



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:29 AM UTC

PDB ID : 4W2I / pdb_00004w2i
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

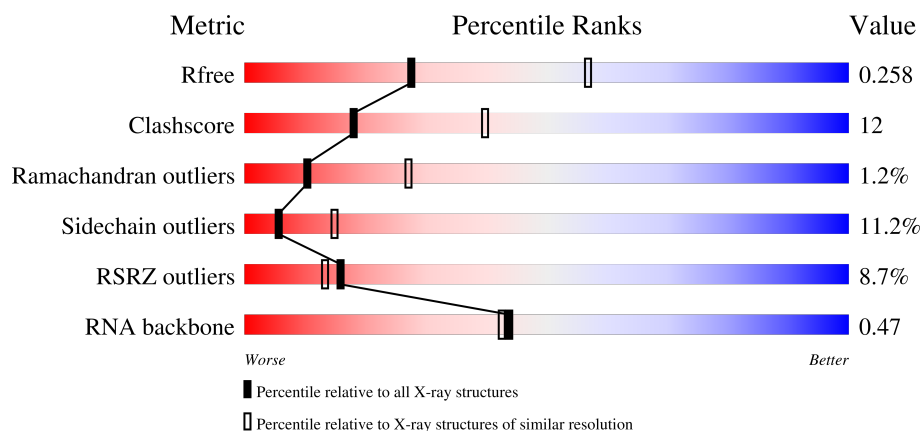
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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

Mol	Chain	Length	Quality of chain
1	AA	1521	4% 51% 37% 11% .
1	CA	1521	7% 46% 42% 11% .
2	AB	256	20% 45% 35% 10% 10%
2	CB	256	29% 41% 37% 11% 10%

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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	

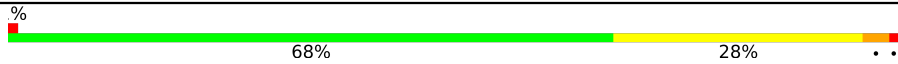
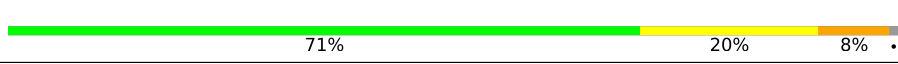
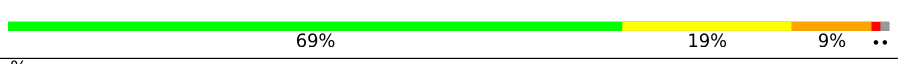
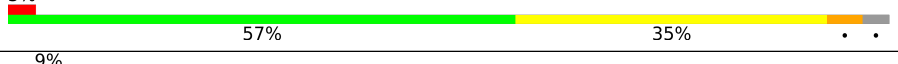
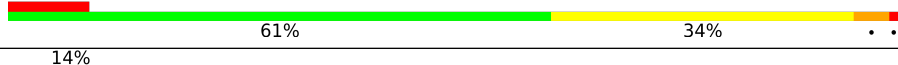
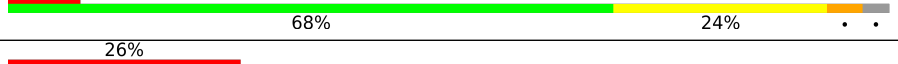
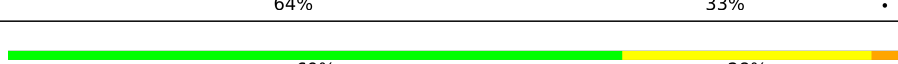
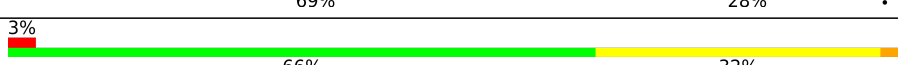
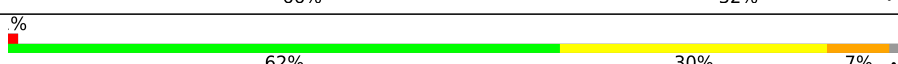
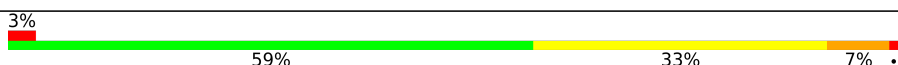
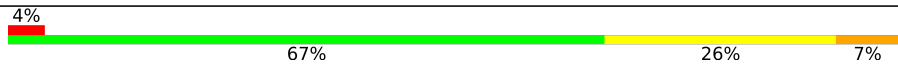
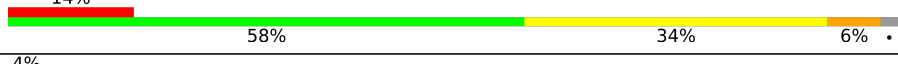
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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	76	
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	77	
24	CX	77	
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	

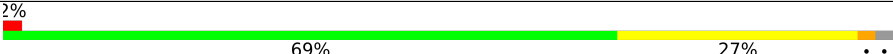
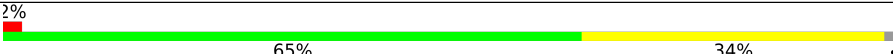
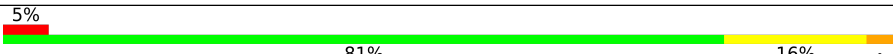
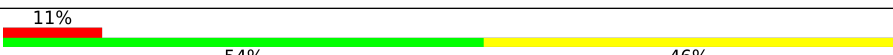
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Mol	Chain	Length	Quality of chain
39	DT	146	
40	BU	118	
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	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	AA	3075	-	-	-	X
56	MG	CA	3054	-	-	-	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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	218	Total	Mg	0	0
			218	218		
56	AD	1	Total	Mg	0	0
			1	1		
56	AE	2	Total	Mg	0	0
			2	2		
56	AF	1	Total	Mg	0	0
			1	1		
56	AM	1	Total	Mg	0	0
			1	1		
56	AN	3	Total	Mg	0	0
			3	3		
56	AO	1	Total	Mg	0	0
			1	1		
56	AV	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AW	4	Total 4	Mg 4	0	0
56	AX	11	Total 11	Mg 11	0	0
56	AY	3	Total 3	Mg 3	0	0
56	BA	785	Total 785	Mg 785	0	0
56	BB	18	Total 18	Mg 18	0	0
56	BD	11	Total 11	Mg 11	0	0
56	BE	8	Total 8	Mg 8	0	0
56	BF	11	Total 11	Mg 11	0	0
56	BG	2	Total 2	Mg 2	0	0
56	BN	6	Total 6	Mg 6	0	0
56	BO	1	Total 1	Mg 1	0	0
56	BP	4	Total 4	Mg 4	0	0
56	BQ	5	Total 5	Mg 5	0	0
56	BR	3	Total 3	Mg 3	0	0
56	BT	1	Total 1	Mg 1	0	0
56	BU	9	Total 9	Mg 9	0	0
56	BV	7	Total 7	Mg 7	0	0
56	BW	4	Total 4	Mg 4	0	0
56	BX	2	Total 2	Mg 2	0	0
56	BY	1	Total 1	Mg 1	0	0
56	BZ	1	Total 1	Mg 1	0	0

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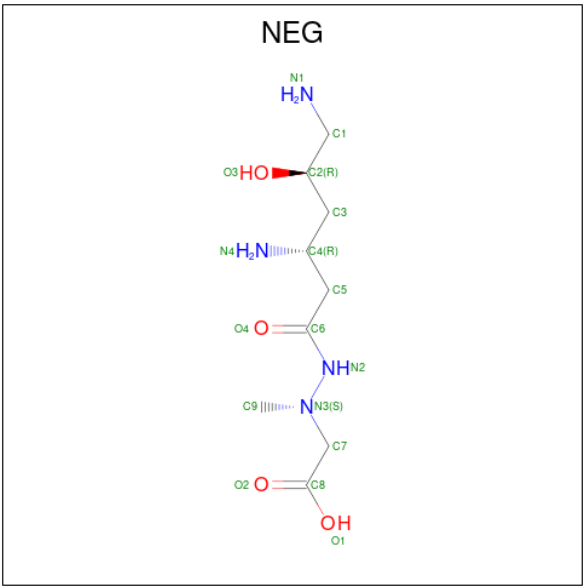
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B0	3	Total 3	Mg 3	0	0
56	B1	1	Total 1	Mg 1	0	0
56	B2	1	Total 1	Mg 1	0	0
56	B3	2	Total 2	Mg 2	0	0
56	B4	1	Total 1	Mg 1	0	0
56	B5	5	Total 5	Mg 5	0	0
56	B6	1	Total 1	Mg 1	0	0
56	B7	4	Total 4	Mg 4	0	0
56	B8	1	Total 1	Mg 1	0	0
56	B9	1	Total 1	Mg 1	0	0
56	CA	172	Total 172	Mg 172	0	0
56	CD	1	Total 1	Mg 1	0	0
56	CE	1	Total 1	Mg 1	0	0
56	CF	1	Total 1	Mg 1	0	0
56	CJ	1	Total 1	Mg 1	0	0
56	CK	1	Total 1	Mg 1	0	0
56	CN	1	Total 1	Mg 1	0	0
56	CT	1	Total 1	Mg 1	0	0
56	CV	1	Total 1	Mg 1	0	0
56	CW	2	Total 2	Mg 2	0	0
56	CX	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CY	1	Total 1	Mg 1	0	0
56	DA	623	Total 623	Mg 623	0	0
56	DB	12	Total 12	Mg 12	0	0
56	DD	9	Total 9	Mg 9	0	0
56	DE	4	Total 4	Mg 4	0	0
56	DF	6	Total 6	Mg 6	0	0
56	DG	1	Total 1	Mg 1	0	0
56	DN	1	Total 1	Mg 1	0	0
56	DO	2	Total 2	Mg 2	0	0
56	DP	1	Total 1	Mg 1	0	0
56	DQ	4	Total 4	Mg 4	0	0
56	DR	2	Total 2	Mg 2	0	0
56	DU	3	Total 3	Mg 3	0	0
56	DV	3	Total 3	Mg 3	0	0
56	DW	4	Total 4	Mg 4	0	0
56	DY	1	Total 1	Mg 1	0	0
56	D0	1	Total 1	Mg 1	0	0
56	D3	1	Total 1	Mg 1	0	0
56	D5	1	Total 1	Mg 1	0	0
56	D7	1	Total 1	Mg 1	0	0
56	D8	1	Total 1	Mg 1	0	0

- Molecule 57 is NEGAMYCIN (CCD ID: NEG) (formula: C₉H₂₀N₄O₄).



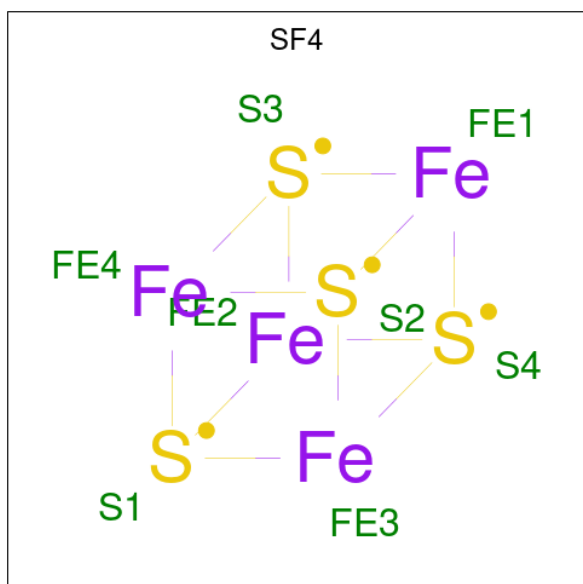
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	9	4	4		
57	AA	1	Total	C	N	O	0	0
			17	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 (CCD ID: SF4) (formula: Fe_4S_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 (CCD ID: ZN) (formula: Zn).

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

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

- Molecule 60 is POTASSIUM ION (CCD ID: 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 2	O 2	0	0
61	AO	1	Total 1	O 1	0	0
61	AV	3	Total 3	O 3	0	0
61	AW	13	Total 13	O 13	0	0
61	AX	11	Total 11	O 11	0	0
61	AY	1	Total 1	O 1	0	0
61	BA	1396	Total 1396	O 1396	0	0
61	BB	34	Total 34	O 34	0	0
61	BD	12	Total 12	O 12	0	0
61	BE	11	Total 11	O 11	0	0
61	BF	5	Total 5	O 5	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0
61	BN	1	Total 1	O 1	0	0
61	BO	2	Total 2	O 2	0	0
61	BP	23	Total 23	O 23	0	0
61	BQ	3	Total 3	O 3	0	0
61	BR	1	Total 1	O 1	0	0
61	BT	2	Total 2	O 2	0	0
61	BU	3	Total 3	O 3	0	0
61	BV	2	Total 2	O 2	0	0

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

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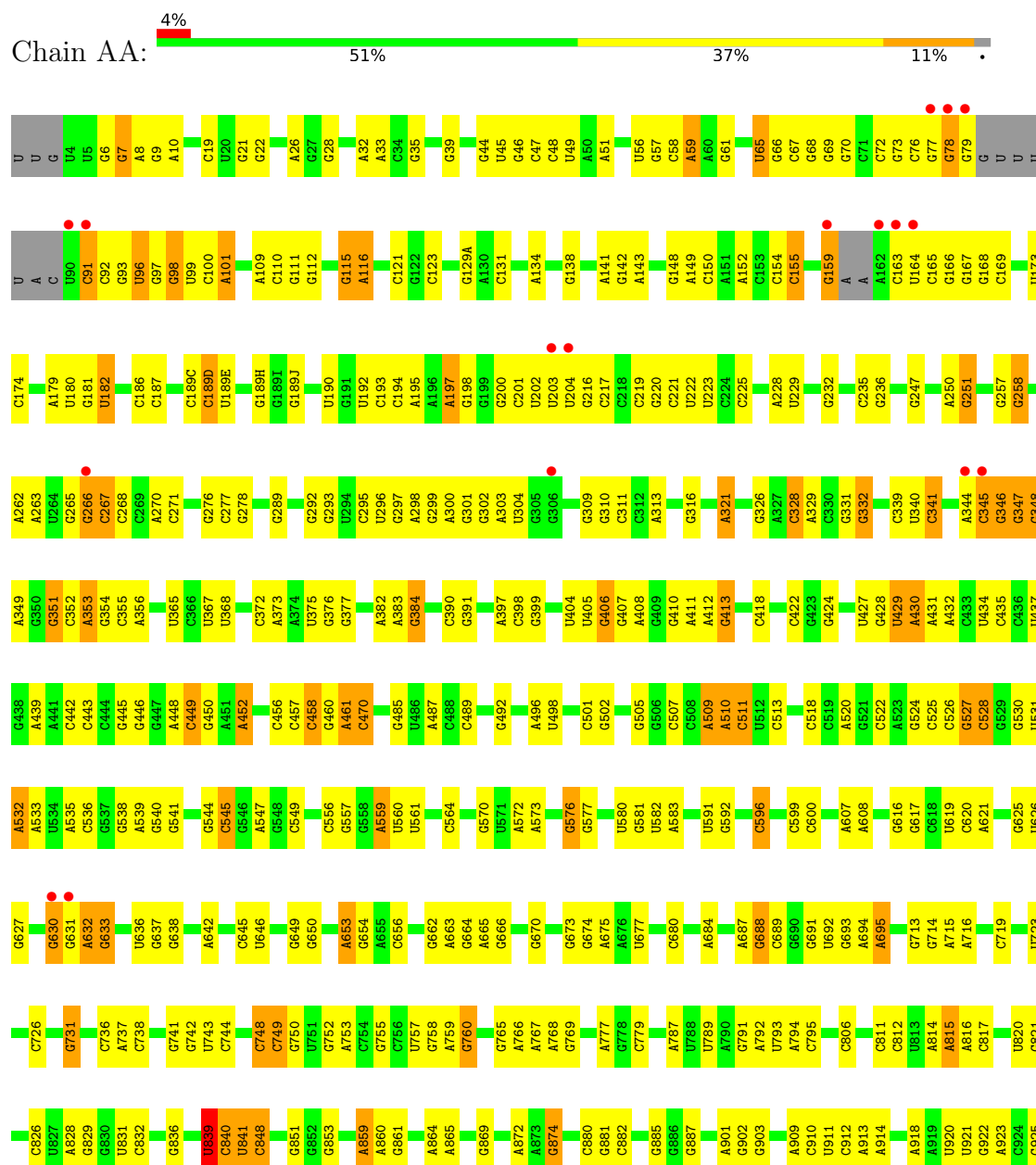
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	DO	2	Total	O	0	0
			2	2		
61	DP	15	Total	O	0	0
			15	15		
61	DQ	1	Total	O	0	0
			1	1		
61	DR	1	Total	O	0	0
			1	1		
61	DU	1	Total	O	0	0
			1	1		
61	DW	1	Total	O	0	0
			1	1		
61	DX	1	Total	O	0	0
			1	1		
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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S Ribosomal RNA





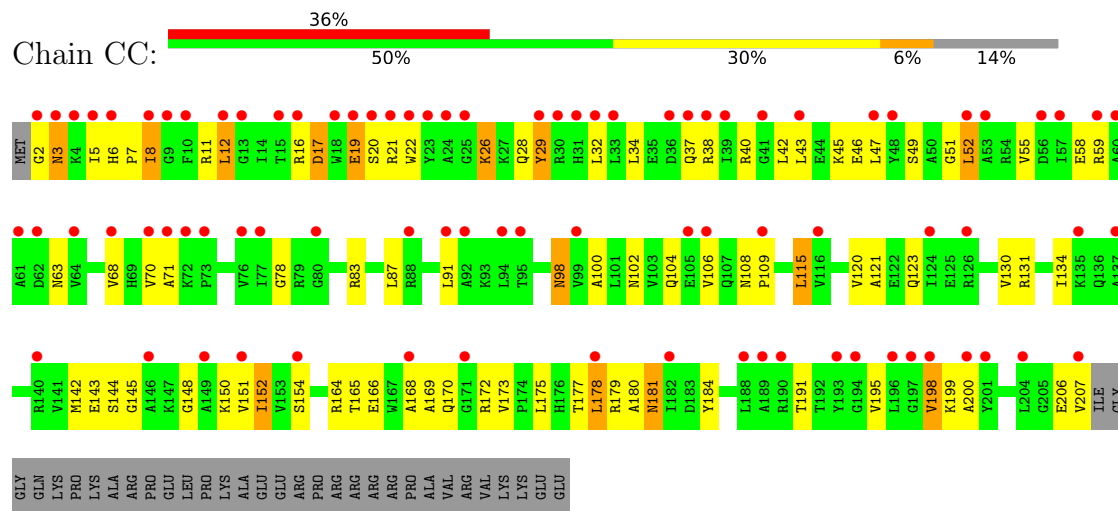


Chain AB:

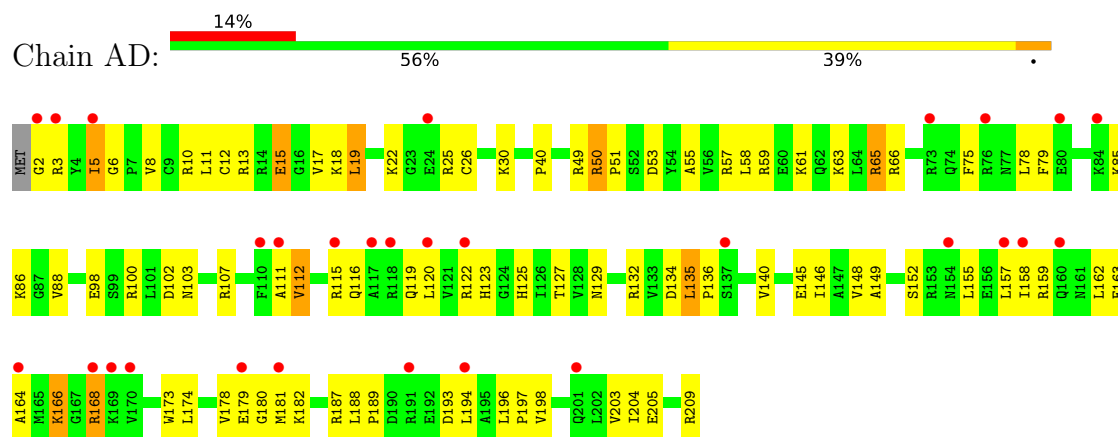


ALA
VAL
ARG
VAL
LYS
LYS
GLU
GLU

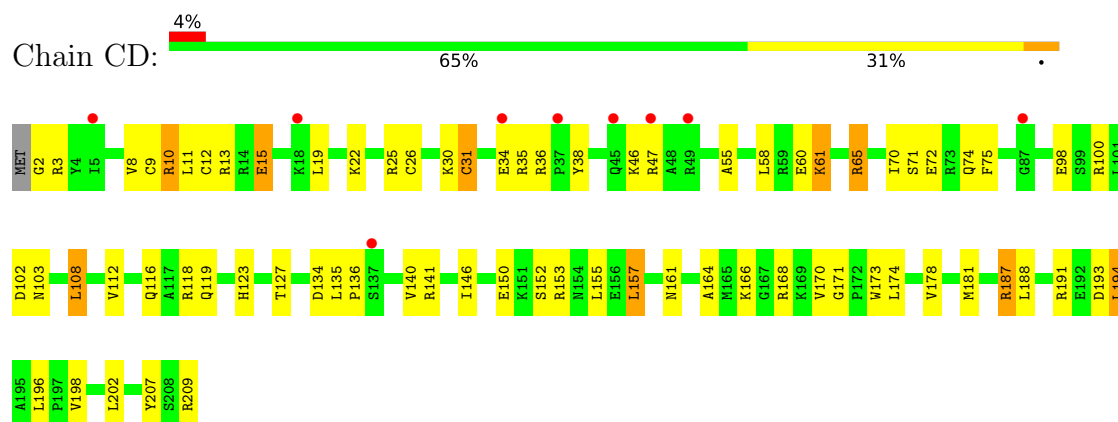
• Molecule 3: 30S Ribosomal Protein S3



• Molecule 4: 30S Ribosomal Protein S4

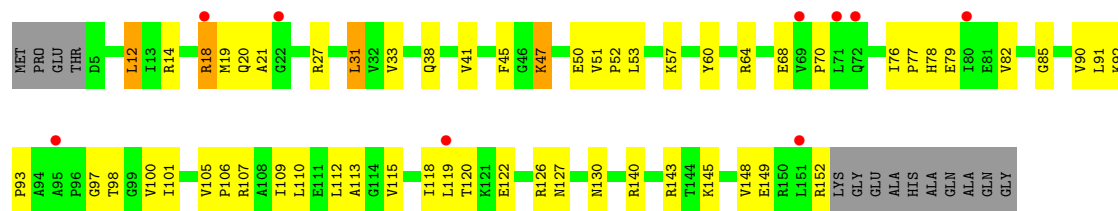


• Molecule 4: 30S Ribosomal Protein S4

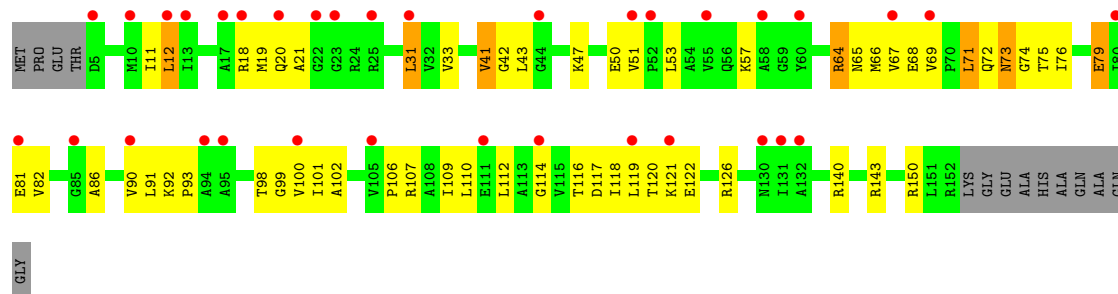


• Molecule 5: 30S Ribosomal Protein S5

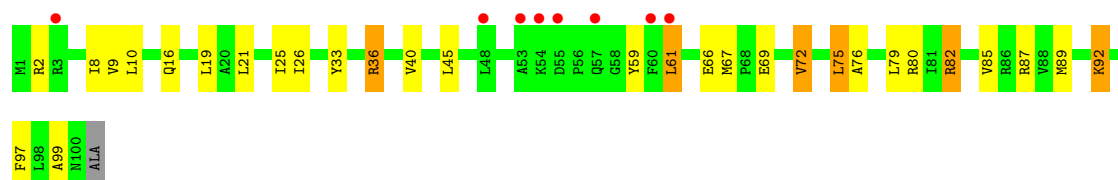




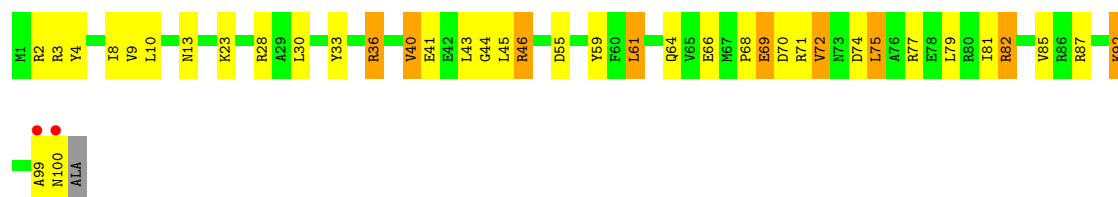
• Molecule 5: 30S Ribosomal Protein S5



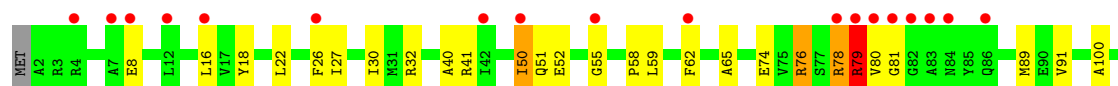
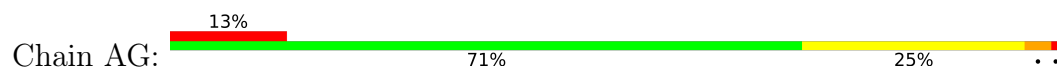
• Molecule 6: 30S Ribosomal Protein S6

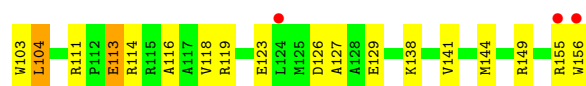


• Molecule 6: 30S Ribosomal Protein S6

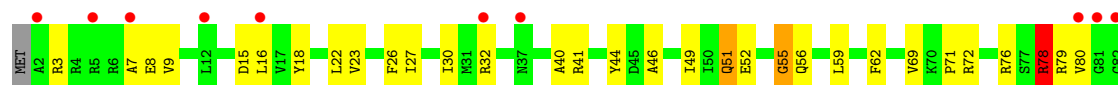


• Molecule 7: 30S Ribosomal Protein S7





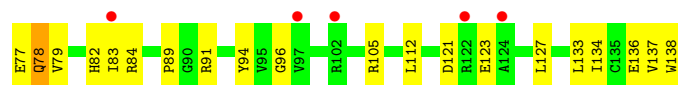
• Molecule 7: 30S Ribosomal Protein S7



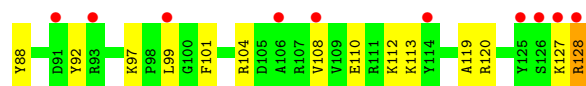
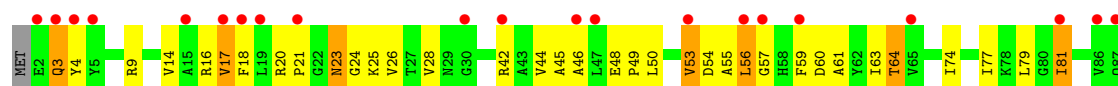
• Molecule 8: 30S Ribosomal Protein S8



• Molecule 8: 30S Ribosomal Protein S8

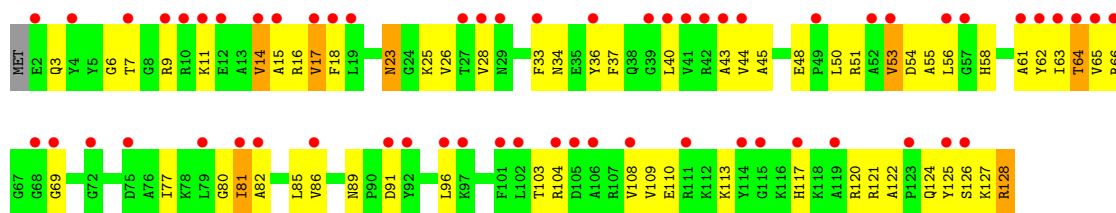


• Molecule 9: 30S Ribosomal Protein S9

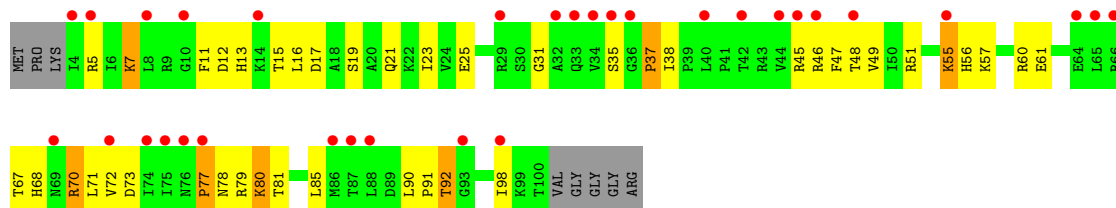


• Molecule 9: 30S Ribosomal Protein S9

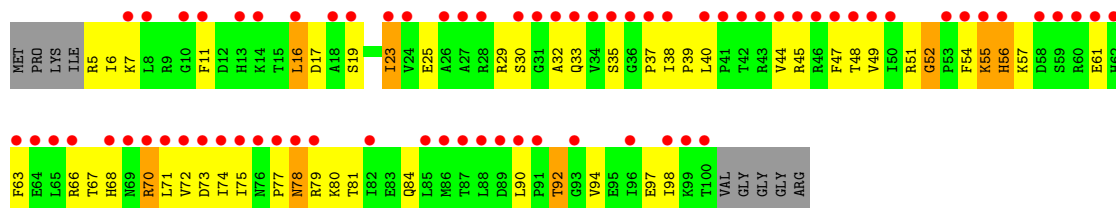
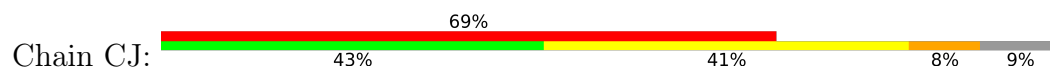




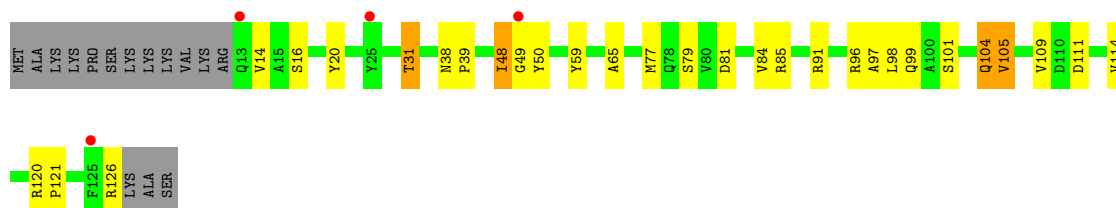
• Molecule 10: 30S Ribosomal Protein S10



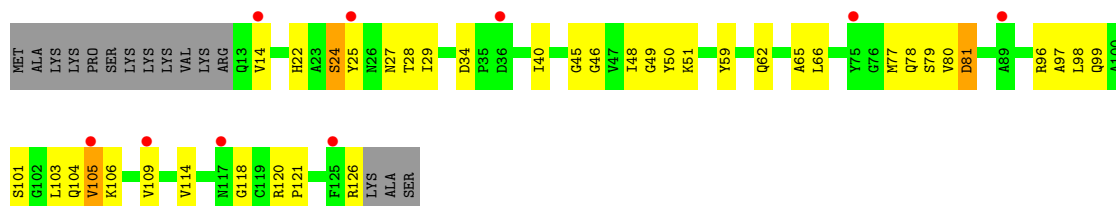
• Molecule 10: 30S Ribosomal Protein S10



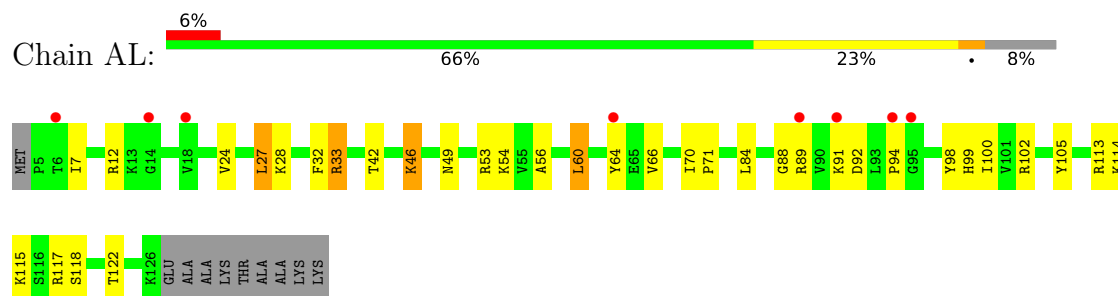
• Molecule 11: 30S Ribosomal Protein S11



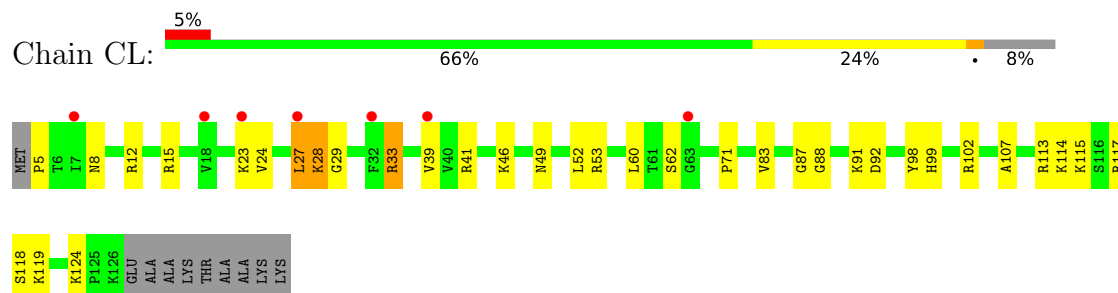
• Molecule 11: 30S Ribosomal Protein S11



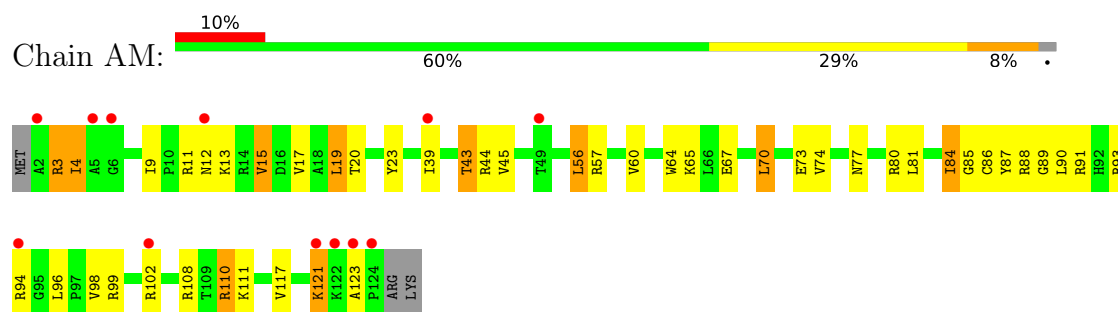
- Molecule 12: 30S Ribosomal Protein S12



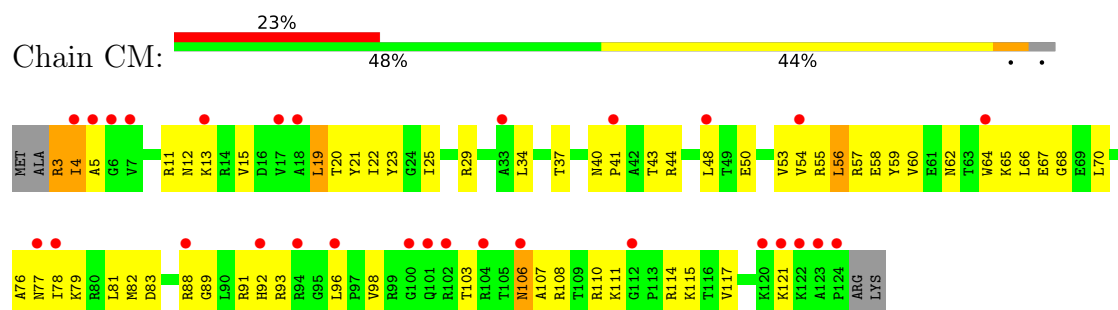
- Molecule 12: 30S Ribosomal Protein S12



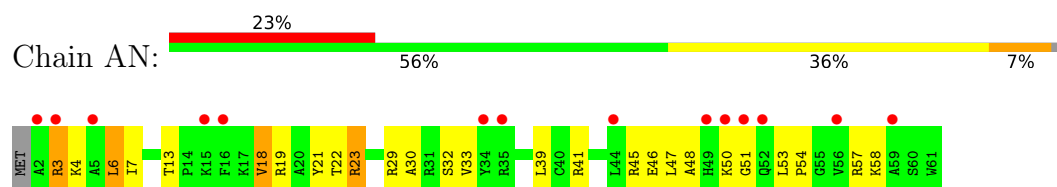
- Molecule 13: 30S Ribosomal Protein S13



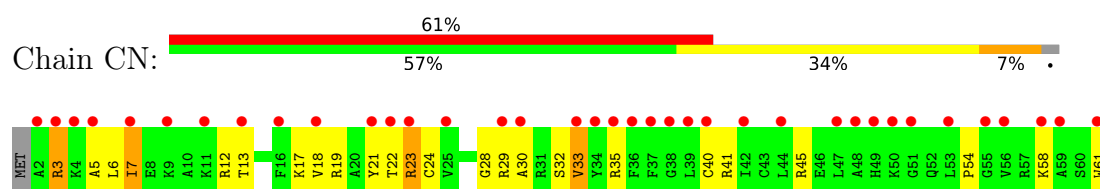
- Molecule 13: 30S Ribosomal Protein S13



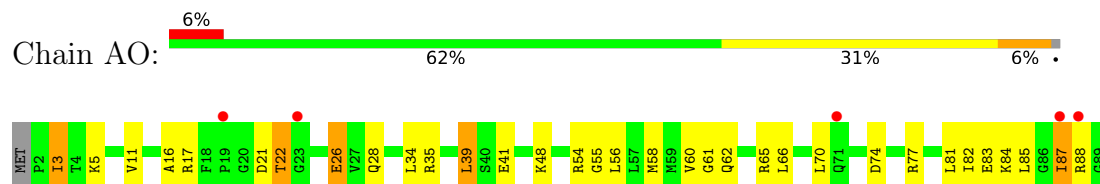
- Molecule 14: 30S Ribosomal Protein S14



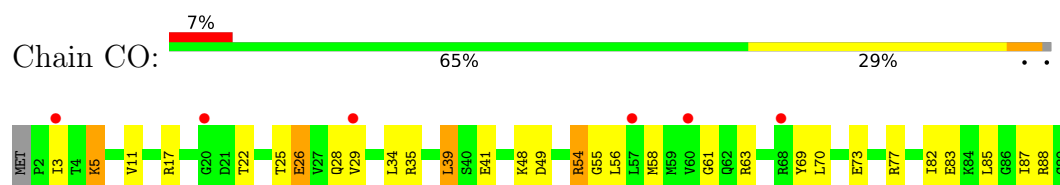
- Molecule 14: 30S Ribosomal Protein S14



