG	BA	3331	1/1	0.81	0.15	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	3486	1/1	0.81	0.12	47,47,47,47	0
56	MG	BA	3060	1/1	0.81	0.32	61,61,61,61	0
56	MG	AA	3178	1/1	0.81	0.11	60,60,60,60	0
56	MG	BQ	3003	1/1	0.81	0.26	67,67,67,67	0
56	MG	BA	3145	1/1	0.81	0.14	41,41,41,41	0
56	MG	DA	3604	1/1	0.82	0.10	58,58,58,58	0
56	MG	DA	3321	1/1	0.82	0.17	58,58,58,58	0
56	MG	CA	3097	1/1	0.82	0.13	66,66,66,66	0
56	MG	BA	3703	1/1	0.82	0.15	56,56,56,56	0
56	MG	BF	310	1/1	0.82	0.20	44,44,44,44	0
56	MG	BA	3256	1/1	0.82	0.25	25,25,25,25	0
56	MG	BA	3706	1/1	0.82	0.17	52,52,52,52	0
56	MG	DA	3474	1/1	0.82	0.14	55,55,55,55	0
56	MG	BA	3680	1/1	0.82	0.15	32,32,32,32	0
56	MG	BA	3438	1/1	0.82	0.15	44,44,44,44	0
56	MG	BA	3165	1/1	0.82	0.13	53,53,53,53	0
56	MG	AA	3146	1/1	0.82	0.21	65,65,65,65	0
56	MG	AA	3092	1/1	0.82	0.17	59,59,59,59	0
56	MG	DA	3175	1/1	0.82	0.18	43,43,43,43	0
56	MG	BA	3714	1/1	0.82	0.17	73,73,73,73	0
56	MG	BA	3577	1/1	0.82	0.19	62,62,62,62	0
56	MG	BA	3183	1/1	0.82	0.73	47,47,47,47	0
56	MG	AM	201	1/1	0.82	0.10	61,61,61,61	0
56	MG	BA	3177	1/1	0.82	0.19	58,58,58,58	0
56	MG	BA	3303	1/1	0.82	0.20	27,27,27,27	0
56	MG	AA	3088	1/1	0.82	0.15	63,63,63,63	0
56	MG	BA	3084	1/1	0.82	0.41	46,46,46,46	0
56	MG	BA	3645	1/1	0.82	0.33	47,47,47,47	0
56	MG	BA	3118	1/1	0.82	0.31	46,46,46,46	0
56	MG	BA	3648	1/1	0.82	0.14	39,39,39,39	0
56	MG	DA	3615	1/1	0.83	0.26	59,59,59,59	0
56	MG	BA	3046	1/1	0.83	0.15	50,50,50,50	0
56	MG	AA	3203	1/1	0.83	0.23	62,62,62,62	0
56	MG	DA	3066	1/1	0.83	0.13	39,39,39,39	0
56	MG	AA	3126	1/1	0.83	0.34	65,65,65,65	0
56	MG	CA	3139	1/1	0.83	0.11	63,63,63,63	0
56	MG	DA	3409	1/1	0.83	0.15	41,41,41,41	0
57	NEG	CA	3174	17/17	0.83	0.29	38,53,68,69	0
56	MG	BB	3011	1/1	0.83	0.13	56,56,56,56	0
56	MG	AO	3101	1/1	0.83	0.19	58,58,58,58	0
56	MG	CA	3121	1/1	0.83	0.14	88,88,88,88	0
56	MG	DQ	3004	1/1	0.83	0.28	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	DA	3159	1/1	0.83	0.14	60,60,60,60	0
56	MG	DA	3093	1/1	0.83	0.11	59,59,59,59	0
56	MG	BA	3561	1/1	0.83	0.22	64,64,64,64	0
56	MG	AA	3074	1/1	0.83	0.29	59,59,59,59	0
56	MG	BA	3421	1/1	0.83	0.12	46,46,46,46	0
56	MG	DA	3084	1/1	0.83	0.20	53,53,53,53	0
56	MG	BA	3045	1/1	0.83	0.20	41,41,41,41	0
56	MG	DA	3144	1/1	0.83	0.11	60,60,60,60	0
56	MG	B4	502	1/1	0.83	0.22	73,73,73,73	0
56	MG	BA	3591	1/1	0.83	0.13	58,58,58,58	0
56	MG	BA	3075	1/1	0.83	0.32	48,48,48,48	0
56	MG	DA	3501	1/1	0.83	0.18	67,67,67,67	0
56	MG	BA	3051	1/1	0.83	0.17	63,63,63,63	0
56	MG	DA	3086	1/1	0.83	0.90	42,42,42,42	0
56	MG	BA	3453	1/1	0.83	0.16	59,59,59,59	0
57	NEG	CA	3172	17/17	0.83	0.23	61,76,83,84	0
56	MG	DA	3578	1/1	0.83	0.10	71,71,71,71	0
56	MG	DA	3621	1/1	0.83	0.42	73,73,73,73	0
56	MG	DA	3108	1/1	0.83	0.17	48,48,48,48	0
56	MG	BA	3693	1/1	0.83	0.19	38,38,38,38	0
56	MG	DA	3107	1/1	0.83	0.17	47,47,47,47	0
56	MG	BA	3628	1/1	0.83	0.18	55,55,55,55	0
56	MG	AV	102	1/1	0.83	0.18	52,52,52,52	0
56	MG	BA	3135	1/1	0.83	0.13	51,51,51,51	0
56	MG	AA	3144	1/1	0.83	0.08	62,62,62,62	0
56	MG	AA	3189	1/1	0.83	0.10	56,56,56,56	0
56	MG	CA	3075	1/1	0.83	0.20	53,53,53,53	0
56	MG	AA	3201	1/1	0.84	0.10	60,60,60,60	0
57	NEG	CA	3173	17/17	0.84	0.31	54,76,85,86	0
56	MG	DA	3053	1/1	0.84	0.21	61,61,61,61	0
56	MG	CA	3020	1/1	0.84	0.15	48,48,48,48	0
56	MG	BA	3373	1/1	0.84	0.12	35,35,35,35	0
56	MG	BA	3530	1/1	0.84	0.10	56,56,56,56	0
56	MG	BA	3213	1/1	0.84	0.14	48,48,48,48	0
56	MG	DA	3176	1/1	0.84	0.15	49,49,49,49	0
56	MG	BA	3179	1/1	0.84	0.25	61,61,61,61	0
56	MG	CA	3054	1/1	0.84	0.16	65,65,65,65	0
56	MG	DA	3157	1/1	0.84	0.22	58,58,58,58	0
56	MG	CA	3039	1/1	0.84	0.14	70,70,70,70	0
56	MG	AA	3011	1/1	0.84	0.18	66,66,66,66	0
56	MG	DA	3142	1/1	0.84	0.27	55,55,55,55	0
56	MG	BA	3462	1/1	0.84	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3119	1/1	0.84	0.17	50,50,50,50	0
56	MG	BA	3181	1/1	0.84	0.17	48,48,48,48	0
56	MG	DA	3467	1/1	0.84	0.25	69,69,69,69	0
56	MG	CA	3025	1/1	0.84	0.16	64,64,64,64	0
56	MG	BA	3545	1/1	0.84	0.18	58,58,58,58	0
56	MG	CA	3016	1/1	0.84	0.09	56,56,56,56	0
56	MG	BA	3546	1/1	0.84	0.12	57,57,57,57	0
56	MG	B9	502	1/1	0.84	0.20	61,61,61,61	0
56	MG	DA	3554	1/1	0.84	0.13	45,45,45,45	0
56	MG	CA	3105	1/1	0.84	0.11	76,76,76,76	0
56	MG	DA	3330	1/1	0.84	0.12	54,54,54,54	0
56	MG	BN	3003	1/1	0.84	0.16	62,62,62,62	0
56	MG	AA	3020	1/1	0.84	0.25	53,53,53,53	0
56	MG	BA	3653	1/1	0.84	0.14	23,23,23,23	0
56	MG	BA	3086	1/1	0.84	0.20	67,67,67,67	0
56	MG	BA	3338	1/1	0.84	0.20	39,39,39,39	0
56	MG	BA	3200	1/1	0.84	0.16	50,50,50,50	0
56	MG	BB	3015	1/1	0.84	0.12	54,54,54,54	0
56	MG	AA	3214	1/1	0.84	0.13	69,69,69,69	0
56	MG	CA	3052	1/1	0.84	0.09	65,65,65,65	0
56	MG	CA	3066	1/1	0.84	0.16	58,58,58,58	0
56	MG	DA	3001	1/1	0.84	0.27	49,49,49,49	0
56	MG	AA	3104	1/1	0.84	0.16	44,44,44,44	0
56	MG	BA	3597	1/1	0.84	0.09	51,51,51,51	0
56	MG	DA	3438	1/1	0.84	0.14	55,55,55,55	0
56	MG	BA	3136	1/1	0.84	0.59	49,49,49,49	0
56	MG	DA	3610	1/1	0.84	0.10	65,65,65,65	0
56	MG	CA	3123	1/1	0.84	0.27	77,77,77,77	0
56	MG	AA	3175	1/1	0.84	0.10	54,54,54,54	0
56	MG	CT	3001	1/1	0.84	0.13	50,50,50,50	0
56	MG	BA	3370	1/1	0.84	0.23	51,51,51,51	0
56	MG	BA	3144	1/1	0.85	0.15	37,37,37,37	0
56	MG	DA	3414	1/1	0.85	0.17	46,46,46,46	0
56	MG	DA	3205	1/1	0.85	0.14	45,45,45,45	0
56	MG	BA	3738	1/1	0.85	0.15	41,41,41,41	0
56	MG	DA	3078	1/1	0.85	0.31	64,64,64,64	0
56	MG	AA	3002	1/1	0.85	0.15	59,59,59,59	0
56	MG	DA	3151	1/1	0.85	0.12	52,52,52,52	0
56	MG	CA	3009	1/1	0.85	0.27	55,55,55,55	0
56	MG	BA	3585	1/1	0.85	0.17	61,61,61,61	0
56	MG	DA	3158	1/1	0.85	0.30	55,55,55,55	0
56	MG	BA	3559	1/1	0.85	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3042	1/1	0.85	0.15	61,61,61,61	0
56	MG	DF	303	1/1	0.85	0.36	46,46,46,46	0
56	MG	DA	3050	1/1	0.85	0.27	60,60,60,60	0
56	MG	BA	3191	1/1	0.85	0.45	50,50,50,50	0
56	MG	DA	3063	1/1	0.85	0.14	52,52,52,52	0
56	MG	BB	3007	1/1	0.85	0.23	84,84,84,84	0
56	MG	CA	3099	1/1	0.85	0.13	82,82,82,82	0
56	MG	BA	3595	1/1	0.85	0.07	65,65,65,65	0
56	MG	AX	3011	1/1	0.85	0.13	62,62,62,62	0
56	MG	BA	3222	1/1	0.85	0.19	60,60,60,60	0
56	MG	AA	3079	1/1	0.85	0.25	66,66,66,66	0
56	MG	BA	3081	1/1	0.85	0.14	61,61,61,61	0
56	MG	BA	3375	1/1	0.85	0.20	52,52,52,52	0
56	MG	DA	3579	1/1	0.85	0.10	69,69,69,69	0
56	MG	BA	3155	1/1	0.85	0.35	63,63,63,63	0
56	MG	BA	3613	1/1	0.85	0.13	53,53,53,53	0
56	MG	DA	3166	1/1	0.85	0.15	57,57,57,57	0
56	MG	DA	3027	1/1	0.85	0.15	43,43,43,43	0
56	MG	AA	3136	1/1	0.85	0.12	59,59,59,59	0
56	MG	DA	3094	1/1	0.85	0.11	55,55,55,55	0
56	MG	DA	3403	1/1	0.85	0.17	54,54,54,54	0
56	MG	DA	3339	1/1	0.85	0.34	46,46,46,46	0
56	MG	CA	3113	1/1	0.85	0.11	79,79,79,79	0
56	MG	AA	3093	1/1	0.85	0.16	58,58,58,58	0
56	MG	BA	3219	1/1	0.85	0.16	39,39,39,39	0
56	MG	AA	3113	1/1	0.85	0.13	57,57,57,57	0
56	MG	BA	3694	1/1	0.85	0.22	57,57,57,57	0
56	MG	DA	3590	1/1	0.85	0.12	61,61,61,61	0
56	MG	DA	3581	1/1	0.85	0.16	67,67,67,67	0
56	MG	BA	3471	1/1	0.85	0.12	33,33,33,33	0
56	MG	BA	3773	1/1	0.85	0.39	43,43,43,43	0
56	MG	CA	3127	1/1	0.85	0.13	69,69,69,69	0
56	MG	BA	3301	1/1	0.85	0.11	55,55,55,55	0
56	MG	DA	3074	1/1	0.85	0.36	49,49,49,49	0
56	MG	CA	3065	1/1	0.85	0.31	73,73,73,73	0
56	MG	DA	3363	1/1	0.85	0.16	61,61,61,61	0
56	MG	BA	3537	1/1	0.85	0.17	55,55,55,55	0
56	MG	DA	3350	1/1	0.86	0.16	61,61,61,61	0
56	MG	AA	3199	1/1	0.86	0.20	68,68,68,68	0
56	MG	CA	3064	1/1	0.86	0.10	67,67,67,67	0
56	MG	BA	3707	1/1	0.86	0.21	62,62,62,62	0
56	MG	BZ	3001	1/1	0.86	0.17	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	3775	1/1	0.86	0.24	47,47,47,47	0
56	MG	BA	3634	1/1	0.86	0.12	50,50,50,50	0
56	MG	DA	3302	1/1	0.86	0.13	38,38,38,38	0
56	MG	DA	3342	1/1	0.86	0.10	55,55,55,55	0
56	MG	BA	3494	1/1	0.86	0.16	41,41,41,41	0
56	MG	BA	3533	1/1	0.86	0.12	27,27,27,27	0
56	MG	BU	204	1/1	0.86	0.27	43,43,43,43	0
57	NEG	CX	3004	17/17	0.86	0.26	32,64,79,84	0
56	MG	CA	3050	1/1	0.86	0.10	55,55,55,55	0
56	MG	AA	3115	1/1	0.86	0.14	61,61,61,61	0
56	MG	BA	3009	1/1	0.86	0.30	41,41,41,41	0
56	MG	BA	3695	1/1	0.86	0.23	39,39,39,39	0
56	MG	BA	3187	1/1	0.86	0.21	42,42,42,42	0
56	MG	BA	3716	1/1	0.86	0.15	48,48,48,48	0
56	MG	DA	3572	1/1	0.86	0.14	70,70,70,70	0
56	MG	DA	3016	1/1	0.86	0.31	34,34,34,34	0
56	MG	BA	3612	1/1	0.86	0.16	65,65,65,65	0
56	MG	BA	3127	1/1	0.86	0.58	38,38,38,38	0
56	MG	BA	3715	1/1	0.86	0.14	48,48,48,48	0
56	MG	DG	3001	1/1	0.86	0.12	55,55,55,55	0
56	MG	DE	303	1/1	0.86	0.17	40,40,40,40	0
56	MG	DA	3533	1/1	0.86	0.13	50,50,50,50	0
56	MG	DA	3283	1/1	0.86	0.10	53,53,53,53	0
56	MG	BA	3109	1/1	0.86	0.16	49,49,49,49	0
56	MG	BN	3001	1/1	0.86	0.62	51,51,51,51	0
56	MG	DA	3247	1/1	0.86	0.08	51,51,51,51	0
56	MG	BA	3180	1/1	0.86	0.14	46,46,46,46	0
56	MG	BA	3281	1/1	0.86	0.09	55,55,55,55	0
56	MG	DA	3377	1/1	0.86	0.11	48,48,48,48	0
56	MG	BA	3704	1/1	0.86	0.14	75,75,75,75	0
56	MG	DD	309	1/1	0.86	0.36	65,65,65,65	0
56	MG	BA	3039	1/1	0.86	0.22	34,34,34,34	0
56	MG	BA	3601	1/1	0.86	0.56	72,72,72,72	0
56	MG	DA	3057	1/1	0.86	0.20	54,54,54,54	0
56	MG	DA	3442	1/1	0.86	0.15	46,46,46,46	0
56	MG	DA	3352	1/1	0.86	0.18	45,45,45,45	0
56	MG	DA	3065	1/1	0.86	0.52	56,56,56,56	0
56	MG	BA	3692	1/1	0.86	0.23	73,73,73,73	0
56	MG	BA	3262	1/1	0.86	0.13	51,51,51,51	0
56	MG	AA	3027	1/1	0.86	0.12	58,58,58,58	0
56	MG	DA	3257	1/1	0.86	0.20	58,58,58,58	0
56	MG	DA	3346	1/1	0.86	0.14	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3148	1/1	0.86	0.11	72,72,72,72	0
56	MG	BA	3700	1/1	0.86	0.13	73,73,73,73	0
56	MG	DA	3606	1/1	0.86	0.12	54,54,54,54	0
56	MG	BA	3406	1/1	0.86	0.13	50,50,50,50	0
56	MG	BA	3609	1/1	0.86	0.15	62,62,62,62	0
56	MG	AA	3031	1/1	0.86	0.15	63,63,63,63	0
56	MG	DA	3562	1/1	0.86	0.09	67,67,67,67	0
56	MG	DA	3462	1/1	0.86	0.12	36,36,36,36	0
56	MG	DA	3153	1/1	0.86	0.13	40,40,40,40	0
56	MG	DA	3133	1/1	0.86	0.15	50,50,50,50	0
56	MG	BA	3526	1/1	0.86	0.18	38,38,38,38	0
56	MG	AA	3130	1/1	0.87	0.21	74,74,74,74	0
56	MG	DA	3522	1/1	0.87	0.12	57,57,57,57	0
56	MG	DA	3216	1/1	0.87	0.28	52,52,52,52	0
56	MG	AA	3208	1/1	0.87	0.28	67,67,67,67	0
56	MG	DA	3353	1/1	0.87	0.06	65,65,65,65	0
56	MG	BA	3631	1/1	0.87	0.17	63,63,63,63	0
56	MG	BA	3395	1/1	0.87	0.13	65,65,65,65	0
56	MG	DA	3173	1/1	0.87	0.25	49,49,49,49	0
56	MG	DA	3616	1/1	0.87	0.13	47,47,47,47	0
57	NEG	CA	3170	17/17	0.87	0.36	58,72,83,86	0
