



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 06:21 am BST

PDB ID : 4W2H  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with pactamycin (co-crystallized), mRNA and deacylated tRNA in the P site  
Authors : Polikanov, Y.S.; Osterman, I.A.; Szal, T.; Tashlitsky, V.N.; Serebryakova, M.V.; Kusochev, P.; Bulkley, D.; Malanicheva, I.A.; Efimenko, T.A.; Efremenkova, O.V.; Konevega, A.L.; Shaw, K.J.; Bogdanov, A.A.; Rodnina, M.V.; Dontsova, O.A.; Mankin, A.S.; Steitz, T.A.; Sergiev, P.V.  
Deposited on : 2014-09-12  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

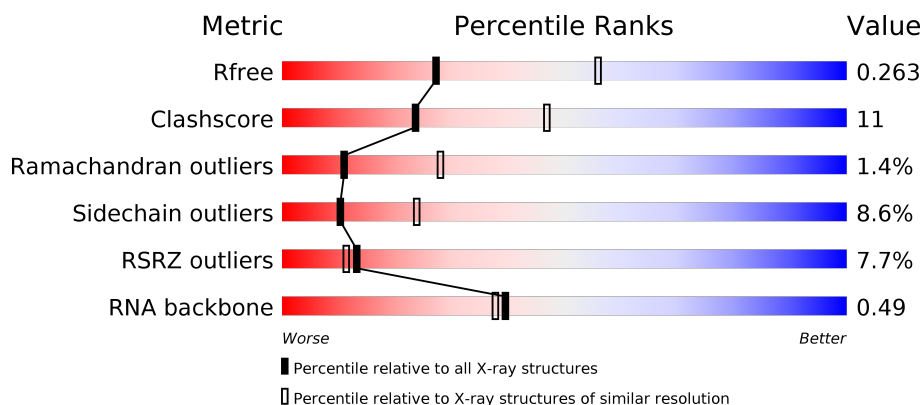
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	<div> <div>0%</div> <div> <div></div> <div>45%</div> <div>40%</div> <div>12%</div> <div>..</div> </div> </div>
1	CA	1521	<div> <div>2%</div> <div> <div></div> <div>44%</div> <div>40%</div> <div>14%</div> <div>..</div> </div> </div>
2	AB	256	<div> <div>4%</div> <div> <div></div> <div>43%</div> <div>36%</div> <div>12%</div> <div>10%</div> </div> </div>
2	CB	256	<div> <div>23%</div> <div> <div></div> <div>43%</div> <div>39%</div> <div>8%</div> <div>10%</div> </div> </div>

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





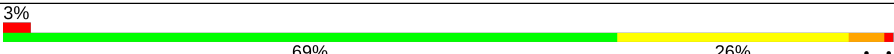
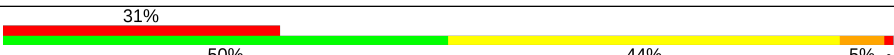
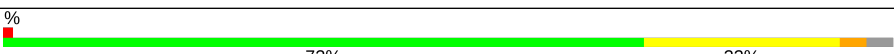
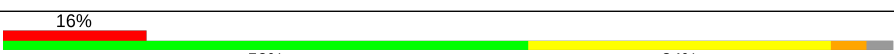
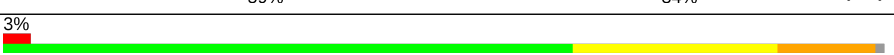

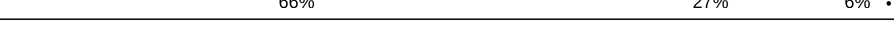


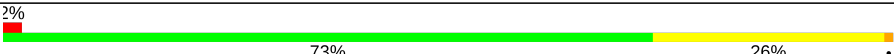

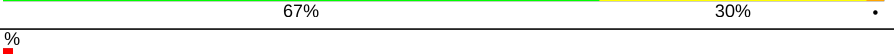




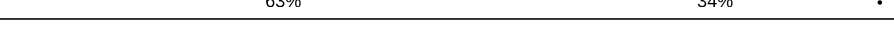


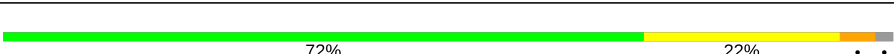

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AX	77	
23	CX	77	
24	AY	76	
24	CY	76	
25	BA	2915	
25	DA	2915	
26	BB	121	
26	DB	121	
27	BD	276	
27	DD	276	

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

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

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	3166	-	-	-	X
56	MG	BA	3048	-	-	-	X
56	MG	BE	306	-	-	-	X
56	MG	CA	3174	-	-	-	X
56	MG	DA	3640	-	-	-	X
56	MG	DA	3647	-	-	-	X
56	MG	DA	3655	-	-	-	X
57	PCY	CA	3176	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 290807 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	1497	Total	C	N	O	P	0	0	0
			32183	14323	5965	10398	1497			
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	120	Total	C	N	O	S		
			937	578	194	163	2	0	0
13	CM	118	Total	C	N	O	S		
			920	566	191	161	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	8	Total	C	N	O	P	0	0	0
			169	76	29	56	8			
22	CV	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	18	Total	C	N	O	P	0	0	0
			385	171	71	125	18			
24	CY	5	Total	C	N	O	P	0	0	0
			104	47	19	33	5			

- 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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	69	Total	C	N	O	S	0	0	0
			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
			511	328	99	82	2			
54	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B4	1	Total	Mg	0	0
			1	1		
56	BA	814	Total	Mg	0	0
			814	814		
56	CA	175	Total	Mg	0	0
			175	175		
56	DQ	3	Total	Mg	0	0
			3	3		
56	D3	1	Total	Mg	0	0
			1	1		
56	DF	5	Total	Mg	0	0
			5	5		
56	B8	2	Total	Mg	0	0
			2	2		
56	BE	7	Total	Mg	0	0
			7	7		
56	DU	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AN	1	Total 1	Mg 1	0	0
56	BP	4	Total 4	Mg 4	0	0
56	AX	9	Total 9	Mg 9	0	0
56	DN	1	Total 1	Mg 1	0	0
56	DD	8	Total 8	Mg 8	0	0
56	B5	4	Total 4	Mg 4	0	0
56	BB	22	Total 22	Mg 22	0	0
56	D8	1	Total 1	Mg 1	0	0
56	AE	3	Total 3	Mg 3	0	0
56	DG	1	Total 1	Mg 1	0	0
56	B9	1	Total 1	Mg 1	0	0
56	BF	9	Total 9	Mg 9	0	0
56	BX	2	Total 2	Mg 2	0	0
56	B2	1	Total 1	Mg 1	0	0
56	AA	190	Total 190	Mg 190	0	0
56	BQ	4	Total 4	Mg 4	0	0
56	CX	2	Total 2	Mg 2	0	0
56	DV	3	Total 3	Mg 3	0	0
56	B6	2	Total 2	Mg 2	0	0
56	AM	1	Total 1	Mg 1	0	0
56	BU	9	Total 9	Mg 9	0	0

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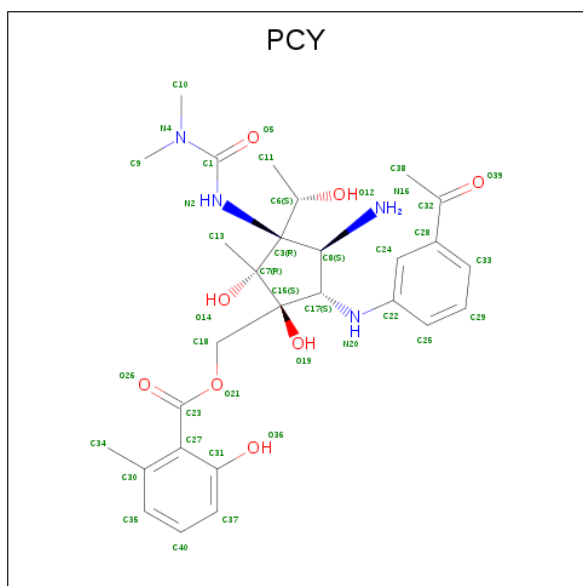
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DR	1	Total 1	Mg 1	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BN	7	Total 7	Mg 7	0	0
56	CT	1	Total 1	Mg 1	0	0
56	D0	2	Total 2	Mg 2	0	0
56	BG	2	Total 2	Mg 2	0	0
56	BY	3	Total 3	Mg 3	0	0
56	DE	5	Total 5	Mg 5	0	0
56	B3	1	Total 1	Mg 1	0	0
56	CJ	1	Total 1	Mg 1	0	0
56	BR	3	Total 3	Mg 3	0	0
56	DA	674	Total 674	Mg 674	0	0
56	DP	2	Total 2	Mg 2	0	0
56	DW	2	Total 2	Mg 2	0	0
56	B7	5	Total 5	Mg 5	0	0
56	CF	1	Total 1	Mg 1	0	0
56	BV	4	Total 4	Mg 4	0	0
56	DO	1	Total 1	Mg 1	0	0
56	BO	1	Total 1	Mg 1	0	0
56	AQ	1	Total 1	Mg 1	0	0
56	D1	1	Total 1	Mg 1	0	0

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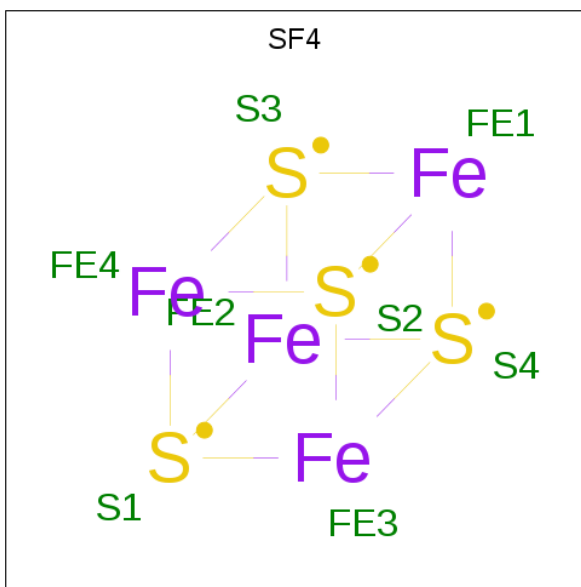
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BZ	2	Total	Mg	0	0
			2	2		
56	DY	1	Total	Mg	0	0
			1	1		
56	BD	9	Total	Mg	0	0
			9	9		
56	B0	5	Total	Mg	0	0
			5	5		
56	CE	2	Total	Mg	0	0
			2	2		
56	BW	4	Total	Mg	0	0
			4	4		
56	AF	1	Total	Mg	0	0
			1	1		
56	DB	10	Total	Mg	0	0
			10	10		

- Molecule 57 is Pactamycin (three-letter code: PCY) (formula:  $C_{28}H_{38}N_4O_8$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	AA	1	Total	C	N	O	0	0
			40	28	4	8		
57	CA	1	Total	C	N	O	0	0
			40	28	4	8		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: 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 (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B5	1	Total	Zn	0	0
			1	1		
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	BY	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	DY	1	Total	Zn	0	0
			1	1		
59	D5	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	D6	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D9	1	Total 1	Zn 1	0	0
59	B6	1	Total 1	Zn 1	0	0

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

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	175	Total 175	O 175	0	0
61	AJ	2	Total 2	O 2	0	0
61	AL	1	Total 1	O 1	0	0
61	AM	1	Total 1	O 1	0	0
61	AO	1	Total 1	O 1	0	0
61	AV	1	Total 1	O 1	0	0
61	AX	8	Total 8	O 8	0	0
61	BA	1294	Total 1294	O 1294	0	0
61	BB	34	Total 34	O 34	0	0
61	BD	16	Total 16	O 16	0	0
61	BE	12	Total 12	O 12	0	0
61	BF	7	Total 7	O 7	0	0
61	BG	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BI	1	Total 1	O 1	0	0
61	BN	1	Total 1	O 1	0	0
61	BO	4	Total 4	O 4	0	0
61	BP	15	Total 15	O 15	0	0
61	BQ	5	Total 5	O 5	0	0
61	BR	1	Total 1	O 1	0	0
61	BU	2	Total 2	O 2	0	0
61	BV	2	Total 2	O 2	0	0
61	BW	3	Total 3	O 3	0	0
61	BX	5	Total 5	O 5	0	0
61	B0	4	Total 4	O 4	0	0
61	B1	1	Total 1	O 1	0	0
61	B3	1	Total 1	O 1	0	0
61	B5	4	Total 4	O 4	0	0
61	B6	1	Total 1	O 1	0	0
61	B7	1	Total 1	O 1	0	0
61	B8	10	Total 10	O 10	0	0
61	CA	137	Total 137	O 137	0	0
61	CD	1	Total 1	O 1	0	0
61	CJ	2	Total 2	O 2	0	0
61	CL	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CN	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0
61	CX	2	Total 2	O 2	0	0
61	DA	924	Total 924	O 924	0	0
61	DB	8	Total 8	O 8	0	0
61	DD	18	Total 18	O 18	0	0
61	DE	9	Total 9	O 9	0	0
61	DF	5	Total 5	O 5	0	0
61	DN	1	Total 1	O 1	0	0
61	DO	1	Total 1	O 1	0	0
61	DP	14	Total 14	O 14	0	0
61	DR	1	Total 1	O 1	0	0
61	DT	1	Total 1	O 1	0	0
61	DU	3	Total 3	O 3	0	0
61	DV	1	Total 1	O 1	0	0
61	DW	1	Total 1	O 1	0	0
61	DX	1	Total 1	O 1	0	0
61	DY	1	Total 1	O 1	0	0
61	D0	7	Total 7	O 7	0	0
61	D1	1	Total 1	O 1	0	0
61	D3	1	Total 1	O 1	0	0

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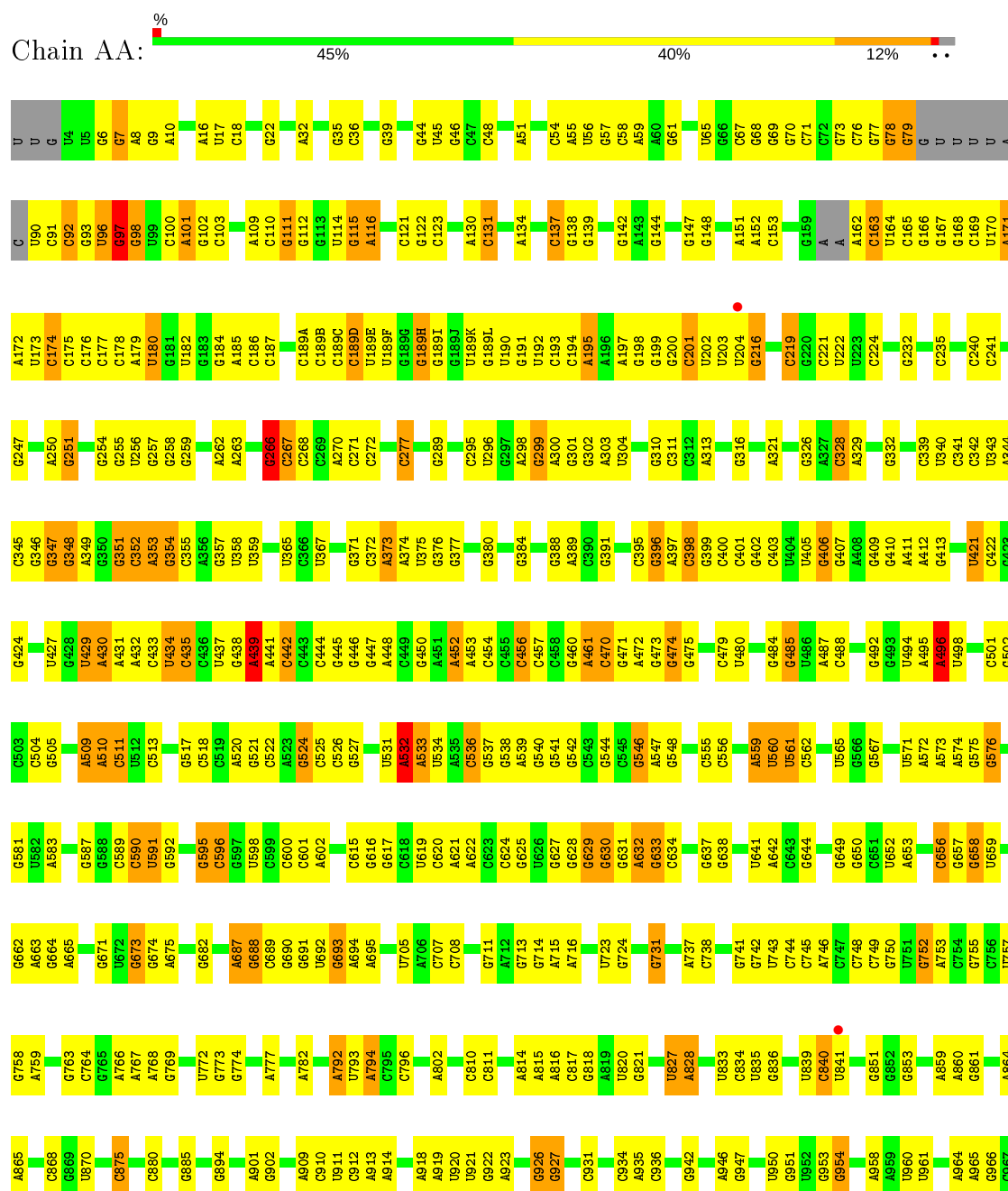
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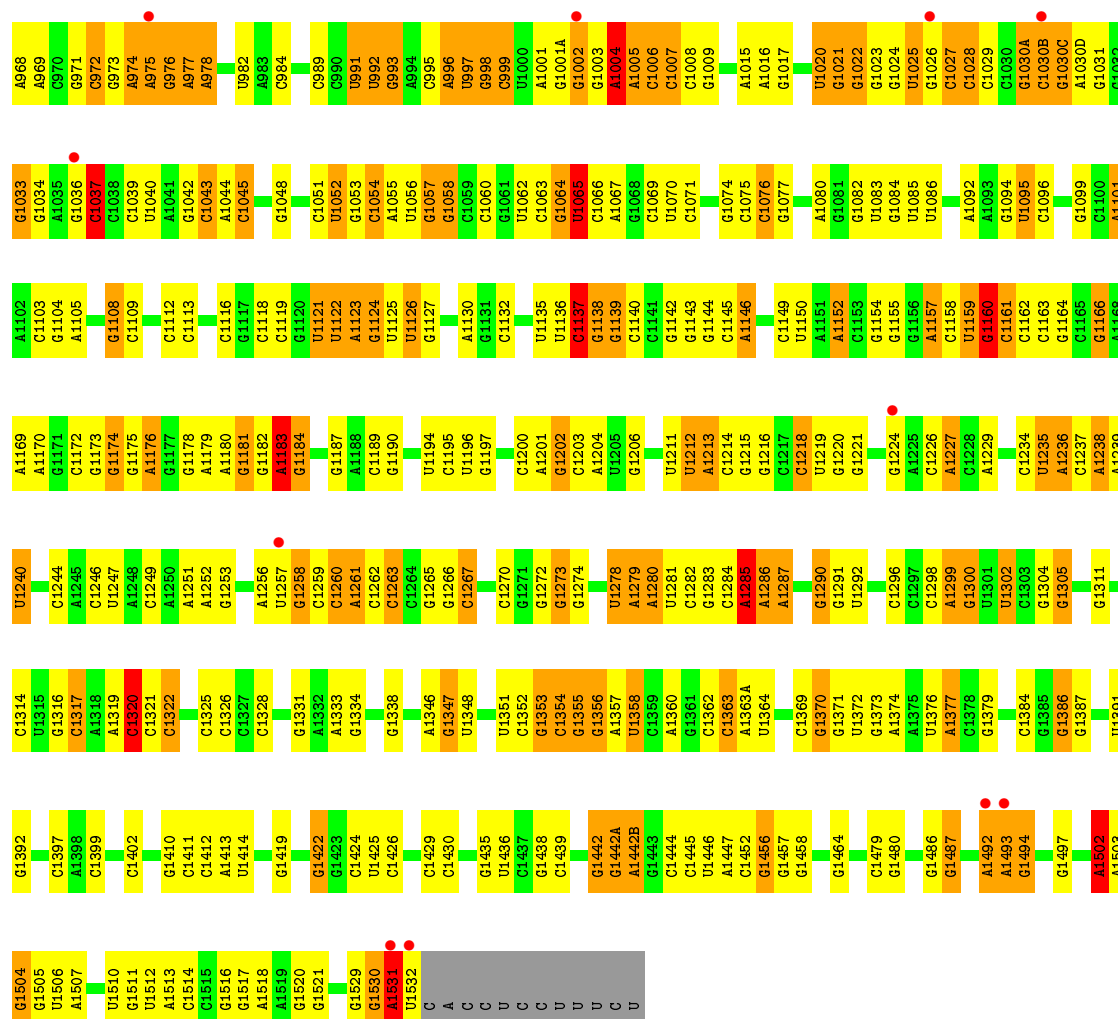
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	D8	4	Total	O	0	0
			4	4		

### 3 Residue-property plots [i](#)

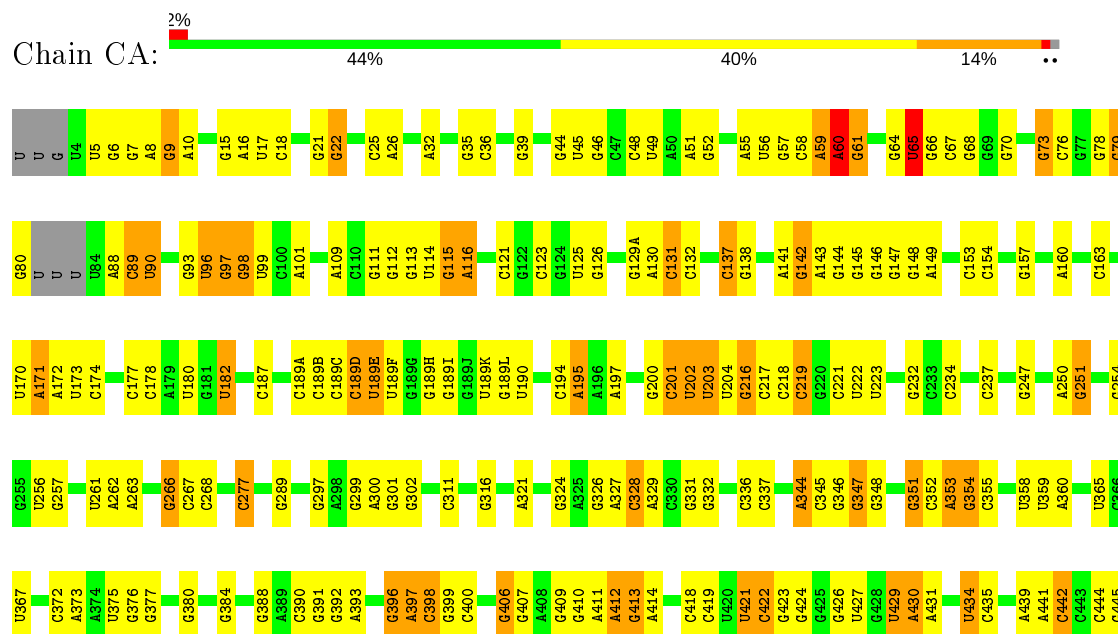
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: 16S Ribosomal RNA






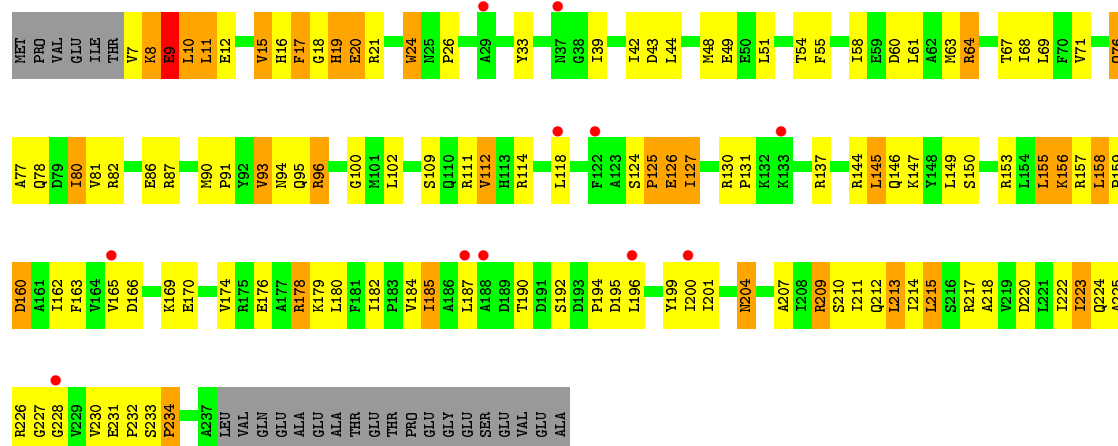
• Molecule 1: 16S Ribosomal RNA



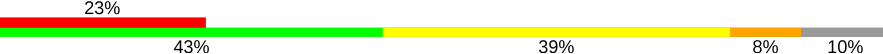
G1470	U1485	G1486	G1487	A1492	A1493	G1494	U1495	G1496	G1497	U1498	A1499	A1502	A1503	G1504	U1505	G1506	A1507	G1508	G1509	U1510	G1511	U1512	C1513	C1514	G1517	G1520	G1521	U1528	G1529	G1530	A1531	U1532	C	A	C	C	U	C	C	U	U	U	U	U	C	U																																																									
A1375	U1376	A1377	G1378	G1379	U1380	U1381	U1382	G1383	G1384	G1385	G1386	G1387	G1388	G1392	G1397	A1398	G1399	G1400	G1401	G1402	G1403	G1410	G1411	G1412	G1413	U1414	G1419	G1422	G1423	G1424	U1425	G1426	U1427	G1428	C1429	G1435	U1436	U1437	U1438	C1439	G1442	A1442A	A1442B	G1443	C1444	C1445	U1446	A1447	G1452	G1456	C1465	C1466	G1469																																																		
G1305	G1309	G1310	G1311	G1312	U1313	C1314	C1315	G1316	G1317	G1318	A1319	G1320	C1321	C1322	G1323	A1324	C1325	G1326	G1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	G1338	A1339	C1342	A1346	G1347	U1348	C1352	G1353	C1354	G1355	A1356	U1357	U1358	C1359	A1360	G1361	G1362	C1363	U1364	C1367	G1370	G1371	U1372	G1373	A1374																																																				
U1240	C1244	A1245	C1246	G1249	A1250	A1251	A1252	G1253	G1254	G1255	A1256	U1257	G1258	G1259	G1260	A1261	C1262	G1263	C1264	G1265	G1266	G1267	A1268	A1269	C1270	G1271	G1272	G1273	G1274	C1277	U1278	A1279	A1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	A1288	A1289	G1290	G1291	U1292	G1293	C1296	G1297	C1298	A1299	G1300	U1301	U1302	C1303	A1238	G1304																																															
A1170	G1171	G1172	G1173	G1174	G1175	A1176	G1177	G1178	A1179	A1180	G1181	G1182	A1183	G1184	G1185	G1186	G1187	G1190	U1196	G1197	G1198	G1199	C1200	A1201	G1202	C1203	A1204	U1205	G1206	C1209	G1210	U1211	U1212	A1213	C1214	G1215	G1216	G1217	G1218	U1219	G1220	G1221	G1222	G1223	G1224	A1225	C1226	A1227	C1228	G1234	U1235	A1236	C1237	A1238	A1239																																																
G1106	C1107	G1108	C1109	G1113	C1114	C1115	G1116	G1117	G1118	C1119	U1122	A1123	G1124	U1125	U1126	G1127	C1128	C1129	A1130	G1131	C1132	G1133	G1134	U1135	U1136	C1137	G1138	G1139	C1140	C1141	G1142	G1143	G1144	C1145	A1146	C1147	U1148	C1149	U1150	A1151	A1152	C1153	G1154	G1155	G1156	A1157	C1158	U1159	G1160	C1161	C1162	G1163	G1164	C1165	A1166	A1168	A1169																																														
G1033	G1034	A1035	G1036	G1037	C1038	C1039	U1040	U1041	C1042	G1043	C1044	C1045	G1048	U1049	G1050	C1051	U1052	G1053	G1054	A1055	U1056	G1057	G1058	G1059	C1060	U1061	U1062	C1063	G1064	U1065	C1066	A1067	G1074	G1075	C1076	G1077	A1080	G1081	G1084	U1085	U1086	A1093	G1094	U1095	C1096	C1097	G1098	G1099	G1100	A1101	A1102	C1103	G1104	A1105																																																	
A977	A978	C979	G980	U981	U982	A983	C984	C985	A986	G987	G988	C989	C990	U991	U992	G993	A996	U997	G998	C999	U1000	A1001	G1002	C1003	A1004	U1005	C1006	C1007	C1008	U1009	G1010	G1011	U1012	G1013	A1014	A1015	A1016	G1017	C1018	C1019	U1020	G1021	G1022	G1023	G1024	U1025	G1026	C1027	C1028	C1029	G1030	C1030A	C1030B	G1030C	A1030D	G1031	C1032																																														
C893	G902	G906	A909	C810	C811	C812	U813	A814	A815	A816	C817	U820	G821	C826	U827	A828	G829	U833	C834	U835	G836	G837	U838	G839	U840	U841	C848	G851	G852	G853	C854	C857	G858	A859	U863	A864	A865	C868	G869	U870	C875	A869	C880	G885	G890	U891	A892	G976	G977	G978	G979	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997																																			
G713	G714	A715	A716	C719	U723	G724	A728	G729	G730	G731	U735	G736	A737	C738	U739	G741	G742	U743	C744	C748	G749	U750	U751	G752	A753	G754	G755	G756	U757	G758	A759	G765	A766	A767	A768	G769	C770	G771	U772	G773	A777	A782	C783	G784	A790	G791	A792	U793	G540	G541	G542	C543	G544	G545	G546	A547	C556	G557	G558	A559	U560	U561	U565	G566	G567	U571	A572	A573	G576	G577	C578	G579	U498	A499	A496	U498	C501	G502	C503	G504	G505	A509	A510	C511	U512	C513	C518	C519	A520	C521	C522	C601	A602	G603	G604	U605	U631	A632	A533	C636	G637	G616	G617

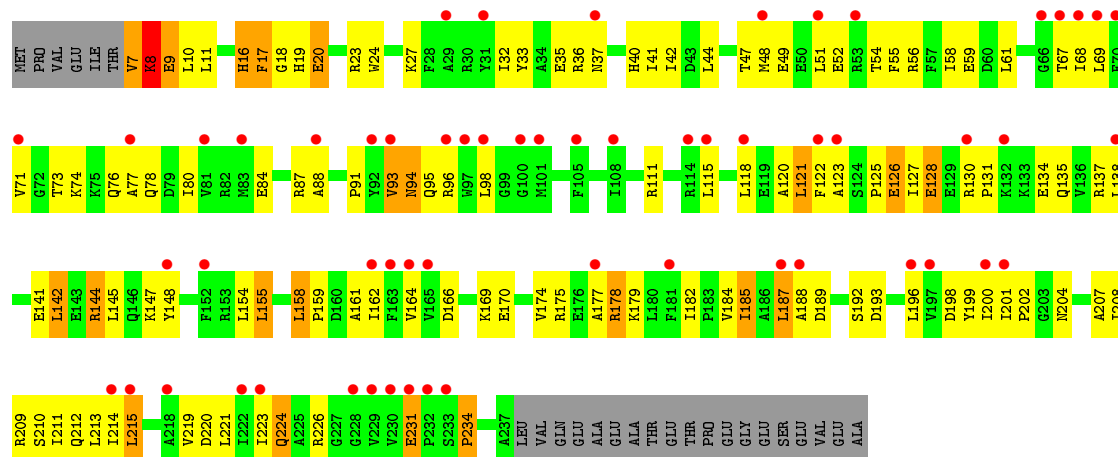
• Molecule 2: 30S Ribosomal Protein S2

Chain AB: 



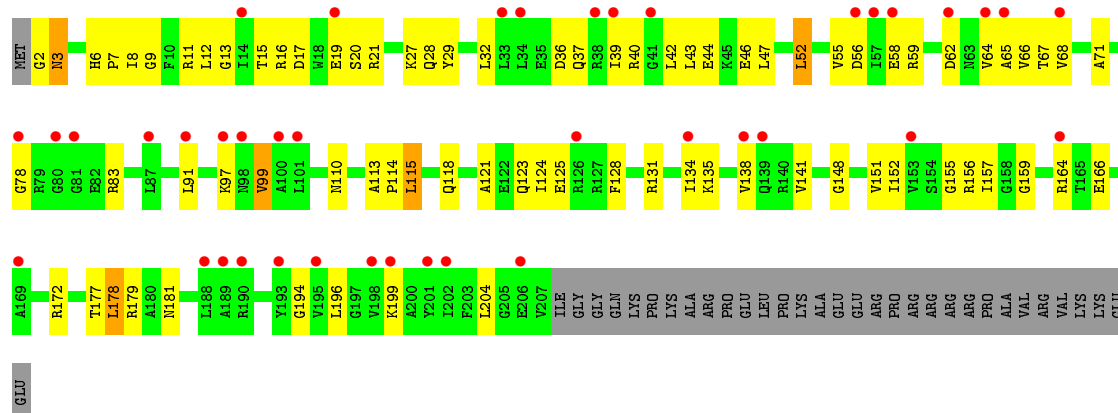
• Molecule 2: 30S Ribosomal Protein S2

Chain CB: 

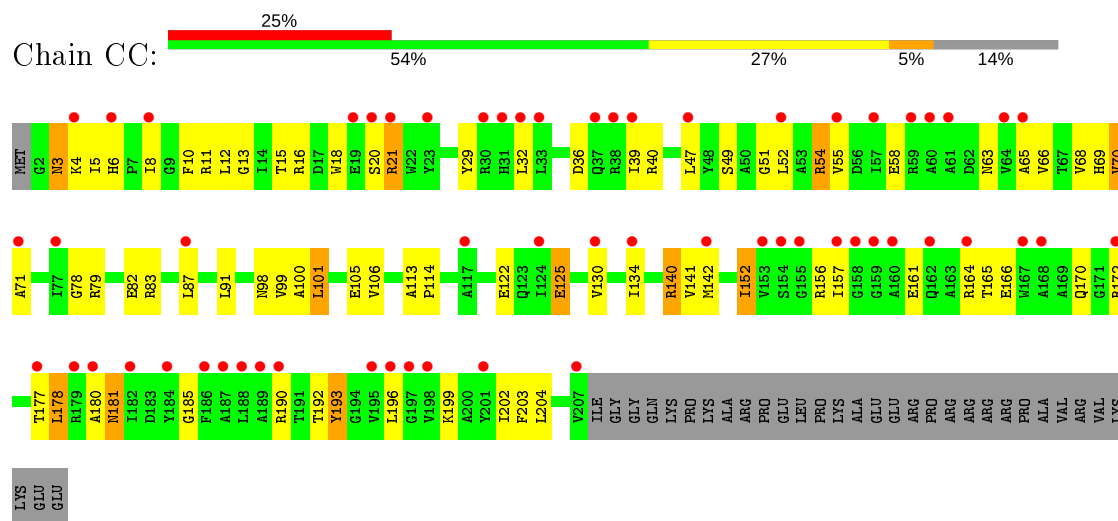


• Molecule 3: 30S Ribosomal Protein S3

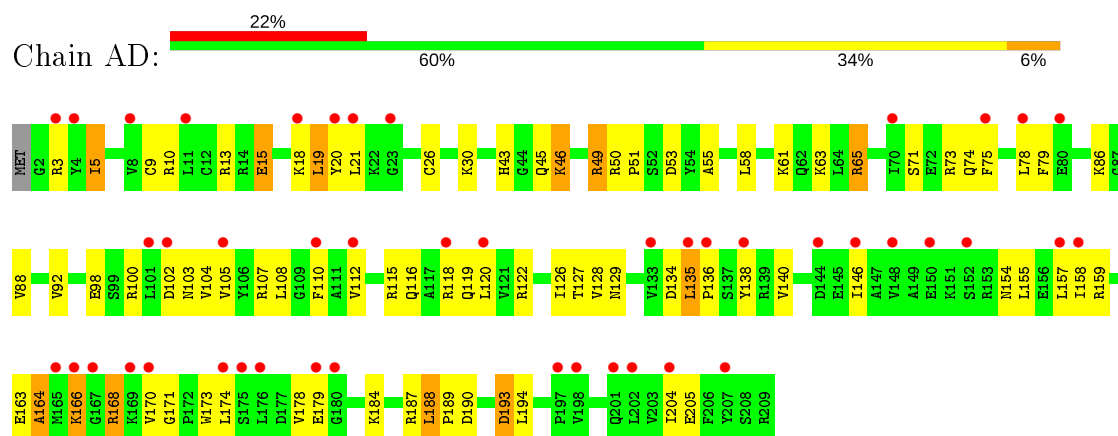
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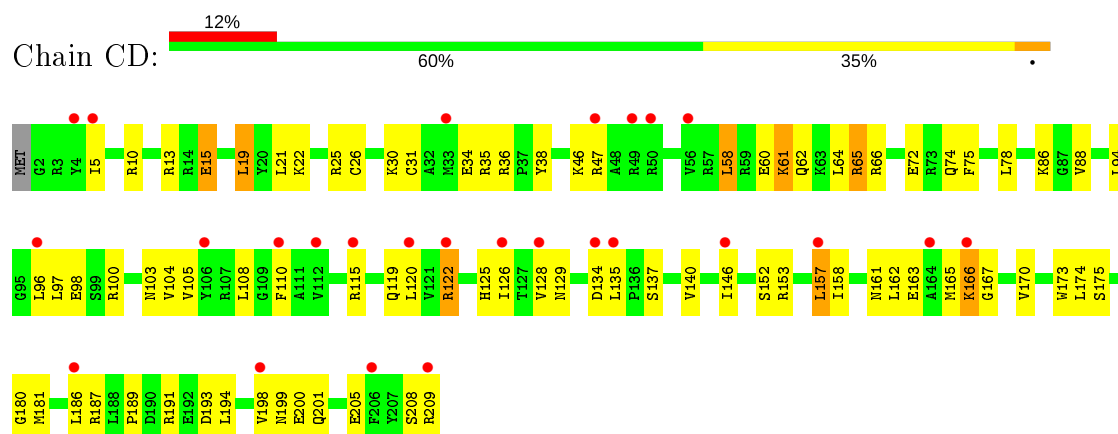
- Molecule 3: 30S Ribosomal Protein S3