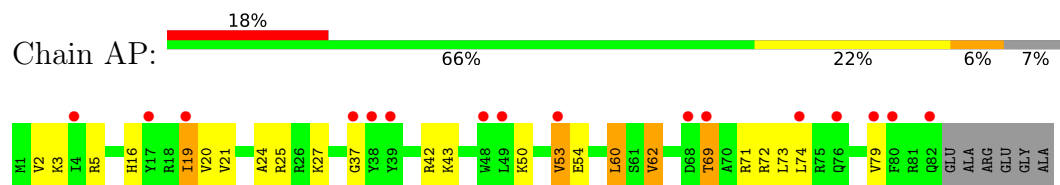
• Molecule 15: 30S Ribosomal Protein S15



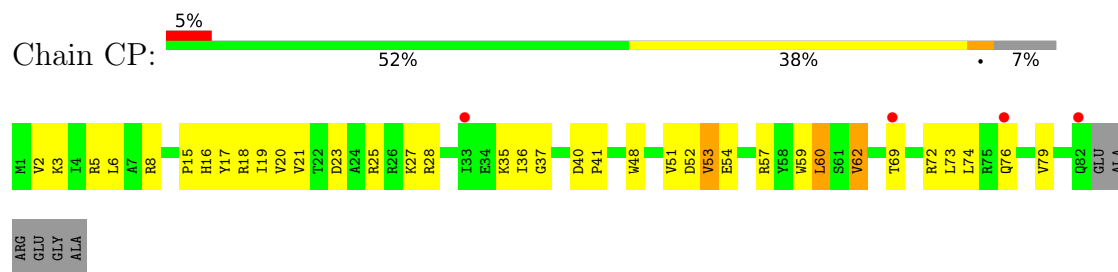
• Molecule 15: 30S Ribosomal Protein S15



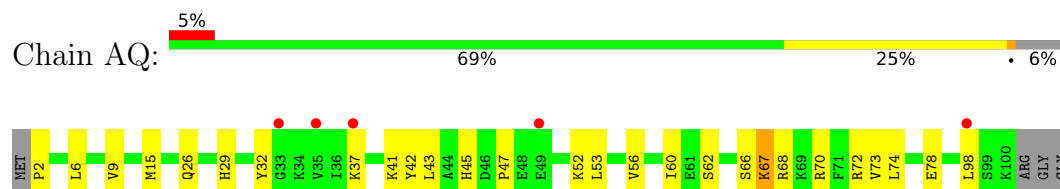
• Molecule 16: 30S Ribosomal Protein S16



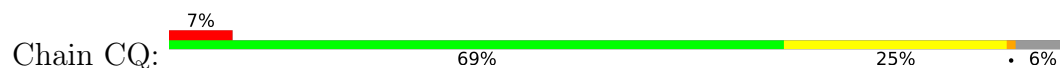
• Molecule 16: 30S Ribosomal Protein S16



• Molecule 17: 30S Ribosomal Protein S17

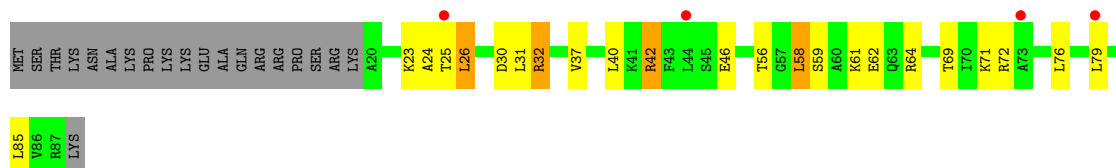


• Molecule 17: 30S Ribosomal Protein S17

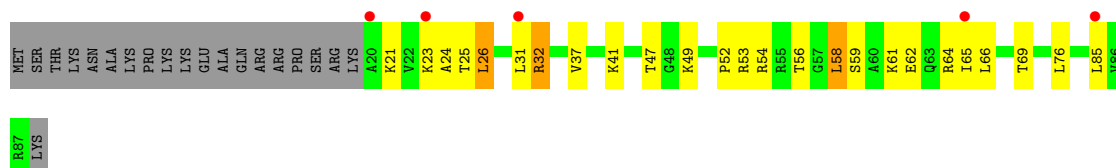




• Molecule 18: 30S Ribosomal Protein S18



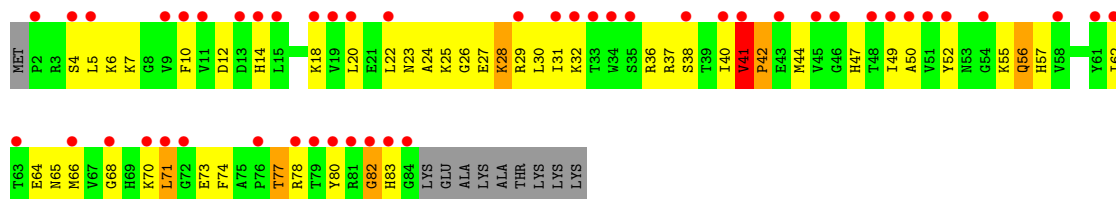
• Molecule 18: 30S Ribosomal Protein S18



• Molecule 19: 30S Ribosomal Protein S19

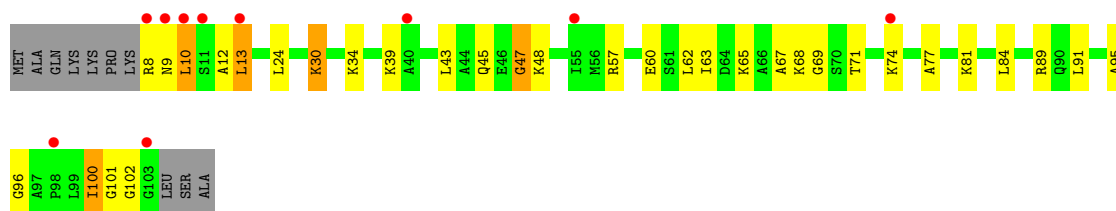


• Molecule 19: 30S Ribosomal Protein S19

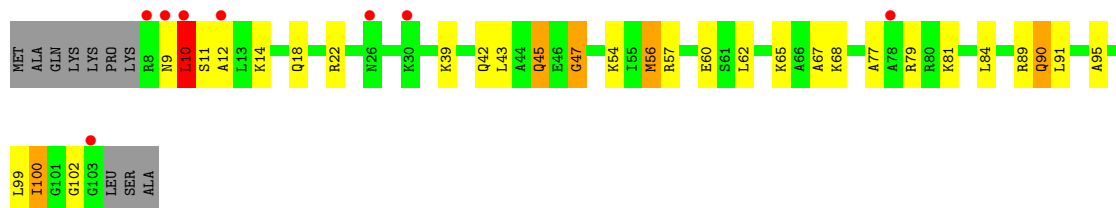


• Molecule 20: 30S Ribosomal Protein S20





● Molecule 20: 30S Ribosomal Protein S20



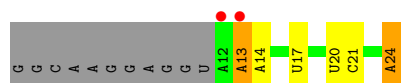
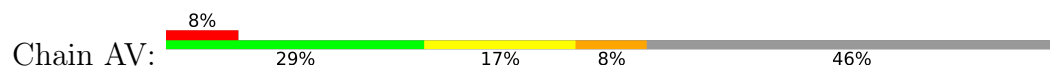
● Molecule 21: 30S Ribosomal Protein THX



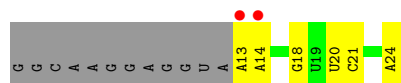
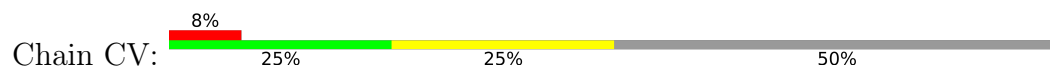
● Molecule 21: 30S Ribosomal Protein THX



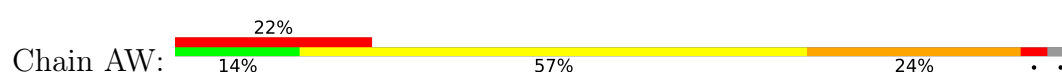
● Molecule 22: mRNA

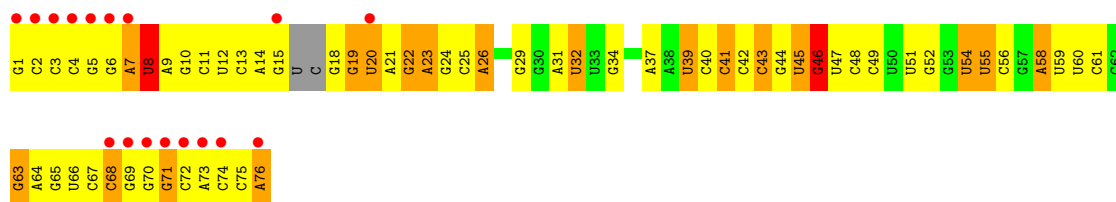


● Molecule 22: mRNA

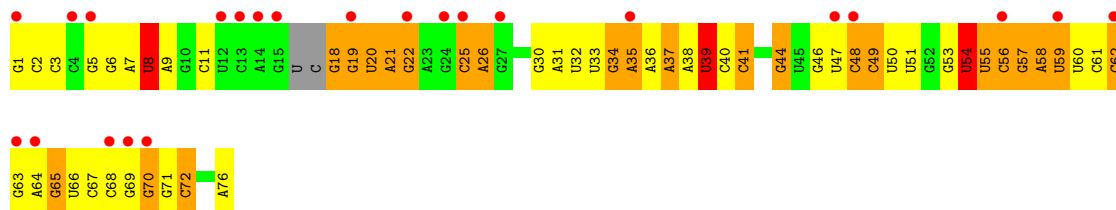
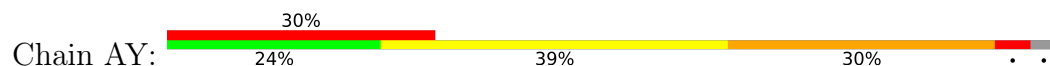


● Molecule 23: A/P-site tRNA

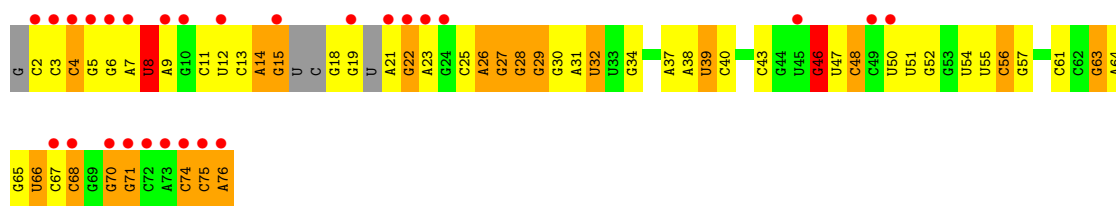
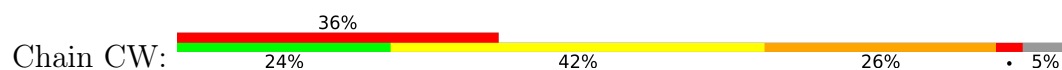




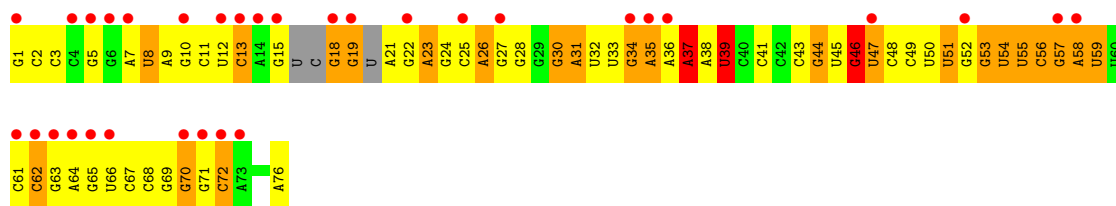
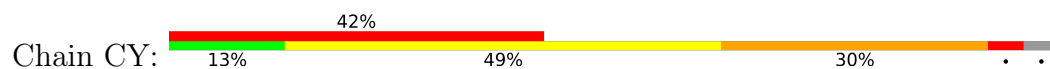
• Molecule 23: A/P-site tRNA



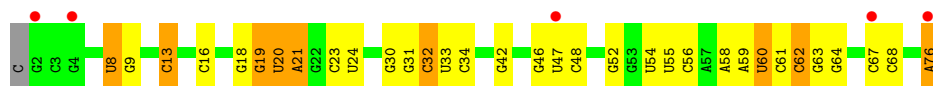
• Molecule 23: A/P-site tRNA



• Molecule 23: A/P-site tRNA

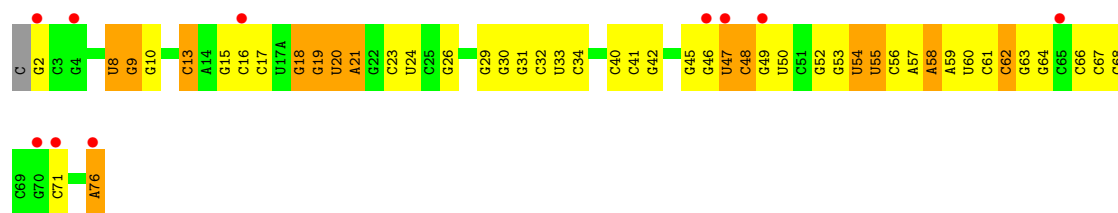


• Molecule 24: E-site tRNA

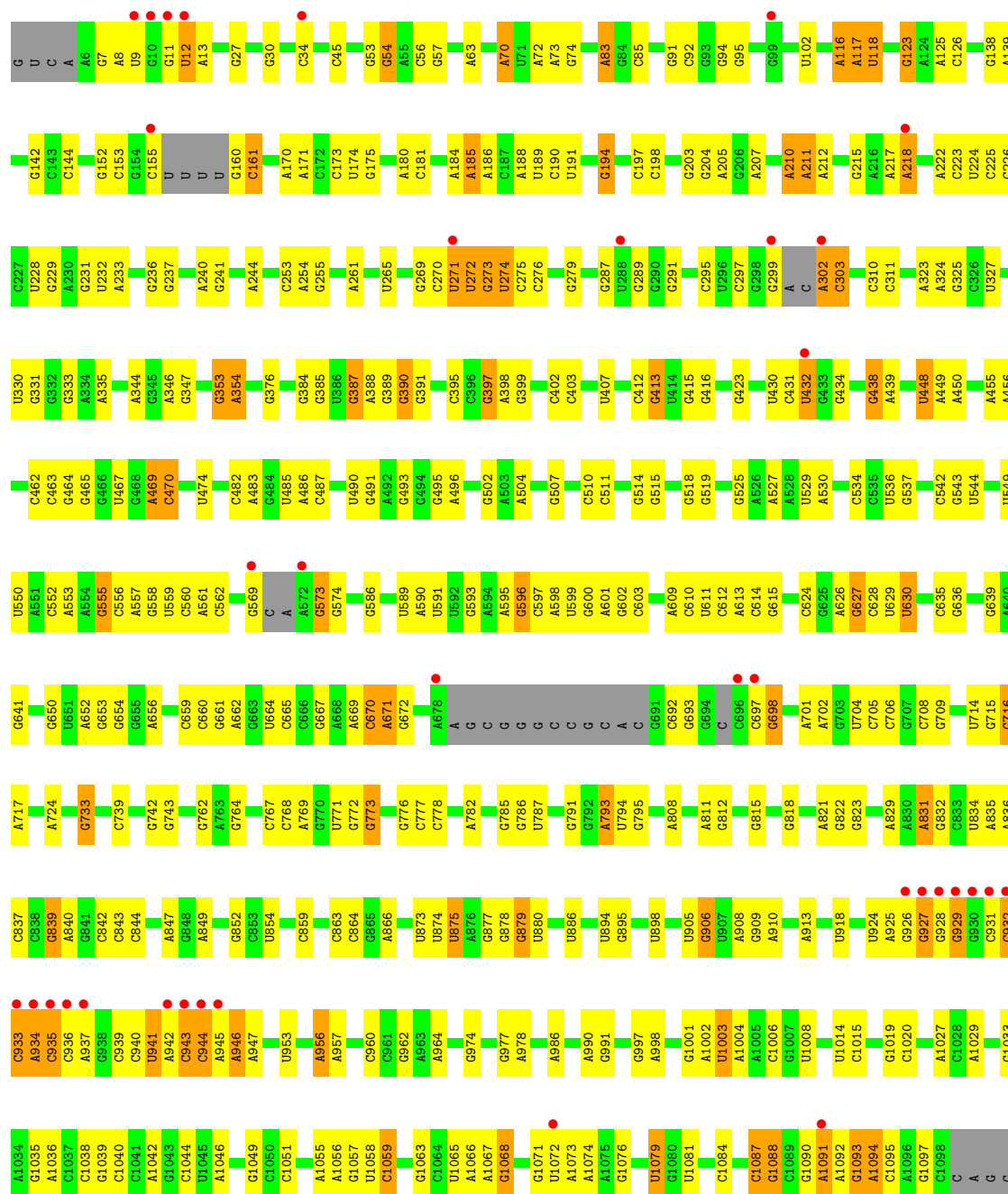


• Molecule 24: E-site tRNA

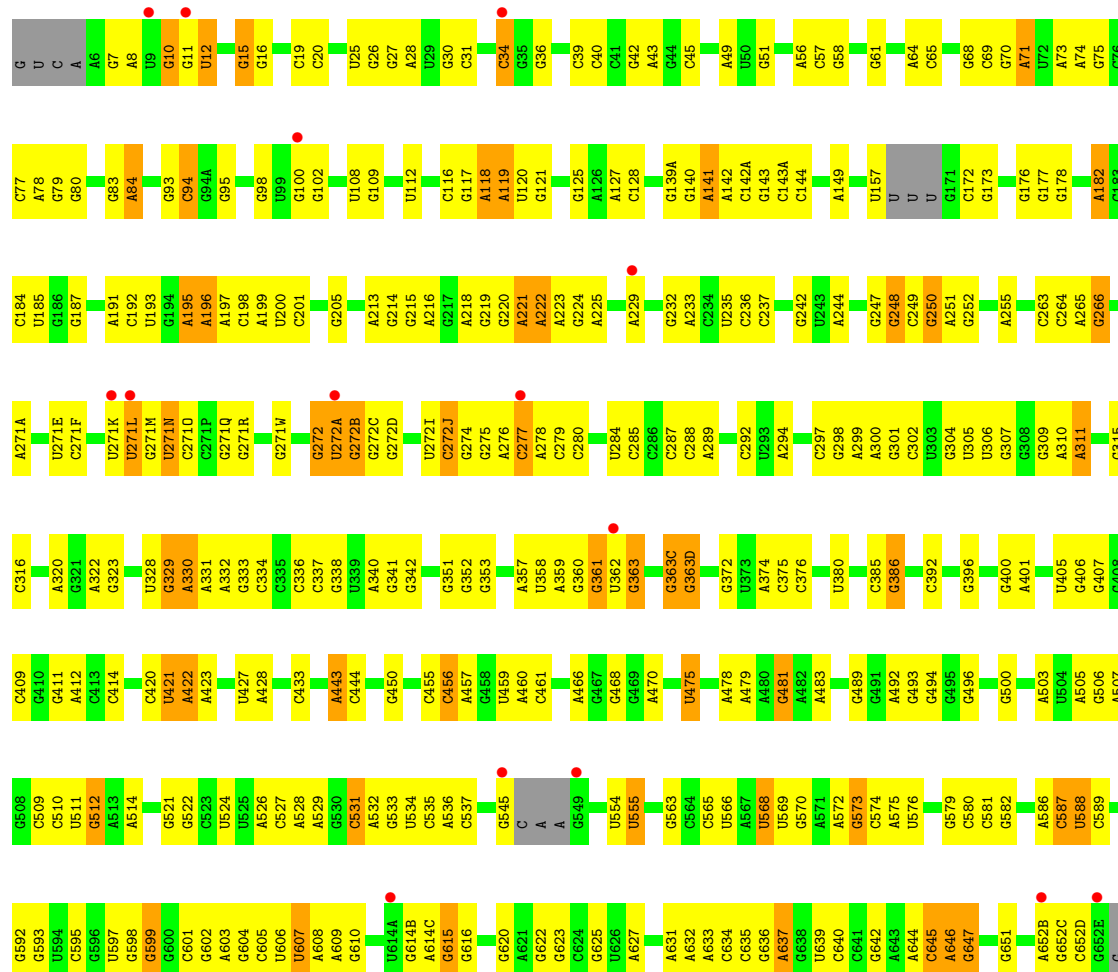




● Molecule 25: 23S Ribosomal RNA



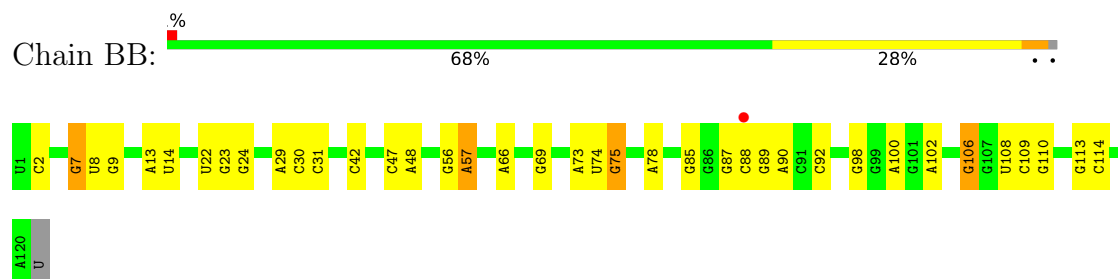




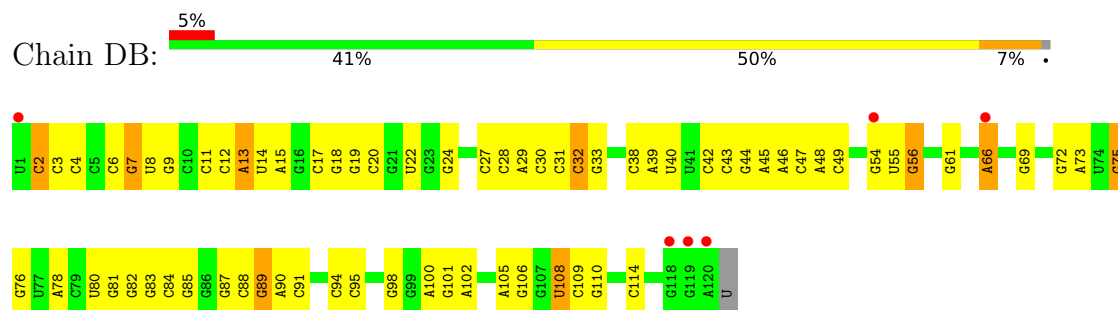
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C1711	C1598	A1509A	G1421	U1329		G1149	A	U1023	A953	C889	C813	G726	C
U1712	A1608	A1509B	G1422	C1330	G1235	C1150	A	G1024	C954	C890	C814		G
U1713	A1609	G1511	A1427	G1337	A1236	C1151	G	U1026	C955	A890	C817	G729	C
G1714	A1610	U1512	C1428	G1338	A1237	C1152	A	U1027	C956	G892	G818	C730	A
G1721	A1611	C1513	G1429	G1339	G1238	C1153	A	A1028	A957	C893	C819	C731	C
A1722	A1612	U1514	U1341	G1340	U1240	C1154	U	A1029	A958	C894	A819		G
U1739	A1613	G1515	U1342	U1241	A1241	A1155	G	G1030	A959	A895	A820	A734	C
A1741	A1614	G1516	G1243	G1244	G1245	G1157	C	G1031	A960	A896	G821		G
G1742	A1615	G1517	G1246	G1247	G1248	G1158	U	A1032	C961	C897	U740		G
C1745A	G1626	C1520	U1352	U1353	A1249	U1159	A	U1033	C962	A899	C825		C
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U1753	U1629	C1522	C145A	C145B	G1251	G1161	A	G1038	C971	C903	U828	G745	G652U
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G1756	A1634	C1536	A1449	U1357	A1254	C1164	U	G1041	C974	U906	U833	C749	U857
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G1758	U1639	G1538	A1452	A1359	G1256	G1166	A	G1043	C976	A910	U839	A752	C659
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A1773	G1643	A1545	G1462	G1366	A1265	G	U	A	C981	C914	U847	A761	G666
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G1799	A1689	U1580	G1487	G1400	G1303	U1204	A	A	A1000	C936	C865	G792	C593
C1800	U1693	G1581	G1488	G1401	G1304	U1205	U	A	A1001	U937	C866	C796	C698
A1801	G1694	A1582	A1490	U1405	C1314	G1206	C	C	G1002	G938	G874	C797	G700
U1802	C1804	C1583	G1492	U1406	C1315	G1207	A	A	G1003	G939	G875	G798	A705
A1803	U1805	A1584	C1493	U1407	U1316	A1210	C	C	C1005	G940	A878	A802	A706
G1812	G1697	C1585	A1494	C1408	U1317	U1211	A	G	U1007	G941	G879		
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G1814	G1699	U1589	U1497	G1410	A1213	C1213	A	C	C1013	G944	G881	C806	G710
A1815	A1700	U1590	A1321	C1320	C1214	U1141	U	A	U1014	G945	C882	U807	G711
G1816	A1701	U1591	G1325	A1326	A1220	U1142	C	C	G1015	G946	G883	G808	G717
G1817	G1702	C1504	G1326	U1326	C1224	A1142A	C	U	U1019	G948	C884		
	G1703	G1594	G1327	U1327	G1225	A1143	U		A1020	C950	C885	U810	

G2867	G2868	G2869	G2870	G2871	G2872	G2876	G2879	G2880	G2881	G2882	U2887	G2883	G2884	G2889	G2891	G2892	G2893	G2894	G2895	G2896	U2897	U	G	A	G	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C
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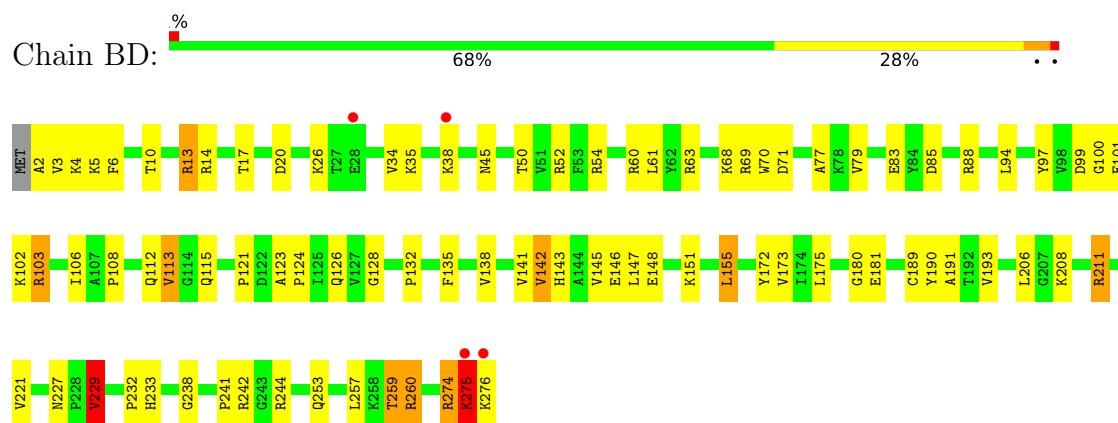
- Molecule 26: 5S Ribosomal RNA



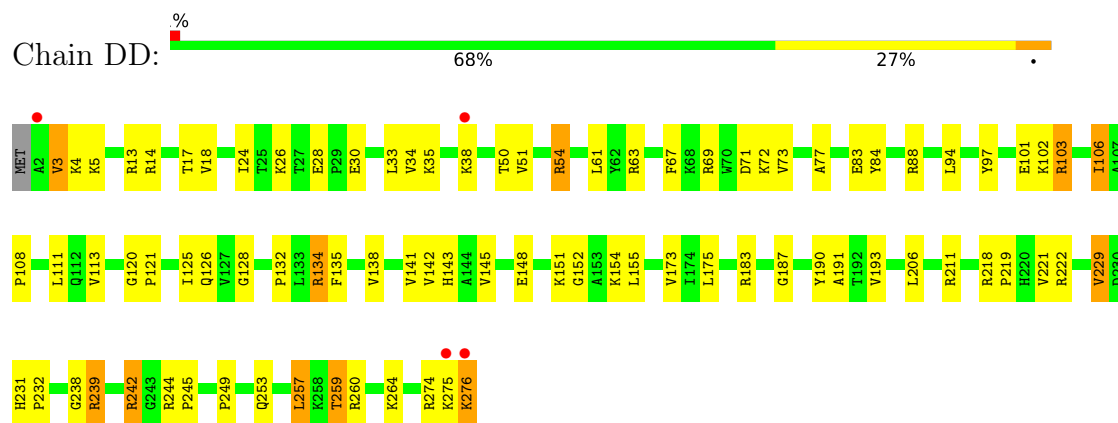
- Molecule 26: 5S Ribosomal RNA



- Molecule 27: 50S Ribosomal Protein L2

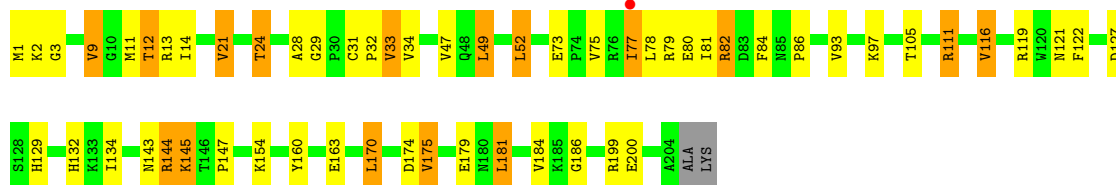


- Molecule 27: 50S Ribosomal Protein L2



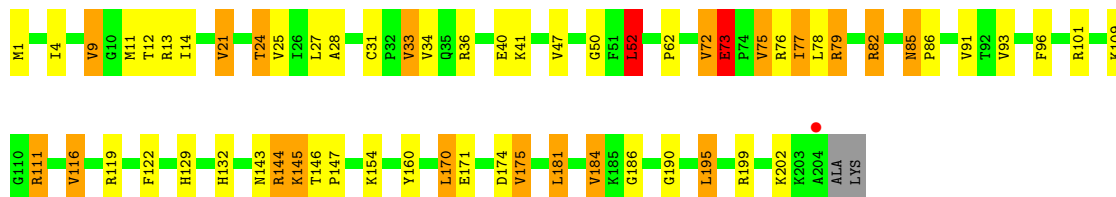
- Molecule 28: 50S Ribosomal Protein L3

Chain BE:  71% 20% 8% .



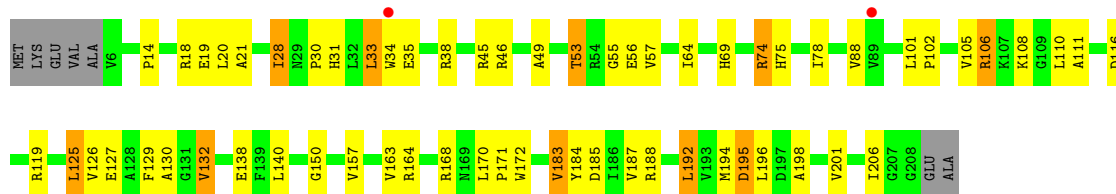
• Molecule 28: 50S Ribosomal Protein L3

Chain DE:  69% 19% 9% ..



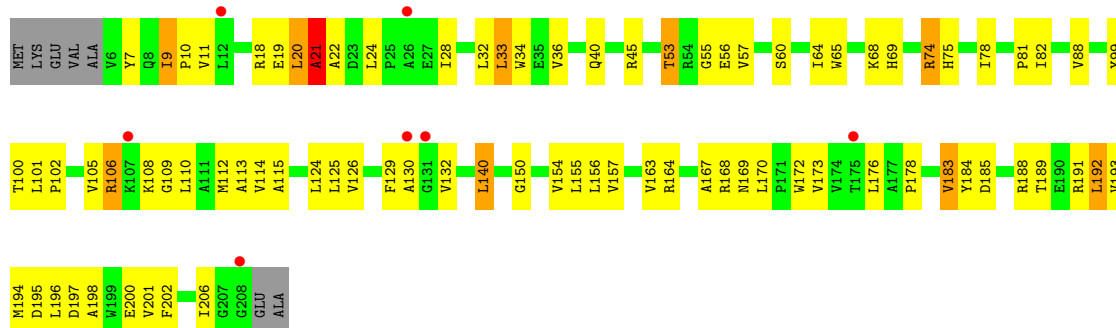
• Molecule 29: 50S Ribosomal Protein L4

Chain BF:  % 67% 25% 5% .



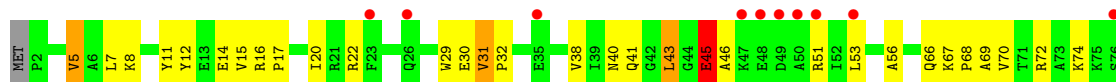
• Molecule 29: 50S Ribosomal Protein L4

Chain DF:  3% 57% 35% ..



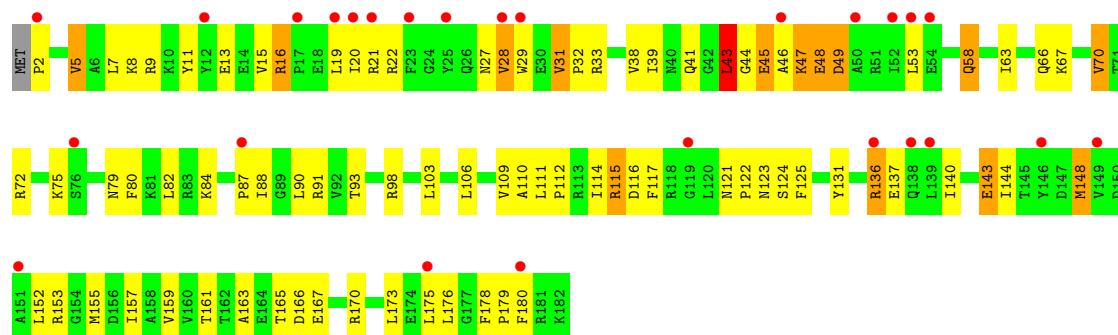
• Molecule 30: 50S Ribosomal Protein L5

Chain BG:  9% 61% 34% ..