56	MG	AA	3021	1/1	0.87	0.15	60,60,60,60	0
56	MG	BA	3484	1/1	0.87	0.13	64,64,64,64	0
56	MG	BA	3784	1/1	0.87	0.09	62,62,62,62	0
56	MG	AA	3017	1/1	0.87	0.14	49,49,49,49	0
56	MG	BA	3054	1/1	0.87	0.17	51,51,51,51	0
56	MG	BA	3415	1/1	0.87	0.12	62,62,62,62	0
56	MG	DA	3593	1/1	0.87	0.23	57,57,57,57	0
56	MG	AX	3006	1/1	0.87	0.14	80,80,80,80	0
56	MG	DA	3022	1/1	0.87	0.24	50,50,50,50	0
56	MG	BA	3449	1/1	0.87	0.16	59,59,59,59	0
56	MG	DA	3550	1/1	0.87	0.11	61,61,61,61	0
56	MG	DA	3595	1/1	0.87	0.12	34,34,34,34	0
56	MG	BA	3108	1/1	0.87	0.38	52,52,52,52	0
56	MG	BA	3201	1/1	0.87	0.24	49,49,49,49	0
56	MG	DA	3291	1/1	0.87	0.15	41,41,41,41	0
56	MG	BB	3005	1/1	0.87	0.19	54,54,54,54	0
56	MG	BA	3013	1/1	0.87	0.19	46,46,46,46	0
56	MG	DA	3193	1/1	0.87	0.09	57,57,57,57	0
56	MG	BA	3558	1/1	0.87	0.16	72,72,72,72	0
56	MG	BA	3360	1/1	0.87	0.21	41,41,41,41	0
56	MG	BA	3400	1/1	0.87	0.15	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	CA	3045	1/1	0.87	0.19	68,68,68,68	0
56	MG	BA	3276	1/1	0.87	0.14	40,40,40,40	0
56	MG	BA	3503	1/1	0.87	0.20	43,43,43,43	0
56	MG	DA	3520	1/1	0.87	0.11	61,61,61,61	0
56	MG	DA	3278	1/1	0.87	0.12	44,44,44,44	0
56	MG	DA	3543	1/1	0.87	0.21	63,63,63,63	0
56	MG	BA	3417	1/1	0.87	0.14	56,56,56,56	0
56	MG	BA	3723	1/1	0.87	0.12	41,41,41,41	0
56	MG	BA	3505	1/1	0.87	0.30	54,54,54,54	0
56	MG	DA	3105	1/1	0.87	0.20	54,54,54,54	0
56	MG	DA	3378	1/1	0.87	0.20	51,51,51,51	0
56	MG	AX	3010	1/1	0.87	0.49	54,54,54,54	0
56	MG	AA	3018	1/1	0.87	0.21	58,58,58,58	0
56	MG	BA	3404	1/1	0.87	0.12	59,59,59,59	0
56	MG	DA	3557	1/1	0.87	0.11	67,67,67,67	0
56	MG	DA	3045	1/1	0.87	0.12	44,44,44,44	0
56	MG	DF	304	1/1	0.87	0.12	48,48,48,48	0
56	MG	BA	3098	1/1	0.87	0.11	51,51,51,51	0
56	MG	DA	3239	1/1	0.87	0.09	61,61,61,61	0
56	MG	BA	3323	1/1	0.87	0.16	60,60,60,60	0
56	MG	DA	3261	1/1	0.87	0.34	60,60,60,60	0
56	MG	BA	3661	1/1	0.87	0.14	61,61,61,61	0
56	MG	BA	3531	1/1	0.87	0.09	56,56,56,56	0
56	MG	BA	3682	1/1	0.87	0.11	73,73,73,73	0
56	MG	B7	104	1/1	0.87	0.20	55,55,55,55	0
56	MG	BA	3243	1/1	0.87	0.17	57,57,57,57	0
56	MG	BA	3757	1/1	0.87	0.29	47,47,47,47	0
56	MG	DA	3006	1/1	0.87	0.36	42,42,42,42	0
56	MG	AX	3004	1/1	0.87	0.22	67,67,67,67	0
56	MG	AA	3193	1/1	0.87	0.25	69,69,69,69	0
56	MG	BA	3467	1/1	0.87	0.21	48,48,48,48	0
56	MG	CA	3026	1/1	0.87	0.19	61,61,61,61	0
56	MG	AA	3215	1/1	0.87	0.24	56,56,56,56	0
56	MG	DA	3249	1/1	0.87	0.10	43,43,43,43	0
56	MG	AA	3059	1/1	0.88	0.21	53,53,53,53	0
56	MG	BA	3725	1/1	0.88	0.09	63,63,63,63	0
56	MG	BA	3242	1/1	0.88	0.21	58,58,58,58	0
56	MG	BA	3012	1/1	0.88	0.11	49,49,49,49	0
56	MG	DA	3049	1/1	0.88	0.16	48,48,48,48	0
56	MG	DA	3564	1/1	0.88	0.14	64,64,64,64	0
56	MG	CA	3131	1/1	0.88	0.09	62,62,62,62	0
56	MG	BA	3143	1/1	0.88	0.37	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3205	1/1	0.88	0.22	45,45,45,45	0
56	MG	BA	3482	1/1	0.88	0.32	27,27,27,27	0
56	MG	DU	3001	1/1	0.88	0.98	61,61,61,61	0
57	NEG	CA	3175	17/17	0.88	0.39	48,61,79,89	0
56	MG	DN	5001	1/1	0.88	0.15	75,75,75,75	0
56	MG	DA	3077	1/1	0.88	0.17	40,40,40,40	0
56	MG	AA	3174	1/1	0.88	0.09	59,59,59,59	0
56	MG	AA	3213	1/1	0.88	0.12	44,44,44,44	0
56	MG	BA	3554	1/1	0.88	0.07	56,56,56,56	0
56	MG	BA	3212	1/1	0.88	0.26	47,47,47,47	0
56	MG	AA	3058	1/1	0.88	0.22	63,63,63,63	0
56	MG	BA	3148	1/1	0.88	0.19	50,50,50,50	0
56	MG	BA	3721	1/1	0.88	0.18	74,74,74,74	0
56	MG	BA	3436	1/1	0.88	0.13	67,67,67,67	0
56	MG	BA	3153	1/1	0.88	0.22	56,56,56,56	0
56	MG	DA	3389	1/1	0.88	0.14	63,63,63,63	0
56	MG	CA	3037	1/1	0.88	0.16	67,67,67,67	0
56	MG	DA	3028	1/1	0.88	0.21	52,52,52,52	0
56	MG	AA	3101	1/1	0.88	0.21	52,52,52,52	0
56	MG	DA	3341	1/1	0.88	0.09	54,54,54,54	0
56	MG	BA	3257	1/1	0.88	0.16	48,48,48,48	0
56	MG	DA	3493	1/1	0.88	0.16	64,64,64,64	0
57	NEG	CW	3002	17/17	0.88	0.31	41,56,78,84	0
56	MG	DA	3566	1/1	0.88	0.12	51,51,51,51	0
56	MG	DA	3620	1/1	0.88	0.17	71,71,71,71	0
56	MG	AA	3186	1/1	0.88	0.17	65,65,65,65	0
56	MG	CA	3125	1/1	0.88	0.08	76,76,76,76	0
56	MG	CA	3100	1/1	0.88	0.10	52,52,52,52	0
56	MG	BA	3622	1/1	0.88	0.21	48,48,48,48	0
56	MG	AA	3121	1/1	0.88	0.10	54,54,54,54	0
56	MG	AA	3040	1/1	0.88	0.10	41,41,41,41	0
56	MG	CA	3146	1/1	0.88	0.14	80,80,80,80	0
56	MG	BA	3586	1/1	0.88	0.25	58,58,58,58	0
56	MG	BA	3007	1/1	0.88	0.35	39,39,39,39	0
56	MG	DA	3349	1/1	0.88	0.12	46,46,46,46	0
56	MG	AA	3050	1/1	0.88	0.13	65,65,65,65	0
56	MG	DB	3001	1/1	0.88	0.25	56,56,56,56	0
56	MG	DA	3433	1/1	0.88	0.11	58,58,58,58	0
56	MG	DA	3212	1/1	0.88	0.27	52,52,52,52	0
56	MG	BA	3211	1/1	0.88	0.20	57,57,57,57	0
56	MG	DW	3004	1/1	0.88	0.21	50,50,50,50	0
56	MG	CA	3095	1/1	0.88	0.08	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3042	1/1	0.88	0.20	54,54,54,54	0
56	MG	BA	3454	1/1	0.88	0.15	43,43,43,43	0
56	MG	BA	3732	1/1	0.88	0.14	57,57,57,57	0
56	MG	BA	3356	1/1	0.88	0.21	24,24,24,24	0
56	MG	BA	3461	1/1	0.88	0.18	21,21,21,21	0
56	MG	AA	3100	1/1	0.88	0.24	53,53,53,53	0
56	MG	BA	3456	1/1	0.88	0.12	63,63,63,63	0
56	MG	BA	3295	1/1	0.88	0.13	66,66,66,66	0
56	MG	DA	3161	1/1	0.88	0.30	57,57,57,57	0
56	MG	AA	3086	1/1	0.88	0.18	53,53,53,53	0
56	MG	BA	3359	1/1	0.88	0.25	43,43,43,43	0
56	MG	BA	3340	1/1	0.88	0.18	34,34,34,34	0
56	MG	DA	3125	1/1	0.88	0.51	56,56,56,56	0
56	MG	CA	3028	1/1	0.88	0.20	53,53,53,53	0
56	MG	BA	3209	1/1	0.88	0.36	57,57,57,57	0
56	MG	DV	3003	1/1	0.88	0.18	62,62,62,62	0
56	MG	DA	3380	1/1	0.88	0.14	43,43,43,43	0
56	MG	BA	3734	1/1	0.88	0.16	24,24,24,24	0
56	MG	DA	3362	1/1	0.88	0.16	22,22,22,22	0
56	MG	BA	3521	1/1	0.88	0.21	28,28,28,28	0
56	MG	BA	3015	1/1	0.88	0.27	52,52,52,52	0
56	MG	DA	3488	1/1	0.88	0.11	66,66,66,66	0
56	MG	BA	3669	1/1	0.88	0.30	45,45,45,45	0
56	MG	AA	3052	1/1	0.88	0.30	52,52,52,52	0
56	MG	DA	3351	1/1	0.89	0.11	40,40,40,40	0
56	MG	BA	3175	1/1	0.89	0.18	44,44,44,44	0
56	MG	AA	3042	1/1	0.89	0.14	52,52,52,52	0
56	MG	DA	3221	1/1	0.89	0.12	56,56,56,56	0
56	MG	BA	3408	1/1	0.89	0.10	71,71,71,71	0
56	MG	AA	3202	1/1	0.89	0.08	63,63,63,63	0
56	MG	BU	201	1/1	0.89	0.33	29,29,29,29	0
56	MG	BA	3258	1/1	0.89	0.18	57,57,57,57	0
56	MG	DA	3425	1/1	0.89	0.14	69,69,69,69	0
56	MG	AA	3122	1/1	0.89	0.13	74,74,74,74	0
56	MG	BD	305	1/1	0.89	0.32	41,41,41,41	0
56	MG	BA	3444	1/1	0.89	0.16	37,37,37,37	0
56	MG	CX	3002	1/1	0.89	0.17	67,67,67,67	0
56	MG	BA	3435	1/1	0.89	0.34	52,52,52,52	0
56	MG	DA	3208	1/1	0.89	0.15	61,61,61,61	0
56	MG	DA	3326	1/1	0.89	0.22	31,31,31,31	0
56	MG	BA	3011	1/1	0.89	0.33	51,51,51,51	0
56	MG	BA	3740	1/1	0.89	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	3223	1/1	0.89	0.19	42,42,42,42	0
56	MG	BA	3445	1/1	0.89	0.24	53,53,53,53	0
56	MG	BA	3649	1/1	0.89	0.27	49,49,49,49	0
57	NEG	AW	3004	17/17	0.89	0.36	37,50,72,73	0
56	MG	BA	3229	1/1	0.89	0.09	38,38,38,38	0
56	MG	DA	3080	1/1	0.89	0.20	48,48,48,48	0
56	MG	DB	3007	1/1	0.89	0.15	67,67,67,67	0
56	MG	DA	3500	1/1	0.89	0.12	56,56,56,56	0
56	MG	CA	3049	1/1	0.89	0.19	54,54,54,54	0
56	MG	BA	3364	1/1	0.89	0.12	50,50,50,50	0
56	MG	AE	3002	1/1	0.89	0.50	67,67,67,67	0
56	MG	DA	3298	1/1	0.89	0.10	57,57,57,57	0
56	MG	DA	3476	1/1	0.89	0.09	62,62,62,62	0
56	MG	DA	3209	1/1	0.89	0.19	52,52,52,52	0
56	MG	BA	3137	1/1	0.89	0.21	41,41,41,41	0
56	MG	CA	3085	1/1	0.89	0.13	60,60,60,60	0
56	MG	DA	3126	1/1	0.89	0.13	51,51,51,51	0
56	MG	AA	3143	1/1	0.89	0.12	57,57,57,57	0
56	MG	CA	3053	1/1	0.89	0.22	63,63,63,63	0
56	MG	BA	3275	1/1	0.89	0.19	45,45,45,45	0
56	MG	BA	3579	1/1	0.89	0.25	57,57,57,57	0
56	MG	CA	3122	1/1	0.89	0.19	70,70,70,70	0
56	MG	CA	3115	1/1	0.89	0.06	58,58,58,58	0
56	MG	BA	3658	1/1	0.89	0.15	41,41,41,41	0
56	MG	DA	3508	1/1	0.89	0.06	68,68,68,68	0
56	MG	BA	3783	1/1	0.89	0.29	36,36,36,36	0
56	MG	BA	3139	1/1	0.89	0.16	52,52,52,52	0
56	MG	BA	3549	1/1	0.89	0.22	53,53,53,53	0
56	MG	DA	3098	1/1	0.89	0.21	61,61,61,61	0
56	MG	BA	3174	1/1	0.89	0.18	52,52,52,52	0
56	MG	BA	3434	1/1	0.89	0.15	65,65,65,65	0
56	MG	DA	3279	1/1	0.89	0.09	51,51,51,51	0
56	MG	BA	3244	1/1	0.89	0.34	53,53,53,53	0
56	MG	BA	3283	1/1	0.89	0.17	39,39,39,39	0
56	MG	BV	204	1/1	0.89	0.18	39,39,39,39	0
56	MG	AA	3176	1/1	0.89	0.18	69,69,69,69	0
56	MG	BA	3510	1/1	0.89	0.17	43,43,43,43	0
56	MG	DA	3504	1/1	0.89	0.12	55,55,55,55	0
56	MG	BA	3233	1/1	0.89	0.13	49,49,49,49	0
56	MG	DA	3603	1/1	0.89	0.21	45,45,45,45	0
56	MG	CA	3018	1/1	0.89	0.15	69,69,69,69	0
56	MG	BA	3178	1/1	0.89	0.22	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	3207	1/1	0.89	0.13	58,58,58,58	0
56	MG	AA	3096	1/1	0.89	0.16	53,53,53,53	0
56	MG	BA	3248	1/1	0.89	0.13	27,27,27,27	0
56	MG	AA	3095	1/1	0.89	0.12	63,63,63,63	0
56	MG	CA	3138	1/1	0.89	0.11	52,52,52,52	0
56	MG	DA	3197	1/1	0.89	0.12	57,57,57,57	0
56	MG	DA	3075	1/1	0.89	0.25	51,51,51,51	0
56	MG	AA	3103	1/1	0.89	0.21	59,59,59,59	0
56	MG	DA	3546	1/1	0.89	0.15	64,64,64,64	0
56	MG	DY	502	1/1	0.89	0.20	86,86,86,86	0
56	MG	BD	303	1/1	0.89	0.34	45,45,45,45	0
56	MG	DA	3619	1/1	0.89	0.21	57,57,57,57	0
56	MG	BA	3630	1/1	0.89	0.14	44,44,44,44	0
56	MG	CA	3057	1/1	0.89	0.20	73,73,73,73	0
56	MG	BA	3625	1/1	0.89	0.14	49,49,49,49	0
60	K	CX	3001	1/1	0.89	0.45	84,84,84,84	0
56	MG	DA	3376	1/1	0.89	0.15	46,46,46,46	0
56	MG	CA	3069	1/1	0.89	0.20	75,75,75,75	0
56	MG	DA	3510	1/1	0.89	0.13	32,32,32,32	0
56	MG	DA	3037	1/1	0.89	0.40	46,46,46,46	0
56	MG	BA	3126	1/1	0.89	0.43	48,48,48,48	0
56	MG	CA	3059	1/1	0.89	0.39	70,70,70,70	0
56	MG	DA	3127	1/1	0.89	0.16	53,53,53,53	0
56	MG	BA	3496	1/1	0.89	0.20	53,53,53,53	0
56	MG	AA	3034	1/1	0.89	0.24	56,56,56,56	0
56	MG	CA	3083	1/1	0.89	0.08	58,58,58,58	0
56	MG	CA	3167	1/1	0.89	0.10	55,55,55,55	0
56	MG	BB	3008	1/1	0.89	0.11	71,71,71,71	0
56	MG	BA	3512	1/1	0.89	0.14	65,65,65,65	0
56	MG	BA	3588	1/1	0.89	0.17	62,62,62,62	0
56	MG	BA	3542	1/1	0.89	0.14	66,66,66,66	0
56	MG	CA	3165	1/1	0.89	0.15	57,57,57,57	0
56	MG	BA	3336	1/1	0.89	0.21	31,31,31,31	0
56	MG	BA	3604	1/1	0.90	0.14	46,46,46,46	0
56	MG	BA	3670	1/1	0.90	0.19	55,55,55,55	0
56	MG	DA	3292	1/1	0.90	0.23	36,36,36,36	0
56	MG	DA	3385	1/1	0.90	0.27	55,55,55,55	0
56	MG	BA	3420	1/1	0.90	0.17	61,61,61,61	0
56	MG	DA	3381	1/1	0.90	0.21	55,55,55,55	0
56	MG	BA	3389	1/1	0.90	0.14	51,51,51,51	0
56	MG	CA	3142	1/1	0.90	0.17	69,69,69,69	0
56	MG	BA	3523	1/1	0.90	0.18	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	3168	1/1	0.90	0.15	57,57,57,57	0