- Molecule 4: 30S Ribosomal Protein S4

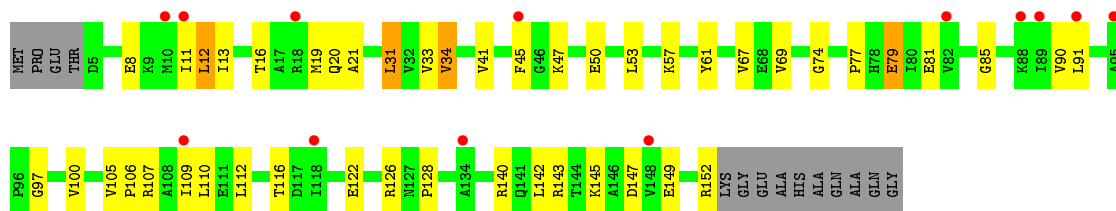


- Molecule 4: 30S Ribosomal Protein S4

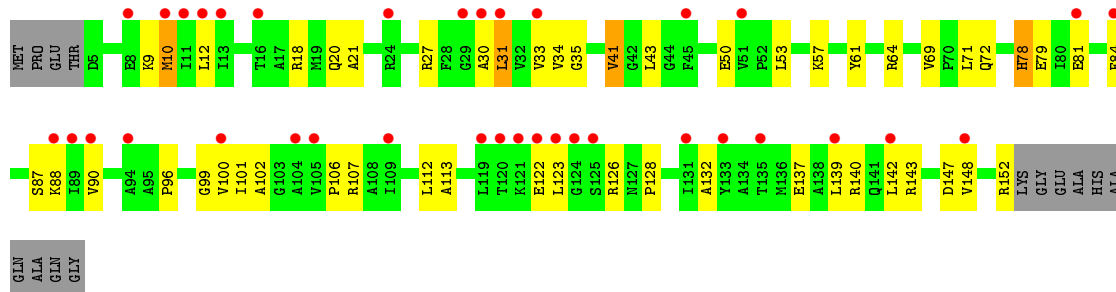


- Molecule 5: 30S Ribosomal Protein S5

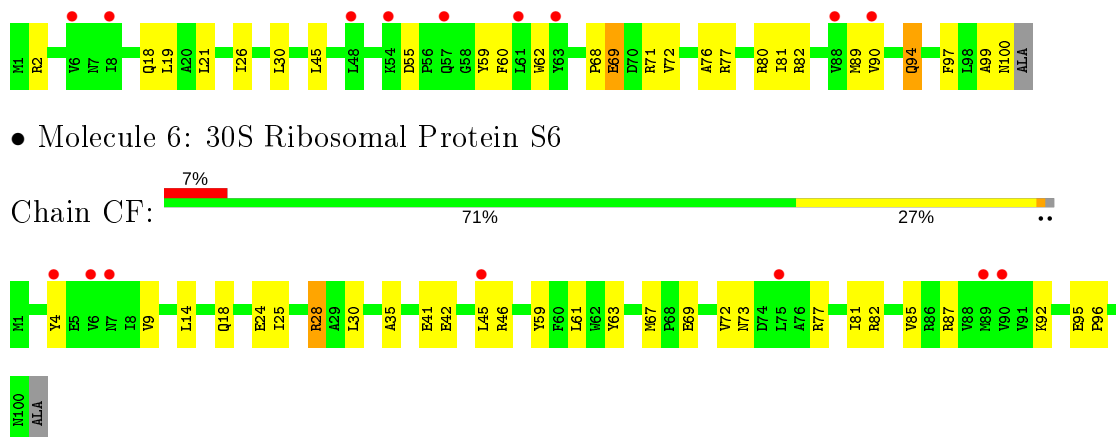
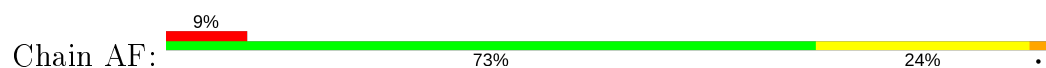




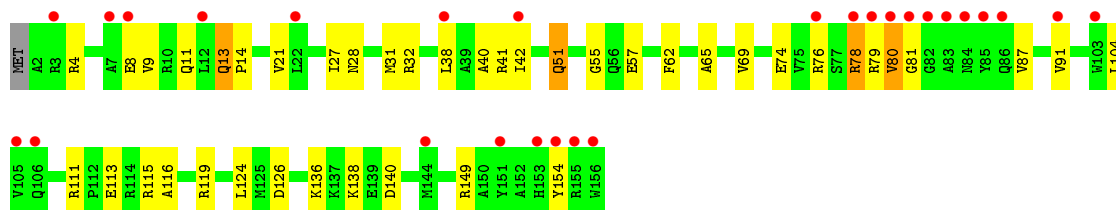
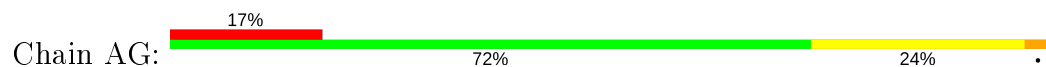
• Molecule 5: 30S Ribosomal Protein S5



• Molecule 6: 30S Ribosomal Protein S6

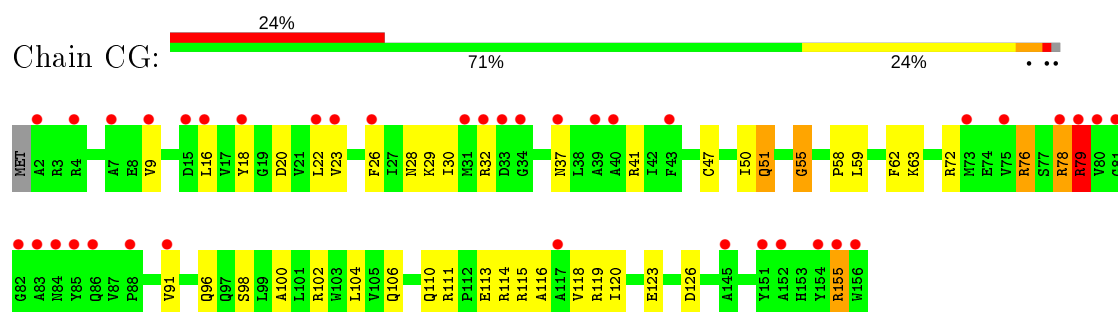


• Molecule 7: 30S Ribosomal Protein S7

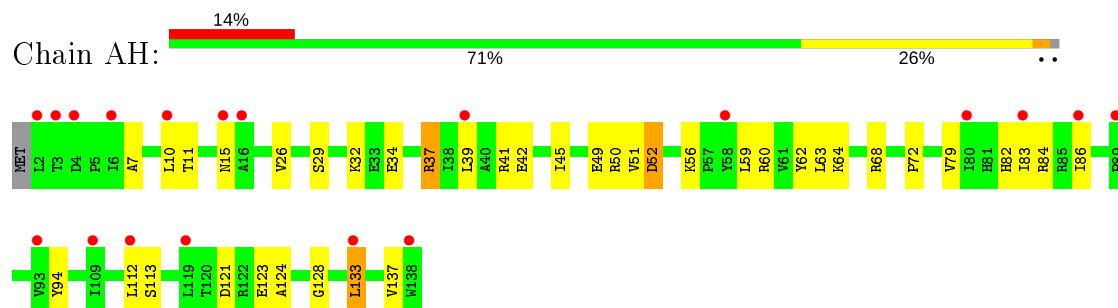


• Molecule 7: 30S Ribosomal Protein S7

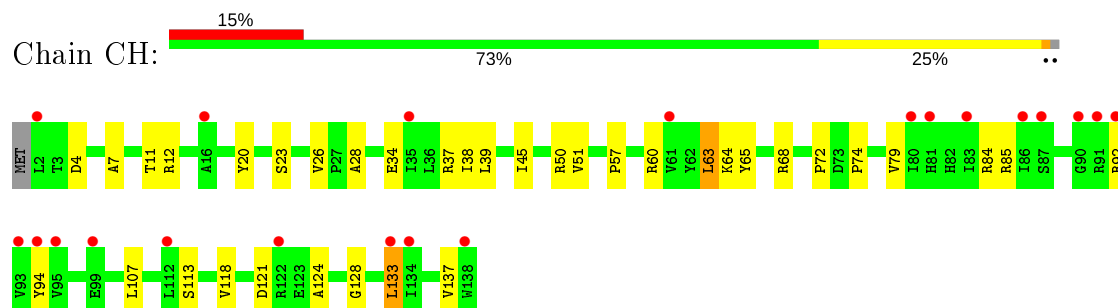




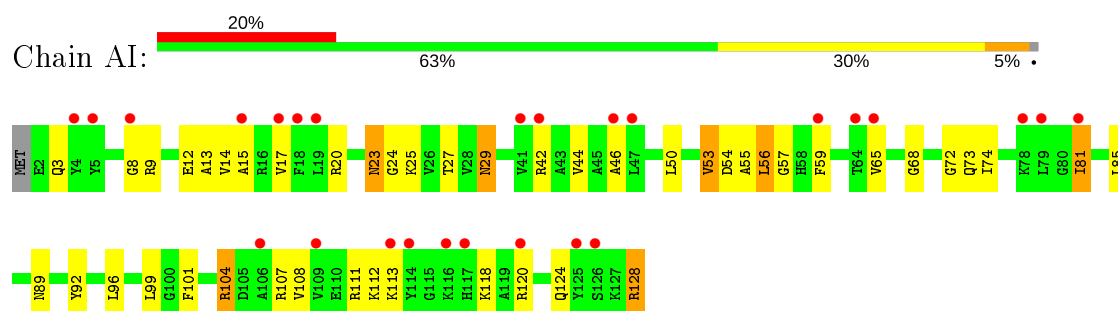
- Molecule 8: 30S Ribosomal Protein S8



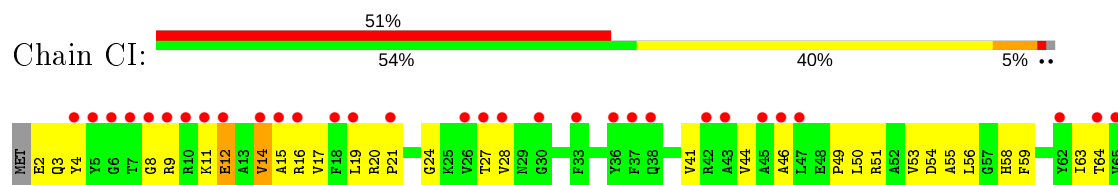
- Molecule 8: 30S Ribosomal Protein S8

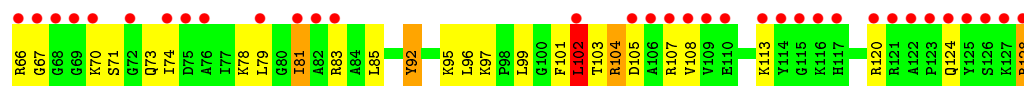


- Molecule 9: 30S Ribosomal Protein S9

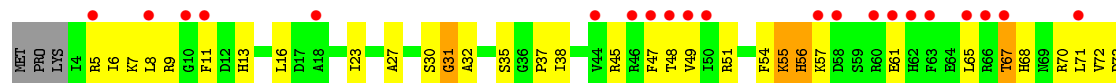


- Molecule 9: 30S Ribosomal Protein S9

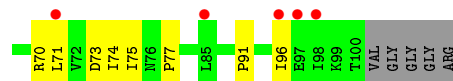
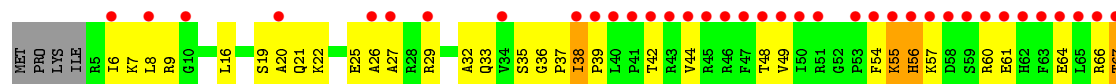
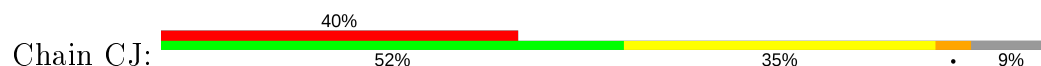




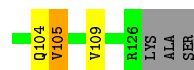
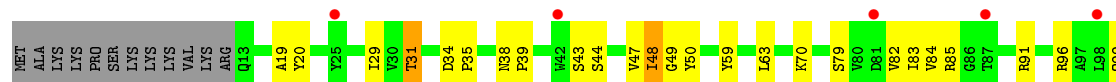
• Molecule 10: 30S Ribosomal Protein S10



• Molecule 10: 30S Ribosomal Protein S10



• Molecule 11: 30S Ribosomal Protein S11

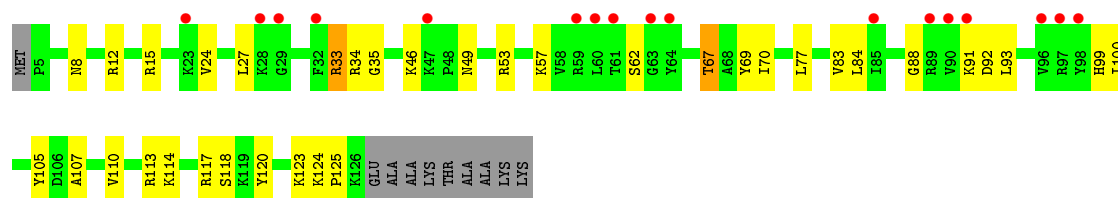


• Molecule 11: 30S Ribosomal Protein S11

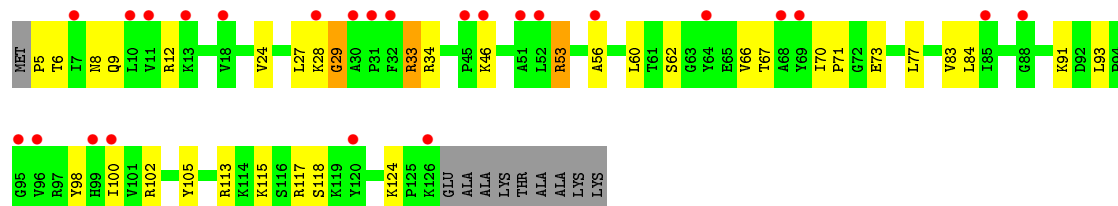


• Molecule 12: 30S Ribosomal Protein S12

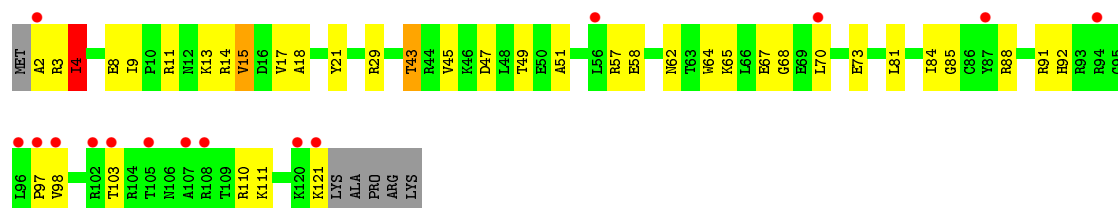




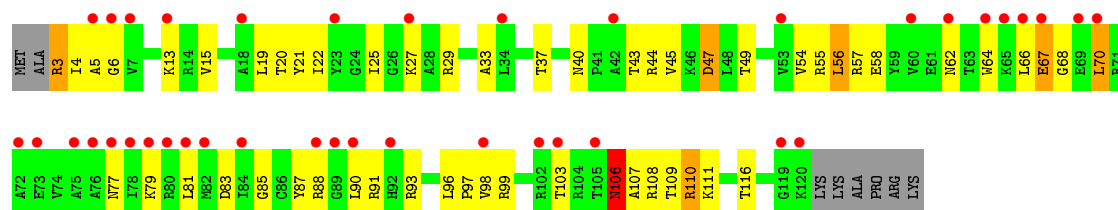
• Molecule 12: 30S Ribosomal Protein S12



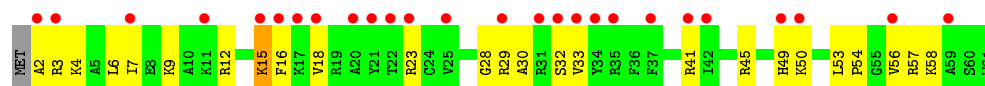
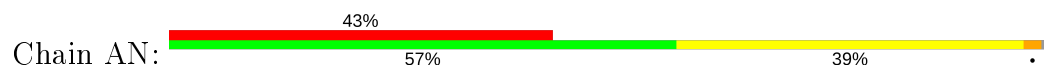
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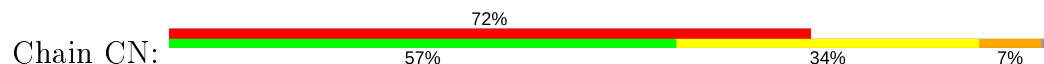
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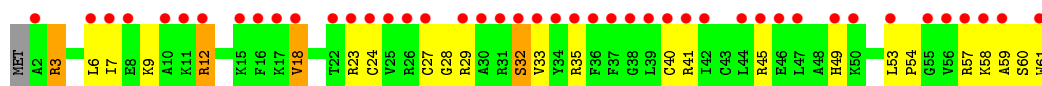


• Molecule 14: 30S Ribosomal Protein S14

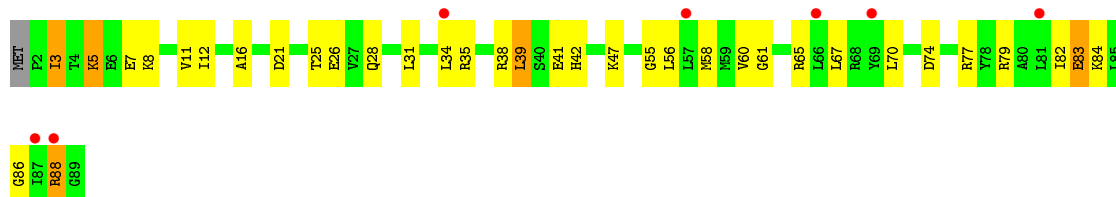


• Molecule 14: 30S Ribosomal Protein S14

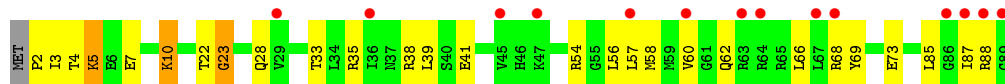




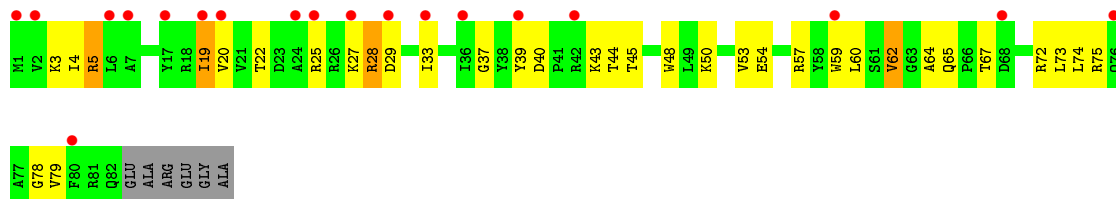
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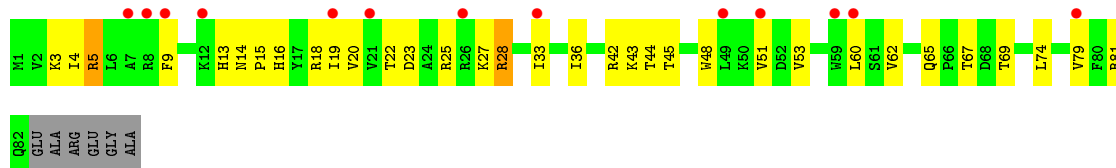
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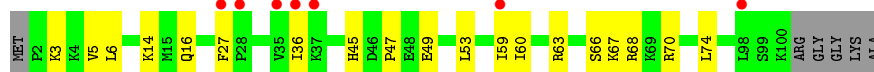
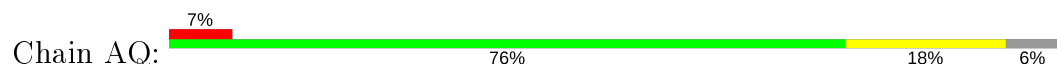
• Molecule 16: 30S Ribosomal Protein S16



• Molecule 16: 30S Ribosomal Protein S16

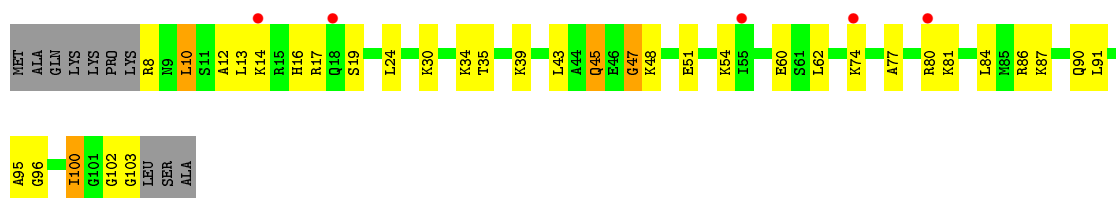


• Molecule 17: 30S Ribosomal Protein S17

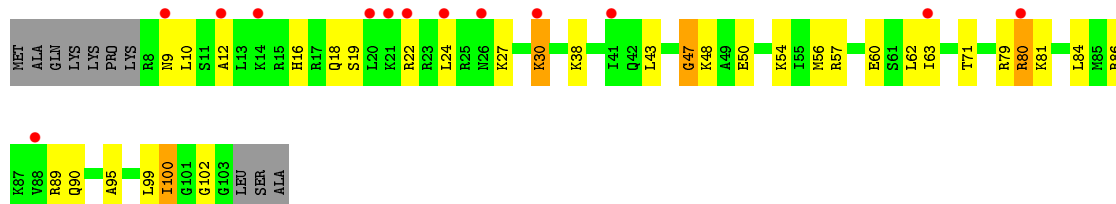


• Molecule 17: 30S Ribosomal Protein S17

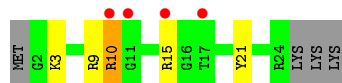




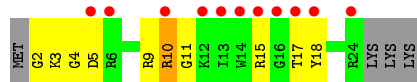
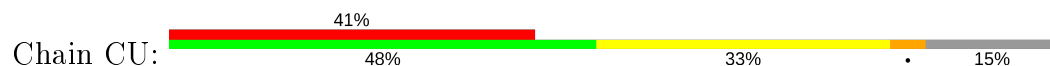
- Molecule 20: 30S Ribosomal Protein S20



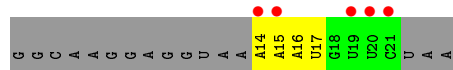
- Molecule 21: 30S Ribosomal Protein THX



- Molecule 21: 30S Ribosomal Protein THX



- Molecule 22: mRNA

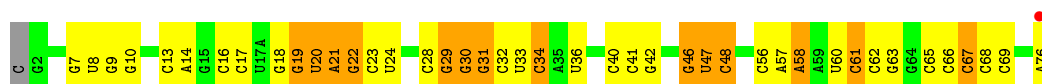


- Molecule 22: mRNA



- Molecule 23: P-site tRNA

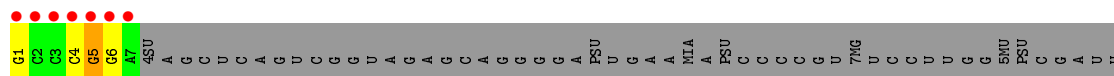




• Molecule 23: P-site tRNA



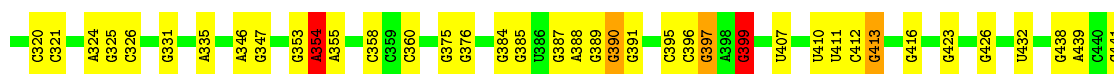
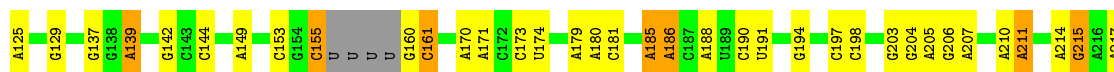
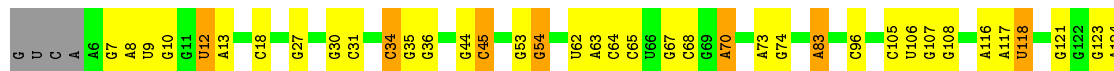
• Molecule 24: E-site tRNA Acceptor Stem



• Molecule 24: E-site tRNA Acceptor Stem



• Molecule 25: 23S Ribosomal RNA



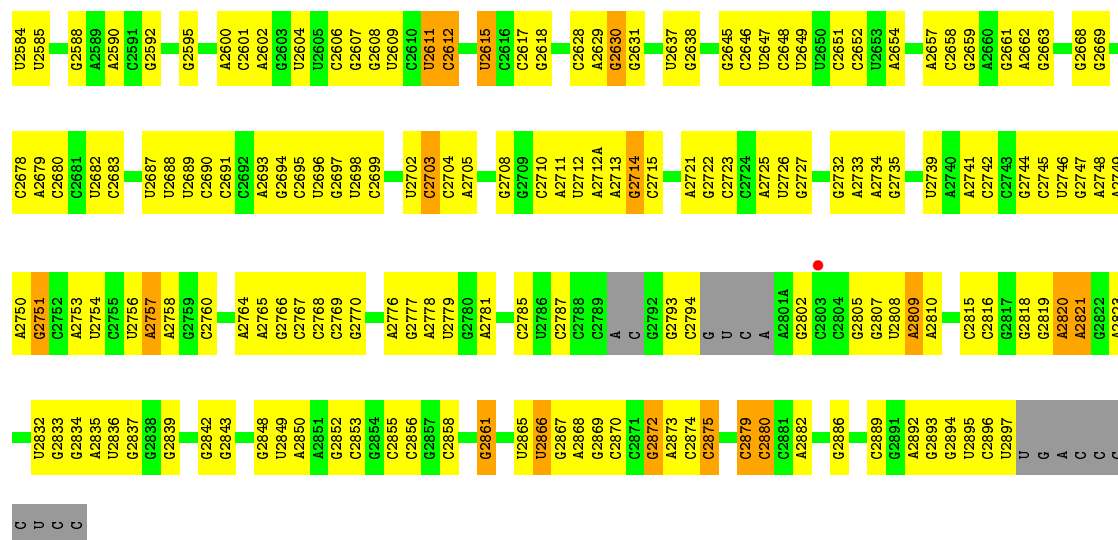
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G1842	U1756	A1630	C1417	A1287	G1182	C	U911	U858	A763	G554	G554	A449
G1845	C1757	A1632	U1418	G1290	G1183	U	A942	C859	A764	G555	G555	A450
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A1847	C1759	C1634	A1541	A1293	A1043	A	C944	A866		G557	G557	
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	G1776	A1654	U1440		A1056	C	A956	G877	C870	C	C	U474
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G1880	G1787	C1677	U1451	G1316	U1213	U	A964	C887	C	G886	G886	C482
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A1906	A1804	G1701	G1476	U1349	U1079	A	G993	G908	G823	C	C	
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	G1807	G1710	A1480	U1359	G1082	A	G998	G909	U611	C612	C612	C511
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G1918	U1809			C1361	U1084	C	G999	G910	A828	G611	G611	G516
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	U1740	G1741	G1513	U1159	G1099	A	G1019	C931	C844	A640	A640	C534
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C1942	G1744	A1616	G1517	G1170	G1269	A	A1029	A934	A849			
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G1830	A1745			A1171		G		C936	G852	G543	G543	U544
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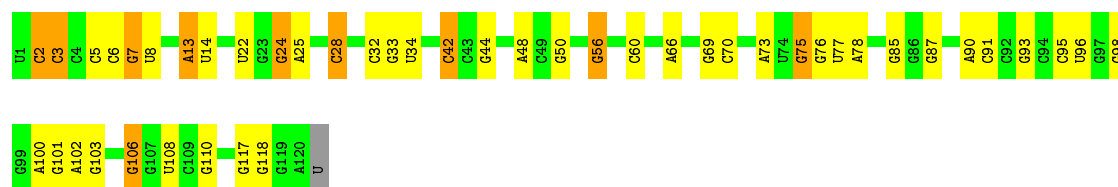


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G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	A2169	A2170	A2171	U2172	A2173	U2174	A2175	G2176	G2177	G2178	G2179	U2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	U2188	U2189	G2192	A2198	G2206	G2207	U2218	G2219	G2224	A2225	G2226	G2227	G2228	G2229	G2234	G2235	G2236	G2237	G2238	G2239	G2240	A2241	G2248	G2252								
G2100	G2101	U2102	G2103	G2104	G2105	G2106	G2107	G2108	U2109	G2110	G2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2121	U2122	G2125	A2126	G2127	G2128	G2129	U2130	G2131	U2132	G2133	A2134	A2135	G2136	G2137	G2138	G2139	G2140	G2141	G2142	U2143	U2144	G2145	G2146	G2147	G2148	G2149	U2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	A2158	G2159	G2160
A2020	G2021	U2022	G2023	G2024	G2025	G2026	G2029	A2030	A2031	G2032	A2033	U2034	G2035	G2036	G2037	G2038	G2039	C2040	U2041	A2042	A2043	C2044	G2045	G2046	A2051	A2054	G2055	G2056	A2057	A2058	A2059	G2060	G2061	A2062	G2063	G2064	G2065	G2066	G2069	U2074	U2075	U2076	G2077	G2078	U2079	G2080	C2081	G2086	G2087	G2094	U2099							
A1927	G1928	G1929	G1930	U1931	A1932	G1933	A1936	A1937	U1938	U1939	U1946	C1947	G1948	U1949	U1955	U1956	U1957	C1958	G1959	U1963	G1964	G1967	A1970	A1971	A1972	A1978	G1979	G1980	A1981	A1989	A1990	C1994	C1995	G1996	G1997	G1998	G1999	G2000	A2001	G2002	C2006	G2010	U2011	U2012	A2013	A2014	A2019											
A1815	G1816	G1822	G1823	G1826	G1827	G1828	G1835	G1836	C1837	G1842	G1846	A1847	A1848	A1849	G1850	C1852	A1859	G1865	A1877	C1878	G1879	G1883	A1889	A1890	C1894	C1895	G1896	G1897	U1898	G1899	A1900	G1906	G1907	G1908	A1912	A1913	C1914	U1915	A1916	U1917	A1918	A1919	G1922	G1923	A2019													
G1705	G1710	C1711	G1716	A1721	A1722	U1723	G1740	A1741	G1742	G1743	G1746	C1751	G1756	A1759	A1762	G1763	G1764	G1772	A1773	U1778	U1779	A1780	A1783	A1784	A1785	A1786	A1789	C1790	A1791	G1792	U1796	C1797	U1798	G1799	G1800	G1801	A1802	A1803	C1804	A1805	A1809	A1810	G1811	A1812	G1813	G1814												
A1610	A1614	G1615	A1616	U1617	A1618	G1626	G1627	G1628	U1629	G1633	G1636	A1637	C1638	U1639	C1640	G1647	G1648	G1651	A1652	G1653	A1654	A1656	A1659	C1660	A1664	G1666	G1667	A1668	C1669	C1670	G1674	G1686	G1687	U1688	A1689	U1692	U1693	G1696	G1697	C1698	A1699	G1699	G1700	A1701	G1702	G1703	G1704											
C1530	C1531	G1532	G1533	U1534	G1536	G1537	G1538	U1539	U1540	G1541	A1542	C1543	C1546	C1547	C1548	C1549	C1550	C1551	A1554	G1557	A1558	G1559	A1566	A1569	U1578	A1579	A1580	G1581	C1582	C1583	C1584	A1586	A1587	C1588	C1589	U1590	G1591	G1592	G1593	G1594	G1595	A1596	A1597	G1598	G1599	C1600	G1601	U1602	C1607	A1608	C1609							
G1447	G1448	A1449	G1450	A1452	U1453	G1455	G1459	U1460	G1461	G1462	G1465	G1466	C1467	A1471	A1472	A1477	G1478	G1482	A1486	G1487	G1492	C1493	A1494	A1495	A1496	U1497	G1498	C1499	G1500	C1505	C1506	A1507	A1508	C1509	A1509A	A1509B	G1510	U1514	G1515	G1519	G1524	G1525	G1526	G1527	A1528	C1445A	G1529											
G1368	G1369	G1370	U1371	U1372	A1373	C1376	G1377	U1378	A1379	A1384	G1385	G1389	U1390	U1391	A1392	A1393	U1396	U1397	C1398	C1399	G1400	U1405	U1406	G1410	A1494	A1411	A1412	U1415	G1416	C1417	G1418	A1419	U1420	G1421	G1422	G1423	G1424	A1427	C1428	G1429	C1430	U1431	A1434	G1435	G1436	C1437	A1445	C1446										