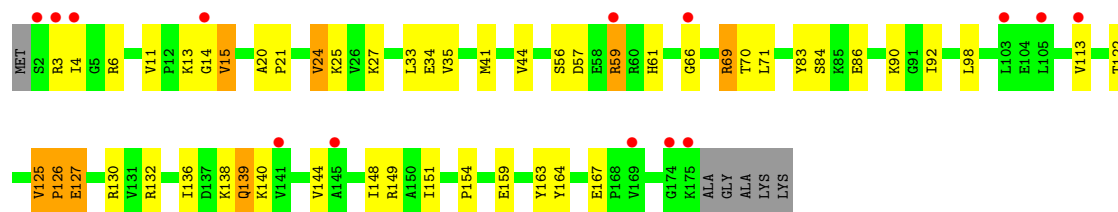




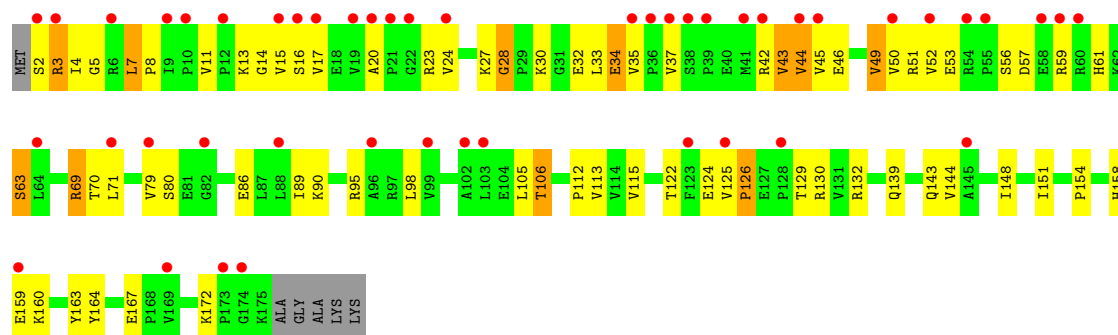
• Molecule 30: 50S Ribosomal Protein L5



• Molecule 31: 50S Ribosomal Protein L6

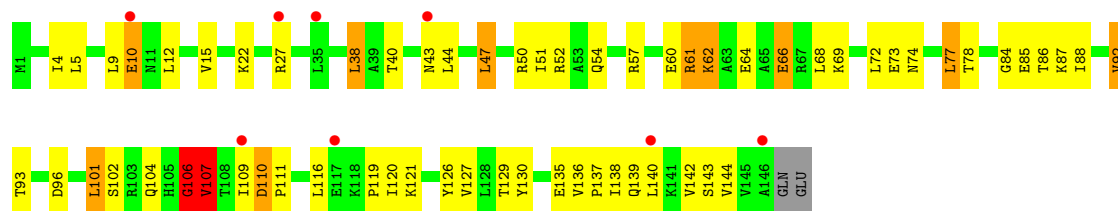


• Molecule 31: 50S Ribosomal Protein L6

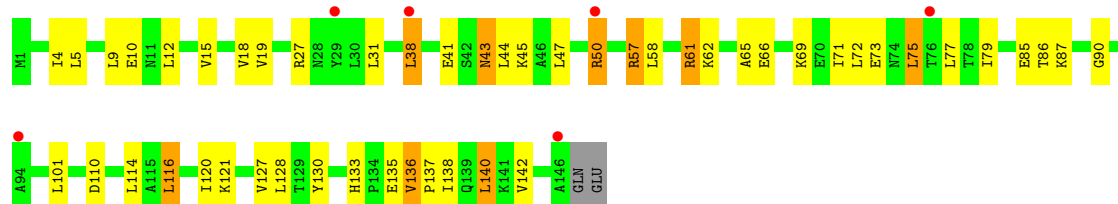


• Molecule 32: 50S Ribosomal Protein L9

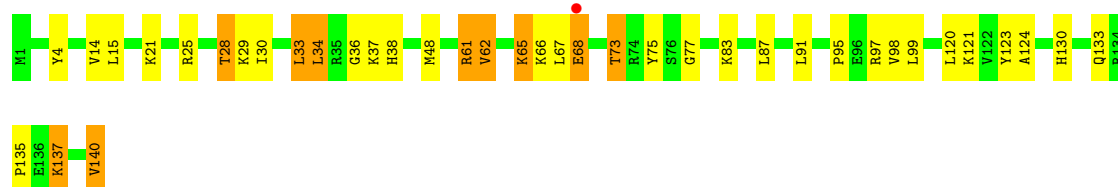
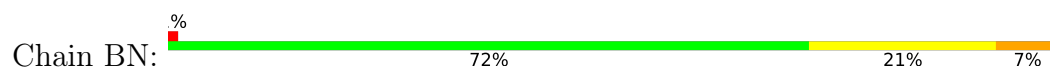




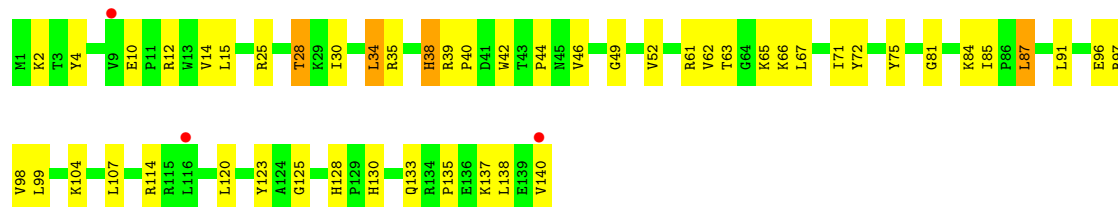
• Molecule 32: 50S Ribosomal Protein L9



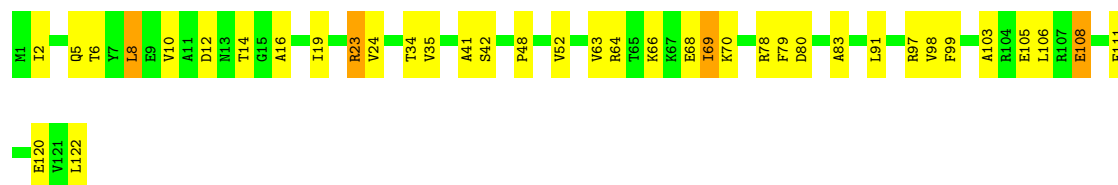
• Molecule 33: 50S Ribosomal Protein L13



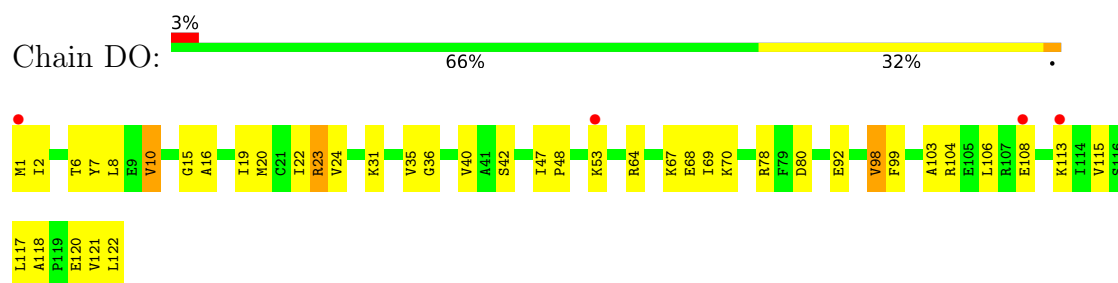
• Molecule 33: 50S Ribosomal Protein L13



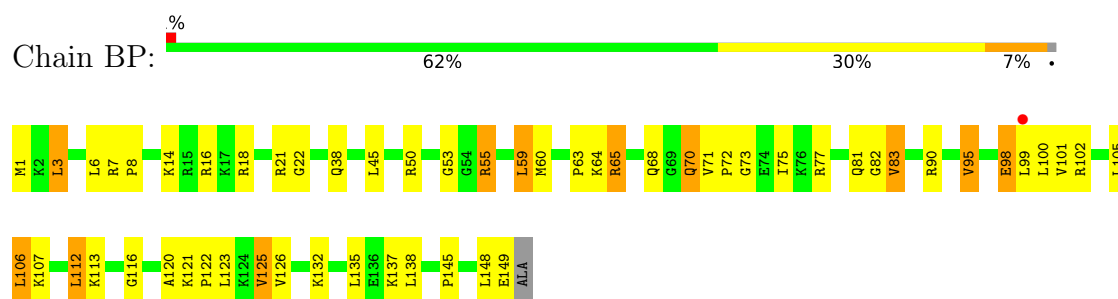
• Molecule 34: 50S Ribosomal Protein L14



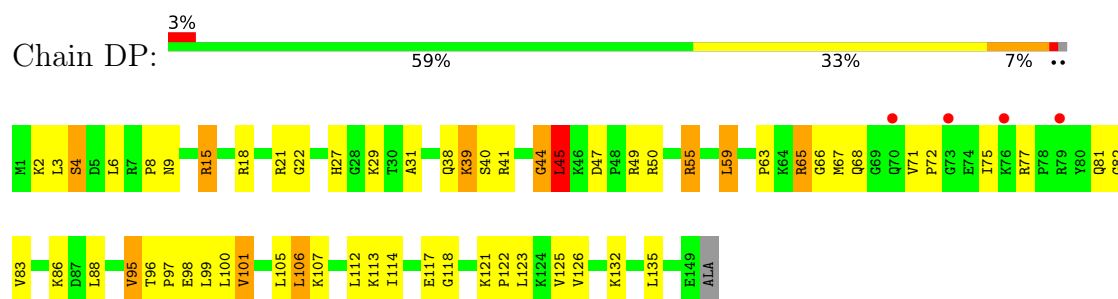
• Molecule 34: 50S Ribosomal Protein L14



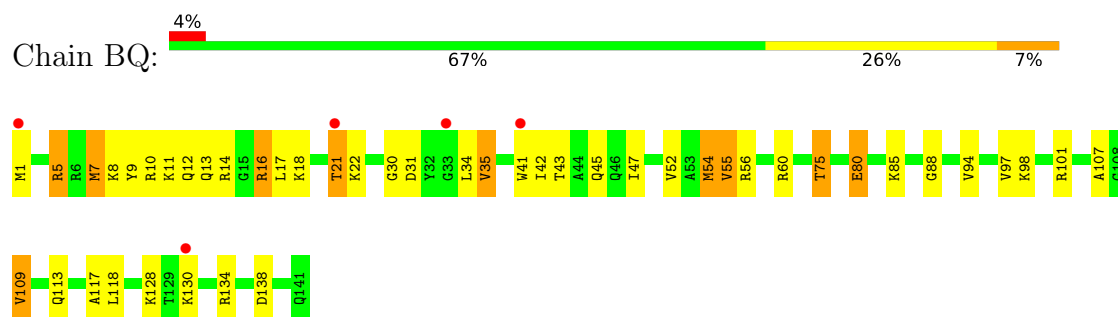
• Molecule 35: 50S Ribosomal Protein L15



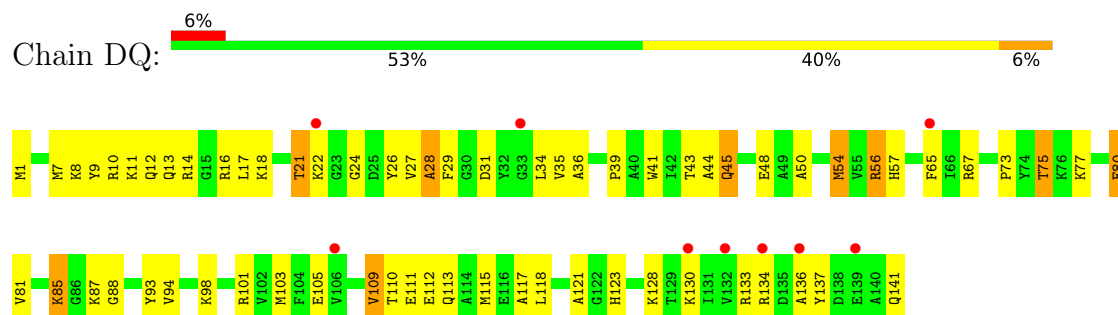
• Molecule 35: 50S Ribosomal Protein L15



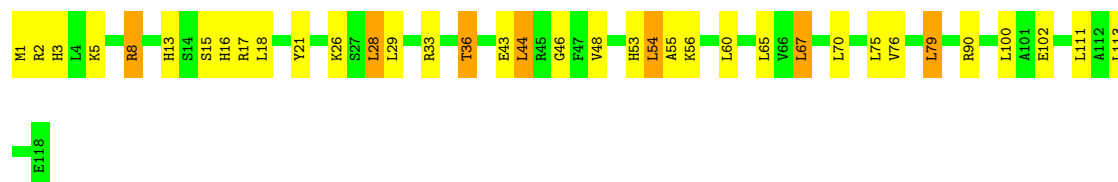
• Molecule 36: 50S Ribosomal Protein L16



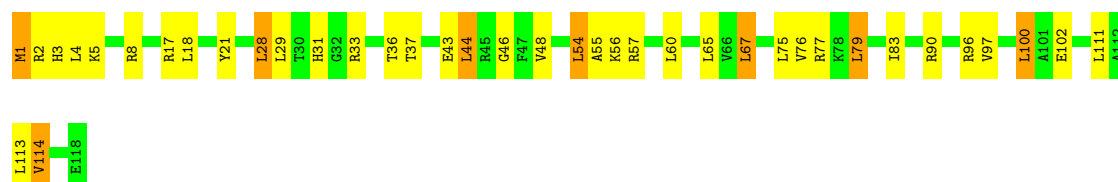
• Molecule 36: 50S Ribosomal Protein L16



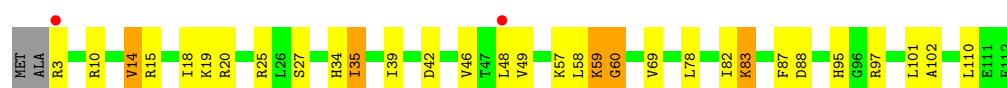
• Molecule 37: 50S Ribosomal Protein L17

Chain BR: 

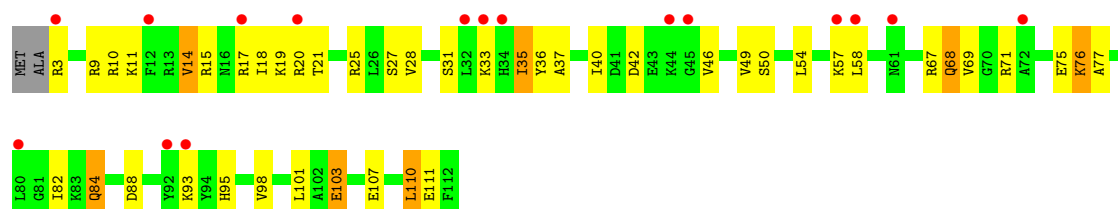
• Molecule 37: 50S Ribosomal Protein L17

Chain DR: 

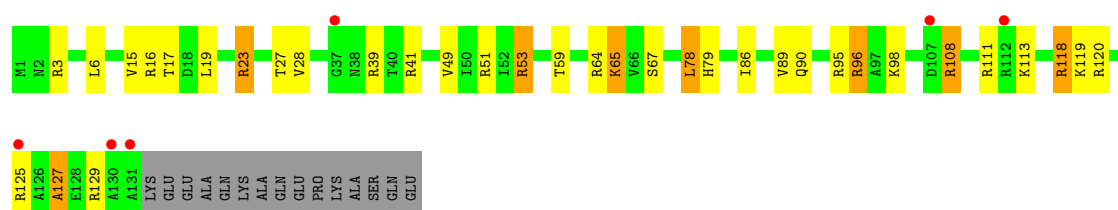
• Molecule 38: 50S Ribosomal Protein L18

Chain BS: 

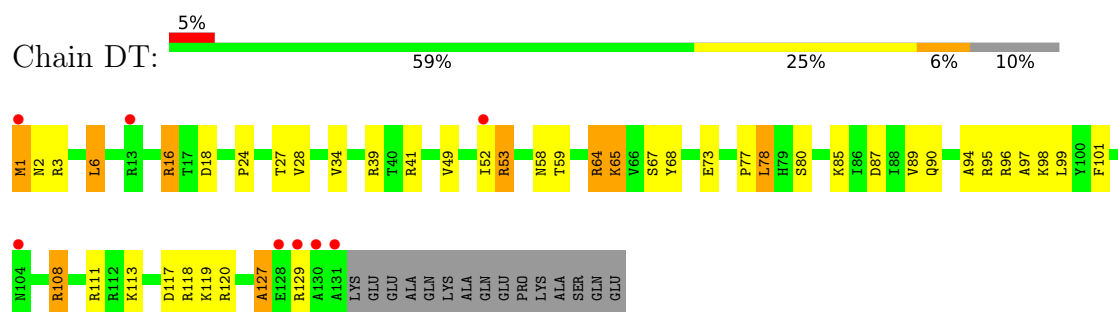
• Molecule 38: 50S Ribosomal Protein L18

Chain DS: 

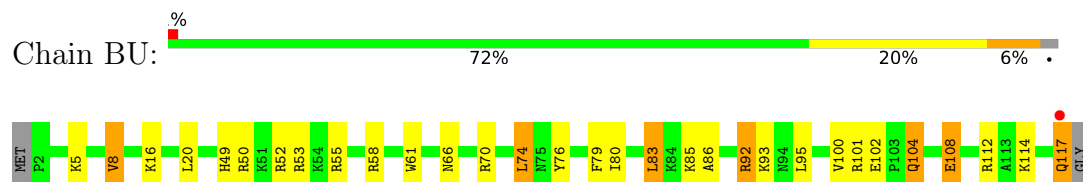
• Molecule 39: 50S Ribosomal Protein L19

Chain BT: 

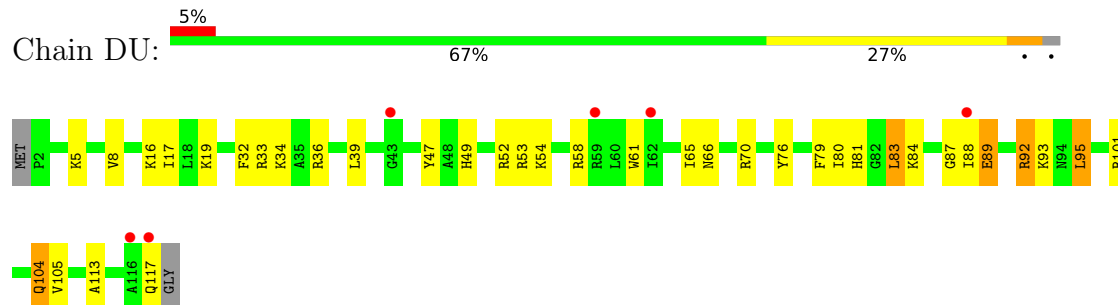
• Molecule 39: 50S Ribosomal Protein L19



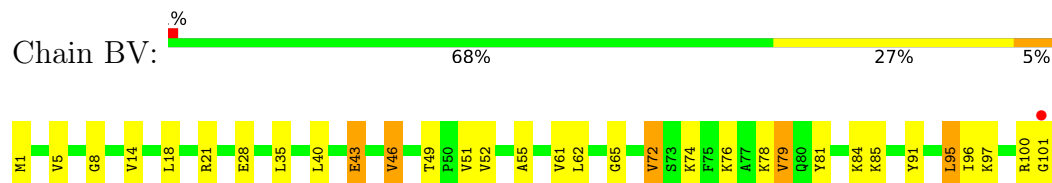
- Molecule 40: 50S Ribosomal Protein L20



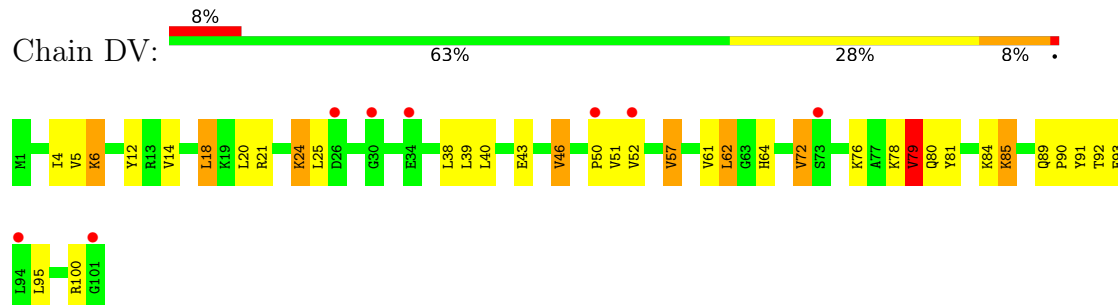
- Molecule 40: 50S Ribosomal Protein L20



- Molecule 41: 50S Ribosomal Protein L21

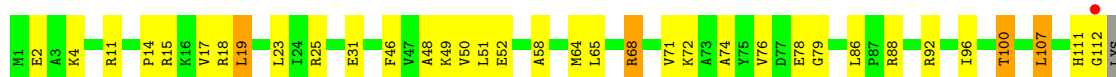


- Molecule 41: 50S Ribosomal Protein L21

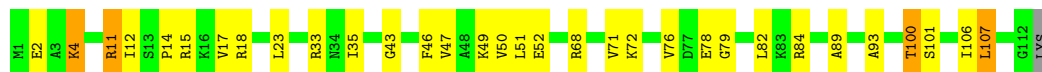


- Molecule 42: 50S Ribosomal Protein L22

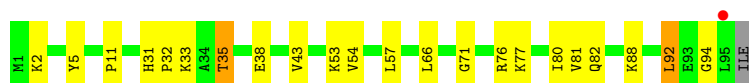
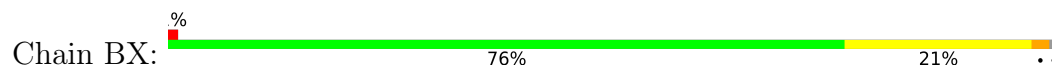




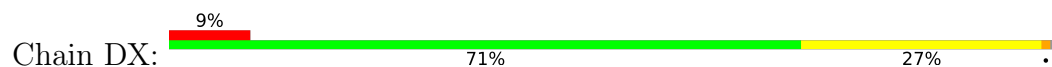
• Molecule 42: 50S Ribosomal Protein L22



• Molecule 43: 50S Ribosomal Protein L23



• Molecule 43: 50S Ribosomal Protein L23

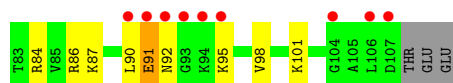
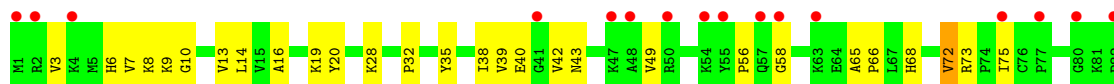


• Molecule 44: 50S Ribosomal Protein L24



GLU
GLU

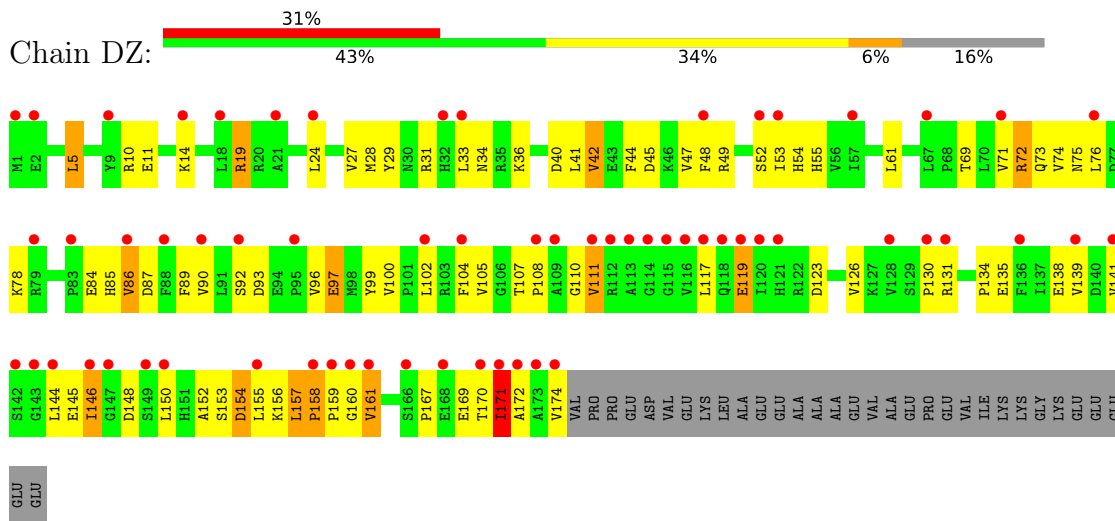
• Molecule 44: 50S Ribosomal Protein L24



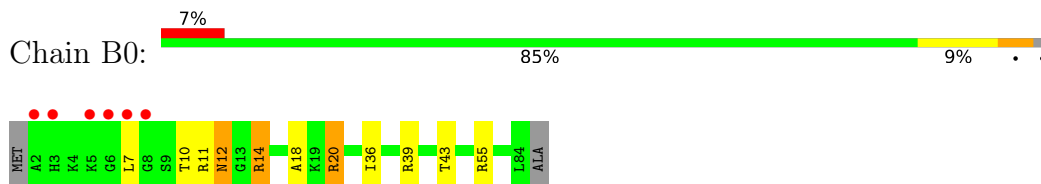
• Molecule 45: 50S Ribosomal Protein L25



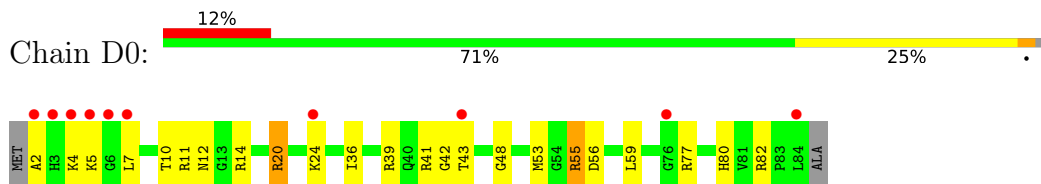
- Molecule 45: 50S Ribosomal Protein L25



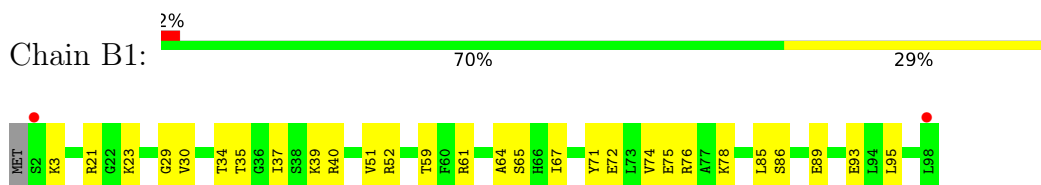
● Molecule 46: 50S Ribosomal Protein L27



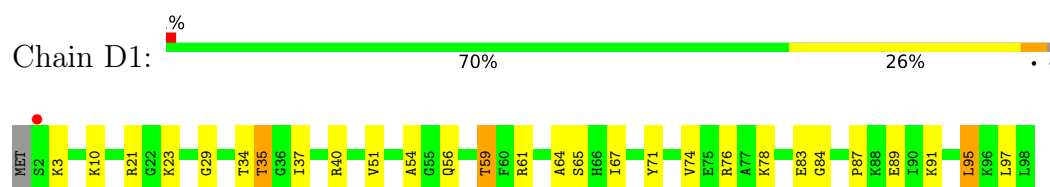
- Molecule 46: 50S Ribosomal Protein L27



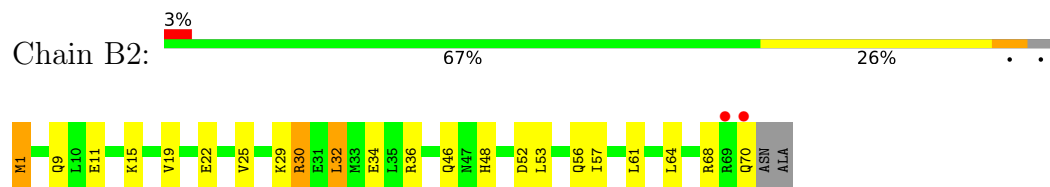
- Molecule 47: 50S Ribosomal Protein L28



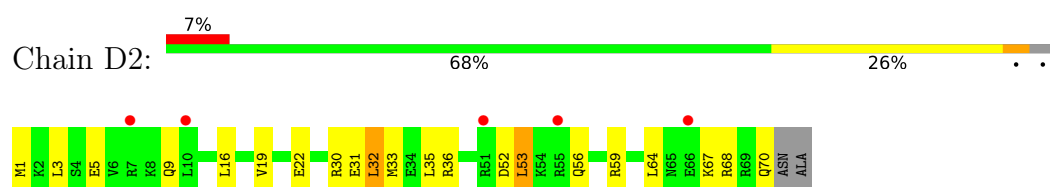
- Molecule 47: 50S Ribosomal Protein L28



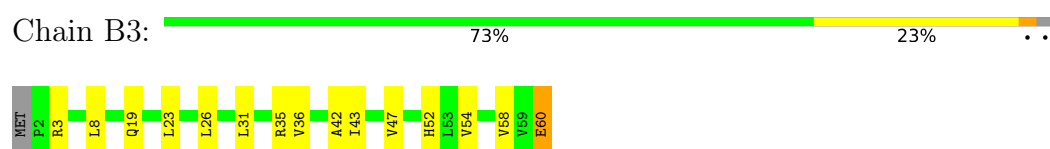
• Molecule 48: 50S Ribosomal Protein L29



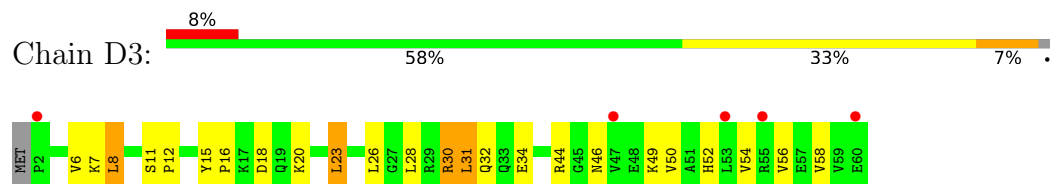
• Molecule 48: 50S Ribosomal Protein L29



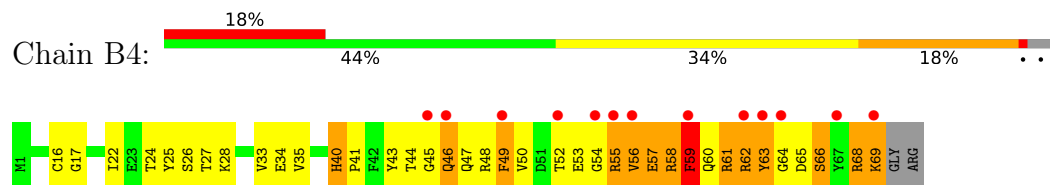
• Molecule 49: 50S Ribosomal Protein L30



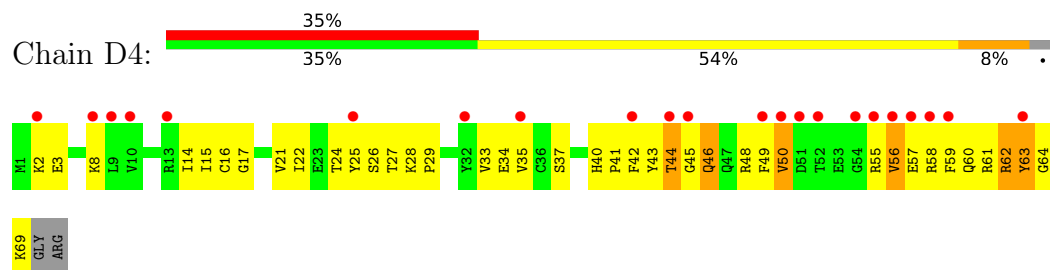
• Molecule 49: 50S Ribosomal Protein L30



• Molecule 50: 50S Ribosomal Protein L31



• Molecule 50: 50S Ribosomal Protein L31



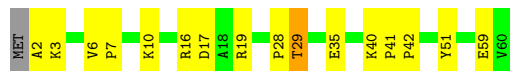
- Molecule 51: 50S Ribosomal Protein L32

Chain B5:  63% 28% 7% .



- Molecule 51: 50S Ribosomal Protein L32

Chain D5:  72% 25% . .



- Molecule 52: 50S Ribosomal Protein L33

Chain B6:  70% 20% 7% .



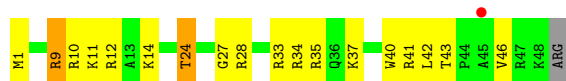
- Molecule 52: 50S Ribosomal Protein L33

Chain D6:  7% 67% 31% .



- Molecule 53: 50S Ribosomal Protein L34

Chain B7:  2% 61% 33% . .



- Molecule 53: 50S Ribosomal Protein L34

Chain D7:  2% 69% 27% . .

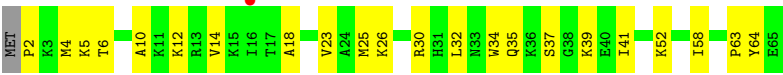


- Molecule 54: 50S Ribosomal Protein L35

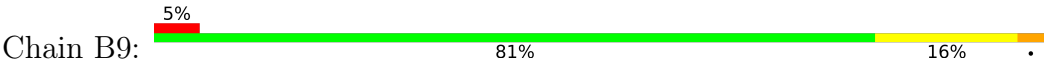
Chain B8:  54% 42% . .



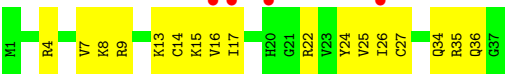
- Molecule 54: 50S Ribosomal Protein L35



● 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, α , β , γ	208.25Å 443.61Å 619.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.25 – 2.70 124.25 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (124.25-2.70) 97.2 (124.25-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.210 , 0.257 0.212 , 0.258	Depositor DCC
R_{free} test set	75600 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	297376	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 7MG, 5MC, K, ZN, PSU, 5MU, NEG, MIA, SF4, 4SU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.25	0/36002	0.45	1/56188 (0.0%)
1	CA	0.24	0/36170	0.46	0/56452
2	AB	0.40	0/1881	1.02	10/2542 (0.4%)
2	CB	0.42	0/1860	1.03	7/2518 (0.3%)
3	AC	0.40	0/1576	0.85	1/2130 (0.0%)
3	CC	0.40	0/1566	0.91	4/2119 (0.2%)
4	AD	0.39	0/1689	0.88	2/2267 (0.1%)
4	CD	0.41	0/1704	0.89	3/2284 (0.1%)
5	AE	0.45	0/1145	0.90	1/1543 (0.1%)
5	CE	0.42	0/1149	0.96	2/1548 (0.1%)
6	AF	0.41	0/819	0.76	0/1111
6	CF	0.39	0/829	0.74	0/1123
7	AG	0.39	0/1250	0.87	1/1679 (0.1%)
7	CG	0.37	0/1254	0.92	4/1683 (0.2%)
8	AH	0.39	0/1108	0.85	0/1494
8	CH	0.38	0/1108	0.85	4/1494 (0.3%)
9	AI	0.40	0/1002	0.91	0/1346
9	CI	0.40	0/997	0.89	1/1343 (0.1%)
10	AJ	0.39	0/722	0.91	1/982 (0.1%)
10	CJ	0.44	0/727	0.97	4/988 (0.4%)
11	AK	0.42	0/844	0.83	0/1145
11	CK	0.42	0/848	0.85	0/1149
12	AL	0.45	0/946	0.81	0/1274
12	CL	0.40	0/946	0.92	3/1274 (0.2%)
13	AM	0.40	0/969	0.93	1/1302 (0.1%)
13	CM	0.40	0/961	0.93	1/1291 (0.1%)
14	AN	0.38	0/501	0.84	2/664 (0.3%)
14	CN	0.41	0/501	0.87	2/664 (0.3%)
15	AO	0.45	0/739	0.87	1/985 (0.1%)
15	CO	0.38	0/739	0.79	0/985
16	AP	0.43	0/697	0.87	1/939 (0.1%)
16	CP	0.41	0/693	0.77	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.39	0/836	0.80	1/1117 (0.1%)
17	CQ	0.37	0/836	0.81	0/1117
18	AR	0.41	0/560	0.79	0/746
18	CR	0.36	0/560	0.78	0/746
19	AS	0.37	0/667	0.90	2/900 (0.2%)
19	CS	0.46	0/661	1.03	3/893 (0.3%)
20	AT	0.38	0/730	0.91	0/965
20	CT	0.41	0/729	0.90	1/965 (0.1%)
21	AU	0.36	0/203	0.87	0/266
21	CU	0.41	0/203	0.83	0/266
22	AV	0.26	0/310	0.37	0/480
22	CV	0.24	0/282	0.42	0/437
23	AW	0.30	1/1602 (0.1%)	0.48	0/2493
23	AY	0.31	1/1602 (0.1%)	0.50	0/2493
23	CW	0.29	0/1556	0.45	0/2418
23	CY	0.31	1/1579 (0.1%)	0.49	0/2455
24	AX	0.31	0/1725	0.47	0/2689
24	CX	0.29	1/1725 (0.1%)	0.46	0/2689
25	BA	0.36	0/68083	0.49	1/106274 (0.0%)
25	DA	0.27	0/67542	0.48	1/105428 (0.0%)
26	BB	0.30	0/2878	0.50	0/4490
26	DB	0.26	0/2878	0.43	0/4490
27	BD	0.56	0/2186	0.91	4/2944 (0.1%)
27	DD	0.49	0/2186	0.88	0/2944
28	BE	0.59	0/1592	0.88	0/2149
28	DE	0.47	0/1592	0.96	9/2149 (0.4%)
29	BF	0.53	0/1619	0.89	0/2193
29	DF	0.43	0/1615	0.90	3/2188 (0.1%)
30	BG	0.42	0/1450	0.87	3/1959 (0.2%)
30	DG	0.39	0/1449	0.93	1/1958 (0.1%)
31	BH	0.49	0/1356	0.86	3/1834 (0.2%)
31	DH	0.43	0/1356	0.97	6/1834 (0.3%)
32	BI	0.41	0/1100	0.95	4/1501 (0.3%)
32	DI	0.39	0/1076	0.88	2/1471 (0.1%)
33	BN	0.52	0/1144	0.83	0/1543
33	DN	0.39	0/1144	0.88	2/1543 (0.1%)
34	BO	0.54	0/943	0.91	0/1269
34	DO	0.42	0/943	0.84	0/1269
35	BP	0.52	0/1152	0.85	2/1533 (0.1%)
35	DP	0.43	0/1152	0.96	5/1533 (0.3%)
36	BQ	0.53	0/1143	0.80	1/1527 (0.1%)
36	DQ	0.44	0/1143	0.85	1/1527 (0.1%)
37	BR	0.55	0/982	0.88	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DR	0.44	0/982	0.81	0/1312
38	BS	0.46	0/887	0.82	0/1180
38	DS	0.37	0/880	0.89	0/1172
39	BT	0.50	0/1105	0.85	0/1477
39	DT	0.41	0/1097	0.80	0/1468
40	BU	0.56	0/977	0.85	0/1301
40	DU	0.39	0/977	0.80	0/1301
41	BV	0.53	0/782	0.85	0/1049
41	DV	0.37	0/782	0.80	0/1049
42	BW	0.59	0/897	0.85	0/1205
42	DW	0.45	0/897	0.81	0/1205
43	BX	0.54	0/764	0.85	0/1025
43	DX	0.44	0/764	0.87	0/1025
44	BY	0.47	0/819	0.90	1/1095 (0.1%)
44	DY	0.38	0/819	0.85	1/1095 (0.1%)
45	BZ	0.45	0/1379	0.99	6/1873 (0.3%)
45	DZ	0.41	0/1390	0.98	5/1890 (0.3%)
46	B0	0.52	0/662	0.90	2/881 (0.2%)
46	D0	0.37	0/662	0.81	2/881 (0.2%)
47	B1	0.52	0/762	0.86	0/1014
47	D1	0.43	0/762	0.85	0/1014
48	B2	0.49	0/590	0.85	0/781
48	D2	0.33	0/590	0.75	0/781
49	B3	0.51	0/474	0.93	0/635
49	D3	0.36	0/469	0.83	0/630
50	B4	0.46	0/571	1.16	7/768 (0.9%)
50	D4	0.46	0/545	0.98	0/737
51	B5	0.57	0/469	0.94	1/635 (0.2%)
51	D5	0.44	0/469	0.82	0/635
52	B6	0.53	0/460	0.77	0/613
52	D6	0.41	0/456	0.70	0/608
53	B7	0.58	0/426	0.78	0/561
53	D7	0.51	0/426	0.81	1/561 (0.2%)
54	B8	0.56	0/525	0.82	0/691
54	D8	0.45	0/525	0.80	0/691
55	B9	0.50	0/310	0.79	0/407
55	D9	0.41	0/310	0.86	0/407
All	All	0.35	4/316673 (0.0%)	0.61	138/474091 (0.0%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AY	8	4SU	O3'-P	5.81	1.62	1.56
23	CY	8	4SU	O3'-P	5.76	1.62	1.56
24	CX	8	4SU	O3'-P	5.19	1.61	1.56
23	AW	8	4SU	O3'-P	5.14	1.61	1.56

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CB	231	GLU	CA-C-N	-12.95	107.78	120.21
2	CB	231	GLU	C-N-CA	-12.95	107.78	120.21
2	AB	231	GLU	CA-C-N	-11.36	109.17	120.31
2	AB	231	GLU	C-N-CA	-11.36	109.17	120.31
45	BZ	107	THR	CA-C-N	9.64	130.03	119.90

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 [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32163	0	16234	556	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CA	32312	0	16308	638	0
2	AB	1846	0	1867	79	0
2	CB	1825	0	1828	100	0
3	AC	1552	0	1546	56	0
3	CC	1542	0	1517	59	0
4	AD	1659	0	1676	66	0
4	CD	1674	0	1714	45	0
5	AE	1129	0	1185	37	0
5	CE	1133	0	1191	40	0
6	AF	806	0	793	23	0
6	CF	816	0	808	29	0
7	AG	1231	0	1238	27	0
7	CG	1235	0	1249	38	0
8	AH	1088	0	1126	35	0
8	CH	1088	0	1126	40	0
9	AI	983	0	986	39	0
9	CI	978	0	966	46	0
10	AJ	709	0	650	32	0
10	CJ	714	0	672	48	0
11	AK	829	0	825	17	0
11	CK	833	0	836	21	0
12	AL	930	0	980	28	0
12	CL	930	0	980	31	0
13	AM	958	0	1002	42	0
13	CM	950	0	988	45	0
14	AN	492	0	529	22	0
14	CN	492	0	529	25	0
15	AO	728	0	760	22	0
15	CO	728	0	760	24	0
16	AP	681	0	697	21	0
16	CP	677	0	686	22	0
17	AQ	823	0	891	18	0
17	CQ	823	0	891	20	0
18	AR	555	0	618	17	0
18	CR	555	0	618	18	0
19	AS	652	0	662	40	0
19	CS	646	0	644	38	0
20	AT	728	0	798	21	0
20	CT	727	0	796	18	0
21	AU	199	0	208	6	0
21	CU	199	0	208	5	0
22	AV	277	0	140	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	252	0	130	6	0
23	AW	1588	0	820	68	0
23	AY	1581	0	805	59	0
23	CW	1541	0	784	46	0
23	CY	1561	0	796	64	0
24	AX	1625	0	828	14	0
24	CX	1625	0	828	31	0
25	BA	60792	0	30654	821	0
25	DA	60311	0	30412	1131	0
26	BB	2573	0	1306	23	0
26	DB	2573	0	1306	65	0
27	BD	2136	0	2218	68	0
27	DD	2136	0	2218	70	0
28	BE	1559	0	1618	36	0
28	DE	1559	0	1618	54	0
29	BF	1584	0	1625	43	0
29	DF	1580	0	1619	64	0
30	BG	1425	0	1443	42	0
30	DG	1424	0	1434	63	0
31	BH	1330	0	1407	31	0
31	DH	1330	0	1407	42	0
32	BI	1085	0	1114	38	0
32	DI	1061	0	1080	22	0
33	BN	1117	0	1184	24	0
33	DN	1117	0	1184	31	0
34	BO	933	0	996	23	0
34	DO	933	0	996	28	0
35	BP	1135	0	1212	48	0
35	DP	1135	0	1212	48	0
36	BQ	1122	0	1179	38	0
36	DQ	1122	0	1179	63	0
37	BR	968	0	1033	20	0
37	DR	968	0	1033	31	0
38	BS	877	0	938	20	0
38	DS	870	0	923	28	0
39	BT	1091	0	1151	23	0
39	DT	1083	0	1136	34	0
40	BU	959	0	1019	27	0
40	DU	959	0	1019	31	0
41	BV	771	0	830	17	0
41	DV	771	0	830	20	0
42	BW	886	0	940	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	DW	886	0	939	18	0
43	BX	750	0	814	17	0
43	DX	750	0	814	18	0
44	BY	806	0	881	28	0
44	DY	806	0	881	29	0
45	BZ	1349	0	1355	52	0
45	DZ	1360	0	1363	65	0
46	B0	653	0	674	13	0
46	D0	653	0	674	22	0
47	B1	755	0	826	18	0
47	D1	755	0	826	18	0
48	B2	588	0	643	11	0
48	D2	588	0	643	12	0
49	B3	469	0	518	6	0
49	D3	464	0	514	16	0
50	B4	558	0	544	30	0
50	D4	532	0	503	30	0
51	B5	455	0	465	15	0
51	D5	455	0	465	11	0
52	B6	453	0	473	10	0
52	D6	449	0	469	10	0
53	B7	418	0	467	20	0
53	D7	418	0	467	13	0
54	B8	517	0	582	26	0
54	D8	517	0	582	17	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
56	B2	1	0	0	0	0
56	B3	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
56	D8	1	0	0	0	0
56	DA	623	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
61	AM	2	0	0	0	0
61	AO	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
61	DD	16	0	0	2	0
61	DE	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
All	All	297376	0	196603	5695	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 5695 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%)	2	5
2	CB	229/256 (90%)	195 (85%)	24 (10%)	10 (4%)	2	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	204/239 (85%)	182 (89%)	18 (9%)	4 (2%)	6	16
3	CC	204/239 (85%)	182 (89%)	19 (9%)	3 (2%)	8	22
4	AD	206/209 (99%)	193 (94%)	12 (6%)	1 (0%)	24	48
4	CD	206/209 (99%)	196 (95%)	8 (4%)	2 (1%)	12	32
5	AE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	18	41
5	CE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	18	41
6	AF	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
6	CF	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	12	32
7	AG	153/156 (98%)	141 (92%)	9 (6%)	3 (2%)	6	16
7	CG	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	6	16
8	AH	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	18	41
8	CH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	18	41
9	AI	125/128 (98%)	113 (90%)	10 (8%)	2 (2%)	7	20
9	CI	125/128 (98%)	112 (90%)	10 (8%)	3 (2%)	4	12
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	1
11	AK	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	6	18
11	CK	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	6	18
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%)	16	37
13	CM	120/126 (95%)	107 (89%)	11 (9%)	2 (2%)	7	19
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%)	10	27
16	AP	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	9	25
16	CP	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	9	25
17	AQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	12	32
18	AR	66/88 (75%)	65 (98%)	0	1 (2%)	8	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CR	66/88 (75%)	65 (98%)	0	1 (2%)	8	22
19	AS	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	4	11
19	CS	81/93 (87%)	69 (85%)	10 (12%)	2 (2%)	4	11
20	AT	94/106 (89%)	86 (92%)	2 (2%)	6 (6%)	1	1
20	CT	94/106 (89%)	87 (93%)	1 (1%)	6 (6%)	1	1
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%)	30	54
27	DD	273/276 (99%)	255 (93%)	16 (6%)	2 (1%)	18	41
28	BE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	24	48
28	DE	202/206 (98%)	195 (96%)	5 (2%)	2 (1%)	12	32
29	BF	201/210 (96%)	199 (99%)	1 (0%)	1 (0%)	24	48
29	DF	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	12	32
30	BG	179/182 (98%)	167 (93%)	10 (6%)	2 (1%)	11	29
30	DG	179/182 (98%)	166 (93%)	10 (6%)	3 (2%)	7	19
31	BH	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21	44
31	DH	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21	44
32	BI	144/148 (97%)	128 (89%)	12 (8%)	4 (3%)	4	9
32	DI	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	9	23
33	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
33	DN	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	18	41
34	BO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16	37
34	DO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
35	BP	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	18	41
35	DP	147/150 (98%)	137 (93%)	7 (5%)	3 (2%)	6	16
36	BQ	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
36	DQ	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	18	41
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%)	14	35
38	DS	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	14	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	BT	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	37
39	DT	129/146 (88%)	124 (96%)	4 (3%)	1 (1%)	16	37
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%)	12	32
41	DV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	32
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%)	12	32
44	DY	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
45	BZ	169/206 (82%)	145 (86%)	21 (12%)	3 (2%)	6	18
45	DZ	172/206 (84%)	153 (89%)	18 (10%)	1 (1%)	21	44
46	B0	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
46	D0	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	10	27
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%)	5	14
54	B8	62/65 (95%)	62 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	10	27