56	MG	DA	3169	1/1	0.90	0.12	61,61,61,61	0
56	MG	CA	3143	1/1	0.90	0.25	59,59,59,59	0
56	MG	CA	3092	1/1	0.90	0.23	55,55,55,55	0
56	MG	CA	3082	1/1	0.90	0.18	41,41,41,41	0
56	MG	BA	3719	1/1	0.90	0.19	49,49,49,49	0
56	MG	BA	3010	1/1	0.90	0.13	58,58,58,58	0
57	NEG	AA	3221	17/17	0.90	0.34	44,57,69,70	0
56	MG	BA	3076	1/1	0.90	0.12	58,58,58,58	0
57	NEG	AA	3217	17/17	0.90	0.27	45,55,78,95	0
56	MG	BA	3049	1/1	0.90	0.23	54,54,54,54	0
56	MG	BA	3080	1/1	0.90	0.30	49,49,49,49	0
56	MG	CA	3044	1/1	0.90	0.16	62,62,62,62	0
56	MG	BA	3196	1/1	0.90	0.15	46,46,46,46	0
56	MG	DA	3112	1/1	0.90	0.12	49,49,49,49	0
56	MG	DD	305	1/1	0.90	0.18	32,32,32,32	0
56	MG	BA	3742	1/1	0.90	0.35	44,44,44,44	0
56	MG	BA	3071	1/1	0.90	0.12	48,48,48,48	0
56	MG	AA	3112	1/1	0.90	0.15	53,53,53,53	0
56	MG	AA	3155	1/1	0.90	0.14	60,60,60,60	0
56	MG	BA	3189	1/1	0.90	0.42	55,55,55,55	0
56	MG	DA	3214	1/1	0.90	0.11	58,58,58,58	0
56	MG	CA	3106	1/1	0.90	0.15	55,55,55,55	0
56	MG	DA	3512	1/1	0.90	0.12	52,52,52,52	0
56	MG	DA	3060	1/1	0.90	0.30	50,50,50,50	0
56	MG	BD	308	1/1	0.90	0.26	42,42,42,42	0
56	MG	DA	3058	1/1	0.90	0.14	48,48,48,48	0
56	MG	CA	3040	1/1	0.90	0.15	70,70,70,70	0
56	MG	AA	3063	1/1	0.90	0.23	56,56,56,56	0
56	MG	DA	3585	1/1	0.90	0.13	55,55,55,55	0
56	MG	BA	3362	1/1	0.90	0.20	25,25,25,25	0
57	NEG	CA	3171	17/17	0.90	0.24	53,72,80,85	0
57	NEG	CA	3177	17/17	0.90	0.24	36,63,74,81	0
56	MG	AA	3008	1/1	0.90	0.18	53,53,53,53	0
56	MG	BA	3253	1/1	0.90	0.17	30,30,30,30	0
56	MG	CA	3116	1/1	0.90	0.17	64,64,64,64	0
56	MG	BA	3749	1/1	0.90	0.12	38,38,38,38	0
56	MG	DA	3070	1/1	0.90	0.12	34,34,34,34	0
56	MG	BB	3003	1/1	0.90	0.16	37,37,37,37	0
56	MG	BQ	3004	1/1	0.90	0.27	48,48,48,48	0
56	MG	BA	3207	1/1	0.90	0.08	52,52,52,52	0
56	MG	AA	3030	1/1	0.90	0.20	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	AA	3094	1/1	0.90	0.30	53,53,53,53	0
56	MG	BA	3300	1/1	0.90	0.17	55,55,55,55	0
56	MG	BD	306	1/1	0.90	0.19	22,22,22,22	0
56	MG	BA	3070	1/1	0.90	0.25	48,48,48,48	0
57	NEG	AA	3222	17/17	0.90	0.29	30,45,63,66	0
56	MG	BA	3147	1/1	0.90	0.09	60,60,60,60	0
56	MG	BA	3689	1/1	0.90	0.19	68,68,68,68	0
57	NEG	AX	3013	17/17	0.90	0.26	29,49,69,70	0
56	MG	BA	3429	1/1	0.90	0.09	71,71,71,71	0
56	MG	AA	3051	1/1	0.90	0.12	64,64,64,64	0
56	MG	DA	3586	1/1	0.90	0.19	49,49,49,49	0
56	MG	BA	3197	1/1	0.90	0.15	46,46,46,46	0
56	MG	BA	3514	1/1	0.90	0.12	50,50,50,50	0
56	MG	BA	3717	1/1	0.90	0.15	34,34,34,34	0
56	MG	BA	3501	1/1	0.90	0.28	74,74,74,74	0
56	MG	BA	3418	1/1	0.90	0.14	57,57,57,57	0
56	MG	DA	3032	1/1	0.90	0.15	40,40,40,40	0
56	MG	DA	3458	1/1	0.90	0.12	56,56,56,56	0
56	MG	BA	3132	1/1	0.90	0.53	42,42,42,42	0
56	MG	DA	3118	1/1	0.90	0.16	50,50,50,50	0
56	MG	DA	3588	1/1	0.90	0.18	57,57,57,57	0
56	MG	BA	3170	1/1	0.90	0.19	30,30,30,30	0
56	MG	DA	3170	1/1	0.90	0.25	39,39,39,39	0
56	MG	BA	3600	1/1	0.90	0.09	59,59,59,59	0
56	MG	BA	3234	1/1	0.90	0.14	52,52,52,52	0
56	MG	CA	3071	1/1	0.90	0.08	58,58,58,58	0
56	MG	CA	3056	1/1	0.90	0.17	74,74,74,74	0
56	MG	BA	3608	1/1	0.90	0.12	68,68,68,68	0
56	MG	BA	3701	1/1	0.90	0.12	66,66,66,66	0
56	MG	CA	3156	1/1	0.90	0.12	58,58,58,58	0
56	MG	DA	3471	1/1	0.90	0.20	58,58,58,58	0
56	MG	BA	3575	1/1	0.90	0.17	48,48,48,48	0
56	MG	DA	3023	1/1	0.90	1.12	44,44,44,44	0
56	MG	DA	3405	1/1	0.90	0.15	76,76,76,76	0
56	MG	BA	3161	1/1	0.90	0.46	40,40,40,40	0
56	MG	BA	3502	1/1	0.90	0.13	62,62,62,62	0
56	MG	B6	101	1/1	0.90	0.11	49,49,49,49	0
56	MG	DA	3089	1/1	0.90	0.10	57,57,57,57	0
56	MG	DA	3549	1/1	0.90	0.23	53,53,53,53	0
56	MG	AA	3124	1/1	0.90	0.16	63,63,63,63	0
56	MG	DA	3431	1/1	0.90	0.16	44,44,44,44	0
56	MG	BA	3728	1/1	0.90	0.10	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	DA	3052	1/1	0.90	0.09	44,44,44,44	0
56	MG	CA	3073	1/1	0.90	0.20	70,70,70,70	0
56	MG	BB	3018	1/1	0.90	0.17	46,46,46,46	0
56	MG	DA	3436	1/1	0.90	0.14	63,63,63,63	0
56	MG	BA	3768	1/1	0.90	0.18	48,48,48,48	0
56	MG	BA	3605	1/1	0.90	0.21	69,69,69,69	0
56	MG	BA	3245	1/1	0.90	0.12	47,47,47,47	0
56	MG	BA	3739	1/1	0.90	0.29	75,75,75,75	0
56	MG	BA	3543	1/1	0.90	0.12	62,62,62,62	0
56	MG	DA	3528	1/1	0.90	0.15	70,70,70,70	0
56	MG	AA	3127	1/1	0.90	0.29	52,52,52,52	0
56	MG	DA	3059	1/1	0.90	0.12	49,49,49,49	0
56	MG	BA	3131	1/1	0.91	0.46	35,35,35,35	0
56	MG	BA	3571	1/1	0.91	0.14	40,40,40,40	0
56	MG	BN	3005	1/1	0.91	0.15	46,46,46,46	0
56	MG	DA	3211	1/1	0.91	0.18	49,49,49,49	0
56	MG	DB	3006	1/1	0.91	0.19	63,63,63,63	0
56	MG	BA	3349	1/1	0.91	0.19	25,25,25,25	0
56	MG	BA	3515	1/1	0.91	0.11	57,57,57,57	0
56	MG	BA	3343	1/1	0.91	0.18	44,44,44,44	0
56	MG	DA	3372	1/1	0.91	0.11	67,67,67,67	0
56	MG	AA	3062	1/1	0.91	0.30	58,58,58,58	0
56	MG	BA	3288	1/1	0.91	0.17	36,36,36,36	0
56	MG	BG	3002	1/1	0.91	0.12	52,52,52,52	0
56	MG	BA	3121	1/1	0.91	0.35	64,64,64,64	0
56	MG	BA	3033	1/1	0.91	0.12	45,45,45,45	0
56	MG	AA	3109	1/1	0.91	0.21	51,51,51,51	0
56	MG	DA	3241	1/1	0.91	0.13	51,51,51,51	0
56	MG	BA	3312	1/1	0.91	0.22	41,41,41,41	0
56	MG	AA	3019	1/1	0.91	0.18	53,53,53,53	0
56	MG	DA	3596	1/1	0.91	0.11	64,64,64,64	0
56	MG	DA	3553	1/1	0.91	0.23	45,45,45,45	0
56	MG	BA	3274	1/1	0.91	0.15	29,29,29,29	0
56	MG	BE	301	1/1	0.91	0.19	36,36,36,36	0
56	MG	DA	3320	1/1	0.91	0.15	53,53,53,53	0
56	MG	BA	3403	1/1	0.91	0.19	53,53,53,53	0
56	MG	BD	311	1/1	0.91	0.72	46,46,46,46	0
56	MG	DU	3003	1/1	0.91	0.32	50,50,50,50	0
56	MG	CA	3162	1/1	0.91	0.07	57,57,57,57	0
56	MG	BA	3724	1/1	0.91	0.14	84,84,84,84	0
56	MG	DF	302	1/1	0.91	0.22	60,60,60,60	0
56	MG	BA	3539	1/1	0.91	0.15	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	B5	104	1/1	0.91	0.42	55,55,55,55	0
56	MG	BA	3261	1/1	0.91	0.21	49,49,49,49	0
56	MG	AA	3195	1/1	0.91	0.19	58,58,58,58	0
56	MG	DA	3167	1/1	0.91	0.77	51,51,51,51	0
56	MG	DA	3012	1/1	0.91	0.21	43,43,43,43	0
56	MG	BA	3534	1/1	0.91	0.21	54,54,54,54	0
56	MG	DA	3262	1/1	0.91	0.16	41,41,41,41	0
56	MG	BA	3182	1/1	0.91	0.91	50,50,50,50	0
56	MG	DA	3366	1/1	0.91	0.15	36,36,36,36	0
56	MG	BA	3652	1/1	0.91	0.21	25,25,25,25	0
57	NEG	AA	3218	17/17	0.91	0.21	57,72,76,91	0
56	MG	DA	3485	1/1	0.91	0.38	60,60,60,60	0
56	MG	DA	3300	1/1	0.91	0.13	27,27,27,27	0
56	MG	AA	3069	1/1	0.91	0.13	59,59,59,59	0
56	MG	BA	3762	1/1	0.91	0.23	58,58,58,58	0
56	MG	AA	3167	1/1	0.91	0.19	71,71,71,71	0
57	NEG	CA	3176	17/17	0.91	0.30	46,65,76,84	0
56	MG	BA	3067	1/1	0.91	0.44	35,35,35,35	0
56	MG	BA	3657	1/1	0.91	0.16	54,54,54,54	0
56	MG	BD	301	1/1	0.91	0.54	45,45,45,45	0
56	MG	DA	3069	1/1	0.91	0.13	49,49,49,49	0
56	MG	DA	3184	1/1	0.91	0.23	56,56,56,56	0
56	MG	BA	3116	1/1	0.91	0.43	68,68,68,68	0
56	MG	AV	103	1/1	0.91	0.13	70,70,70,70	0
56	MG	BA	3755	1/1	0.91	0.16	42,42,42,42	0
56	MG	AE	3001	1/1	0.91	0.09	77,77,77,77	0
56	MG	BX	101	1/1	0.91	0.15	48,48,48,48	0
56	MG	BA	3231	1/1	0.91	0.17	42,42,42,42	0
57	NEG	AA	3219	17/17	0.91	0.30	61,71,78,79	0
56	MG	BA	3506	1/1	0.91	0.05	43,43,43,43	0
56	MG	AA	3140	1/1	0.91	0.21	61,61,61,61	0
56	MG	DA	3286	1/1	0.91	0.14	39,39,39,39	0
56	MG	BA	3382	1/1	0.91	0.19	30,30,30,30	0
56	MG	CA	3155	1/1	0.91	0.18	61,61,61,61	0
56	MG	BA	3675	1/1	0.91	0.28	39,39,39,39	0
56	MG	AA	3066	1/1	0.91	0.11	53,53,53,53	0
56	MG	DA	3584	1/1	0.91	0.16	45,45,45,45	0
56	MG	AX	3007	1/1	0.91	0.24	66,66,66,66	0
56	MG	DA	3318	1/1	0.91	0.08	60,60,60,60	0
56	MG	DA	3109	1/1	0.91	0.34	47,47,47,47	0
56	MG	DA	3149	1/1	0.91	0.18	48,48,48,48	0
56	MG	BA	3651	1/1	0.91	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3412	1/1	0.91	0.34	52,52,52,52	0
56	MG	CA	3130	1/1	0.91	0.11	70,70,70,70	0
56	MG	DR	3002	1/1	0.91	0.10	55,55,55,55	0
56	MG	CF	3001	1/1	0.91	0.17	44,44,44,44	0
56	MG	BA	3620	1/1	0.91	0.21	42,42,42,42	0
56	MG	DA	3097	1/1	0.91	0.14	52,52,52,52	0
56	MG	CA	3119	1/1	0.91	0.14	84,84,84,84	0
56	MG	BA	3492	1/1	0.91	0.14	33,33,33,33	0
56	MG	BA	3290	1/1	0.91	0.19	61,61,61,61	0
56	MG	AA	3089	1/1	0.91	0.17	54,54,54,54	0
56	MG	DA	3117	1/1	0.91	0.10	46,46,46,46	0
56	MG	AA	3117	1/1	0.91	0.14	66,66,66,66	0
56	MG	DA	3482	1/1	0.91	0.15	42,42,42,42	0
56	MG	DA	3569	1/1	0.91	0.11	75,75,75,75	0
56	MG	BA	3623	1/1	0.91	0.15	59,59,59,59	0
56	MG	AA	3197	1/1	0.91	0.11	64,64,64,64	0
56	MG	AA	3038	1/1	0.91	0.25	56,56,56,56	0
56	MG	BA	3279	1/1	0.91	0.14	52,52,52,52	0
56	MG	AA	3084	1/1	0.91	0.12	53,53,53,53	0
56	MG	BA	3621	1/1	0.91	0.26	48,48,48,48	0
56	MG	BA	3572	1/1	0.91	0.13	55,55,55,55	0
56	MG	DA	3219	1/1	0.91	0.10	35,35,35,35	0
56	MG	CA	3013	1/1	0.91	0.14	52,52,52,52	0
56	MG	BA	3019	1/1	0.91	0.31	38,38,38,38	0
56	MG	DA	3025	1/1	0.91	0.71	49,49,49,49	0
56	MG	AA	3190	1/1	0.91	0.08	61,61,61,61	0
56	MG	B0	103	1/1	0.91	0.14	61,61,61,61	0
56	MG	DA	3203	1/1	0.91	0.18	46,46,46,46	0
56	MG	DA	3397	1/1	0.91	0.12	50,50,50,50	0
56	MG	BA	3036	1/1	0.91	0.21	50,50,50,50	0
56	MG	DA	3517	1/1	0.91	0.29	60,60,60,60	0
56	MG	DA	3182	1/1	0.91	0.11	52,52,52,52	0
56	MG	AA	3170	1/1	0.91	0.07	66,66,66,66	0
56	MG	CA	3120	1/1	0.91	0.12	70,70,70,70	0
56	MG	BA	3225	1/1	0.91	0.17	43,43,43,43	0
56	MG	BA	3504	1/1	0.91	0.23	57,57,57,57	0
56	MG	BA	3111	1/1	0.91	0.31	45,45,45,45	0
56	MG	BA	3522	1/1	0.91	0.25	59,59,59,59	0
56	MG	AA	3153	1/1	0.91	0.19	44,44,44,44	0
56	MG	BA	3468	1/1	0.91	0.14	31,31,31,31	0
56	MG	AA	3137	1/1	0.91	0.16	49,49,49,49	0
56	MG	BA	3477	1/1	0.91	0.20	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	3565	1/1	0.91	0.16	48,48,48,48	0
56	MG	AA	3194	1/1	0.91	0.07	66,66,66,66	0
56	MG	DA	3386	1/1	0.91	0.14	59,59,59,59	0
56	MG	BA	3260	1/1	0.91	0.28	52,52,52,52	0
56	MG	BA	3490	1/1	0.91	0.07	66,66,66,66	0
56	MG	DA	3308	1/1	0.91	0.25	57,57,57,57	0
56	MG	BA	3335	1/1	0.91	0.12	50,50,50,50	0
56	MG	CA	3014	1/1	0.91	0.09	46,46,46,46	0
56	MG	CA	3062	1/1	0.91	0.22	65,65,65,65	0
56	MG	DB	3011	1/1	0.91	0.14	49,49,49,49	0
56	MG	AA	3156	1/1	0.91	0.08	65,65,65,65	0
56	MG	DA	3542	1/1	0.91	0.12	65,65,65,65	0
56	MG	BA	3683	1/1	0.92	0.19	50,50,50,50	0
56	MG	BA	3667	1/1	0.92	0.12	64,64,64,64	0
56	MG	BA	3068	1/1	0.92	0.77	56,56,56,56	0
56	MG	DA	3622	1/1	0.92	0.37	61,61,61,61	0
56	MG	BA	3252	1/1	0.92	0.27	61,61,61,61	0
56	MG	BA	3437	1/1	0.92	0.10	55,55,55,55	0
56	MG	BR	201	1/1	0.92	0.55	40,40,40,40	0
56	MG	AX	3005	1/1	0.92	0.12	66,66,66,66	0
56	MG	DA	3013	1/1	0.92	0.14	49,49,49,49	0
56	MG	DB	3009	1/1	0.92	0.12	70,70,70,70	0
56	MG	DD	302	1/1	0.92	0.44	40,40,40,40	0
56	MG	DA	3452	1/1	0.92	0.15	44,44,44,44	0