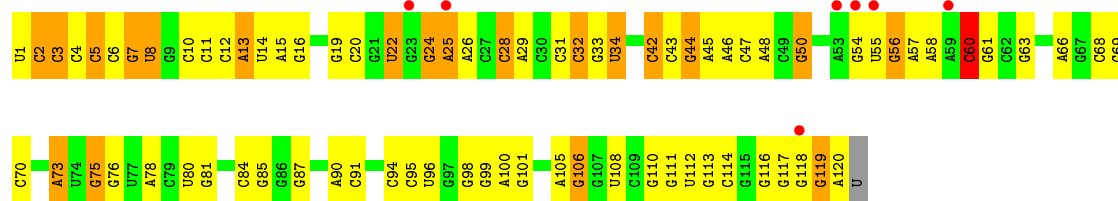
• Molecule 26: 5S Ribosomal RNA

Chain BB: 61% 30% 8%



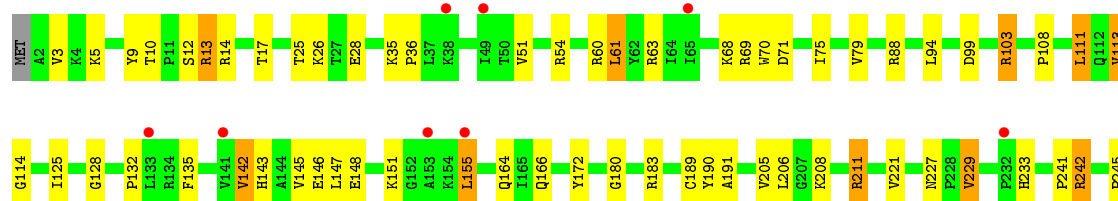
• Molecule 26: 5S Ribosomal RNA

Chain DB: 6% 35% 47% 17%



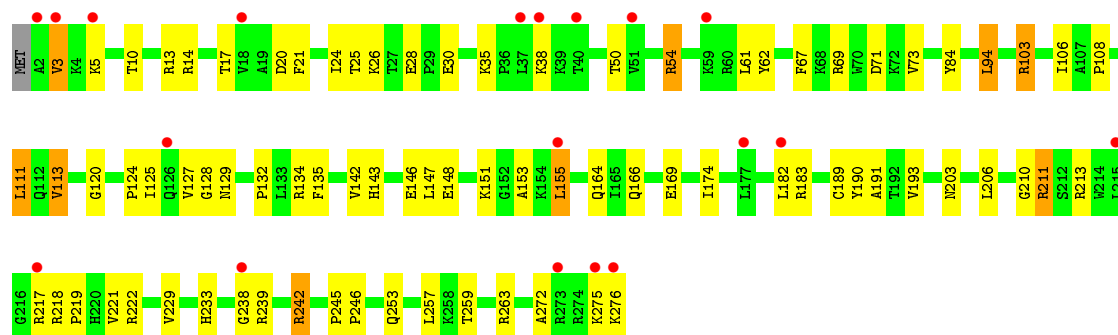
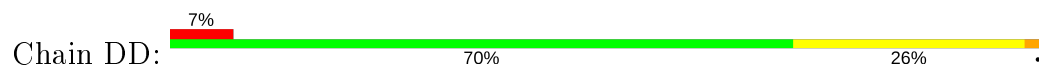
• Molecule 27: 50S Ribosomal Protein L2

Chain BD: 4% 73% 23%

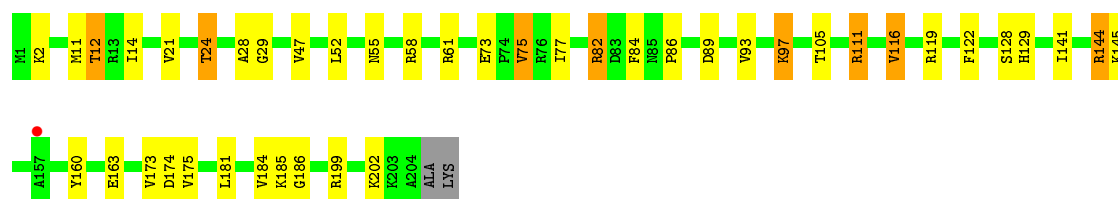
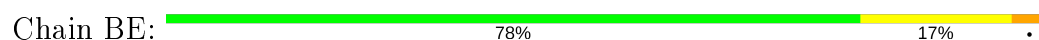




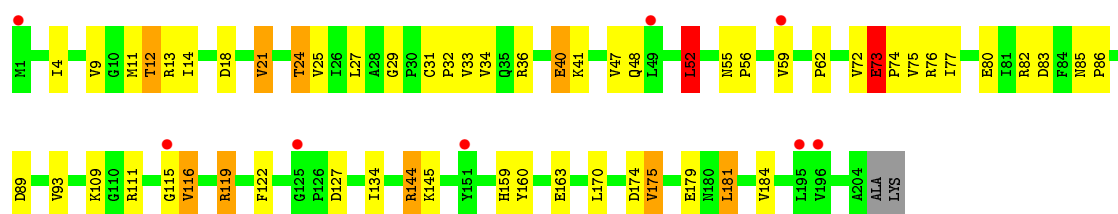
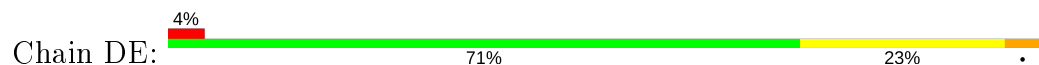
• Molecule 27: 50S Ribosomal Protein L2



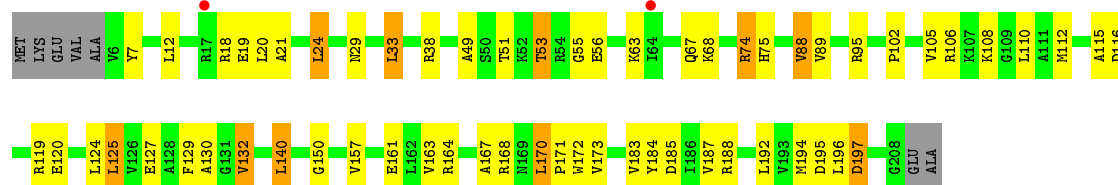
• Molecule 28: 50S Ribosomal Protein L3



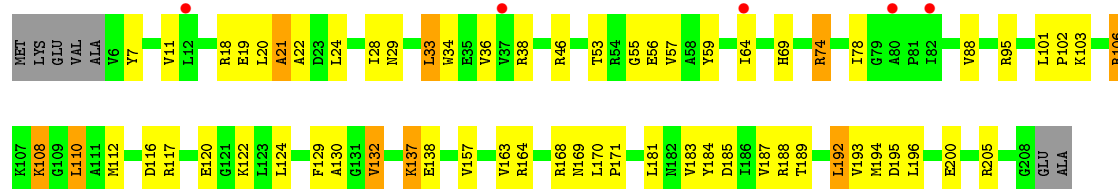
• Molecule 28: 50S Ribosomal Protein L3



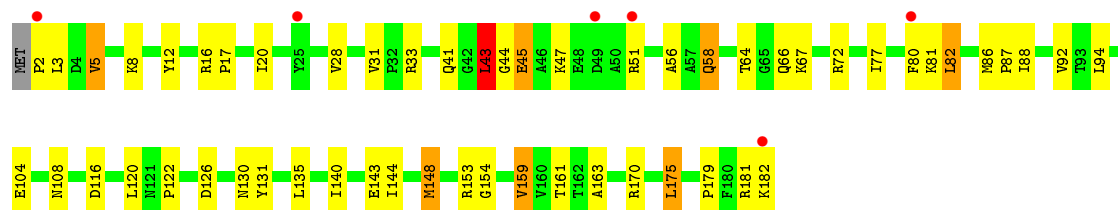
• Molecule 29: 50S Ribosomal Protein L4



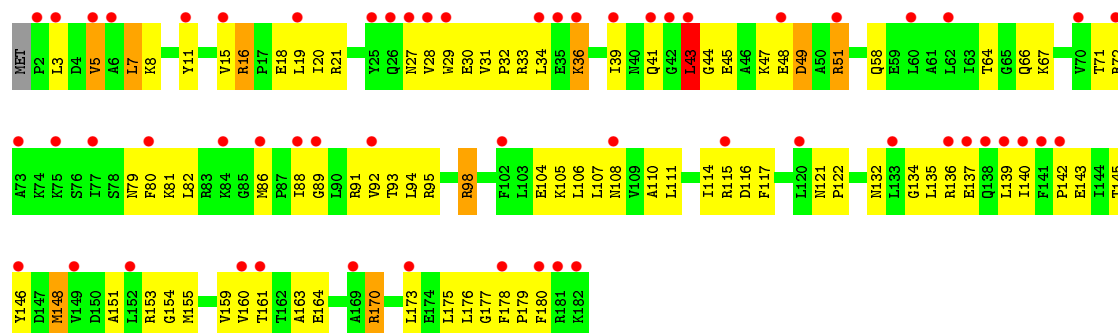
• Molecule 29: 50S Ribosomal Protein L4



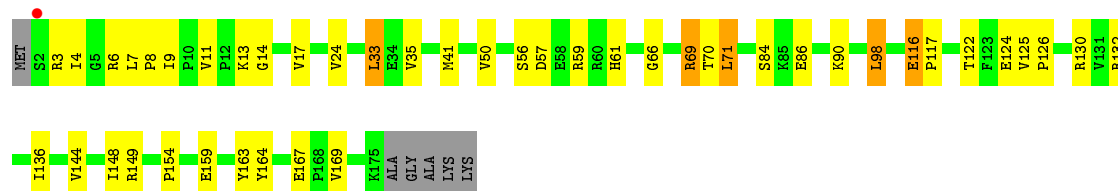
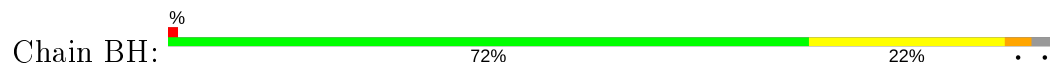
• Molecule 30: 50S Ribosomal Protein L5



• Molecule 30: 50S Ribosomal Protein L5

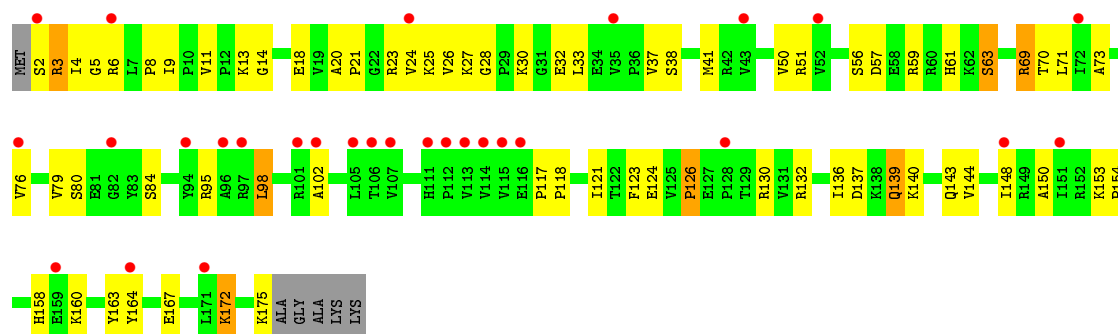


• Molecule 31: 50S Ribosomal Protein L6

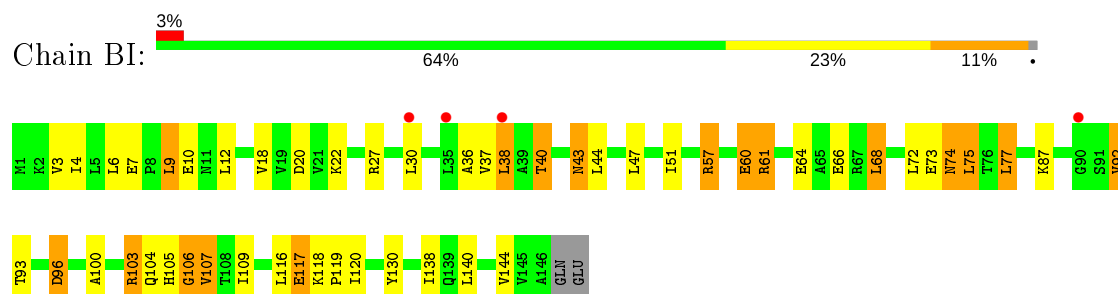


• Molecule 31: 50S Ribosomal Protein L6

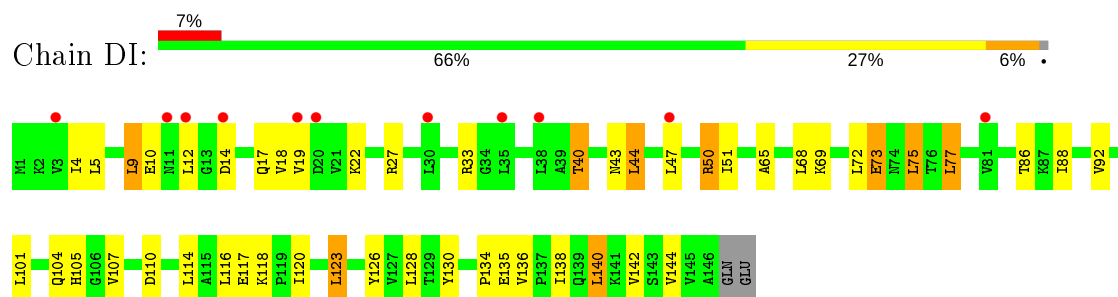




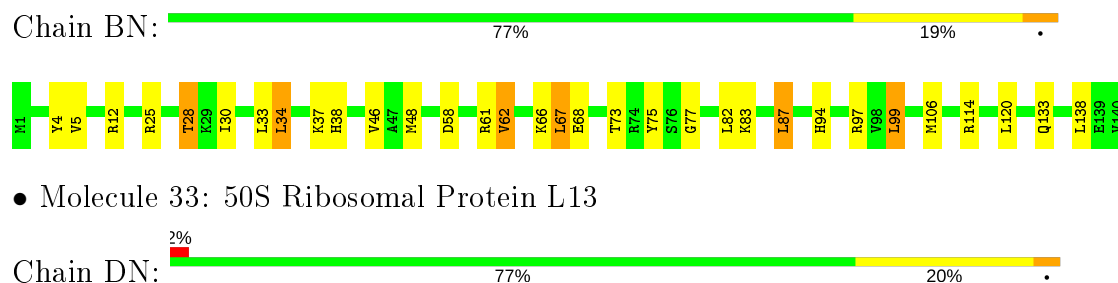
• Molecule 32: 50S Ribosomal Protein L9



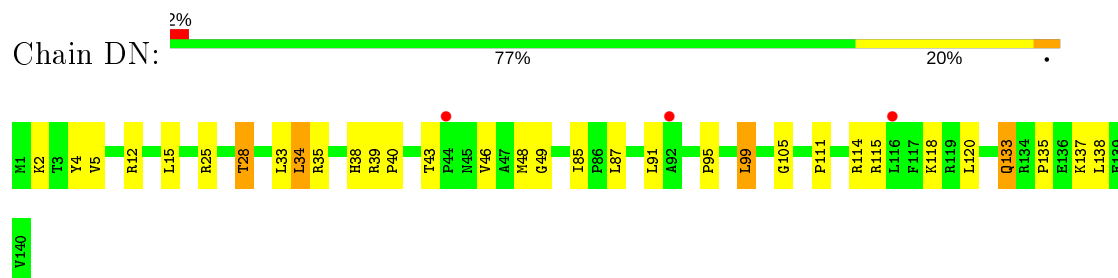
• Molecule 32: 50S Ribosomal Protein L9



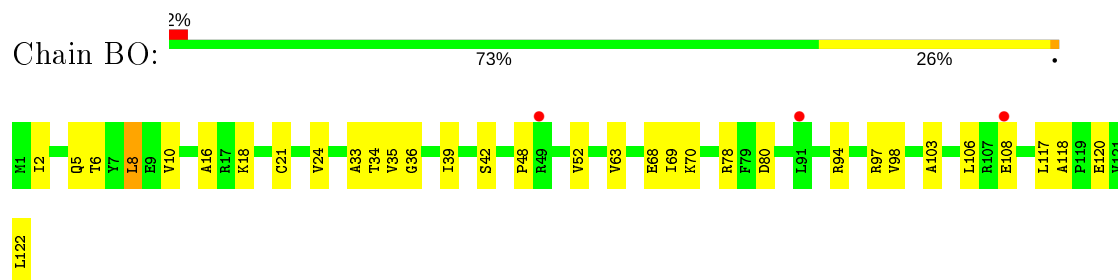
• Molecule 33: 50S Ribosomal Protein L13



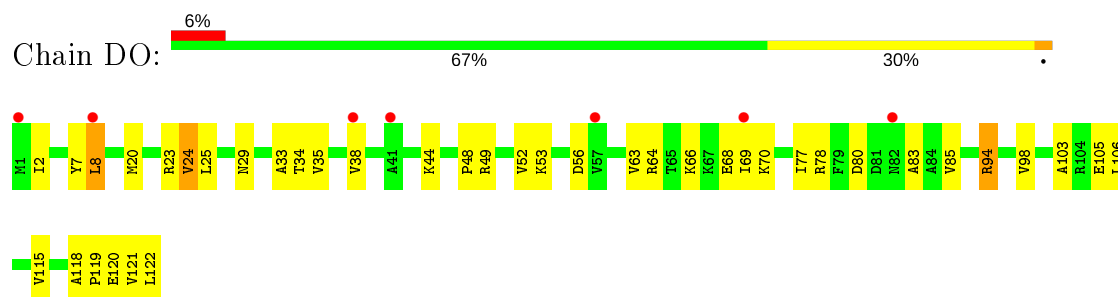
• Molecule 33: 50S Ribosomal Protein L13



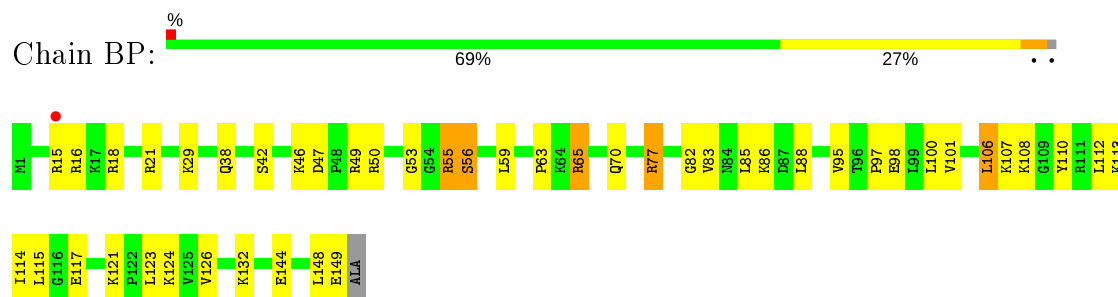
• Molecule 34: 50S Ribosomal Protein L14



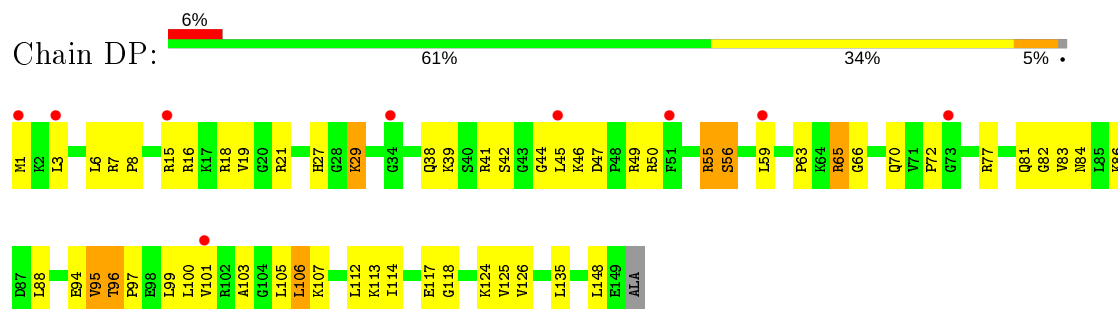
• Molecule 34: 50S Ribosomal Protein L14



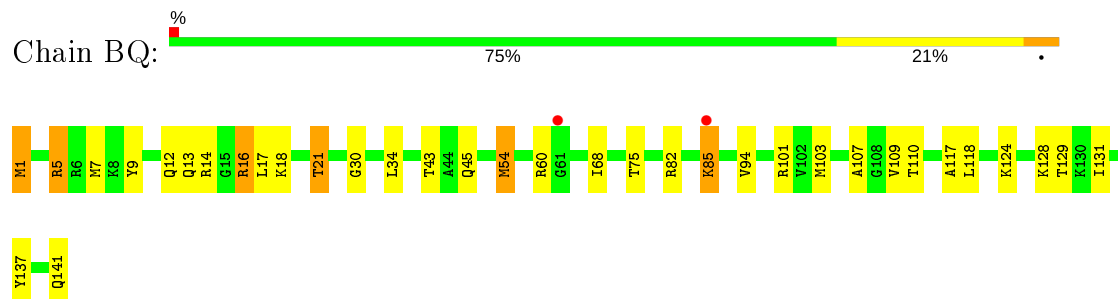
• Molecule 35: 50S Ribosomal Protein L15



• Molecule 35: 50S Ribosomal Protein L15

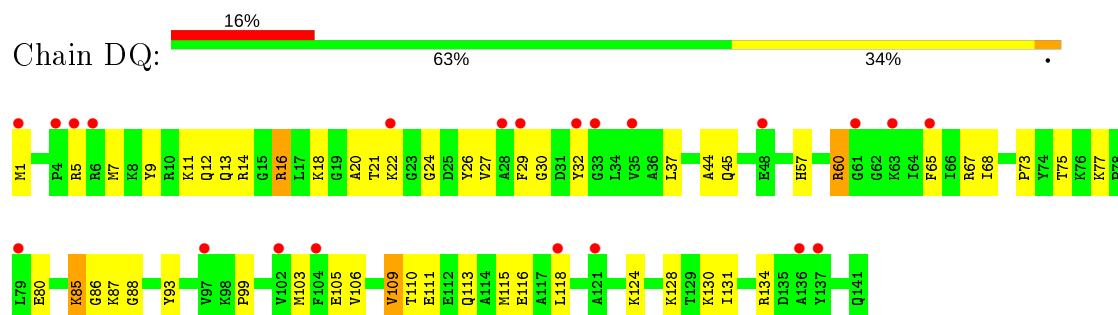


• Molecule 36: 50S Ribosomal Protein L16

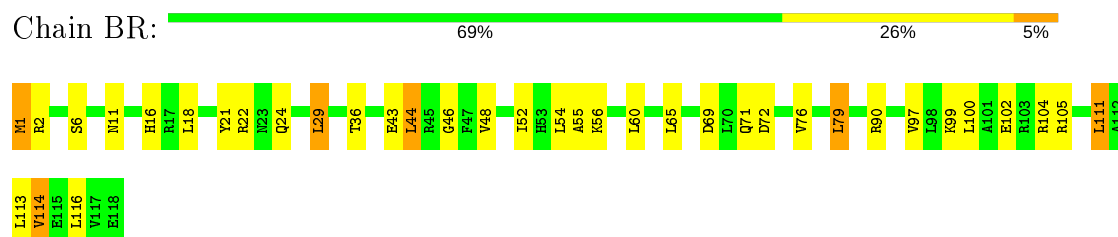




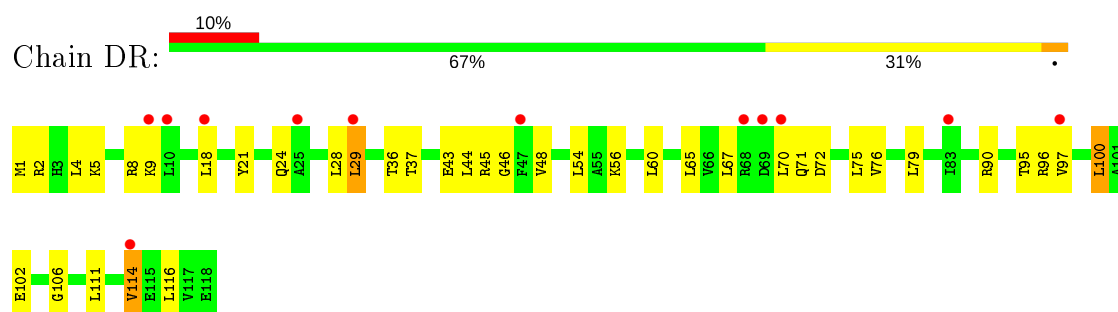
- Molecule 36: 50S Ribosomal Protein L16



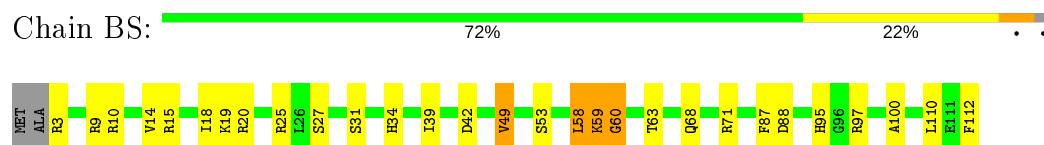
- Molecule 37: 50S Ribosomal Protein L17



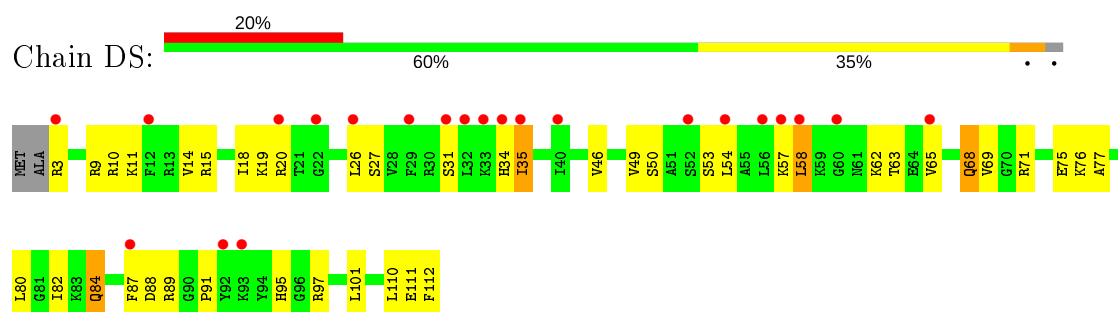
- Molecule 37: 50S Ribosomal Protein L17



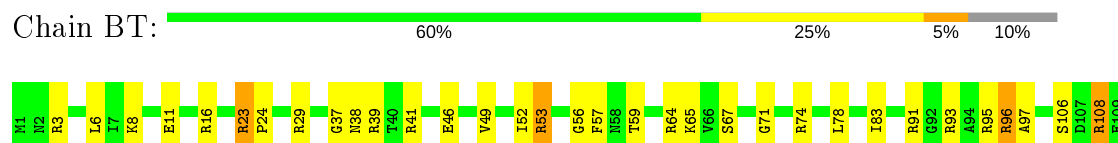
- Molecule 38: 50S Ribosomal Protein L18



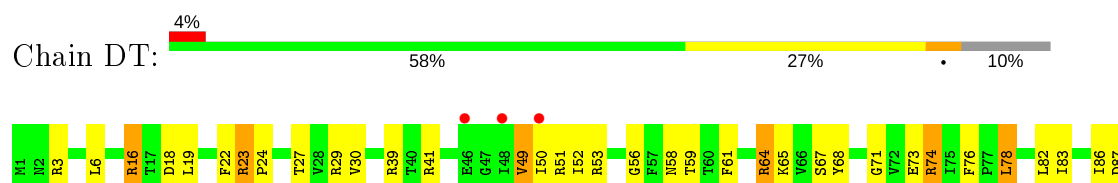
- Molecule 38: 50S Ribosomal Protein L18



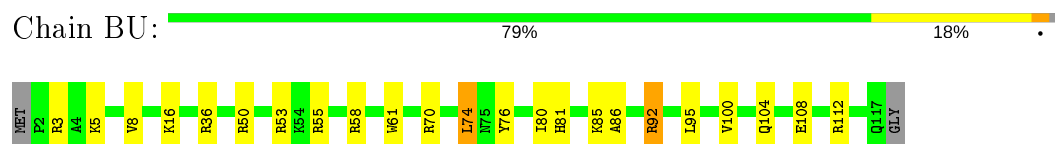
- Molecule 39: 50S Ribosomal Protein L19



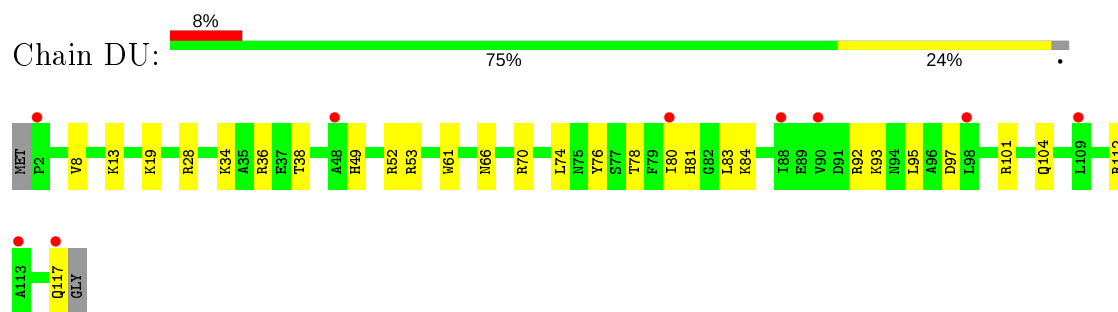
- Molecule 39: 50S Ribosomal Protein L19



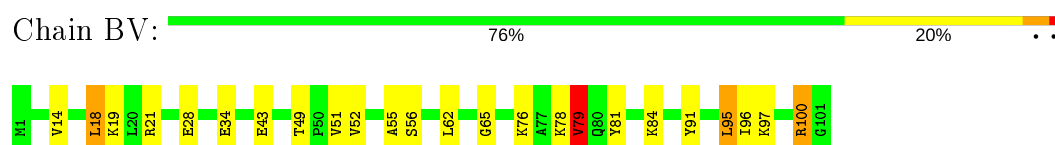
- Molecule 40: 50S Ribosomal Protein L20



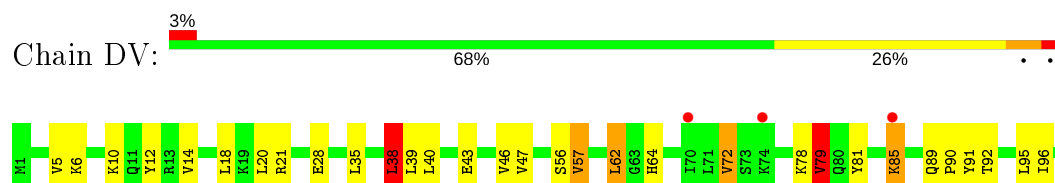
- Molecule 40: 50S Ribosomal Protein L20




- Molecule 41: 50S Ribosomal Protein L21

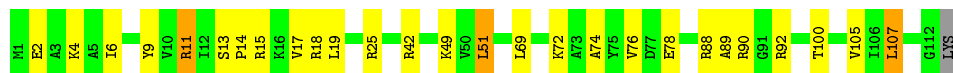


- Molecule 41: 50S Ribosomal Protein L21




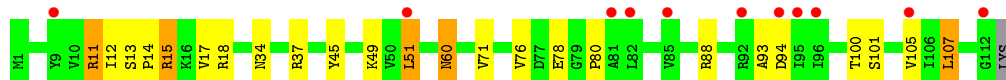
- Molecule 42: 50S Ribosomal Protein L22

Chain BW:  75% 21% ..



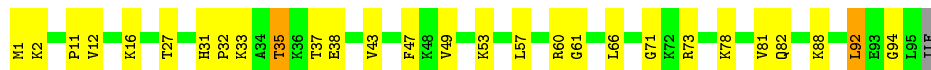
- Molecule 42: 50S Ribosomal Protein L22

Chain DW:  10% 78% 17% ..



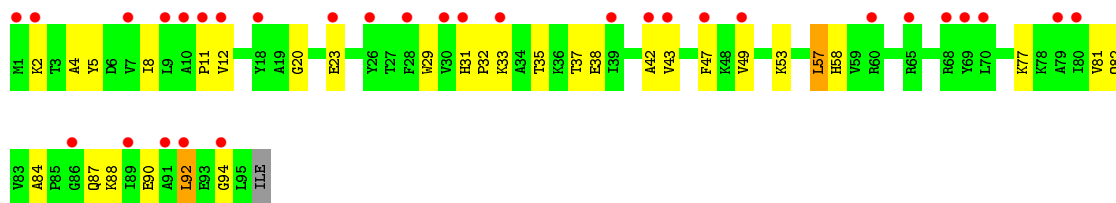
- Molecule 43: 50S Ribosomal Protein L23

Chain BX:  70% 27% ..



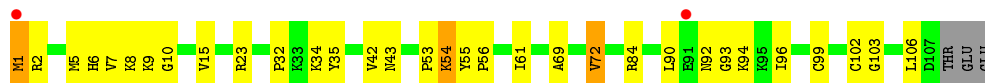
- Molecule 43: 50S Ribosomal Protein L23

Chain DX:  32% 67% 30% ..



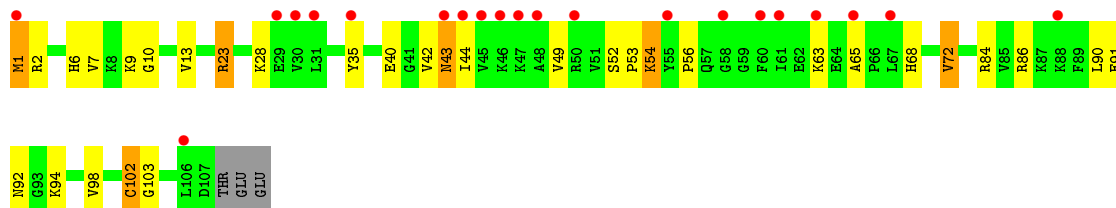
- Molecule 44: 50S Ribosomal Protein L24

Chain BY:  2% 68% 26% ..



- Molecule 44: 50S Ribosomal Protein L24

Chain DY:  19% 68% 24% 5% .