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%)	157 (82%)	35 (18%)	2	5
2	CB	187/220 (85%)	156 (83%)	31 (17%)	2	6
3	AC	143/188 (76%)	128 (90%)	15 (10%)	6	17
3	CC	140/188 (74%)	123 (88%)	17 (12%)	5	12
4	AD	170/181 (94%)	158 (93%)	12 (7%)	13	33
4	CD	173/181 (96%)	157 (91%)	16 (9%)	8	22
5	AE	113/123 (92%)	101 (89%)	12 (11%)	6	17
5	CE	114/123 (93%)	100 (88%)	14 (12%)	4	12
6	AF	83/90 (92%)	76 (92%)	7 (8%)	10	26
6	CF	85/90 (94%)	73 (86%)	12 (14%)	3	9
7	AG	119/127 (94%)	107 (90%)	12 (10%)	7	18
7	CG	120/127 (94%)	110 (92%)	10 (8%)	10	26
8	AH	114/119 (96%)	109 (96%)	5 (4%)	25	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	114/119 (96%)	104 (91%)	10 (9%)	9	23
9	AI	90/99 (91%)	78 (87%)	12 (13%)	4	10
9	CI	89/99 (90%)	78 (88%)	11 (12%)	4	11
10	AJ	66/92 (72%)	61 (92%)	5 (8%)	12	30
10	CJ	69/92 (75%)	63 (91%)	6 (9%)	9	24
11	AK	82/99 (83%)	72 (88%)	10 (12%)	5	12
11	CK	83/99 (84%)	73 (88%)	10 (12%)	5	12
12	AL	97/109 (89%)	93 (96%)	4 (4%)	27	56
12	CL	97/109 (89%)	93 (96%)	4 (4%)	27	56
13	AM	93/101 (92%)	81 (87%)	12 (13%)	4	10
13	CM	92/101 (91%)	82 (89%)	10 (11%)	6	16
14	AN	49/50 (98%)	40 (82%)	9 (18%)	1	4
14	CN	49/50 (98%)	42 (86%)	7 (14%)	3	8
15	AO	78/80 (98%)	70 (90%)	8 (10%)	7	18
15	CO	78/80 (98%)	71 (91%)	7 (9%)	9	23
16	AP	69/74 (93%)	60 (87%)	9 (13%)	4	10
16	CP	68/74 (92%)	61 (90%)	7 (10%)	7	18
17	AQ	94/97 (97%)	87 (93%)	7 (7%)	13	32
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	20	46
18	AR	59/77 (77%)	51 (86%)	8 (14%)	3	9
18	CR	59/77 (77%)	53 (90%)	6 (10%)	7	18
19	AS	69/80 (86%)	63 (91%)	6 (9%)	9	24
19	CS	67/80 (84%)	59 (88%)	8 (12%)	5	13
20	AT	70/82 (85%)	63 (90%)	7 (10%)	7	19
20	CT	70/82 (85%)	64 (91%)	6 (9%)	10	25
21	AU	18/22 (82%)	16 (89%)	2 (11%)	6	15
21	CU	18/22 (82%)	17 (94%)	1 (6%)	19	44
27	BD	215/218 (99%)	195 (91%)	20 (9%)	8	21
27	DD	215/218 (99%)	194 (90%)	21 (10%)	7	19
28	BE	164/166 (99%)	140 (85%)	24 (15%)	3	8
28	DE	164/166 (99%)	141 (86%)	23 (14%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BF	160/166 (96%)	143 (89%)	17 (11%)	6	17
29	DF	159/166 (96%)	144 (91%)	15 (9%)	8	21
30	BG	143/156 (92%)	127 (89%)	16 (11%)	6	15
30	DG	142/156 (91%)	122 (86%)	20 (14%)	3	9
31	BH	144/148 (97%)	133 (92%)	11 (8%)	12	30
31	DH	144/148 (97%)	125 (87%)	19 (13%)	4	10
32	BI	110/124 (89%)	86 (78%)	24 (22%)	1	3
32	DI	104/124 (84%)	84 (81%)	20 (19%)	1	4
33	BN	118/119 (99%)	99 (84%)	19 (16%)	2	6
33	DN	118/119 (99%)	104 (88%)	14 (12%)	5	13
34	BO	100/100 (100%)	93 (93%)	7 (7%)	14	34
34	DO	100/100 (100%)	93 (93%)	7 (7%)	14	34
35	BP	115/116 (99%)	99 (86%)	16 (14%)	3	9
35	DP	115/116 (99%)	98 (85%)	17 (15%)	3	8
36	BQ	111/111 (100%)	98 (88%)	13 (12%)	5	13
36	DQ	111/111 (100%)	98 (88%)	13 (12%)	5	13
37	BR	101/101 (100%)	84 (83%)	17 (17%)	2	6
37	DR	101/101 (100%)	84 (83%)	17 (17%)	2	6
38	BS	87/88 (99%)	78 (90%)	9 (10%)	7	18
38	DS	85/88 (97%)	71 (84%)	14 (16%)	2	6
39	BT	115/127 (91%)	102 (89%)	13 (11%)	5	14
39	DT	113/127 (89%)	99 (88%)	14 (12%)	4	11
40	BU	93/94 (99%)	84 (90%)	9 (10%)	8	20
40	DU	93/94 (99%)	85 (91%)	8 (9%)	10	25
41	BV	80/82 (98%)	67 (84%)	13 (16%)	2	6
41	DV	80/82 (98%)	66 (82%)	14 (18%)	2	5
42	BW	90/92 (98%)	81 (90%)	9 (10%)	7	19
42	DW	90/92 (98%)	82 (91%)	8 (9%)	9	23
43	BX	77/78 (99%)	71 (92%)	6 (8%)	11	29
43	DX	77/78 (99%)	73 (95%)	4 (5%)	21	47
44	BY	85/91 (93%)	79 (93%)	6 (7%)	13	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	DY	85/91 (93%)	83 (98%)	2 (2%)	43	72
45	BZ	145/179 (81%)	127 (88%)	18 (12%)	4	11
45	DZ	145/179 (81%)	123 (85%)	22 (15%)	3	7
46	B0	65/67 (97%)	62 (95%)	3 (5%)	24	51
46	D0	65/67 (97%)	61 (94%)	4 (6%)	16	39
47	B1	80/83 (96%)	73 (91%)	7 (9%)	9	23
47	D1	80/83 (96%)	73 (91%)	7 (9%)	9	23
48	B2	65/67 (97%)	58 (89%)	7 (11%)	6	16
48	D2	65/67 (97%)	59 (91%)	6 (9%)	8	22
49	B3	51/52 (98%)	45 (88%)	6 (12%)	5	13
49	D3	50/52 (96%)	42 (84%)	8 (16%)	2	6
50	B4	60/63 (95%)	49 (82%)	11 (18%)	2	5
50	D4	53/63 (84%)	44 (83%)	9 (17%)	2	6
51	B5	50/52 (96%)	44 (88%)	6 (12%)	5	12
51	D5	50/52 (96%)	46 (92%)	4 (8%)	11	28
52	B6	51/52 (98%)	47 (92%)	4 (8%)	11	29
52	D6	50/52 (96%)	47 (94%)	3 (6%)	17	41
53	B7	41/42 (98%)	36 (88%)	5 (12%)	5	12
53	D7	41/42 (98%)	40 (98%)	1 (2%)	43	72
54	B8	54/55 (98%)	49 (91%)	5 (9%)	8	21
54	D8	54/55 (98%)	47 (87%)	7 (13%)	4	10
55	B9	34/34 (100%)	32 (94%)	2 (6%)	18	42
55	D9	34/34 (100%)	32 (94%)	2 (6%)	18	42
All	All	9321/10066 (93%)	8280 (89%)	1041 (11%)	6	15

5 of 1041 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	DT	78	LEU
41	DV	100	ARG
39	DT	65	LYS
55	D9	26	ILE
38	BS	83	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 154 such sidechains are listed below:

Mol	Chain	Res	Type
16	CP	76	GLN
43	DX	82	GLN
20	CT	45	GLN
32	DI	43	ASN
47	D1	56	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1493/1521 (98%)	281 (18%)	27 (1%)
1	CA	1501/1521 (98%)	281 (18%)	24 (1%)
22	AV	12/24 (50%)	2 (16%)	0
22	CV	11/24 (45%)	2 (18%)	0
23	AW	72/76 (94%)	31 (43%)	1 (1%)
23	AY	73/76 (96%)	33 (45%)	4 (5%)
23	CW	69/76 (90%)	30 (43%)	2 (2%)
23	CY	71/76 (93%)	32 (45%)	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%)	456 (16%)	28 (0%)
25	DA	2791/2915 (95%)	520 (18%)	29 (1%)
26	BB	119/121 (98%)	13 (10%)	2 (1%)
26	DB	119/121 (98%)	14 (11%)	0
All	All	9295/9620 (96%)	1737 (18%)	121 (1%)

5 of 1737 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	2418	U
25	DA	1913	A
1	CA	560	U

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Mol	Chain	Res	Type
25	DA	1653	G
25	DA	2602	A

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$
24	PSU	AX	55	24	18,21,22	1.38	2 (11%)	21,30,33	2.04	4 (19%)
23	PSU	CW	55	23	18,21,22	1.43	2 (11%)	21,30,33	1.95	3 (14%)
23	PSU	AY	32	23	18,21,22	1.35	2 (11%)	21,30,33	2.05	4 (19%)
23	4SU	CY	8	23	18,21,22	1.79	4 (22%)	25,30,33	2.13	5 (20%)
23	MIA	AW	37	23	28,31,32	2.31	6 (21%)	38,44,47	2.84	14 (36%)
23	4SU	AY	8	23	18,21,22	1.69	4 (22%)	25,30,33	1.82	4 (16%)
23	7MG	CY	46	23	23,26,27	1.41	5 (21%)	27,39,42	2.46	5 (18%)
23	5MU	CW	54	23	19,22,23	1.36	4 (21%)	27,32,35	1.69	6 (22%)
24	5MC	CX	32	24	19,22,23	1.69	3 (15%)	26,32,35	1.30	3 (11%)
23	PSU	CY	39	23	18,21,22	1.39	2 (11%)	21,30,33	2.30	3 (14%)
24	4SU	CX	8	24	18,21,22	2.18	5 (27%)	25,30,33	1.50	6 (24%)
24	5MU	AX	54	24	19,22,23	1.36	4 (21%)	27,32,35	1.97	7 (25%)
23	PSU	AW	39	23	18,21,22	1.44	3 (16%)	21,30,33	1.65	4 (19%)
23	7MG	CW	46	23	23,26,27	1.30	4 (17%)	27,39,42	2.71	7 (25%)
23	PSU	AY	55	23	18,21,22	1.34	2 (11%)	21,30,33	2.11	4 (19%)
23	PSU	CW	39	23	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
23	4SU	AW	8	23	18,21,22	1.76	4 (22%)	25,30,33	1.81	5 (20%)
23	PSU	CY	32	23	18,21,22	1.36	2 (11%)	21,30,33	1.90	4 (19%)
23	5MU	AW	54	23	19,22,23	1.40	5 (26%)	27,32,35	1.91	6 (22%)
23	PSU	AW	32	23	18,21,22	1.36	2 (11%)	21,30,33	1.88	3 (14%)
23	7MG	AW	46	23	23,26,27	1.38	5 (21%)	27,39,42	2.54	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	MIA	AY	37	23	21,24,32	1.63	3 (14%)	30,35,47	1.98	9 (30%)
23	PSU	AY	39	23	18,21,22	1.57	4 (22%)	21,30,33	2.14	5 (23%)
23	4SU	CW	8	23	18,21,22	1.68	4 (22%)	25,30,33	2.34	5 (20%)
23	PSU	CW	32	23	18,21,22	1.38	2 (11%)	21,30,33	1.95	3 (14%)
24	5MC	AX	32	24	19,22,23	1.59	3 (15%)	26,32,35	1.26	2 (7%)
23	MIA	CY	37	23	21,24,32	1.67	4 (19%)	30,35,47	2.03	8 (26%)
24	5MU	CX	54	24	19,22,23	1.39	4 (21%)	27,32,35	2.29	8 (29%)
23	7MG	AY	46	23	23,26,27	1.37	4 (17%)	27,39,42	2.65	7 (25%)
24	PSU	CX	55	24	18,21,22	1.37	2 (11%)	21,30,33	1.92	5 (23%)
23	5MU	AY	54	23	19,22,23	1.53	5 (26%)	27,32,35	1.65	6 (22%)
23	PSU	CY	55	23	18,21,22	1.49	3 (16%)	21,30,33	1.94	5 (23%)
23	MIA	CW	37	23	21,24,32	1.57	4 (19%)	30,35,47	2.11	8 (26%)
23	5MU	CY	54	23	19,22,23	1.39	5 (26%)	27,32,35	2.19	8 (29%)
24	4SU	AX	8	24	18,21,22	2.34	5 (27%)	25,30,33	1.61	5 (20%)
23	PSU	AW	55	23	18,21,22	1.31	2 (11%)	21,30,33	1.78	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
23	PSU	AY	32	23	-	0/7/25/26	0/2/2/2
23	4SU	CY	8	23	-	2/7/25/26	0/2/2/2
23	MIA	AW	37	23	-	1/15/33/34	0/3/3/3
23	4SU	AY	8	23	-	2/7/25/26	0/2/2/2
23	7MG	CY	46	23	-	2/7/37/38	0/3/3/3
23	5MU	CW	54	23	-	0/7/25/26	0/2/2/2
24	5MC	CX	32	24	-	0/7/25/26	0/2/2/2
23	PSU	CY	39	23	-	2/7/25/26	0/2/2/2
24	4SU	CX	8	24	-	1/7/25/26	0/2/2/2
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	2/7/37/38	0/3/3/3
23	PSU	AY	55	23	-	2/7/25/26	0/2/2/2
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2

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

The worst 5 of 126 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C2-S10	-6.96	1.70	1.75
23	AW	37	MIA	C13-C14	6.78	1.52	1.32
24	CX	32	5MC	C5-C4	6.09	1.48	1.44
24	AX	8	4SU	C4-N3	-5.83	1.31	1.37
24	AX	32	5MC	C5-C4	5.49	1.48	1.44

The worst 5 of 196 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	37	MIA	C12-C13-C14	-10.43	108.30	127.01
23	AY	46	7MG	N9-C4-N3	9.05	138.72	125.46
23	CW	46	7MG	N9-C4-N3	8.86	138.44	125.46
23	AW	46	7MG	N9-C4-N3	8.24	137.53	125.46
23	CY	46	7MG	N9-C4-N3	7.84	136.95	125.46

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	37	MIA	C12-C13-C14-C16
23	AY	46	7MG	C2'-C1'-N9-C8
23	AY	55	PSU	C2'-C1'-C5-C4
23	CY	54	5MU	C3'-C4'-C5'-O5'
23	CY	54	5MU	O4'-C4'-C5'-O5'

There are no ring outliers.

24 monomers are involved in 46 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides 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	CA	3170	56	14,16,16	7.77	1 (7%)	12,20,20	1.09	1 (8%)
58	SF4	CD	302	4	0,12,12	-	-	-	-	-
57	NEG	CA	3176	-	14,16,16	7.71	1 (7%)	12,20,20	1.50	2 (16%)
57	NEG	CA	3171	-	14,16,16	7.30	1 (7%)	12,20,20	2.55	3 (25%)
57	NEG	AA	3222	-	14,16,16	7.58	1 (7%)	12,20,20	1.66	1 (8%)
57	NEG	AA	3216	56	14,16,16	7.98	1 (7%)	12,20,20	2.29	2 (16%)
57	NEG	CX	3004	-	14,16,16	7.66	1 (7%)	12,20,20	2.04	2 (16%)
57	NEG	CA	3174	-	14,16,16	7.12	1 (7%)	12,20,20	4.26	4 (33%)
57	NEG	CA	3173	-	14,16,16	7.54	1 (7%)	12,20,20	2.16	2 (16%)
57	NEG	CA	3175	-	14,16,16	7.82	1 (7%)	12,20,20	2.37	4 (33%)
57	NEG	AA	3218	56	14,16,16	7.74	1 (7%)	12,20,20	1.92	3 (25%)
57	NEG	AA	3220	-	14,16,16	7.21	1 (7%)	12,20,20	2.09	4 (33%)
57	NEG	AA	3221	-	14,16,16	8.17	1 (7%)	12,20,20	1.59	1 (8%)
57	NEG	CA	3177	-	14,16,16	6.82	1 (7%)	12,20,20	3.84	5 (41%)
57	NEG	CW	3002	-	14,16,16	7.34	1 (7%)	12,20,20	1.38	2 (16%)
57	NEG	AW	3004	-	14,16,16	7.31	1 (7%)	12,20,20	1.34	1 (8%)
57	NEG	AX	3013	-	14,16,16	8.09	2 (14%)	12,20,20	2.53	3 (25%)
57	NEG	AA	3217	-	14,16,16	7.23	1 (7%)	12,20,20	2.25	3 (25%)
57	NEG	AA	3219	-	14,16,16	7.42	1 (7%)	12,20,20	2.31	3 (25%)
58	SF4	AD	501	4	0,12,12	-	-	-	-	-
57	NEG	CA	3172	-	14,16,16	7.93	1 (7%)	12,20,20	2.14	2 (16%)

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	CA	3170	56	-	5/18/18/18	-
58	SF4	CD	302	4	-	-	0/6/5/5
57	NEG	CA	3176	-	-	3/18/18/18	-
57	NEG	CA	3171	-	-	4/18/18/18	-
57	NEG	AA	3222	-	-	3/18/18/18	-
57	NEG	AA	3216	56	-	3/18/18/18	-
57	NEG	CX	3004	-	-	5/18/18/18	-
57	NEG	CA	3174	-	-	1/18/18/18	-
57	NEG	CA	3173	-	-	4/18/18/18	-
57	NEG	CA	3175	-	-	7/18/18/18	-
57	NEG	AA	3218	56	-	4/18/18/18	-
57	NEG	AA	3220	-	-	5/18/18/18	-
57	NEG	AA	3221	-	-	6/18/18/18	-
57	NEG	CA	3177	-	-	4/18/18/18	-
57	NEG	CW	3002	-	-	1/18/18/18	-
57	NEG	AW	3004	-	-	3/18/18/18	-
57	NEG	AX	3013	-	-	7/18/18/18	-
57	NEG	AA	3217	-	-	3/18/18/18	-
57	NEG	AA	3219	-	-	4/18/18/18	-
58	SF4	AD	501	4	-	-	0/6/5/5
57	NEG	CA	3172	-	-	4/18/18/18	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AA	3221	NEG	N2-N3	-30.41	1.11	1.41
57	AX	3013	NEG	N2-N3	-30.05	1.11	1.41
57	AA	3216	NEG	N2-N3	-29.74	1.11	1.41
57	CA	3172	NEG	N2-N3	-29.54	1.12	1.41
57	CA	3175	NEG	N2-N3	-29.11	1.12	1.41

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	CA	3174	NEG	C9-N3-N2	10.94	119.34	109.09
57	CA	3177	NEG	C9-N3-N2	9.82	118.29	109.09
57	CA	3174	NEG	C6-N2-N3	8.14	128.42	120.29
57	AA	3216	NEG	C9-N3-N2	6.96	115.60	109.09
57	CA	3177	NEG	C6-N2-N3	6.92	127.21	120.29

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	AA	3217	NEG	N3-C7-C8-O1
57	AA	3217	NEG	N3-C7-C8-O2
57	AA	3219	NEG	N3-C7-C8-O1
57	AA	3219	NEG	N3-C7-C8-O2
57	AA	3220	NEG	C6-N2-N3-C7

There are no ring outliers.

15 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	CA	3171	NEG	1	0
57	AA	3216	NEG	7	0
57	CX	3004	NEG	5	0
57	CA	3174	NEG	5	0
57	CA	3173	NEG	2	0
57	CA	3175	NEG	3	0
57	AA	3218	NEG	1	0
57	AA	3220	NEG	4	0
57	AA	3221	NEG	4	0
57	CA	3177	NEG	2	0
57	CW	3002	NEG	1	0
57	AW	3004	NEG	2	0
57	AX	3013	NEG	3	0
57	AA	3217	NEG	1	0
57	AA	3219	NEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	AA	1496/1521 (98%)	0.48	64 (4%)	40 36	36, 68, 97, 112	0
1	CA	1503/1521 (98%)	0.66	100 (6%)	24 21	38, 71, 97, 111	0
2	AB	231/256 (90%)	1.30	52 (22%)	2 2	67, 83, 93, 99	0
2	CB	231/256 (90%)	1.69	73 (31%)	1 1	69, 85, 94, 100	0
3	AC	206/239 (86%)	1.25	39 (18%)	3 3	65, 78, 88, 96	0
3	CC	206/239 (86%)	1.85	85 (41%)	0 0	68, 80, 90, 96	0
4	AD	208/209 (99%)	1.04	29 (13%)	6 5	53, 68, 80, 87	0
4	CD	208/209 (99%)	0.82	9 (4%)	40 36	54, 67, 80, 90	0
5	AE	148/162 (91%)	0.79	9 (6%)	27 24	54, 70, 81, 86	0
5	CE	148/162 (91%)	1.46	34 (22%)	2 2	57, 72, 82, 88	0
6	AF	100/101 (99%)	1.05	8 (8%)	18 15	53, 67, 78, 87	0
6	CF	100/101 (99%)	0.65	2 (2%)	65 62	54, 68, 80, 87	0
7	AG	155/156 (99%)	1.10	21 (13%)	7 6	62, 75, 86, 95	0
7	CG	155/156 (99%)	0.98	17 (10%)	10 9	63, 77, 86, 99	0
8	AH	137/138 (99%)	0.98	10 (7%)	21 18	57, 70, 78, 85	0
8	CH	137/138 (99%)	1.08	12 (8%)	15 13	60, 72, 81, 85	0
9	AI	127/128 (99%)	1.55	31 (24%)	2 1	57, 82, 90, 94	0
9	CI	127/128 (99%)	2.05	60 (47%)	0 0	65, 84, 91, 95	0
10	AJ	97/105 (92%)	1.70	32 (32%)	1 1	63, 85, 94, 98	0
10	CJ	96/105 (91%)	2.59	72 (75%)	0 0	65, 86, 94, 99	0
11	AK	114/129 (88%)	0.68	4 (3%)	47 43	47, 66, 78, 84	0
11	CK	114/129 (88%)	0.71	9 (7%)	18 16	49, 68, 79, 85	0
12	AL	122/132 (92%)	0.55	8 (6%)	24 21	48, 57, 69, 79	0
12	CL	122/132 (92%)	0.91	7 (5%)	29 26	50, 60, 71, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9
13	AM	123/126 (97%)	0.97	12 (9%) 13 11	52, 70, 84, 96	0
13	CM	122/126 (96%)	1.59	29 (23%) 2 1	70, 83, 93, 99	0
14	AN	60/61 (98%)	1.57	14 (23%) 2 2	64, 77, 83, 89	0
14	CN	60/61 (98%)	2.62	37 (61%) 0 0	67, 80, 87, 90	0
15	AO	88/89 (98%)	0.76	5 (5%) 29 26	49, 66, 77, 84	0
15	CO	88/89 (98%)	0.78	6 (6%) 23 20	51, 67, 79, 85	0
16	AP	82/88 (93%)	1.34	16 (19%) 3 2	53, 67, 78, 82	0
16	CP	82/88 (93%)	1.07	4 (4%) 35 31	54, 66, 77, 82	0
17	AQ	99/105 (94%)	0.91	5 (5%) 33 29	53, 69, 81, 83	0
17	CQ	99/105 (94%)	0.85	7 (7%) 22 19	55, 70, 81, 85	0
18	AR	68/88 (77%)	0.74	4 (5%) 28 25	54, 67, 80, 82	0
18	CR	68/88 (77%)	0.83	5 (7%) 20 18	54, 69, 81, 85	0
19	AS	83/93 (89%)	1.29	17 (20%) 2 2	68, 80, 88, 97	0
19	CS	83/93 (89%)	2.31	48 (57%) 0 0	71, 82, 91, 97	0
20	AT	96/106 (90%)	0.88	10 (10%) 11 10	57, 69, 85, 90	0
20	CT	96/106 (90%)	0.89	8 (8%) 17 14	56, 69, 85, 90	0
21	AU	23/27 (85%)	1.23	4 (17%) 4 3	62, 71, 78, 81	0
21	CU	23/27 (85%)	1.93	9 (39%) 1 0	65, 74, 80, 83	0
22	AV	13/24 (54%)	0.79	2 (15%) 5 4	51, 61, 91, 97	0
22	CV	12/24 (50%)	1.24	2 (16%) 4 3	55, 65, 91, 92	0
23	AW	67/76 (88%)	1.46	17 (25%) 1 1	50, 93, 102, 108	0
23	AY	67/76 (88%)	1.61	23 (34%) 1 1	37, 101, 106, 107	0
23	CW	65/76 (85%)	2.02	27 (41%) 0 0	69, 100, 108, 110	0
23	CY	66/76 (86%)	1.82	32 (48%) 0 0	40, 101, 106, 107	0
24	AX	72/77 (93%)	0.67	5 (6%) 23 20	45, 69, 85, 96	0
24	CX	72/77 (93%)	1.02	10 (13%) 6 5	46, 72, 87, 98	0
25	BA	2822/2915 (96%)	-0.15	117 (4%) 41 37	22, 42, 94, 110	0
25	DA	2800/2915 (96%)	0.01	114 (4%) 41 37	25, 47, 96, 113	0
26	BB	120/121 (99%)	0.29	1 (0%) 82 81	41, 61, 72, 92	0
26	DB	120/121 (99%)	0.94	6 (5%) 34 30	48, 67, 78, 93	0
27	BD	275/276 (99%)	0.08	4 (1%) 72 70	21, 38, 55, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DD	275/276 (99%)	0.08	4 (1%) 72 70	23, 41, 57, 85	0
28	BE	204/206 (99%)	0.21	1 (0%) 87 86	19, 45, 67, 84	0
28	DE	204/206 (99%)	0.12	1 (0%) 87 86	22, 49, 69, 84	0
29	BF	203/210 (96%)	0.26	2 (0%) 79 78	23, 50, 74, 95	0
29	DF	203/210 (96%)	0.38	7 (3%) 48 44	25, 55, 77, 95	0
30	BG	181/182 (99%)	0.83	17 (9%) 14 12	52, 68, 82, 94	0
30	DG	181/182 (99%)	1.26	26 (14%) 6 5	57, 72, 84, 92	0
31	BH	174/180 (96%)	0.93	14 (8%) 18 15	51, 69, 80, 87	0
31	DH	174/180 (96%)	1.48	47 (27%) 1 1	57, 74, 84, 88	0
32	BI	146/148 (98%)	0.88	8 (5%) 30 27	45, 71, 84, 88	0
32	DI	146/148 (98%)	0.85	6 (4%) 41 37	46, 72, 84, 89	0
33	BN	140/140 (100%)	0.43	1 (0%) 84 83	32, 48, 69, 78	0
33	DN	140/140 (100%)	0.60	3 (2%) 63 61	38, 53, 72, 79	0
34	BO	122/122 (100%)	-0.19	0 100 100	23, 39, 59, 65	0
34	DO	122/122 (100%)	0.54	4 (3%) 49 45	43, 58, 72, 84	0
35	BP	149/150 (99%)	0.44	1 (0%) 84 83	23, 53, 76, 82	0
35	DP	149/150 (99%)	0.52	4 (2%) 56 53	28, 57, 78, 83	0
36	BQ	141/141 (100%)	0.65	5 (3%) 47 43	32, 53, 69, 81	0
36	DQ	141/141 (100%)	0.97	9 (6%) 25 22	36, 58, 73, 82	0
37	BR	118/118 (100%)	-0.19	0 100 100	19, 33, 48, 59	0
37	DR	118/118 (100%)	0.24	0 100 100	32, 51, 65, 78	0
38	BS	110/112 (98%)	0.06	2 (1%) 67 65	36, 50, 67, 72	0
38	DS	110/112 (98%)	1.26	16 (14%) 6 5	64, 77, 88, 94	0
39	BT	131/146 (89%)	0.04	6 (4%) 37 34	28, 41, 69, 88	0
39	DT	131/146 (89%)	0.72	8 (6%) 27 24	45, 60, 78, 88	0
40	BU	116/118 (98%)	-0.40	1 (0%) 81 80	17, 29, 43, 67	0
40	DU	116/118 (98%)	0.78	6 (5%) 33 29	36, 64, 80, 89	0
41	BV	101/101 (100%)	-0.32	1 (0%) 79 78	18, 36, 55, 73	0
41	DV	101/101 (100%)	0.98	8 (7%) 18 16	42, 77, 87, 93	0
42	BW	112/113 (99%)	-0.39	1 (0%) 81 80	17, 29, 52, 89	0
42	DW	112/113 (99%)	0.28	0 100 100	35, 49, 71, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BX	95/96 (98%)	-0.25	1 (1%) 78 76	15, 33, 65, 84	0
43	DX	95/96 (98%)	0.73	9 (9%) 14 11	38, 57, 76, 84	0
44	BY	107/110 (97%)	0.20	4 (3%) 45 41	33, 48, 75, 84	0
44	DY	107/110 (97%)	1.29	25 (23%) 2 2	54, 70, 86, 93	0
45	BZ	171/206 (83%)	1.14	30 (17%) 4 3	38, 69, 102, 108	0
45	DZ	174/206 (84%)	1.96	63 (36%) 1 0	71, 88, 101, 108	0
46	B0	83/85 (97%)	0.10	6 (7%) 21 18	25, 37, 67, 83	0
46	D0	83/85 (97%)	1.17	10 (12%) 9 7	46, 69, 81, 91	0
47	B1	97/98 (98%)	0.12	2 (2%) 63 61	19, 40, 69, 76	0
47	D1	97/98 (98%)	0.19	1 (1%) 79 78	33, 53, 77, 79	0
48	B2	70/72 (97%)	0.06	2 (2%) 53 50	32, 42, 62, 80	0
48	D2	70/72 (97%)	0.95	5 (7%) 22 19	54, 70, 81, 84	0
49	B3	59/60 (98%)	-0.16	0 100 100	22, 36, 55, 80	0
49	D3	59/60 (98%)	0.88	5 (8%) 16 14	52, 67, 82, 85	0
50	B4	69/71 (97%)	0.87	13 (18%) 3 3	53, 73, 93, 94	0
50	D4	69/71 (97%)	1.80	25 (36%) 1 0	76, 87, 99, 107	0
51	B5	59/60 (98%)	-0.46	0 100 100	18, 31, 46, 68	0
51	D5	59/60 (98%)	0.20	0 100 100	28, 50, 68, 77	0
52	B6	53/54 (98%)	-0.16	0 100 100	29, 40, 59, 67	0
52	D6	53/54 (98%)	0.86	4 (7%) 20 17	47, 61, 75, 79	0
53	B7	48/49 (97%)	-0.24	1 (2%) 63 61	16, 25, 55, 66	0
53	D7	48/49 (97%)	0.03	1 (2%) 63 61	28, 37, 62, 71	0
54	B8	64/65 (98%)	-0.35	0 100 100	23, 32, 43, 58	0
54	D8	64/65 (98%)	0.51	1 (1%) 70 68	43, 57, 65, 71	0
55	B9	37/37 (100%)	0.33	2 (5%) 31 27	31, 50, 69, 75	0
55	D9	37/37 (100%)	1.12	4 (10%) 11 9	49, 60, 73, 77	0
All	All	20900/21748 (96%)	0.54	1810 (8%) 16 13	15, 62, 92, 113	0

The worst 5 of 1810 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	CN	38	GLY	8.6
7	CG	82	GLY	8.4

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Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	8.4
45	DZ	116	VAL	7.8
13	CM	123	ALA	7.6