56	MG	BA	3562	1/1	0.92	0.42	37,37,37,37	0
56	MG	AA	3090	1/1	0.92	0.28	50,50,50,50	0
56	MG	BA	3202	1/1	0.92	0.25	41,41,41,41	0
56	MG	BA	3671	1/1	0.92	0.17	33,33,33,33	0
56	MG	BA	3402	1/1	0.92	0.19	67,67,67,67	0
56	MG	BF	306	1/1	0.92	0.47	41,41,41,41	0
56	MG	BA	3102	1/1	0.92	0.35	47,47,47,47	0
56	MG	BA	3690	1/1	0.92	0.16	44,44,44,44	0
56	MG	BA	3686	1/1	0.92	0.12	61,61,61,61	0
56	MG	DA	3325	1/1	0.92	0.13	32,32,32,32	0
56	MG	AA	3198	1/1	0.92	0.13	82,82,82,82	0
56	MG	BA	3140	1/1	0.92	0.52	41,41,41,41	0
56	MG	AA	3210	1/1	0.92	0.10	65,65,65,65	0
56	MG	DA	3248	1/1	0.92	0.10	39,39,39,39	0
56	MG	AA	3116	1/1	0.92	0.14	57,57,57,57	0
56	MG	B8	101	1/1	0.92	0.19	35,35,35,35	0
56	MG	DA	3345	1/1	0.92	0.10	57,57,57,57	0
56	MG	DA	3465	1/1	0.92	0.23	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	AA	3023	1/1	0.92	0.13	51,51,51,51	0
56	MG	BA	3192	1/1	0.92	0.32	56,56,56,56	0
56	MG	AA	3163	1/1	0.92	0.20	53,53,53,53	0
56	MG	B3	3002	1/1	0.92	0.13	65,65,65,65	0
56	MG	DA	3613	1/1	0.92	0.10	57,57,57,57	0
56	MG	BX	102	1/1	0.92	0.29	40,40,40,40	0
56	MG	DA	3002	1/1	0.92	0.13	51,51,51,51	0
56	MG	BA	3712	1/1	0.92	0.13	35,35,35,35	0
56	MG	BA	3003	1/1	0.92	0.26	43,43,43,43	0
56	MG	DQ	3002	1/1	0.92	0.13	50,50,50,50	0
56	MG	DA	3172	1/1	0.92	0.18	56,56,56,56	0
56	MG	BA	3681	1/1	0.92	0.22	47,47,47,47	0
56	MG	DA	3609	1/1	0.92	0.14	47,47,47,47	0
56	MG	BA	3355	1/1	0.92	0.17	26,26,26,26	0
56	MG	CA	3084	1/1	0.92	0.12	46,46,46,46	0
56	MG	CA	3168	1/1	0.92	0.26	62,62,62,62	0
56	MG	BA	3498	1/1	0.92	0.05	70,70,70,70	0
56	MG	DA	3489	1/1	0.92	0.07	53,53,53,53	0
56	MG	BA	3381	1/1	0.92	0.17	33,33,33,33	0
56	MG	BA	3339	1/1	0.92	0.16	31,31,31,31	0
56	MG	CA	3118	1/1	0.92	0.21	61,61,61,61	0
56	MG	BA	3473	1/1	0.92	0.21	31,31,31,31	0
56	MG	B5	102	1/1	0.92	0.57	42,42,42,42	0
56	MG	BA	3366	1/1	0.92	0.16	23,23,23,23	0
56	MG	CA	3180	1/1	0.92	0.12	61,61,61,61	0
56	MG	DA	3530	1/1	0.92	0.22	69,69,69,69	0
56	MG	DA	3009	1/1	0.92	0.11	46,46,46,46	0
56	MG	BA	3570	1/1	0.92	0.18	57,57,57,57	0
56	MG	BA	3333	1/1	0.92	0.11	39,39,39,39	0
56	MG	BA	3160	1/1	0.92	0.65	58,58,58,58	0
56	MG	DA	3580	1/1	0.92	0.09	44,44,44,44	0
56	MG	BA	3735	1/1	0.92	0.13	41,41,41,41	0
56	MG	DA	3011	1/1	0.92	0.13	46,46,46,46	0
56	MG	CA	3093	1/1	0.92	0.09	57,57,57,57	0
56	MG	DA	3333	1/1	0.92	0.07	53,53,53,53	0
56	MG	DA	3328	1/1	0.92	0.17	49,49,49,49	0
56	MG	DA	3289	1/1	0.92	0.17	23,23,23,23	0
56	MG	DB	3010	1/1	0.92	0.23	72,72,72,72	0
56	MG	DA	3294	1/1	0.92	0.08	53,53,53,53	0
56	MG	BA	3746	1/1	0.92	0.10	71,71,71,71	0
56	MG	AA	3150	1/1	0.92	0.20	58,58,58,58	0
56	MG	DA	3597	1/1	0.92	0.24	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	DA	3582	1/1	0.92	0.15	65,65,65,65	0
56	MG	AA	3141	1/1	0.92	0.18	67,67,67,67	0
56	MG	CA	3017	1/1	0.92	0.27	53,53,53,53	0
56	MG	D8	5001	1/1	0.92	0.16	52,52,52,52	0
56	MG	DA	3561	1/1	0.92	0.18	65,65,65,65	0
56	MG	AN	504	1/1	0.92	0.20	56,56,56,56	0
56	MG	BA	3450	1/1	0.92	0.15	59,59,59,59	0
56	MG	BA	3249	1/1	0.92	0.20	33,33,33,33	0
56	MG	BE	308	1/1	0.92	0.12	34,34,34,34	0
56	MG	BA	3363	1/1	0.92	0.15	53,53,53,53	0
56	MG	BA	3677	1/1	0.92	0.21	63,63,63,63	0
56	MG	AA	3152	1/1	0.92	0.09	63,63,63,63	0
56	MG	BY	502	1/1	0.92	0.15	60,60,60,60	0
56	MG	DA	3369	1/1	0.92	0.19	47,47,47,47	0
56	MG	BA	3399	1/1	0.92	0.25	62,62,62,62	0
56	MG	DA	3481	1/1	0.92	0.16	51,51,51,51	0
56	MG	BA	3035	1/1	0.92	0.22	25,25,25,25	0
56	MG	DA	3332	1/1	0.92	0.13	46,46,46,46	0
56	MG	DA	3106	1/1	0.92	0.26	56,56,56,56	0
56	MG	DA	3082	1/1	0.92	0.08	48,48,48,48	0
56	MG	BA	3113	1/1	0.92	0.94	44,44,44,44	0
56	MG	BA	3061	1/1	0.92	0.32	48,48,48,48	0
56	MG	AA	3171	1/1	0.92	0.15	56,56,56,56	0
56	MG	DA	3435	1/1	0.92	0.25	59,59,59,59	0
56	MG	DA	3612	1/1	0.92	0.57	38,38,38,38	0
56	MG	DA	3338	1/1	0.92	0.10	60,60,60,60	0
56	MG	AA	3145	1/1	0.92	0.23	36,36,36,36	0
56	MG	BA	3185	1/1	0.92	0.30	38,38,38,38	0
56	MG	DA	3419	1/1	0.92	0.07	59,59,59,59	0
56	MG	DA	3483	1/1	0.92	0.07	64,64,64,64	0
56	MG	BA	3560	1/1	0.92	0.25	47,47,47,47	0
56	MG	BA	3142	1/1	0.92	0.32	47,47,47,47	0
56	MG	AA	3007	1/1	0.92	0.23	49,49,49,49	0
56	MG	BA	3568	1/1	0.92	0.20	39,39,39,39	0
56	MG	CA	3081	1/1	0.92	0.11	51,51,51,51	0
56	MG	BE	307	1/1	0.92	0.08	71,71,71,71	0
56	MG	BA	3088	1/1	0.92	0.40	46,46,46,46	0
56	MG	BA	3361	1/1	0.92	0.17	29,29,29,29	0
56	MG	AA	3046	1/1	0.92	0.21	50,50,50,50	0
56	MG	AA	3006	1/1	0.92	0.23	57,57,57,57	0
56	MG	BA	3412	1/1	0.92	0.15	50,50,50,50	0
56	MG	AA	3184	1/1	0.92	0.09	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3722	1/1	0.92	0.12	46,46,46,46	0
56	MG	BA	3294	1/1	0.92	0.16	45,45,45,45	0
56	MG	DA	3044	1/1	0.92	0.25	60,60,60,60	0
56	MG	DA	3134	1/1	0.92	0.26	60,60,60,60	0
56	MG	BA	3297	1/1	0.92	0.16	45,45,45,45	0
56	MG	AA	3009	1/1	0.92	0.23	64,64,64,64	0
56	MG	DA	3574	1/1	0.92	0.13	68,68,68,68	0
56	MG	BA	3705	1/1	0.92	0.16	52,52,52,52	0
56	MG	BA	3309	1/1	0.92	0.15	41,41,41,41	0
56	MG	DA	3150	1/1	0.92	0.17	49,49,49,49	0
56	MG	DB	3004	1/1	0.92	0.14	54,54,54,54	0
56	MG	DA	3225	1/1	0.92	0.15	56,56,56,56	0
56	MG	BA	3409	1/1	0.92	0.15	43,43,43,43	0
56	MG	AA	3134	1/1	0.92	0.17	73,73,73,73	0
56	MG	CA	3159	1/1	0.92	0.17	60,60,60,60	0
56	MG	BA	3044	1/1	0.92	0.14	39,39,39,39	0
56	MG	BA	3215	1/1	0.92	0.15	47,47,47,47	0
56	MG	AA	3177	1/1	0.92	0.22	66,66,66,66	0
56	MG	BA	3374	1/1	0.92	0.19	34,34,34,34	0
56	MG	BA	3764	1/1	0.92	0.17	26,26,26,26	0
56	MG	DW	3001	1/1	0.92	0.52	45,45,45,45	0
56	MG	BA	3567	1/1	0.92	0.09	35,35,35,35	0
56	MG	DA	3116	1/1	0.92	0.08	58,58,58,58	0
56	MG	DA	3523	1/1	0.92	0.33	62,62,62,62	0
56	MG	DA	3395	1/1	0.92	0.21	40,40,40,40	0
56	MG	BA	3483	1/1	0.92	0.19	50,50,50,50	0
56	MG	DA	3130	1/1	0.92	0.23	52,52,52,52	0
56	MG	BA	3090	1/1	0.92	0.23	40,40,40,40	0
56	MG	DA	3140	1/1	0.92	0.20	36,36,36,36	0
56	MG	BA	3557	1/1	0.92	0.11	58,58,58,58	0
56	MG	DA	3068	1/1	0.92	0.34	52,52,52,52	0
56	MG	BA	3781	1/1	0.92	0.23	42,42,42,42	0
56	MG	AA	3149	1/1	0.92	0.08	71,71,71,71	0
56	MG	CA	3079	1/1	0.92	0.12	61,61,61,61	0
56	MG	CA	3046	1/1	0.92	0.22	68,68,68,68	0
56	MG	CA	3111	1/1	0.92	0.12	69,69,69,69	0
56	MG	DA	3223	1/1	0.92	0.14	63,63,63,63	0
56	MG	BA	3032	1/1	0.92	0.22	32,32,32,32	0
56	MG	BA	3146	1/1	0.92	0.17	36,36,36,36	0
56	MG	BB	3013	1/1	0.93	0.24	46,46,46,46	0
56	MG	DA	3177	1/1	0.93	0.23	54,54,54,54	0
56	MG	DA	3003	1/1	0.93	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3304	1/1	0.93	0.18	21,21,21,21	0
60	K	AX	3001	1/1	0.93	0.28	73,73,73,73	0
56	MG	BA	3240	1/1	0.93	0.19	43,43,43,43	0
56	MG	BA	3391	1/1	0.93	0.13	36,36,36,36	0
56	MG	DA	3429	1/1	0.93	0.14	57,57,57,57	0
56	MG	BA	3440	1/1	0.93	0.33	41,41,41,41	0
56	MG	BA	3241	1/1	0.93	0.22	59,59,59,59	0
56	MG	DA	3441	1/1	0.93	0.10	39,39,39,39	0
56	MG	BA	3056	1/1	0.93	0.26	26,26,26,26	0
56	MG	BA	3619	1/1	0.93	0.11	49,49,49,49	0
59	ZN	D6	501	1/1	0.93	0.20	70,70,70,70	0
56	MG	BA	3353	1/1	0.93	0.16	27,27,27,27	0
56	MG	DA	3539	1/1	0.93	0.20	64,64,64,64	0
56	MG	DA	3454	1/1	0.93	0.12	47,47,47,47	0
56	MG	AW	3001	1/1	0.93	0.12	67,67,67,67	0
56	MG	CA	3087	1/1	0.93	0.17	65,65,65,65	0
56	MG	BA	3416	1/1	0.93	0.17	53,53,53,53	0
56	MG	DA	3017	1/1	0.93	0.26	46,46,46,46	0
56	MG	DA	3124	1/1	0.93	0.12	43,43,43,43	0
56	MG	BB	3012	1/1	0.93	0.10	42,42,42,42	0
56	MG	BA	3419	1/1	0.93	0.20	50,50,50,50	0
56	MG	B0	101	1/1	0.93	0.40	49,49,49,49	0
56	MG	DA	3200	1/1	0.93	0.09	52,52,52,52	0
56	MG	DA	3178	1/1	0.93	0.09	45,45,45,45	0
56	MG	BA	3159	1/1	0.93	0.14	45,45,45,45	0
56	MG	DA	3152	1/1	0.93	0.27	53,53,53,53	0
56	MG	BA	3062	1/1	0.93	0.32	35,35,35,35	0
56	MG	DA	3160	1/1	0.93	0.52	51,51,51,51	0
56	MG	CA	3110	1/1	0.93	0.19	62,62,62,62	0
56	MG	BA	3337	1/1	0.93	0.15	25,25,25,25	0
56	MG	BA	3001	1/1	0.93	0.17	23,23,23,23	0
56	MG	BA	3569	1/1	0.93	0.12	44,44,44,44	0
56	MG	DA	3055	1/1	0.93	0.12	44,44,44,44	0
56	MG	AA	3047	1/1	0.93	0.25	68,68,68,68	0
56	MG	AA	3154	1/1	0.93	0.12	67,67,67,67	0
56	MG	BA	3603	1/1	0.93	0.24	28,28,28,28	0
56	MG	BA	3313	1/1	0.93	0.13	32,32,32,32	0
56	MG	BA	3087	1/1	0.93	0.13	63,63,63,63	0
56	MG	DA	3187	1/1	0.93	0.16	41,41,41,41	0
56	MG	BA	3476	1/1	0.93	0.21	37,37,37,37	0
56	MG	BA	3663	1/1	0.93	0.16	26,26,26,26	0
56	MG	DF	305	1/1	0.93	0.45	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	AY	3002	1/1	0.93	0.13	70,70,70,70	0
56	MG	BA	3358	1/1	0.93	0.14	30,30,30,30	0
56	MG	DA	3227	1/1	0.93	0.10	47,47,47,47	0
56	MG	BA	3310	1/1	0.93	0.11	41,41,41,41	0
56	MG	BA	3765	1/1	0.93	0.15	59,59,59,59	0
56	MG	CA	3150	1/1	0.93	0.08	80,80,80,80	0
56	MG	BA	3439	1/1	0.93	0.20	15,15,15,15	0
56	MG	BA	3117	1/1	0.93	0.45	41,41,41,41	0
56	MG	BA	3528	1/1	0.93	0.16	29,29,29,29	0
56	MG	AA	3191	1/1	0.93	0.18	49,49,49,49	0
56	MG	BB	3004	1/1	0.93	0.13	64,64,64,64	0
56	MG	BA	3718	1/1	0.93	0.17	49,49,49,49	0
56	MG	BA	3643	1/1	0.93	0.47	38,38,38,38	0
56	MG	DA	3297	1/1	0.93	0.50	70,70,70,70	0
56	MG	CA	3010	1/1	0.93	0.21	60,60,60,60	0
56	MG	CA	3027	1/1	0.93	0.15	64,64,64,64	0
56	MG	CA	3029	1/1	0.93	0.15	37,37,37,37	0
56	MG	BA	3598	1/1	0.93	0.07	58,58,58,58	0
56	MG	DA	3432	1/1	0.93	0.11	43,43,43,43	0
56	MG	BA	3407	1/1	0.93	0.22	44,44,44,44	0
56	MG	DA	3264	1/1	0.93	0.12	44,44,44,44	0
56	MG	CA	3114	1/1	0.93	0.09	52,52,52,52	0
56	MG	BP	203	1/1	0.93	0.18	37,37,37,37	0
56	MG	DR	3001	1/1	0.93	0.66	55,55,55,55	0
56	MG	CA	3147	1/1	0.93	0.12	51,51,51,51	0
56	MG	DA	3393	1/1	0.93	0.19	53,53,53,53	0
56	MG	DA	3445	1/1	0.93	0.30	50,50,50,50	0
56	MG	BA	3664	1/1	0.93	0.17	25,25,25,25	0
56	MG	DA	3315	1/1	0.93	0.09	28,28,28,28	0
56	MG	BA	3141	1/1	0.93	0.42	55,55,55,55	0
56	MG	BA	3344	1/1	0.93	0.19	36,36,36,36	0
56	MG	BA	3540	1/1	0.93	0.11	28,28,28,28	0
56	MG	BA	3266	1/1	0.93	0.13	38,38,38,38	0
56	MG	DA	3165	1/1	0.93	0.18	69,69,69,69	0
56	MG	DA	3304	1/1	0.93	0.12	32,32,32,32	0
56	MG	DA	3498	1/1	0.93	0.15	66,66,66,66	0
56	MG	BA	3401	1/1	0.93	0.59	67,67,67,67	0
56	MG	BA	3442	1/1	0.93	0.14	31,31,31,31	0
56	MG	DA	3047	1/1	0.93	0.16	46,46,46,46	0
56	MG	BA	3365	1/1	0.93	0.09	47,47,47,47	0
56	MG	DA	3466	1/1	0.93	0.20	46,46,46,46	0
56	MG	DA	3033	1/1	0.93	0.19	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	3443	1/1	0.93	0.15	49,49,49,49	0
56	MG	DA	3113	1/1	0.93	0.27	51,51,51,51	0
56	MG	DA	3284	1/1	0.93	0.26	40,40,40,40	0
56	MG	DA	3251	1/1	0.93	0.33	47,47,47,47	0