- Molecule 45: 50S Ribosomal Protein L25

Response	Percentage
Yes	50%
No	30%
Don't know	17%



Frequency	Percentage
Daily	14%
Often	51%
Sometimes	29%
Never	16%



Frequency	Percentage
Very often	8%
Often	80%
Sometimes	15%
Rarely	••
Never	••



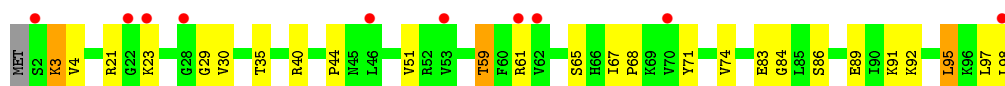
Response	Percentage
Yes, the U.S. is a democracy	27%
No, the U.S. is not a democracy	75%



Frequency	Percentage
5%	5%
74%	74%
20%	20%



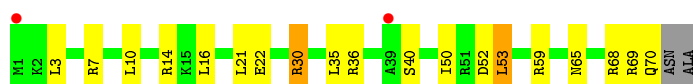
Response	Percentage
Yes	10%
No	72%
Don't know	23%



• Molecule 48: 50S Ribosomal Protein L29



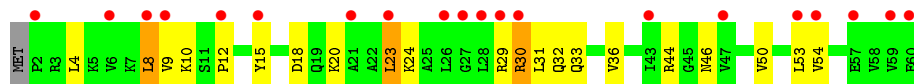
• Molecule 48: 50S Ribosomal Protein L29



• Molecule 49: 50S Ribosomal Protein L30



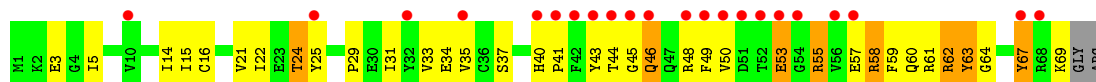
• Molecule 49: 50S Ribosomal Protein L30



• Molecule 50: 50S Ribosomal Protein L31



• Molecule 50: 50S Ribosomal Protein L31

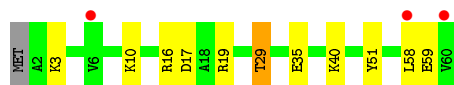
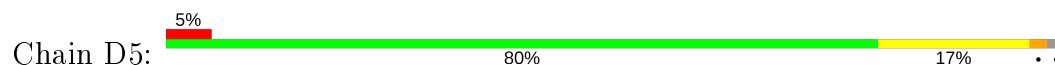


• Molecule 51: 50S Ribosomal Protein L32





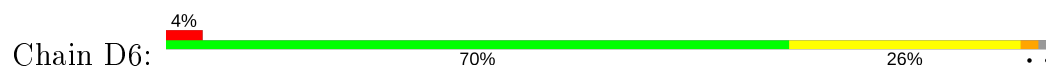
- Molecule 51: 50S Ribosomal Protein L32



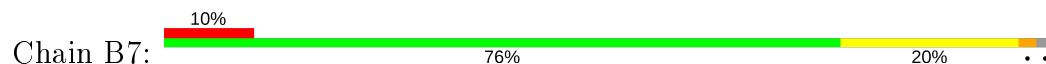
- Molecule 52: 50S Ribosomal Protein L33



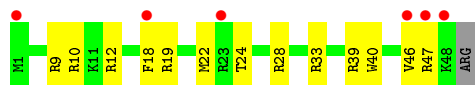
- Molecule 52: 50S Ribosomal Protein L33



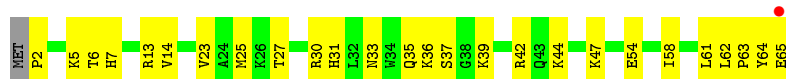
- Molecule 53: 50S Ribosomal Protein L34



- Molecule 53: 50S Ribosomal Protein L34

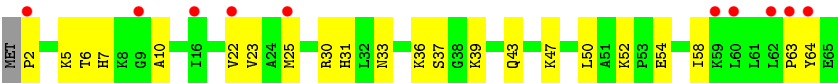


- Molecule 54: 50S Ribosomal Protein L35

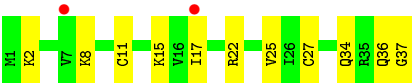


- Molecule 54: 50S Ribosomal Protein L35

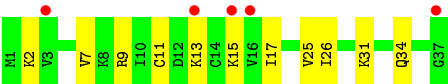




• Molecule 55: 50S Ribosomal Protein L36



• Molecule 55: 50S Ribosomal Protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.93Å 446.95Å 619.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	144.86 – 2.70 254.67 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (144.86-2.70) 99.6 (254.67-2.70)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.215 , 0.262 0.215 , 0.263	Depositor DCC
$R_{free}$ test set	78302 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.5	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 59.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	290807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AA	1.31	15/36024 (0.0%)	1.16	60/56222 (0.1%)
1	CA	0.43	0/36170	0.97	61/56452 (0.1%)
2	AB	0.34	0/1881	0.62	1/2542 (0.0%)
2	CB	0.35	0/1860	0.62	1/2518 (0.0%)
3	AC	0.30	0/1576	0.51	0/2130
3	CC	0.33	0/1566	0.59	1/2119 (0.0%)
4	AD	0.31	0/1689	0.55	0/2267
4	CD	0.31	0/1704	0.55	0/2284
5	AE	0.31	0/1145	0.53	0/1543
5	CE	0.33	0/1149	0.57	0/1548
6	AF	0.30	0/819	0.52	0/1111
6	CF	0.32	0/829	0.54	0/1123
7	AG	0.29	0/1250	0.50	0/1679
7	CG	0.31	0/1254	0.53	0/1683
8	AH	0.30	0/1108	0.52	0/1494
8	CH	0.29	0/1108	0.52	0/1494
9	AI	0.29	0/1002	0.55	0/1346
9	CI	0.33	0/997	0.58	1/1343 (0.1%)
10	AJ	0.29	0/722	0.54	0/982
10	CJ	0.34	0/727	0.59	0/988
11	AK	0.32	0/844	0.51	0/1145
11	CK	0.30	0/848	0.53	0/1149
12	AL	0.33	0/946	0.51	0/1274
12	CL	0.33	0/946	0.60	1/1274 (0.1%)
13	AM	0.29	0/947	0.58	0/1272
13	CM	0.31	0/930	0.55	0/1250
14	AN	0.31	0/501	0.54	0/664
14	CN	0.34	0/501	0.52	0/664
15	AO	0.31	0/739	0.53	0/985
15	CO	0.32	0/739	0.53	0/985
16	AP	0.31	0/697	0.53	0/939
16	CP	0.32	0/693	0.51	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.32	0/836	0.52	0/1117
17	CQ	0.31	0/836	0.48	0/1117
18	AR	0.32	0/560	0.53	0/746
18	CR	0.30	0/560	0.51	0/746
19	AS	0.31	0/667	0.53	0/900
19	CS	0.33	0/661	0.65	1/893 (0.1%)
20	AT	0.31	0/730	0.56	0/965
20	CT	0.29	0/729	0.53	0/965
21	AU	0.29	0/203	0.51	0/266
21	CU	0.35	0/203	0.55	0/266
22	AV	0.56	0/188	1.13	0/290
22	CV	0.62	0/122	1.18	0/188
23	AX	0.56	2/1725 (0.1%)	1.16	18/2689 (0.7%)
23	CX	0.55	1/1725 (0.1%)	1.20	18/2689 (0.7%)
24	AY	0.72	1/428 (0.2%)	0.91	0/661
24	CY	0.48	0/115	1.02	0/176
25	BA	0.67	6/68083 (0.0%)	1.04	144/106274 (0.1%)
25	DA	0.51	3/67542 (0.0%)	1.00	78/105428 (0.1%)
26	BB	0.51	0/2878	0.91	0/4490
26	DB	0.57	0/2878	1.01	2/4490 (0.0%)
27	BD	0.44	0/2186	0.60	0/2944
27	DD	0.39	0/2186	0.59	0/2944
28	BE	0.45	0/1592	0.60	0/2149
28	DE	0.38	0/1592	0.62	0/2149
29	BF	0.43	0/1619	0.58	0/2193
29	DF	0.36	0/1615	0.59	0/2188
30	BG	0.33	0/1450	0.55	1/1959 (0.1%)
30	DG	0.36	0/1449	0.57	0/1958
31	BH	0.36	0/1356	0.54	0/1834
31	DH	0.34	0/1356	0.54	0/1834
32	BI	0.32	0/1100	0.58	0/1501
32	DI	0.32	0/1076	0.57	0/1471
33	BN	0.39	0/1144	0.54	0/1543
33	DN	0.36	0/1144	0.57	0/1543
34	BO	0.45	0/943	0.59	1/1269 (0.1%)
34	DO	0.37	0/943	0.60	1/1269 (0.1%)
35	BP	0.42	0/1152	0.60	0/1533
35	DP	0.38	0/1152	0.64	1/1533 (0.1%)
36	BQ	0.44	0/1143	0.58	0/1527
36	DQ	0.36	0/1143	0.57	0/1527
37	BR	0.44	0/982	0.66	0/1312
37	DR	0.33	0/982	0.57	0/1312
38	BS	0.39	0/887	0.62	0/1180

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DS	0.33	0/880	0.55	0/1172
39	BT	0.38	0/1105	0.60	0/1477
39	DT	0.35	0/1097	0.57	1/1468 (0.1%)
40	BU	0.48	0/977	0.61	0/1301
40	DU	0.33	0/977	0.53	0/1301
41	BV	0.44	0/782	0.64	0/1049
41	DV	0.34	0/782	0.55	1/1049 (0.1%)
42	BW	0.50	0/897	0.62	0/1205
42	DW	0.34	0/897	0.53	0/1205
43	BX	0.45	0/764	0.58	0/1025
43	DX	0.34	0/764	0.54	1/1025 (0.1%)
44	BY	0.40	0/819	0.62	0/1095
44	DY	0.33	0/819	0.57	0/1095
45	BZ	0.35	0/1379	0.62	0/1873
45	DZ	0.31	0/1390	0.54	0/1890
46	B0	0.45	0/662	0.65	0/881
46	D0	0.33	0/662	0.55	0/881
47	B1	0.40	0/762	0.55	0/1014
47	D1	0.36	0/762	0.56	0/1014
48	B2	0.39	0/590	0.59	0/781
48	D2	0.29	0/590	0.50	0/781
49	B3	0.41	0/474	0.59	0/635
49	D3	0.30	0/469	0.53	0/630
50	B4	0.36	0/571	0.68	0/768
50	D4	0.34	0/545	0.62	0/737
51	B5	0.50	1/469 (0.2%)	0.77	0/635
51	D5	0.35	0/469	0.59	1/635 (0.2%)
52	B6	0.60	1/460 (0.2%)	0.67	1/613 (0.2%)
52	D6	0.36	0/456	0.52	0/608
53	B7	0.48	0/426	0.62	0/561
53	D7	0.37	0/426	0.57	0/561
54	B8	0.44	0/519	0.61	0/684
54	D8	0.36	0/525	0.54	0/691
55	B9	0.50	0/310	0.65	1/407 (0.2%)
55	D9	0.38	0/310	0.62	0/407
All	All	0.65	30/310558 (0.0%)	0.94	397/464586 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
7	CG	0	2
38	BS	0	1
50	B4	0	1
50	D4	0	1
All	All	0	6

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	439	A	C5-C4	145.31	2.40	1.38
1	AA	496	A	C6-N1	114.63	2.15	1.35
1	AA	439	A	N3-C4	59.27	1.70	1.34
1	AA	496	A	C2-N3	54.84	1.82	1.33
1	AA	439	A	C6-N1	53.24	1.72	1.35

The worst 5 of 397 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	496	A	C2-N3-C4	97.04	159.12	110.60
1	AA	496	A	N1-C2-N3	-89.99	84.31	129.30
1	AA	496	A	C5-C6-N6	-36.75	94.30	123.70
1	AA	496	A	C5-C6-N1	31.98	133.69	117.70
1	AA	496	A	C4-C5-C6	-28.65	102.68	117.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	439	A	Sidechain
50	B4	59	PHE	Peptide
38	BS	58	LEU	Peptide
7	CG	78	ARG	Peptide
7	CG	79	ARG	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32183	0	16244	640	0
1	CA	32312	0	16308	675	0
2	AB	1846	0	1867	88	0
2	CB	1825	0	1828	91	0
3	AC	1552	0	1546	53	0
3	CC	1542	0	1517	52	0
4	AD	1659	0	1676	71	0
4	CD	1674	0	1714	52	0
5	AE	1129	0	1185	32	0
5	CE	1133	0	1191	37	0
6	AF	806	0	793	19	0
6	CF	816	0	808	16	0
7	AG	1231	0	1238	22	0
7	CG	1235	0	1249	37	0
8	AH	1088	0	1126	28	0
8	CH	1088	0	1126	26	0
9	AI	983	0	986	30	0
9	CI	978	0	966	47	0
10	AJ	709	0	650	34	0
10	CJ	714	0	672	34	0
11	AK	829	0	825	20	0
11	CK	833	0	836	16	0
12	AL	930	0	980	25	0
12	CL	930	0	980	28	0
13	AM	937	0	977	27	0
13	CM	920	0	950	37	0
14	AN	492	0	529	21	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	23	0
16	CP	677	0	686	17	0
17	AQ	823	0	891	11	0
17	CQ	823	0	891	10	0
18	AR	555	0	618	13	0
18	CR	555	0	618	12	0
19	AS	652	0	662	25	0
19	CS	646	0	644	39	0
20	AT	728	0	798	21	0
20	CT	727	0	796	16	0
21	AU	199	0	208	4	0
21	CU	199	0	208	9	0
22	AV	169	0	86	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	109	0	55	5	0
23	AX	1625	0	828	21	0
23	CX	1625	0	829	27	0
24	AY	385	0	199	11	0
24	CY	104	0	56	6	0
25	BA	60792	0	30653	698	0
25	DA	60311	0	30414	981	0
26	BB	2573	0	1306	23	0
26	DB	2573	0	1306	73	0
27	BD	2136	0	2218	60	0
27	DD	2136	0	2218	66	0
28	BE	1559	0	1618	27	0
28	DE	1559	0	1618	41	0
29	BF	1584	0	1625	45	0
29	DF	1580	0	1619	51	0
30	BG	1425	0	1443	43	0
30	DG	1424	0	1434	67	0
31	BH	1330	0	1407	24	0
31	DH	1330	0	1407	49	0
32	BI	1085	0	1114	35	0
32	DI	1061	0	1080	30	0
33	BN	1117	0	1183	19	0
33	DN	1117	0	1184	17	0
34	BO	933	0	996	23	0
34	DO	933	0	996	29	0
35	BP	1135	0	1212	34	0
35	DP	1135	0	1212	53	0
36	BQ	1122	0	1179	26	0
36	DQ	1122	0	1179	37	0
37	BR	968	0	1033	20	0
37	DR	968	0	1033	25	0
38	BS	877	0	938	26	0
38	DS	870	0	923	29	0
39	BT	1091	0	1151	38	0
39	DT	1083	0	1136	36	0
40	BU	959	0	1019	18	0
40	DU	959	0	1019	18	0
41	BV	771	0	830	13	0
41	DV	771	0	830	20	0
42	BW	886	0	940	18	0
42	DW	886	0	940	16	0
43	BX	750	0	814	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DX	750	0	814	18	0
44	BY	806	0	881	21	0
44	DY	806	0	881	21	0
45	BZ	1349	0	1355	45	0
45	DZ	1360	0	1363	44	0
46	B0	653	0	674	15	0
46	D0	653	0	674	22	0
47	B1	755	0	826	21	0
47	D1	755	0	826	19	0
48	B2	588	0	643	10	0
48	D2	588	0	643	12	0
49	B3	469	0	518	10	0
49	D3	464	0	514	12	0
50	B4	558	0	544	36	0
50	D4	532	0	503	27	0
51	B5	455	0	465	9	0
51	D5	455	0	465	9	0
52	B6	453	0	473	10	0
52	D6	449	0	469	10	0
53	B7	418	0	467	7	0
53	D7	418	0	467	9	0
54	B8	511	0	571	22	0
54	D8	517	0	582	16	0
55	B9	307	0	335	8	0
55	D9	307	0	335	7	0
56	AA	190	0	0	0	0
56	AD	1	0	0	0	0
56	AE	3	0	0	0	0
56	AF	1	0	0	0	0
56	AM	1	0	0	0	0
56	AN	1	0	0	0	0
56	AQ	1	0	0	0	0
56	AX	9	0	0	0	0
56	B0	5	0	0	0	0
56	B2	1	0	0	0	0
56	B3	1	0	0	0	0
56	B4	1	0	0	0	0
56	B5	4	0	0	0	0
56	B6	2	0	0	0	0
56	B7	5	0	0	0	0
56	B8	2	0	0	0	0
56	B9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BA	814	0	0	0	0
56	BB	22	0	0	0	0
56	BD	9	0	0	0	0
56	BE	7	0	0	0	0
56	BF	9	0	0	0	0
56	BG	2	0	0	0	0
56	BN	7	0	0	0	0
56	BO	1	0	0	0	0
56	BP	4	0	0	0	0
56	BQ	4	0	0	0	0
56	BR	3	0	0	0	0
56	BU	9	0	0	0	0
56	BV	4	0	0	0	0
56	BW	4	0	0	0	0
56	BX	2	0	0	0	0
56	BY	3	0	0	0	0
56	BZ	2	0	0	0	0
56	CA	175	0	0	0	0
56	CE	2	0	0	0	0
56	CF	1	0	0	0	0
56	CJ	1	0	0	0	0
56	CT	1	0	0	0	0
56	CX	2	0	0	0	0
56	D0	2	0	0	0	0
56	D1	1	0	0	0	0
56	D3	1	0	0	0	0
56	D8	1	0	0	0	0
56	DA	674	0	0	0	0
56	DB	10	0	0	0	0
56	DD	8	0	0	0	0
56	DE	5	0	0	0	0
56	DF	5	0	0	0	0
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	1	0	0	0	0
56	DP	2	0	0	0	0
56	DQ	3	0	0	0	0
56	DR	1	0	0	0	0
56	DU	4	0	0	0	0
56	DV	3	0	0	0	0
56	DW	2	0	0	0	0
56	DY	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AA	40	0	38	6	0
57	CA	40	0	38	4	0
58	AD	8	0	0	1	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	175	0	0	13	0
61	AJ	2	0	0	0	0
61	AL	1	0	0	0	0
61	AM	1	0	0	0	0
61	AO	1	0	0	0	0
61	AV	1	0	0	0	0
61	AX	8	0	0	0	0
61	B0	4	0	0	0	0
61	B1	1	0	0	0	0
61	B3	1	0	0	0	0
61	B5	4	0	0	1	0
61	B6	1	0	0	0	0
61	B7	1	0	0	0	0
61	B8	10	0	0	1	0
61	BA	1294	0	0	49	0
61	BB	34	0	0	1	0
61	BD	16	0	0	1	0
61	BE	12	0	0	1	0
61	BF	7	0	0	1	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BN	1	0	0	0	0
61	BO	4	0	0	0	0
61	BP	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BQ	5	0	0	0	0
61	BR	1	0	0	0	0
61	BU	2	0	0	0	0
61	BV	2	0	0	0	0
61	BW	3	0	0	0	0
61	BX	5	0	0	0	0
61	CA	137	0	0	12	0
61	CD	1	0	0	0	0
61	CJ	2	0	0	0	0
61	CL	1	0	0	1	0
61	CN	1	0	0	0	0
61	CT	1	0	0	0	0
61	CX	2	0	0	0	0
61	D0	7	0	0	0	0
61	D1	1	0	0	0	0
61	D3	1	0	0	0	0
61	D8	4	0	0	0	0
61	DA	924	0	0	75	0
61	DB	8	0	0	0	0
61	DD	18	0	0	3	0
61	DE	9	0	0	1	0
61	DF	5	0	0	0	0
61	DN	1	0	0	0	0
61	DO	1	0	0	0	0
61	DP	14	0	0	1	0
61	DR	1	0	0	0	0
61	DT	1	0	0	0	0
61	DU	3	0	0	0	0
61	DV	1	0	0	0	0
61	DW	1	0	0	0	0
61	DX	1	0	0	0	0
61	DY	1	0	0	0	0
All	All	290807	0	193177	5129	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 11.

The worst 5 of 5129 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:439:A:N3	1:AA:439:A:C2	1.68	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:439:A:C5	1:AA:439:A:C6	1.79	1.62
1:AA:439:A:N3	1:AA:439:A:C4	1.70	1.56
1:AA:439:A:N1	1:AA:439:A:C6	1.72	1.55
1:AA:439:A:N1	1:AA:439:A:C2	1.70	1.54

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	194 (85%)	24 (10%)	11 (5%)	2	4
2	CB	229/256 (90%)	195 (85%)	24 (10%)	10 (4%)	2	5
3	AC	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	15	37
3	CC	204/239 (85%)	178 (87%)	23 (11%)	3 (2%)	10	26
4	AD	206/209 (99%)	189 (92%)	15 (7%)	2 (1%)	15	37
4	CD	206/209 (99%)	190 (92%)	14 (7%)	2 (1%)	15	37
5	AE	146/162 (90%)	139 (95%)	5 (3%)	2 (1%)	11	28
5	CE	146/162 (90%)	136 (93%)	8 (6%)	2 (1%)	11	28
6	AF	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
6	CF	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
7	AG	153/156 (98%)	139 (91%)	11 (7%)	3 (2%)	7	19
7	CG	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	22	46
8	AH	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
8	CH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	22	46
9	AI	125/128 (98%)	107 (86%)	14 (11%)	4 (3%)	4	9
9	CI	125/128 (98%)	109 (87%)	12 (10%)	4 (3%)	4	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	95/105 (90%)	80 (84%)	9 (10%)	6 (6%)	1	2
10	CJ	94/105 (90%)	83 (88%)	6 (6%)	5 (5%)	2	3
11	AK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	8	21
11	CK	112/129 (87%)	101 (90%)	8 (7%)	3 (3%)	5	12
12	AL	120/132 (91%)	111 (92%)	9 (8%)	0	100	100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
13	AM	118/126 (94%)	103 (87%)	13 (11%)	2 (2%)	9	23
13	CM	116/126 (92%)	101 (87%)	11 (10%)	4 (3%)	3	8
14	AN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
14	CN	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	AO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	CO	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	13	32
16	AP	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
16	CP	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	12	30
17	AQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
17	CQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
18	AR	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
18	CR	66/88 (75%)	64 (97%)	1 (2%)	1 (2%)	10	26
19	AS	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
19	CS	81/93 (87%)	68 (84%)	11 (14%)	2 (2%)	5	14
20	AT	94/106 (89%)	82 (87%)	6 (6%)	6 (6%)	1	2
20	CT	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	2	3
21	AU	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
21	CU	21/27 (78%)	16 (76%)	4 (19%)	1 (5%)	2	4
27	BD	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	34	60
27	DD	273/276 (99%)	257 (94%)	14 (5%)	2 (1%)	22	46
28	BE	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	54
28	DE	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	15	37
29	BF	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	29	54
29	DF	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	15	37
30	BG	179/182 (98%)	165 (92%)	11 (6%)	3 (2%)	9	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	DG	179/182 (98%)	161 (90%)	14 (8%)	4 (2%)	6	17
31	BH	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	25	50
31	DH	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	25	50
32	BI	144/148 (97%)	129 (90%)	12 (8%)	3 (2%)	7	18
32	DI	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	11	28
33	BN	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
33	DN	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	22	46
34	BO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	19	43
34	DO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
35	BP	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	22	46
35	DP	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22	46
36	BQ	139/141 (99%)	132 (95%)	6 (4%)	1 (1%)	22	46
36	DQ	139/141 (99%)	132 (95%)	5 (4%)	2 (1%)	11	28
37	BR	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
37	DR	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	17	40
38	BS	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	17	40
38	DS	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	17	40
39	BT	129/146 (88%)	122 (95%)	5 (4%)	2 (2%)	9	24
39	DT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
40	BU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
40	DU	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
41	BV	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	7	19
41	DV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	37
42	BW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
42	DW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
43	BX	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	14	34
43	DX	93/96 (97%)	88 (95%)	3 (3%)	2 (2%)	6	17
44	BY	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	8	20
44	DY	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	15	37
45	BZ	169/206 (82%)	147 (87%)	18 (11%)	4 (2%)	6	15
45	DZ	172/206 (84%)	154 (90%)	17 (10%)	1 (1%)	25	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	B0	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	13	32
46	D0	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
47	B1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	34
47	D1	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	34
48	B2	68/72 (94%)	68 (100%)	0	0	100	100
48	D2	68/72 (94%)	68 (100%)	0	0	100	100
49	B3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
49	D3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	B4	67/71 (94%)	50 (75%)	10 (15%)	7 (10%)	0	0
50	D4	67/71 (94%)	53 (79%)	7 (10%)	7 (10%)	0	0
51	B5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
51	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
52	B6	51/54 (94%)	49 (96%)	1 (2%)	1 (2%)	7	19
52	D6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
53	B7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
53	D7	46/49 (94%)	45 (98%)	0	1 (2%)	6	17
54	B8	62/65 (95%)	62 (100%)	0	0	100	100
54	D8	62/65 (95%)	62 (100%)	0	0	100	100
55	B9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
55	D9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
All	All	11402/12128 (94%)	10561 (93%)	687 (6%)	154 (1%)	11	28

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	10	LEU
2	AB	125	PRO
4	AD	166	LYS
7	AG	80	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%)	158 (82%)	34 (18%)	2	4
2	CB	187/220 (85%)	161 (86%)	26 (14%)	3	8
3	AC	143/188 (76%)	134 (94%)	9 (6%)	18	40
3	CC	140/188 (74%)	127 (91%)	13 (9%)	9	21
4	AD	170/181 (94%)	154 (91%)	16 (9%)	8	20
4	CD	173/181 (96%)	158 (91%)	15 (9%)	10	23
5	AE	113/123 (92%)	106 (94%)	7 (6%)	18	40
5	CE	114/123 (93%)	103 (90%)	11 (10%)	8	19
6	AF	83/90 (92%)	79 (95%)	4 (5%)	25	53
6	CF	85/90 (94%)	82 (96%)	3 (4%)	36	65
7	AG	119/127 (94%)	108 (91%)	11 (9%)	9	21
7	CG	120/127 (94%)	113 (94%)	7 (6%)	20	43
8	AH	114/119 (96%)	108 (95%)	6 (5%)	22	48
8	CH	114/119 (96%)	109 (96%)	5 (4%)	28	56
9	AI	90/99 (91%)	79 (88%)	11 (12%)	5	11
9	CI	89/99 (90%)	81 (91%)	8 (9%)	9	22
10	AJ	66/92 (72%)	63 (96%)	3 (4%)	27	55
10	CJ	69/92 (75%)	64 (93%)	5 (7%)	14	34
11	AK	82/99 (83%)	78 (95%)	4 (5%)	25	52
11	CK	83/99 (84%)	79 (95%)	4 (5%)	25	53
12	AL	97/109 (89%)	92 (95%)	5 (5%)	23	49
12	CL	97/109 (89%)	93 (96%)	4 (4%)	30	59
13	AM	91/101 (90%)	83 (91%)	8 (9%)	10	23
13	CM	89/101 (88%)	80 (90%)	9 (10%)	7	17
14	AN	49/50 (98%)	43 (88%)	6 (12%)	5	11
14	CN	49/50 (98%)	42 (86%)	7 (14%)	3	8
15	AO	78/80 (98%)	68 (87%)	10 (13%)	4	10
15	CO	78/80 (98%)	73 (94%)	5 (6%)	17	39
16	AP	69/74 (93%)	59 (86%)	10 (14%)	3	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	CP	68/74 (92%)	60 (88%)	8 (12%)	5	12
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	17	39
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	22	48
18	AR	59/77 (77%)	54 (92%)	5 (8%)	10	24
18	CR	59/77 (77%)	55 (93%)	4 (7%)	16	36
19	AS	69/80 (86%)	63 (91%)	6 (9%)	10	23
19	CS	67/80 (84%)	58 (87%)	9 (13%)	4	9
20	AT	70/82 (85%)	62 (89%)	8 (11%)	5	13
20	CT	70/82 (85%)	62 (89%)	8 (11%)	5	13
21	AU	18/22 (82%)	16 (89%)	2 (11%)	6	14
21	CU	18/22 (82%)	17 (94%)	1 (6%)	21	45
27	BD	215/218 (99%)	200 (93%)	15 (7%)	15	35
27	DD	215/218 (99%)	200 (93%)	15 (7%)	15	35
28	BE	164/166 (99%)	150 (92%)	14 (8%)	10	24
28	DE	164/166 (99%)	147 (90%)	17 (10%)	7	16
29	BF	160/166 (96%)	145 (91%)	15 (9%)	8	20
29	DF	159/166 (96%)	144 (91%)	15 (9%)	8	20
30	BG	143/156 (92%)	128 (90%)	15 (10%)	7	16
30	DG	142/156 (91%)	128 (90%)	14 (10%)	8	18
31	BH	144/148 (97%)	133 (92%)	11 (8%)	13	30
31	DH	144/148 (97%)	134 (93%)	10 (7%)	15	35
32	BI	110/124 (89%)	88 (80%)	22 (20%)	1	3
32	DI	104/124 (84%)	90 (86%)	14 (14%)	4	9
33	BN	118/119 (99%)	103 (87%)	15 (13%)	4	10
33	DN	118/119 (99%)	106 (90%)	12 (10%)	7	17
34	BO	100/100 (100%)	95 (95%)	5 (5%)	24	51
34	DO	100/100 (100%)	96 (96%)	4 (4%)	31	60
35	BP	115/116 (99%)	105 (91%)	10 (9%)	10	23
35	DP	115/116 (99%)	106 (92%)	9 (8%)	12	29
36	BQ	111/111 (100%)	100 (90%)	11 (10%)	8	18
36	DQ	111/111 (100%)	103 (93%)	8 (7%)	14	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	BR	101/101 (100%)	87 (86%)	14 (14%)	3	8
37	DR	101/101 (100%)	88 (87%)	13 (13%)	4	10
38	BS	87/88 (99%)	83 (95%)	4 (5%)	27	54
38	DS	85/88 (97%)	77 (91%)	8 (9%)	8	20
39	BT	115/127 (91%)	106 (92%)	9 (8%)	12	29
39	DT	113/127 (89%)	104 (92%)	9 (8%)	12	27
40	BU	93/94 (99%)	87 (94%)	6 (6%)	17	38
40	DU	93/94 (99%)	87 (94%)	6 (6%)	17	38
41	BV	80/82 (98%)	72 (90%)	8 (10%)	7	18
41	DV	80/82 (98%)	72 (90%)	8 (10%)	7	18
42	BW	90/92 (98%)	85 (94%)	5 (6%)	21	45
42	DW	90/92 (98%)	84 (93%)	6 (7%)	16	37
43	BX	77/78 (99%)	73 (95%)	4 (5%)	23	49
43	DX	77/78 (99%)	73 (95%)	4 (5%)	23	49
44	BY	85/91 (93%)	81 (95%)	4 (5%)	26	54
44	DY	85/91 (93%)	78 (92%)	7 (8%)	11	26
45	BZ	145/179 (81%)	131 (90%)	14 (10%)	8	19
45	DZ	145/179 (81%)	132 (91%)	13 (9%)	9	22
46	B0	65/67 (97%)	62 (95%)	3 (5%)	27	54
46	D0	65/67 (97%)	62 (95%)	3 (5%)	27	54
47	B1	80/83 (96%)	74 (92%)	6 (8%)	13	31
47	D1	80/83 (96%)	75 (94%)	5 (6%)	18	40
48	B2	65/67 (97%)	61 (94%)	4 (6%)	18	40
48	D2	65/67 (97%)	60 (92%)	5 (8%)	13	30
49	B3	51/52 (98%)	46 (90%)	5 (10%)	8	18
49	D3	50/52 (96%)	45 (90%)	5 (10%)	7	18
50	B4	60/63 (95%)	51 (85%)	9 (15%)	3	7
50	D4	53/63 (84%)	46 (87%)	7 (13%)	4	9
51	B5	50/52 (96%)	42 (84%)	8 (16%)	2	6
51	D5	50/52 (96%)	47 (94%)	3 (6%)	19	42
52	B6	51/52 (98%)	45 (88%)	6 (12%)	5	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	D6	50/52 (96%)	49 (98%)	1 (2%)	55	81
53	B7	41/42 (98%)	38 (93%)	3 (7%)	14	33
53	D7	41/42 (98%)	41 (100%)	0	100	100
54	B8	53/55 (96%)	49 (92%)	4 (8%)	13	31
54	D8	54/55 (98%)	52 (96%)	2 (4%)	34	63
55	B9	34/34 (100%)	33 (97%)	1 (3%)	42	71
55	D9	34/34 (100%)	33 (97%)	1 (3%)	42	71
All	All	9315/10066 (92%)	8513 (91%)	802 (9%)	10	24

5 of 802 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BZ	61	LEU
3	CC	21	ARG
42	DW	15	ARG
46	B0	20	ARG
52	B6	4	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 147 such sidechains are listed below:

Mol	Chain	Res	Type
49	B3	32	GLN
4	CD	123	HIS
41	DV	80	GLN
52	B6	20	ASN
3	CC	28	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1494/1521 (98%)	363 (24%)	26 (1%)
1	CA	1501/1521 (98%)	372 (24%)	32 (2%)
22	AV	7/24 (29%)	0	0
22	CV	4/24 (16%)	1 (25%)	0
23	AX	75/77 (97%)	25 (33%)	0
23	CX	75/77 (97%)	23 (30%)	0
24	AY	16/76 (21%)	7 (43%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	CY	4/76 (5%)	0	0
25	BA	2814/2915 (96%)	473 (16%)	31 (1%)
25	DA	2791/2915 (95%)	523 (18%)	27 (0%)
26	BB	119/121 (98%)	24 (20%)	0
26	DB	119/121 (98%)	25 (21%)	0
All	All	9019/9468 (95%)	1836 (20%)	116 (1%)

5 of 1836 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	22	G
1	AA	32	A

5 of 116 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2442	A
1	CA	560	U
25	DA	1913	A
25	BA	2701	U
1	CA	65	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	5MU	AX	54	23	15,22,23	1.11	2 (13%)	16,32,35	2.39	2 (12%)
23	PSU	CX	55	23	17,21,22	1.53	2 (11%)	20,30,33	3.21	6 (30%)
23	5MC	AX	32	23	15,22,23	1.38	1 (6%)	19,32,35	1.53	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	4SU	CX	8	23	14,21,22	1.16	2 (14%)	15,30,33	2.77	3 (20%)
23	5MU	CX	54	23	15,22,23	1.12	2 (13%)	16,32,35	2.03	2 (12%)
23	PSU	AX	55	23	17,21,22	1.72	3 (17%)	20,30,33	3.25	6 (30%)
23	4SU	AX	8	23	14,21,22	1.49	2 (14%)	15,30,33	2.76	2 (13%)
23	5MC	CX	32	23	15,22,23	1.24	1 (6%)	19,32,35	1.39	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	5MU	AX	54	23	-	0/5/25/26	0/2/2/2
23	PSU	CX	55	23	-	0/7/25/26	0/2/2/2
23	5MC	AX	32	23	-	0/5/25/26	0/2/2/2
23	4SU	CX	8	23	-	0/5/25/26	0/2/2/2
23	5MU	CX	54	23	-	0/5/25/26	0/2/2/2
23	PSU	AX	55	23	-	0/7/25/26	0/2/2/2
23	4SU	AX	8	23	-	0/5/25/26	0/2/2/2
23	5MC	CX	32	23	-	0/5/25/26	0/2/2/2

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AX	55	PSU	C5-C1'	-5.21	1.47	1.52
23	AX	32	5MC	C5-C4	4.91	1.49	1.41
23	CX	32	5MC	C5-C4	4.41	1.48	1.41
23	AX	8	4SU	C4-S4	-4.15	1.59	1.67
23	CX	55	PSU	C5-C1'	-4.13	1.48	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AX	8	4SU	C2-N3-C4	9.61	129.08	115.15
23	CX	8	4SU	C2-N3-C4	9.00	128.20	115.15
23	AX	54	5MU	C4-N3-C2	9.00	122.74	115.14
23	CX	55	PSU	N1-C2-N3	-8.55	121.63	128.43
23	AX	55	PSU	N1-C2-N3	-8.49	121.68	128.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AX	32	5MC	1	0
23	CX	8	4SU	1	0
23	CX	54	5MU	1	0
23	AX	8	4SU	1	0
23	CX	32	5MC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2061 ligands modelled in this entry, 2057 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	SF4	CD	501	4	0,12,12	0.00	-	-		
57	PCY	AA	3191	-	36,42,42	1.85	5 (13%)	41,65,65	1.52	8 (19%)
57	PCY	CA	3176	-	36,42,42	1.68	5 (13%)	41,65,65	0.96	3 (7%)
58	SF4	AD	501	4	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	CD	501	4	-	-	0/6/5/5
57	PCY	AA	3191	-	-	18/33/67/67	0/3/3/3
57	PCY	CA	3176	-	-	7/33/67/67	0/3/3/3
58	SF4	AD	501	4	-	-	0/6/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	AA	3191	PCY	C34-C30	-5.67	1.39	1.51
57	AA	3191	PCY	C28-C32	-5.48	1.39	1.49
57	CA	3176	PCY	C34-C30	-5.38	1.40	1.51
57	CA	3176	PCY	C28-C32	-4.82	1.40	1.49
57	AA	3191	PCY	C17-N20	4.68	1.51	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	AA	3191	PCY	O21-C18-C15	4.06	115.29	107.79
57	AA	3191	PCY	O21-C23-C27	4.01	121.35	112.33
57	AA	3191	PCY	C18-O21-C23	-2.79	110.93	116.57
57	CA	3176	PCY	C10-N4-C9	2.46	123.39	115.77
57	AA	3191	PCY	C30-C27-C23	2.43	127.43	120.47

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	AA	3191	PCY	N2-C3-C6-C11
57	AA	3191	PCY	N2-C3-C6-O12
57	AA	3191	PCY	C7-C3-C6-C11
57	AA	3191	PCY	C7-C3-C6-O12
57	AA	3191	PCY	C8-C3-C6-C11

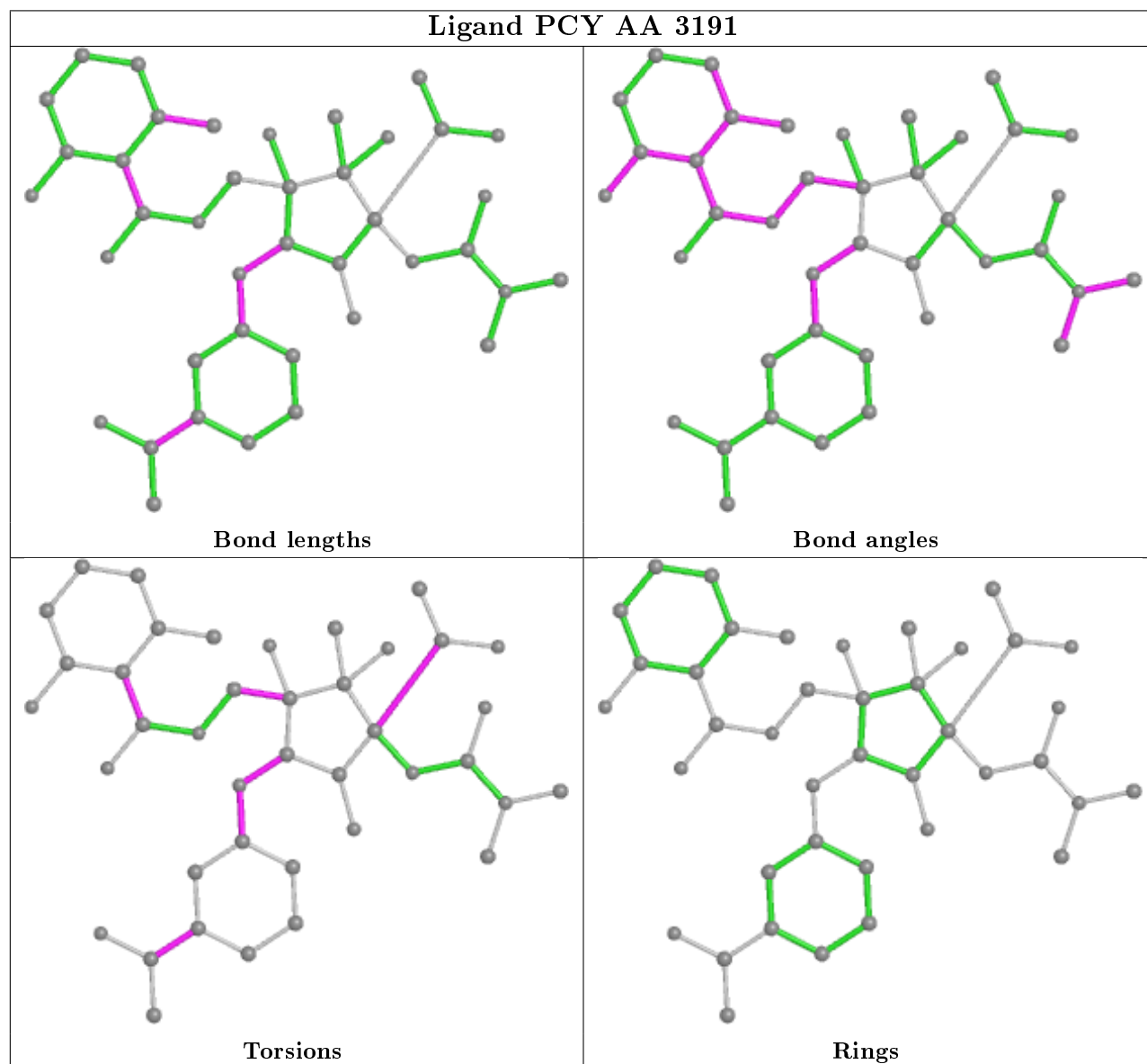
There are no ring outliers.