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, 95th 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 ²)	Q<0.9
23	7MG	CY	46	24/25	0.46	0.17	91,105,113,139	0
23	7MG	CW	46	24/25	0.51	0.18	93,104,114,127	0
23	PSU	CY	55	20/21	0.54	0.19	91,104,118,129	0
23	7MG	AW	46	24/25	0.59	0.15	74,94,116,138	0
23	4SU	CY	8	20/21	0.59	0.15	95,103,122,140	0
23	7MG	AY	46	24/25	0.63	0.14	92,100,111,135	0
23	4SU	CW	8	20/21	0.64	0.16	85,105,116,130	0
23	5MU	CY	54	21/22	0.65	0.17	88,99,111,135	0
23	PSU	AY	55	20/21	0.65	0.14	88,103,115,132	0
23	PSU	CY	32	20/21	0.69	0.14	83,95,100,107	0
23	PSU	CW	55	20/21	0.69	0.14	76,95,105,108	0
23	5MU	AY	54	21/22	0.70	0.14	85,97,115,141	0
23	PSU	CY	39	20/21	0.71	0.14	79,92,100,112	0
23	4SU	AY	8	20/21	0.72	0.11	99,105,115,127	0
23	4SU	AW	8	20/21	0.76	0.14	81,89,100,121	0
23	MIA	AY	37	22/30	0.76	0.17	82,91,103,118	0
23	MIA	CY	37	22/30	0.77	0.12	75,93,102,117	0
23	PSU	AW	55	20/21	0.80	0.13	57,85,93,93	0
24	PSU	CX	55	20/21	0.81	0.12	62,70,83,92	0
23	PSU	CW	32	20/21	0.84	0.17	62,82,97,97	0
23	PSU	AY	39	20/21	0.86	0.14	76,89,100,102	0
23	5MU	CW	54	21/22	0.87	0.13	72,81,90,93	0
23	PSU	AY	32	20/21	0.88	0.12	83,93,99,105	0
24	4SU	CX	8	20/21	0.88	0.14	73,82,90,90	0
24	5MC	CX	32	21/22	0.89	0.12	63,72,77,80	0
24	5MU	CX	54	21/22	0.89	0.12	69,80,89,95	0
24	PSU	AX	55	20/21	0.91	0.10	60,68,83,92	0
24	5MU	AX	54	21/22	0.92	0.10	60,70,77,80	0
23	MIA	CW	37	22/30	0.92	0.11	53,72,83,85	0
23	5MU	AW	54	21/22	0.93	0.10	57,76,85,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	PSU	CW	39	20/21	0.93	0.14	62,79,88,94	0
24	4SU	AX	8	20/21	0.94	0.10	47,62,81,87	0
24	5MC	AX	32	21/22	0.95	0.11	38,56,66,77	0
23	PSU	AW	32	20/21	0.95	0.09	39,59,64,65	0
23	MIA	AW	37	29/30	0.96	0.10	36,49,67,72	0
23	PSU	AW	39	20/21	0.96	0.08	37,57,68,72	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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	3578	1/1	0.49	0.19	71,71,71,71	0
56	MG	DA	3601	1/1	0.50	0.18	75,75,75,75	0
56	MG	AY	3003	1/1	0.51	0.28	78,78,78,78	0
56	MG	DA	3572	1/1	0.53	0.14	70,70,70,70	0
56	MG	BA	3737	1/1	0.59	0.22	68,68,68,68	0
56	MG	CA	3126	1/1	0.60	0.28	76,76,76,76	0
56	MG	DA	3365	1/1	0.62	0.23	54,54,54,54	0
56	MG	DY	502	1/1	0.62	0.19	86,86,86,86	0
56	MG	AA	3168	1/1	0.63	0.17	76,76,76,76	0
56	MG	DA	3417	1/1	0.63	0.26	71,71,71,71	0
56	MG	DA	3605	1/1	0.64	0.14	53,53,53,53	0
56	MG	BA	3692	1/1	0.64	0.26	73,73,73,73	0
56	MG	BA	3322	1/1	0.65	0.27	58,58,58,58	0
56	MG	CA	3054	1/1	0.65	0.50	65,65,65,65	0
56	MG	BA	3453	1/1	0.66	0.14	59,59,59,59	0
56	MG	AA	3198	1/1	0.66	0.23	82,82,82,82	0
56	MG	BA	3703	1/1	0.67	0.17	56,56,56,56	0
56	MG	DA	3042	1/1	0.67	0.19	71,71,71,71	0
56	MG	BA	3550	1/1	0.67	0.40	74,74,74,74	0
56	MG	AA	3179	1/1	0.67	0.19	85,85,85,85	0
56	MG	DA	3522	1/1	0.67	0.27	57,57,57,57	0
56	MG	CA	3007	1/1	0.68	0.26	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	CA	3124	1/1	0.68	0.36	90,90,90,90	0
56	MG	BA	3558	1/1	0.69	0.22	72,72,72,72	0
56	MG	CA	3075	1/1	0.69	0.20	53,53,53,53	0
56	MG	DA	3569	1/1	0.69	0.32	75,75,75,75	0
56	MG	BA	3714	1/1	0.69	0.26	73,73,73,73	0
56	MG	DA	3501	1/1	0.70	0.35	67,67,67,67	0
56	MG	CA	3145	1/1	0.70	0.20	62,62,62,62	0
56	MG	AY	3001	1/1	0.71	0.30	92,92,92,92	0
56	MG	DA	3242	1/1	0.71	0.12	56,56,56,56	0
56	MG	AA	3113	1/1	0.72	0.19	57,57,57,57	0
56	MG	CJ	5001	1/1	0.72	0.20	75,75,75,75	0
56	MG	CA	3051	1/1	0.72	0.27	78,78,78,78	0
56	MG	DA	3517	1/1	0.72	0.17	60,60,60,60	0
56	MG	CA	3143	1/1	0.72	0.29	59,59,59,59	0
56	MG	DA	3526	1/1	0.72	0.22	64,64,64,64	0
56	MG	BA	3327	1/1	0.73	0.25	74,74,74,74	0
56	MG	CA	3125	1/1	0.73	0.19	76,76,76,76	0
56	MG	BA	3154	1/1	0.73	0.27	58,58,58,58	0
56	MG	BA	3480	1/1	0.73	0.19	29,29,29,29	0
56	MG	DD	309	1/1	0.73	0.15	65,65,65,65	0
56	MG	BB	3015	1/1	0.73	0.12	54,54,54,54	0
56	MG	BA	3700	1/1	0.74	0.26	73,73,73,73	0
56	MG	AA	3093	1/1	0.74	0.19	58,58,58,58	0
56	MG	DA	3528	1/1	0.74	0.23	70,70,70,70	0
56	MG	CA	3036	1/1	0.74	0.21	69,69,69,69	0
56	MG	CA	3113	1/1	0.74	0.16	79,79,79,79	0
56	MG	BB	3007	1/1	0.75	0.14	84,84,84,84	0
56	MG	BA	3508	1/1	0.75	0.16	61,61,61,61	0
56	MG	BA	3544	1/1	0.75	0.23	57,57,57,57	0
56	MG	AX	3006	1/1	0.75	0.30	80,80,80,80	0
56	MG	DB	3009	1/1	0.75	0.24	70,70,70,70	0
56	MG	BA	3400	1/1	0.75	0.20	53,53,53,53	0
56	MG	BA	3608	1/1	0.75	0.21	68,68,68,68	0
56	MG	BA	3555	1/1	0.76	0.17	49,49,49,49	0
56	MG	CA	3150	1/1	0.76	0.18	80,80,80,80	0
56	MG	BA	3532	1/1	0.76	0.20	73,73,73,73	0
56	MG	AA	3188	1/1	0.76	0.17	69,69,69,69	0
56	MG	AY	3002	1/1	0.76	0.19	70,70,70,70	0
56	MG	DA	3247	1/1	0.76	0.10	51,51,51,51	0
56	MG	DA	3330	1/1	0.76	0.14	54,54,54,54	0
56	MG	DA	3349	1/1	0.76	0.15	46,46,46,46	0
56	MG	BA	3751	1/1	0.76	0.17	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	3602	1/1	0.76	0.20	62,62,62,62	0
56	MG	BA	3760	1/1	0.76	0.26	78,78,78,78	0
56	MG	DA	3433	1/1	0.76	0.11	58,58,58,58	0
56	MG	DA	3489	1/1	0.76	0.11	53,53,53,53	0
56	MG	DA	3491	1/1	0.76	0.12	69,69,69,69	0
56	MG	BA	3419	1/1	0.77	0.16	50,50,50,50	0
56	MG	AA	3112	1/1	0.77	0.21	53,53,53,53	0
56	MG	DA	3079	1/1	0.77	0.24	60,60,60,60	0
56	MG	DA	3163	1/1	0.77	0.28	63,63,63,63	0
56	MG	AA	3075	1/1	0.77	0.56	81,81,81,81	0
56	MG	BA	3610	1/1	0.77	0.28	64,64,64,64	0
56	MG	AA	3122	1/1	0.77	0.12	74,74,74,74	0
56	MG	AA	3206	1/1	0.77	0.19	62,62,62,62	0
56	MG	CA	3134	1/1	0.77	0.15	78,78,78,78	0
56	MG	DA	3411	1/1	0.77	0.16	43,43,43,43	0
56	MG	CA	3027	1/1	0.77	0.16	64,64,64,64	0
56	MG	AA	3138	1/1	0.77	0.20	73,73,73,73	0
56	MG	DA	3621	1/1	0.77	0.20	73,73,73,73	0
56	MG	DA	3463	1/1	0.77	0.13	53,53,53,53	0
56	MG	DA	3476	1/1	0.77	0.15	62,62,62,62	0
56	MG	AA	3014	1/1	0.77	0.16	64,64,64,64	0
56	MG	CA	3046	1/1	0.78	0.36	68,68,68,68	0
56	MG	DA	3036	1/1	0.78	0.13	48,48,48,48	0
56	MG	AX	3002	1/1	0.78	0.35	71,71,71,71	0
56	MG	AA	3192	1/1	0.78	0.17	71,71,71,71	0
56	MG	BA	3168	1/1	0.78	0.22	57,57,57,57	0
56	MG	BA	3591	1/1	0.78	0.18	58,58,58,58	0
56	MG	CA	3121	1/1	0.78	0.14	88,88,88,88	0
56	MG	DA	3553	1/1	0.78	0.30	45,45,45,45	0
56	MG	DA	3257	1/1	0.78	0.18	58,58,58,58	0
56	MG	CA	3123	1/1	0.78	0.28	77,77,77,77	0
56	MG	BA	3771	1/1	0.78	0.18	73,73,73,73	0
56	MG	AA	3183	1/1	0.78	0.18	63,63,63,63	0
56	MG	AA	3008	1/1	0.78	0.25	53,53,53,53	0
56	MG	BB	3016	1/1	0.78	0.21	63,63,63,63	0
56	MG	BA	3519	1/1	0.78	0.21	56,56,56,56	0
56	MG	BA	3331	1/1	0.78	0.15	51,51,51,51	0
56	MG	DA	3470	1/1	0.78	0.21	65,65,65,65	0
56	MG	BA	3395	1/1	0.78	0.17	65,65,65,65	0
56	MG	BA	3307	1/1	0.79	0.12	57,57,57,57	0
56	MG	DA	3524	1/1	0.79	0.21	58,58,58,58	0
56	MG	BA	3445	1/1	0.79	0.28	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3081	1/1	0.79	0.15	61,61,61,61	0
56	MG	DA	3425	1/1	0.79	0.38	69,69,69,69	0
56	MG	DA	3085	1/1	0.79	0.21	65,65,65,65	0
56	MG	DA	3436	1/1	0.79	0.17	63,63,63,63	0
56	MG	DA	3094	1/1	0.79	0.15	55,55,55,55	0
56	MG	DA	3581	1/1	0.79	0.29	67,67,67,67	0
56	MG	BA	3470	1/1	0.79	0.29	46,46,46,46	0
56	MG	BA	3730	1/1	0.79	0.15	45,45,45,45	0
56	MG	DA	3483	1/1	0.79	0.12	64,64,64,64	0
56	MG	CA	3068	1/1	0.79	0.23	77,77,77,77	0
56	MG	BA	3731	1/1	0.79	0.14	57,57,57,57	0
56	MG	CA	3004	1/1	0.79	0.17	69,69,69,69	0
56	MG	BA	3402	1/1	0.79	0.20	67,67,67,67	0
57	NEG	CA	3171	17/17	0.79	0.23	53,72,80,85	0
56	MG	BA	3682	1/1	0.80	0.29	73,73,73,73	0
56	MG	BP	204	1/1	0.80	0.18	54,54,54,54	0
56	MG	BA	3735	1/1	0.80	0.12	41,41,41,41	0
56	MG	BA	3736	1/1	0.80	0.12	73,73,73,73	0
56	MG	DA	3561	1/1	0.80	0.14	65,65,65,65	0
56	MG	CA	3021	1/1	0.80	0.22	66,66,66,66	0
56	MG	DA	3090	1/1	0.80	0.33	67,67,67,67	0
56	MG	BA	3435	1/1	0.80	0.14	52,52,52,52	0
56	MG	AA	3106	1/1	0.80	0.18	62,62,62,62	0
56	MG	DA	3178	1/1	0.80	0.12	45,45,45,45	0
56	MG	DA	3200	1/1	0.80	0.26	52,52,52,52	0
56	MG	BA	3539	1/1	0.80	0.18	58,58,58,58	0
56	MG	BA	3707	1/1	0.80	0.25	62,62,62,62	0
56	MG	BA	3484	1/1	0.80	0.27	64,64,64,64	0
56	MG	DA	3513	1/1	0.80	0.11	58,58,58,58	0
56	MG	CA	3148	1/1	0.80	0.19	72,72,72,72	0
57	NEG	AA	3217	17/17	0.80	0.20	45,55,78,95	0
56	MG	AA	3082	1/1	0.80	0.33	70,70,70,70	0
56	MG	CA	3069	1/1	0.81	0.30	75,75,75,75	0
56	MG	AA	3186	1/1	0.81	0.31	65,65,65,65	0
56	MG	BA	3373	1/1	0.81	0.17	35,35,35,35	0
56	MG	BA	3243	1/1	0.81	0.26	57,57,57,57	0
56	MG	BA	3303	1/1	0.81	0.16	27,27,27,27	0
56	MG	BA	3401	1/1	0.81	0.13	67,67,67,67	0
56	MG	BN	3002	1/1	0.81	0.14	53,53,53,53	0
56	MG	BA	3710	1/1	0.81	0.24	51,51,51,51	0
56	MG	DA	3276	1/1	0.81	0.11	57,57,57,57	0
56	MG	BU	201	1/1	0.81	0.20	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	DA	3340	1/1	0.81	0.16	60,60,60,60	0
56	MG	DA	3562	1/1	0.81	0.14	67,67,67,67	0
56	MG	DA	3564	1/1	0.81	0.22	64,64,64,64	0
56	MG	CA	3139	1/1	0.81	0.22	63,63,63,63	0
56	MG	BA	3580	1/1	0.81	0.15	61,61,61,61	0
56	MG	DA	3573	1/1	0.81	0.12	69,69,69,69	0
56	MG	DA	3381	1/1	0.81	0.18	55,55,55,55	0
56	MG	BA	3723	1/1	0.81	0.14	41,41,41,41	0
56	MG	AA	3003	1/1	0.81	0.30	79,79,79,79	0
56	MG	AA	3136	1/1	0.81	0.18	59,59,59,59	0
56	MG	CA	3159	1/1	0.81	0.25	60,60,60,60	0
56	MG	AA	3030	1/1	0.81	0.28	65,65,65,65	0
56	MG	DA	3459	1/1	0.81	0.09	63,63,63,63	0
56	MG	BA	3634	1/1	0.81	0.12	50,50,50,50	0
56	MG	DO	201	1/1	0.81	0.17	59,59,59,59	0
56	MG	BA	3638	1/1	0.81	0.12	47,47,47,47	0
56	MG	BA	3741	1/1	0.81	0.15	68,68,68,68	0
56	MG	BA	3652	1/1	0.81	0.14	25,25,25,25	0
57	NEG	CA	3174	17/17	0.81	0.22	38,53,68,69	0
56	MG	AA	3047	1/1	0.82	0.22	68,68,68,68	0
56	MG	B4	502	1/1	0.82	0.24	73,73,73,73	0
56	MG	DA	3001	1/1	0.82	0.13	49,49,49,49	0
56	MG	BA	3566	1/1	0.82	0.11	28,28,28,28	0
56	MG	DA	3039	1/1	0.82	0.12	50,50,50,50	0
56	MG	BA	3543	1/1	0.82	0.20	62,62,62,62	0
56	MG	DA	3054	1/1	0.82	0.12	59,59,59,59	0
56	MG	AF	3001	1/1	0.82	0.14	48,48,48,48	0
56	MG	DA	3081	1/1	0.82	0.17	53,53,53,53	0
56	MG	CA	3026	1/1	0.82	0.15	61,61,61,61	0
56	MG	BA	3725	1/1	0.82	0.24	63,63,63,63	0
56	MG	CA	3128	1/1	0.82	0.37	72,72,72,72	0
56	MG	BA	3727	1/1	0.82	0.21	57,57,57,57	0
56	MG	DA	3582	1/1	0.82	0.21	65,65,65,65	0
56	MG	DA	3466	1/1	0.82	0.12	46,46,46,46	0
56	MG	BA	3429	1/1	0.82	0.13	71,71,71,71	0
56	MG	DA	3474	1/1	0.82	0.17	55,55,55,55	0
56	MG	DA	3180	1/1	0.82	0.23	50,50,50,50	0
56	MG	BA	3153	1/1	0.82	0.29	56,56,56,56	0
56	MG	DA	3220	1/1	0.82	0.11	45,45,45,45	0
56	MG	DE	302	1/1	0.82	0.11	30,30,30,30	0
56	MG	DA	3221	1/1	0.82	0.13	56,56,56,56	0
56	MG	BA	3702	1/1	0.82	0.18	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3630	1/1	0.82	0.15	44,44,44,44	0
56	MG	DA	3514	1/1	0.82	0.12	67,67,67,67	0
56	MG	BR	202	1/1	0.82	0.17	51,51,51,51	0
57	NEG	CX	3004	17/17	0.82	0.15	32,64,79,84	0
56	MG	BA	3134	1/1	0.83	0.22	57,57,57,57	0
56	MG	BA	3724	1/1	0.83	0.17	84,84,84,84	0
56	MG	CA	3055	1/1	0.83	0.24	63,63,63,63	0
56	MG	AA	3202	1/1	0.83	0.17	63,63,63,63	0
56	MG	BA	3639	1/1	0.83	0.21	55,55,55,55	0
56	MG	DA	3287	1/1	0.83	0.24	50,50,50,50	0
56	MG	DA	3291	1/1	0.83	0.17	41,41,41,41	0
56	MG	AA	3068	1/1	0.83	0.40	70,70,70,70	0
56	MG	CA	3098	1/1	0.83	0.17	59,59,59,59	0
56	MG	DA	3342	1/1	0.83	0.13	55,55,55,55	0
56	MG	CA	3110	1/1	0.83	0.29	62,62,62,62	0
56	MG	DA	3354	1/1	0.83	0.16	56,56,56,56	0
56	MG	BA	3515	1/1	0.83	0.12	57,57,57,57	0
56	MG	DA	3050	1/1	0.83	0.31	60,60,60,60	0
56	MG	CA	3118	1/1	0.83	0.24	61,61,61,61	0
56	MG	BA	3689	1/1	0.83	0.23	68,68,68,68	0
56	MG	BA	3157	1/1	0.83	0.30	59,59,59,59	0
56	MG	DA	3597	1/1	0.83	0.21	56,56,56,56	0
56	MG	DA	3430	1/1	0.83	0.12	51,51,51,51	0
56	MG	BA	3586	1/1	0.83	0.10	58,58,58,58	0
56	MG	BA	3356	1/1	0.83	0.15	24,24,24,24	0
56	MG	DA	3091	1/1	0.83	0.13	57,57,57,57	0
56	MG	DB	3005	1/1	0.83	0.51	77,77,77,77	0
56	MG	DB	3007	1/1	0.83	0.23	67,67,67,67	0
56	MG	BA	3600	1/1	0.83	0.14	59,59,59,59	0
56	MG	DA	3114	1/1	0.83	0.19	53,53,53,53	0
56	MG	DA	3122	1/1	0.83	0.34	71,71,71,71	0
56	MG	DA	3131	1/1	0.83	0.30	63,63,63,63	0
56	MG	DQ	3004	1/1	0.83	0.17	65,65,65,65	0
56	MG	AA	3210	1/1	0.83	0.24	65,65,65,65	0
56	MG	BA	3077	1/1	0.83	0.21	59,59,59,59	0
56	MG	CA	3136	1/1	0.83	0.18	73,73,73,73	0
57	NEG	CA	3172	17/17	0.83	0.18	61,76,83,84	0
56	MG	AX	3012	1/1	0.83	0.30	66,66,66,66	0
57	NEG	CA	3177	17/17	0.83	0.18	36,63,74,81	0
56	MG	CA	3048	1/1	0.83	0.26	54,54,54,54	0
56	MG	DA	3166	1/1	0.84	0.19	57,57,57,57	0
56	MG	DA	3176	1/1	0.84	0.09	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	3633	1/1	0.84	0.10	58,58,58,58	0
56	MG	CA	3011	1/1	0.84	0.31	71,71,71,71	0
56	MG	DA	3195	1/1	0.84	0.21	56,56,56,56	0
56	MG	AA	3042	1/1	0.84	0.13	52,52,52,52	0
56	MG	AA	3044	1/1	0.84	0.26	67,67,67,67	0
56	MG	AA	3004	1/1	0.84	0.15	67,67,67,67	0
56	MG	DA	3226	1/1	0.84	0.12	70,70,70,70	0
56	MG	CA	3141	1/1	0.84	0.21	61,61,61,61	0
56	MG	BA	3295	1/1	0.84	0.16	66,66,66,66	0
56	MG	DA	3545	1/1	0.84	0.13	68,68,68,68	0
56	MG	BA	3662	1/1	0.84	0.14	56,56,56,56	0
56	MG	BA	3740	1/1	0.84	0.12	49,49,49,49	0
56	MG	BA	3086	1/1	0.84	0.22	67,67,67,67	0
56	MG	BA	3502	1/1	0.84	0.10	62,62,62,62	0
56	MG	AA	3027	1/1	0.84	0.16	58,58,58,58	0
56	MG	CA	3056	1/1	0.84	0.18	74,74,74,74	0
56	MG	BA	3585	1/1	0.84	0.19	61,61,61,61	0
56	MG	BA	3415	1/1	0.84	0.13	62,62,62,62	0
56	MG	CA	3073	1/1	0.84	0.32	70,70,70,70	0
56	MG	AA	3074	1/1	0.84	0.41	59,59,59,59	0
56	MG	DA	3596	1/1	0.84	0.13	64,64,64,64	0
56	MG	CA	3087	1/1	0.84	0.14	65,65,65,65	0
56	MG	DA	3599	1/1	0.84	0.23	72,72,72,72	0
56	MG	DA	3385	1/1	0.84	0.20	55,55,55,55	0
56	MG	DA	3394	1/1	0.84	0.12	50,50,50,50	0
56	MG	DA	3604	1/1	0.84	0.24	58,58,58,58	0
56	MG	DA	3398	1/1	0.84	0.22	73,73,73,73	0
56	MG	DA	3620	1/1	0.84	0.21	71,71,71,71	0
56	MG	DA	3405	1/1	0.84	0.16	76,76,76,76	0
56	MG	DA	3059	1/1	0.84	0.10	49,49,49,49	0
56	MG	CA	3090	1/1	0.84	0.16	70,70,70,70	0
56	MG	CA	3097	1/1	0.84	0.13	66,66,66,66	0
56	MG	DA	3429	1/1	0.84	0.17	57,57,57,57	0
56	MG	DA	3082	1/1	0.84	0.15	48,48,48,48	0
56	MG	BA	3527	1/1	0.84	0.12	58,58,58,58	0
56	MG	BE	308	1/1	0.84	0.14	34,34,34,34	0
56	MG	DA	3437	1/1	0.84	0.11	47,47,47,47	0
56	MG	D5	502	1/1	0.84	0.13	50,50,50,50	0
56	MG	BA	3530	1/1	0.84	0.10	56,56,56,56	0
57	NEG	AA	3222	17/17	0.84	0.18	30,45,63,66	0
56	MG	BA	3713	1/1	0.84	0.39	68,68,68,68	0
56	MG	AA	3011	1/1	0.84	0.22	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	BA	3613	1/1	0.84	0.16	53,53,53,53	0
56	MG	BA	3628	1/1	0.84	0.17	55,55,55,55	0
56	MG	BA	3155	1/1	0.84	0.28	63,63,63,63	0
56	MG	CA	3131	1/1	0.85	0.20	62,62,62,62	0
56	MG	AA	3154	1/1	0.85	0.17	67,67,67,67	0
56	MG	BA	3681	1/1	0.85	0.19	47,47,47,47	0
56	MG	DA	3397	1/1	0.85	0.11	50,50,50,50	0
56	MG	AA	3155	1/1	0.85	0.22	60,60,60,60	0
56	MG	DA	3144	1/1	0.85	0.20	60,60,60,60	0
56	MG	CA	3057	1/1	0.85	0.12	73,73,73,73	0
56	MG	BA	3601	1/1	0.85	0.21	72,72,72,72	0
56	MG	DA	3577	1/1	0.85	0.19	72,72,72,72	0
56	MG	BA	3482	1/1	0.85	0.23	27,27,27,27	0
56	MG	DA	3426	1/1	0.85	0.19	53,53,53,53	0
56	MG	BA	3338	1/1	0.85	0.15	39,39,39,39	0
56	MG	BA	3340	1/1	0.85	0.17	34,34,34,34	0
56	MG	BA	3503	1/1	0.85	0.16	43,43,43,43	0
56	MG	AA	3015	1/1	0.85	0.19	56,56,56,56	0
56	MG	CA	3012	1/1	0.85	0.22	56,56,56,56	0
56	MG	BA	3370	1/1	0.85	0.10	51,51,51,51	0
56	MG	CA	3105	1/1	0.85	0.16	76,76,76,76	0
56	MG	BA	3712	1/1	0.85	0.12	35,35,35,35	0
56	MG	BA	3572	1/1	0.85	0.19	55,55,55,55	0
56	MG	BB	3001	1/1	0.85	0.20	56,56,56,56	0
56	MG	DB	3001	1/1	0.85	0.24	56,56,56,56	0
56	MG	DA	3058	1/1	0.85	0.10	48,48,48,48	0
56	MG	DA	3283	1/1	0.85	0.11	53,53,53,53	0
56	MG	CA	3040	1/1	0.85	0.17	70,70,70,70	0
56	MG	CA	3122	1/1	0.85	0.21	70,70,70,70	0
56	MG	DA	3318	1/1	0.85	0.10	60,60,60,60	0
56	MG	DA	3508	1/1	0.85	0.10	68,68,68,68	0
56	MG	DA	3323	1/1	0.85	0.13	44,44,44,44	0
56	MG	CA	3042	1/1	0.85	0.20	61,61,61,61	0
56	MG	CA	3043	1/1	0.85	0.26	56,56,56,56	0
56	MG	AA	3069	1/1	0.85	0.29	59,59,59,59	0
56	MG	DA	3086	1/1	0.85	0.28	42,42,42,42	0
56	MG	BA	3389	1/1	0.85	0.13	51,51,51,51	0
56	MG	AA	3193	1/1	0.85	0.19	69,69,69,69	0
56	MG	DA	3533	1/1	0.85	0.14	50,50,50,50	0
56	MG	DA	3534	1/1	0.85	0.28	59,59,59,59	0
56	MG	DA	3540	1/1	0.85	0.10	65,65,65,65	0
56	MG	DA	3460	1/1	0.86	0.10	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	3257	1/1	0.86	0.14	48,48,48,48	0
56	MG	BA	3687	1/1	0.86	0.24	56,56,56,56	0
56	MG	BE	301	1/1	0.86	0.15	36,36,36,36	0
56	MG	DA	3151	1/1	0.86	0.21	52,52,52,52	0
56	MG	AE	3002	1/1	0.86	0.18	67,67,67,67	0
56	MG	BG	3002	1/1	0.86	0.09	52,52,52,52	0
56	MG	DA	3175	1/1	0.86	0.21	43,43,43,43	0
56	MG	AA	3174	1/1	0.86	0.10	59,59,59,59	0
56	MG	DA	3500	1/1	0.86	0.12	56,56,56,56	0
56	MG	BA	3694	1/1	0.86	0.12	57,57,57,57	0
56	MG	BA	3697	1/1	0.86	0.08	34,34,34,34	0
56	MG	BA	3304	1/1	0.86	0.15	21,21,21,21	0
56	MG	DA	3197	1/1	0.86	0.10	57,57,57,57	0
56	MG	DA	3199	1/1	0.86	0.35	57,57,57,57	0
56	MG	BA	3438	1/1	0.86	0.15	44,44,44,44	0
56	MG	DA	3207	1/1	0.86	0.18	58,58,58,58	0
56	MG	BA	3442	1/1	0.86	0.11	31,31,31,31	0
56	MG	CA	3005	1/1	0.86	0.20	62,62,62,62	0
56	MG	DA	3223	1/1	0.86	0.20	63,63,63,63	0
56	MG	BA	3444	1/1	0.86	0.13	37,37,37,37	0
56	MG	BA	3577	1/1	0.86	0.17	62,62,62,62	0
56	MG	DA	3542	1/1	0.86	0.11	65,65,65,65	0
56	MG	AN	502	1/1	0.86	0.25	56,56,56,56	0
56	MG	DA	3252	1/1	0.86	0.09	43,43,43,43	0
56	MG	BA	3109	1/1	0.86	0.17	49,49,49,49	0
56	MG	CA	3142	1/1	0.86	0.25	69,69,69,69	0
56	MG	BA	3112	1/1	0.86	0.12	50,50,50,50	0
56	MG	DA	3285	1/1	0.86	0.12	43,43,43,43	0
56	MG	BA	3715	1/1	0.86	0.11	48,48,48,48	0
56	MG	CA	3028	1/1	0.86	0.23	53,53,53,53	0
56	MG	DA	3574	1/1	0.86	0.13	68,68,68,68	0
56	MG	DA	3575	1/1	0.86	0.21	58,58,58,58	0
56	MG	DA	3298	1/1	0.86	0.12	57,57,57,57	0
56	MG	DA	3311	1/1	0.86	0.14	54,54,54,54	0
56	MG	BA	3329	1/1	0.86	0.13	57,57,57,57	0
56	MG	DA	3322	1/1	0.86	0.09	46,46,46,46	0
56	MG	AA	3176	1/1	0.86	0.20	69,69,69,69	0
56	MG	AA	3088	1/1	0.86	0.19	63,63,63,63	0
56	MG	CX	3003	1/1	0.86	0.15	64,64,64,64	0
56	MG	CY	3001	1/1	0.86	0.18	63,63,63,63	0
56	MG	DA	3345	1/1	0.86	0.12	57,57,57,57	0
56	MG	DA	3603	1/1	0.86	0.19	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3494	1/1	0.86	0.15	41,41,41,41	0
56	MG	AA	3128	1/1	0.86	0.22	60,60,60,60	0
56	MG	DA	3606	1/1	0.86	0.11	54,54,54,54	0
56	MG	AA	3159	1/1	0.86	0.12	70,70,70,70	0
56	MG	DA	3377	1/1	0.86	0.12	48,48,48,48	0
56	MG	BA	3615	1/1	0.86	0.34	41,41,41,41	0
56	MG	BA	3504	1/1	0.86	0.30	57,57,57,57	0
56	MG	AA	3209	1/1	0.86	0.22	62,62,62,62	0
56	MG	BA	3512	1/1	0.86	0.12	65,65,65,65	0
56	MG	AA	3146	1/1	0.86	0.23	65,65,65,65	0
56	MG	DA	3061	1/1	0.86	0.12	63,63,63,63	0
56	MG	BA	3746	1/1	0.86	0.26	71,71,71,71	0
56	MG	BA	3189	1/1	0.86	0.17	55,55,55,55	0
56	MG	DR	3002	1/1	0.86	0.12	55,55,55,55	0
56	MG	BA	3755	1/1	0.86	0.13	42,42,42,42	0
56	MG	BA	3199	1/1	0.86	0.33	55,55,55,55	0
56	MG	BA	3765	1/1	0.86	0.15	59,59,59,59	0
57	NEG	AA	3220	17/17	0.86	0.13	29,49,59,65	0
56	MG	BA	3208	1/1	0.86	0.14	47,47,47,47	0
56	MG	CA	3093	1/1	0.86	0.14	57,57,57,57	0
56	MG	BA	3242	1/1	0.86	0.23	58,58,58,58	0
56	MG	DA	3103	1/1	0.86	0.17	60,60,60,60	0
57	NEG	CA	3175	17/17	0.86	0.25	48,61,79,89	0
56	MG	DA	3458	1/1	0.86	0.09	56,56,56,56	0
56	MG	BA	3031	1/1	0.86	0.21	49,49,49,49	0
56	MG	AA	3029	1/1	0.87	0.17	60,60,60,60	0
56	MG	BA	3247	1/1	0.87	0.14	49,49,49,49	0
56	MG	AA	3203	1/1	0.87	0.32	62,62,62,62	0
56	MG	BA	3559	1/1	0.87	0.13	66,66,66,66	0
56	MG	DA	3488	1/1	0.87	0.23	66,66,66,66	0
56	MG	BA	3561	1/1	0.87	0.12	64,64,64,64	0
56	MG	BA	3069	1/1	0.87	0.24	46,46,46,46	0
56	MG	DA	3496	1/1	0.87	0.25	51,51,51,51	0
56	MG	BA	3300	1/1	0.87	0.14	55,55,55,55	0
56	MG	AA	3048	1/1	0.87	0.25	55,55,55,55	0
56	MG	AA	3130	1/1	0.87	0.23	74,74,74,74	0
56	MG	BA	3582	1/1	0.87	0.16	63,63,63,63	0
56	MG	BA	3305	1/1	0.87	0.26	61,61,61,61	0
56	MG	BA	3465	1/1	0.87	0.14	20,20,20,20	0
56	MG	CA	3025	1/1	0.87	0.23	64,64,64,64	0
56	MG	DA	3523	1/1	0.87	0.15	62,62,62,62	0
56	MG	BA	3588	1/1	0.87	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3246	1/1	0.87	0.18	53,53,53,53	0
56	MG	AA	3134	1/1	0.87	0.24	73,73,73,73	0
56	MG	CA	3146	1/1	0.87	0.25	80,80,80,80	0
56	MG	BA	3597	1/1	0.87	0.12	51,51,51,51	0
56	MG	DA	3539	1/1	0.87	0.11	64,64,64,64	0
56	MG	CA	3031	1/1	0.87	0.26	71,71,71,71	0
56	MG	CA	3152	1/1	0.87	0.15	58,58,58,58	0
56	MG	CA	3153	1/1	0.87	0.16	62,62,62,62	0
56	MG	DA	3550	1/1	0.87	0.17	61,61,61,61	0
56	MG	AA	3224	1/1	0.87	0.18	61,61,61,61	0
56	MG	AA	3050	1/1	0.87	0.15	65,65,65,65	0
56	MG	BA	3729	1/1	0.87	0.22	55,55,55,55	0
56	MG	BA	3602	1/1	0.87	0.11	61,61,61,61	0
56	MG	CA	3045	1/1	0.87	0.27	68,68,68,68	0
56	MG	DA	3030	1/1	0.87	0.18	54,54,54,54	0
56	MG	AA	3111	1/1	0.87	0.13	65,65,65,65	0
56	MG	DA	3329	1/1	0.87	0.16	62,62,62,62	0
56	MG	AA	3184	1/1	0.87	0.17	75,75,75,75	0
56	MG	BA	3333	1/1	0.87	0.10	39,39,39,39	0
56	MG	CA	3052	1/1	0.87	0.17	65,65,65,65	0
56	MG	AA	3139	1/1	0.87	0.18	50,50,50,50	0
56	MG	DA	3348	1/1	0.87	0.13	46,46,46,46	0
56	MG	DA	3057	1/1	0.87	0.19	54,54,54,54	0
56	MG	BA	3616	1/1	0.87	0.09	43,43,43,43	0
56	MG	DA	3363	1/1	0.87	0.12	61,61,61,61	0
56	MG	AX	3004	1/1	0.87	0.20	67,67,67,67	0
56	MG	DA	3367	1/1	0.87	0.09	44,44,44,44	0
56	MG	DA	3369	1/1	0.87	0.14	47,47,47,47	0
56	MG	AX	3005	1/1	0.87	0.22	66,66,66,66	0
56	MG	DA	3066	1/1	0.87	0.10	39,39,39,39	0
56	MG	CA	3067	1/1	0.87	0.18	57,57,57,57	0
56	MG	DA	3615	1/1	0.87	0.25	59,59,59,59	0
56	MG	AA	3041	1/1	0.87	0.19	64,64,64,64	0
56	MG	BA	3183	1/1	0.87	0.24	47,47,47,47	0
56	MG	BA	3637	1/1	0.87	0.21	34,34,34,34	0
56	MG	AX	3009	1/1	0.87	0.22	72,72,72,72	0
56	MG	DA	3087	1/1	0.87	0.10	49,49,49,49	0
56	MG	AA	3149	1/1	0.87	0.12	71,71,71,71	0
56	MG	DA	3422	1/1	0.87	0.31	52,52,52,52	0
56	MG	AA	3087	1/1	0.87	0.17	59,59,59,59	0
56	MG	DA	3093	1/1	0.87	0.15	59,59,59,59	0
56	MG	BA	3209	1/1	0.87	0.23	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	BB	3013	1/1	0.87	0.17	46,46,46,46	0
56	MG	BA	3670	1/1	0.87	0.25	55,55,55,55	0
56	MG	D0	101	1/1	0.87	0.17	73,73,73,73	0
56	MG	CA	3103	1/1	0.87	0.16	78,78,78,78	0
56	MG	BA	3235	1/1	0.87	0.23	65,65,65,65	0
57	NEG	AA	3218	17/17	0.87	0.16	57,72,76,91	0
56	MG	DA	3442	1/1	0.87	0.14	46,46,46,46	0
56	MG	DA	3453	1/1	0.87	0.20	77,77,77,77	0
56	MG	DA	3456	1/1	0.87	0.10	50,50,50,50	0
56	MG	AA	3116	1/1	0.87	0.14	57,57,57,57	0
57	NEG	CA	3173	17/17	0.87	0.16	54,76,85,86	0
56	MG	BE	307	1/1	0.87	0.18	71,71,71,71	0
56	MG	CA	3117	1/1	0.87	0.26	71,71,71,71	0
56	MG	BA	3418	1/1	0.87	0.15	57,57,57,57	0
57	NEG	CW	3002	17/17	0.87	0.20	41,56,78,84	0
56	MG	DA	3169	1/1	0.87	0.17	61,61,61,61	0
56	MG	BA	3505	1/1	0.88	0.16	54,54,54,54	0
56	MG	BD	303	1/1	0.88	0.18	45,45,45,45	0
56	MG	CA	3120	1/1	0.88	0.19	70,70,70,70	0
56	MG	AA	3208	1/1	0.88	0.33	67,67,67,67	0
56	MG	DA	3184	1/1	0.88	0.35	56,56,56,56	0
56	MG	BA	3509	1/1	0.88	0.16	46,46,46,46	0
56	MG	DA	3494	1/1	0.88	0.17	55,55,55,55	0
56	MG	BA	3653	1/1	0.88	0.10	23,23,23,23	0
56	MG	BA	3323	1/1	0.88	0.29	60,60,60,60	0
56	MG	BA	3665	1/1	0.88	0.11	45,45,45,45	0
56	MG	BO	5001	1/1	0.88	0.15	70,70,70,70	0
56	MG	AA	3020	1/1	0.88	0.29	53,53,53,53	0
56	MG	AA	3032	1/1	0.88	0.19	62,62,62,62	0
56	MG	BA	3521	1/1	0.88	0.16	28,28,28,28	0
56	MG	DA	3224	1/1	0.88	0.17	27,27,27,27	0
56	MG	BA	3526	1/1	0.88	0.13	38,38,38,38	0
56	MG	B6	101	1/1	0.88	0.20	49,49,49,49	0
56	MG	BA	3118	1/1	0.88	0.13	46,46,46,46	0
56	MG	AA	3126	1/1	0.88	0.18	65,65,65,65	0
56	MG	BA	3151	1/1	0.88	0.26	51,51,51,51	0
56	MG	CA	3009	1/1	0.88	0.24	55,55,55,55	0