56	MG	DA	3250	1/1	0.93	0.15	37,37,37,37	0
56	MG	BA	3066	1/1	0.93	0.41	40,40,40,40	0
56	MG	AA	3048	1/1	0.93	0.14	55,55,55,55	0
56	MG	CA	3129	1/1	0.93	0.20	49,49,49,49	0
56	MG	BA	3254	1/1	0.93	0.11	56,56,56,56	0
56	MG	BA	3465	1/1	0.93	0.21	20,20,20,20	0
56	MG	BA	3713	1/1	0.93	0.21	68,68,68,68	0
56	MG	AA	3033	1/1	0.93	0.31	45,45,45,45	0
56	MG	AA	3224	1/1	0.93	0.19	61,61,61,61	0
56	MG	AA	3043	1/1	0.93	0.11	62,62,62,62	0
56	MG	DA	3007	1/1	0.93	0.17	53,53,53,53	0
56	MG	DA	3406	1/1	0.93	0.20	48,48,48,48	0
56	MG	AA	3165	1/1	0.93	0.14	51,51,51,51	0
56	MG	DA	3185	1/1	0.93	0.24	53,53,53,53	0
56	MG	DA	3275	1/1	0.93	0.13	51,51,51,51	0
56	MG	BA	3584	1/1	0.93	0.20	47,47,47,47	0
56	MG	BA	3459	1/1	0.93	0.21	56,56,56,56	0
56	MG	AA	3080	1/1	0.93	0.26	58,58,58,58	0
56	MG	CA	3060	1/1	0.93	0.15	58,58,58,58	0
56	MG	BA	3203	1/1	0.93	0.30	51,51,51,51	0
56	MG	DA	3400	1/1	0.93	0.13	61,61,61,61	0
56	MG	BA	3100	1/1	0.93	0.35	46,46,46,46	0
56	MG	BA	3264	1/1	0.93	0.19	19,19,19,19	0
56	MG	DA	3100	1/1	0.93	0.16	45,45,45,45	0
56	MG	BA	3040	1/1	0.93	0.13	60,60,60,60	0
56	MG	BA	3041	1/1	0.93	0.26	51,51,51,51	0
56	MG	CA	3048	1/1	0.93	0.25	54,54,54,54	0
56	MG	CA	3154	1/1	0.93	0.14	62,62,62,62	0
56	MG	DA	3545	1/1	0.93	0.13	68,68,68,68	0
56	MG	BA	3581	1/1	0.93	0.14	47,47,47,47	0
56	MG	BA	3460	1/1	0.93	0.42	45,45,45,45	0
56	MG	CA	3074	1/1	0.93	0.09	62,62,62,62	0
56	MG	BA	3332	1/1	0.93	0.20	48,48,48,48	0
56	MG	DA	3475	1/1	0.93	0.16	32,32,32,32	0
56	MG	BA	3048	1/1	0.93	0.14	56,56,56,56	0
56	MG	D5	502	1/1	0.93	0.54	50,50,50,50	0
56	MG	BA	3387	1/1	0.93	0.29	43,43,43,43	0
56	MG	BA	3485	1/1	0.93	0.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3594	1/1	0.93	0.14	52,52,52,52	0
56	MG	AA	3138	1/1	0.93	0.08	73,73,73,73	0
56	MG	BG	3001	1/1	0.93	0.19	42,42,42,42	0
56	MG	BA	3063	1/1	0.93	0.15	39,39,39,39	0
56	MG	DE	304	1/1	0.93	0.14	45,45,45,45	0
56	MG	CA	3038	1/1	0.93	0.13	31,31,31,31	0
56	MG	CA	3141	1/1	0.93	0.20	61,61,61,61	0
56	MG	AA	3070	1/1	0.93	0.12	31,31,31,31	0
56	MG	DA	3019	1/1	0.93	0.11	40,40,40,40	0
56	MG	BA	3627	1/1	0.93	0.20	52,52,52,52	0
56	MG	AA	3029	1/1	0.93	0.15	60,60,60,60	0
56	MG	DD	301	1/1	0.93	0.22	44,44,44,44	0
56	MG	DA	3171	1/1	0.93	0.16	41,41,41,41	0
56	MG	DA	3430	1/1	0.93	0.10	51,51,51,51	0
56	MG	BB	3014	1/1	0.93	0.16	39,39,39,39	0
56	MG	BA	3771	1/1	0.93	0.10	73,73,73,73	0
56	MG	BA	3760	1/1	0.93	0.12	78,78,78,78	0
56	MG	BA	3124	1/1	0.93	0.26	33,33,33,33	0
56	MG	BV	207	1/1	0.93	0.30	42,42,42,42	0
56	MG	CA	3133	1/1	0.93	0.22	67,67,67,67	0
56	MG	DA	3548	1/1	0.93	0.13	67,67,67,67	0
56	MG	CA	3067	1/1	0.93	0.20	57,57,57,57	0
56	MG	AA	3010	1/1	0.93	0.14	22,22,22,22	0
56	MG	BN	3004	1/1	0.93	0.78	60,60,60,60	0
56	MG	BA	3372	1/1	0.93	0.20	33,33,33,33	0
56	MG	DA	3479	1/1	0.93	0.12	52,52,52,52	0
56	MG	AA	3039	1/1	0.93	0.19	57,57,57,57	0
56	MG	BF	307	1/1	0.93	0.20	46,46,46,46	0
56	MG	BA	3158	1/1	0.93	0.19	47,47,47,47	0
56	MG	BA	3702	1/1	0.93	0.18	60,60,60,60	0
56	MG	BA	3685	1/1	0.93	0.22	43,43,43,43	0
56	MG	DA	3329	1/1	0.93	0.09	62,62,62,62	0
57	NEG	AA	3220	17/17	0.93	0.26	29,49,59,65	0
56	MG	CA	3158	1/1	0.93	0.13	72,72,72,72	0
56	MG	DA	3460	1/1	0.93	0.08	64,64,64,64	0
56	MG	BA	3491	1/1	0.93	0.16	52,52,52,52	0
56	MG	BA	3184	1/1	0.93	0.18	33,33,33,33	0
56	MG	BA	3394	1/1	0.93	0.17	53,53,53,53	0
56	MG	DE	302	1/1	0.93	0.20	30,30,30,30	0
56	MG	BB	3009	1/1	0.93	0.14	49,49,49,49	0
56	MG	DA	3088	1/1	0.93	0.17	39,39,39,39	0
56	MG	DA	3421	1/1	0.93	0.14	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3164	1/1	0.93	0.12	71,71,71,71	0
56	MG	CA	3178	1/1	0.93	0.09	54,54,54,54	0
56	MG	BA	3198	1/1	0.93	0.28	35,35,35,35	0
56	MG	CA	3047	1/1	0.93	0.28	56,56,56,56	0
56	MG	BA	3587	1/1	0.93	0.36	58,58,58,58	0
56	MG	BA	3447	1/1	0.93	0.12	38,38,38,38	0
56	MG	DU	3002	1/1	0.93	0.80	58,58,58,58	0
56	MG	BA	3710	1/1	0.93	0.15	51,51,51,51	0
56	MG	BA	3636	1/1	0.93	0.22	61,61,61,61	0
56	MG	BA	3095	1/1	0.93	0.32	39,39,39,39	0
56	MG	DA	3587	1/1	0.93	0.16	45,45,45,45	0
56	MG	BA	3367	1/1	0.93	0.11	58,58,58,58	0
56	MG	BA	3103	1/1	0.94	0.16	45,45,45,45	0
56	MG	AN	503	1/1	0.94	0.14	59,59,59,59	0
56	MG	DW	3003	1/1	0.94	0.58	71,71,71,71	0
56	MG	BA	3311	1/1	0.94	0.18	34,34,34,34	0
56	MG	DA	3111	1/1	0.94	0.11	49,49,49,49	0
56	MG	BA	3092	1/1	0.94	0.12	27,27,27,27	0
56	MG	BA	3218	1/1	0.94	0.10	52,52,52,52	0
56	MG	BA	3441	1/1	0.94	0.12	37,37,37,37	0
56	MG	BA	3590	1/1	0.94	0.18	38,38,38,38	0
56	MG	B7	102	1/1	0.94	0.47	40,40,40,40	0
56	MG	DA	3120	1/1	0.94	0.18	42,42,42,42	0
56	MG	DA	3446	1/1	0.94	0.18	52,52,52,52	0
56	MG	CA	3153	1/1	0.94	0.24	62,62,62,62	0
56	MG	BA	3443	1/1	0.94	0.15	50,50,50,50	0
56	MG	AA	3005	1/1	0.94	0.36	55,55,55,55	0
56	MG	BA	3615	1/1	0.94	0.72	41,41,41,41	0
56	MG	BA	3047	1/1	0.94	0.13	51,51,51,51	0
56	MG	BF	301	1/1	0.94	0.41	39,39,39,39	0
56	MG	DA	3492	1/1	0.94	0.43	51,51,51,51	0
56	MG	DA	3559	1/1	0.94	0.09	49,49,49,49	0
56	MG	DA	3527	1/1	0.94	0.17	67,67,67,67	0
56	MG	AA	3160	1/1	0.94	0.22	70,70,70,70	0
56	MG	DA	3355	1/1	0.94	0.12	53,53,53,53	0
56	MG	DA	3407	1/1	0.94	0.24	41,41,41,41	0
56	MG	BA	3551	1/1	0.94	0.15	56,56,56,56	0
56	MG	DA	3217	1/1	0.94	0.12	43,43,43,43	0
56	MG	CA	3163	1/1	0.94	0.15	49,49,49,49	0
56	MG	BN	3006	1/1	0.94	0.63	54,54,54,54	0
56	MG	DA	3056	1/1	0.94	0.08	51,51,51,51	0
56	MG	AA	3157	1/1	0.94	0.16	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	BA	3566	1/1	0.94	0.15	28,28,28,28	0
56	MG	CA	3076	1/1	0.94	0.15	54,54,54,54	0
56	MG	AA	3205	1/1	0.94	0.07	66,66,66,66	0
56	MG	DA	3570	1/1	0.94	0.10	62,62,62,62	0
56	MG	AA	3073	1/1	0.94	0.23	60,60,60,60	0
56	MG	BA	3352	1/1	0.94	0.15	22,22,22,22	0
56	MG	CW	3001	1/1	0.94	0.65	69,69,69,69	0
56	MG	BA	3110	1/1	0.94	0.72	49,49,49,49	0
56	MG	DA	3295	1/1	0.94	0.18	34,34,34,34	0
56	MG	AW	3002	1/1	0.94	0.20	54,54,54,54	0
56	MG	BA	3287	1/1	0.94	0.14	21,21,21,21	0
56	MG	AA	3083	1/1	0.94	0.17	57,57,57,57	0
56	MG	BA	3573	1/1	0.94	0.13	53,53,53,53	0
56	MG	CA	3063	1/1	0.94	0.18	59,59,59,59	0
56	MG	BA	3172	1/1	0.94	0.30	58,58,58,58	0
56	MG	DA	3469	1/1	0.94	0.05	56,56,56,56	0
56	MG	DA	3196	1/1	0.94	0.14	49,49,49,49	0
56	MG	BA	3326	1/1	0.94	0.09	50,50,50,50	0
56	MG	BB	3006	1/1	0.94	0.13	46,46,46,46	0
56	MG	BA	3509	1/1	0.94	0.16	46,46,46,46	0
56	MG	BA	3469	1/1	0.94	0.18	49,49,49,49	0
56	MG	AA	3013	1/1	0.94	0.12	66,66,66,66	0
56	MG	DA	3128	1/1	0.94	0.22	45,45,45,45	0
56	MG	BQ	3001	1/1	0.94	0.98	52,52,52,52	0
56	MG	BA	3383	1/1	0.94	0.21	49,49,49,49	0
56	MG	DA	3228	1/1	0.94	0.15	29,29,29,29	0
56	MG	AA	3139	1/1	0.94	0.20	50,50,50,50	0
56	MG	DA	3129	1/1	0.94	0.15	42,42,42,42	0
56	MG	DA	3018	1/1	0.94	0.15	29,29,29,29	0
56	MG	BA	3499	1/1	0.94	0.12	57,57,57,57	0
56	MG	AA	3161	1/1	0.94	0.07	59,59,59,59	0
56	MG	AA	3060	1/1	0.94	0.14	42,42,42,42	0
56	MG	D7	101	1/1	0.94	0.48	33,33,33,33	0
56	MG	BA	3687	1/1	0.94	0.18	56,56,56,56	0
56	MG	BA	3624	1/1	0.94	0.11	50,50,50,50	0
56	MG	BA	3271	1/1	0.94	0.26	39,39,39,39	0
56	MG	BA	3428	1/1	0.94	0.22	42,42,42,42	0
56	MG	BA	3152	1/1	0.94	0.19	48,48,48,48	0
56	MG	DA	3136	1/1	0.94	0.15	35,35,35,35	0
56	MG	DA	3186	1/1	0.94	0.47	41,41,41,41	0
56	MG	DA	3076	1/1	0.94	0.20	34,34,34,34	0
56	MG	CA	3098	1/1	0.94	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3535	1/1	0.94	0.16	46,46,46,46	0
56	MG	DA	3043	1/1	0.94	0.16	49,49,49,49	0
56	MG	BA	3093	1/1	0.94	0.23	39,39,39,39	0
56	MG	BA	3053	1/1	0.94	0.15	56,56,56,56	0
56	MG	DA	3368	1/1	0.94	0.17	48,48,48,48	0
56	MG	BA	3640	1/1	0.94	0.11	61,61,61,61	0
56	MG	BA	3552	1/1	0.94	0.18	32,32,32,32	0
56	MG	DA	3618	1/1	0.94	0.10	57,57,57,57	0
56	MG	DA	3102	1/1	0.94	0.10	50,50,50,50	0
56	MG	DA	3220	1/1	0.94	0.08	45,45,45,45	0
56	MG	CA	3135	1/1	0.94	0.43	75,75,75,75	0
56	MG	B7	103	1/1	0.94	0.15	69,69,69,69	0
56	MG	CA	3035	1/1	0.94	0.29	52,52,52,52	0
56	MG	AA	3024	1/1	0.94	0.11	49,49,49,49	0
56	MG	CA	3103	1/1	0.94	0.20	78,78,78,78	0
56	MG	DA	3290	1/1	0.94	0.20	36,36,36,36	0
56	MG	DA	3215	1/1	0.94	0.22	53,53,53,53	0
56	MG	BA	3265	1/1	0.94	0.25	55,55,55,55	0
56	MG	BA	3064	1/1	0.94	0.34	46,46,46,46	0
56	MG	BA	3316	1/1	0.94	0.20	58,58,58,58	0
56	MG	CA	3086	1/1	0.94	0.20	53,53,53,53	0
56	MG	DA	3354	1/1	0.94	0.10	56,56,56,56	0
56	MG	BU	205	1/1	0.94	0.63	39,39,39,39	0
56	MG	DA	3411	1/1	0.94	0.41	43,43,43,43	0
56	MG	AA	3077	1/1	0.94	0.06	69,69,69,69	0
56	MG	DA	3600	1/1	0.94	0.24	55,55,55,55	0
56	MG	BA	3171	1/1	0.94	0.10	58,58,58,58	0
56	MG	CA	3102	1/1	0.94	0.11	48,48,48,48	0
56	MG	AA	3085	1/1	0.94	0.12	63,63,63,63	0
56	MG	DA	3343	1/1	0.94	0.11	57,57,57,57	0
56	MG	BA	3470	1/1	0.94	0.24	46,46,46,46	0
56	MG	DA	3229	1/1	0.94	0.16	49,49,49,49	0
56	MG	BA	3014	1/1	0.94	0.17	46,46,46,46	0
56	MG	DA	3529	1/1	0.94	0.11	55,55,55,55	0
56	MG	DA	3146	1/1	0.94	0.13	50,50,50,50	0
56	MG	BA	3481	1/1	0.94	0.18	32,32,32,32	0
56	MG	BA	3008	1/1	0.94	0.23	27,27,27,27	0
56	MG	DA	3571	1/1	0.94	0.14	49,49,49,49	0
56	MG	AA	3067	1/1	0.94	0.31	53,53,53,53	0
56	MG	BV	202	1/1	0.94	0.40	34,34,34,34	0
56	MG	DA	3623	1/1	0.94	0.66	48,48,48,48	0
56	MG	BA	3149	1/1	0.94	0.19	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	3022	1/1	0.94	0.11	53,53,53,53	0
56	MG	DA	3031	1/1	0.94	0.21	51,51,51,51	0
56	MG	DA	3480	1/1	0.94	0.19	48,48,48,48	0
56	MG	BA	3105	1/1	0.94	0.30	43,43,43,43	0
56	MG	AA	3211	1/1	0.94	0.23	41,41,41,41	0
56	MG	DA	3607	1/1	0.94	0.05	60,60,60,60	0
56	MG	DA	3174	1/1	0.94	0.10	42,42,42,42	0
56	MG	BA	3025	1/1	0.94	0.33	37,37,37,37	0
56	MG	BA	3052	1/1	0.94	0.20	34,34,34,34	0
56	MG	BA	3644	1/1	0.94	0.31	34,34,34,34	0
56	MG	BW	202	1/1	0.94	0.18	43,43,43,43	0
56	MG	B5	101	1/1	0.94	0.62	42,42,42,42	0
56	MG	BA	3405	1/1	0.94	0.15	47,47,47,47	0
56	MG	DA	3245	1/1	0.94	0.13	28,28,28,28	0
56	MG	AA	3212	1/1	0.94	0.15	33,33,33,33	0
56	MG	AA	3147	1/1	0.94	0.09	47,47,47,47	0
56	MG	AA	3169	1/1	0.94	0.11	57,57,57,57	0
56	MG	DA	3324	1/1	0.94	0.19	46,46,46,46	0
56	MG	DA	3143	1/1	0.94	0.13	35,35,35,35	0
56	MG	DA	3232	1/1	0.94	0.09	57,57,57,57	0
56	MG	BW	201	1/1	0.94	0.20	45,45,45,45	0
56	MG	BA	3055	1/1	0.94	0.22	30,30,30,30	0
56	MG	DA	3394	1/1	0.94	0.11	50,50,50,50	0
56	MG	BA	3754	1/1	0.94	0.21	36,36,36,36	0
56	MG	DA	3459	1/1	0.94	0.11	63,63,63,63	0
56	MG	AA	3118	1/1	0.94	0.12	40,40,40,40	0
56	MG	DA	3293	1/1	0.94	0.13	59,59,59,59	0