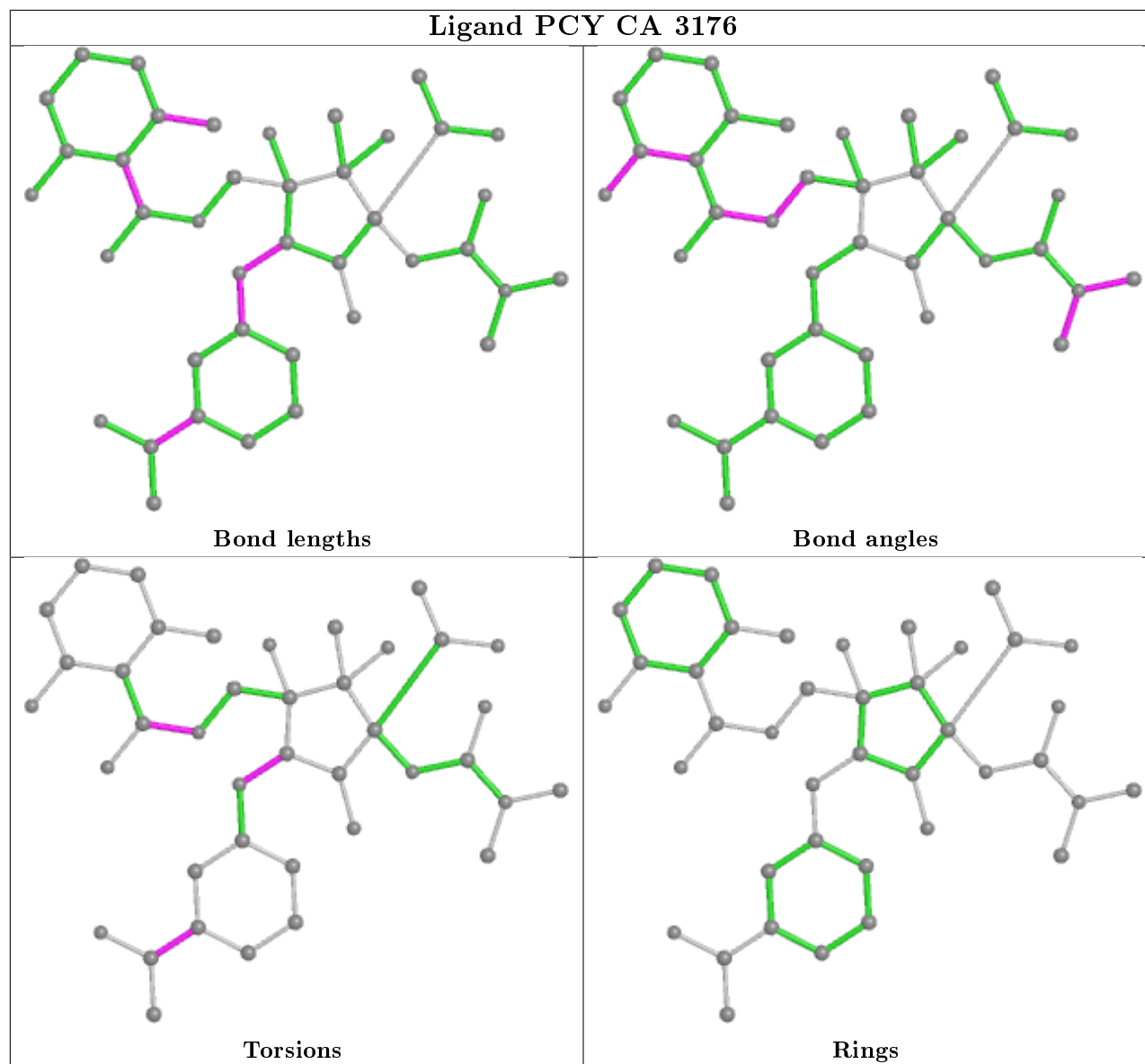
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	3191	PCY	6	0
57	CA	3176	PCY	4	0
58	AD	501	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1497/1521 (98%)	0.03	13 (0%) 84 85	40, 76, 97, 113	0
1	CA	1503/1521 (98%)	0.02	29 (1%) 66 69	42, 77, 97, 113	0
2	AB	231/256 (90%)	0.30	11 (4%) 30 28	71, 85, 93, 98	0
2	CB	231/256 (90%)	1.18	58 (25%) 0 0	71, 86, 94, 98	0
3	AC	206/239 (86%)	1.02	40 (19%) 1 0	69, 83, 91, 95	0
3	CC	206/239 (86%)	1.33	59 (28%) 0 0	69, 84, 92, 96	0
4	AD	208/209 (99%)	1.16	46 (22%) 0 0	60, 76, 86, 91	0
4	CD	208/209 (99%)	0.97	26 (12%) 3 3	60, 76, 84, 89	0
5	AE	148/162 (91%)	0.91	13 (8%) 10 8	56, 72, 81, 88	0
5	CE	148/162 (91%)	1.23	36 (24%) 0 0	58, 74, 83, 89	0
6	AF	100/101 (99%)	0.66	9 (9%) 9 7	61, 74, 82, 85	0
6	CF	100/101 (99%)	0.46	7 (7%) 16 14	62, 75, 83, 86	0
7	AG	155/156 (99%)	1.09	27 (17%) 1 1	69, 79, 89, 98	0
7	CG	155/156 (99%)	1.30	38 (24%) 0 0	70, 80, 90, 99	0
8	AH	137/138 (99%)	0.85	19 (13%) 2 2	61, 74, 81, 85	0
8	CH	137/138 (99%)	0.92	21 (15%) 2 1	63, 75, 83, 88	0
9	AI	127/128 (99%)	1.11	26 (20%) 1 0	63, 85, 91, 94	0
9	CI	127/128 (99%)	2.24	65 (51%) 0 0	70, 86, 92, 96	0
10	AJ	97/105 (92%)	1.18	25 (25%) 0 0	73, 87, 94, 97	0
10	CJ	96/105 (91%)	1.95	42 (43%) 0 0	76, 89, 95, 96	0
11	AK	114/129 (88%)	0.57	5 (4%) 34 33	52, 72, 84, 87	0
11	CK	114/129 (88%)	0.38	5 (4%) 34 33	54, 74, 84, 87	0
12	AL	122/132 (92%)	0.64	17 (13%) 2 2	52, 67, 77, 81	0
12	CL	122/132 (92%)	1.19	25 (20%) 1 0	53, 67, 76, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	120/126 (95%)	0.86	15 (12%)	3 3	53, 75, 85, 93	0
13	CM	118/126 (93%)	1.60	39 (33%)	0 0	71, 88, 94, 98	0
14	AN	60/61 (98%)	1.81	26 (43%)	0 0	74, 80, 88, 90	0
14	CN	60/61 (98%)	3.46	44 (73%)	0 0	75, 83, 88, 92	0
15	AO	88/89 (98%)	0.76	7 (7%)	12 10	55, 69, 81, 85	0
15	CO	88/89 (98%)	1.06	14 (15%)	1 1	58, 71, 82, 86	0
16	AP	82/88 (93%)	1.25	19 (23%)	0 0	64, 75, 84, 91	0
16	CP	82/88 (93%)	1.06	13 (15%)	1 1	63, 73, 83, 89	0
17	AQ	99/105 (94%)	0.76	7 (7%)	16 14	55, 70, 79, 81	0
17	CQ	99/105 (94%)	1.57	35 (35%)	0 0	58, 71, 80, 84	0
18	AR	68/88 (77%)	0.59	5 (7%)	14 12	62, 74, 84, 89	0
18	CR	68/88 (77%)	0.63	5 (7%)	14 12	64, 74, 84, 91	0
19	AS	83/93 (89%)	0.85	6 (7%)	15 13	75, 85, 93, 94	0
19	CS	83/93 (89%)	1.94	39 (46%)	0 0	78, 87, 93, 96	0
20	AT	96/106 (90%)	0.60	5 (5%)	27 25	63, 72, 82, 87	0
20	CT	96/106 (90%)	0.66	13 (13%)	3 2	61, 73, 82, 87	0
21	AU	23/27 (85%)	1.10	4 (17%)	1 1	71, 77, 79, 81	0
21	CU	23/27 (85%)	2.26	11 (47%)	0 0	72, 79, 81, 83	0
22	AV	8/24 (33%)	3.57	5 (62%)	0 0	62, 89, 94, 97	0
22	CV	5/24 (20%)	2.64	3 (60%)	0 0	65, 73, 91, 96	0
23	AX	72/77 (93%)	0.18	1 (1%)	75 77	40, 71, 88, 98	0
23	CX	72/77 (93%)	0.12	3 (4%)	36 35	43, 74, 90, 97	0
24	AY	18/76 (23%)	3.72	13 (72%)	0 0	62, 104, 109, 109	0
24	CY	5/76 (6%)	5.80	5 (100%)	0 0	74, 101, 102, 106	0
25	BA	2822/2915 (96%)	0.54	51 (1%)	68 70	18, 41, 91, 109	0
25	DA	2800/2915 (96%)	-0.04	52 (1%)	66 69	22, 45, 91, 112	0
26	BB	120/121 (99%)	0.36	0	100 100	31, 63, 75, 88	0
26	DB	120/121 (99%)	-0.03	7 (5%)	23 22	38, 69, 81, 91	0
27	BD	275/276 (99%)	0.74	10 (3%)	42 42	20, 39, 58, 77	0
27	DD	275/276 (99%)	0.70	19 (6%)	16 15	22, 42, 60, 78	0
28	BE	204/206 (99%)	0.63	1 (0%)	91 92	19, 44, 64, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DE	204/206 (99%)	0.51	8 (3%) 39 38	22, 48, 66, 86	0
29	BF	203/210 (96%)	0.61	2 (0%) 82 83	21, 50, 74, 91	0
29	DF	203/210 (96%)	0.45	5 (2%) 57 59	24, 55, 77, 90	0
30	BG	181/182 (99%)	0.58	6 (3%) 46 46	55, 71, 83, 96	0
30	DG	181/182 (99%)	1.48	57 (31%) 0 0	60, 75, 84, 95	0
31	BH	174/180 (96%)	0.52	1 (0%) 89 91	45, 64, 75, 84	0
31	DH	174/180 (96%)	0.85	29 (16%) 1 1	53, 68, 79, 86	0
32	BI	146/148 (98%)	0.33	4 (2%) 54 55	48, 75, 84, 88	0
32	DI	146/148 (98%)	0.33	11 (7%) 14 12	51, 75, 84, 88	0
33	BN	140/140 (100%)	0.67	0 100 100	28, 45, 69, 79	0
33	DN	140/140 (100%)	0.50	3 (2%) 63 65	33, 49, 71, 81	0
34	BO	122/122 (100%)	0.64	3 (2%) 57 59	31, 45, 63, 70	0
34	DO	122/122 (100%)	0.56	7 (5%) 23 22	34, 48, 64, 70	0
35	BP	149/150 (99%)	0.62	1 (0%) 87 89	18, 53, 74, 82	0
35	DP	149/150 (99%)	0.60	9 (6%) 21 20	20, 56, 76, 84	0
36	BQ	141/141 (100%)	0.69	2 (1%) 75 77	29, 48, 65, 77	0
36	DQ	141/141 (100%)	1.06	22 (15%) 2 1	32, 52, 69, 78	0
37	BR	118/118 (100%)	0.46	0 100 100	19, 32, 49, 62	0
37	DR	118/118 (100%)	0.94	12 (10%) 6 5	35, 53, 66, 78	0
38	BS	110/112 (98%)	0.32	0 100 100	30, 47, 65, 70	0
38	DS	110/112 (98%)	1.20	22 (20%) 1 0	63, 77, 88, 93	0
39	BT	131/146 (89%)	0.33	0 100 100	30, 43, 71, 85	0
39	DT	131/146 (89%)	0.51	6 (4%) 32 31	43, 59, 78, 88	0
40	BU	116/118 (98%)	0.38	0 100 100	15, 27, 48, 62	0
40	DU	116/118 (98%)	0.82	9 (7%) 13 11	38, 59, 76, 87	0
41	BV	101/101 (100%)	0.22	0 100 100	14, 35, 57, 76	0
41	DV	101/101 (100%)	0.44	3 (2%) 50 51	43, 71, 84, 90	0
42	BW	112/113 (99%)	0.35	0 100 100	17, 28, 50, 75	0
42	DW	112/113 (99%)	0.89	11 (9%) 7 5	34, 50, 68, 92	0
43	BX	95/96 (98%)	0.36	0 100 100	17, 35, 65, 78	0
43	DX	95/96 (98%)	1.61	31 (32%) 0 0	44, 62, 77, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BY	107/110 (97%)	0.38	2 (1%) 66 69	28, 47, 67, 85	0
44	DY	107/110 (97%)	1.24	21 (19%) 1 0	51, 72, 83, 88	0
45	BZ	171/206 (83%)	0.25	1 (0%) 89 91	36, 62, 81, 90	0
45	DZ	174/206 (84%)	1.08	28 (16%) 1 1	66, 83, 93, 96	0
46	B0	83/85 (97%)	0.72	7 (8%) 11 9	12, 33, 66, 84	0
46	D0	83/85 (97%)	1.79	23 (27%) 0 0	34, 64, 78, 91	0
47	B1	97/98 (98%)	0.68	5 (5%) 27 25	19, 43, 69, 72	0
47	D1	97/98 (98%)	0.90	10 (10%) 6 5	37, 57, 78, 82	0
48	B2	70/72 (97%)	0.33	0 100 100	30, 46, 63, 77	0
48	D2	70/72 (97%)	0.53	2 (2%) 51 52	56, 71, 80, 85	0
49	B3	59/60 (98%)	0.28	0 100 100	20, 31, 56, 83	0
49	D3	59/60 (98%)	1.65	20 (33%) 0 0	47, 62, 77, 91	0
50	B4	69/71 (97%)	0.73	6 (8%) 10 8	55, 77, 92, 99	0
50	D4	69/71 (97%)	1.52	22 (31%) 0 0	77, 91, 99, 105	0
51	B5	59/60 (98%)	0.47	2 (3%) 45 45	11, 28, 53, 67	0
51	D5	59/60 (98%)	0.50	3 (5%) 28 26	27, 52, 68, 81	0
52	B6	53/54 (98%)	0.26	0 100 100	27, 39, 56, 67	0
52	D6	53/54 (98%)	0.32	2 (3%) 40 39	45, 62, 73, 79	0
53	B7	48/49 (97%)	0.79	5 (10%) 6 4	16, 23, 52, 68	0
53	D7	48/49 (97%)	1.02	6 (12%) 3 3	29, 40, 64, 77	0
54	B8	64/65 (98%)	0.64	1 (1%) 72 74	24, 31, 43, 61	0
54	D8	64/65 (98%)	1.14	10 (15%) 2 1	44, 53, 63, 72	0
55	B9	37/37 (100%)	0.68	2 (5%) 25 24	28, 45, 67, 72	0
55	D9	37/37 (100%)	1.09	5 (13%) 3 2	44, 55, 68, 75	0
All	All	20640/21596 (95%)	0.56	1586 (7%) 13 11	11, 64, 91, 113	0