56	MG	DA	3260	1/1	0.88	0.13	36,36,36,36	0
56	MG	BA	3695	1/1	0.88	0.14	39,39,39,39	0
56	MG	DA	3541	1/1	0.88	0.29	46,46,46,46	0
56	MG	CA	3147	1/1	0.88	0.10	51,51,51,51	0
56	MG	AA	3017	1/1	0.88	0.16	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	3546	1/1	0.88	0.12	64,64,64,64	0
56	MG	BA	3343	1/1	0.88	0.13	44,44,44,44	0
56	MG	BA	3701	1/1	0.88	0.23	66,66,66,66	0
56	MG	DA	3554	1/1	0.88	0.14	45,45,45,45	0
56	MG	DA	3294	1/1	0.88	0.14	53,53,53,53	0
56	MG	AA	3095	1/1	0.88	0.14	63,63,63,63	0
56	MG	DA	3302	1/1	0.88	0.11	38,38,38,38	0
56	MG	DA	3565	1/1	0.88	0.14	48,48,48,48	0
56	MG	AA	3177	1/1	0.88	0.12	66,66,66,66	0
56	MG	BA	3156	1/1	0.88	0.20	64,64,64,64	0
56	MG	AV	102	1/1	0.88	0.21	52,52,52,52	0
56	MG	BA	3394	1/1	0.88	0.12	53,53,53,53	0
56	MG	AW	3001	1/1	0.88	0.17	67,67,67,67	0
56	MG	AA	3096	1/1	0.88	0.27	53,53,53,53	0
56	MG	BA	3570	1/1	0.88	0.31	57,57,57,57	0
56	MG	BA	3721	1/1	0.88	0.14	74,74,74,74	0
56	MG	BA	3187	1/1	0.88	0.14	42,42,42,42	0
56	MG	DA	3593	1/1	0.88	0.15	57,57,57,57	0
56	MG	DA	3047	1/1	0.88	0.10	46,46,46,46	0
56	MG	CA	3047	1/1	0.88	0.33	56,56,56,56	0
56	MG	DA	3598	1/1	0.88	0.38	63,63,63,63	0
56	MG	AA	3180	1/1	0.88	0.21	67,67,67,67	0
56	MG	AA	3101	1/1	0.88	0.20	52,52,52,52	0
56	MG	AA	3102	1/1	0.88	0.14	50,50,50,50	0
56	MG	AA	3019	1/1	0.88	0.19	53,53,53,53	0
56	MG	BA	3420	1/1	0.88	0.14	61,61,61,61	0
56	MG	BA	3215	1/1	0.88	0.16	47,47,47,47	0
56	MG	AA	3080	1/1	0.88	0.34	58,58,58,58	0
56	MG	AA	3058	1/1	0.88	0.28	63,63,63,63	0
56	MG	DA	3616	1/1	0.88	0.14	47,47,47,47	0
56	MG	DA	3617	1/1	0.88	0.26	55,55,55,55	0
56	MG	AA	3150	1/1	0.88	0.17	58,58,58,58	0
56	MG	AA	3196	1/1	0.88	0.17	66,66,66,66	0
56	MG	CA	3070	1/1	0.88	0.23	52,52,52,52	0
56	MG	BA	3256	1/1	0.88	0.15	25,25,25,25	0
56	MG	DA	3406	1/1	0.88	0.25	48,48,48,48	0
56	MG	DA	3409	1/1	0.88	0.10	41,41,41,41	0
56	MG	AA	3151	1/1	0.88	0.24	65,65,65,65	0
56	MG	CA	3080	1/1	0.88	0.21	62,62,62,62	0
56	MG	BA	3259	1/1	0.88	0.14	32,32,32,32	0
56	MG	DP	201	1/1	0.88	0.19	50,50,50,50	0
56	MG	BA	3294	1/1	0.88	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3047	1/1	0.88	0.15	51,51,51,51	0
56	MG	DU	3001	1/1	0.88	0.26	61,61,61,61	0
56	MG	DA	3109	1/1	0.88	0.12	47,47,47,47	0
56	MG	BA	3048	1/1	0.88	0.22	56,56,56,56	0
56	MG	DA	3119	1/1	0.88	0.14	50,50,50,50	0
56	MG	AA	3152	1/1	0.88	0.16	63,63,63,63	0
56	MG	DA	3125	1/1	0.88	0.25	56,56,56,56	0
57	NEG	AA	3219	17/17	0.88	0.16	61,71,78,79	0
56	MG	CA	3101	1/1	0.88	0.10	64,64,64,64	0
57	NEG	AA	3221	17/17	0.88	0.17	44,57,69,70	0
56	MG	DA	3135	1/1	0.88	0.31	44,44,44,44	0
57	NEG	CA	3170	17/17	0.88	0.20	58,72,83,86	0
56	MG	BA	3074	1/1	0.88	0.20	58,58,58,58	0
56	MG	DA	3147	1/1	0.88	0.08	49,49,49,49	0
56	MG	AA	3153	1/1	0.88	0.17	44,44,44,44	0
56	MG	CA	3109	1/1	0.88	0.20	67,67,67,67	0
56	MG	AA	3083	1/1	0.88	0.18	57,57,57,57	0
56	MG	DA	3167	1/1	0.88	0.38	51,51,51,51	0
56	MG	BA	3310	1/1	0.88	0.10	41,41,41,41	0
56	MG	DA	3473	1/1	0.88	0.10	60,60,60,60	0
56	MG	AN	503	1/1	0.89	0.16	59,59,59,59	0
56	MG	BB	3012	1/1	0.89	0.08	42,42,42,42	0
56	MG	BA	3631	1/1	0.89	0.20	63,63,63,63	0
56	MG	BA	3335	1/1	0.89	0.12	50,50,50,50	0
56	MG	CA	3119	1/1	0.89	0.16	84,84,84,84	0
56	MG	BA	3053	1/1	0.89	0.12	56,56,56,56	0
56	MG	BD	301	1/1	0.89	0.25	45,45,45,45	0
56	MG	DA	3188	1/1	0.89	0.20	61,61,61,61	0
56	MG	BA	3636	1/1	0.89	0.11	61,61,61,61	0
56	MG	DA	3498	1/1	0.89	0.16	66,66,66,66	0
56	MG	AN	504	1/1	0.89	0.22	56,56,56,56	0
56	MG	BA	3070	1/1	0.89	0.11	48,48,48,48	0
56	MG	DA	3502	1/1	0.89	0.14	47,47,47,47	0
56	MG	BA	3348	1/1	0.89	0.14	35,35,35,35	0
56	MG	DA	3205	1/1	0.89	0.08	45,45,45,45	0
56	MG	BF	307	1/1	0.89	0.13	46,46,46,46	0
56	MG	BA	3644	1/1	0.89	0.15	34,34,34,34	0
56	MG	DA	3520	1/1	0.89	0.14	61,61,61,61	0
56	MG	BA	3351	1/1	0.89	0.19	61,61,61,61	0
56	MG	BA	3071	1/1	0.89	0.20	48,48,48,48	0
56	MG	BA	3660	1/1	0.89	0.17	44,44,44,44	0
56	MG	BR	201	1/1	0.89	0.25	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	AA	3086	1/1	0.89	0.16	53,53,53,53	0
56	MG	BA	3524	1/1	0.89	0.11	44,44,44,44	0
56	MG	B2	3001	1/1	0.89	0.12	54,54,54,54	0
56	MG	BA	3233	1/1	0.89	0.12	49,49,49,49	0
56	MG	BA	3675	1/1	0.89	0.16	39,39,39,39	0
56	MG	BA	3378	1/1	0.89	0.18	24,24,24,24	0
56	MG	BA	3381	1/1	0.89	0.13	33,33,33,33	0
56	MG	AV	103	1/1	0.89	0.19	70,70,70,70	0
56	MG	BA	3537	1/1	0.89	0.17	55,55,55,55	0
56	MG	BA	3241	1/1	0.89	0.26	59,59,59,59	0
56	MG	DA	3290	1/1	0.89	0.15	36,36,36,36	0
56	MG	CA	3154	1/1	0.89	0.28	62,62,62,62	0
56	MG	CA	3156	1/1	0.89	0.13	58,58,58,58	0
56	MG	DA	3297	1/1	0.89	0.11	70,70,70,70	0
56	MG	BA	3078	1/1	0.89	0.10	48,48,48,48	0
56	MG	CA	3016	1/1	0.89	0.21	56,56,56,56	0
56	MG	AA	3059	1/1	0.89	0.24	53,53,53,53	0
56	MG	BA	3546	1/1	0.89	0.14	57,57,57,57	0
56	MG	DA	3320	1/1	0.89	0.16	53,53,53,53	0
56	MG	BA	3698	1/1	0.89	0.16	59,59,59,59	0
56	MG	DA	3028	1/1	0.89	0.09	52,52,52,52	0
56	MG	AA	3103	1/1	0.89	0.16	59,59,59,59	0
56	MG	BA	3551	1/1	0.89	0.21	56,56,56,56	0
56	MG	DA	3579	1/1	0.89	0.12	69,69,69,69	0
56	MG	DA	3338	1/1	0.89	0.09	60,60,60,60	0
56	MG	BA	3254	1/1	0.89	0.12	56,56,56,56	0
56	MG	BA	3403	1/1	0.89	0.19	53,53,53,53	0
56	MG	DA	3344	1/1	0.89	0.07	54,54,54,54	0
56	MG	BA	3704	1/1	0.89	0.09	75,75,75,75	0
56	MG	BA	3706	1/1	0.89	0.13	52,52,52,52	0
56	MG	BA	3089	1/1	0.89	0.35	46,46,46,46	0
56	MG	DA	3352	1/1	0.89	0.13	45,45,45,45	0
56	MG	AA	3140	1/1	0.89	0.10	61,61,61,61	0
56	MG	DA	3355	1/1	0.89	0.12	53,53,53,53	0
56	MG	AA	3144	1/1	0.89	0.08	62,62,62,62	0
56	MG	BA	3276	1/1	0.89	0.16	40,40,40,40	0
56	MG	AA	3145	1/1	0.89	0.20	36,36,36,36	0
56	MG	DA	3614	1/1	0.89	0.08	34,34,34,34	0
56	MG	BA	3430	1/1	0.89	0.18	48,48,48,48	0
56	MG	DA	3373	1/1	0.89	0.23	51,51,51,51	0
56	MG	DA	3376	1/1	0.89	0.14	46,46,46,46	0
56	MG	DA	3068	1/1	0.89	0.15	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	DA	3078	1/1	0.89	0.14	64,64,64,64	0
56	MG	DA	3622	1/1	0.89	0.12	61,61,61,61	0
56	MG	AA	3057	1/1	0.89	0.24	58,58,58,58	0
56	MG	DB	3002	1/1	0.89	0.15	58,58,58,58	0
56	MG	DB	3003	1/1	0.89	0.10	62,62,62,62	0
56	MG	CA	3053	1/1	0.89	0.34	63,63,63,63	0
56	MG	BA	3147	1/1	0.89	0.23	60,60,60,60	0
56	MG	AA	3160	1/1	0.89	0.21	70,70,70,70	0
56	MG	BA	3152	1/1	0.89	0.17	48,48,48,48	0
56	MG	AA	3215	1/1	0.89	0.22	56,56,56,56	0
56	MG	BA	3590	1/1	0.89	0.15	38,38,38,38	0
56	MG	BA	3447	1/1	0.89	0.11	38,38,38,38	0
56	MG	BA	3596	1/1	0.89	0.11	52,52,52,52	0
56	MG	AA	3164	1/1	0.89	0.18	71,71,71,71	0
56	MG	BA	3460	1/1	0.89	0.23	45,45,45,45	0
56	MG	AA	3190	1/1	0.89	0.17	61,61,61,61	0
56	MG	BA	3312	1/1	0.89	0.14	41,41,41,41	0
56	MG	BA	3002	1/1	0.89	0.12	36,36,36,36	0
56	MG	D8	5001	1/1	0.89	0.17	52,52,52,52	0
56	MG	DA	3121	1/1	0.89	0.11	33,33,33,33	0
56	MG	BA	3019	1/1	0.89	0.16	38,38,38,38	0
56	MG	BA	3483	1/1	0.89	0.15	50,50,50,50	0
56	MG	BA	3159	1/1	0.89	0.13	45,45,45,45	0
56	MG	DA	3444	1/1	0.89	0.11	59,59,59,59	0
56	MG	DA	3450	1/1	0.89	0.09	50,50,50,50	0
57	NEG	AW	3004	17/17	0.89	0.15	37,50,72,73	0
57	NEG	AX	3013	17/17	0.89	0.17	29,49,69,70	0
56	MG	BA	3757	1/1	0.89	0.17	47,47,47,47	0
56	MG	DA	3139	1/1	0.89	0.32	59,59,59,59	0
56	MG	AA	3117	1/1	0.89	0.18	66,66,66,66	0
56	MG	BA	3618	1/1	0.89	0.17	64,64,64,64	0
56	MG	DA	3148	1/1	0.89	0.14	53,53,53,53	0
56	MG	BA	3620	1/1	0.89	0.18	42,42,42,42	0
56	MG	CA	3106	1/1	0.89	0.14	55,55,55,55	0
56	MG	AA	3170	1/1	0.89	0.12	66,66,66,66	0
56	MG	DA	3472	1/1	0.89	0.11	40,40,40,40	0
56	MG	CA	3013	1/1	0.90	0.07	52,52,52,52	0
56	MG	BA	3299	1/1	0.90	0.07	53,53,53,53	0
56	MG	CA	3018	1/1	0.90	0.18	69,69,69,69	0
56	MG	BA	3492	1/1	0.90	0.11	33,33,33,33	0
56	MG	BA	3205	1/1	0.90	0.12	45,45,45,45	0
56	MG	DA	3238	1/1	0.90	0.09	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	3241	1/1	0.90	0.17	51,51,51,51	0
56	MG	AA	3115	1/1	0.90	0.23	61,61,61,61	0
56	MG	BA	3716	1/1	0.90	0.13	48,48,48,48	0
56	MG	BA	3391	1/1	0.90	0.10	36,36,36,36	0
56	MG	DA	3518	1/1	0.90	0.17	57,57,57,57	0
56	MG	CA	3155	1/1	0.90	0.25	61,61,61,61	0
56	MG	AA	3207	1/1	0.90	0.16	57,57,57,57	0
56	MG	BA	3605	1/1	0.90	0.28	69,69,69,69	0
56	MG	CA	3168	1/1	0.90	0.20	62,62,62,62	0
56	MG	DA	3279	1/1	0.90	0.07	51,51,51,51	0
56	MG	DA	3527	1/1	0.90	0.16	67,67,67,67	0
56	MG	BA	3213	1/1	0.90	0.17	48,48,48,48	0
56	MG	CN	101	1/1	0.90	0.20	69,69,69,69	0
56	MG	BA	3609	1/1	0.90	0.14	62,62,62,62	0
56	MG	BA	3306	1/1	0.90	0.14	51,51,51,51	0
56	MG	AO	3101	1/1	0.90	0.15	58,58,58,58	0
56	MG	DA	3013	1/1	0.90	0.17	49,49,49,49	0
56	MG	DA	3025	1/1	0.90	0.23	49,49,49,49	0
56	MG	BA	3221	1/1	0.90	0.16	47,47,47,47	0
56	MG	DA	3029	1/1	0.90	0.14	52,52,52,52	0
56	MG	BA	3223	1/1	0.90	0.13	42,42,42,42	0
56	MG	BA	3407	1/1	0.90	0.12	44,44,44,44	0
56	MG	AA	3063	1/1	0.90	0.27	56,56,56,56	0
56	MG	DA	3558	1/1	0.90	0.13	48,48,48,48	0
56	MG	BA	3522	1/1	0.90	0.27	59,59,59,59	0
56	MG	BA	3416	1/1	0.90	0.10	53,53,53,53	0
56	MG	DA	3048	1/1	0.90	0.20	58,58,58,58	0
56	MG	BA	3417	1/1	0.90	0.14	56,56,56,56	0
56	MG	BA	3234	1/1	0.90	0.29	52,52,52,52	0
56	MG	BA	3753	1/1	0.90	0.20	76,76,76,76	0
56	MG	BA	3754	1/1	0.90	0.17	36,36,36,36	0
56	MG	CA	3061	1/1	0.90	0.19	61,61,61,61	0
56	MG	CA	3064	1/1	0.90	0.27	67,67,67,67	0
56	MG	DA	3062	1/1	0.90	0.09	49,49,49,49	0
56	MG	CA	3065	1/1	0.90	0.39	73,73,73,73	0
56	MG	BA	3325	1/1	0.90	0.12	42,42,42,42	0
56	MG	BA	3756	1/1	0.90	0.17	56,56,56,56	0
56	MG	AA	3092	1/1	0.90	0.26	59,59,59,59	0
56	MG	DA	3588	1/1	0.90	0.18	57,57,57,57	0
56	MG	DA	3590	1/1	0.90	0.10	61,61,61,61	0
56	MG	DA	3360	1/1	0.90	0.16	47,47,47,47	0
56	MG	AA	3099	1/1	0.90	0.13	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	AA	3031	1/1	0.90	0.14	63,63,63,63	0
56	MG	AA	3167	1/1	0.90	0.14	71,71,71,71	0
56	MG	CA	3076	1/1	0.90	0.14	54,54,54,54	0
56	MG	CA	3079	1/1	0.90	0.16	61,61,61,61	0
56	MG	AA	3201	1/1	0.90	0.10	60,60,60,60	0
56	MG	CA	3081	1/1	0.90	0.18	51,51,51,51	0
56	MG	BA	3174	1/1	0.90	0.09	52,52,52,52	0
56	MG	BA	3180	1/1	0.90	0.08	46,46,46,46	0
56	MG	DA	3393	1/1	0.90	0.19	53,53,53,53	0
56	MG	AA	3127	1/1	0.90	0.26	52,52,52,52	0
56	MG	DA	3105	1/1	0.90	0.22	54,54,54,54	0
56	MG	BA	3554	1/1	0.90	0.10	56,56,56,56	0
56	MG	AA	3094	1/1	0.90	0.30	53,53,53,53	0
56	MG	DA	3116	1/1	0.90	0.06	58,58,58,58	0
56	MG	BA	3450	1/1	0.90	0.16	59,59,59,59	0
56	MG	AX	3010	1/1	0.90	0.17	54,54,54,54	0
56	MG	CA	3104	1/1	0.90	0.14	51,51,51,51	0
56	MG	DA	3418	1/1	0.90	0.16	55,55,55,55	0
56	MG	BA	3354	1/1	0.90	0.20	39,39,39,39	0
56	MG	DA	3130	1/1	0.90	0.29	52,52,52,52	0
56	MG	BA	3563	1/1	0.90	0.17	43,43,43,43	0
56	MG	DA	3427	1/1	0.90	0.28	61,61,61,61	0
56	MG	DB	3010	1/1	0.90	0.34	72,72,72,72	0
56	MG	BA	3686	1/1	0.90	0.23	61,61,61,61	0
56	MG	BA	3461	1/1	0.90	0.11	21,21,21,21	0
56	MG	DE	304	1/1	0.90	0.10	45,45,45,45	0
56	MG	DF	304	1/1	0.90	0.10	48,48,48,48	0
56	MG	BA	3464	1/1	0.90	0.23	53,53,53,53	0
56	MG	BN	3001	1/1	0.90	0.14	51,51,51,51	0
56	MG	DQ	3002	1/1	0.90	0.08	50,50,50,50	0
56	MG	BA	3691	1/1	0.90	0.13	60,60,60,60	0
56	MG	DA	3439	1/1	0.90	0.23	58,58,58,58	0
56	MG	DA	3441	1/1	0.90	0.09	39,39,39,39	0
56	MG	DU	3003	1/1	0.90	0.09	50,50,50,50	0
56	MG	DV	3003	1/1	0.90	0.14	62,62,62,62	0
56	MG	BA	3283	1/1	0.90	0.08	39,39,39,39	0
56	MG	DA	3161	1/1	0.90	0.13	57,57,57,57	0
56	MG	DA	3447	1/1	0.90	0.15	49,49,49,49	0
56	MG	BA	3573	1/1	0.90	0.13	53,53,53,53	0
56	MG	BA	3574	1/1	0.90	0.24	60,60,60,60	0
56	MG	BA	3576	1/1	0.90	0.14	56,56,56,56	0
56	MG	BA	3359	1/1	0.90	0.17	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	BY	502	1/1	0.90	0.14	60,60,60,60	0
56	MG	BA	3579	1/1	0.90	0.12	57,57,57,57	0
56	MG	DA	3462	1/1	0.90	0.08	36,36,36,36	0
56	MG	BA	3471	1/1	0.90	0.11	33,33,33,33	0
56	MG	BA	3475	1/1	0.90	0.15	52,52,52,52	0
56	MG	B7	104	1/1	0.90	0.12	55,55,55,55	0
56	MG	CA	3133	1/1	0.90	0.22	67,67,67,67	0
56	MG	BA	3584	1/1	0.90	0.11	47,47,47,47	0
56	MG	BA	3479	1/1	0.90	0.19	36,36,36,36	0
56	MG	BA	3360	1/1	0.90	0.21	41,41,41,41	0
56	MG	BA	3195	1/1	0.90	0.30	53,53,53,53	0
56	MG	BA	3148	1/1	0.90	0.15	50,50,50,50	0
56	MG	BA	3711	1/1	0.90	0.11	51,51,51,51	0
56	MG	DA	3216	1/1	0.90	0.12	52,52,52,52	0
56	MG	BA	3567	1/1	0.91	0.08	35,35,35,35	0
56	MG	DA	3461	1/1	0.91	0.08	49,49,49,49	0
56	MG	BA	3569	1/1	0.91	0.11	44,44,44,44	0
56	MG	BA	3690	1/1	0.91	0.11	44,44,44,44	0
56	MG	DA	3465	1/1	0.91	0.21	52,52,52,52	0
56	MG	BA	3087	1/1	0.91	0.08	63,63,63,63	0
56	MG	DA	3165	1/1	0.91	0.26	69,69,69,69	0
56	MG	BA	3466	1/1	0.91	0.24	52,52,52,52	0
56	MG	BA	3468	1/1	0.91	0.08	31,31,31,31	0
56	MG	DA	3168	1/1	0.91	0.23	41,41,41,41	0
56	MG	BX	101	1/1	0.91	0.16	48,48,48,48	0
56	MG	DA	3172	1/1	0.91	0.15	56,56,56,56	0
56	MG	DA	3485	1/1	0.91	0.13	60,60,60,60	0
56	MG	BA	3281	1/1	0.91	0.14	55,55,55,55	0
56	MG	BA	3363	1/1	0.91	0.19	53,53,53,53	0
56	MG	DA	3490	1/1	0.91	0.08	49,49,49,49	0
56	MG	DA	3177	1/1	0.91	0.14	54,54,54,54	0
56	MG	BA	3364	1/1	0.91	0.12	50,50,50,50	0
56	MG	DA	3495	1/1	0.91	0.10	57,57,57,57	0
56	MG	BA	3477	1/1	0.91	0.15	35,35,35,35	0
56	MG	AA	3105	1/1	0.91	0.09	66,66,66,66	0
56	MG	BA	3285	1/1	0.91	0.16	55,55,55,55	0
56	MG	DA	3193	1/1	0.91	0.17	57,57,57,57	0
56	MG	BA	3290	1/1	0.91	0.17	61,61,61,61	0
56	MG	DA	3504	1/1	0.91	0.14	55,55,55,55	0
56	MG	BA	3108	1/1	0.91	0.09	52,52,52,52	0
56	MG	BA	3387	1/1	0.91	0.16	43,43,43,43	0
56	MG	BA	3015	1/1	0.91	0.16	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	3298	1/1	0.91	0.12	24,24,24,24	0
56	MG	BA	3496	1/1	0.91	0.11	53,53,53,53	0
56	MG	DA	3213	1/1	0.91	0.10	58,58,58,58	0
56	MG	AA	3100	1/1	0.91	0.15	53,53,53,53	0
56	MG	BA	3201	1/1	0.91	0.20	49,49,49,49	0
56	MG	BA	3599	1/1	0.91	0.17	59,59,59,59	0
56	MG	BA	3399	1/1	0.91	0.19	62,62,62,62	0
56	MG	CA	3149	1/1	0.91	0.19	61,61,61,61	0
56	MG	BA	3113	1/1	0.91	0.52	44,44,44,44	0
56	MG	DA	3532	1/1	0.91	0.17	53,53,53,53	0
56	MG	DA	3232	1/1	0.91	0.18	57,57,57,57	0
56	MG	DA	3233	1/1	0.91	0.17	40,40,40,40	0
56	MG	AA	3132	1/1	0.91	0.14	75,75,75,75	0
56	MG	BA	3040	1/1	0.91	0.28	60,60,60,60	0
56	MG	BA	3211	1/1	0.91	0.29	57,57,57,57	0
56	MG	BA	3406	1/1	0.91	0.15	50,50,50,50	0
56	MG	CA	3037	1/1	0.91	0.31	67,67,67,67	0
56	MG	BA	3135	1/1	0.91	0.15	51,51,51,51	0
56	MG	DA	3548	1/1	0.91	0.17	67,67,67,67	0
56	MG	CA	3162	1/1	0.91	0.14	57,57,57,57	0
56	MG	CA	3163	1/1	0.91	0.12	49,49,49,49	0
56	MG	DA	3270	1/1	0.91	0.15	47,47,47,47	0
56	MG	DA	3274	1/1	0.91	0.12	43,43,43,43	0
56	MG	DA	3275	1/1	0.91	0.10	51,51,51,51	0
56	MG	CA	3164	1/1	0.91	0.17	65,65,65,65	0
56	MG	CA	3167	1/1	0.91	0.10	55,55,55,55	0
56	MG	DA	3282	1/1	0.91	0.19	43,43,43,43	0
56	MG	DA	3568	1/1	0.91	0.11	61,61,61,61	0
56	MG	BA	3412	1/1	0.91	0.13	50,50,50,50	0
56	MG	DA	3284	1/1	0.91	0.21	40,40,40,40	0
56	MG	BA	3309	1/1	0.91	0.09	41,41,41,41	0
56	MG	CA	3044	1/1	0.91	0.15	62,62,62,62	0
56	MG	CW	3001	1/1	0.91	0.15	69,69,69,69	0
56	MG	CX	3002	1/1	0.91	0.26	67,67,67,67	0
56	MG	BA	3523	1/1	0.91	0.10	39,39,39,39	0
56	MG	BA	3734	1/1	0.91	0.10	24,24,24,24	0
56	MG	BA	3045	1/1	0.91	0.10	41,41,41,41	0
56	MG	DA	3002	1/1	0.91	0.10	51,51,51,51	0
56	MG	DA	3585	1/1	0.91	0.10	55,55,55,55	0
56	MG	DA	3306	1/1	0.91	0.07	57,57,57,57	0
56	MG	DA	3589	1/1	0.91	0.20	55,55,55,55	0
56	MG	DA	3003	1/1	0.91	0.25	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	3217	1/1	0.91	0.21	66,66,66,66	0
56	MG	DA	3023	1/1	0.91	0.39	44,44,44,44	0
56	MG	CA	3049	1/1	0.91	0.14	54,54,54,54	0
56	MG	AA	3107	1/1	0.91	0.24	66,66,66,66	0
56	MG	BA	3738	1/1	0.91	0.12	41,41,41,41	0
56	MG	BA	3149	1/1	0.91	0.23	57,57,57,57	0
56	MG	DA	3334	1/1	0.91	0.19	51,51,51,51	0
56	MG	BA	3227	1/1	0.91	0.11	38,38,38,38	0
56	MG	BA	3742	1/1	0.91	0.11	44,44,44,44	0
56	MG	BA	3534	1/1	0.91	0.09	54,54,54,54	0
56	MG	BA	3749	1/1	0.91	0.10	38,38,38,38	0
56	MG	CA	3060	1/1	0.91	0.10	58,58,58,58	0
56	MG	AA	3120	1/1	0.91	0.17	72,72,72,72	0
56	MG	BA	3049	1/1	0.91	0.24	54,54,54,54	0
56	MG	DA	3350	1/1	0.91	0.08	61,61,61,61	0
56	MG	DA	3619	1/1	0.91	0.27	57,57,57,57	0
56	MG	DA	3055	1/1	0.91	0.17	44,44,44,44	0
56	MG	DA	3056	1/1	0.91	0.09	51,51,51,51	0
56	MG	BA	3542	1/1	0.91	0.22	66,66,66,66	0
56	MG	DA	3623	1/1	0.91	0.13	48,48,48,48	0
56	MG	AA	3214	1/1	0.91	0.25	69,69,69,69	0
56	MG	AA	3121	1/1	0.91	0.10	54,54,54,54	0
56	MG	BA	3641	1/1	0.91	0.18	46,46,46,46	0
56	MG	AA	3002	1/1	0.91	0.21	59,59,59,59	0
56	MG	BA	3651	1/1	0.91	0.08	38,38,38,38	0
56	MG	BA	3548	1/1	0.91	0.13	50,50,50,50	0
56	MG	DA	3072	1/1	0.91	0.27	60,60,60,60	0
56	MG	DB	3012	1/1	0.91	0.16	61,61,61,61	0
56	MG	BA	3776	1/1	0.91	0.40	52,52,52,52	0
56	MG	BA	3337	1/1	0.91	0.09	25,25,25,25	0
56	MG	BB	3003	1/1	0.91	0.07	37,37,37,37	0
56	MG	DF	302	1/1	0.91	0.23	60,60,60,60	0
56	MG	BB	3005	1/1	0.91	0.13	54,54,54,54	0
56	MG	DG	3001	1/1	0.91	0.13	55,55,55,55	0
56	MG	CA	3086	1/1	0.91	0.10	53,53,53,53	0
56	MG	BA	3655	1/1	0.91	0.11	29,29,29,29	0
56	MG	CA	3088	1/1	0.91	0.14	48,48,48,48	0
56	MG	DQ	3003	1/1	0.91	0.20	64,64,64,64	0
56	MG	BA	3656	1/1	0.91	0.13	34,34,34,34	0
56	MG	CA	3092	1/1	0.91	0.18	55,55,55,55	0
56	MG	BA	3658	1/1	0.91	0.14	41,41,41,41	0
56	MG	CA	3094	1/1	0.91	0.17	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	DA	3098	1/1	0.91	0.23	61,61,61,61	0
56	MG	CA	3096	1/1	0.91	0.18	51,51,51,51	0
56	MG	AA	3225	1/1	0.91	0.10	55,55,55,55	0
56	MG	DA	3106	1/1	0.91	0.27	56,56,56,56	0
56	MG	AA	3178	1/1	0.91	0.19	60,60,60,60	0
57	NEG	AA	3216	17/17	0.91	0.15	34,56,70,74	0
56	MG	CA	3099	1/1	0.91	0.09	82,82,82,82	0
56	MG	CA	3100	1/1	0.91	0.07	52,52,52,52	0
56	MG	BA	3449	1/1	0.91	0.15	59,59,59,59	0
56	MG	DA	3120	1/1	0.91	0.09	42,42,42,42	0
56	MG	BA	3668	1/1	0.91	0.11	42,42,42,42	0
56	MG	AA	3199	1/1	0.91	0.24	68,68,68,68	0
56	MG	DA	3124	1/1	0.91	0.18	43,43,43,43	0
56	MG	AA	3124	1/1	0.91	0.16	63,63,63,63	0
56	MG	BA	3676	1/1	0.91	0.14	55,55,55,55	0
56	MG	DA	3443	1/1	0.91	0.11	49,49,49,49	0
56	MG	CA	3107	1/1	0.91	0.14	63,63,63,63	0
56	MG	AA	3043	1/1	0.91	0.27	62,62,62,62	0
56	MG	BA	3258	1/1	0.91	0.10	57,57,57,57	0
56	MG	DA	3140	1/1	0.91	0.20	36,36,36,36	0
57	NEG	CA	3176	17/17	0.91	0.18	46,65,76,84	0
56	MG	CA	3111	1/1	0.91	0.30	69,69,69,69	0
56	MG	DA	3146	1/1	0.91	0.17	50,50,50,50	0
56	MG	AA	3091	1/1	0.91	0.23	62,62,62,62	0
56	MG	AA	3067	1/1	0.92	0.30	53,53,53,53	0
56	MG	DA	3471	1/1	0.92	0.16	58,58,58,58	0
56	MG	CA	3039	1/1	0.92	0.21	70,70,70,70	0
56	MG	CA	3157	1/1	0.92	0.13	57,57,57,57	0
56	MG	CA	3158	1/1	0.92	0.19	72,72,72,72	0
56	MG	DA	3475	1/1	0.92	0.11	32,32,32,32	0
56	MG	BA	3739	1/1	0.92	0.10	75,75,75,75	0
56	MG	DA	3206	1/1	0.92	0.18	45,45,45,45	0
56	MG	DA	3484	1/1	0.92	0.09	59,59,59,59	0
56	MG	BA	3462	1/1	0.92	0.13	59,59,59,59	0
56	MG	BA	3649	1/1	0.92	0.22	49,49,49,49	0
56	MG	BA	3365	1/1	0.92	0.12	47,47,47,47	0
56	MG	AA	3197	1/1	0.92	0.17	64,64,64,64	0
56	MG	BA	3748	1/1	0.92	0.10	63,63,63,63	0
56	MG	CA	3179	1/1	0.92	0.16	53,53,53,53	0
56	MG	AA	3141	1/1	0.92	0.15	67,67,67,67	0
56	MG	BA	3750	1/1	0.92	0.19	52,52,52,52	0
56	MG	BA	3375	1/1	0.92	0.10	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	3210	1/1	0.92	0.18	34,34,34,34	0
56	MG	BA	3564	1/1	0.92	0.11	49,49,49,49	0
56	MG	BA	3145	1/1	0.92	0.12	41,41,41,41	0
56	MG	BA	3212	1/1	0.92	0.25	47,47,47,47	0
56	MG	DA	3243	1/1	0.92	0.09	42,42,42,42	0
56	MG	DA	3244	1/1	0.92	0.17	58,58,58,58	0
56	MG	BA	3051	1/1	0.92	0.18	63,63,63,63	0
56	MG	BA	3758	1/1	0.92	0.08	38,38,38,38	0
56	MG	DA	3008	1/1	0.92	0.08	38,38,38,38	0
56	MG	DA	3010	1/1	0.92	0.09	55,55,55,55	0
56	MG	DA	3012	1/1	0.92	0.06	43,43,43,43	0
56	MG	DA	3261	1/1	0.92	0.10	60,60,60,60	0
56	MG	DA	3267	1/1	0.92	0.12	42,42,42,42	0
56	MG	BA	3667	1/1	0.92	0.21	64,64,64,64	0
56	MG	CA	3058	1/1	0.92	0.18	64,64,64,64	0
56	MG	DA	3024	1/1	0.92	0.27	43,43,43,43	0
56	MG	CA	3059	1/1	0.92	0.48	70,70,70,70	0
56	MG	DA	3027	1/1	0.92	0.18	43,43,43,43	0
56	MG	BA	3214	1/1	0.92	0.18	64,64,64,64	0
56	MG	BA	3393	1/1	0.92	0.17	48,48,48,48	0
56	MG	BA	3775	1/1	0.92	0.16	47,47,47,47	0
56	MG	AA	3009	1/1	0.92	0.08	64,64,64,64	0
56	MG	DA	3037	1/1	0.92	0.11	46,46,46,46	0
56	MG	BA	3780	1/1	0.92	0.29	45,45,45,45	0
56	MG	BA	3054	1/1	0.92	0.15	51,51,51,51	0
56	MG	DA	3292	1/1	0.92	0.14	36,36,36,36	0
56	MG	AA	3007	1/1	0.92	0.09	49,49,49,49	0
56	MG	AM	201	1/1	0.92	0.09	61,61,61,61	0
56	MG	AA	3045	1/1	0.92	0.48	68,68,68,68	0
56	MG	DA	3300	1/1	0.92	0.09	27,27,27,27	0
56	MG	CA	3074	1/1	0.92	0.11	62,62,62,62	0
56	MG	BB	3008	1/1	0.92	0.11	71,71,71,71	0
56	MG	DA	3308	1/1	0.92	0.10	57,57,57,57	0
56	MG	AA	3054	1/1	0.92	0.18	46,46,46,46	0
56	MG	DA	3317	1/1	0.92	0.07	47,47,47,47	0
56	MG	AA	3077	1/1	0.92	0.10	69,69,69,69	0
56	MG	DA	3571	1/1	0.92	0.15	49,49,49,49	0
56	MG	AA	3108	1/1	0.92	0.13	59,59,59,59	0
56	MG	DA	3321	1/1	0.92	0.21	58,58,58,58	0
56	MG	BA	3080	1/1	0.92	0.21	49,49,49,49	0
56	MG	CA	3082	1/1	0.92	0.16	41,41,41,41	0
56	MG	CA	3085	1/1	0.92	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3007	1/1	0.92	0.13	39,39,39,39	0
56	MG	DA	3333	1/1	0.92	0.08	53,53,53,53	0
56	MG	BA	3328	1/1	0.92	0.12	56,56,56,56	0
56	MG	BD	307	1/1	0.92	0.17	38,38,38,38	0
56	MG	DA	3584	1/1	0.92	0.08	45,45,45,45	0
56	MG	BD	308	1/1	0.92	0.12	42,42,42,42	0
56	MG	BA	3011	1/1	0.92	0.12	51,51,51,51	0
56	MG	BE	303	1/1	0.92	0.32	61,61,61,61	0
56	MG	BE	304	1/1	0.92	0.12	42,42,42,42	0
56	MG	DA	3346	1/1	0.92	0.07	29,29,29,29	0
56	MG	DA	3595	1/1	0.92	0.14	34,34,34,34	0
56	MG	BA	3696	1/1	0.92	0.12	38,38,38,38	0
56	MG	BA	3510	1/1	0.92	0.10	43,43,43,43	0
56	MG	BA	3246	1/1	0.92	0.12	57,57,57,57	0
56	MG	BA	3514	1/1	0.92	0.10	50,50,50,50	0
56	MG	DA	3353	1/1	0.92	0.07	65,65,65,65	0
56	MG	AA	3189	1/1	0.92	0.15	56,56,56,56	0
56	MG	BA	3518	1/1	0.92	0.15	25,25,25,25	0
56	MG	BN	3004	1/1	0.92	0.32	60,60,60,60	0
56	MG	DA	3361	1/1	0.92	0.18	45,45,45,45	0
56	MG	DA	3096	1/1	0.92	0.19	29,29,29,29	0
56	MG	DA	3611	1/1	0.92	0.07	53,53,53,53	0
56	MG	DA	3613	1/1	0.92	0.15	57,57,57,57	0
56	MG	AA	3109	1/1	0.92	0.14	51,51,51,51	0
56	MG	BA	3097	1/1	0.92	0.22	33,33,33,33	0
56	MG	DA	3368	1/1	0.92	0.09	48,48,48,48	0
56	MG	BA	3705	1/1	0.92	0.09	52,52,52,52	0
56	MG	DA	3371	1/1	0.92	0.11	68,68,68,68	0
56	MG	BA	3424	1/1	0.92	0.11	51,51,51,51	0
56	MG	DA	3108	1/1	0.92	0.12	48,48,48,48	0
56	MG	BA	3030	1/1	0.92	0.18	50,50,50,50	0
56	MG	BU	208	1/1	0.92	0.19	35,35,35,35	0
56	MG	DA	3384	1/1	0.92	0.26	55,55,55,55	0
56	MG	AA	3175	1/1	0.92	0.11	54,54,54,54	0
56	MG	BA	3434	1/1	0.92	0.10	65,65,65,65	0
56	MG	BZ	3001	1/1	0.92	0.21	52,52,52,52	0
56	MG	DB	3006	1/1	0.92	0.07	63,63,63,63	0
56	MG	DA	3395	1/1	0.92	0.14	40,40,40,40	0
56	MG	B0	103	1/1	0.92	0.14	61,61,61,61	0
56	MG	BA	3611	1/1	0.92	0.13	23,23,23,23	0
56	MG	DA	3401	1/1	0.92	0.09	50,50,50,50	0
56	MG	BA	3341	1/1	0.92	0.11	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	B5	101	1/1	0.92	0.32	42,42,42,42	0
56	MG	DA	3126	1/1	0.92	0.14	51,51,51,51	0
56	MG	DF	301	1/1	0.92	0.09	49,49,49,49	0
56	MG	DA	3127	1/1	0.92	0.20	53,53,53,53	0
56	MG	DA	3414	1/1	0.92	0.13	46,46,46,46	0
56	MG	B5	104	1/1	0.92	0.13	55,55,55,55	0
56	MG	BA	3191	1/1	0.92	0.22	50,50,50,50	0
56	MG	BA	3260	1/1	0.92	0.13	52,52,52,52	0
56	MG	CA	3001	1/1	0.92	0.09	59,59,59,59	0
56	MG	BA	3617	1/1	0.92	0.10	46,46,46,46	0
56	MG	CA	3127	1/1	0.92	0.12	69,69,69,69	0
56	MG	BA	3717	1/1	0.92	0.10	34,34,34,34	0
56	MG	BA	3533	1/1	0.92	0.08	27,27,27,27	0