56	MG	DA	3347	1/1	0.94	0.15	53,53,53,53	0
56	MG	AA	3054	1/1	0.94	0.17	46,46,46,46	0
56	MG	DA	3536	1/1	0.94	0.14	39,39,39,39	0
56	MG	BA	3780	1/1	0.94	0.52	45,45,45,45	0
56	MG	BA	3114	1/1	0.94	0.61	49,49,49,49	0
59	ZN	D9	501	1/1	0.94	0.09	82,82,82,82	0
56	MG	DA	3422	1/1	0.94	0.18	52,52,52,52	0
56	MG	DA	3384	1/1	0.94	0.21	55,55,55,55	0
56	MG	BA	3565	1/1	0.94	0.12	50,50,50,50	0
56	MG	BA	3596	1/1	0.94	0.15	52,52,52,52	0
56	MG	BA	3193	1/1	0.94	0.14	24,24,24,24	0
56	MG	BA	3772	1/1	0.94	0.15	52,52,52,52	0
56	MG	DA	3558	1/1	0.94	0.35	48,48,48,48	0
56	MG	DA	3038	1/1	0.94	0.15	56,56,56,56	0
56	MG	AA	3065	1/1	0.94	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	NEG	AA	3216	17/17	0.94	0.31	34,56,70,74	0
56	MG	DA	3497	1/1	0.94	0.14	27,27,27,27	0
56	MG	DA	3238	1/1	0.94	0.11	40,40,40,40	0
56	MG	BA	3378	1/1	0.94	0.21	24,24,24,24	0
56	MG	BA	3507	1/1	0.94	0.15	53,53,53,53	0
56	MG	DA	3202	1/1	0.94	0.15	51,51,51,51	0
56	MG	BA	3479	1/1	0.94	0.27	36,36,36,36	0
56	MG	BA	3679	1/1	0.94	0.16	47,47,47,47	0
56	MG	DA	3418	1/1	0.94	0.11	55,55,55,55	0
56	MG	DA	3511	1/1	0.94	0.12	62,62,62,62	0
56	MG	DF	306	1/1	0.94	1.20	55,55,55,55	0
56	MG	DA	3434	1/1	0.94	0.31	46,46,46,46	0
56	MG	BA	3425	1/1	0.94	0.13	31,31,31,31	0
56	MG	DA	3337	1/1	0.94	0.13	42,42,42,42	0
56	MG	BU	202	1/1	0.94	0.45	32,32,32,32	0
56	MG	BA	3246	1/1	0.94	0.15	57,57,57,57	0
56	MG	DA	3555	1/1	0.94	0.22	48,48,48,48	0
56	MG	BV	205	1/1	0.94	0.71	37,37,37,37	0
56	MG	BA	3696	1/1	0.94	0.12	38,38,38,38	0
56	MG	BA	3151	1/1	0.94	0.36	51,51,51,51	0
56	MG	DA	3273	1/1	0.94	0.17	36,36,36,36	0
56	MG	CY	3001	1/1	0.94	0.15	63,63,63,63	0
56	MG	CD	301	1/1	0.94	0.12	67,67,67,67	0
56	MG	BA	3285	1/1	0.94	0.20	55,55,55,55	0
56	MG	BA	3697	1/1	0.94	0.13	34,34,34,34	0
56	MG	DA	3447	1/1	0.94	0.17	49,49,49,49	0
56	MG	BA	3563	1/1	0.94	0.20	43,43,43,43	0
56	MG	DA	3451	1/1	0.94	0.23	56,56,56,56	0
56	MG	DA	3305	1/1	0.94	0.16	42,42,42,42	0
56	MG	BA	3377	1/1	0.94	0.20	39,39,39,39	0
56	MG	BA	3777	1/1	0.94	0.55	40,40,40,40	0
56	MG	AA	3180	1/1	0.94	0.12	67,67,67,67	0
56	MG	CA	3006	1/1	0.94	0.27	50,50,50,50	0
56	MG	BA	3602	1/1	0.94	0.11	61,61,61,61	0
56	MG	BA	3431	1/1	0.94	0.15	54,54,54,54	0
56	MG	DA	3524	1/1	0.94	0.09	58,58,58,58	0
56	MG	DA	3258	1/1	0.94	0.10	24,24,24,24	0
56	MG	DA	3361	1/1	0.94	0.35	45,45,45,45	0
56	MG	BA	3350	1/1	0.94	0.11	43,43,43,43	0
56	MG	DA	3449	1/1	0.94	0.34	49,49,49,49	0
56	MG	DA	3162	1/1	0.94	0.39	45,45,45,45	0
56	MG	BB	3017	1/1	0.94	0.14	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	3182	1/1	0.94	0.20	76,76,76,76	0
56	MG	CA	3117	1/1	0.94	0.18	71,71,71,71	0
56	MG	BA	3691	1/1	0.94	0.09	60,60,60,60	0
56	MG	BA	3424	1/1	0.94	0.22	51,51,51,51	0
56	MG	DA	3285	1/1	0.94	0.12	43,43,43,43	0
56	MG	CA	3072	1/1	0.94	0.17	57,57,57,57	0
56	MG	DA	3256	1/1	0.94	0.17	48,48,48,48	0
56	MG	BA	3688	1/1	0.94	0.12	24,24,24,24	0
56	MG	BA	3698	1/1	0.94	0.10	59,59,59,59	0
56	MG	DA	3611	1/1	0.94	0.09	53,53,53,53	0
56	MG	BA	3614	1/1	0.94	0.14	54,54,54,54	0
56	MG	AA	3151	1/1	0.95	0.18	65,65,65,65	0
56	MG	D3	3001	1/1	0.95	0.61	70,70,70,70	0
56	MG	DA	3201	1/1	0.95	0.17	56,56,56,56	0
56	MG	DA	3560	1/1	0.95	0.49	59,59,59,59	0
56	MG	DA	3035	1/1	0.95	0.17	39,39,39,39	0
56	MG	DA	3137	1/1	0.95	0.13	57,57,57,57	0
56	MG	CX	3003	1/1	0.95	0.19	64,64,64,64	0
56	MG	BA	3371	1/1	0.95	0.19	50,50,50,50	0
56	MG	BA	3319	1/1	0.95	0.17	38,38,38,38	0
56	MG	CA	3078	1/1	0.95	0.12	41,41,41,41	0
56	MG	BA	3216	1/1	0.95	0.14	53,53,53,53	0
56	MG	AA	3207	1/1	0.95	0.13	57,57,57,57	0
56	MG	AA	3057	1/1	0.95	0.19	58,58,58,58	0
56	MG	BA	3464	1/1	0.95	0.21	53,53,53,53	0
56	MG	BA	3606	1/1	0.95	0.16	62,62,62,62	0
56	MG	BA	3727	1/1	0.95	0.09	57,57,57,57	0
56	MG	CA	3140	1/1	0.95	0.27	49,49,49,49	0
56	MG	CA	3132	1/1	0.95	0.19	54,54,54,54	0
56	MG	BF	303	1/1	0.95	0.19	36,36,36,36	0
56	MG	CA	3012	1/1	0.95	0.13	56,56,56,56	0
56	MG	DA	3181	1/1	0.95	0.28	50,50,50,50	0
56	MG	BA	3547	1/1	0.95	0.17	47,47,47,47	0
56	MG	BA	3379	1/1	0.95	0.18	22,22,22,22	0
56	MG	DA	3502	1/1	0.95	0.12	47,47,47,47	0
56	MG	DA	3064	1/1	0.95	0.22	52,52,52,52	0
56	MG	AN	502	1/1	0.95	0.22	56,56,56,56	0
56	MG	AA	3055	1/1	0.95	0.10	40,40,40,40	0
56	MG	BA	3607	1/1	0.95	0.21	45,45,45,45	0
56	MG	DA	3544	1/1	0.95	0.12	49,49,49,49	0
56	MG	BA	3354	1/1	0.95	0.27	39,39,39,39	0
56	MG	CA	3008	1/1	0.95	0.11	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	DB	3002	1/1	0.95	0.20	58,58,58,58	0
56	MG	BA	3226	1/1	0.95	0.25	32,32,32,32	0
56	MG	CA	3034	1/1	0.95	0.22	46,46,46,46	0
56	MG	DA	3014	1/1	0.95	0.11	37,37,37,37	0
56	MG	BD	307	1/1	0.95	0.38	38,38,38,38	0
56	MG	DA	3334	1/1	0.95	0.23	51,51,51,51	0
56	MG	DA	3541	1/1	0.95	0.17	46,46,46,46	0
56	MG	DA	3404	1/1	0.95	0.12	36,36,36,36	0
56	MG	DA	3083	1/1	0.95	0.50	46,46,46,46	0
56	MG	BA	3753	1/1	0.95	0.12	76,76,76,76	0
56	MG	DA	3599	1/1	0.95	0.10	72,72,72,72	0
56	MG	BA	3328	1/1	0.95	0.10	56,56,56,56	0
56	MG	DQ	3003	1/1	0.95	0.58	64,64,64,64	0
56	MG	AA	3022	1/1	0.95	0.09	58,58,58,58	0
56	MG	CA	3041	1/1	0.95	0.16	63,63,63,63	0
56	MG	BA	3518	1/1	0.95	0.17	25,25,25,25	0
56	MG	BA	3123	1/1	0.95	0.58	39,39,39,39	0
56	MG	DA	3516	1/1	0.95	0.14	35,35,35,35	0
56	MG	B0	102	1/1	0.95	0.09	54,54,54,54	0
56	MG	BA	3004	1/1	0.95	0.09	25,25,25,25	0
56	MG	BA	3564	1/1	0.95	0.15	49,49,49,49	0
56	MG	BA	3089	1/1	0.95	0.59	46,46,46,46	0
56	MG	BA	3314	1/1	0.95	0.14	41,41,41,41	0
56	MG	BF	311	1/1	0.95	0.08	60,60,60,60	0
56	MG	BA	3541	1/1	0.95	0.35	31,31,31,31	0
56	MG	DA	3299	1/1	0.95	0.12	40,40,40,40	0
59	ZN	CN	102	1/1	0.95	0.09	82,82,82,82	0
56	MG	DA	3464	1/1	0.95	0.15	51,51,51,51	0
56	MG	DA	3255	1/1	0.95	0.12	50,50,50,50	0
56	MG	BA	3028	1/1	0.95	0.55	48,48,48,48	0
56	MG	DA	3067	1/1	0.95	0.09	52,52,52,52	0
56	MG	BA	3150	1/1	0.95	0.18	47,47,47,47	0
56	MG	DA	3312	1/1	0.95	0.14	40,40,40,40	0
56	MG	BA	3169	1/1	0.95	0.18	28,28,28,28	0
56	MG	BA	3302	1/1	0.95	0.11	46,46,46,46	0
56	MG	DA	3505	1/1	0.95	0.18	41,41,41,41	0
56	MG	DA	3267	1/1	0.95	0.14	42,42,42,42	0
56	MG	BA	3474	1/1	0.95	0.17	37,37,37,37	0
56	MG	BA	3194	1/1	0.95	0.27	40,40,40,40	0
56	MG	BA	3296	1/1	0.95	0.10	47,47,47,47	0
56	MG	BA	3083	1/1	0.95	0.20	30,30,30,30	0
56	MG	CA	3043	1/1	0.95	0.14	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	DA	3383	1/1	0.95	0.20	40,40,40,40	0
56	MG	DA	3236	1/1	0.95	0.14	59,59,59,59	0
56	MG	B3	3001	1/1	0.95	0.33	41,41,41,41	0
56	MG	BA	3744	1/1	0.95	0.15	27,27,27,27	0
56	MG	DA	3062	1/1	0.95	0.31	49,49,49,49	0
56	MG	BA	3466	1/1	0.95	0.29	52,52,52,52	0
56	MG	DA	3145	1/1	0.95	0.26	61,61,61,61	0
56	MG	AA	3098	1/1	0.95	0.17	59,59,59,59	0
56	MG	CA	3128	1/1	0.95	0.08	72,72,72,72	0
56	MG	BA	3611	1/1	0.95	0.20	23,23,23,23	0
56	MG	DA	3323	1/1	0.95	0.10	44,44,44,44	0
56	MG	BE	302	1/1	0.95	0.20	28,28,28,28	0
56	MG	BA	3156	1/1	0.95	0.16	64,64,64,64	0
56	MG	DD	303	1/1	0.95	0.27	60,60,60,60	0
56	MG	BA	3578	1/1	0.95	0.15	49,49,49,49	0
56	MG	BA	3750	1/1	0.95	0.19	52,52,52,52	0
56	MG	DA	3301	1/1	0.95	0.09	60,60,60,60	0
56	MG	DA	3387	1/1	0.95	0.13	47,47,47,47	0
56	MG	AA	3053	1/1	0.95	0.15	41,41,41,41	0
56	MG	DA	3415	1/1	0.95	0.58	45,45,45,45	0
56	MG	DA	3041	1/1	0.95	0.40	51,51,51,51	0
56	MG	BA	3495	1/1	0.95	0.32	44,44,44,44	0
56	MG	BA	3513	1/1	0.95	0.17	42,42,42,42	0
56	MG	BA	3632	1/1	0.95	0.15	53,53,53,53	0
56	MG	DA	3164	1/1	0.95	0.06	58,58,58,58	0
56	MG	BA	3065	1/1	0.95	0.24	33,33,33,33	0
56	MG	BA	3413	1/1	0.95	0.19	53,53,53,53	0
56	MG	DA	3046	1/1	0.95	0.17	30,30,30,30	0
56	MG	DA	3358	1/1	0.95	0.12	51,51,51,51	0
56	MG	BF	309	1/1	0.95	0.49	40,40,40,40	0
56	MG	BA	3497	1/1	0.95	0.23	24,24,24,24	0
56	MG	BQ	3005	1/1	0.95	0.50	49,49,49,49	0
56	MG	DA	3402	1/1	0.95	0.10	57,57,57,57	0
56	MG	BA	3157	1/1	0.95	0.34	59,59,59,59	0
56	MG	BA	3711	1/1	0.95	0.13	51,51,51,51	0
56	MG	BA	3306	1/1	0.95	0.20	51,51,51,51	0
56	MG	BA	3073	1/1	0.95	0.17	25,25,25,25	0
56	MG	DA	3456	1/1	0.95	0.11	50,50,50,50	0
56	MG	DA	3410	1/1	0.95	0.09	37,37,37,37	0
56	MG	BA	3318	1/1	0.95	0.08	36,36,36,36	0
56	MG	DA	3568	1/1	0.95	0.11	61,61,61,61	0
56	MG	DA	3190	1/1	0.95	0.10	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	3296	1/1	0.95	0.14	38,38,38,38	0
56	MG	BA	3390	1/1	0.95	0.22	26,26,26,26	0
56	MG	BA	3034	1/1	0.95	0.15	34,34,34,34	0
56	MG	AA	3078	1/1	0.95	0.18	59,59,59,59	0
56	MG	CA	3157	1/1	0.95	0.13	57,57,57,57	0
56	MG	DA	3121	1/1	0.95	0.11	33,33,33,33	0
56	MG	BA	3228	1/1	0.95	0.32	51,51,51,51	0
56	MG	DA	3316	1/1	0.95	0.38	48,48,48,48	0
56	MG	AA	3162	1/1	0.95	0.08	70,70,70,70	0
56	MG	BA	3676	1/1	0.95	0.14	55,55,55,55	0
56	MG	AA	3108	1/1	0.95	0.08	59,59,59,59	0
56	MG	DA	3040	1/1	0.95	0.12	47,47,47,47	0
56	MG	DA	3617	1/1	0.95	0.38	55,55,55,55	0
56	MG	BD	310	1/1	0.95	0.29	45,45,45,45	0
56	MG	DA	3021	1/1	0.95	0.35	44,44,44,44	0
56	MG	CA	3019	1/1	0.95	0.24	45,45,45,45	0
56	MG	BA	3280	1/1	0.95	0.22	25,25,25,25	0
56	MG	BA	3133	1/1	0.95	0.29	43,43,43,43	0
56	MG	DA	3455	1/1	0.95	0.29	50,50,50,50	0
56	MG	AA	3110	1/1	0.95	0.15	53,53,53,53	0
56	MG	BA	3756	1/1	0.95	0.12	56,56,56,56	0
56	MG	BA	3348	1/1	0.95	0.24	35,35,35,35	0
56	MG	BA	3660	1/1	0.95	0.17	44,44,44,44	0
56	MG	DA	3552	1/1	0.95	0.13	43,43,43,43	0
56	MG	DA	3373	1/1	0.95	0.22	51,51,51,51	0
56	MG	BA	3486	1/1	0.95	0.21	30,30,30,30	0
56	MG	CA	3032	1/1	0.95	0.24	52,52,52,52	0
56	MG	BA	3748	1/1	0.95	0.19	63,63,63,63	0
56	MG	DA	3359	1/1	0.95	0.15	54,54,54,54	0
56	MG	BA	3668	1/1	0.95	0.29	42,42,42,42	0
56	MG	BA	3341	1/1	0.95	0.17	59,59,59,59	0
56	MG	BA	3259	1/1	0.95	0.16	32,32,32,32	0
56	MG	DA	3008	1/1	0.95	0.14	38,38,38,38	0
56	MG	BA	3057	1/1	0.95	0.57	48,48,48,48	0
56	MG	AA	3173	1/1	0.95	0.11	55,55,55,55	0
56	MG	BU	206	1/1	0.95	0.88	54,54,54,54	0
56	MG	BA	3173	1/1	0.95	0.45	46,46,46,46	0
56	MG	DA	3507	1/1	0.95	0.20	54,54,54,54	0
56	MG	BA	3163	1/1	0.95	0.19	57,57,57,57	0
56	MG	DA	3468	1/1	0.95	0.05	54,54,54,54	0
56	MG	BA	3583	1/1	0.95	0.12	46,46,46,46	0
56	MG	BA	3589	1/1	0.95	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	DA	3551	1/1	0.95	0.18	66,66,66,66	0
56	MG	DA	3141	1/1	0.95	0.32	56,56,56,56	0
56	MG	BA	3022	1/1	0.95	0.50	41,41,41,41	0
56	MG	DA	3538	1/1	0.95	0.07	50,50,50,50	0
56	MG	BA	3305	1/1	0.95	0.26	61,61,61,61	0
56	MG	DA	3360	1/1	0.95	0.20	47,47,47,47	0
56	MG	BA	3674	1/1	0.95	0.15	42,42,42,42	0