The worst 5 of 1586 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	CG	82	GLY	12.8
2	CB	165	VAL	10.4
1	CA	1030(B)	C	9.9
13	AM	2	ALA	9.8
10	CJ	47	PHE	9.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	4SU	CX	8	20/21	0.90	0.15	73,81,98,100	0
23	PSU	CX	55	20/21	0.91	0.12	56,73,80,86	0
23	5MU	CX	54	21/22	0.93	0.18	69,80,93,106	0
23	5MU	AX	54	21/22	0.94	0.16	60,72,80,91	0
23	PSU	AX	55	20/21	0.95	0.17	56,70,78,80	0
23	5MC	CX	32	21/22	0.95	0.21	66,75,83,86	0
23	5MC	AX	32	21/22	0.96	0.24	38,59,69,83	0
23	4SU	AX	8	20/21	0.96	0.18	47,67,77,84	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3098	1/1	0.38	0.14	71,71,71,71	0
56	MG	DA	3655	1/1	0.40	1.89	74,74,74,74	0
56	MG	BA	3703	1/1	0.52	0.21	57,57,57,57	0
56	MG	BB	205	1/1	0.56	0.18	76,76,76,76	0
56	MG	CA	3043	1/1	0.59	0.14	67,67,67,67	0
56	MG	CX	3002	1/1	0.62	0.16	81,81,81,81	0
56	MG	CA	3081	1/1	0.62	0.16	58,58,58,58	0
56	MG	BA	3237	1/1	0.63	0.32	63,63,63,63	0
56	MG	DA	3242	1/1	0.65	0.16	68,68,68,68	0
56	MG	DA	3484	1/1	0.65	0.16	32,32,32,32	0
56	MG	CA	3084	1/1	0.66	0.14	71,71,71,71	0
56	MG	CA	3158	1/1	0.66	0.14	75,75,75,75	0
56	MG	AA	3038	1/1	0.67	0.20	61,61,61,61	0
56	MG	BA	3044	1/1	0.68	0.29	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	BB	209	1/1	0.68	0.19	69,69,69,69	0
56	MG	AA	3034	1/1	0.68	0.19	70,70,70,70	0
56	MG	BA	3547	1/1	0.68	0.14	64,64,64,64	0
56	MG	AA	3125	1/1	0.68	0.35	72,72,72,72	0
56	MG	DA	3192	1/1	0.69	0.16	57,57,57,57	0
56	MG	AA	3147	1/1	0.69	0.14	72,72,72,72	0
56	MG	CA	3045	1/1	0.70	0.26	68,68,68,68	0
56	MG	DW	201	1/1	0.71	0.28	67,67,67,67	0
56	MG	CA	3078	1/1	0.71	0.15	64,64,64,64	0
56	MG	DA	3649	1/1	0.71	0.23	53,53,53,53	0
56	MG	AA	3020	1/1	0.72	0.14	71,71,71,71	0
56	MG	CA	3079	1/1	0.72	0.16	67,67,67,67	0
56	MG	DA	3222	1/1	0.73	0.14	46,46,46,46	0
56	MG	BA	3813	1/1	0.73	0.09	58,58,58,58	0
56	MG	BA	3325	1/1	0.73	0.15	51,51,51,51	0
56	MG	BA	3241	1/1	0.73	0.13	45,45,45,45	0
56	MG	AA	3166	1/1	0.73	0.48	74,74,74,74	0
59	ZN	D4	501	1/1	0.73	0.07	151,151,151,151	0
56	MG	CA	3006	1/1	0.73	0.18	59,59,59,59	0
56	MG	DA	3647	1/1	0.73	0.45	53,53,53,53	0
56	MG	BB	211	1/1	0.74	0.17	81,81,81,81	0
56	MG	BA	3059	1/1	0.74	0.14	49,49,49,49	0
56	MG	DA	3536	1/1	0.74	0.10	44,44,44,44	0
56	MG	DA	3533	1/1	0.74	0.14	52,52,52,52	0
56	MG	DE	303	1/1	0.74	0.40	62,62,62,62	0
56	MG	DA	3640	1/1	0.74	0.43	64,64,64,64	0
56	MG	CA	3082	1/1	0.74	0.23	73,73,73,73	0
56	MG	CA	3001	1/1	0.74	0.09	59,59,59,59	0
56	MG	AA	3184	1/1	0.74	0.12	66,66,66,66	0
56	MG	BE	306	1/1	0.74	0.71	93,93,93,93	0
56	MG	BA	3514	1/1	0.74	0.15	45,45,45,45	0
56	MG	DA	3110	1/1	0.75	0.15	64,64,64,64	0
56	MG	DA	3488	1/1	0.75	0.19	51,51,51,51	0
56	MG	B7	104	1/1	0.75	0.19	64,64,64,64	0
56	MG	BA	3139	1/1	0.75	0.34	53,53,53,53	0
56	MG	DA	3627	1/1	0.75	0.18	64,64,64,64	0
56	MG	BA	3221	1/1	0.75	0.13	39,39,39,39	0
56	MG	DA	3080	1/1	0.76	0.16	49,49,49,49	0
56	MG	CA	3148	1/1	0.76	0.11	88,88,88,88	0
56	MG	CA	3171	1/1	0.77	0.18	65,65,65,65	0
56	MG	CJ	5001	1/1	0.77	0.11	94,94,94,94	0
56	MG	CA	3107	1/1	0.77	0.18	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3605	1/1	0.77	0.17	44,44,44,44	0
56	MG	CA	3053	1/1	0.77	0.18	55,55,55,55	0
56	MG	AA	3170	1/1	0.77	0.12	73,73,73,73	0
56	MG	BA	3048	1/1	0.77	0.43	47,47,47,47	0
56	MG	DA	3026	1/1	0.77	0.22	52,52,52,52	0
56	MG	AX	3002	1/1	0.78	0.18	69,69,69,69	0
56	MG	BA	3099	1/1	0.78	0.22	67,67,67,67	0
56	MG	DA	3210	1/1	0.78	0.20	53,53,53,53	0
56	MG	BZ	301	1/1	0.78	0.23	58,58,58,58	0
56	MG	DA	3423	1/1	0.78	0.15	56,56,56,56	0
56	MG	AA	3067	1/1	0.78	0.19	72,72,72,72	0
56	MG	BA	3292	1/1	0.78	0.27	40,40,40,40	0
56	MG	CA	3083	1/1	0.78	0.17	72,72,72,72	0
56	MG	AA	3169	1/1	0.78	0.26	73,73,73,73	0
56	MG	BA	3092	1/1	0.78	0.22	53,53,53,53	0
56	MG	BA	3657	1/1	0.78	0.15	52,52,52,52	0
56	MG	CA	3124	1/1	0.78	0.20	75,75,75,75	0
56	MG	B2	3001	1/1	0.79	0.20	49,49,49,49	0
56	MG	AA	3124	1/1	0.79	0.10	71,71,71,71	0
56	MG	BA	3447	1/1	0.79	0.15	59,59,59,59	0
56	MG	DA	3074	1/1	0.79	0.11	56,56,56,56	0
56	MG	DA	3255	1/1	0.79	0.12	62,62,62,62	0
56	MG	CE	201	1/1	0.79	0.20	73,73,73,73	0
56	MG	BA	3172	1/1	0.79	0.24	52,52,52,52	0
56	MG	BA	3498	1/1	0.79	0.20	43,43,43,43	0
56	MG	DA	3019	1/1	0.79	0.14	48,48,48,48	0
56	MG	BA	3028	1/1	0.79	0.24	52,52,52,52	0
56	MG	DA	3097	1/1	0.79	0.27	57,57,57,57	0
56	MG	CA	3174	1/1	0.79	0.56	80,80,80,80	0
56	MG	AA	3062	1/1	0.79	0.20	67,67,67,67	0
56	MG	CT	3001	1/1	0.79	0.14	59,59,59,59	0
57	PCY	CA	3176	40/40	0.80	0.43	72,89,98,102	0
56	MG	BA	3512	1/1	0.80	0.32	47,47,47,47	0
56	MG	BA	3375	1/1	0.80	0.13	38,38,38,38	0
56	MG	AA	3059	1/1	0.80	0.15	64,64,64,64	0
56	MG	CA	3016	1/1	0.80	0.15	53,53,53,53	0
56	MG	BU	206	1/1	0.80	1.07	61,61,61,61	0
56	MG	DA	3032	1/1	0.80	0.17	47,47,47,47	0
56	MG	BA	3711	1/1	0.80	0.40	51,51,51,51	0
56	MG	BA	3294	1/1	0.80	0.36	67,67,67,67	0
56	MG	BA	3521	1/1	0.80	0.29	29,29,29,29	0
56	MG	DA	3402	1/1	0.80	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BZ	302	1/1	0.80	0.26	56,56,56,56	0
56	MG	BA	3290	1/1	0.80	0.34	50,50,50,50	0
56	MG	BA	3692	1/1	0.80	0.12	51,51,51,51	0
56	MG	AA	3185	1/1	0.80	0.19	61,61,61,61	0
56	MG	DA	3603	1/1	0.80	0.19	55,55,55,55	0
56	MG	DA	3653	1/1	0.80	0.18	32,32,32,32	0
56	MG	DA	3469	1/1	0.80	0.10	53,53,53,53	0
56	MG	AA	3040	1/1	0.80	0.13	72,72,72,72	0
56	MG	CA	3092	1/1	0.80	0.25	61,61,61,61	0
56	MG	DA	3657	1/1	0.80	0.19	56,56,56,56	0
56	MG	BA	3288	1/1	0.81	0.11	44,44,44,44	0
56	MG	DA	3024	1/1	0.81	0.61	37,37,37,37	0
56	MG	BA	3030	1/1	0.81	0.15	40,40,40,40	0
56	MG	BA	3199	1/1	0.81	0.44	51,51,51,51	0
56	MG	BA	3607	1/1	0.81	0.17	51,51,51,51	0
56	MG	CA	3009	1/1	0.81	0.27	66,66,66,66	0
56	MG	CA	3011	1/1	0.81	0.13	69,69,69,69	0
56	MG	AF	3001	1/1	0.81	0.16	56,56,56,56	0
56	MG	DA	3644	1/1	0.81	0.12	40,40,40,40	0
56	MG	BA	3296	1/1	0.81	0.21	47,47,47,47	0
56	MG	CA	3097	1/1	0.81	0.22	64,64,64,64	0
56	MG	BA	3050	1/1	0.81	0.16	46,46,46,46	0
56	MG	AA	3094	1/1	0.81	0.12	66,66,66,66	0
56	MG	AA	3049	1/1	0.81	0.28	64,64,64,64	0
56	MG	DA	3083	1/1	0.81	0.20	63,63,63,63	0
56	MG	CA	3129	1/1	0.81	0.11	69,69,69,69	0
56	MG	DA	3455	1/1	0.81	0.20	46,46,46,46	0
56	MG	DA	3389	1/1	0.81	0.10	50,50,50,50	0
56	MG	AA	3084	1/1	0.81	0.11	62,62,62,62	0
56	MG	DB	3001	1/1	0.81	0.17	77,77,77,77	0
56	MG	CA	3131	1/1	0.81	0.14	81,81,81,81	0
56	MG	DA	3286	1/1	0.82	0.15	54,54,54,54	0
56	MG	DV	3003	1/1	0.82	0.10	55,55,55,55	0
56	MG	DA	3043	1/1	0.82	0.11	52,52,52,52	0
56	MG	DA	3586	1/1	0.82	0.12	39,39,39,39	0
56	MG	BA	3256	1/1	0.82	0.24	54,54,54,54	0
56	MG	AA	3048	1/1	0.82	0.22	59,59,59,59	0
56	MG	CA	3067	1/1	0.82	0.18	72,72,72,72	0
56	MG	BA	3111	1/1	0.82	0.09	57,57,57,57	0
56	MG	AA	3171	1/1	0.82	0.17	67,67,67,67	0
56	MG	DA	3612	1/1	0.82	0.16	58,58,58,58	0
56	MG	BA	3040	1/1	0.82	0.20	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	3069	1/1	0.82	0.13	55,55,55,55	0
56	MG	BA	3475	1/1	0.82	0.12	45,45,45,45	0
56	MG	BA	3109	1/1	0.82	0.21	56,56,56,56	0
56	MG	CA	3022	1/1	0.83	0.18	60,60,60,60	0
56	MG	DA	3643	1/1	0.83	0.18	49,49,49,49	0
56	MG	DA	3087	1/1	0.83	0.32	50,50,50,50	0
56	MG	DF	302	1/1	0.83	0.28	44,44,44,44	0
56	MG	DA	3062	1/1	0.83	0.16	51,51,51,51	0
56	MG	DA	3037	1/1	0.83	0.16	34,34,34,34	0
56	MG	BB	206	1/1	0.83	0.32	58,58,58,58	0
56	MG	DA	3033	1/1	0.83	0.55	54,54,54,54	0
56	MG	AA	3100	1/1	0.83	0.13	66,66,66,66	0
57	PCY	AA	3191	40/40	0.83	0.43	59,86,97,99	0
56	MG	BA	3525	1/1	0.83	0.23	23,23,23,23	0
56	MG	DA	3164	1/1	0.83	0.20	47,47,47,47	0
56	MG	DA	3673	1/1	0.83	0.52	68,68,68,68	0
56	MG	CA	3032	1/1	0.83	0.10	57,57,57,57	0
56	MG	CA	3089	1/1	0.83	0.09	67,67,67,67	0
56	MG	AA	3076	1/1	0.83	0.16	56,56,56,56	0
56	MG	DA	3075	1/1	0.83	0.30	43,43,43,43	0
56	MG	BA	3168	1/1	0.83	0.23	39,39,39,39	0
56	MG	DA	3115	1/1	0.83	0.12	46,46,46,46	0
56	MG	BA	3437	1/1	0.83	0.24	61,61,61,61	0
56	MG	DA	3180	1/1	0.83	0.77	58,58,58,58	0
56	MG	CA	3087	1/1	0.83	0.12	62,62,62,62	0
56	MG	AX	3003	1/1	0.83	0.23	66,66,66,66	0
56	MG	BA	3604	1/1	0.83	0.25	46,46,46,46	0
56	MG	DA	3181	1/1	0.83	0.18	54,54,54,54	0
56	MG	DA	3607	1/1	0.83	0.17	63,63,63,63	0
56	MG	DD	308	1/1	0.84	0.80	72,72,72,72	0
56	MG	AX	3009	1/1	0.84	0.15	74,74,74,74	0
56	MG	BA	3389	1/1	0.84	0.18	56,56,56,56	0
56	MG	DA	3036	1/1	0.84	0.09	46,46,46,46	0
56	MG	BA	3455	1/1	0.84	0.14	32,32,32,32	0
56	MG	DA	3660	1/1	0.84	0.08	28,28,28,28	0
56	MG	DA	3491	1/1	0.84	0.12	42,42,42,42	0
56	MG	AA	3163	1/1	0.84	0.17	58,58,58,58	0
56	MG	AA	3157	1/1	0.84	0.19	84,84,84,84	0
56	MG	BA	3135	1/1	0.84	0.12	61,61,61,61	0
56	MG	B4	502	1/1	0.84	0.10	77,77,77,77	0
56	MG	AX	3007	1/1	0.84	0.13	69,69,69,69	0
56	MG	BA	3327	1/1	0.84	0.18	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3616	1/1	0.84	0.15	51,51,51,51	0
56	MG	DA	3502	1/1	0.84	0.09	48,48,48,48	0
56	MG	BA	3598	1/1	0.84	0.29	53,53,53,53	0
56	MG	DA	3203	1/1	0.84	0.11	50,50,50,50	0
56	MG	BA	3545	1/1	0.84	0.14	36,36,36,36	0
56	MG	BA	3088	1/1	0.84	0.54	49,49,49,49	0
56	MG	DA	3109	1/1	0.84	0.11	68,68,68,68	0
56	MG	DA	3208	1/1	0.84	0.19	44,44,44,44	0
56	MG	DA	3101	1/1	0.84	0.27	55,55,55,55	0
56	MG	BA	3672	1/1	0.84	0.11	62,62,62,62	0
56	MG	AA	3134	1/1	0.84	0.14	65,65,65,65	0
56	MG	BA	3175	1/1	0.84	0.28	57,57,57,57	0
56	MG	DA	3241	1/1	0.84	0.12	48,48,48,48	0
56	MG	CA	3036	1/1	0.84	0.18	72,72,72,72	0
56	MG	CA	3159	1/1	0.84	0.12	71,71,71,71	0
56	MG	DA	3285	1/1	0.84	0.15	52,52,52,52	0
56	MG	DA	3494	1/1	0.84	0.31	57,57,57,57	0
56	MG	BA	3392	1/1	0.84	0.21	41,41,41,41	0
56	MG	CA	3002	1/1	0.84	0.09	62,62,62,62	0
56	MG	DA	3593	1/1	0.84	0.11	50,50,50,50	0
56	MG	CA	3152	1/1	0.84	0.23	54,54,54,54	0
56	MG	DA	3126	1/1	0.84	0.21	46,46,46,46	0
56	MG	BA	3097	1/1	0.84	0.18	52,52,52,52	0
56	MG	BA	3276	1/1	0.84	0.16	42,42,42,42	0
56	MG	DA	3031	1/1	0.85	0.11	44,44,44,44	0
56	MG	DA	3572	1/1	0.85	0.06	68,68,68,68	0
56	MG	DA	3194	1/1	0.85	0.12	54,54,54,54	0
56	MG	CA	3050	1/1	0.85	0.17	52,52,52,52	0
56	MG	BA	3673	1/1	0.85	0.15	28,28,28,28	0
56	MG	DA	3100	1/1	0.85	0.12	66,66,66,66	0
56	MG	DA	3034	1/1	0.85	0.12	45,45,45,45	0
56	MG	CA	3021	1/1	0.85	0.21	65,65,65,65	0
56	MG	AA	3153	1/1	0.85	0.12	81,81,81,81	0
56	MG	DA	3570	1/1	0.85	0.19	59,59,59,59	0
56	MG	BA	3696	1/1	0.85	0.10	45,45,45,45	0
56	MG	DB	3003	1/1	0.85	0.19	56,56,56,56	0
56	MG	BA	3026	1/1	0.85	0.26	49,49,49,49	0
56	MG	DA	3466	1/1	0.85	0.28	66,66,66,66	0
56	MG	DA	3500	1/1	0.85	0.11	51,51,51,51	0
56	MG	BA	3457	1/1	0.85	0.17	47,47,47,47	0
56	MG	BA	3786	1/1	0.85	0.18	58,58,58,58	0
56	MG	BA	3585	1/1	0.85	0.08	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3044	1/1	0.85	0.15	49,49,49,49	0
56	MG	BA	3319	1/1	0.85	0.17	39,39,39,39	0
56	MG	BA	3700	1/1	0.85	0.13	53,53,53,53	0
56	MG	DA	3467	1/1	0.85	0.14	48,48,48,48	0
56	MG	BA	3093	1/1	0.85	0.16	48,48,48,48	0
56	MG	BA	3079	1/1	0.85	0.34	49,49,49,49	0
56	MG	DA	3420	1/1	0.85	0.13	40,40,40,40	0
56	MG	CA	3077	1/1	0.85	0.18	61,61,61,61	0
56	MG	DE	304	1/1	0.85	0.14	40,40,40,40	0
56	MG	DA	3409	1/1	0.85	0.14	55,55,55,55	0
56	MG	DA	3090	1/1	0.85	0.11	48,48,48,48	0
56	MG	BA	3580	1/1	0.85	0.21	48,48,48,48	0
56	MG	BA	3019	1/1	0.85	0.14	39,39,39,39	0
56	MG	CA	3168	1/1	0.85	0.15	60,60,60,60	0
56	MG	CA	3125	1/1	0.85	0.10	63,63,63,63	0
56	MG	BA	3103	1/1	0.85	0.17	44,44,44,44	0
56	MG	DA	3347	1/1	0.85	0.13	46,46,46,46	0
56	MG	CA	3049	1/1	0.85	0.17	71,71,71,71	0
56	MG	BA	3016	1/1	0.85	0.12	37,37,37,37	0
56	MG	AE	201	1/1	0.85	0.20	64,64,64,64	0
56	MG	BA	3480	1/1	0.85	0.12	50,50,50,50	0
56	MG	BA	3018	1/1	0.85	0.22	63,63,63,63	0
56	MG	BA	3185	1/1	0.85	0.18	52,52,52,52	0
56	MG	DA	3556	1/1	0.85	0.16	55,55,55,55	0
56	MG	DA	3342	1/1	0.85	0.06	46,46,46,46	0
56	MG	BA	3636	1/1	0.85	0.21	52,52,52,52	0
56	MG	CA	3138	1/1	0.85	0.16	65,65,65,65	0
56	MG	AA	3047	1/1	0.85	0.17	63,63,63,63	0
56	MG	BA	3505	1/1	0.86	0.24	33,33,33,33	0
56	MG	DA	3229	1/1	0.86	0.10	64,64,64,64	0
56	MG	DA	3588	1/1	0.86	0.10	65,65,65,65	0
59	ZN	CN	501	1/1	0.86	0.10	103,103,103,103	0
56	MG	BA	3249	1/1	0.86	0.28	40,40,40,40	0
56	MG	BF	308	1/1	0.86	0.37	45,45,45,45	0
56	MG	DA	3244	1/1	0.86	0.26	59,59,59,59	0
56	MG	BA	3468	1/1	0.86	0.15	45,45,45,45	0
56	MG	BA	3460	1/1	0.86	0.15	58,58,58,58	0
56	MG	CA	3029	1/1	0.86	0.09	58,58,58,58	0
56	MG	DA	3125	1/1	0.86	0.19	40,40,40,40	0
56	MG	DA	3042	1/1	0.86	0.11	46,46,46,46	0
56	MG	BA	3120	1/1	0.86	0.20	50,50,50,50	0
56	MG	AA	3079	1/1	0.86	0.21	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	CA	3105	1/1	0.86	0.12	51,51,51,51	0
56	MG	DA	3264	1/1	0.86	0.18	50,50,50,50	0
56	MG	DA	3294	1/1	0.86	0.08	36,36,36,36	0
56	MG	BA	3609	1/1	0.86	0.14	54,54,54,54	0
56	MG	BA	3381	1/1	0.86	0.13	45,45,45,45	0
56	MG	AE	203	1/1	0.86	0.76	73,73,73,73	0
56	MG	BA	3741	1/1	0.86	0.14	50,50,50,50	0
56	MG	BA	3555	1/1	0.86	0.15	61,61,61,61	0
56	MG	DD	301	1/1	0.86	0.24	43,43,43,43	0
56	MG	AA	3177	1/1	0.86	0.10	80,80,80,80	0
56	MG	DA	3527	1/1	0.86	0.20	61,61,61,61	0
56	MG	BA	3233	1/1	0.86	0.18	61,61,61,61	0
56	MG	CA	3142	1/1	0.86	0.13	81,81,81,81	0
56	MG	BA	3617	1/1	0.86	0.26	44,44,44,44	0
56	MG	BA	3017	1/1	0.86	0.17	52,52,52,52	0
56	MG	DA	3269	1/1	0.86	0.15	54,54,54,54	0
56	MG	DA	3138	1/1	0.86	0.22	63,63,63,63	0
56	MG	DB	3002	1/1	0.86	0.15	58,58,58,58	0
56	MG	DA	3372	1/1	0.86	0.13	24,24,24,24	0
56	MG	BA	3027	1/1	0.86	0.12	45,45,45,45	0
56	MG	AA	3015	1/1	0.86	0.12	65,65,65,65	0
56	MG	CA	3047	1/1	0.86	0.12	59,59,59,59	0
56	MG	BA	3083	1/1	0.86	0.19	51,51,51,51	0
56	MG	BG	3001	1/1	0.86	0.21	51,51,51,51	0
56	MG	CA	3041	1/1	0.86	0.17	62,62,62,62	0
56	MG	DA	3152	1/1	0.86	0.24	62,62,62,62	0
56	MG	DA	3248	1/1	0.86	0.14	49,49,49,49	0
56	MG	AA	3167	1/1	0.86	0.15	61,61,61,61	0
56	MG	DA	3245	1/1	0.86	0.15	47,47,47,47	0
56	MG	DA	3291	1/1	0.86	0.13	41,41,41,41	0
56	MG	CA	3100	1/1	0.86	0.08	69,69,69,69	0
56	MG	BA	3558	1/1	0.86	0.21	57,57,57,57	0
56	MG	DA	3433	1/1	0.86	0.13	34,34,34,34	0
56	MG	BB	210	1/1	0.86	0.24	55,55,55,55	0
56	MG	DA	3468	1/1	0.86	0.15	37,37,37,37	0
56	MG	BA	3690	1/1	0.86	0.18	52,52,52,52	0
56	MG	BN	3002	1/1	0.86	0.24	57,57,57,57	0
56	MG	BA	3745	1/1	0.86	0.24	58,58,58,58	0
56	MG	DA	3079	1/1	0.86	0.12	32,32,32,32	0
56	MG	DA	3162	1/1	0.87	0.23	37,37,37,37	0
56	MG	BA	3218	1/1	0.87	0.20	34,34,34,34	0
56	MG	DA	3370	1/1	0.87	0.10	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3387	1/1	0.87	0.14	45,45,45,45	0
56	MG	DA	3619	1/1	0.87	0.23	54,54,54,54	0
56	MG	BA	3693	1/1	0.87	0.14	74,74,74,74	0
56	MG	BA	3137	1/1	0.87	0.42	40,40,40,40	0
56	MG	BA	3490	1/1	0.87	0.12	60,60,60,60	0
56	MG	AA	3006	1/1	0.87	0.30	71,71,71,71	0
56	MG	DA	3277	1/1	0.87	0.18	54,54,54,54	0
56	MG	BA	3002	1/1	0.87	0.17	57,57,57,57	0
56	MG	BA	3706	1/1	0.87	0.11	63,63,63,63	0
56	MG	BA	3238	1/1	0.87	0.32	41,41,41,41	0
56	MG	DA	3485	1/1	0.87	0.16	43,43,43,43	0
56	MG	CA	3117	1/1	0.87	0.11	58,58,58,58	0
56	MG	DA	3225	1/1	0.87	0.11	49,49,49,49	0
56	MG	DA	3537	1/1	0.87	0.14	58,58,58,58	0
56	MG	DA	3493	1/1	0.87	0.15	63,63,63,63	0
56	MG	DA	3482	1/1	0.87	0.13	42,42,42,42	0
56	MG	BA	3807	1/1	0.87	0.71	66,66,66,66	0
56	MG	AA	3187	1/1	0.87	0.12	54,54,54,54	0
56	MG	DA	3107	1/1	0.87	0.12	43,43,43,43	0
56	MG	DA	3001	1/1	0.87	0.24	40,40,40,40	0
56	MG	DA	3053	1/1	0.87	0.51	37,37,37,37	0
56	MG	BA	3076	1/1	0.87	0.34	34,34,34,34	0
56	MG	DA	3060	1/1	0.87	0.15	48,48,48,48	0
56	MG	CA	3014	1/1	0.87	0.13	57,57,57,57	0
56	MG	DA	3236	1/1	0.87	0.11	42,42,42,42	0
56	MG	BA	3198	1/1	0.87	0.22	28,28,28,28	0
56	MG	CA	3144	1/1	0.87	0.06	68,68,68,68	0
56	MG	BA	3677	1/1	0.87	0.17	56,56,56,56	0
56	MG	BA	3434	1/1	0.87	0.25	40,40,40,40	0
56	MG	DA	3146	1/1	0.87	0.19	49,49,49,49	0
56	MG	BA	3430	1/1	0.87	0.15	31,31,31,31	0
56	MG	BA	3277	1/1	0.87	0.27	54,54,54,54	0
56	MG	DA	3331	1/1	0.87	0.08	49,49,49,49	0
56	MG	CA	3020	1/1	0.87	0.12	46,46,46,46	0
56	MG	AA	3026	1/1	0.87	0.10	71,71,71,71	0
56	MG	DA	3541	1/1	0.87	0.12	40,40,40,40	0
56	MG	AA	3180	1/1	0.87	0.14	49,49,49,49	0
56	MG	AA	3045	1/1	0.87	0.32	54,54,54,54	0
56	MG	DA	3624	1/1	0.87	0.49	46,46,46,46	0
56	MG	BA	3624	1/1	0.87	0.13	37,37,37,37	0
56	MG	CA	3030	1/1	0.87	0.18	56,56,56,56	0
56	MG	BN	3007	1/1	0.87	0.20	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3704	1/1	0.87	0.33	36,36,36,36	0
56	MG	DA	3054	1/1	0.87	0.10	39,39,39,39	0
56	MG	BA	3806	1/1	0.87	0.70	33,33,33,33	0
56	MG	DA	3256	1/1	0.87	0.12	46,46,46,46	0
56	MG	CA	3071	1/1	0.87	0.10	57,57,57,57	0
56	MG	AA	3021	1/1	0.87	0.13	62,62,62,62	0
56	MG	DA	3343	1/1	0.87	0.17	42,42,42,42	0
56	MG	BA	3228	1/1	0.87	0.21	56,56,56,56	0
56	MG	DA	3652	1/1	0.87	0.13	53,53,53,53	0
56	MG	B9	502	1/1	0.87	0.21	47,47,47,47	0
56	MG	DB	3006	1/1	0.87	0.10	60,60,60,60	0
56	MG	BA	3698	1/1	0.87	0.17	50,50,50,50	0
56	MG	DA	3168	1/1	0.88	0.07	47,47,47,47	0
56	MG	DA	3129	1/1	0.88	0.20	42,42,42,42	0
56	MG	DA	3459	1/1	0.88	0.11	44,44,44,44	0
56	MG	DA	3070	1/1	0.88	0.11	51,51,51,51	0
56	MG	DA	3163	1/1	0.88	0.13	54,54,54,54	0
56	MG	AA	3005	1/1	0.88	0.22	77,77,77,77	0
56	MG	DA	3562	1/1	0.88	0.22	72,72,72,72	0
56	MG	BA	3553	1/1	0.88	0.14	53,53,53,53	0
56	MG	AA	3139	1/1	0.88	0.16	72,72,72,72	0
56	MG	DA	3221	1/1	0.88	0.12	52,52,52,52	0
56	MG	CA	3143	1/1	0.88	0.13	77,77,77,77	0
56	MG	BA	3131	1/1	0.88	0.35	39,39,39,39	0
56	MG	AE	202	1/1	0.88	0.07	74,74,74,74	0
56	MG	DA	3018	1/1	0.88	0.22	51,51,51,51	0
56	MG	BA	3427	1/1	0.88	0.26	52,52,52,52	0
56	MG	BA	3063	1/1	0.88	0.26	54,54,54,54	0
56	MG	BA	3006	1/1	0.88	0.25	52,52,52,52	0
56	MG	BQ	204	1/1	0.88	0.19	43,43,43,43	0
56	MG	BA	3054	1/1	0.88	0.23	43,43,43,43	0
56	MG	BV	204	1/1	0.88	0.22	47,47,47,47	0
56	MG	AA	3001	1/1	0.88	0.17	77,77,77,77	0
56	MG	DA	3281	1/1	0.88	0.15	49,49,49,49	0
56	MG	BA	3112	1/1	0.88	0.20	42,42,42,42	0
56	MG	BA	3499	1/1	0.88	0.21	19,19,19,19	0
56	MG	BA	3259	1/1	0.88	0.22	59,59,59,59	0
56	MG	BA	3720	1/1	0.88	0.11	45,45,45,45	0
56	MG	DA	3338	1/1	0.88	0.19	43,43,43,43	0
56	MG	BA	3351	1/1	0.88	0.19	59,59,59,59	0
56	MG	DG	3001	1/1	0.88	0.07	57,57,57,57	0
56	MG	CA	3005	1/1	0.88	0.10	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3156	1/1	0.88	0.12	67,67,67,67	0
56	MG	AA	3043	1/1	0.88	0.12	76,76,76,76	0
56	MG	DA	3630	1/1	0.88	0.10	51,51,51,51	0
56	MG	BA	3062	1/1	0.88	0.17	48,48,48,48	0
56	MG	BA	3114	1/1	0.88	0.15	34,34,34,34	0
56	MG	CA	3019	1/1	0.88	0.06	62,62,62,62	0
56	MG	AA	3107	1/1	0.88	0.13	63,63,63,63	0
56	MG	BA	3404	1/1	0.88	0.23	23,23,23,23	0
56	MG	DA	3103	1/1	0.88	0.08	71,71,71,71	0
56	MG	DA	3238	1/1	0.88	0.13	54,54,54,54	0
56	MG	DA	3114	1/1	0.88	0.11	55,55,55,55	0
56	MG	BA	3232	1/1	0.88	0.18	51,51,51,51	0
56	MG	AA	3122	1/1	0.88	0.22	80,80,80,80	0
56	MG	BA	3801	1/1	0.88	0.27	39,39,39,39	0
56	MG	BA	3678	1/1	0.88	0.47	35,35,35,35	0
56	MG	DA	3479	1/1	0.88	0.19	35,35,35,35	0
56	MG	DA	3623	1/1	0.88	0.41	66,66,66,66	0
56	MG	BA	3626	1/1	0.88	0.13	43,43,43,43	0
56	MG	AA	3179	1/1	0.88	0.27	61,61,61,61	0
56	MG	CA	3024	1/1	0.88	0.11	58,58,58,58	0
56	MG	AA	3073	1/1	0.88	0.22	71,71,71,71	0
56	MG	AA	3080	1/1	0.88	0.24	71,71,71,71	0
56	MG	DA	3122	1/1	0.88	0.08	53,53,53,53	0
56	MG	DA	3016	1/1	0.88	0.32	42,42,42,42	0
56	MG	BA	3721	1/1	0.88	0.17	9,9,9,9	0
56	MG	BA	3055	1/1	0.88	0.20	55,55,55,55	0
56	MG	DA	3364	1/1	0.88	0.21	57,57,57,57	0
56	MG	BG	3002	1/1	0.88	0.08	50,50,50,50	0
56	MG	BA	3440	1/1	0.88	0.24	29,29,29,29	0
56	MG	DA	3366	1/1	0.88	0.11	38,38,38,38	0
56	MG	DA	3426	1/1	0.88	0.10	39,39,39,39	0
56	MG	BA	3066	1/1	0.88	0.16	52,52,52,52	0
56	MG	CA	3120	1/1	0.88	0.10	65,65,65,65	0
56	MG	BA	3755	1/1	0.88	0.16	52,52,52,52	0
56	MG	DA	3017	1/1	0.88	0.12	56,56,56,56	0
56	MG	DA	3132	1/1	0.88	0.15	54,54,54,54	0
56	MG	BP	203	1/1	0.88	0.14	49,49,49,49	0
56	MG	CA	3052	1/1	0.88	0.13	69,69,69,69	0
56	MG	DA	3249	1/1	0.88	0.22	65,65,65,65	0
56	MG	DA	3276	1/1	0.88	0.14	54,54,54,54	0
56	MG	DA	3230	1/1	0.88	0.13	52,52,52,52	0
56	MG	BA	3125	1/1	0.88	0.48	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	3507	1/1	0.88	0.30	57,57,57,57	0
56	MG	BA	3588	1/1	0.89	0.12	29,29,29,29	0
56	MG	DA	3392	1/1	0.89	0.09	50,50,50,50	0
56	MG	BA	3126	1/1	0.89	0.26	47,47,47,47	0
56	MG	BA	3165	1/1	0.89	0.17	50,50,50,50	0
56	MG	DA	3292	1/1	0.89	0.18	40,40,40,40	0
56	MG	BA	3101	1/1	0.89	0.10	39,39,39,39	0
56	MG	AA	3074	1/1	0.89	0.12	51,51,51,51	0
56	MG	AA	3176	1/1	0.89	0.31	57,57,57,57	0
56	MG	CA	3145	1/1	0.89	0.09	68,68,68,68	0
56	MG	DA	3472	1/1	0.89	0.11	60,60,60,60	0
56	MG	BA	3649	1/1	0.89	0.10	44,44,44,44	0
56	MG	DA	3165	1/1	0.89	0.12	42,42,42,42	0
56	MG	DA	3324	1/1	0.89	0.21	32,32,32,32	0
56	MG	AQ	3001	1/1	0.89	0.19	52,52,52,52	0
56	MG	DA	3282	1/1	0.89	0.16	42,42,42,42	0
56	MG	BA	3506	1/1	0.89	0.14	31,31,31,31	0
56	MG	DA	3592	1/1	0.89	0.11	40,40,40,40	0
56	MG	BA	3471	1/1	0.89	0.19	27,27,27,27	0
56	MG	AA	3168	1/1	0.89	0.11	57,57,57,57	0
56	MG	BA	3539	1/1	0.89	0.27	29,29,29,29	0
56	MG	BA	3295	1/1	0.89	0.23	49,49,49,49	0
56	MG	BA	3567	1/1	0.89	0.17	45,45,45,45	0
56	MG	BF	304	1/1	0.89	0.13	35,35,35,35	0
56	MG	BA	3659	1/1	0.89	0.16	67,67,67,67	0
56	MG	CA	3033	1/1	0.89	0.15	60,60,60,60	0
56	MG	DA	3258	1/1	0.89	0.17	51,51,51,51	0
56	MG	BA	3768	1/1	0.89	0.10	61,61,61,61	0
56	MG	DA	3185	1/1	0.89	0.07	55,55,55,55	0
56	MG	DA	3046	1/1	0.89	0.13	56,56,56,56	0
56	MG	BA	3284	1/1	0.89	0.27	33,33,33,33	0
56	MG	BA	3154	1/1	0.89	0.32	37,37,37,37	0
56	MG	DP	202	1/1	0.89	0.38	55,55,55,55	0
56	MG	DA	3076	1/1	0.89	0.35	39,39,39,39	0
56	MG	AA	3150	1/1	0.89	0.13	66,66,66,66	0
56	MG	DA	3130	1/1	0.89	0.19	54,54,54,54	0
56	MG	CA	3073	1/1	0.89	0.10	55,55,55,55	0
56	MG	BA	3503	1/1	0.89	0.25	64,64,64,64	0
56	MG	AA	3121	1/1	0.89	0.13	33,33,33,33	0
56	MG	BA	3105	1/1	0.89	0.17	39,39,39,39	0
56	MG	DA	3224	1/1	0.89	0.43	47,47,47,47	0
56	MG	BA	3793	1/1	0.89	0.40	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	3231	1/1	0.89	0.16	51,51,51,51	0
56	MG	DA	3142	1/1	0.89	0.10	50,50,50,50	0
56	MG	BA	3212	1/1	0.89	0.17	26,26,26,26	0
56	MG	BA	3551	1/1	0.89	0.15	49,49,49,49	0
56	MG	DA	3111	1/1	0.89	0.25	53,53,53,53	0
56	MG	DA	3400	1/1	0.89	0.21	56,56,56,56	0
56	MG	BA	3534	1/1	0.89	0.16	44,44,44,44	0
56	MG	DA	3267	1/1	0.89	0.15	41,41,41,41	0
56	MG	DA	3524	1/1	0.89	0.20	59,59,59,59	0
56	MG	BA	3522	1/1	0.89	0.19	16,16,16,16	0
56	MG	DA	3606	1/1	0.89	0.09	48,48,48,48	0
56	MG	BA	3435	1/1	0.89	0.19	26,26,26,26	0
56	MG	DA	3035	1/1	0.89	0.08	40,40,40,40	0
56	MG	AA	3089	1/1	0.89	0.14	57,57,57,57	0
56	MG	BA	3691	1/1	0.89	0.10	68,68,68,68	0
56	MG	CA	3015	1/1	0.89	0.10	58,58,58,58	0
56	MG	DA	3583	1/1	0.89	0.09	56,56,56,56	0
56	MG	DA	3085	1/1	0.89	0.11	38,38,38,38	0
56	MG	DA	3626	1/1	0.89	0.28	56,56,56,56	0
56	MG	DA	3437	1/1	0.89	0.15	36,36,36,36	0
56	MG	BA	3359	1/1	0.89	0.23	40,40,40,40	0
56	MG	DA	3064	1/1	0.89	0.28	56,56,56,56	0
56	MG	AA	3068	1/1	0.89	0.24	62,62,62,62	0
56	MG	DA	3212	1/1	0.89	0.07	54,54,54,54	0
56	MG	DD	302	1/1	0.89	0.44	73,73,73,73	0
56	MG	BU	201	1/1	0.89	0.23	36,36,36,36	0
56	MG	AA	3025	1/1	0.89	0.24	69,69,69,69	0
56	MG	AA	3066	1/1	0.89	0.13	58,58,58,58	0
56	MG	BE	301	1/1	0.89	0.19	27,27,27,27	0
56	MG	DA	3314	1/1	0.89	0.08	45,45,45,45	0
56	MG	DA	3175	1/1	0.89	0.44	51,51,51,51	0
56	MG	BA	3804	1/1	0.89	0.13	35,35,35,35	0
56	MG	BA	3682	1/1	0.89	0.30	39,39,39,39	0
56	MG	BA	3744	1/1	0.89	0.16	61,61,61,61	0
56	MG	CA	3064	1/1	0.89	0.07	59,59,59,59	0
56	MG	BA	3583	1/1	0.89	0.14	56,56,56,56	0
56	MG	BA	3057	1/1	0.89	0.10	53,53,53,53	0
56	MG	DA	3187	1/1	0.89	0.22	51,51,51,51	0
56	MG	DA	3228	1/1	0.89	0.10	46,46,46,46	0
56	MG	BA	3326	1/1	0.89	0.14	22,22,22,22	0
56	MG	DA	3002	1/1	0.89	0.27	55,55,55,55	0
56	MG	DA	3226	1/1	0.89	0.17	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	AA	3096	1/1	0.89	0.23	60,60,60,60	0
56	MG	CA	3063	1/1	0.89	0.10	70,70,70,70	0
56	MG	AA	3014	1/1	0.90	0.09	62,62,62,62	0
56	MG	DA	3082	1/1	0.90	0.17	40,40,40,40	0