56	MG	DA	3432	1/1	0.92	0.13	43,43,43,43	0
56	MG	DV	3001	1/1	0.92	0.10	75,75,75,75	0
56	MG	BA	3261	1/1	0.92	0.15	49,49,49,49	0
56	MG	BA	3625	1/1	0.92	0.15	49,49,49,49	0
56	MG	BA	3265	1/1	0.92	0.23	55,55,55,55	0
56	MG	DA	3438	1/1	0.92	0.15	55,55,55,55	0
56	MG	BA	3726	1/1	0.92	0.14	61,61,61,61	0
56	MG	CA	3140	1/1	0.92	0.12	49,49,49,49	0
56	MG	BA	3446	1/1	0.92	0.20	40,40,40,40	0
56	MG	CA	3017	1/1	0.92	0.25	53,53,53,53	0
56	MG	BA	3541	1/1	0.92	0.28	31,31,31,31	0
56	MG	DA	3445	1/1	0.92	0.09	50,50,50,50	0
56	MG	CA	3019	1/1	0.92	0.11	45,45,45,45	0
56	MG	BA	3355	1/1	0.92	0.11	26,26,26,26	0
56	MG	DA	3451	1/1	0.92	0.15	56,56,56,56	0
56	MG	DA	3173	1/1	0.92	0.10	49,49,49,49	0
56	MG	BA	3111	1/1	0.92	0.11	45,45,45,45	0
56	MG	BA	3733	1/1	0.92	0.10	78,78,78,78	0
56	MG	AA	3079	1/1	0.92	0.27	66,66,66,66	0
56	MG	BA	3200	1/1	0.92	0.08	50,50,50,50	0
56	MG	CA	3151	1/1	0.92	0.12	59,59,59,59	0
56	MG	DA	3183	1/1	0.92	0.13	57,57,57,57	0
56	MG	BA	3459	1/1	0.92	0.13	56,56,56,56	0
56	MG	CA	3032	1/1	0.92	0.20	52,52,52,52	0
56	MG	AX	3003	1/1	0.92	0.12	74,74,74,74	0
56	MG	DA	3469	1/1	0.92	0.10	56,56,56,56	0
59	ZN	D4	501	1/1	0.92	0.07	137,137,137,137	0
60	K	AX	3001	1/1	0.92	0.11	73,73,73,73	0
60	K	CX	3001	1/1	0.92	0.15	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AW	3002	1/1	0.93	0.17	54,54,54,54	0
56	MG	BA	3033	1/1	0.93	0.12	45,45,45,45	0
56	MG	DA	3196	1/1	0.93	0.18	49,49,49,49	0
56	MG	CA	3033	1/1	0.93	0.13	44,44,44,44	0
56	MG	CA	3034	1/1	0.93	0.22	46,46,46,46	0
56	MG	CA	3160	1/1	0.93	0.20	53,53,53,53	0
56	MG	CA	3035	1/1	0.93	0.27	52,52,52,52	0
56	MG	DA	3467	1/1	0.93	0.15	69,69,69,69	0
56	MG	DA	3468	1/1	0.93	0.08	54,54,54,54	0
56	MG	BA	3036	1/1	0.93	0.24	50,50,50,50	0
56	MG	AW	3003	1/1	0.93	0.16	44,44,44,44	0
56	MG	DA	3212	1/1	0.93	0.13	52,52,52,52	0
56	MG	CA	3165	1/1	0.93	0.21	57,57,57,57	0
56	MG	DA	3214	1/1	0.93	0.20	58,58,58,58	0
56	MG	BA	3116	1/1	0.93	0.16	68,68,68,68	0
56	MG	DA	3219	1/1	0.93	0.06	35,35,35,35	0
56	MG	AA	3046	1/1	0.93	0.19	50,50,50,50	0
56	MG	DA	3479	1/1	0.93	0.11	52,52,52,52	0
56	MG	CA	3169	1/1	0.93	0.20	49,49,49,49	0
56	MG	BA	3046	1/1	0.93	0.21	50,50,50,50	0
56	MG	CD	301	1/1	0.93	0.09	67,67,67,67	0
56	MG	DA	3486	1/1	0.93	0.10	47,47,47,47	0
56	MG	DA	3225	1/1	0.93	0.23	56,56,56,56	0
56	MG	AA	3061	1/1	0.93	0.11	44,44,44,44	0
56	MG	BA	3137	1/1	0.93	0.13	41,41,41,41	0
56	MG	BA	3643	1/1	0.93	0.23	38,38,38,38	0
56	MG	DA	3237	1/1	0.93	0.08	42,42,42,42	0
56	MG	BA	3139	1/1	0.93	0.17	52,52,52,52	0
56	MG	DA	3239	1/1	0.93	0.11	61,61,61,61	0
56	MG	BA	3645	1/1	0.93	0.18	47,47,47,47	0
56	MG	DA	3499	1/1	0.93	0.10	60,60,60,60	0
56	MG	BA	3222	1/1	0.93	0.19	60,60,60,60	0
56	MG	BA	3545	1/1	0.93	0.10	58,58,58,58	0
56	MG	BA	3141	1/1	0.93	0.20	55,55,55,55	0
56	MG	BA	3761	1/1	0.93	0.21	65,65,65,65	0
56	MG	DA	3007	1/1	0.93	0.29	53,53,53,53	0
56	MG	DA	3510	1/1	0.93	0.09	32,32,32,32	0
56	MG	BA	3224	1/1	0.93	0.23	55,55,55,55	0
56	MG	DA	3253	1/1	0.93	0.21	57,57,57,57	0
56	MG	DA	3515	1/1	0.93	0.09	56,56,56,56	0
56	MG	DA	3254	1/1	0.93	0.10	53,53,53,53	0
56	MG	DA	3255	1/1	0.93	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	AA	3062	1/1	0.93	0.25	58,58,58,58	0
56	MG	BA	3773	1/1	0.93	0.17	43,43,43,43	0
56	MG	BA	3231	1/1	0.93	0.14	42,42,42,42	0
56	MG	AA	3125	1/1	0.93	0.10	53,53,53,53	0
56	MG	BA	3451	1/1	0.93	0.13	53,53,53,53	0
56	MG	BA	3783	1/1	0.93	0.16	36,36,36,36	0
56	MG	AA	3035	1/1	0.93	0.17	69,69,69,69	0
56	MG	BB	3002	1/1	0.93	0.24	51,51,51,51	0
56	MG	DA	3277	1/1	0.93	0.09	52,52,52,52	0
56	MG	CA	3063	1/1	0.93	0.19	59,59,59,59	0
56	MG	BA	3663	1/1	0.93	0.13	26,26,26,26	0
56	MG	BA	3342	1/1	0.93	0.11	43,43,43,43	0
56	MG	CA	3066	1/1	0.93	0.25	58,58,58,58	0
56	MG	BA	3560	1/1	0.93	0.15	47,47,47,47	0
56	MG	DA	3543	1/1	0.93	0.13	63,63,63,63	0
56	MG	DA	3544	1/1	0.93	0.17	49,49,49,49	0
56	MG	AX	3007	1/1	0.93	0.32	66,66,66,66	0
56	MG	DA	3044	1/1	0.93	0.42	60,60,60,60	0
56	MG	DA	3046	1/1	0.93	0.14	30,30,30,30	0
56	MG	BA	3345	1/1	0.93	0.12	20,20,20,20	0
56	MG	DA	3293	1/1	0.93	0.12	59,59,59,59	0
56	MG	AA	3110	1/1	0.93	0.09	53,53,53,53	0
56	MG	DA	3555	1/1	0.93	0.21	48,48,48,48	0
56	MG	BA	3565	1/1	0.93	0.12	50,50,50,50	0
56	MG	BA	3677	1/1	0.93	0.09	63,63,63,63	0
56	MG	BB	3017	1/1	0.93	0.10	48,48,48,48	0
56	MG	DA	3563	1/1	0.93	0.11	45,45,45,45	0
56	MG	BB	3018	1/1	0.93	0.08	46,46,46,46	0
56	MG	BA	3060	1/1	0.93	0.10	61,61,61,61	0
56	MG	BA	3063	1/1	0.93	0.08	39,39,39,39	0
56	MG	BA	3568	1/1	0.93	0.13	39,39,39,39	0
56	MG	DA	3570	1/1	0.93	0.09	62,62,62,62	0
56	MG	DA	3316	1/1	0.93	0.11	48,48,48,48	0
56	MG	DA	3060	1/1	0.93	0.14	50,50,50,50	0
56	MG	BA	3244	1/1	0.93	0.35	53,53,53,53	0
56	MG	AE	3001	1/1	0.93	0.07	77,77,77,77	0
56	MG	AX	3011	1/1	0.93	0.17	62,62,62,62	0
56	MG	BA	3248	1/1	0.93	0.10	27,27,27,27	0
56	MG	BA	3252	1/1	0.93	0.20	61,61,61,61	0
56	MG	DA	3325	1/1	0.93	0.06	32,32,32,32	0
56	MG	DA	3073	1/1	0.93	0.15	50,50,50,50	0
56	MG	DA	3075	1/1	0.93	0.11	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	3332	1/1	0.93	0.12	46,46,46,46	0
56	MG	DA	3076	1/1	0.93	0.24	34,34,34,34	0
56	MG	DA	3077	1/1	0.93	0.08	40,40,40,40	0
56	MG	BA	3693	1/1	0.93	0.10	38,38,38,38	0
56	MG	BF	301	1/1	0.93	0.18	39,39,39,39	0
56	MG	DA	3592	1/1	0.93	0.08	57,57,57,57	0
56	MG	BF	303	1/1	0.93	0.11	36,36,36,36	0
56	MG	BF	306	1/1	0.93	0.30	41,41,41,41	0
56	MG	AA	3098	1/1	0.93	0.22	59,59,59,59	0
56	MG	BF	311	1/1	0.93	0.23	60,60,60,60	0
56	MG	AA	3129	1/1	0.93	0.12	77,77,77,77	0
56	MG	AA	3006	1/1	0.93	0.08	57,57,57,57	0
56	MG	BA	3161	1/1	0.93	0.14	40,40,40,40	0
56	MG	AA	3200	1/1	0.93	0.16	61,61,61,61	0
56	MG	BA	3171	1/1	0.93	0.13	58,58,58,58	0
56	MG	AA	3026	1/1	0.93	0.20	68,68,68,68	0
56	MG	DA	3097	1/1	0.93	0.19	52,52,52,52	0
56	MG	BQ	3001	1/1	0.93	0.39	52,52,52,52	0
56	MG	DA	3610	1/1	0.93	0.07	65,65,65,65	0
56	MG	BQ	3005	1/1	0.93	0.14	49,49,49,49	0
56	MG	DA	3612	1/1	0.93	0.22	38,38,38,38	0
56	MG	BA	3263	1/1	0.93	0.19	47,47,47,47	0
56	MG	BA	3587	1/1	0.93	0.14	58,58,58,58	0
56	MG	DA	3366	1/1	0.93	0.12	36,36,36,36	0
56	MG	BA	3495	1/1	0.93	0.15	44,44,44,44	0
56	MG	BA	3177	1/1	0.93	0.15	58,58,58,58	0
56	MG	CA	3112	1/1	0.93	0.23	59,59,59,59	0
56	MG	DA	3370	1/1	0.93	0.17	49,49,49,49	0
56	MG	BV	207	1/1	0.93	0.17	42,42,42,42	0
56	MG	CA	3114	1/1	0.93	0.11	52,52,52,52	0
56	MG	DA	3374	1/1	0.93	0.15	52,52,52,52	0
56	MG	BA	3498	1/1	0.93	0.07	70,70,70,70	0
56	MG	BA	3592	1/1	0.93	0.18	61,61,61,61	0
56	MG	DA	3378	1/1	0.93	0.22	51,51,51,51	0
56	MG	DA	3380	1/1	0.93	0.10	43,43,43,43	0
56	MG	BA	3500	1/1	0.93	0.10	37,37,37,37	0
56	MG	BA	3501	1/1	0.93	0.13	74,74,74,74	0
56	MG	DB	3008	1/1	0.93	0.09	62,62,62,62	0
56	MG	AA	3013	1/1	0.93	0.12	66,66,66,66	0
56	MG	DA	3387	1/1	0.93	0.12	47,47,47,47	0
56	MG	B3	3001	1/1	0.93	0.14	41,41,41,41	0
56	MG	DD	301	1/1	0.93	0.25	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	DD	307	1/1	0.93	0.21	56,56,56,56	0
56	MG	DD	308	1/1	0.93	0.20	45,45,45,45	0
56	MG	BA	3182	1/1	0.93	0.33	50,50,50,50	0
56	MG	DA	3129	1/1	0.93	0.18	42,42,42,42	0
56	MG	BA	3084	1/1	0.93	0.14	46,46,46,46	0
56	MG	BA	3186	1/1	0.93	0.30	59,59,59,59	0
56	MG	BA	3604	1/1	0.93	0.16	46,46,46,46	0
56	MG	DF	303	1/1	0.93	0.12	46,46,46,46	0
56	MG	DA	3403	1/1	0.93	0.19	54,54,54,54	0
56	MG	DF	305	1/1	0.93	0.11	45,45,45,45	0
56	MG	DF	306	1/1	0.93	0.38	55,55,55,55	0
56	MG	DA	3137	1/1	0.93	0.07	57,57,57,57	0
56	MG	DA	3138	1/1	0.93	0.09	46,46,46,46	0
56	MG	DA	3407	1/1	0.93	0.19	41,41,41,41	0
56	MG	BA	3287	1/1	0.93	0.07	21,21,21,21	0
56	MG	BA	3719	1/1	0.93	0.15	49,49,49,49	0
56	MG	DA	3413	1/1	0.93	0.13	40,40,40,40	0
56	MG	BA	3606	1/1	0.93	0.19	62,62,62,62	0
56	MG	DA	3416	1/1	0.93	0.07	39,39,39,39	0
56	MG	DU	3002	1/1	0.93	0.35	58,58,58,58	0
56	MG	AA	3182	1/1	0.93	0.11	76,76,76,76	0
56	MG	BA	3012	1/1	0.93	0.12	49,49,49,49	0
56	MG	DA	3421	1/1	0.93	0.12	55,55,55,55	0
56	MG	CA	3135	1/1	0.93	0.16	75,75,75,75	0
56	MG	AA	3073	1/1	0.93	0.25	60,60,60,60	0
56	MG	D3	3001	1/1	0.93	0.20	70,70,70,70	0
56	MG	DA	3158	1/1	0.93	0.11	55,55,55,55	0
56	MG	CA	3138	1/1	0.93	0.14	52,52,52,52	0
56	MG	CA	3010	1/1	0.93	0.15	60,60,60,60	0
56	MG	BA	3091	1/1	0.93	0.24	43,43,43,43	0
56	MG	DA	3431	1/1	0.93	0.12	44,44,44,44	0
56	MG	BA	3612	1/1	0.93	0.20	65,65,65,65	0
56	MG	AA	3028	1/1	0.93	0.18	46,46,46,46	0
56	MG	CA	3014	1/1	0.93	0.10	46,46,46,46	0
56	MG	BA	3614	1/1	0.93	0.14	54,54,54,54	0
56	MG	BA	3105	1/1	0.93	0.09	43,43,43,43	0
56	MG	BA	3408	1/1	0.93	0.15	71,71,71,71	0
56	MG	DA	3174	1/1	0.93	0.08	42,42,42,42	0
56	MG	BA	3107	1/1	0.93	0.30	49,49,49,49	0
56	MG	CA	3020	1/1	0.93	0.08	48,48,48,48	0
56	MG	BA	3413	1/1	0.93	0.15	53,53,53,53	0
56	MG	CA	3024	1/1	0.93	0.16	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	3446	1/1	0.93	0.07	52,52,52,52	0
56	MG	BA	3202	1/1	0.93	0.10	41,41,41,41	0
56	MG	DA	3449	1/1	0.93	0.14	49,49,49,49	0
56	MG	DA	3181	1/1	0.93	0.35	50,50,50,50	0
56	MG	AA	3033	1/1	0.93	0.28	45,45,45,45	0
56	MG	BA	3626	1/1	0.93	0.12	40,40,40,40	0
56	MG	DA	3187	1/1	0.93	0.08	41,41,41,41	0
56	MG	BA	3207	1/1	0.93	0.14	52,52,52,52	0
56	MG	BA	3396	1/1	0.94	0.10	24,24,24,24	0
56	MG	DA	3031	1/1	0.94	0.15	51,51,51,51	0
56	MG	DA	3035	1/1	0.94	0.19	39,39,39,39	0
56	MG	BA	3593	1/1	0.94	0.24	53,53,53,53	0
56	MG	DA	3481	1/1	0.94	0.16	51,51,51,51	0
56	MG	DA	3482	1/1	0.94	0.12	42,42,42,42	0
56	MG	BF	308	1/1	0.94	0.28	40,40,40,40	0
56	MG	CA	3077	1/1	0.94	0.10	36,36,36,36	0
56	MG	DA	3041	1/1	0.94	0.09	51,51,51,51	0
56	MG	AA	3097	1/1	0.94	0.19	45,45,45,45	0
56	MG	DA	3249	1/1	0.94	0.08	43,43,43,43	0
56	MG	AA	3213	1/1	0.94	0.12	44,44,44,44	0
56	MG	BA	3598	1/1	0.94	0.11	58,58,58,58	0
56	MG	BA	3061	1/1	0.94	0.18	48,48,48,48	0
56	MG	DA	3493	1/1	0.94	0.14	64,64,64,64	0
56	MG	CA	3083	1/1	0.94	0.06	58,58,58,58	0
56	MG	DA	3256	1/1	0.94	0.15	48,48,48,48	0
56	MG	AA	3023	1/1	0.94	0.11	51,51,51,51	0
56	MG	BN	3005	1/1	0.94	0.11	46,46,46,46	0
56	MG	BN	3006	1/1	0.94	0.20	54,54,54,54	0
56	MG	BA	3708	1/1	0.94	0.06	7,7,7,7	0
56	MG	AA	3024	1/1	0.94	0.08	49,49,49,49	0
56	MG	DA	3271	1/1	0.94	0.12	51,51,51,51	0
56	MG	BA	3404	1/1	0.94	0.06	59,59,59,59	0
56	MG	BQ	3003	1/1	0.94	0.10	67,67,67,67	0
56	MG	BA	3405	1/1	0.94	0.09	47,47,47,47	0
56	MG	BA	3511	1/1	0.94	0.12	31,31,31,31	0
56	MG	AA	3114	1/1	0.94	0.19	66,66,66,66	0
56	MG	DA	3065	1/1	0.94	0.14	56,56,56,56	0
56	MG	BT	201	1/1	0.94	0.25	49,49,49,49	0
56	MG	DA	3067	1/1	0.94	0.08	52,52,52,52	0
56	MG	BA	3513	1/1	0.94	0.13	42,42,42,42	0
56	MG	DA	3069	1/1	0.94	0.19	49,49,49,49	0
56	MG	DA	3071	1/1	0.94	0.20	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	BU	206	1/1	0.94	0.32	54,54,54,54	0
56	MG	AA	3085	1/1	0.94	0.25	63,63,63,63	0
56	MG	BV	204	1/1	0.94	0.10	39,39,39,39	0
56	MG	AA	3021	1/1	0.94	0.24	60,60,60,60	0
56	MG	DA	3529	1/1	0.94	0.09	55,55,55,55	0
56	MG	DA	3530	1/1	0.94	0.18	69,69,69,69	0
56	MG	BW	201	1/1	0.94	0.17	45,45,45,45	0
56	MG	BA	3076	1/1	0.94	0.07	58,58,58,58	0
56	MG	BA	3311	1/1	0.94	0.17	34,34,34,34	0
56	MG	DA	3536	1/1	0.94	0.10	39,39,39,39	0
56	MG	DA	3538	1/1	0.94	0.08	50,50,50,50	0
56	MG	DA	3080	1/1	0.94	0.18	48,48,48,48	0
56	MG	DA	3305	1/1	0.94	0.12	42,42,42,42	0
56	MG	CA	3108	1/1	0.94	0.20	56,56,56,56	0
56	MG	AA	3158	1/1	0.94	0.16	62,62,62,62	0
56	MG	BA	3313	1/1	0.94	0.07	32,32,32,32	0
56	MG	BA	3318	1/1	0.94	0.06	36,36,36,36	0
56	MG	AA	3137	1/1	0.94	0.10	49,49,49,49	0
56	MG	DA	3089	1/1	0.94	0.23	57,57,57,57	0
56	MG	AA	3071	1/1	0.94	0.15	52,52,52,52	0
56	MG	AA	3161	1/1	0.94	0.07	59,59,59,59	0
56	MG	BA	3619	1/1	0.94	0.09	49,49,49,49	0
56	MG	BA	3421	1/1	0.94	0.09	46,46,46,46	0
56	MG	DA	3095	1/1	0.94	0.11	54,54,54,54	0
56	MG	DA	3556	1/1	0.94	0.12	48,48,48,48	0
56	MG	DA	3326	1/1	0.94	0.10	31,31,31,31	0
56	MG	B7	103	1/1	0.94	0.12	69,69,69,69	0
56	MG	BA	3531	1/1	0.94	0.10	56,56,56,56	0
56	MG	B9	502	1/1	0.94	0.17	61,61,61,61	0
56	MG	DA	3100	1/1	0.94	0.22	45,45,45,45	0
56	MG	AA	3162	1/1	0.94	0.14	70,70,70,70	0
56	MG	DA	3567	1/1	0.94	0.10	52,52,52,52	0
56	MG	CA	3002	1/1	0.94	0.12	65,65,65,65	0
56	MG	AA	3194	1/1	0.94	0.10	66,66,66,66	0
56	MG	DA	3107	1/1	0.94	0.11	47,47,47,47	0
56	MG	DA	3343	1/1	0.94	0.12	57,57,57,57	0
56	MG	BA	3629	1/1	0.94	0.15	62,62,62,62	0
56	MG	CA	3006	1/1	0.94	0.25	50,50,50,50	0
56	MG	DA	3110	1/1	0.94	0.08	30,30,30,30	0
56	MG	DA	3111	1/1	0.94	0.06	49,49,49,49	0
56	MG	DA	3112	1/1	0.94	0.28	49,49,49,49	0
56	MG	BA	3240	1/1	0.94	0.14	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	3115	1/1	0.94	0.06	51,51,51,51	0
56	MG	BA	3023	1/1	0.94	0.08	38,38,38,38	0
56	MG	DA	3117	1/1	0.94	0.09	46,46,46,46	0
56	MG	CA	3129	1/1	0.94	0.15	49,49,49,49	0
56	MG	DA	3359	1/1	0.94	0.10	54,54,54,54	0
56	MG	BA	3165	1/1	0.94	0.10	53,53,53,53	0
56	MG	CA	3132	1/1	0.94	0.10	54,54,54,54	0
56	MG	AA	3163	1/1	0.94	0.29	53,53,53,53	0
56	MG	BA	3439	1/1	0.94	0.09	15,15,15,15	0
56	MG	AA	3037	1/1	0.94	0.20	55,55,55,55	0
56	MG	BA	3172	1/1	0.94	0.14	58,58,58,58	0
56	MG	BA	3092	1/1	0.94	0.06	27,27,27,27	0
56	MG	BA	3640	1/1	0.94	0.17	61,61,61,61	0
56	MG	BA	3032	1/1	0.94	0.15	32,32,32,32	0
56	MG	BA	3547	1/1	0.94	0.14	47,47,47,47	0
56	MG	DA	3372	1/1	0.94	0.07	67,67,67,67	0
56	MG	BA	3178	1/1	0.94	0.20	43,43,43,43	0
56	MG	BA	3549	1/1	0.94	0.14	53,53,53,53	0
56	MG	DA	3375	1/1	0.94	0.22	42,42,42,42	0
56	MG	CA	3144	1/1	0.94	0.10	54,54,54,54	0
56	MG	BA	3646	1/1	0.94	0.22	48,48,48,48	0
56	MG	DA	3607	1/1	0.94	0.09	60,60,60,60	0
56	MG	DA	3608	1/1	0.94	0.07	47,47,47,47	0
56	MG	BA	3647	1/1	0.94	0.13	48,48,48,48	0
56	MG	DA	3141	1/1	0.94	0.14	56,56,56,56	0
56	MG	DA	3142	1/1	0.94	0.16	55,55,55,55	0
56	MG	DA	3382	1/1	0.94	0.28	53,53,53,53	0
56	MG	BA	3253	1/1	0.94	0.11	30,30,30,30	0
56	MG	DA	3145	1/1	0.94	0.13	61,61,61,61	0
56	MG	BA	3098	1/1	0.94	0.08	51,51,51,51	0
56	MG	DA	3389	1/1	0.94	0.15	63,63,63,63	0
56	MG	DA	3618	1/1	0.94	0.16	57,57,57,57	0
56	MG	DA	3390	1/1	0.94	0.16	48,48,48,48	0
56	MG	BA	3255	1/1	0.94	0.28	56,56,56,56	0
56	MG	BA	3104	1/1	0.94	0.36	44,44,44,44	0
56	MG	BA	3762	1/1	0.94	0.15	58,58,58,58	0
56	MG	DA	3152	1/1	0.94	0.25	53,53,53,53	0
56	MG	DA	3153	1/1	0.94	0.06	40,40,40,40	0
56	MG	DA	3400	1/1	0.94	0.10	61,61,61,61	0
56	MG	AA	3039	1/1	0.94	0.20	57,57,57,57	0
56	MG	BA	3770	1/1	0.94	0.09	20,20,20,20	0
56	MG	AA	3060	1/1	0.94	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3164	1/1	0.94	0.15	58,58,58,58	0
56	MG	BA	3772	1/1	0.94	0.10	52,52,52,52	0
56	MG	AA	3169	1/1	0.94	0.09	57,57,57,57	0
56	MG	BA	3042	1/1	0.94	0.11	54,54,54,54	0
56	MG	DB	3011	1/1	0.94	0.08	49,49,49,49	0
56	MG	BA	3661	1/1	0.94	0.13	61,61,61,61	0
56	MG	CA	3041	1/1	0.94	0.14	63,63,63,63	0
56	MG	AA	3143	1/1	0.94	0.10	57,57,57,57	0
56	MG	BA	3362	1/1	0.94	0.12	25,25,25,25	0
56	MG	BA	3784	1/1	0.94	0.09	62,62,62,62	0
56	MG	DA	3419	1/1	0.94	0.16	59,59,59,59	0
56	MG	DE	303	1/1	0.94	0.11	40,40,40,40	0
56	MG	BA	3785	1/1	0.94	0.24	42,42,42,42	0
56	MG	BA	3262	1/1	0.94	0.10	51,51,51,51	0
56	MG	DA	3423	1/1	0.94	0.15	34,34,34,34	0
56	MG	DA	3424	1/1	0.94	0.19	35,35,35,35	0
56	MG	BA	3467	1/1	0.94	0.14	48,48,48,48	0
56	MG	AA	3173	1/1	0.94	0.24	55,55,55,55	0
56	MG	DA	3179	1/1	0.94	0.25	61,61,61,61	0
56	MG	BA	3197	1/1	0.94	0.20	46,46,46,46	0
56	MG	BA	3367	1/1	0.94	0.12	58,58,58,58	0
56	MG	AA	3040	1/1	0.94	0.07	41,41,41,41	0
56	MG	CF	3001	1/1	0.94	0.14	44,44,44,44	0
56	MG	BA	3371	1/1	0.94	0.14	50,50,50,50	0
56	MG	DA	3434	1/1	0.94	0.13	46,46,46,46	0
56	MG	DA	3435	1/1	0.94	0.20	59,59,59,59	0
56	MG	BA	3278	1/1	0.94	0.10	48,48,48,48	0
56	MG	DA	3190	1/1	0.94	0.17	58,58,58,58	0
56	MG	DA	3191	1/1	0.94	0.18	35,35,35,35	0
56	MG	CT	3001	1/1	0.94	0.13	50,50,50,50	0
56	MG	AA	3078	1/1	0.94	0.24	59,59,59,59	0
56	MG	DW	3003	1/1	0.94	0.11	71,71,71,71	0
56	MG	DW	3004	1/1	0.94	0.06	50,50,50,50	0
56	MG	AA	3022	1/1	0.94	0.17	58,58,58,58	0
56	MG	BA	3119	1/1	0.94	0.11	44,44,44,44	0
56	MG	BA	3688	1/1	0.94	0.08	24,24,24,24	0
56	MG	BA	3127	1/1	0.94	0.19	38,38,38,38	0
56	MG	DA	3202	1/1	0.94	0.21	51,51,51,51	0
56	MG	BA	3486	1/1	0.94	0.13	30,30,30,30	0
56	MG	BA	3490	1/1	0.94	0.06	66,66,66,66	0
56	MG	BA	3491	1/1	0.94	0.10	52,52,52,52	0
56	MG	DA	3208	1/1	0.94	0.32	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3209	1/1	0.94	0.18	52,52,52,52	0
56	MG	DA	3455	1/1	0.94	0.17	50,50,50,50	0
56	MG	DA	3211	1/1	0.94	0.34	49,49,49,49	0
56	MG	BA	3388	1/1	0.94	0.11	40,40,40,40	0
56	MG	BA	3128	1/1	0.94	0.11	46,46,46,46	0
56	MG	DA	3011	1/1	0.94	0.10	46,46,46,46	0
56	MG	BA	3132	1/1	0.94	0.16	42,42,42,42	0
56	MG	AA	3147	1/1	0.94	0.10	47,47,47,47	0
56	MG	DA	3015	1/1	0.94	0.19	49,49,49,49	0
56	MG	DA	3016	1/1	0.94	0.15	34,34,34,34	0
56	MG	DA	3022	1/1	0.94	0.10	50,50,50,50	0
56	MG	BA	3589	1/1	0.94	0.08	41,41,41,41	0
56	MG	BA	3297	1/1	0.94	0.10	45,45,45,45	0
56	MG	AA	3049	1/1	0.94	0.15	59,59,59,59	0
56	MG	DA	3229	1/1	0.94	0.11	49,49,49,49	0
56	MG	CA	3071	1/1	0.94	0.19	58,58,58,58	0
56	MG	CA	3072	1/1	0.94	0.13	57,57,57,57	0
56	MG	BF	305	1/1	0.94	0.20	40,40,40,40	0
56	MG	BA	3520	1/1	0.95	0.14	25,25,25,25	0
56	MG	DA	3492	1/1	0.95	0.12	51,51,51,51	0
56	MG	DA	3088	1/1	0.95	0.08	39,39,39,39	0
56	MG	B3	3002	1/1	0.95	0.10	65,65,65,65	0
56	MG	BA	3144	1/1	0.95	0.11	37,37,37,37	0
56	MG	BA	3216	1/1	0.95	0.15	53,53,53,53	0
56	MG	DA	3497	1/1	0.95	0.08	27,27,27,27	0
56	MG	B5	103	1/1	0.95	0.15	51,51,51,51	0
56	MG	BA	3732	1/1	0.95	0.13	57,57,57,57	0
56	MG	BA	3623	1/1	0.95	0.08	59,59,59,59	0
56	MG	B7	102	1/1	0.95	0.20	40,40,40,40	0
56	MG	BA	3034	1/1	0.95	0.09	34,34,34,34	0
56	MG	BA	3035	1/1	0.95	0.13	25,25,25,25	0
56	MG	DA	3507	1/1	0.95	0.09	54,54,54,54	0
56	MG	BA	3627	1/1	0.95	0.09	52,52,52,52	0
56	MG	DA	3301	1/1	0.95	0.10	60,60,60,60	0
56	MG	DA	3511	1/1	0.95	0.10	62,62,62,62	0
56	MG	DA	3102	1/1	0.95	0.08	50,50,50,50	0
56	MG	DA	3304	1/1	0.95	0.08	32,32,32,32	0
56	MG	AA	3072	1/1	0.95	0.20	48,48,48,48	0
56	MG	CA	3130	1/1	0.95	0.19	70,70,70,70	0
56	MG	BA	3085	1/1	0.95	0.12	50,50,50,50	0
56	MG	DA	3310	1/1	0.95	0.08	39,39,39,39	0
56	MG	CA	3003	1/1	0.95	0.14	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	3312	1/1	0.95	0.11	40,40,40,40	0
56	MG	DA	3314	1/1	0.95	0.06	46,46,46,46	0
56	MG	BA	3039	1/1	0.95	0.15	34,34,34,34	0
56	MG	BA	3225	1/1	0.95	0.06	43,43,43,43	0
56	MG	BA	3632	1/1	0.95	0.15	53,53,53,53	0
56	MG	BA	3226	1/1	0.95	0.12	32,32,32,32	0
56	MG	CA	3008	1/1	0.95	0.11	45,45,45,45	0
56	MG	AA	3148	1/1	0.95	0.17	50,50,50,50	0
56	MG	BA	3635	1/1	0.95	0.07	56,56,56,56	0
56	MG	BA	3428	1/1	0.95	0.15	42,42,42,42	0
56	MG	BA	3229	1/1	0.95	0.06	38,38,38,38	0
56	MG	DA	3328	1/1	0.95	0.14	49,49,49,49	0
56	MG	BA	3088	1/1	0.95	0.10	46,46,46,46	0
56	MG	BA	3431	1/1	0.95	0.08	54,54,54,54	0
56	MG	AA	3191	1/1	0.95	0.09	49,49,49,49	0
56	MG	BA	3090	1/1	0.95	0.15	40,40,40,40	0
56	MG	DA	3123	1/1	0.95	0.12	40,40,40,40	0
56	MG	BA	3436	1/1	0.95	0.12	67,67,67,67	0
56	MG	DA	3339	1/1	0.95	0.16	46,46,46,46	0
56	MG	AA	3053	1/1	0.95	0.09	41,41,41,41	0
56	MG	DA	3341	1/1	0.95	0.08	54,54,54,54	0
56	MG	DA	3549	1/1	0.95	0.16	53,53,53,53	0
56	MG	BA	3236	1/1	0.95	0.07	34,34,34,34	0
56	MG	DA	3552	1/1	0.95	0.09	43,43,43,43	0
56	MG	AA	3010	1/1	0.95	0.06	22,22,22,22	0
56	MG	DA	3128	1/1	0.95	0.16	45,45,45,45	0
56	MG	CA	3022	1/1	0.95	0.12	53,53,53,53	0
56	MG	BA	3094	1/1	0.95	0.36	49,49,49,49	0
56	MG	DA	3557	1/1	0.95	0.16	67,67,67,67	0
56	MG	BA	3096	1/1	0.95	0.07	29,29,29,29	0
56	MG	DA	3559	1/1	0.95	0.10	49,49,49,49	0
56	MG	BA	3336	1/1	0.95	0.11	31,31,31,31	0
56	MG	BA	3769	1/1	0.95	0.12	52,52,52,52	0
56	MG	BA	3163	1/1	0.95	0.20	57,57,57,57	0
56	MG	BA	3448	1/1	0.95	0.27	60,60,60,60	0
56	MG	BA	3001	1/1	0.95	0.09	23,23,23,23	0
56	MG	BA	3245	1/1	0.95	0.09	47,47,47,47	0
56	MG	BA	3774	1/1	0.95	0.30	32,32,32,32	0
56	MG	CA	3161	1/1	0.95	0.15	59,59,59,59	0
56	MG	AA	3211	1/1	0.95	0.15	41,41,41,41	0
56	MG	BA	3659	1/1	0.95	0.11	24,24,24,24	0
56	MG	BA	3777	1/1	0.95	0.31	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	BA	3778	1/1	0.95	0.07	36,36,36,36	0
56	MG	DA	3149	1/1	0.95	0.25	48,48,48,48	0
56	MG	BA	3099	1/1	0.95	0.12	58,58,58,58	0
56	MG	DA	3576	1/1	0.95	0.12	46,46,46,46	0
56	MG	BA	3456	1/1	0.95	0.10	63,63,63,63	0
56	MG	BA	3562	1/1	0.95	0.18	37,37,37,37	0
56	MG	DA	3156	1/1	0.95	0.19	45,45,45,45	0
56	MG	BA	3100	1/1	0.95	0.12	46,46,46,46	0
56	MG	DA	3159	1/1	0.95	0.25	60,60,60,60	0
56	MG	DA	3583	1/1	0.95	0.10	44,44,44,44	0
56	MG	BA	3664	1/1	0.95	0.07	25,25,25,25	0
56	MG	CE	3001	1/1	0.95	0.12	73,73,73,73	0
56	MG	DA	3587	1/1	0.95	0.11	45,45,45,45	0
56	MG	BA	3344	1/1	0.95	0.10	36,36,36,36	0
56	MG	BA	3249	1/1	0.95	0.10	33,33,33,33	0
56	MG	CK	3001	1/1	0.95	0.12	47,47,47,47	0
56	MG	DA	3591	1/1	0.95	0.12	46,46,46,46	0
56	MG	DA	3379	1/1	0.95	0.14	38,38,38,38	0
56	MG	BA	3250	1/1	0.95	0.15	40,40,40,40	0
56	MG	DA	3594	1/1	0.95	0.18	52,52,52,52	0
56	MG	BA	3350	1/1	0.95	0.07	43,43,43,43	0
56	MG	BA	3671	1/1	0.95	0.07	33,33,33,33	0
56	MG	DA	3383	1/1	0.95	0.19	40,40,40,40	0
56	MG	CA	3050	1/1	0.95	0.10	55,55,55,55	0
56	MG	BB	3009	1/1	0.95	0.09	49,49,49,49	0
56	MG	DA	3600	1/1	0.95	0.13	55,55,55,55	0
56	MG	DA	3386	1/1	0.95	0.12	59,59,59,59	0
56	MG	BA	3672	1/1	0.95	0.23	37,37,37,37	0
56	MG	BA	3103	1/1	0.95	0.08	45,45,45,45	0
56	MG	AA	3056	1/1	0.95	0.19	56,56,56,56	0
56	MG	BA	3009	1/1	0.95	0.15	41,41,41,41	0
56	MG	DA	3006	1/1	0.95	0.20	42,42,42,42	0
56	MG	AA	3195	1/1	0.95	0.15	58,58,58,58	0
56	MG	BA	3469	1/1	0.95	0.14	49,49,49,49	0
56	MG	DA	3609	1/1	0.95	0.09	47,47,47,47	0
56	MG	BA	3683	1/1	0.95	0.26	50,50,50,50	0
56	MG	BA	3685	1/1	0.95	0.07	43,43,43,43	0
56	MG	BD	304	1/1	0.95	0.11	50,50,50,50	0
56	MG	DA	3402	1/1	0.95	0.13	57,57,57,57	0
56	MG	AA	3018	1/1	0.95	0.07	58,58,58,58	0
56	MG	BA	3056	1/1	0.95	0.15	26,26,26,26	0
56	MG	BA	3474	1/1	0.95	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3019	1/1	0.95	0.08	40,40,40,40	0
56	MG	DA	3192	1/1	0.95	0.17	49,49,49,49	0
56	MG	DA	3410	1/1	0.95	0.06	37,37,37,37	0
56	MG	BA	3361	1/1	0.95	0.08	29,29,29,29	0
56	MG	DA	3412	1/1	0.95	0.09	52,52,52,52	0
56	MG	DA	3194	1/1	0.95	0.14	52,52,52,52	0
56	MG	BA	3057	1/1	0.95	0.15	48,48,48,48	0
56	MG	BA	3059	1/1	0.95	0.07	40,40,40,40	0
56	MG	BA	3583	1/1	0.95	0.09	46,46,46,46	0
56	MG	BA	3013	1/1	0.95	0.22	46,46,46,46	0
56	MG	BA	3014	1/1	0.95	0.11	46,46,46,46	0
56	MG	BF	304	1/1	0.95	0.23	37,37,37,37	0
56	MG	DA	3204	1/1	0.95	0.09	47,47,47,47	0
56	MG	AA	3038	1/1	0.95	0.27	56,56,56,56	0
56	MG	BA	3064	1/1	0.95	0.11	46,46,46,46	0
56	MG	DA	3033	1/1	0.95	0.12	43,43,43,43	0
56	MG	BA	3264	1/1	0.95	0.09	19,19,19,19	0
56	MG	BA	3121	1/1	0.95	0.13	64,64,64,64	0
56	MG	DA	3210	1/1	0.95	0.14	35,35,35,35	0
56	MG	DD	302	1/1	0.95	0.08	40,40,40,40	0
56	MG	BF	310	1/1	0.95	0.07	44,44,44,44	0
56	MG	DA	3038	1/1	0.95	0.14	56,56,56,56	0
56	MG	BA	3699	1/1	0.95	0.06	39,39,39,39	0
56	MG	CA	3078	1/1	0.95	0.07	41,41,41,41	0
56	MG	DA	3215	1/1	0.95	0.29	53,53,53,53	0
56	MG	BA	3266	1/1	0.95	0.07	38,38,38,38	0
56	MG	BA	3271	1/1	0.95	0.16	39,39,39,39	0
56	MG	DA	3045	1/1	0.95	0.06	44,44,44,44	0
56	MG	BA	3274	1/1	0.95	0.07	29,29,29,29	0
56	MG	BN	3003	1/1	0.95	0.13	62,62,62,62	0
56	MG	BA	3384	1/1	0.95	0.08	43,43,43,43	0
56	MG	DA	3049	1/1	0.95	0.07	48,48,48,48	0
56	MG	CA	3084	1/1	0.95	0.11	46,46,46,46	0