56	MG	DA	3478	1/1	0.95	0.08	54,54,54,54	0
56	MG	BA	3662	1/1	0.95	0.11	56,56,56,56	0
56	MG	BA	3397	1/1	0.95	0.15	29,29,29,29	0
56	MG	CA	3104	1/1	0.95	0.17	51,51,51,51	0
56	MG	BA	3342	1/1	0.95	0.16	43,43,43,43	0
56	MG	BA	3270	1/1	0.95	0.13	47,47,47,47	0
56	MG	BE	304	1/1	0.95	0.50	42,42,42,42	0
56	MG	BA	3286	1/1	0.95	0.08	48,48,48,48	0
56	MG	BF	305	1/1	0.95	0.46	40,40,40,40	0
56	MG	AA	3204	1/1	0.95	0.21	44,44,44,44	0
56	MG	DA	3277	1/1	0.95	0.14	52,52,52,52	0
56	MG	BA	3224	1/1	0.95	0.16	55,55,55,55	0
56	MG	DA	3477	1/1	0.95	0.18	41,41,41,41	0
56	MG	BA	3206	1/1	0.95	0.31	49,49,49,49	0
56	MG	BA	3699	1/1	0.95	0.12	39,39,39,39	0
56	MG	AA	3076	1/1	0.95	0.17	45,45,45,45	0
56	MG	AA	3129	1/1	0.95	0.06	77,77,77,77	0
56	MG	DA	3473	1/1	0.95	0.10	60,60,60,60	0
56	MG	BA	3758	1/1	0.95	0.14	38,38,38,38	0
56	MG	BA	3527	1/1	0.95	0.23	58,58,58,58	0
56	MG	AA	3097	1/1	0.95	0.17	45,45,45,45	0
56	MG	BA	3325	1/1	0.95	0.13	42,42,42,42	0
56	MG	BB	3002	1/1	0.96	0.28	51,51,51,51	0
56	MG	BA	3475	1/1	0.96	0.17	52,52,52,52	0
56	MG	DA	3370	1/1	0.96	0.14	49,49,49,49	0
56	MG	BA	3385	1/1	0.96	0.20	50,50,50,50	0
56	MG	CA	3149	1/1	0.96	0.10	61,61,61,61	0
56	MG	DA	3310	1/1	0.96	0.07	39,39,39,39	0
56	MG	BU	209	1/1	0.96	0.64	41,41,41,41	0
56	MG	DA	3155	1/1	0.96	0.15	53,53,53,53	0
56	MG	BA	3029	1/1	0.96	0.33	44,44,44,44	0
56	MG	DA	3608	1/1	0.96	0.09	47,47,47,47	0
56	MG	AW	3005	1/1	0.96	0.12	52,52,52,52	0
56	MG	BA	3380	1/1	0.96	0.18	59,59,59,59	0
56	MG	CA	3094	1/1	0.96	0.21	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	3432	1/1	0.96	0.13	48,48,48,48	0
56	MG	DA	3188	1/1	0.96	0.12	61,61,61,61	0
56	MG	DA	3364	1/1	0.96	0.20	54,54,54,54	0
56	MG	DA	3132	1/1	0.96	0.09	39,39,39,39	0
56	MG	DA	3496	1/1	0.96	0.27	51,51,51,51	0
56	MG	DA	3243	1/1	0.96	0.22	42,42,42,42	0
56	MG	DA	3026	1/1	0.96	0.11	24,24,24,24	0
56	MG	DA	3204	1/1	0.96	0.13	47,47,47,47	0
56	MG	DA	3206	1/1	0.96	0.17	45,45,45,45	0
56	MG	CA	3112	1/1	0.96	0.28	59,59,59,59	0
56	MG	BA	3745	1/1	0.96	0.16	27,27,27,27	0
56	MG	BA	3167	1/1	0.96	0.19	28,28,28,28	0
56	MG	AA	3056	1/1	0.96	0.10	56,56,56,56	0
56	MG	BF	308	1/1	0.96	0.73	40,40,40,40	0
56	MG	BP	202	1/1	0.96	0.32	36,36,36,36	0
56	MG	DA	3156	1/1	0.96	0.23	45,45,45,45	0
56	MG	BA	3393	1/1	0.96	0.17	48,48,48,48	0
56	MG	DA	3356	1/1	0.96	0.09	47,47,47,47	0
56	MG	DA	3367	1/1	0.96	0.20	44,44,44,44	0
56	MG	DA	3602	1/1	0.96	0.19	62,62,62,62	0
56	MG	DA	3461	1/1	0.96	0.14	49,49,49,49	0
56	MG	BA	3293	1/1	0.96	0.18	40,40,40,40	0
56	MG	BA	3770	1/1	0.96	0.19	20,20,20,20	0
56	MG	DA	3272	1/1	0.96	0.17	43,43,43,43	0
56	MG	DA	3189	1/1	0.96	0.20	42,42,42,42	0
56	MG	AA	3196	1/1	0.96	0.18	66,66,66,66	0
56	MG	DA	3317	1/1	0.96	0.05	47,47,47,47	0
56	MG	AA	3072	1/1	0.96	0.20	48,48,48,48	0
56	MG	BA	3635	1/1	0.96	0.19	56,56,56,56	0
56	MG	BA	3778	1/1	0.96	0.14	36,36,36,36	0
56	MG	CA	3151	1/1	0.96	0.14	59,59,59,59	0
56	MG	BA	3091	1/1	0.96	0.63	43,43,43,43	0
56	MG	AA	3181	1/1	0.96	0.10	65,65,65,65	0
56	MG	BA	3345	1/1	0.96	0.19	20,20,20,20	0
56	MG	DA	3532	1/1	0.96	0.16	53,53,53,53	0
56	MG	DA	3439	1/1	0.96	0.10	58,58,58,58	0
56	MG	AA	3107	1/1	0.96	0.18	66,66,66,66	0
56	MG	CA	3107	1/1	0.96	0.14	63,63,63,63	0
56	MG	BA	3164	1/1	0.96	0.54	33,33,33,33	0
56	MG	BA	3430	1/1	0.96	0.17	48,48,48,48	0
56	MG	DA	3154	1/1	0.96	0.12	43,43,43,43	0
56	MG	AA	3172	1/1	0.96	0.32	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3376	1/1	0.96	0.17	23,23,23,23	0
56	MG	AA	3091	1/1	0.96	0.21	62,62,62,62	0
56	MG	DA	3210	1/1	0.96	0.21	35,35,35,35	0
56	MG	BA	3096	1/1	0.96	0.16	29,29,29,29	0
56	MG	BA	3308	1/1	0.96	0.21	38,38,38,38	0
56	MG	BA	3221	1/1	0.96	0.19	47,47,47,47	0
56	MG	DA	3494	1/1	0.96	0.21	55,55,55,55	0
56	MG	BA	3220	1/1	0.96	0.26	45,45,45,45	0
56	MG	BA	3766	1/1	0.96	0.20	43,43,43,43	0
56	MG	DA	3095	1/1	0.96	0.08	54,54,54,54	0
56	MG	AV	101	1/1	0.96	0.10	47,47,47,47	0
56	MG	BA	3487	1/1	0.96	0.20	37,37,37,37	0
56	MG	DA	3115	1/1	0.96	0.08	51,51,51,51	0
56	MG	DA	3589	1/1	0.96	0.13	55,55,55,55	0
56	MG	DA	3503	1/1	0.96	0.07	58,58,58,58	0
56	MG	AA	3223	1/1	0.96	0.12	52,52,52,52	0
56	MG	DA	3253	1/1	0.96	0.20	57,57,57,57	0
56	MG	BO	5001	1/1	0.96	0.22	70,70,70,70	0
56	MG	BA	3388	1/1	0.96	0.17	40,40,40,40	0
56	MG	BA	3433	1/1	0.96	0.15	48,48,48,48	0
56	MG	DA	3531	1/1	0.96	0.12	40,40,40,40	0
56	MG	CA	3166	1/1	0.96	0.11	42,42,42,42	0
56	MG	BW	204	1/1	0.96	0.48	41,41,41,41	0
56	MG	AD	502	1/1	0.96	0.25	58,58,58,58	0
56	MG	BA	3291	1/1	0.96	0.20	26,26,26,26	0
56	MG	DA	3270	1/1	0.96	0.23	47,47,47,47	0
56	MG	DA	3444	1/1	0.96	0.17	59,59,59,59	0
56	MG	DA	3303	1/1	0.96	0.12	44,44,44,44	0
56	MG	AA	3061	1/1	0.96	0.17	44,44,44,44	0
56	MG	AA	3026	1/1	0.96	0.11	68,68,68,68	0
56	MG	DA	3263	1/1	0.96	0.06	48,48,48,48	0
56	MG	DA	3331	1/1	0.96	0.14	46,46,46,46	0
56	MG	BA	3446	1/1	0.96	0.22	40,40,40,40	0
56	MG	BV	206	1/1	0.96	0.17	38,38,38,38	0
56	MG	AA	3114	1/1	0.96	0.19	66,66,66,66	0
56	MG	BA	3659	1/1	0.96	0.19	24,24,24,24	0
56	MG	CA	3015	1/1	0.96	0.10	45,45,45,45	0
56	MG	DA	3535	1/1	0.96	0.10	38,38,38,38	0
56	MG	DA	3424	1/1	0.96	0.31	35,35,35,35	0
56	MG	BA	3166	1/1	0.96	0.15	47,47,47,47	0
56	MG	DA	3139	1/1	0.96	0.24	59,59,59,59	0
56	MG	CA	3077	1/1	0.96	0.17	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	3210	1/1	0.96	0.42	34,34,34,34	0
56	MG	DA	3484	1/1	0.96	0.06	59,59,59,59	0
56	MG	AA	3125	1/1	0.96	0.20	53,53,53,53	0
56	MG	AA	3123	1/1	0.96	0.15	25,25,25,25	0
56	MG	DA	3110	1/1	0.96	0.09	30,30,30,30	0
56	MG	AA	3119	1/1	0.96	0.17	36,36,36,36	0
56	MG	BA	3448	1/1	0.96	0.20	60,60,60,60	0
56	MG	BA	3050	1/1	0.96	0.18	34,34,34,34	0
56	MG	BA	3347	1/1	0.96	0.19	26,26,26,26	0
56	MG	DA	3408	1/1	0.96	0.10	25,25,25,25	0
56	MG	DA	3348	1/1	0.96	0.15	46,46,46,46	0
56	MG	BA	3500	1/1	0.96	0.11	37,37,37,37	0
56	MG	BA	3524	1/1	0.96	0.17	44,44,44,44	0
56	MG	BA	3752	1/1	0.96	0.22	48,48,48,48	0
56	MG	DA	3222	1/1	0.96	0.10	46,46,46,46	0
56	MG	BA	3396	1/1	0.96	0.16	24,24,24,24	0
56	MG	BA	3478	1/1	0.96	0.19	36,36,36,36	0
56	MG	BF	304	1/1	0.96	0.48	37,37,37,37	0
56	MG	BA	3776	1/1	0.96	1.10	52,52,52,52	0
56	MG	BA	3085	1/1	0.96	0.19	50,50,50,50	0
56	MG	DA	3487	1/1	0.96	0.14	37,37,37,37	0
56	MG	BA	3204	1/1	0.96	0.30	35,35,35,35	0
56	MG	DA	3282	1/1	0.96	0.14	43,43,43,43	0
56	MG	BA	3269	1/1	0.96	0.15	40,40,40,40	0
56	MG	BP	201	1/1	0.96	0.42	36,36,36,36	0
56	MG	BA	3129	1/1	0.96	0.36	49,49,49,49	0
56	MG	DA	3240	1/1	0.96	0.15	36,36,36,36	0
56	MG	AA	3081	1/1	0.96	0.19	52,52,52,52	0
56	MG	DA	3260	1/1	0.96	0.19	36,36,36,36	0
56	MG	AA	3064	1/1	0.96	0.13	47,47,47,47	0
56	MG	BA	3520	1/1	0.96	0.23	25,25,25,25	0
56	MG	CW	3003	1/1	0.96	0.10	64,64,64,64	0
56	MG	BA	3058	1/1	0.96	0.14	23,23,23,23	0
56	MG	CA	3011	1/1	0.96	0.25	71,71,71,71	0
56	MG	AA	3200	1/1	0.96	0.14	61,61,61,61	0
56	MG	CA	3070	1/1	0.96	0.33	52,52,52,52	0
56	MG	DA	3547	1/1	0.96	0.51	41,41,41,41	0
56	MG	DA	3423	1/1	0.96	0.18	34,34,34,34	0
56	MG	DB	3012	1/1	0.96	0.08	61,61,61,61	0
56	MG	DD	304	1/1	0.96	0.44	56,56,56,56	0
56	MG	DA	3307	1/1	0.96	0.10	28,28,28,28	0
56	MG	DA	3288	1/1	0.96	0.15	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	AA	3071	1/1	0.96	0.13	52,52,52,52	0
56	MG	DA	3556	1/1	0.96	0.41	48,48,48,48	0
56	MG	DA	3420	1/1	0.96	0.08	40,40,40,40	0
56	MG	DB	3003	1/1	0.96	0.12	62,62,62,62	0
56	MG	DA	3274	1/1	0.96	0.20	43,43,43,43	0
56	MG	BA	3398	1/1	0.96	0.18	37,37,37,37	0
56	MG	BA	3128	1/1	0.96	0.39	46,46,46,46	0
56	MG	DA	3391	1/1	0.96	0.14	40,40,40,40	0
56	MG	DA	3592	1/1	0.96	0.10	57,57,57,57	0
56	MG	CA	3088	1/1	0.96	0.15	48,48,48,48	0
56	MG	CA	3096	1/1	0.96	0.16	51,51,51,51	0
56	MG	BA	3263	1/1	0.96	0.10	47,47,47,47	0
56	MG	D0	101	1/1	0.96	0.17	73,73,73,73	0
56	MG	DA	3309	1/1	0.97	0.10	42,42,42,42	0
56	MG	BA	3351	1/1	0.97	0.16	61,61,61,61	0
56	MG	DA	3268	1/1	0.97	0.19	53,53,53,53	0
56	MG	DA	3440	1/1	0.97	0.12	49,49,49,49	0
56	MG	DA	3427	1/1	0.97	0.08	61,61,61,61	0
56	MG	DA	3254	1/1	0.97	0.12	53,53,53,53	0
56	MG	BA	3273	1/1	0.97	0.17	36,36,36,36	0
56	MG	BA	3769	1/1	0.97	0.34	52,52,52,52	0
56	MG	BA	3138	1/1	0.97	0.17	50,50,50,50	0
56	MG	DA	3401	1/1	0.97	0.12	50,50,50,50	0
56	MG	DA	3357	1/1	0.97	0.12	44,44,44,44	0
56	MG	DA	3396	1/1	0.97	0.10	27,27,27,27	0
56	MG	BE	305	1/1	0.97	0.28	38,38,38,38	0
56	MG	DA	3168	1/1	0.97	0.27	41,41,41,41	0
56	MG	BA	3115	1/1	0.97	0.17	13,13,13,13	0
56	MG	BA	3027	1/1	0.97	0.44	41,41,41,41	0
56	MG	DA	3392	1/1	0.97	0.16	34,34,34,34	0
56	MG	CA	3101	1/1	0.97	0.19	64,64,64,64	0
56	MG	BA	3493	1/1	0.97	0.14	29,29,29,29	0
56	MG	BA	3321	1/1	0.97	0.18	43,43,43,43	0
56	MG	CA	3108	1/1	0.97	0.10	56,56,56,56	0
56	MG	DA	3413	1/1	0.97	0.25	40,40,40,40	0
56	MG	BA	3130	1/1	0.97	0.30	44,44,44,44	0
56	MG	DA	3457	1/1	0.97	0.23	46,46,46,46	0
56	MG	DA	3534	1/1	0.97	0.18	59,59,59,59	0
56	MG	CA	3080	1/1	0.97	0.13	62,62,62,62	0
56	MG	DA	3194	1/1	0.97	0.13	52,52,52,52	0
56	MG	DA	3235	1/1	0.97	0.09	29,29,29,29	0
56	MG	BA	3250	1/1	0.97	0.19	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3265	1/1	0.97	0.17	47,47,47,47	0
56	MG	DA	3281	1/1	0.97	0.12	39,39,39,39	0
56	MG	BA	3641	1/1	0.97	0.26	46,46,46,46	0
56	MG	BD	302	1/1	0.97	0.30	33,33,33,33	0
56	MG	DA	3071	1/1	0.97	0.32	43,43,43,43	0
56	MG	BA	3642	1/1	0.97	0.29	38,38,38,38	0
56	MG	BA	3411	1/1	0.97	0.24	49,49,49,49	0
56	MG	BA	3747	1/1	0.97	0.23	50,50,50,50	0
56	MG	DA	3024	1/1	0.97	0.54	43,43,43,43	0
56	MG	BA	3037	1/1	0.97	0.22	33,33,33,33	0
56	MG	DA	3092	1/1	0.97	0.12	43,43,43,43	0
56	MG	DA	3135	1/1	0.97	0.27	44,44,44,44	0
56	MG	DA	3237	1/1	0.97	0.09	42,42,42,42	0
56	MG	BA	3617	1/1	0.97	0.06	46,46,46,46	0
56	MG	BA	3020	1/1	0.97	0.45	32,32,32,32	0
56	MG	DA	3563	1/1	0.97	0.06	45,45,45,45	0
56	MG	AA	3133	1/1	0.97	0.12	35,35,35,35	0
56	MG	BA	3574	1/1	0.97	0.26	60,60,60,60	0
56	MG	BA	3392	1/1	0.97	0.14	17,17,17,17	0
56	MG	BA	3386	1/1	0.97	0.20	36,36,36,36	0
56	MG	BA	3647	1/1	0.97	0.15	48,48,48,48	0
56	MG	CA	3089	1/1	0.97	0.25	46,46,46,46	0
56	MG	DA	3416	1/1	0.97	0.13	39,39,39,39	0
56	MG	BA	3472	1/1	0.97	0.40	43,43,43,43	0
59	ZN	DY	501	1/1	0.97	0.13	88,88,88,88	0
56	MG	BA	3079	1/1	0.97	0.25	40,40,40,40	0
56	MG	DA	3335	1/1	0.97	0.07	41,41,41,41	0
56	MG	AA	3025	1/1	0.97	0.25	54,54,54,54	0
56	MG	BA	3655	1/1	0.97	0.15	29,29,29,29	0
56	MG	BA	3119	1/1	0.97	0.34	44,44,44,44	0