56	MG	DA	3670	1/1	0.90	0.18	49,49,49,49	0
56	MG	AX	3006	1/1	0.90	0.11	71,71,71,71	0
56	MG	BA	3699	1/1	0.90	0.12	48,48,48,48	0
56	MG	DA	3010	1/1	0.90	0.14	45,45,45,45	0
56	MG	DA	3609	1/1	0.90	0.11	61,61,61,61	0
56	MG	DA	3416	1/1	0.90	0.13	22,22,22,22	0
56	MG	BA	3739	1/1	0.90	0.27	46,46,46,46	0
56	MG	DA	3049	1/1	0.90	0.13	53,53,53,53	0
56	MG	BA	3666	1/1	0.90	0.13	47,47,47,47	0
56	MG	BA	3571	1/1	0.90	0.13	46,46,46,46	0
56	MG	BA	3554	1/1	0.90	0.15	24,24,24,24	0
56	MG	BA	3461	1/1	0.90	0.09	62,62,62,62	0
56	MG	BA	3767	1/1	0.90	0.23	57,57,57,57	0
56	MG	BA	3161	1/1	0.90	0.48	46,46,46,46	0
56	MG	DA	3567	1/1	0.90	0.06	57,57,57,57	0
56	MG	BA	3394	1/1	0.90	0.20	20,20,20,20	0
56	MG	DA	3405	1/1	0.90	0.12	41,41,41,41	0
56	MG	AA	3138	1/1	0.90	0.09	73,73,73,73	0
56	MG	CA	3151	1/1	0.90	0.20	60,60,60,60	0
56	MG	DA	3057	1/1	0.90	0.32	55,55,55,55	0
56	MG	DA	3332	1/1	0.90	0.22	50,50,50,50	0
56	MG	D1	101	1/1	0.90	0.10	50,50,50,50	0
56	MG	AA	3161	1/1	0.90	0.20	59,59,59,59	0
56	MG	DA	3113	1/1	0.90	0.13	50,50,50,50	0
56	MG	CA	3139	1/1	0.90	0.15	69,69,69,69	0
56	MG	DA	3179	1/1	0.90	0.20	57,57,57,57	0
56	MG	CA	3013	1/1	0.90	0.10	54,54,54,54	0
56	MG	DA	3441	1/1	0.90	0.06	30,30,30,30	0
56	MG	DA	3280	1/1	0.90	0.07	62,62,62,62	0
56	MG	BA	3687	1/1	0.90	0.22	53,53,53,53	0
56	MG	AA	3002	1/1	0.90	0.09	63,63,63,63	0
56	MG	BX	101	1/1	0.90	0.23	36,36,36,36	0
56	MG	BB	218	1/1	0.90	0.16	31,31,31,31	0
56	MG	DA	3213	1/1	0.90	0.42	46,46,46,46	0
56	MG	DA	3135	1/1	0.90	0.14	46,46,46,46	0
56	MG	BA	3266	1/1	0.90	0.21	27,27,27,27	0
56	MG	CA	3068	1/1	0.90	0.23	64,64,64,64	0
56	MG	DA	3363	1/1	0.90	0.15	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	3283	1/1	0.90	0.16	30,30,30,30	0
56	MG	BA	3594	1/1	0.90	0.17	33,33,33,33	0
56	MG	DA	3521	1/1	0.90	0.45	55,55,55,55	0
56	MG	DA	3358	1/1	0.90	0.14	28,28,28,28	0
56	MG	AN	502	1/1	0.90	0.17	56,56,56,56	0
56	MG	DA	3424	1/1	0.90	0.08	41,41,41,41	0
56	MG	BA	3340	1/1	0.90	0.11	40,40,40,40	0
56	MG	BA	3548	1/1	0.90	0.13	40,40,40,40	0
56	MG	DA	3651	1/1	0.90	0.12	40,40,40,40	0
56	MG	BA	3225	1/1	0.90	0.19	31,31,31,31	0
56	MG	DA	3613	1/1	0.90	0.07	55,55,55,55	0
56	MG	AM	201	1/1	0.90	0.06	59,59,59,59	0
56	MG	DA	3266	1/1	0.90	0.18	56,56,56,56	0
56	MG	DA	3668	1/1	0.90	1.77	51,51,51,51	0
56	MG	AA	3140	1/1	0.90	0.17	36,36,36,36	0
56	MG	DA	3589	1/1	0.90	0.06	53,53,53,53	0
56	MG	DA	3014	1/1	0.90	0.15	43,43,43,43	0
56	MG	BA	3193	1/1	0.90	0.34	62,62,62,62	0
56	MG	BA	3671	1/1	0.90	0.19	59,59,59,59	0
56	MG	BA	3315	1/1	0.90	0.23	59,59,59,59	0
56	MG	AA	3022	1/1	0.90	0.10	54,54,54,54	0
56	MG	BA	3651	1/1	0.90	0.34	52,52,52,52	0
56	MG	DA	3199	1/1	0.90	0.10	55,55,55,55	0
56	MG	BA	3614	1/1	0.90	0.21	59,59,59,59	0
56	MG	AA	3141	1/1	0.90	0.24	50,50,50,50	0
56	MG	DA	3608	1/1	0.90	0.20	47,47,47,47	0
56	MG	CA	3008	1/1	0.90	0.26	60,60,60,60	0
56	MG	DA	3159	1/1	0.90	0.10	42,42,42,42	0
56	MG	BA	3452	1/1	0.90	0.29	55,55,55,55	0
56	MG	DA	3123	1/1	0.90	0.14	52,52,52,52	0
56	MG	AA	3064	1/1	0.90	0.21	54,54,54,54	0
56	MG	DA	3591	1/1	0.90	0.10	59,59,59,59	0
56	MG	B5	102	1/1	0.90	0.38	45,45,45,45	0
56	MG	B0	103	1/1	0.90	0.20	38,38,38,38	0
56	MG	DA	3218	1/1	0.90	0.27	30,30,30,30	0
56	MG	AA	3007	1/1	0.90	0.12	54,54,54,54	0
56	MG	BA	3264	1/1	0.90	0.34	45,45,45,45	0
56	MG	BA	3082	1/1	0.90	0.26	55,55,55,55	0
56	MG	CA	3044	1/1	0.90	0.10	44,44,44,44	0
56	MG	DA	3124	1/1	0.90	0.09	50,50,50,50	0
56	MG	DA	3360	1/1	0.90	0.13	37,37,37,37	0
56	MG	DA	3605	1/1	0.90	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3194	1/1	0.90	0.17	62,62,62,62	0
56	MG	BA	3200	1/1	0.90	0.18	41,41,41,41	0
56	MG	DA	3663	1/1	0.90	0.13	37,37,37,37	0
56	MG	AA	3004	1/1	0.90	0.19	66,66,66,66	0
56	MG	DA	3395	1/1	0.90	0.10	33,33,33,33	0
56	MG	BA	3663	1/1	0.90	0.23	65,65,65,65	0
56	MG	BA	3219	1/1	0.90	0.14	62,62,62,62	0
56	MG	BA	3401	1/1	0.90	0.20	34,34,34,34	0
56	MG	DA	3377	1/1	0.90	0.15	62,62,62,62	0
56	MG	CA	3115	1/1	0.90	0.09	60,60,60,60	0
56	MG	CA	3149	1/1	0.90	0.24	74,74,74,74	0
56	MG	DA	3510	1/1	0.90	0.18	55,55,55,55	0
56	MG	BA	3384	1/1	0.90	0.18	63,63,63,63	0
56	MG	AA	3029	1/1	0.90	0.18	43,43,43,43	0
56	MG	DA	3599	1/1	0.90	0.07	47,47,47,47	0
56	MG	BA	3160	1/1	0.90	0.42	40,40,40,40	0
56	MG	BA	3396	1/1	0.90	0.12	41,41,41,41	0
56	MG	AA	3011	1/1	0.90	0.21	56,56,56,56	0
56	MG	DA	3559	1/1	0.90	0.16	61,61,61,61	0
56	MG	BA	3747	1/1	0.90	0.33	33,33,33,33	0
56	MG	BA	3610	1/1	0.90	0.18	39,39,39,39	0
56	MG	BA	3509	1/1	0.90	0.12	39,39,39,39	0
56	MG	BA	3010	1/1	0.91	0.15	41,41,41,41	0
56	MG	AA	3120	1/1	0.91	0.12	49,49,49,49	0
56	MG	BA	3586	1/1	0.91	0.11	60,60,60,60	0
56	MG	BA	3478	1/1	0.91	0.14	59,59,59,59	0
56	MG	BA	3377	1/1	0.91	0.11	48,48,48,48	0
56	MG	BA	3532	1/1	0.91	0.29	30,30,30,30	0
56	MG	BA	3431	1/1	0.91	0.13	63,63,63,63	0
56	MG	BA	3416	1/1	0.91	0.17	36,36,36,36	0
56	MG	DA	3638	1/1	0.91	0.12	42,42,42,42	0
56	MG	BA	3462	1/1	0.91	0.18	49,49,49,49	0
56	MG	B7	103	1/1	0.91	0.20	35,35,35,35	0
56	MG	DA	3313	1/1	0.91	0.05	46,46,46,46	0
56	MG	BA	3746	1/1	0.91	0.16	55,55,55,55	0
56	MG	DA	3333	1/1	0.91	0.09	51,51,51,51	0
56	MG	DA	3063	1/1	0.91	0.08	54,54,54,54	0
56	MG	BA	3064	1/1	0.91	0.17	33,33,33,33	0
56	MG	BA	3731	1/1	0.91	0.14	26,26,26,26	0
56	MG	DU	3004	1/1	0.91	0.19	59,59,59,59	0
56	MG	AA	3044	1/1	0.91	0.24	55,55,55,55	0
56	MG	BA	3068	1/1	0.91	0.24	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3149	1/1	0.91	0.12	68,68,68,68	0
56	MG	CA	3136	1/1	0.91	0.08	55,55,55,55	0
56	MG	BA	3128	1/1	0.91	0.14	44,44,44,44	0
56	MG	DA	3597	1/1	0.91	0.09	49,49,49,49	0
56	MG	CA	3069	1/1	0.91	0.06	59,59,59,59	0
56	MG	DA	3274	1/1	0.91	0.07	54,54,54,54	0
56	MG	BA	3759	1/1	0.91	0.07	36,36,36,36	0
56	MG	AA	3039	1/1	0.91	0.16	46,46,46,46	0
56	MG	BU	204	1/1	0.91	0.31	43,43,43,43	0
56	MG	DA	3538	1/1	0.91	0.14	44,44,44,44	0
56	MG	DA	3202	1/1	0.91	0.44	52,52,52,52	0
56	MG	BA	3324	1/1	0.91	0.19	42,42,42,42	0
56	MG	AA	3083	1/1	0.91	0.13	53,53,53,53	0
56	MG	BA	3258	1/1	0.91	0.27	61,61,61,61	0
56	MG	DA	3086	1/1	0.91	0.45	36,36,36,36	0
56	MG	B5	103	1/1	0.91	0.16	41,41,41,41	0
56	MG	DA	3440	1/1	0.91	0.12	51,51,51,51	0
56	MG	DA	3415	1/1	0.91	0.14	59,59,59,59	0
56	MG	DA	3247	1/1	0.91	0.19	34,34,34,34	0
56	MG	DA	3499	1/1	0.91	0.06	61,61,61,61	0
56	MG	BA	3674	1/1	0.91	0.17	55,55,55,55	0
56	MG	BA	3419	1/1	0.91	0.17	25,25,25,25	0
56	MG	BA	3592	1/1	0.91	0.10	64,64,64,64	0
56	MG	DA	3182	1/1	0.91	0.08	43,43,43,43	0
56	MG	BA	3479	1/1	0.91	0.13	53,53,53,53	0
56	MG	DU	3003	1/1	0.91	0.46	53,53,53,53	0
56	MG	CA	3104	1/1	0.91	0.09	60,60,60,60	0
56	MG	CA	3085	1/1	0.91	0.21	73,73,73,73	0
56	MG	BA	3025	1/1	0.91	0.11	48,48,48,48	0
56	MG	BA	3751	1/1	0.91	0.36	55,55,55,55	0
56	MG	BA	3679	1/1	0.91	0.22	56,56,56,56	0
56	MG	CA	3025	1/1	0.91	0.20	61,61,61,61	0
56	MG	BA	3529	1/1	0.91	0.20	25,25,25,25	0
56	MG	DA	3200	1/1	0.91	0.11	57,57,57,57	0
56	MG	BA	3157	1/1	0.91	0.83	36,36,36,36	0
56	MG	DR	5001	1/1	0.91	0.12	51,51,51,51	0
56	MG	DA	3454	1/1	0.91	0.09	56,56,56,56	0
56	MG	BA	3576	1/1	0.91	0.17	36,36,36,36	0
56	MG	DA	3150	1/1	0.91	0.18	52,52,52,52	0
56	MG	DA	3316	1/1	0.91	0.09	34,34,34,34	0
56	MG	DA	3438	1/1	0.91	0.14	55,55,55,55	0
56	MG	BA	3034	1/1	0.91	0.17	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3725	1/1	0.91	0.20	44,44,44,44	0
56	MG	BA	3464	1/1	0.91	0.16	46,46,46,46	0
56	MG	BA	3495	1/1	0.91	0.14	58,58,58,58	0
56	MG	DA	3118	1/1	0.91	0.14	43,43,43,43	0
56	MG	BA	3169	1/1	0.91	0.41	50,50,50,50	0
56	MG	DB	3005	1/1	0.91	0.14	48,48,48,48	0
56	MG	DA	3391	1/1	0.91	0.10	44,44,44,44	0
56	MG	DA	3270	1/1	0.91	0.25	56,56,56,56	0
56	MG	BF	305	1/1	0.91	0.12	45,45,45,45	0
56	MG	BA	3248	1/1	0.91	0.20	52,52,52,52	0
56	MG	DP	201	1/1	0.91	0.14	58,58,58,58	0
56	MG	CA	3061	1/1	0.91	0.25	64,64,64,64	0
56	MG	BA	3647	1/1	0.91	0.21	49,49,49,49	0
56	MG	BA	3247	1/1	0.91	0.17	50,50,50,50	0
56	MG	BA	3014	1/1	0.91	0.25	38,38,38,38	0
56	MG	BQ	201	1/1	0.91	0.23	35,35,35,35	0
56	MG	BY	201	1/1	0.91	0.23	52,52,52,52	0
56	MG	B6	102	1/1	0.91	0.19	51,51,51,51	0
56	MG	BA	3144	1/1	0.91	0.32	43,43,43,43	0
56	MG	CA	3155	1/1	0.91	0.08	76,76,76,76	0
56	MG	AA	3037	1/1	0.91	0.19	46,46,46,46	0
56	MG	BA	3760	1/1	0.91	0.17	43,43,43,43	0
56	MG	BA	3305	1/1	0.91	0.13	46,46,46,46	0
56	MG	DA	3260	1/1	0.91	0.11	55,55,55,55	0
56	MG	BA	3562	1/1	0.91	0.27	44,44,44,44	0
56	MG	DA	3149	1/1	0.91	0.62	37,37,37,37	0
56	MG	BA	3204	1/1	0.91	0.15	55,55,55,55	0
56	MG	BB	221	1/1	0.91	0.12	43,43,43,43	0
56	MG	DA	3574	1/1	0.91	0.09	55,55,55,55	0
56	MG	BA	3222	1/1	0.91	0.11	48,48,48,48	0
56	MG	BA	3369	1/1	0.91	0.20	40,40,40,40	0
56	MG	CA	3132	1/1	0.91	0.21	55,55,55,55	0
56	MG	BA	3737	1/1	0.91	0.10	70,70,70,70	0
56	MG	AA	3189	1/1	0.91	0.24	62,62,62,62	0
56	MG	BA	3621	1/1	0.91	0.15	39,39,39,39	0
56	MG	DA	3102	1/1	0.91	0.26	49,49,49,49	0
56	MG	BA	3211	1/1	0.91	0.28	41,41,41,41	0
56	MG	BA	3368	1/1	0.91	0.21	35,35,35,35	0
56	MG	AA	3050	1/1	0.91	0.22	77,77,77,77	0
56	MG	DA	3412	1/1	0.91	0.11	56,56,56,56	0
56	MG	DA	3211	1/1	0.91	0.09	53,53,53,53	0
56	MG	DA	3508	1/1	0.91	0.08	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3354	1/1	0.91	0.05	48,48,48,48	0
56	MG	DA	3116	1/1	0.91	0.10	48,48,48,48	0
56	MG	BA	3689	1/1	0.91	0.10	53,53,53,53	0
56	MG	BA	3102	1/1	0.91	0.22	61,61,61,61	0
56	MG	AA	3173	1/1	0.91	0.21	60,60,60,60	0
56	MG	DA	3099	1/1	0.91	0.17	45,45,45,45	0
56	MG	DA	3073	1/1	0.91	0.08	55,55,55,55	0
56	MG	BA	3422	1/1	0.91	0.16	53,53,53,53	0
56	MG	DA	3547	1/1	0.91	0.14	45,45,45,45	0
56	MG	DA	3131	1/1	0.91	0.19	52,52,52,52	0
56	MG	BA	3697	1/1	0.91	0.12	46,46,46,46	0
56	MG	BR	201	1/1	0.91	0.26	40,40,40,40	0
56	MG	BA	3342	1/1	0.91	0.10	33,33,33,33	0
56	MG	BA	3467	1/1	0.91	0.18	49,49,49,49	0
56	MG	BA	3622	1/1	0.91	0.14	29,29,29,29	0
56	MG	CA	3096	1/1	0.91	0.15	65,65,65,65	0
56	MG	AA	3102	1/1	0.91	0.24	64,64,64,64	0
56	MG	BA	3020	1/1	0.91	0.13	36,36,36,36	0
56	MG	DA	3041	1/1	0.91	0.09	56,56,56,56	0
56	MG	BF	302	1/1	0.91	0.25	56,56,56,56	0
56	MG	BA	3518	1/1	0.91	0.17	65,65,65,65	0
56	MG	DA	3504	1/1	0.91	0.09	41,41,41,41	0
56	MG	DA	3553	1/1	0.91	0.06	46,46,46,46	0
56	MG	DA	3195	1/1	0.91	0.24	58,58,58,58	0
56	MG	BA	3618	1/1	0.91	0.17	56,56,56,56	0
56	MG	BA	3179	1/1	0.91	0.23	41,41,41,41	0
56	MG	BA	3395	1/1	0.91	0.21	36,36,36,36	0
56	MG	BA	3086	1/1	0.91	0.55	49,49,49,49	0
56	MG	DA	3375	1/1	0.91	0.13	37,37,37,37	0
56	MG	BA	3578	1/1	0.91	0.20	20,20,20,20	0
56	MG	CA	3042	1/1	0.91	0.13	70,70,70,70	0
56	MG	BA	3771	1/1	0.91	0.20	52,52,52,52	0
56	MG	BA	3504	1/1	0.92	0.13	40,40,40,40	0
56	MG	BA	3358	1/1	0.92	0.12	40,40,40,40	0
56	MG	CA	3059	1/1	0.92	0.12	75,75,75,75	0
56	MG	BA	3643	1/1	0.92	0.15	58,58,58,58	0
56	MG	B0	101	1/1	0.92	0.09	55,55,55,55	0
56	MG	BA	3110	1/1	0.92	0.17	46,46,46,46	0
56	MG	BA	3186	1/1	0.92	0.14	47,47,47,47	0
56	MG	BA	3577	1/1	0.92	0.24	18,18,18,18	0
56	MG	DA	3341	1/1	0.92	0.23	67,67,67,67	0
56	MG	CA	3103	1/1	0.92	0.11	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3164	1/1	0.92	0.24	51,51,51,51	0
56	MG	CA	3017	1/1	0.92	0.14	76,76,76,76	0
56	MG	DA	3318	1/1	0.92	0.07	33,33,33,33	0
56	MG	DA	3345	1/1	0.92	0.23	38,38,38,38	0
56	MG	BA	3162	1/1	0.92	0.34	53,53,53,53	0
56	MG	BA	3192	1/1	0.92	0.21	53,53,53,53	0
56	MG	BA	3728	1/1	0.92	0.30	60,60,60,60	0
56	MG	BA	3785	1/1	0.92	0.13	81,81,81,81	0
56	MG	DA	3197	1/1	0.92	0.83	55,55,55,55	0
56	MG	BA	3774	1/1	0.92	0.09	37,37,37,37	0
56	MG	BA	3787	1/1	0.92	0.16	57,57,57,57	0
56	MG	AA	3151	1/1	0.92	0.12	56,56,56,56	0
56	MG	BA	3766	1/1	0.92	0.17	59,59,59,59	0
56	MG	BA	3776	1/1	0.92	0.10	48,48,48,48	0
56	MG	BA	3667	1/1	0.92	0.19	39,39,39,39	0
56	MG	B5	101	1/1	0.92	0.42	39,39,39,39	0
56	MG	BA	3213	1/1	0.92	0.20	35,35,35,35	0
56	MG	AA	3097	1/1	0.92	0.18	71,71,71,71	0
56	MG	DA	3610	1/1	0.92	0.17	49,49,49,49	0
56	MG	DA	3544	1/1	0.92	0.22	39,39,39,39	0
56	MG	DA	3283	1/1	0.92	0.14	43,43,43,43	0
56	MG	DA	3495	1/1	0.92	0.15	39,39,39,39	0
56	MG	DD	307	1/1	0.92	0.40	50,50,50,50	0
56	MG	BA	3477	1/1	0.92	0.12	59,59,59,59	0
56	MG	DA	3576	1/1	0.92	0.09	50,50,50,50	0
56	MG	DA	3590	1/1	0.92	0.09	66,66,66,66	0
56	MG	BA	3397	1/1	0.92	0.14	25,25,25,25	0
56	MG	DA	3453	1/1	0.92	0.21	56,56,56,56	0
56	MG	BA	3207	1/1	0.92	0.32	44,44,44,44	0
56	MG	BA	3322	1/1	0.92	0.28	48,48,48,48	0
56	MG	AA	3069	1/1	0.92	0.15	52,52,52,52	0
56	MG	BA	3263	1/1	0.92	0.25	56,56,56,56	0
56	MG	CA	3080	1/1	0.92	0.10	56,56,56,56	0
56	MG	BA	3738	1/1	0.92	0.26	60,60,60,60	0
56	MG	CA	3169	1/1	0.92	0.10	52,52,52,52	0
56	MG	BA	3041	1/1	0.92	0.25	35,35,35,35	0
56	MG	AA	3070	1/1	0.92	0.12	65,65,65,65	0
56	MG	AA	3109	1/1	0.92	0.13	67,67,67,67	0
56	MG	BA	3773	1/1	0.92	0.13	38,38,38,38	0
56	MG	DA	3545	1/1	0.92	0.09	51,51,51,51	0
56	MG	BA	3380	1/1	0.92	0.11	36,36,36,36	0
56	MG	BF	306	1/1	0.92	0.52	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3108	1/1	0.92	0.24	64,64,64,64	0
56	MG	DA	3056	1/1	0.92	0.14	60,60,60,60	0
56	MG	DA	3209	1/1	0.92	0.28	46,46,46,46	0
56	MG	CA	3054	1/1	0.92	0.12	70,70,70,70	0
56	MG	BA	3122	1/1	0.92	0.42	46,46,46,46	0
56	MG	BA	3360	1/1	0.92	0.14	21,21,21,21	0
56	MG	BA	3279	1/1	0.92	0.24	45,45,45,45	0
56	MG	BA	3262	1/1	0.92	0.27	54,54,54,54	0
56	MG	BA	3770	1/1	0.92	0.14	47,47,47,47	0
56	MG	DW	202	1/1	0.92	0.43	46,46,46,46	0
56	MG	DA	3628	1/1	0.92	0.08	47,47,47,47	0
56	MG	CF	3001	1/1	0.92	0.10	55,55,55,55	0
56	MG	AA	3128	1/1	0.92	0.12	67,67,67,67	0
56	MG	D8	5001	1/1	0.92	0.19	52,52,52,52	0
56	MG	BA	3646	1/1	0.92	0.20	57,57,57,57	0
56	MG	DA	3096	1/1	0.92	0.82	48,48,48,48	0
56	MG	AA	3087	1/1	0.92	0.26	53,53,53,53	0
56	MG	BA	3151	1/1	0.92	0.26	37,37,37,37	0
56	MG	CA	3072	1/1	0.92	0.22	62,62,62,62	0
56	MG	BA	3648	1/1	0.92	0.26	65,65,65,65	0
56	MG	BU	205	1/1	0.92	0.26	43,43,43,43	0
56	MG	BA	3250	1/1	0.92	0.28	42,42,42,42	0
56	MG	DA	3565	1/1	0.92	0.09	45,45,45,45	0
56	MG	DA	3452	1/1	0.92	0.10	37,37,37,37	0
56	MG	BA	3790	1/1	0.92	0.23	29,29,29,29	0
56	MG	B8	102	1/1	0.92	0.15	41,41,41,41	0
56	MG	DA	3388	1/1	0.92	0.14	52,52,52,52	0
56	MG	BA	3531	1/1	0.92	0.28	43,43,43,43	0
56	MG	DA	3376	1/1	0.92	0.15	51,51,51,51	0
56	MG	DA	3497	1/1	0.92	0.13	36,36,36,36	0
56	MG	DA	3431	1/1	0.92	0.09	64,64,64,64	0
56	MG	BA	3439	1/1	0.92	0.14	71,71,71,71	0
56	MG	BA	3217	1/1	0.92	0.20	47,47,47,47	0
56	MG	DA	3147	1/1	0.92	0.12	53,53,53,53	0
56	MG	DA	3369	1/1	0.92	0.10	37,37,37,37	0
56	MG	DA	3322	1/1	0.92	0.12	53,53,53,53	0
56	MG	BB	202	1/1	0.92	0.20	45,45,45,45	0
56	MG	DA	3089	1/1	0.92	0.12	47,47,47,47	0
56	MG	DB	3004	1/1	0.92	0.14	53,53,53,53	0
56	MG	DA	3184	1/1	0.92	0.09	49,49,49,49	0
56	MG	DA	3039	1/1	0.92	0.11	44,44,44,44	0
56	MG	AA	3012	1/1	0.92	0.14	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	DB	3008	1/1	0.92	0.13	64,64,64,64	0
56	MG	BA	3808	1/1	0.92	0.09	40,40,40,40	0
56	MG	DA	3357	1/1	0.92	0.09	38,38,38,38	0
56	MG	CA	3106	1/1	0.92	0.08	58,58,58,58	0
56	MG	DA	3189	1/1	0.92	0.13	41,41,41,41	0
56	MG	BA	3149	1/1	0.92	0.39	36,36,36,36	0
56	MG	DA	3310	1/1	0.92	0.20	49,49,49,49	0
56	MG	DA	3193	1/1	0.92	0.08	46,46,46,46	0
56	MG	BA	3459	1/1	0.92	0.20	47,47,47,47	0
56	MG	BA	3148	1/1	0.92	0.08	49,49,49,49	0
56	MG	DA	3153	1/1	0.92	0.17	38,38,38,38	0
56	MG	BU	208	1/1	0.92	0.23	28,28,28,28	0
56	MG	B0	102	1/1	0.92	0.17	50,50,50,50	0
56	MG	DA	3272	1/1	0.92	0.10	45,45,45,45	0
56	MG	BA	3089	1/1	0.92	0.30	42,42,42,42	0
56	MG	BB	220	1/1	0.92	0.10	51,51,51,51	0
56	MG	BA	3346	1/1	0.92	0.15	29,29,29,29	0
56	MG	BA	3033	1/1	0.92	0.60	42,42,42,42	0
56	MG	DA	3295	1/1	0.92	0.10	30,30,30,30	0
56	MG	AA	3127	1/1	0.92	0.12	79,79,79,79	0
56	MG	DA	3299	1/1	0.92	0.13	40,40,40,40	0
56	MG	AA	3055	1/1	0.92	0.19	69,69,69,69	0
56	MG	BA	3039	1/1	0.92	0.25	58,58,58,58	0
56	MG	BA	3627	1/1	0.92	0.13	57,57,57,57	0
56	MG	BA	3740	1/1	0.92	0.15	35,35,35,35	0
56	MG	BA	3350	1/1	0.92	0.21	28,28,28,28	0
56	MG	DA	3578	1/1	0.92	0.06	40,40,40,40	0
56	MG	BA	3717	1/1	0.92	0.14	54,54,54,54	0
56	MG	DA	3006	1/1	0.92	0.19	58,58,58,58	0
56	MG	DA	3419	1/1	0.92	0.12	45,45,45,45	0
56	MG	DA	3393	1/1	0.92	0.20	48,48,48,48	0
56	MG	BA	3650	1/1	0.92	0.14	48,48,48,48	0
56	MG	BA	3253	1/1	0.92	0.19	47,47,47,47	0
56	MG	BA	3252	1/1	0.92	0.15	44,44,44,44	0
56	MG	BA	3367	1/1	0.92	0.15	34,34,34,34	0
56	MG	BA	3638	1/1	0.92	0.11	56,56,56,56	0
56	MG	DA	3549	1/1	0.92	0.14	32,32,32,32	0
56	MG	DA	3666	1/1	0.92	0.59	47,47,47,47	0
56	MG	DA	3385	1/1	0.92	0.10	32,32,32,32	0
56	MG	DA	3422	1/1	0.92	0.11	51,51,51,51	0
56	MG	BA	3575	1/1	0.92	0.18	27,27,27,27	0
56	MG	CA	3058	1/1	0.92	0.06	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3287	1/1	0.92	0.07	39,39,39,39	0
56	MG	DA	3020	1/1	0.92	0.16	32,32,32,32	0
56	MG	DA	3227	1/1	0.92	0.40	49,49,49,49	0
56	MG	CA	3165	1/1	0.92	0.13	60,60,60,60	0
56	MG	BA	3779	1/1	0.92	0.15	45,45,45,45	0
56	MG	DA	3634	1/1	0.92	0.28	61,61,61,61	0
56	MG	CA	3113	1/1	0.92	0.16	49,49,49,49	0
56	MG	DA	3300	1/1	0.92	0.10	41,41,41,41	0
56	MG	AA	3174	1/1	0.93	0.06	54,54,54,54	0
56	MG	BA	3196	1/1	0.93	0.16	40,40,40,40	0
56	MG	DA	3191	1/1	0.93	0.16	46,46,46,46	0
56	MG	BA	3143	1/1	0.93	0.27	39,39,39,39	0
56	MG	BA	3138	1/1	0.93	0.45	40,40,40,40	0
56	MG	AA	3019	1/1	0.93	0.21	66,66,66,66	0
56	MG	DA	3503	1/1	0.93	0.09	31,31,31,31	0
56	MG	CA	3023	1/1	0.93	0.12	39,39,39,39	0
56	MG	BA	3652	1/1	0.93	0.13	61,61,61,61	0
56	MG	BA	3081	1/1	0.93	0.14	33,33,33,33	0
56	MG	CA	3003	1/1	0.93	0.12	51,51,51,51	0
56	MG	BA	3795	1/1	0.93	0.27	43,43,43,43	0
56	MG	BA	3330	1/1	0.93	0.13	52,52,52,52	0
59	ZN	B4	501	1/1	0.93	0.12	99,99,99,99	0
56	MG	AA	3072	1/1	0.93	0.14	45,45,45,45	0
56	MG	DA	3489	1/1	0.93	0.14	45,45,45,45	0
56	MG	AD	502	1/1	0.93	0.18	56,56,56,56	0
56	MG	DA	3071	1/1	0.93	0.09	48,48,48,48	0
56	MG	BA	3492	1/1	0.93	0.16	47,47,47,47	0
56	MG	BA	3251	1/1	0.93	0.38	52,52,52,52	0
56	MG	DA	3639	1/1	0.93	0.06	52,52,52,52	0
56	MG	DA	3584	1/1	0.93	0.14	31,31,31,31	0
56	MG	BA	3597	1/1	0.93	0.11	40,40,40,40	0
56	MG	BA	3772	1/1	0.93	0.18	56,56,56,56	0
56	MG	BA	3214	1/1	0.93	0.29	44,44,44,44	0
56	MG	DA	3534	1/1	0.93	0.15	67,67,67,67	0
56	MG	DA	3059	1/1	0.93	0.16	40,40,40,40	0
56	MG	DA	3177	1/1	0.93	0.12	46,46,46,46	0
56	MG	BA	3606	1/1	0.93	0.08	67,67,67,67	0
56	MG	DA	3161	1/1	0.93	0.13	37,37,37,37	0
56	MG	BF	303	1/1	0.93	0.31	43,43,43,43	0
56	MG	BA	3633	1/1	0.93	0.25	59,59,59,59	0
56	MG	DV	3002	1/1	0.93	0.64	48,48,48,48	0
56	MG	DA	3528	1/1	0.93	0.08	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3783	1/1	0.93	0.15	43,43,43,43	0
56	MG	DA	3143	1/1	0.93	0.61	36,36,36,36	0
56	MG	BA	3265	1/1	0.93	0.09	49,49,49,49	0
56	MG	DA	3563	1/1	0.93	0.14	61,61,61,61	0
56	MG	BA	3426	1/1	0.93	0.18	20,20,20,20	0
56	MG	BA	3224	1/1	0.93	0.44	50,50,50,50	0
56	MG	DA	3012	1/1	0.93	0.10	39,39,39,39	0
56	MG	DA	3134	1/1	0.93	0.07	48,48,48,48	0
56	MG	BA	3408	1/1	0.93	0.14	21,21,21,21	0
56	MG	BA	3045	1/1	0.93	0.17	38,38,38,38	0
56	MG	DA	3571	1/1	0.93	0.12	51,51,51,51	0
56	MG	DA	3665	1/1	0.93	0.42	48,48,48,48	0
56	MG	CA	3018	1/1	0.93	0.09	52,52,52,52	0
56	MG	BA	3318	1/1	0.93	0.16	25,25,25,25	0
56	MG	DO	5001	1/1	0.93	0.12	55,55,55,55	0
56	MG	DA	3141	1/1	0.93	0.12	46,46,46,46	0
59	ZN	DY	501	1/1	0.93	0.16	97,97,97,97	0
56	MG	CA	3099	1/1	0.93	0.09	58,58,58,58	0
56	MG	DB	3010	1/1	0.93	0.20	53,53,53,53	0
56	MG	AA	3188	1/1	0.93	0.12	49,49,49,49	0
56	MG	CA	3134	1/1	0.93	0.13	65,65,65,65	0
56	MG	DA	3251	1/1	0.93	0.12	46,46,46,46	0
56	MG	DA	3575	1/1	0.93	0.14	51,51,51,51	0
56	MG	BA	3156	1/1	0.93	0.20	32,32,32,32	0
56	MG	DA	3442	1/1	0.93	0.09	37,37,37,37	0
56	MG	BA	3713	1/1	0.93	0.18	26,26,26,26	0
56	MG	DA	3622	1/1	0.93	0.14	35,35,35,35	0
56	MG	BA	3302	1/1	0.93	0.20	24,24,24,24	0
56	MG	DA	3298	1/1	0.93	0.12	55,55,55,55	0
56	MG	BD	3308	1/1	0.93	0.64	60,60,60,60	0
56	MG	DA	3383	1/1	0.93	0.11	31,31,31,31	0
56	MG	BA	3159	1/1	0.93	0.24	40,40,40,40	0
56	MG	BA	3100	1/1	0.93	0.26	53,53,53,53	0
56	MG	BA	3417	1/1	0.93	0.17	32,32,32,32	0
56	MG	BA	3629	1/1	0.93	0.16	57,57,57,57	0
56	MG	BA	3599	1/1	0.93	0.11	45,45,45,45	0
56	MG	BA	3420	1/1	0.93	0.30	46,46,46,46	0
56	MG	BA	3523	1/1	0.93	0.25	47,47,47,47	0
56	MG	DA	3555	1/1	0.93	0.08	56,56,56,56	0
56	MG	DA	3396	1/1	0.93	0.16	47,47,47,47	0
56	MG	BA	3590	1/1	0.93	0.15	60,60,60,60	0
56	MG	CA	3160	1/1	0.93	0.17	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	3554	1/1	0.93	0.09	47,47,47,47	0
56	MG	DA	3335	1/1	0.93	0.11	43,43,43,43	0
56	MG	DA	3095	1/1	0.93	0.11	43,43,43,43	0
56	MG	DE	305	1/1	0.93	0.14	38,38,38,38	0
56	MG	AA	3172	1/1	0.93	0.22	55,55,55,55	0
56	MG	DA	3058	1/1	0.93	0.37	50,50,50,50	0
56	MG	BA	3091	1/1	0.93	0.20	40,40,40,40	0
56	MG	BW	202	1/1	0.93	0.20	41,41,41,41	0
56	MG	BA	3559	1/1	0.93	0.04	59,59,59,59	0
56	MG	CA	3091	1/1	0.93	0.20	70,70,70,70	0
56	MG	DA	3173	1/1	0.93	0.20	51,51,51,51	0
56	MG	BA	3714	1/1	0.93	0.36	41,41,41,41	0
56	MG	BA	3272	1/1	0.93	0.14	22,22,22,22	0
56	MG	CA	3127	1/1	0.93	0.17	65,65,65,65	0
56	MG	DA	3465	1/1	0.93	0.16	49,49,49,49	0
56	MG	BB	207	1/1	0.93	0.18	39,39,39,39	0
56	MG	BA	3337	1/1	0.93	0.25	46,46,46,46	0
56	MG	BR	202	1/1	0.93	0.22	42,42,42,42	0
56	MG	BA	3227	1/1	0.93	0.18	34,34,34,34	0
56	MG	DA	3568	1/1	0.93	0.12	66,66,66,66	0
56	MG	BA	3174	1/1	0.93	0.16	50,50,50,50	0
56	MG	DA	3457	1/1	0.93	0.16	43,43,43,43	0
56	MG	BA	3060	1/1	0.93	0.27	26,26,26,26	0
56	MG	BA	3780	1/1	0.93	0.23	54,54,54,54	0
56	MG	BB	216	1/1	0.93	0.11	63,63,63,63	0
56	MG	BA	3281	1/1	0.93	0.15	56,56,56,56	0
56	MG	DA	3253	1/1	0.93	0.11	47,47,47,47	0
56	MG	DA	3268	1/1	0.93	0.13	56,56,56,56	0
56	MG	BA	3425	1/1	0.93	0.14	48,48,48,48	0
56	MG	AA	3133	1/1	0.93	0.23	66,66,66,66	0
56	MG	BA	3582	1/1	0.93	0.20	19,19,19,19	0
56	MG	DA	3104	1/1	0.93	0.16	39,39,39,39	0
56	MG	BA	3065	1/1	0.93	0.20	41,41,41,41	0
56	MG	AA	3142	1/1	0.93	0.09	46,46,46,46	0
56	MG	DA	3305	1/1	0.93	0.12	45,45,45,45	0
56	MG	DA	3413	1/1	0.93	0.08	34,34,34,34	0
56	MG	BA	3613	1/1	0.93	0.18	55,55,55,55	0
56	MG	BA	3061	1/1	0.93	0.30	49,49,49,49	0
56	MG	AA	3160	1/1	0.93	0.14	54,54,54,54	0
56	MG	DA	3279	1/1	0.93	0.11	54,54,54,54	0
56	MG	AA	3031	1/1	0.93	0.12	54,54,54,54	0
56	MG	DA	3140	1/1	0.93	0.35	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3299	1/1	0.93	0.16	44,44,44,44	0
56	MG	CA	3173	1/1	0.93	0.10	58,58,58,58	0
56	MG	DA	3564	1/1	0.93	0.10	50,50,50,50	0
56	MG	BA	3723	1/1	0.93	0.15	25,25,25,25	0
56	MG	CA	3026	1/1	0.93	0.12	55,55,55,55	0
56	MG	DA	3648	1/1	0.93	0.18	31,31,31,31	0
56	MG	BA	3595	1/1	0.93	0.62	43,43,43,43	0
56	MG	BA	3724	1/1	0.93	0.17	25,25,25,25	0
56	MG	BA	3612	1/1	0.93	0.16	58,58,58,58	0
56	MG	BA	3013	1/1	0.93	0.17	26,26,26,26	0
56	MG	BA	3163	1/1	0.93	0.33	34,34,34,34	0
56	MG	DA	3460	1/1	0.93	0.10	42,42,42,42	0
56	MG	DA	3061	1/1	0.93	0.20	41,41,41,41	0
56	MG	AA	3143	1/1	0.93	0.09	57,57,57,57	0
56	MG	BA	3563	1/1	0.93	0.09	44,44,44,44	0
56	MG	AA	3042	1/1	0.93	0.10	55,55,55,55	0
56	MG	AA	3154	1/1	0.93	0.10	50,50,50,50	0
56	MG	DB	3009	1/1	0.93	0.12	58,58,58,58	0
56	MG	BA	3254	1/1	0.93	0.15	55,55,55,55	0
56	MG	DA	3309	1/1	0.93	0.32	46,46,46,46	0
56	MG	BA	3096	1/1	0.93	0.30	61,61,61,61	0
56	MG	BA	3314	1/1	0.93	0.12	44,44,44,44	0
56	MG	DA	3458	1/1	0.93	0.08	57,57,57,57	0
56	MG	DA	3319	1/1	0.93	0.27	52,52,52,52	0
56	MG	DA	3374	1/1	0.93	0.07	31,31,31,31	0
56	MG	BA	3399	1/1	0.93	0.16	61,61,61,61	0
56	MG	BA	3520	1/1	0.93	0.17	50,50,50,50	0
56	MG	DF	303	1/1	0.93	0.08	52,52,52,52	0
56	MG	BA	3566	1/1	0.93	0.19	50,50,50,50	0
56	MG	BA	3722	1/1	0.93	0.19	17,17,17,17	0
56	MG	AA	3145	1/1	0.93	0.12	65,65,65,65	0
56	MG	DA	3522	1/1	0.93	0.28	53,53,53,53	0
56	MG	DA	3418	1/1	0.93	0.11	44,44,44,44	0
56	MG	BA	3443	1/1	0.93	0.17	27,27,27,27	0
56	MG	BA	3347	1/1	0.93	0.16	37,37,37,37	0
56	MG	BA	3694	1/1	0.93	0.14	54,54,54,54	0
56	MG	DA	3617	1/1	0.93	0.10	45,45,45,45	0