56	MG	DN	5001	1/1	0.95	0.08	75,75,75,75	0
56	MG	DA	3228	1/1	0.95	0.10	29,29,29,29	0
56	MG	DA	3052	1/1	0.95	0.17	44,44,44,44	0
56	MG	DA	3053	1/1	0.95	0.18	61,61,61,61	0
56	MG	BA	3125	1/1	0.95	0.15	34,34,34,34	0
56	MG	BA	3497	1/1	0.95	0.10	24,24,24,24	0
56	MG	BA	3018	1/1	0.95	0.15	36,36,36,36	0
56	MG	BP	203	1/1	0.95	0.09	37,37,37,37	0
56	MG	BA	3279	1/1	0.95	0.10	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	3181	1/1	0.95	0.12	65,65,65,65	0
56	MG	BA	3203	1/1	0.95	0.27	51,51,51,51	0
56	MG	BQ	3004	1/1	0.95	0.23	48,48,48,48	0
56	MG	BA	3130	1/1	0.95	0.10	44,44,44,44	0
56	MG	DA	3063	1/1	0.95	0.09	52,52,52,52	0
56	MG	BA	3286	1/1	0.95	0.05	48,48,48,48	0
56	MG	BA	3206	1/1	0.95	0.24	49,49,49,49	0
56	MG	BA	3506	1/1	0.95	0.07	43,43,43,43	0
56	MG	BA	3288	1/1	0.95	0.09	36,36,36,36	0
56	MG	BU	204	1/1	0.95	0.11	43,43,43,43	0
56	MG	AA	3005	1/1	0.95	0.25	55,55,55,55	0
56	MG	AA	3012	1/1	0.95	0.17	43,43,43,43	0
56	MG	DA	3258	1/1	0.95	0.05	24,24,24,24	0
56	MG	DA	3259	1/1	0.95	0.09	50,50,50,50	0
56	MG	BA	3075	1/1	0.95	0.11	48,48,48,48	0
56	MG	BV	205	1/1	0.95	0.31	37,37,37,37	0
56	MG	DA	3263	1/1	0.95	0.08	48,48,48,48	0
56	MG	DA	3264	1/1	0.95	0.10	44,44,44,44	0
56	MG	DA	3265	1/1	0.95	0.09	47,47,47,47	0
56	MG	BA	3136	1/1	0.95	0.20	49,49,49,49	0
56	MG	DA	3268	1/1	0.95	0.18	53,53,53,53	0
56	MG	DA	3480	1/1	0.95	0.13	48,48,48,48	0
56	MG	AA	3157	1/1	0.95	0.11	46,46,46,46	0
56	MG	AA	3172	1/1	0.95	0.14	44,44,44,44	0
56	MG	BX	102	1/1	0.95	0.10	40,40,40,40	0
56	MG	AA	3081	1/1	0.95	0.14	52,52,52,52	0
56	MG	BA	3301	1/1	0.95	0.07	55,55,55,55	0
56	MG	BA	3143	1/1	0.95	0.20	35,35,35,35	0
56	MG	DA	3487	1/1	0.95	0.07	37,37,37,37	0
56	MG	DA	3278	1/1	0.95	0.07	44,44,44,44	0
56	MG	B1	101	1/1	0.95	0.26	45,45,45,45	0
56	MG	BA	3728	1/1	0.95	0.09	65,65,65,65	0
56	MG	AA	3090	1/1	0.96	0.27	50,50,50,50	0
56	MG	BA	3669	1/1	0.96	0.12	45,45,45,45	0
56	MG	BA	3146	1/1	0.96	0.07	36,36,36,36	0
56	MG	DA	3505	1/1	0.96	0.07	41,41,41,41	0
56	MG	BA	3067	1/1	0.96	0.11	35,35,35,35	0
56	MG	BA	3068	1/1	0.96	0.22	56,56,56,56	0
56	MG	DA	3509	1/1	0.96	0.11	38,38,38,38	0
56	MG	DA	3315	1/1	0.96	0.05	28,28,28,28	0
56	MG	BB	3004	1/1	0.96	0.13	64,64,64,64	0
56	MG	BA	3674	1/1	0.96	0.18	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3280	1/1	0.96	0.10	25,25,25,25	0
56	MG	CA	3038	1/1	0.96	0.10	31,31,31,31	0
56	MG	DA	3516	1/1	0.96	0.08	35,35,35,35	0
56	MG	BA	3101	1/1	0.96	0.14	36,36,36,36	0
56	MG	BA	3150	1/1	0.96	0.06	47,47,47,47	0
56	MG	DA	3519	1/1	0.96	0.05	78,78,78,78	0
56	MG	DA	3136	1/1	0.96	0.13	35,35,35,35	0
56	MG	DA	3324	1/1	0.96	0.14	46,46,46,46	0
56	MG	CA	3166	1/1	0.96	0.05	42,42,42,42	0
56	MG	BB	3010	1/1	0.96	0.14	51,51,51,51	0
56	MG	BA	3678	1/1	0.96	0.09	41,41,41,41	0
56	MG	BA	3679	1/1	0.96	0.07	47,47,47,47	0
56	MG	BB	3014	1/1	0.96	0.05	39,39,39,39	0
56	MG	DA	3331	1/1	0.96	0.04	46,46,46,46	0
56	MG	CA	3180	1/1	0.96	0.17	61,61,61,61	0
56	MG	BA	3680	1/1	0.96	0.08	32,32,32,32	0
56	MG	BA	3472	1/1	0.96	0.11	43,43,43,43	0
56	MG	DA	3337	1/1	0.96	0.05	42,42,42,42	0
56	MG	BA	3473	1/1	0.96	0.12	31,31,31,31	0
56	MG	BA	3578	1/1	0.96	0.10	49,49,49,49	0
56	MG	AA	3171	1/1	0.96	0.09	56,56,56,56	0
56	MG	BA	3372	1/1	0.96	0.11	33,33,33,33	0
56	MG	DA	3150	1/1	0.96	0.09	49,49,49,49	0
56	MG	BA	3581	1/1	0.96	0.07	47,47,47,47	0
56	MG	CV	101	1/1	0.96	0.14	56,56,56,56	0
56	MG	BD	305	1/1	0.96	0.11	41,41,41,41	0
56	MG	BD	306	1/1	0.96	0.14	22,22,22,22	0
56	MG	DA	3347	1/1	0.96	0.08	53,53,53,53	0
56	MG	DA	3157	1/1	0.96	0.20	58,58,58,58	0
56	MG	BA	3003	1/1	0.96	0.07	43,43,43,43	0
56	MG	BA	3219	1/1	0.96	0.10	39,39,39,39	0
56	MG	DA	3551	1/1	0.96	0.11	66,66,66,66	0
56	MG	BD	311	1/1	0.96	0.27	46,46,46,46	0
56	MG	BA	3377	1/1	0.96	0.13	39,39,39,39	0
56	MG	BA	3481	1/1	0.96	0.12	32,32,32,32	0
56	MG	BA	3037	1/1	0.96	0.28	33,33,33,33	0
56	MG	DA	3358	1/1	0.96	0.07	51,51,51,51	0
56	MG	BA	3380	1/1	0.96	0.15	59,59,59,59	0
56	MG	BA	3106	1/1	0.96	0.12	42,42,42,42	0
56	MG	CA	3062	1/1	0.96	0.34	65,65,65,65	0
56	MG	DA	3560	1/1	0.96	0.10	59,59,59,59	0
56	MG	DA	3362	1/1	0.96	0.10	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3485	1/1	0.96	0.08	25,25,25,25	0
56	MG	DA	3364	1/1	0.96	0.25	54,54,54,54	0
56	MG	DA	3170	1/1	0.96	0.27	39,39,39,39	0
56	MG	BA	3382	1/1	0.96	0.11	30,30,30,30	0
56	MG	DA	3566	1/1	0.96	0.09	51,51,51,51	0
56	MG	BA	3487	1/1	0.96	0.13	37,37,37,37	0
56	MG	BA	3073	1/1	0.96	0.16	25,25,25,25	0
56	MG	BA	3386	1/1	0.96	0.19	36,36,36,36	0
56	MG	DA	3017	1/1	0.96	0.07	46,46,46,46	0
56	MG	AA	3185	1/1	0.96	0.19	51,51,51,51	0
56	MG	BA	3296	1/1	0.96	0.11	47,47,47,47	0
56	MG	AD	502	1/1	0.96	0.26	58,58,58,58	0
56	MG	BA	3390	1/1	0.96	0.13	26,26,26,26	0
56	MG	BG	3001	1/1	0.96	0.12	42,42,42,42	0
56	MG	DA	3182	1/1	0.96	0.11	52,52,52,52	0
56	MG	BA	3041	1/1	0.96	0.08	51,51,51,51	0
56	MG	BA	3392	1/1	0.96	0.07	17,17,17,17	0
56	MG	DA	3186	1/1	0.96	0.16	41,41,41,41	0
56	MG	BA	3499	1/1	0.96	0.08	57,57,57,57	0
56	MG	BA	3603	1/1	0.96	0.14	28,28,28,28	0
56	MG	BA	3160	1/1	0.96	0.17	58,58,58,58	0
56	MG	DA	3032	1/1	0.96	0.08	40,40,40,40	0
56	MG	BA	3228	1/1	0.96	0.30	51,51,51,51	0
56	MG	DA	3586	1/1	0.96	0.12	49,49,49,49	0
56	MG	AA	3052	1/1	0.96	0.12	52,52,52,52	0
56	MG	BA	3302	1/1	0.96	0.10	46,46,46,46	0
56	MG	BP	201	1/1	0.96	0.14	36,36,36,36	0
56	MG	BP	202	1/1	0.96	0.14	36,36,36,36	0
56	MG	BA	3230	1/1	0.96	0.21	53,53,53,53	0
56	MG	DA	3040	1/1	0.96	0.08	47,47,47,47	0
56	MG	BA	3044	1/1	0.96	0.14	39,39,39,39	0
56	MG	DA	3201	1/1	0.96	0.23	56,56,56,56	0
56	MG	BA	3114	1/1	0.96	0.22	49,49,49,49	0
56	MG	DA	3203	1/1	0.96	0.13	46,46,46,46	0
56	MG	DA	3043	1/1	0.96	0.09	49,49,49,49	0
56	MG	BA	3166	1/1	0.96	0.12	47,47,47,47	0
56	MG	BA	3115	1/1	0.96	0.07	13,13,13,13	0
56	MG	BA	3308	1/1	0.96	0.17	38,38,38,38	0
56	MG	DA	3404	1/1	0.96	0.07	36,36,36,36	0
56	MG	BA	3720	1/1	0.96	0.06	28,28,28,28	0
56	MG	BA	3079	1/1	0.96	0.23	40,40,40,40	0
56	MG	BR	203	1/1	0.96	0.18	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3722	1/1	0.96	0.10	46,46,46,46	0
56	MG	CA	3095	1/1	0.96	0.06	47,47,47,47	0
56	MG	BA	3239	1/1	0.96	0.17	30,30,30,30	0
56	MG	AA	3034	1/1	0.96	0.33	56,56,56,56	0
56	MG	AA	3066	1/1	0.96	0.07	53,53,53,53	0
56	MG	BA	3409	1/1	0.96	0.11	43,43,43,43	0
56	MG	DA	3415	1/1	0.96	0.28	45,45,45,45	0
56	MG	BA	3120	1/1	0.96	0.13	45,45,45,45	0
56	MG	BA	3621	1/1	0.96	0.07	48,48,48,48	0
56	MG	CA	3102	1/1	0.96	0.08	48,48,48,48	0
56	MG	DA	3222	1/1	0.96	0.10	46,46,46,46	0
56	MG	BV	206	1/1	0.96	0.09	38,38,38,38	0
56	MG	BA	3622	1/1	0.96	0.08	48,48,48,48	0
56	MG	BA	3317	1/1	0.96	0.10	47,47,47,47	0
56	MG	BW	202	1/1	0.96	0.13	43,43,43,43	0
56	MG	DA	3064	1/1	0.96	0.17	52,52,52,52	0
56	MG	BW	203	1/1	0.96	0.08	42,42,42,42	0
56	MG	BW	204	1/1	0.96	0.17	41,41,41,41	0
56	MG	BA	3083	1/1	0.96	0.13	30,30,30,30	0
56	MG	DA	3234	1/1	0.96	0.10	42,42,42,42	0
56	MG	DA	3236	1/1	0.96	0.09	59,59,59,59	0
56	MG	BA	3319	1/1	0.96	0.12	38,38,38,38	0
56	MG	BA	3123	1/1	0.96	0.28	39,39,39,39	0
56	MG	BA	3181	1/1	0.96	0.10	48,48,48,48	0
56	MG	DA	3240	1/1	0.96	0.12	36,36,36,36	0
56	MG	BA	3324	1/1	0.96	0.08	44,44,44,44	0
56	MG	BA	3525	1/1	0.96	0.06	40,40,40,40	0
56	MG	DA	3074	1/1	0.96	0.13	49,49,49,49	0
56	MG	CA	3115	1/1	0.96	0.06	58,58,58,58	0
56	MG	DA	3440	1/1	0.96	0.12	49,49,49,49	0
56	MG	CA	3116	1/1	0.96	0.07	64,64,64,64	0
56	MG	BA	3124	1/1	0.96	0.07	33,33,33,33	0
56	MG	DD	303	1/1	0.96	0.08	60,60,60,60	0
56	MG	DD	304	1/1	0.96	0.11	56,56,56,56	0
56	MG	DD	305	1/1	0.96	0.19	32,32,32,32	0
56	MG	BA	3326	1/1	0.96	0.08	50,50,50,50	0
56	MG	DA	3251	1/1	0.96	0.10	47,47,47,47	0
56	MG	BA	3422	1/1	0.96	0.12	45,45,45,45	0
56	MG	AA	3076	1/1	0.96	0.13	45,45,45,45	0
56	MG	BA	3184	1/1	0.96	0.15	33,33,33,33	0
56	MG	BA	3126	1/1	0.96	0.20	48,48,48,48	0
56	MG	DA	3083	1/1	0.96	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DA	3084	1/1	0.96	0.15	53,53,53,53	0
56	MG	DA	3452	1/1	0.96	0.09	44,44,44,44	0
56	MG	AX	3008	1/1	0.96	0.14	52,52,52,52	0
56	MG	BA	3332	1/1	0.96	0.22	48,48,48,48	0
56	MG	BA	3432	1/1	0.96	0.07	48,48,48,48	0
56	MG	DA	3457	1/1	0.96	0.10	46,46,46,46	0
56	MG	AA	3118	1/1	0.96	0.06	40,40,40,40	0
56	MG	DA	3262	1/1	0.96	0.08	41,41,41,41	0
56	MG	AA	3051	1/1	0.96	0.10	64,64,64,64	0
56	MG	BA	3752	1/1	0.96	0.09	48,48,48,48	0
56	MG	BA	3192	1/1	0.96	0.10	56,56,56,56	0
56	MG	DA	3266	1/1	0.96	0.12	61,61,61,61	0
56	MG	BA	3131	1/1	0.96	0.20	35,35,35,35	0
56	MG	BA	3196	1/1	0.96	0.06	46,46,46,46	0
56	MG	DA	3269	1/1	0.96	0.09	46,46,46,46	0
56	MG	BA	3440	1/1	0.96	0.09	41,41,41,41	0
56	MG	BA	3339	1/1	0.96	0.07	31,31,31,31	0
56	MG	DV	3002	1/1	0.96	0.18	51,51,51,51	0
56	MG	DA	3273	1/1	0.96	0.08	36,36,36,36	0
56	MG	AA	3165	1/1	0.96	0.10	51,51,51,51	0
56	MG	BA	3650	1/1	0.96	0.06	38,38,38,38	0
56	MG	DA	3099	1/1	0.96	0.14	39,39,39,39	0
56	MG	BA	3025	1/1	0.96	0.19	37,37,37,37	0
56	MG	DA	3101	1/1	0.96	0.08	28,28,28,28	0
56	MG	BA	3026	1/1	0.96	0.13	41,41,41,41	0
56	MG	DA	3477	1/1	0.96	0.12	41,41,41,41	0
56	MG	BA	3028	1/1	0.96	0.21	48,48,48,48	0
56	MG	DA	3104	1/1	0.96	0.19	49,49,49,49	0
56	MG	BA	3768	1/1	0.96	0.14	48,48,48,48	0
56	MG	AA	3166	1/1	0.96	0.12	43,43,43,43	0
56	MG	DA	3286	1/1	0.96	0.13	39,39,39,39	0
56	MG	BA	3138	1/1	0.96	0.16	50,50,50,50	0
56	MG	DA	3289	1/1	0.96	0.10	23,23,23,23	0
56	MG	BA	3657	1/1	0.96	0.16	54,54,54,54	0
56	MG	BA	3346	1/1	0.96	0.08	28,28,28,28	0
56	MG	AA	3131	1/1	0.96	0.12	63,63,63,63	0
56	MG	BA	3140	1/1	0.96	0.14	41,41,41,41	0
56	MG	BA	3095	1/1	0.96	0.17	39,39,39,39	0
56	MG	DA	3296	1/1	0.96	0.09	38,38,38,38	0
56	MG	DA	3113	1/1	0.96	0.21	51,51,51,51	0
56	MG	AA	3089	1/1	0.96	0.22	54,54,54,54	0
56	MG	DA	3299	1/1	0.96	0.08	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	BA	3269	1/1	0.96	0.16	40,40,40,40	0
56	MG	BA	3270	1/1	0.96	0.12	47,47,47,47	0
56	MG	BA	3779	1/1	0.96	0.12	52,52,52,52	0
56	MG	AA	3104	1/1	0.96	0.12	44,44,44,44	0
59	ZN	D9	501	1/1	0.96	0.06	82,82,82,82	0
56	MG	BA	3781	1/1	0.96	0.07	42,42,42,42	0
56	MG	BA	3272	1/1	0.96	0.14	41,41,41,41	0
56	MG	BA	3185	1/1	0.97	0.14	38,38,38,38	0
56	MG	BA	3321	1/1	0.97	0.06	43,43,43,43	0
56	MG	BA	3379	1/1	0.97	0.11	22,22,22,22	0
56	MG	B0	101	1/1	0.97	0.10	49,49,49,49	0
56	MG	BA	3050	1/1	0.97	0.07	34,34,34,34	0
56	MG	DA	3009	1/1	0.97	0.15	46,46,46,46	0
56	MG	AA	3187	1/1	0.97	0.09	56,56,56,56	0
56	MG	BA	3188	1/1	0.97	0.25	41,41,41,41	0
56	MG	DA	3408	1/1	0.97	0.05	25,25,25,25	0
56	MG	AA	3036	1/1	0.97	0.07	24,24,24,24	0
56	MG	CA	3089	1/1	0.97	0.17	46,46,46,46	0
56	MG	DA	3014	1/1	0.97	0.09	37,37,37,37	0
56	MG	BA	3454	1/1	0.97	0.05	43,43,43,43	0
56	MG	DA	3132	1/1	0.97	0.07	39,39,39,39	0
56	MG	DA	3133	1/1	0.97	0.06	50,50,50,50	0
56	MG	DA	3134	1/1	0.97	0.12	60,60,60,60	0
56	MG	BA	3385	1/1	0.97	0.11	50,50,50,50	0
56	MG	BA	3457	1/1	0.97	0.06	46,46,46,46	0
56	MG	DA	3018	1/1	0.97	0.06	29,29,29,29	0
56	MG	B5	102	1/1	0.97	0.23	42,42,42,42	0
56	MG	BA	3528	1/1	0.97	0.06	29,29,29,29	0
56	MG	DA	3272	1/1	0.97	0.09	43,43,43,43	0
56	MG	BA	3529	1/1	0.97	0.20	57,57,57,57	0
56	MG	B5	106	1/1	0.97	0.07	55,55,55,55	0
56	MG	BA	3458	1/1	0.97	0.14	52,52,52,52	0
56	MG	DA	3143	1/1	0.97	0.08	35,35,35,35	0
56	MG	BA	3273	1/1	0.97	0.06	36,36,36,36	0
56	MG	DA	3428	1/1	0.97	0.21	50,50,50,50	0
56	MG	BA	3020	1/1	0.97	0.13	32,32,32,32	0
56	MG	BA	3055	1/1	0.97	0.14	30,30,30,30	0
56	MG	DA	3280	1/1	0.97	0.08	26,26,26,26	0
56	MG	B8	101	1/1	0.97	0.08	35,35,35,35	0
56	MG	BA	3277	1/1	0.97	0.09	40,40,40,40	0
56	MG	BB	3006	1/1	0.97	0.04	46,46,46,46	0
56	MG	BA	3535	1/1	0.97	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BA	3536	1/1	0.97	0.12	30,30,30,30	0
56	MG	BA	3330	1/1	0.97	0.09	35,35,35,35	0
56	MG	DA	3288	1/1	0.97	0.09	43,43,43,43	0
56	MG	BA	3232	1/1	0.97	0.26	44,44,44,44	0
56	MG	DA	3154	1/1	0.97	0.06	43,43,43,43	0
56	MG	DA	3155	1/1	0.97	0.26	53,53,53,53	0
56	MG	BA	3193	1/1	0.97	0.04	24,24,24,24	0
56	MG	BA	3194	1/1	0.97	0.07	40,40,40,40	0
56	MG	BA	3334	1/1	0.97	0.04	23,23,23,23	0
56	MG	BA	3624	1/1	0.97	0.08	50,50,50,50	0
56	MG	DA	3160	1/1	0.97	0.20	51,51,51,51	0
56	MG	BA	3021	1/1	0.97	0.09	32,32,32,32	0
56	MG	DA	3448	1/1	0.97	0.08	40,40,40,40	0
56	MG	DA	3162	1/1	0.97	0.15	45,45,45,45	0
56	MG	BA	3102	1/1	0.97	0.10	47,47,47,47	0
56	MG	BA	3709	1/1	0.97	0.08	42,42,42,42	0
56	MG	BA	3397	1/1	0.97	0.12	29,29,29,29	0
56	MG	BA	3238	1/1	0.97	0.39	35,35,35,35	0
56	MG	DA	3454	1/1	0.97	0.10	47,47,47,47	0
56	MG	CA	3015	1/1	0.97	0.04	45,45,45,45	0
56	MG	BA	3129	1/1	0.97	0.12	49,49,49,49	0
56	MG	BA	3198	1/1	0.97	0.12	35,35,35,35	0
56	MG	BA	3022	1/1	0.97	0.24	41,41,41,41	0
56	MG	DA	3171	1/1	0.97	0.06	41,41,41,41	0
56	MG	DA	3051	1/1	0.97	0.14	54,54,54,54	0
56	MG	DA	3313	1/1	0.97	0.12	46,46,46,46	0
56	MG	BA	3476	1/1	0.97	0.14	37,37,37,37	0
56	MG	BA	3552	1/1	0.97	0.11	32,32,32,32	0
56	MG	DA	3464	1/1	0.97	0.07	51,51,51,51	0
56	MG	BA	3058	1/1	0.97	0.13	23,23,23,23	0
56	MG	BA	3718	1/1	0.97	0.11	49,49,49,49	0
56	MG	CA	3023	1/1	0.97	0.07	54,54,54,54	0
56	MG	BE	302	1/1	0.97	0.06	28,28,28,28	0
56	MG	BA	3478	1/1	0.97	0.10	36,36,36,36	0
56	MG	BA	3293	1/1	0.97	0.07	40,40,40,40	0
56	MG	BE	305	1/1	0.97	0.11	38,38,38,38	0
56	MG	BA	3008	1/1	0.97	0.05	27,27,27,27	0
56	MG	CA	3029	1/1	0.97	0.13	37,37,37,37	0
56	MG	CA	3030	1/1	0.97	0.20	51,51,51,51	0
56	MG	DA	3185	1/1	0.97	0.23	53,53,53,53	0
56	MG	BA	3082	1/1	0.97	0.14	27,27,27,27	0
56	MG	AA	3055	1/1	0.97	0.09	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	BA	3010	1/1	0.97	0.18	58,58,58,58	0
56	MG	CA	3137	1/1	0.97	0.07	52,52,52,52	0
56	MG	BA	3347	1/1	0.97	0.12	26,26,26,26	0
56	MG	BA	3642	1/1	0.97	0.20	38,38,38,38	0
56	MG	DA	3070	1/1	0.97	0.10	34,34,34,34	0
56	MG	BA	3062	1/1	0.97	0.12	35,35,35,35	0
56	MG	BA	3349	1/1	0.97	0.09	25,25,25,25	0
56	MG	BA	3110	1/1	0.97	0.19	49,49,49,49	0
56	MG	BA	3489	1/1	0.97	0.06	43,43,43,43	0
56	MG	BA	3170	1/1	0.97	0.09	30,30,30,30	0
56	MG	BA	3648	1/1	0.97	0.08	39,39,39,39	0
56	MG	BA	3352	1/1	0.97	0.10	22,22,22,22	0
56	MG	BA	3353	1/1	0.97	0.09	27,27,27,27	0
56	MG	BA	3571	1/1	0.97	0.07	40,40,40,40	0
56	MG	DE	301	1/1	0.97	0.32	50,50,50,50	0
56	MG	BA	3493	1/1	0.97	0.08	29,29,29,29	0
56	MG	BA	3043	1/1	0.97	0.06	34,34,34,34	0
56	MG	BA	3027	1/1	0.97	0.10	41,41,41,41	0
56	MG	BA	3575	1/1	0.97	0.10	48,48,48,48	0
56	MG	BA	3173	1/1	0.97	0.10	46,46,46,46	0
56	MG	BA	3358	1/1	0.97	0.09	30,30,30,30	0
56	MG	BA	3423	1/1	0.97	0.17	43,43,43,43	0
56	MG	BA	3745	1/1	0.97	0.09	27,27,27,27	0
56	MG	DA	3357	1/1	0.97	0.07	44,44,44,44	0
56	MG	BA	3065	1/1	0.97	0.14	33,33,33,33	0
56	MG	BA	3175	1/1	0.97	0.08	44,44,44,44	0
56	MG	BQ	3002	1/1	0.97	0.16	41,41,41,41	0
56	MG	DO	202	1/1	0.97	0.11	57,57,57,57	0
56	MG	BA	3176	1/1	0.97	0.15	41,41,41,41	0
56	MG	DQ	3001	1/1	0.97	0.06	57,57,57,57	0
56	MG	BA	3142	1/1	0.97	0.14	47,47,47,47	0
56	MG	DA	3217	1/1	0.97	0.05	43,43,43,43	0
56	MG	DA	3218	1/1	0.97	0.07	53,53,53,53	0
56	MG	DR	3001	1/1	0.97	0.17	55,55,55,55	0
56	MG	BA	3066	1/1	0.97	0.17	40,40,40,40	0
56	MG	DA	3512	1/1	0.97	0.07	52,52,52,52	0
56	MG	BA	3179	1/1	0.97	0.09	61,61,61,61	0
56	MG	BA	3666	1/1	0.97	0.04	11,11,11,11	0
56	MG	BA	3218	1/1	0.97	0.14	52,52,52,52	0
56	MG	AA	3119	1/1	0.97	0.10	36,36,36,36	0
56	MG	BA	3507	1/1	0.97	0.12	53,53,53,53	0
56	MG	DW	3002	1/1	0.97	0.17	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BU	202	1/1	0.97	0.26	32,32,32,32	0
56	MG	BA	3368	1/1	0.97	0.08	56,56,56,56	0
56	MG	DA	3227	1/1	0.97	0.07	47,47,47,47	0
56	MG	CA	3178	1/1	0.97	0.06	54,54,54,54	0
56	MG	BU	205	1/1	0.97	0.17	39,39,39,39	0
56	MG	DA	3230	1/1	0.97	0.12	23,23,23,23	0
56	MG	D7	101	1/1	0.97	0.20	33,33,33,33	0
56	MG	AA	3016	1/1	0.97	0.13	48,48,48,48	0
56	MG	AA	3204	1/1	0.97	0.17	44,44,44,44	0
56	MG	BU	209	1/1	0.97	0.27	41,41,41,41	0
56	MG	BV	201	1/1	0.97	0.08	26,26,26,26	0
56	MG	BV	202	1/1	0.97	0.17	34,34,34,34	0
56	MG	DA	3531	1/1	0.97	0.11	40,40,40,40	0
56	MG	BA	3673	1/1	0.97	0.11	22,22,22,22	0
56	MG	BA	3314	1/1	0.97	0.04	41,41,41,41	0
56	MG	AA	3205	1/1	0.97	0.06	66,66,66,66	0
56	MG	DA	3535	1/1	0.97	0.04	38,38,38,38	0
56	MG	BA	3766	1/1	0.97	0.07	43,43,43,43	0
56	MG	BA	3443	1/1	0.97	0.08	50,50,50,50	0
56	MG	CW	3003	1/1	0.97	0.07	64,64,64,64	0
56	MG	DA	3388	1/1	0.97	0.06	49,49,49,49	0
56	MG	BA	3594	1/1	0.97	0.12	37,37,37,37	0
56	MG	BA	3374	1/1	0.97	0.11	34,34,34,34	0
56	MG	DA	3391	1/1	0.97	0.11	40,40,40,40	0
56	MG	AA	3084	1/1	0.97	0.21	53,53,53,53	0
56	MG	DA	3248	1/1	0.97	0.07	39,39,39,39	0
56	MG	DA	3118	1/1	0.97	0.17	50,50,50,50	0
59	ZN	CN	102	1/1	0.97	0.06	82,82,82,82	0
56	MG	DA	3547	1/1	0.97	0.12	41,41,41,41	0
56	MG	DA	3396	1/1	0.97	0.07	27,27,27,27	0
56	MG	DA	3250	1/1	0.97	0.10	37,37,37,37	0
56	MG	BA	3516	1/1	0.97	0.10	36,36,36,36	0
56	MG	AA	3025	1/1	0.98	0.35	54,54,54,54	0
56	MG	BA	3220	1/1	0.98	0.08	45,45,45,45	0
56	MG	AW	3005	1/1	0.98	0.05	52,52,52,52	0
56	MG	BA	3441	1/1	0.98	0.06	37,37,37,37	0
56	MG	BA	3267	1/1	0.98	0.15	14,14,14,14	0
56	MG	BA	3398	1/1	0.98	0.06	37,37,37,37	0
56	MG	DA	3537	1/1	0.98	0.05	53,53,53,53	0
56	MG	BA	3488	1/1	0.98	0.04	28,28,28,28	0
56	MG	AA	3064	1/1	0.98	0.07	47,47,47,47	0
56	MG	BA	3162	1/1	0.98	0.06	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	DB	3004	1/1	0.98	0.14	54,54,54,54	0
56	MG	AA	3065	1/1	0.98	0.05	40,40,40,40	0
56	MG	BA	3204	1/1	0.98	0.09	35,35,35,35	0
56	MG	BA	3684	1/1	0.98	0.07	39,39,39,39	0
56	MG	DA	3295	1/1	0.98	0.12	34,34,34,34	0
56	MG	BA	3366	1/1	0.98	0.06	23,23,23,23	0
56	MG	DA	3020	1/1	0.98	0.09	33,33,33,33	0
56	MG	DA	3021	1/1	0.98	0.06	44,44,44,44	0
56	MG	BA	3538	1/1	0.98	0.06	43,43,43,43	0
56	MG	BA	3164	1/1	0.98	0.21	33,33,33,33	0
56	MG	BA	3540	1/1	0.98	0.06	28,28,28,28	0
56	MG	DA	3092	1/1	0.98	0.07	43,43,43,43	0
56	MG	DA	3303	1/1	0.98	0.07	44,44,44,44	0
56	MG	BU	203	1/1	0.98	0.11	34,34,34,34	0
56	MG	AA	3070	1/1	0.98	0.04	31,31,31,31	0
56	MG	BA	3369	1/1	0.98	0.11	23,23,23,23	0
56	MG	DA	3307	1/1	0.98	0.04	28,28,28,28	0
56	MG	BA	3452	1/1	0.98	0.04	41,41,41,41	0
56	MG	DA	3309	1/1	0.98	0.05	42,42,42,42	0
56	MG	BA	3275	1/1	0.98	0.10	45,45,45,45	0
56	MG	DA	3392	1/1	0.98	0.09	34,34,34,34	0
56	MG	BA	3006	1/1	0.98	0.04	26,26,26,26	0
56	MG	BA	3251	1/1	0.98	0.10	51,51,51,51	0
56	MG	BA	3747	1/1	0.98	0.06	50,50,50,50	0
56	MG	DA	3034	1/1	0.98	0.04	35,35,35,35	0
56	MG	DA	3478	1/1	0.98	0.05	54,54,54,54	0
56	MG	BV	203	1/1	0.98	0.08	31,31,31,31	0
56	MG	BD	302	1/1	0.98	0.07	33,33,33,33	0
56	MG	DA	3399	1/1	0.98	0.11	35,35,35,35	0
56	MG	BA	3595	1/1	0.98	0.06	65,65,65,65	0
56	MG	BA	3411	1/1	0.98	0.07	49,49,49,49	0
56	MG	DA	3319	1/1	0.98	0.07	21,21,21,21	0
56	MG	BA	3167	1/1	0.98	0.14	28,28,28,28	0
56	MG	DA	3245	1/1	0.98	0.05	28,28,28,28	0
56	MG	BA	3117	1/1	0.98	0.12	41,41,41,41	0
56	MG	AA	3001	1/1	0.98	0.10	37,37,37,37	0
56	MG	BA	3038	1/1	0.98	0.10	31,31,31,31	0
56	MG	BD	309	1/1	0.98	0.18	39,39,39,39	0
56	MG	BA	3282	1/1	0.98	0.04	59,59,59,59	0
56	MG	BA	3016	1/1	0.98	0.04	22,22,22,22	0
56	MG	DA	3580	1/1	0.98	0.07	44,44,44,44	0
56	MG	BA	3284	1/1	0.98	0.07	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	3556	1/1	0.98	0.15	50,50,50,50	0
56	MG	BA	3557	1/1	0.98	0.09	58,58,58,58	0
56	MG	DW	3001	1/1	0.98	0.16	45,45,45,45	0
56	MG	B0	102	1/1	0.98	0.07	54,54,54,54	0
56	MG	BA	3315	1/1	0.98	0.08	40,40,40,40	0
56	MG	BA	3607	1/1	0.98	0.08	45,45,45,45	0
56	MG	BA	3316	1/1	0.98	0.09	58,58,58,58	0
56	MG	BA	3763	1/1	0.98	0.11	10,10,10,10	0
56	MG	BF	302	1/1	0.98	0.24	29,29,29,29	0
56	MG	DA	3420	1/1	0.98	0.05	40,40,40,40	0
56	MG	DA	3503	1/1	0.98	0.06	58,58,58,58	0
56	MG	DA	3189	1/1	0.98	0.06	42,42,42,42	0
56	MG	BA	3764	1/1	0.98	0.10	26,26,26,26	0
56	MG	BA	3383	1/1	0.98	0.19	49,49,49,49	0
56	MG	BA	3052	1/1	0.98	0.05	34,34,34,34	0
56	MG	BA	3767	1/1	0.98	0.07	31,31,31,31	0
56	MG	BA	3093	1/1	0.98	0.06	39,39,39,39	0
56	MG	BA	3425	1/1	0.98	0.07	31,31,31,31	0
56	MG	BF	309	1/1	0.98	0.13	40,40,40,40	0
56	MG	BA	3017	1/1	0.98	0.05	32,32,32,32	0
56	MG	DA	3198	1/1	0.98	0.14	32,32,32,32	0
56	MG	BA	3320	1/1	0.98	0.04	28,28,28,28	0
56	MG	DA	3351	1/1	0.98	0.04	40,40,40,40	0
56	MG	BA	3237	1/1	0.98	0.15	43,43,43,43	0
56	MG	BA	3029	1/1	0.98	0.13	44,44,44,44	0
56	MG	BA	3292	1/1	0.98	0.11	26,26,26,26	0
56	MG	BA	3433	1/1	0.98	0.06	48,48,48,48	0
56	MG	DA	3521	1/1	0.98	0.13	29,29,29,29	0
56	MG	DA	3356	1/1	0.98	0.05	47,47,47,47	0
56	MG	AA	3212	1/1	0.98	0.10	33,33,33,33	0
56	MG	BA	3158	1/1	0.98	0.05	47,47,47,47	0
58	SF4	CD	302	8/8	0.98	0.05	51,66,73,73	0
59	ZN	B4	501	1/1	0.98	0.05	86,86,86,86	0
56	MG	BA	3357	1/1	0.98	0.11	29,29,29,29	0
56	MG	DA	3004	1/1	0.98	0.11	18,18,18,18	0
59	ZN	D6	501	1/1	0.98	0.05	70,70,70,70	0
56	MG	DA	3005	1/1	0.98	0.11	39,39,39,39	0
56	MG	DA	3281	1/1	0.98	0.09	39,39,39,39	0
56	MG	BA	3437	1/1	0.98	0.04	55,55,55,55	0
56	MG	BA	3743	1/1	0.99	0.04	18,18,18,18	0
56	MG	BA	3744	1/1	0.99	0.08	27,27,27,27	0
56	MG	BA	3190	1/1	0.99	0.34	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	3291	1/1	0.99	0.12	26,26,26,26	0
56	MG	AV	101	1/1	0.99	0.04	47,47,47,47	0
56	MG	BU	207	1/1	0.99	0.20	22,22,22,22	0
56	MG	CA	3091	1/1	0.99	0.11	45,45,45,45	0
56	MG	B7	101	1/1	0.99	0.06	35,35,35,35	0
56	MG	BA	3426	1/1	0.99	0.07	29,29,29,29	0
56	MG	BA	3427	1/1	0.99	0.05	22,22,22,22	0
56	MG	AA	3123	1/1	0.99	0.07	25,25,25,25	0
56	MG	BA	3517	1/1	0.99	0.11	26,26,26,26	0
56	MG	BA	3024	1/1	0.99	0.14	19,19,19,19	0
56	MG	AA	3142	1/1	0.99	0.05	38,38,38,38	0
56	MG	DD	306	1/1	0.99	0.19	35,35,35,35	0
56	MG	BA	3410	1/1	0.99	0.05	33,33,33,33	0
56	MG	BA	3376	1/1	0.99	0.07	23,23,23,23	0
56	MG	DA	3327	1/1	0.99	0.03	32,32,32,32	0
56	MG	BA	3782	1/1	0.99	0.13	48,48,48,48	0
56	MG	DA	3525	1/1	0.99	0.04	33,33,33,33	0
56	MG	AA	3133	1/1	0.99	0.06	35,35,35,35	0
56	MG	BA	3169	1/1	0.99	0.12	28,28,28,28	0
56	MG	BD	310	1/1	0.99	0.06	45,45,45,45	0
56	MG	BA	3414	1/1	0.99	0.08	26,26,26,26	0
56	MG	BA	3759	1/1	0.99	0.06	29,29,29,29	0
56	MG	BA	3133	1/1	0.99	0.05	43,43,43,43	0
56	MG	DA	3335	1/1	0.99	0.03	41,41,41,41	0
56	MG	DA	3336	1/1	0.99	0.03	30,30,30,30	0
56	MG	BA	3122	1/1	0.99	0.04	42,42,42,42	0
56	MG	BA	3072	1/1	0.99	0.06	42,42,42,42	0
56	MG	AA	3223	1/1	0.99	0.04	52,52,52,52	0
56	MG	BE	306	1/1	0.99	0.10	15,15,15,15	0
56	MG	DA	3026	1/1	0.99	0.06	24,24,24,24	0
58	SF4	AD	501	8/8	0.99	0.06	52,60,68,71	0
56	MG	DA	3231	1/1	0.99	0.03	54,54,54,54	0
59	ZN	AN	501	1/1	0.99	0.05	65,65,65,65	0
56	MG	AA	3156	1/1	0.99	0.04	65,65,65,65	0
59	ZN	B5	105	1/1	0.99	0.10	52,52,52,52	0
56	MG	BA	3463	1/1	0.99	0.07	34,34,34,34	0
59	ZN	DY	501	1/1	0.99	0.04	88,88,88,88	0
56	MG	BA	3004	1/1	0.99	0.02	25,25,25,25	0
59	ZN	D5	501	1/1	0.99	0.05	57,57,57,57	0
56	MG	DA	3235	1/1	0.99	0.04	29,29,29,29	0
56	MG	BA	3005	1/1	0.99	0.06	41,41,41,41	0
56	MG	BA	3289	1/1	0.99	0.05	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	BB	3011	1/1	0.99	0.05	56,56,56,56	0
59	ZN	B9	501	1/1	1.00	0.04	47,47,47,47	0
56	MG	BA	3455	1/1	1.00	0.05	28,28,28,28	0
56	MG	AA	3135	1/1	1.00	0.03	34,34,34,34	0
56	MG	BA	3553	1/1	1.00	0.09	49,49,49,49	0
56	MG	BA	3654	1/1	1.00	0.04	24,24,24,24	0
59	ZN	BY	501	1/1	1.00	0.03	60,60,60,60	0
56	MG	DA	3506	1/1	1.00	0.07	37,37,37,37	0
56	MG	BA	3268	1/1	1.00	0.09	40,40,40,40	0
59	ZN	B6	102	1/1	1.00	0.03	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.