56	MG	B5	106	1/1	0.97	0.15	55,55,55,55	0
56	MG	BA	3629	1/1	0.97	0.17	62,62,62,62	0
56	MG	BA	3708	1/1	0.97	0.13	7,7,7,7	0
56	MG	DA	3020	1/1	0.97	0.13	33,33,33,33	0
56	MG	CA	3161	1/1	0.97	0.10	59,59,59,59	0
56	MG	BA	3626	1/1	0.97	0.12	40,40,40,40	0
56	MG	DA	3379	1/1	0.97	0.18	38,38,38,38	0
56	MG	DA	3246	1/1	0.97	0.09	53,53,53,53	0
56	MG	BA	3743	1/1	0.97	0.15	18,18,18,18	0
56	MG	BA	3230	1/1	0.97	0.20	53,53,53,53	0
56	MG	DA	3374	1/1	0.97	0.13	52,52,52,52	0
56	MG	DA	3072	1/1	0.97	0.19	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3259	1/1	0.97	0.12	50,50,50,50	0
56	MG	DA	3450	1/1	0.97	0.08	50,50,50,50	0
56	MG	BU	203	1/1	0.97	0.28	34,34,34,34	0
56	MG	DA	3371	1/1	0.97	0.21	68,68,68,68	0
56	MG	AA	3028	1/1	0.97	0.23	46,46,46,46	0
56	MG	DD	308	1/1	0.97	0.56	45,45,45,45	0
56	MG	AA	3132	1/1	0.97	0.19	75,75,75,75	0
56	MG	BA	3422	1/1	0.97	0.12	45,45,45,45	0
56	MG	BA	3023	1/1	0.97	0.32	38,38,38,38	0
56	MG	BA	3650	1/1	0.97	0.10	38,38,38,38	0
56	MG	CE	3001	1/1	0.97	0.14	73,73,73,73	0
56	MG	DA	3390	1/1	0.97	0.14	48,48,48,48	0
56	MG	BA	3369	1/1	0.97	0.19	23,23,23,23	0
56	MG	DA	3266	1/1	0.97	0.24	61,61,61,61	0
56	MG	DF	301	1/1	0.97	0.16	49,49,49,49	0
56	MG	BA	3426	1/1	0.97	0.15	29,29,29,29	0
56	MG	BA	3190	1/1	0.97	0.67	35,35,35,35	0
56	MG	BD	304	1/1	0.97	0.41	50,50,50,50	0
56	MG	DA	3123	1/1	0.97	0.39	40,40,40,40	0
56	MG	BF	302	1/1	0.97	0.45	29,29,29,29	0
56	MG	BA	3774	1/1	0.97	0.64	32,32,32,32	0
56	MG	DO	202	1/1	0.97	0.10	57,57,57,57	0
56	MG	BA	3489	1/1	0.97	0.09	43,43,43,43	0
56	MG	DD	306	1/1	0.97	0.55	35,35,35,35	0
56	MG	BA	3556	1/1	0.97	0.20	50,50,50,50	0
56	MG	BA	3112	1/1	0.97	0.07	50,50,50,50	0
56	MG	BA	3043	1/1	0.97	0.17	34,34,34,34	0
56	MG	BA	3346	1/1	0.97	0.17	28,28,28,28	0
56	MG	DD	307	1/1	0.97	0.33	56,56,56,56	0
56	MG	DA	3090	1/1	0.97	0.21	67,67,67,67	0
56	MG	DA	3191	1/1	0.97	0.19	35,35,35,35	0
56	MG	DA	3537	1/1	0.97	0.21	53,53,53,53	0
56	MG	BA	3427	1/1	0.97	0.17	22,22,22,22	0
56	MG	BQ	3002	1/1	0.97	0.23	41,41,41,41	0
56	MG	CK	3001	1/1	0.97	0.17	47,47,47,47	0
56	MG	AA	3209	1/1	0.97	0.09	62,62,62,62	0
56	MG	B1	101	1/1	0.97	0.71	45,45,45,45	0
56	MG	BA	3576	1/1	0.97	0.10	56,56,56,56	0
56	MG	DA	3319	1/1	0.97	0.13	21,21,21,21	0
56	MG	DA	3327	1/1	0.97	0.12	32,32,32,32	0
56	MG	BA	3298	1/1	0.97	0.26	24,24,24,24	0
56	MG	BA	3357	1/1	0.97	0.18	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3144	1/1	0.97	0.13	54,54,54,54	0
56	MG	AX	3012	1/1	0.97	0.22	66,66,66,66	0
56	MG	DA	3518	1/1	0.97	0.06	57,57,57,57	0
56	MG	DA	3231	1/1	0.97	0.10	54,54,54,54	0
56	MG	BA	3125	1/1	0.97	0.37	34,34,34,34	0
56	MG	BA	3672	1/1	0.97	0.34	37,37,37,37	0
56	MG	CA	3152	1/1	0.97	0.19	58,58,58,58	0
56	MG	BV	201	1/1	0.97	0.24	26,26,26,26	0
56	MG	BA	3094	1/1	0.97	0.78	49,49,49,49	0
56	MG	BA	3782	1/1	0.97	0.37	48,48,48,48	0
56	MG	DA	3015	1/1	0.97	0.45	49,49,49,49	0
56	MG	AA	3158	1/1	0.97	0.14	62,62,62,62	0
56	MG	DA	3344	1/1	0.97	0.07	54,54,54,54	0
56	MG	BA	3284	1/1	0.97	0.19	35,35,35,35	0
56	MG	DA	3004	1/1	0.97	0.18	18,18,18,18	0
56	MG	AA	3102	1/1	0.97	0.17	50,50,50,50	0
56	MG	BA	3104	1/1	0.97	0.95	44,44,44,44	0
56	MG	DA	3567	1/1	0.97	0.07	52,52,52,52	0
56	MG	CA	3030	1/1	0.97	0.20	51,51,51,51	0
56	MG	DA	3519	1/1	0.97	0.06	78,78,78,78	0
56	MG	BA	3488	1/1	0.97	0.12	28,28,28,28	0
56	MG	DA	3448	1/1	0.97	0.18	40,40,40,40	0
56	MG	DA	3382	1/1	0.97	0.14	53,53,53,53	0
56	MG	BA	3292	1/1	0.97	0.15	26,26,26,26	0
56	MG	CA	3033	1/1	0.97	0.19	44,44,44,44	0
56	MG	DA	3525	1/1	0.97	0.07	33,33,33,33	0
56	MG	BA	3282	1/1	0.97	0.08	59,59,59,59	0
56	MG	DB	3008	1/1	0.97	0.10	62,62,62,62	0
56	MG	BA	3457	1/1	0.97	0.10	46,46,46,46	0
56	MG	DA	3034	1/1	0.97	0.20	35,35,35,35	0
56	MG	BA	3678	1/1	0.97	0.14	41,41,41,41	0
56	MG	CA	3023	1/1	0.97	0.11	54,54,54,54	0
56	MG	BA	3278	1/1	0.97	0.12	48,48,48,48	0
56	MG	BA	3511	1/1	0.97	0.19	31,31,31,31	0
56	MG	BA	3785	1/1	0.97	0.52	42,42,42,42	0
56	MG	DA	3598	1/1	0.97	0.24	63,63,63,63	0
56	MG	BR	203	1/1	0.97	0.25	36,36,36,36	0
56	MG	DA	3233	1/1	0.97	0.23	40,40,40,40	0
56	MG	BA	3299	1/1	0.97	0.07	53,53,53,53	0
56	MG	AW	3003	1/1	0.97	0.21	44,44,44,44	0
56	MG	CA	3024	1/1	0.97	0.07	53,53,53,53	0
56	MG	DA	3104	1/1	0.97	0.25	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3280	1/1	0.97	0.15	26,26,26,26	0
56	MG	BA	3451	1/1	0.98	0.21	53,53,53,53	0
56	MG	BA	3463	1/1	0.98	0.16	34,34,34,34	0
56	MG	CA	3091	1/1	0.98	0.17	45,45,45,45	0
56	MG	AA	3012	1/1	0.98	0.21	43,43,43,43	0
56	MG	BA	3317	1/1	0.98	0.13	47,47,47,47	0
56	MG	BA	3410	1/1	0.98	0.18	33,33,33,33	0
56	MG	BA	3236	1/1	0.98	0.16	34,34,34,34	0
56	MG	DA	3252	1/1	0.98	0.09	43,43,43,43	0
56	MG	BA	3021	1/1	0.98	0.31	32,32,32,32	0
56	MG	DA	3096	1/1	0.98	0.21	29,29,29,29	0
56	MG	DA	3230	1/1	0.98	0.12	23,23,23,23	0
56	MG	BT	201	1/1	0.98	0.19	49,49,49,49	0
56	MG	BA	3289	1/1	0.98	0.14	24,24,24,24	0
56	MG	BA	3315	1/1	0.98	0.11	40,40,40,40	0
56	MG	BA	3516	1/1	0.98	0.20	36,36,36,36	0
56	MG	AA	3142	1/1	0.98	0.13	38,38,38,38	0
59	ZN	BY	501	1/1	0.98	0.20	60,60,60,60	0
56	MG	AA	3187	1/1	0.98	0.15	56,56,56,56	0
56	MG	BA	3452	1/1	0.98	0.10	41,41,41,41	0
56	MG	BA	3268	1/1	0.98	0.19	40,40,40,40	0
56	MG	DV	3001	1/1	0.98	0.34	75,75,75,75	0
56	MG	BA	3082	1/1	0.98	0.17	27,27,27,27	0
56	MG	BA	3709	1/1	0.98	0.20	42,42,42,42	0
56	MG	DA	3005	1/1	0.98	0.15	39,39,39,39	0
56	MG	BA	3238	1/1	0.98	0.63	35,35,35,35	0
56	MG	DA	3509	1/1	0.98	0.13	38,38,38,38	0
56	MG	AA	3037	1/1	0.98	0.13	55,55,55,55	0
56	MG	BA	3330	1/1	0.98	0.18	35,35,35,35	0
56	MG	DA	3521	1/1	0.98	0.16	29,29,29,29	0
56	MG	BA	3458	1/1	0.98	0.21	52,52,52,52	0
56	MG	BA	3594	1/1	0.98	0.15	37,37,37,37	0
56	MG	BA	3423	1/1	0.98	0.23	43,43,43,43	0
56	MG	BU	207	1/1	0.98	0.39	22,22,22,22	0
56	MG	BA	3759	1/1	0.98	0.17	29,29,29,29	0
56	MG	BA	3237	1/1	0.98	0.38	43,43,43,43	0
56	MG	CA	3179	1/1	0.98	0.16	53,53,53,53	0
56	MG	BW	203	1/1	0.98	0.22	42,42,42,42	0
56	MG	BA	3654	1/1	0.98	0.17	24,24,24,24	0
56	MG	AA	3185	1/1	0.98	0.21	51,51,51,51	0
56	MG	DA	3591	1/1	0.98	0.13	46,46,46,46	0
56	MG	BA	3767	1/1	0.98	0.14	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AX	3008	1/1	0.98	0.17	52,52,52,52	0
56	MG	DA	3375	1/1	0.98	0.16	42,42,42,42	0
56	MG	CN	101	1/1	0.98	0.19	69,69,69,69	0
56	MG	BA	3272	1/1	0.98	0.20	41,41,41,41	0
56	MG	DA	3428	1/1	0.98	0.20	50,50,50,50	0
56	MG	DE	301	1/1	0.98	0.90	50,50,50,50	0
56	MG	BA	3538	1/1	0.98	0.10	43,43,43,43	0
56	MG	BA	3324	1/1	0.98	0.16	44,44,44,44	0
56	MG	CV	101	1/1	0.98	0.17	56,56,56,56	0
56	MG	AA	3016	1/1	0.98	0.11	48,48,48,48	0
56	MG	BA	3517	1/1	0.98	0.23	26,26,26,26	0
56	MG	CA	3164	1/1	0.98	0.19	65,65,65,65	0
56	MG	BA	3593	1/1	0.98	0.20	53,53,53,53	0
56	MG	BA	3720	1/1	0.98	0.10	28,28,28,28	0
56	MG	BA	3255	1/1	0.98	0.22	56,56,56,56	0
56	MG	BA	3368	1/1	0.98	0.12	56,56,56,56	0
59	ZN	AN	501	1/1	0.98	0.20	65,65,65,65	0
56	MG	BA	3525	1/1	0.98	0.20	40,40,40,40	0
56	MG	BA	3106	1/1	0.98	0.43	42,42,42,42	0
56	MG	BA	3455	1/1	0.98	0.13	28,28,28,28	0
56	MG	DA	3269	1/1	0.98	0.11	46,46,46,46	0
56	MG	BA	3251	1/1	0.98	0.13	51,51,51,51	0
56	MG	DQ	3001	1/1	0.98	0.11	57,57,57,57	0
56	MG	DA	3313	1/1	0.98	0.18	46,46,46,46	0
56	MG	BA	3017	1/1	0.98	0.13	32,32,32,32	0
56	MG	BD	309	1/1	0.98	0.64	39,39,39,39	0
56	MG	BE	306	1/1	0.98	0.21	15,15,15,15	0
56	MG	AA	3001	1/1	0.98	0.15	37,37,37,37	0
56	MG	DA	3198	1/1	0.98	0.22	32,32,32,32	0
56	MG	AA	3036	1/1	0.98	0.16	24,24,24,24	0
56	MG	AA	3131	1/1	0.98	0.22	63,63,63,63	0
56	MG	DA	3051	1/1	0.98	0.14	54,54,54,54	0
56	MG	BA	3188	1/1	0.98	0.54	41,41,41,41	0
56	MG	BA	3162	1/1	0.98	0.16	37,37,37,37	0
56	MG	DA	3099	1/1	0.98	0.20	39,39,39,39	0
56	MG	B7	101	1/1	0.98	0.21	35,35,35,35	0
56	MG	DA	3399	1/1	0.98	0.16	35,35,35,35	0
56	MG	DA	3101	1/1	0.98	0.09	28,28,28,28	0
56	MG	BB	3010	1/1	0.98	0.19	51,51,51,51	0
56	MG	BA	3120	1/1	0.98	0.40	45,45,45,45	0
56	MG	BA	3684	1/1	0.98	0.08	39,39,39,39	0
56	MG	CA	3160	1/1	0.98	0.22	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	DA	3506	1/1	0.98	0.14	37,37,37,37	0
56	MG	BA	3384	1/1	0.98	0.14	43,43,43,43	0
56	MG	BA	3005	1/1	0.98	0.13	41,41,41,41	0
56	MG	DA	3244	1/1	0.98	0.27	58,58,58,58	0
56	MG	BA	3553	1/1	0.98	0.11	49,49,49,49	0
56	MG	CA	3109	1/1	0.98	0.14	67,67,67,67	0
56	MG	BA	3239	1/1	0.98	0.30	30,30,30,30	0
59	ZN	B4	501	1/1	0.98	0.18	86,86,86,86	0
56	MG	BA	3072	1/1	0.98	0.16	42,42,42,42	0
56	MG	BA	3122	1/1	0.98	0.25	42,42,42,42	0
56	MG	AA	3120	1/1	0.98	0.12	72,72,72,72	0
56	MG	BA	3026	1/1	0.98	0.38	41,41,41,41	0
56	MG	BA	3277	1/1	0.98	0.17	40,40,40,40	0
56	MG	DV	3002	1/1	0.98	0.70	51,51,51,51	0
56	MG	BA	3320	1/1	0.98	0.15	28,28,28,28	0
56	MG	DA	3336	1/1	0.98	0.12	30,30,30,30	0
56	MG	DA	3576	1/1	0.98	0.13	46,46,46,46	0
56	MG	DA	3234	1/1	0.98	0.13	42,42,42,42	0
56	MG	BA	3016	1/1	0.98	0.21	22,22,22,22	0
56	MG	BU	208	1/1	0.98	0.36	35,35,35,35	0
56	MG	BA	3529	1/1	0.98	0.17	57,57,57,57	0
56	MG	BA	3101	1/1	0.98	0.28	36,36,36,36	0
56	MG	DW	3002	1/1	0.98	0.40	32,32,32,32	0
56	MG	DA	3499	1/1	0.99	0.17	60,60,60,60	0
56	MG	BA	3673	1/1	0.99	0.28	22,22,22,22	0
56	MG	BA	3414	1/1	0.99	0.16	26,26,26,26	0
56	MG	BA	3107	1/1	0.99	0.73	49,49,49,49	0
56	MG	AA	3135	1/1	0.99	0.11	34,34,34,34	0
56	MG	BA	3334	1/1	0.99	0.18	23,23,23,23	0
56	MG	BA	3666	1/1	0.99	0.18	11,11,11,11	0
59	ZN	B6	102	1/1	0.99	0.23	43,43,43,43	0
56	MG	BA	3038	1/1	0.99	0.17	31,31,31,31	0
56	MG	BA	3267	1/1	0.99	0.20	14,14,14,14	0
56	MG	CA	3137	1/1	0.99	0.08	52,52,52,52	0
56	MG	CA	3169	1/1	0.99	0.19	49,49,49,49	0
56	MG	BA	3024	1/1	0.99	0.19	19,19,19,19	0
59	ZN	D5	501	1/1	0.99	0.21	57,57,57,57	0
58	SF4	CD	302	8/8	0.99	0.17	51,66,73,73	0
56	MG	BA	3592	1/1	0.99	0.18	61,61,61,61	0
56	MG	BA	3763	1/1	0.99	0.19	10,10,10,10	0
56	MG	AA	3148	1/1	0.99	0.18	50,50,50,50	0
56	MG	DA	3271	1/1	0.99	0.23	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	ZN	B9	501	1/1	0.99	0.21	47,47,47,47	0
58	SF4	AD	501	8/8	0.99	0.18	52,60,68,71	0
56	MG	AA	3166	1/1	0.99	0.19	43,43,43,43	0
59	ZN	B5	105	1/1	0.99	0.26	52,52,52,52	0
56	MG	BA	3006	1/1	0.99	0.14	26,26,26,26	0
56	MG	DA	3388	1/1	0.99	0.15	49,49,49,49	0
56	MG	BA	3232	1/1	0.99	0.28	44,44,44,44	0
56	MG	BV	203	1/1	0.99	0.28	31,31,31,31	0
56	MG	BA	3018	1/1	0.99	0.47	36,36,36,36	0
56	MG	BA	3536	1/1	0.99	0.25	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.