56	MG	BA	3178	1/1	0.93	0.65	42,42,42,42	0
56	MG	BA	3133	1/1	0.93	0.16	48,48,48,48	0
56	MG	BA	3538	1/1	0.93	0.18	26,26,26,26	0
56	MG	CA	3121	1/1	0.93	0.16	81,81,81,81	0
56	MG	DA	3490	1/1	0.93	0.12	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3121	1/1	0.94	0.43	45,45,45,45	0
56	MG	DA	3183	1/1	0.94	0.13	40,40,40,40	0
56	MG	BA	3049	1/1	0.94	0.13	34,34,34,34	0
56	MG	BA	3308	1/1	0.94	0.12	49,49,49,49	0
56	MG	DA	3631	1/1	0.94	0.10	57,57,57,57	0
56	MG	DA	3051	1/1	0.94	0.08	45,45,45,45	0
56	MG	BA	3637	1/1	0.94	0.10	54,54,54,54	0
56	MG	DA	3220	1/1	0.94	0.07	50,50,50,50	0
56	MG	DA	3259	1/1	0.94	0.15	53,53,53,53	0
56	MG	AA	3036	1/1	0.94	0.19	69,69,69,69	0
56	MG	DA	3445	1/1	0.94	0.16	50,50,50,50	0
56	MG	BB	204	1/1	0.94	0.14	42,42,42,42	0
56	MG	DA	3429	1/1	0.94	0.13	45,45,45,45	0
56	MG	DA	3535	1/1	0.94	0.07	59,59,59,59	0
56	MG	CA	3126	1/1	0.94	0.09	57,57,57,57	0
56	MG	DA	3361	1/1	0.94	0.11	25,25,25,25	0
56	MG	DA	3463	1/1	0.94	0.06	32,32,32,32	0
56	MG	BA	3494	1/1	0.94	0.13	47,47,47,47	0
56	MG	BA	3072	1/1	0.94	0.15	58,58,58,58	0
56	MG	BA	3732	1/1	0.94	0.17	41,41,41,41	0
56	MG	DA	3252	1/1	0.94	0.10	38,38,38,38	0
56	MG	BA	3702	1/1	0.94	0.23	53,53,53,53	0
56	MG	AA	3158	1/1	0.94	0.09	71,71,71,71	0
56	MG	DA	3025	1/1	0.94	0.14	52,52,52,52	0
56	MG	DA	3604	1/1	0.94	0.14	47,47,47,47	0
56	MG	DA	3091	1/1	0.94	0.11	46,46,46,46	0
56	MG	BA	3402	1/1	0.94	0.14	25,25,25,25	0
56	MG	DA	3067	1/1	0.94	0.12	45,45,45,45	0
56	MG	BA	3798	1/1	0.94	0.09	51,51,51,51	0
56	MG	BA	3719	1/1	0.94	0.16	36,36,36,36	0
56	MG	DA	3008	1/1	0.94	0.14	40,40,40,40	0
56	MG	BA	3240	1/1	0.94	0.10	30,30,30,30	0
56	MG	DA	3625	1/1	0.94	0.18	56,56,56,56	0
56	MG	BA	3449	1/1	0.94	0.19	32,32,32,32	0
56	MG	BA	3600	1/1	0.94	0.17	50,50,50,50	0
56	MG	DA	3410	1/1	0.94	0.10	46,46,46,46	0
56	MG	AA	3052	1/1	0.94	0.15	49,49,49,49	0
56	MG	CA	3004	1/1	0.94	0.09	67,67,67,67	0
56	MG	DA	3284	1/1	0.94	0.18	37,37,37,37	0
56	MG	DA	3516	1/1	0.94	0.28	52,52,52,52	0
56	MG	DA	3398	1/1	0.94	0.14	52,52,52,52	0
56	MG	DA	3611	1/1	0.94	0.20	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	3639	1/1	0.94	0.15	54,54,54,54	0
56	MG	DA	3072	1/1	0.94	0.13	52,52,52,52	0
56	MG	DA	3297	1/1	0.94	0.12	24,24,24,24	0
56	MG	BA	3260	1/1	0.94	0.10	42,42,42,42	0
56	MG	DA	3178	1/1	0.94	0.28	53,53,53,53	0
56	MG	DA	3551	1/1	0.94	0.07	47,47,47,47	0
56	MG	DA	3365	1/1	0.94	0.08	56,56,56,56	0
56	MG	BA	3466	1/1	0.94	0.19	44,44,44,44	0
56	MG	DA	3659	1/1	0.94	0.48	39,39,39,39	0
56	MG	DA	3015	1/1	0.94	0.54	48,48,48,48	0
56	MG	DA	3386	1/1	0.94	0.08	23,23,23,23	0
56	MG	BA	3335	1/1	0.94	0.20	42,42,42,42	0
56	MG	DA	3262	1/1	0.94	0.07	46,46,46,46	0
56	MG	AA	3016	1/1	0.94	0.14	55,55,55,55	0
56	MG	BA	3540	1/1	0.94	0.11	57,57,57,57	0
56	MG	DA	3581	1/1	0.94	0.10	35,35,35,35	0
56	MG	BA	3764	1/1	0.94	0.21	44,44,44,44	0
56	MG	DA	3435	1/1	0.94	0.15	55,55,55,55	0
56	MG	CA	3093	1/1	0.94	0.18	65,65,65,65	0
56	MG	BA	3130	1/1	0.94	0.56	41,41,41,41	0
56	MG	CA	3164	1/1	0.94	0.07	73,73,73,73	0
56	MG	BA	3166	1/1	0.94	0.16	46,46,46,46	0
56	MG	AA	3095	1/1	0.94	0.12	50,50,50,50	0
56	MG	AA	3017	1/1	0.94	0.13	69,69,69,69	0
56	MG	DA	3560	1/1	0.94	0.07	47,47,47,47	0
56	MG	BA	3323	1/1	0.94	0.15	43,43,43,43	0
56	MG	BA	3510	1/1	0.94	0.11	42,42,42,42	0
56	MG	BA	3075	1/1	0.94	0.18	21,21,21,21	0
56	MG	DA	3038	1/1	0.94	0.15	28,28,28,28	0
56	MG	BA	3683	1/1	0.94	0.15	43,43,43,43	0
56	MG	DA	3569	1/1	0.94	0.24	59,59,59,59	0
56	MG	BA	3312	1/1	0.94	0.18	35,35,35,35	0
56	MG	BA	3124	1/1	0.94	0.20	35,35,35,35	0
56	MG	BA	3056	1/1	0.94	0.23	50,50,50,50	0
56	MG	BA	3799	1/1	0.94	0.56	50,50,50,50	0
56	MG	DA	3511	1/1	0.94	0.14	54,54,54,54	0
56	MG	DQ	3003	1/1	0.94	0.50	52,52,52,52	0
56	MG	DA	3237	1/1	0.94	0.19	43,43,43,43	0
56	MG	BA	3561	1/1	0.94	0.18	55,55,55,55	0
56	MG	AA	3058	1/1	0.94	0.12	61,61,61,61	0
56	MG	DA	3308	1/1	0.94	0.10	49,49,49,49	0
56	MG	BA	3715	1/1	0.94	0.25	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3517	1/1	0.94	0.11	49,49,49,49	0
56	MG	AA	3086	1/1	0.94	0.10	48,48,48,48	0
56	MG	CA	3057	1/1	0.94	0.12	52,52,52,52	0
56	MG	AA	3057	1/1	0.94	0.20	66,66,66,66	0
56	MG	BA	3080	1/1	0.94	0.26	51,51,51,51	0
56	MG	DA	3427	1/1	0.94	0.07	45,45,45,45	0
56	MG	DA	3539	1/1	0.94	0.09	38,38,38,38	0
56	MG	AA	3119	1/1	0.94	0.04	65,65,65,65	0
56	MG	AA	3162	1/1	0.94	0.15	59,59,59,59	0
56	MG	CA	3090	1/1	0.94	0.21	67,67,67,67	0
56	MG	DU	3002	1/1	0.94	0.44	52,52,52,52	0
56	MG	AA	3056	1/1	0.94	0.26	54,54,54,54	0
56	MG	BA	3778	1/1	0.94	0.11	41,41,41,41	0
56	MG	BA	3150	1/1	0.94	0.19	56,56,56,56	0
56	MG	BA	3433	1/1	0.94	0.17	31,31,31,31	0
56	MG	DA	3275	1/1	0.94	0.09	58,58,58,58	0
56	MG	DA	3430	1/1	0.94	0.11	52,52,52,52	0
56	MG	BA	3484	1/1	0.94	0.16	51,51,51,51	0
56	MG	BA	3366	1/1	0.94	0.11	42,42,42,42	0
56	MG	CA	3112	1/1	0.94	0.10	56,56,56,56	0
56	MG	BA	3501	1/1	0.94	0.13	43,43,43,43	0
56	MG	CX	3003	1/1	0.94	0.16	58,58,58,58	0
56	MG	CA	3154	1/1	0.94	0.19	54,54,54,54	0
56	MG	DF	305	1/1	0.94	0.45	44,44,44,44	0
56	MG	BA	3117	1/1	0.94	0.35	35,35,35,35	0
56	MG	BA	3707	1/1	0.94	0.10	43,43,43,43	0
56	MG	BA	3456	1/1	0.94	0.12	32,32,32,32	0
56	MG	BA	3382	1/1	0.94	0.13	41,41,41,41	0
56	MG	DA	3273	1/1	0.94	0.10	39,39,39,39	0
56	MG	DA	3325	1/1	0.94	0.24	37,37,37,37	0
56	MG	BD	3301	1/1	0.94	0.27	37,37,37,37	0
56	MG	DA	3158	1/1	0.94	0.19	30,30,30,30	0
56	MG	BA	3593	1/1	0.94	0.18	47,47,47,47	0
56	MG	BA	3587	1/1	0.94	0.09	54,54,54,54	0
56	MG	DA	3447	1/1	0.94	0.14	41,41,41,41	0
56	MG	CA	3116	1/1	0.94	0.08	54,54,54,54	0
56	MG	DA	3434	1/1	0.94	0.12	27,27,27,27	0
56	MG	BA	3119	1/1	0.94	0.22	29,29,29,29	0
56	MG	BA	3757	1/1	0.94	0.17	45,45,45,45	0
56	MG	AA	3030	1/1	0.94	0.12	63,63,63,63	0
56	MG	DA	3098	1/1	0.94	0.09	57,57,57,57	0
56	MG	DA	3350	1/1	0.94	0.07	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	3240	1/1	0.94	0.09	42,42,42,42	0
56	MG	AA	3155	1/1	0.94	0.10	49,49,49,49	0
56	MG	AA	3054	1/1	0.94	0.07	62,62,62,62	0
56	MG	DA	3596	1/1	0.94	0.07	65,65,65,65	0
56	MG	BA	3748	1/1	0.94	0.10	69,69,69,69	0
56	MG	DA	3170	1/1	0.94	0.22	46,46,46,46	0
56	MG	BA	3418	1/1	0.94	0.16	34,34,34,34	0
56	MG	DA	3201	1/1	0.94	0.20	64,64,64,64	0
56	MG	BA	3579	1/1	0.94	0.26	43,43,43,43	0
56	MG	DA	3594	1/1	0.94	0.18	54,54,54,54	0
56	MG	DA	3156	1/1	0.94	0.13	50,50,50,50	0
56	MG	DA	3425	1/1	0.94	0.12	52,52,52,52	0
56	MG	AA	3071	1/1	0.94	0.15	51,51,51,51	0
56	MG	DA	3288	1/1	0.94	0.10	48,48,48,48	0
56	MG	BW	201	1/1	0.94	0.25	45,45,45,45	0
56	MG	DA	3337	1/1	0.94	0.13	44,44,44,44	0
56	MG	BA	3239	1/1	0.94	0.17	40,40,40,40	0
56	MG	DA	3615	1/1	0.94	0.09	50,50,50,50	0
56	MG	CA	3027	1/1	0.94	0.18	61,61,61,61	0
56	MG	CA	3088	1/1	0.94	0.15	66,66,66,66	0
56	MG	BA	3182	1/1	0.94	0.19	21,21,21,21	0
56	MG	DA	3579	1/1	0.94	0.15	52,52,52,52	0
56	MG	BA	3268	1/1	0.94	0.32	57,57,57,57	0
56	MG	DA	3023	1/1	0.94	0.19	44,44,44,44	0
56	MG	BA	3777	1/1	0.94	0.15	44,44,44,44	0
56	MG	BA	3310	1/1	0.94	0.17	42,42,42,42	0
56	MG	BA	3695	1/1	0.94	0.28	37,37,37,37	0
56	MG	AA	3008	1/1	0.94	0.14	56,56,56,56	0
56	MG	BA	3073	1/1	0.94	0.20	45,45,45,45	0
56	MG	BA	3242	1/1	0.94	0.10	47,47,47,47	0
56	MG	BA	3021	1/1	0.94	0.17	22,22,22,22	0
56	MG	DA	3030	1/1	0.94	0.09	46,46,46,46	0
56	MG	BA	3524	1/1	0.94	0.16	53,53,53,53	0
56	MG	B5	105	1/1	0.94	0.14	66,66,66,66	0
56	MG	BA	3537	1/1	0.94	0.19	21,21,21,21	0
56	MG	BA	3789	1/1	0.94	0.29	37,37,37,37	0
56	MG	BA	3735	1/1	0.94	0.15	20,20,20,20	0
56	MG	BA	3261	1/1	0.94	0.10	46,46,46,46	0
56	MG	DA	3304	1/1	0.94	0.14	40,40,40,40	0
56	MG	AA	3041	1/1	0.94	0.08	64,64,64,64	0
56	MG	BA	3220	1/1	0.94	0.32	40,40,40,40	0
56	MG	BB	219	1/1	0.94	0.10	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3190	1/1	0.94	0.24	50,50,50,50	0
56	MG	BA	3129	1/1	0.94	0.55	38,38,38,38	0
56	MG	DA	3387	1/1	0.94	0.24	39,39,39,39	0
56	MG	BA	3307	1/1	0.94	0.30	50,50,50,50	0
56	MG	DV	3001	1/1	0.94	0.17	61,61,61,61	0
56	MG	BA	3634	1/1	0.94	0.20	47,47,47,47	0
56	MG	DA	3219	1/1	0.94	0.11	36,36,36,36	0
56	MG	BF	309	1/1	0.94	0.10	45,45,45,45	0
56	MG	DE	302	1/1	0.94	0.12	33,33,33,33	0
56	MG	BA	3763	1/1	0.94	0.11	39,39,39,39	0
56	MG	DA	3093	1/1	0.94	0.39	54,54,54,54	0
56	MG	BA	3410	1/1	0.94	0.26	31,31,31,31	0
56	MG	BA	3071	1/1	0.94	0.16	40,40,40,40	0
56	MG	AA	3105	1/1	0.94	0.14	71,71,71,71	0
56	MG	DA	3443	1/1	0.94	0.11	38,38,38,38	0
56	MG	AA	3182	1/1	0.94	0.14	64,64,64,64	0
56	MG	BA	3317	1/1	0.94	0.21	41,41,41,41	0
56	MG	DA	3379	1/1	0.94	0.09	50,50,50,50	0
59	ZN	AN	501	1/1	0.94	0.15	86,86,86,86	0
56	MG	DA	3582	1/1	0.94	0.14	64,64,64,64	0
56	MG	BA	3411	1/1	0.94	0.26	30,30,30,30	0
56	MG	DA	3436	1/1	0.94	0.11	70,70,70,70	0
56	MG	CA	3040	1/1	0.94	0.14	45,45,45,45	0
56	MG	BN	3003	1/1	0.94	0.19	44,44,44,44	0
56	MG	BA	3153	1/1	0.94	0.14	50,50,50,50	0
56	MG	DA	3486	1/1	0.94	0.34	50,50,50,50	0
56	MG	AA	3009	1/1	0.94	0.11	24,24,24,24	0
56	MG	CA	3123	1/1	0.94	0.16	67,67,67,67	0
56	MG	BA	3210	1/1	0.94	0.24	43,43,43,43	0
56	MG	BA	3067	1/1	0.94	0.20	49,49,49,49	0
56	MG	BA	3012	1/1	0.94	0.34	33,33,33,33	0
56	MG	BA	3158	1/1	0.94	0.30	40,40,40,40	0
56	MG	BA	3116	1/1	0.94	0.11	35,35,35,35	0
56	MG	DA	3206	1/1	0.94	0.09	46,46,46,46	0
56	MG	DA	3176	1/1	0.94	0.34	44,44,44,44	0
56	MG	DA	3151	1/1	0.94	0.09	33,33,33,33	0
56	MG	BA	3229	1/1	0.94	0.32	44,44,44,44	0
56	MG	D0	101	1/1	0.95	0.16	50,50,50,50	0
56	MG	BA	3454	1/1	0.95	0.12	29,29,29,29	0
56	MG	BD	3306	1/1	0.95	0.44	38,38,38,38	0
56	MG	BE	302	1/1	0.95	0.29	40,40,40,40	0
56	MG	BA	3493	1/1	0.95	0.11	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	3602	1/1	0.95	0.17	51,51,51,51	0
56	MG	DA	3518	1/1	0.95	0.13	58,58,58,58	0
56	MG	DA	3068	1/1	0.95	0.34	47,47,47,47	0
56	MG	DF	301	1/1	0.95	0.16	47,47,47,47	0
56	MG	DA	3171	1/1	0.95	0.14	53,53,53,53	0
56	MG	DA	3642	1/1	0.95	0.09	48,48,48,48	0
56	MG	DA	3633	1/1	0.95	0.06	56,56,56,56	0
56	MG	BA	3047	1/1	0.95	0.12	43,43,43,43	0
56	MG	AA	3104	1/1	0.95	0.25	70,70,70,70	0
56	MG	DD	303	1/1	0.95	0.57	51,51,51,51	0
56	MG	BA	3206	1/1	0.95	0.22	37,37,37,37	0
56	MG	BO	5001	1/1	0.95	0.11	55,55,55,55	0
56	MG	DA	3473	1/1	0.95	0.09	30,30,30,30	0
56	MG	AA	3024	1/1	0.95	0.20	55,55,55,55	0
56	MG	BA	3809	1/1	0.95	0.12	41,41,41,41	0
56	MG	CA	3150	1/1	0.95	0.12	47,47,47,47	0
56	MG	DA	3411	1/1	0.95	0.25	46,46,46,46	0
56	MG	BA	3574	1/1	0.95	0.17	28,28,28,28	0
56	MG	BA	3344	1/1	0.95	0.21	55,55,55,55	0
56	MG	DA	3439	1/1	0.95	0.20	46,46,46,46	0
56	MG	DA	3662	1/1	0.95	0.14	38,38,38,38	0
56	MG	DA	3198	1/1	0.95	0.30	49,49,49,49	0
56	MG	AA	3091	1/1	0.95	0.16	40,40,40,40	0
56	MG	DN	5001	1/1	0.95	0.10	54,54,54,54	0
56	MG	BA	3015	1/1	0.95	0.14	50,50,50,50	0
56	MG	AA	3010	1/1	0.95	0.12	63,63,63,63	0
56	MG	BA	3497	1/1	0.95	0.13	44,44,44,44	0
56	MG	AA	3175	1/1	0.95	0.10	66,66,66,66	0
56	MG	DA	3172	1/1	0.95	0.11	31,31,31,31	0
56	MG	BP	204	1/1	0.95	0.15	54,54,54,54	0
56	MG	AA	3099	1/1	0.95	0.21	47,47,47,47	0
56	MG	DA	3312	1/1	0.95	0.09	41,41,41,41	0
56	MG	BA	3750	1/1	0.95	0.25	42,42,42,42	0
56	MG	BQ	202	1/1	0.95	0.26	37,37,37,37	0
56	MG	BA	3107	1/1	0.95	0.18	50,50,50,50	0
56	MG	BA	3270	1/1	0.95	0.29	40,40,40,40	0
56	MG	BA	3188	1/1	0.95	0.20	46,46,46,46	0
56	MG	BA	3176	1/1	0.95	0.10	44,44,44,44	0
56	MG	BA	3412	1/1	0.95	0.27	19,19,19,19	0
56	MG	BA	3363	1/1	0.95	0.09	66,66,66,66	0
56	MG	DA	3128	1/1	0.95	0.35	57,57,57,57	0
56	MG	BA	3796	1/1	0.95	0.29	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3670	1/1	0.95	0.14	47,47,47,47	0
56	MG	BA	3550	1/1	0.95	0.14	25,25,25,25	0
56	MG	BA	3244	1/1	0.95	0.52	39,39,39,39	0
56	MG	CA	3055	1/1	0.95	0.20	55,55,55,55	0
56	MG	DA	3632	1/1	0.95	0.11	50,50,50,50	0
56	MG	DA	3190	1/1	0.95	0.14	41,41,41,41	0
56	MG	BA	3705	1/1	0.95	0.25	28,28,28,28	0
56	MG	BA	3814	1/1	0.95	0.27	42,42,42,42	0
56	MG	DA	3585	1/1	0.95	0.21	43,43,43,43	0
56	MG	BA	3641	1/1	0.95	0.08	54,54,54,54	0
56	MG	DA	3543	1/1	0.95	0.14	52,52,52,52	0
56	MG	DA	3404	1/1	0.95	0.09	40,40,40,40	0
56	MG	BA	3743	1/1	0.95	0.15	43,43,43,43	0
56	MG	CA	3156	1/1	0.95	0.16	41,41,41,41	0
56	MG	DA	3446	1/1	0.95	0.17	44,44,44,44	0
56	MG	DA	3661	1/1	0.95	0.22	54,54,54,54	0
56	MG	BA	3177	1/1	0.95	0.30	44,44,44,44	0
56	MG	BA	3029	1/1	0.95	0.18	30,30,30,30	0
56	MG	DA	3401	1/1	0.95	0.08	43,43,43,43	0
56	MG	AX	3004	1/1	0.95	0.12	53,53,53,53	0
56	MG	AA	3046	1/1	0.95	0.15	56,56,56,56	0
56	MG	BA	3267	1/1	0.95	0.14	45,45,45,45	0
56	MG	BA	3429	1/1	0.95	0.16	23,23,23,23	0
56	MG	AX	3010	1/1	0.95	0.09	59,59,59,59	0
56	MG	BA	3348	1/1	0.95	0.19	24,24,24,24	0
56	MG	DA	3326	1/1	0.95	0.17	47,47,47,47	0
56	MG	BA	3357	1/1	0.95	0.19	46,46,46,46	0
56	MG	DA	3340	1/1	0.95	0.10	30,30,30,30	0
56	MG	BA	3257	1/1	0.95	0.20	54,54,54,54	0
56	MG	BA	3189	1/1	0.95	0.23	46,46,46,46	0
56	MG	DA	3257	1/1	0.95	0.22	57,57,57,57	0
56	MG	BA	3205	1/1	0.95	0.38	40,40,40,40	0
56	MG	BA	3716	1/1	0.95	0.37	39,39,39,39	0
56	MG	BA	3556	1/1	0.95	0.11	48,48,48,48	0
56	MG	BA	3123	1/1	0.95	0.23	28,28,28,28	0
56	MG	AA	3103	1/1	0.95	0.17	48,48,48,48	0
56	MG	BA	3269	1/1	0.95	0.21	42,42,42,42	0
56	MG	DA	3307	1/1	0.95	0.13	27,27,27,27	0
56	MG	BA	3361	1/1	0.95	0.16	61,61,61,61	0
56	MG	DA	3290	1/1	0.95	0.10	46,46,46,46	0
56	MG	AA	3130	1/1	0.95	0.06	56,56,56,56	0
56	MG	BA	3236	1/1	0.95	0.36	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3007	1/1	0.95	0.10	35,35,35,35	0
56	MG	BD	3307	1/1	0.95	1.03	56,56,56,56	0
56	MG	BA	3090	1/1	0.95	0.22	27,27,27,27	0
56	MG	BA	3752	1/1	0.95	0.08	32,32,32,32	0
56	MG	BV	203	1/1	0.95	0.48	31,31,31,31	0
56	MG	BB	208	1/1	0.95	0.11	36,36,36,36	0
56	MG	AA	3113	1/1	0.95	0.07	67,67,67,67	0
56	MG	BA	3094	1/1	0.95	0.17	44,44,44,44	0
56	MG	BA	3393	1/1	0.95	0.17	22,22,22,22	0
56	MG	DA	3650	1/1	0.95	0.16	46,46,46,46	0
56	MG	AA	3165	1/1	0.95	0.08	49,49,49,49	0
56	MG	DA	3621	1/1	0.95	0.25	50,50,50,50	0
56	MG	CA	3098	1/1	0.95	0.15	44,44,44,44	0
56	MG	CA	3075	1/1	0.95	0.20	67,67,67,67	0
56	MG	CA	3048	1/1	0.95	0.12	77,77,77,77	0
56	MG	BA	3373	1/1	0.95	0.09	42,42,42,42	0
56	MG	BA	3589	1/1	0.95	0.18	42,42,42,42	0
56	MG	DA	3664	1/1	0.95	0.86	50,50,50,50	0
56	MG	BA	3761	1/1	0.95	0.21	53,53,53,53	0
56	MG	BA	3570	1/1	0.95	0.23	35,35,35,35	0
56	MG	BA	3453	1/1	0.95	0.19	52,52,52,52	0
56	MG	BA	3686	1/1	0.95	0.13	41,41,41,41	0
56	MG	BA	3797	1/1	0.95	0.16	19,19,19,19	0
56	MG	BA	3146	1/1	0.95	0.13	19,19,19,19	0
56	MG	DA	3399	1/1	0.95	0.11	55,55,55,55	0
56	MG	AA	3023	1/1	0.95	0.18	48,48,48,48	0
56	MG	BA	3684	1/1	0.95	0.18	51,51,51,51	0
56	MG	CA	3065	1/1	0.95	0.17	64,64,64,64	0
56	MG	BA	3533	1/1	0.95	0.18	38,38,38,38	0
56	MG	DA	3580	1/1	0.95	0.08	46,46,46,46	0
56	MG	DA	3148	1/1	0.95	0.42	43,43,43,43	0
60	K	CX	3001	1/1	0.95	0.31	77,77,77,77	0
56	MG	BA	3406	1/1	0.95	0.09	32,32,32,32	0
56	MG	BA	3611	1/1	0.95	0.11	45,45,45,45	0
56	MG	BA	3275	1/1	0.95	0.16	34,34,34,34	0
56	MG	DA	3616	1/1	0.95	0.25	43,43,43,43	0
56	MG	DA	3566	1/1	0.95	0.09	62,62,62,62	0
56	MG	BA	3378	1/1	0.95	0.13	47,47,47,47	0
56	MG	AX	3008	1/1	0.95	0.19	37,37,37,37	0
56	MG	BB	215	1/1	0.95	0.20	35,35,35,35	0
56	MG	CA	3166	1/1	0.95	0.16	52,52,52,52	0
56	MG	BA	3414	1/1	0.95	0.22	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3701	1/1	0.95	0.20	20,20,20,20	0
56	MG	AA	3112	1/1	0.95	0.14	60,60,60,60	0
56	MG	BA	3765	1/1	0.95	0.09	53,53,53,53	0
56	MG	DA	3428	1/1	0.95	0.05	26,26,26,26	0
56	MG	DA	3557	1/1	0.95	0.17	44,44,44,44	0
56	MG	BA	3565	1/1	0.95	0.09	43,43,43,43	0
56	MG	BA	3541	1/1	0.95	0.17	55,55,55,55	0
56	MG	BN	3005	1/1	0.95	0.21	35,35,35,35	0
56	MG	CA	3128	1/1	0.95	0.14	68,68,68,68	0
56	MG	BA	3669	1/1	0.95	0.11	36,36,36,36	0
56	MG	DA	3003	1/1	0.95	0.12	48,48,48,48	0
56	MG	BA	3132	1/1	0.95	0.22	49,49,49,49	0
56	MG	BA	3662	1/1	0.95	0.17	52,52,52,52	0
56	MG	BA	3197	1/1	0.95	0.82	51,51,51,51	0
56	MG	AA	3078	1/1	0.95	0.07	72,72,72,72	0
56	MG	BA	3642	1/1	0.95	0.15	36,36,36,36	0
56	MG	B0	105	1/1	0.95	0.07	64,64,64,64	0
56	MG	DA	3658	1/1	0.95	0.33	55,55,55,55	0
56	MG	DA	3278	1/1	0.95	0.14	37,37,37,37	0
56	MG	DA	3050	1/1	0.95	0.10	37,37,37,37	0
56	MG	B6	101	1/1	0.95	0.20	47,47,47,47	0
56	MG	AA	3152	1/1	0.95	0.08	48,48,48,48	0
56	MG	BA	3628	1/1	0.95	0.11	34,34,34,34	0
56	MG	BA	3405	1/1	0.95	0.19	22,22,22,22	0
56	MG	DA	3501	1/1	0.95	0.08	46,46,46,46	0
56	MG	DA	3449	1/1	0.95	0.10	33,33,33,33	0
56	MG	DA	3303	1/1	0.95	0.15	55,55,55,55	0
56	MG	CA	3074	1/1	0.95	0.11	57,57,57,57	0
56	MG	DA	3480	1/1	0.95	0.14	38,38,38,38	0
56	MG	CA	3086	1/1	0.95	0.13	76,76,76,76	0
56	MG	BA	3274	1/1	0.95	0.20	51,51,51,51	0
56	MG	AA	3131	1/1	0.95	0.14	29,29,29,29	0
56	MG	DA	3382	1/1	0.95	0.14	31,31,31,31	0
56	MG	BA	3584	1/1	0.95	0.22	34,34,34,34	0
56	MG	BA	3474	1/1	0.95	0.18	20,20,20,20	0
56	MG	DA	3513	1/1	0.95	0.09	30,30,30,30	0
56	MG	BA	3202	1/1	0.95	0.29	38,38,38,38	0
56	MG	DA	3481	1/1	0.95	0.12	24,24,24,24	0
56	MG	BA	3297	1/1	0.95	0.15	46,46,46,46	0
56	MG	CA	3012	1/1	0.95	0.12	51,51,51,51	0
56	MG	DA	3520	1/1	0.95	0.06	44,44,44,44	0
56	MG	BA	3489	1/1	0.95	0.32	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3007	1/1	0.95	0.08	43,43,43,43	0
56	MG	DA	3235	1/1	0.95	0.15	35,35,35,35	0
56	MG	BA	3031	1/1	0.95	0.23	28,28,28,28	0
56	MG	BA	3106	1/1	0.95	0.17	44,44,44,44	0
56	MG	BD	3304	1/1	0.95	0.09	25,25,25,25	0
56	MG	CA	3007	1/1	0.95	0.20	42,42,42,42	0
56	MG	BA	3141	1/1	0.95	0.13	42,42,42,42	0
56	MG	AA	3013	1/1	0.95	0.07	57,57,57,57	0
56	MG	BA	3313	1/1	0.96	0.16	34,34,34,34	0
56	MG	BA	3376	1/1	0.96	0.12	43,43,43,43	0
56	MG	BA	3053	1/1	0.96	0.22	23,23,23,23	0
56	MG	BA	3386	1/1	0.96	0.15	47,47,47,47	0
56	MG	DA	3160	1/1	0.96	0.20	38,38,38,38	0
56	MG	AA	3123	1/1	0.96	0.18	51,51,51,51	0
56	MG	BA	3171	1/1	0.96	0.19	54,54,54,54	0
56	MG	BA	3681	1/1	0.96	0.16	50,50,50,50	0
56	MG	BA	3271	1/1	0.96	0.14	38,38,38,38	0
56	MG	AA	3090	1/1	0.96	0.23	41,41,41,41	0
56	MG	DA	3352	1/1	0.96	0.11	27,27,27,27	0
56	MG	BA	3469	1/1	0.96	0.13	41,41,41,41	0
56	MG	BA	3432	1/1	0.96	0.12	35,35,35,35	0
56	MG	BA	3058	1/1	0.96	0.13	27,27,27,27	0
60	K	AX	3001	1/1	0.96	0.15	65,65,65,65	0
56	MG	BA	3370	1/1	0.96	0.13	27,27,27,27	0
56	MG	BA	3311	1/1	0.96	0.17	23,23,23,23	0
56	MG	BN	3006	1/1	0.96	0.54	47,47,47,47	0
56	MG	BA	3736	1/1	0.96	0.08	42,42,42,42	0
56	MG	BB	222	1/1	0.96	0.19	50,50,50,50	0
56	MG	BA	3658	1/1	0.96	0.16	51,51,51,51	0
56	MG	AA	3082	1/1	0.96	0.34	51,51,51,51	0
56	MG	AA	3126	1/1	0.96	0.17	57,57,57,57	0
56	MG	DA	3233	1/1	0.96	0.13	40,40,40,40	0
56	MG	DA	3451	1/1	0.96	0.15	20,20,20,20	0
56	MG	BA	3710	1/1	0.96	0.27	28,28,28,28	0
56	MG	BD	3303	1/1	0.96	0.17	33,33,33,33	0
56	MG	DA	3356	1/1	0.96	0.17	37,37,37,37	0
56	MG	BA	3810	1/1	0.96	0.23	43,43,43,43	0
56	MG	BA	3781	1/1	0.96	0.24	47,47,47,47	0
56	MG	DA	3092	1/1	0.96	0.36	48,48,48,48	0
56	MG	AA	3116	1/1	0.96	0.12	32,32,32,32	0
56	MG	BX	102	1/1	0.96	0.15	36,36,36,36	0
56	MG	BA	3569	1/1	0.96	0.16	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3316	1/1	0.96	0.23	25,25,25,25	0
56	MG	BA	3450	1/1	0.96	0.15	10,10,10,10	0
56	MG	BA	3287	1/1	0.96	0.27	28,28,28,28	0
56	MG	DA	3301	1/1	0.96	0.11	51,51,51,51	0
56	MG	BA	3754	1/1	0.96	0.10	60,60,60,60	0
56	MG	AA	3065	1/1	0.96	0.08	55,55,55,55	0
56	MG	CA	3062	1/1	0.96	0.18	67,67,67,67	0
56	MG	BA	3660	1/1	0.96	0.17	51,51,51,51	0
56	MG	DA	3620	1/1	0.96	0.17	59,59,59,59	0
56	MG	DA	3397	1/1	0.96	0.09	30,30,30,30	0
56	MG	BA	3536	1/1	0.96	0.23	36,36,36,36	0
56	MG	BA	3022	1/1	0.96	0.14	25,25,25,25	0
56	MG	DA	3344	1/1	0.96	0.18	46,46,46,46	0
56	MG	BB	217	1/1	0.96	0.16	41,41,41,41	0
56	MG	DA	3667	1/1	0.96	0.14	66,66,66,66	0
56	MG	CA	3102	1/1	0.96	0.12	49,49,49,49	0
56	MG	BA	3549	1/1	0.96	0.15	36,36,36,36	0
56	MG	DA	3421	1/1	0.96	0.07	31,31,31,31	0
56	MG	AA	3106	1/1	0.96	0.10	61,61,61,61	0
56	MG	DA	3381	1/1	0.96	0.19	34,34,34,34	0
56	MG	AA	3081	1/1	0.96	0.23	51,51,51,51	0
56	MG	BA	3246	1/1	0.96	0.12	47,47,47,47	0
56	MG	DA	3311	1/1	0.96	0.12	19,19,19,19	0
56	MG	BA	3483	1/1	0.96	0.20	41,41,41,41	0
56	MG	DA	3674	1/1	0.96	0.80	43,43,43,43	0
56	MG	DA	3496	1/1	0.96	0.42	35,35,35,35	0
56	MG	DA	3106	1/1	0.96	0.06	52,52,52,52	0
56	MG	BA	3775	1/1	0.96	0.07	34,34,34,34	0
56	MG	BA	3591	1/1	0.96	0.13	48,48,48,48	0
56	MG	AA	3144	1/1	0.96	0.10	59,59,59,59	0
56	MG	AA	3148	1/1	0.96	0.09	58,58,58,58	0
56	MG	CA	3039	1/1	0.96	0.15	55,55,55,55	0
56	MG	CA	3111	1/1	0.96	0.10	56,56,56,56	0
56	MG	BA	3304	1/1	0.96	0.12	37,37,37,37	0
56	MG	BA	3216	1/1	0.96	0.10	62,62,62,62	0
56	MG	CA	3122	1/1	0.96	0.10	65,65,65,65	0
56	MG	DA	3243	1/1	0.96	0.15	47,47,47,47	0
56	MG	BA	3136	1/1	0.96	0.29	42,42,42,42	0
56	MG	DA	3265	1/1	0.96	0.18	37,37,37,37	0
56	MG	DA	3011	1/1	0.96	0.53	51,51,51,51	0
56	MG	DA	3444	1/1	0.96	0.12	46,46,46,46	0
56	MG	BA	3635	1/1	0.96	0.08	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3803	1/1	0.96	0.17	33,33,33,33	0
56	MG	BA	3791	1/1	0.96	0.18	18,18,18,18	0
56	MG	BA	3615	1/1	0.96	0.08	60,60,60,60	0
56	MG	BA	3564	1/1	0.96	0.18	50,50,50,50	0
56	MG	DD	306	1/1	0.96	0.84	48,48,48,48	0
56	MG	B8	101	1/1	0.96	0.15	36,36,36,36	0
56	MG	DA	3169	1/1	0.96	0.18	44,44,44,44	0
56	MG	BA	3482	1/1	0.96	0.14	42,42,42,42	0
56	MG	BA	3603	1/1	0.96	0.20	42,42,42,42	0
56	MG	DA	3339	1/1	0.96	0.12	60,60,60,60	0
56	MG	BA	3365	1/1	0.96	0.28	37,37,37,37	0
56	MG	BA	3640	1/1	0.96	0.21	42,42,42,42	0
56	MG	BE	304	1/1	0.96	0.50	43,43,43,43	0
56	MG	CA	3066	1/1	0.96	0.11	47,47,47,47	0
56	MG	BA	3379	1/1	0.96	0.18	39,39,39,39	0
56	MG	BA	3303	1/1	0.96	0.32	37,37,37,37	0
56	MG	BA	3235	1/1	0.96	0.22	26,26,26,26	0
56	MG	BA	3668	1/1	0.96	0.21	48,48,48,48	0
56	MG	DA	3028	1/1	0.96	0.54	45,45,45,45	0
56	MG	DA	3672	1/1	0.96	0.28	59,59,59,59	0
56	MG	BA	3321	1/1	0.96	0.19	21,21,21,21	0
56	MG	DA	3108	1/1	0.96	0.21	46,46,46,46	0
56	MG	BA	3568	1/1	0.96	0.23	26,26,26,26	0
56	MG	BA	3203	1/1	0.96	0.50	38,38,38,38	0
56	MG	BA	3383	1/1	0.96	0.19	20,20,20,20	0
56	MG	DA	3119	1/1	0.96	0.09	40,40,40,40	0
56	MG	BA	3355	1/1	0.96	0.26	28,28,28,28	0
56	MG	DA	3052	1/1	0.96	0.19	26,26,26,26	0
56	MG	BA	3008	1/1	0.96	0.15	26,26,26,26	0
56	MG	BA	3655	1/1	0.96	0.14	54,54,54,54	0
56	MG	DA	3144	1/1	0.96	0.16	39,39,39,39	0
56	MG	CA	3056	1/1	0.96	0.11	60,60,60,60	0
56	MG	DA	3078	1/1	0.96	0.19	35,35,35,35	0
56	MG	BA	3442	1/1	0.96	0.13	36,36,36,36	0
56	MG	DA	3367	1/1	0.96	0.15	55,55,55,55	0
56	MG	DA	3378	1/1	0.96	0.10	34,34,34,34	0
56	MG	DA	3600	1/1	0.96	0.14	43,43,43,43	0
56	MG	BA	3353	1/1	0.96	0.21	49,49,49,49	0
56	MG	BA	3446	1/1	0.96	0.20	31,31,31,31	0
56	MG	CA	3146	1/1	0.96	0.20	65,65,65,65	0
56	MG	DA	3587	1/1	0.96	0.12	52,52,52,52	0
56	MG	B0	104	1/1	0.96	0.18	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3243	1/1	0.96	0.31	56,56,56,56	0
56	MG	BA	3502	1/1	0.96	0.11	20,20,20,20	0
56	MG	B7	101	1/1	0.96	0.24	47,47,47,47	0
56	MG	BA	3301	1/1	0.96	0.10	48,48,48,48	0
56	MG	DY	502	1/1	0.96	0.15	58,58,58,58	0
56	MG	BA	3544	1/1	0.96	0.31	45,45,45,45	0
56	MG	DA	3614	1/1	0.96	0.16	61,61,61,61	0
56	MG	DA	3509	1/1	0.96	0.13	55,55,55,55	0
56	MG	B7	105	1/1	0.96	0.27	46,46,46,46	0
56	MG	BA	3664	1/1	0.96	0.19	17,17,17,17	0
56	MG	BA	3762	1/1	0.96	0.16	53,53,53,53	0
56	MG	BA	3515	1/1	0.96	0.17	35,35,35,35	0
56	MG	BE	305	1/1	0.96	0.21	19,19,19,19	0
56	MG	AA	3114	1/1	0.96	0.17	45,45,45,45	0
56	MG	AA	3146	1/1	0.96	0.13	53,53,53,53	0
56	MG	BA	3733	1/1	0.96	0.09	46,46,46,46	0
56	MG	BA	3444	1/1	0.96	0.22	43,43,43,43	0
56	MG	CA	3147	1/1	0.96	0.13	70,70,70,70	0
56	MG	BA	3756	1/1	0.96	0.06	56,56,56,56	0
56	MG	DA	3293	1/1	0.96	0.14	57,57,57,57	0
56	MG	CA	3051	1/1	0.96	0.15	55,55,55,55	0
56	MG	BA	3596	1/1	0.96	0.08	68,68,68,68	0
56	MG	DA	3406	1/1	0.96	0.12	33,33,33,33	0
56	MG	BA	3230	1/1	0.96	0.51	36,36,36,36	0
56	MG	DQ	3001	1/1	0.96	0.07	45,45,45,45	0
56	MG	BA	3338	1/1	0.96	0.20	43,43,43,43	0
56	MG	DA	3548	1/1	0.96	0.16	55,55,55,55	0
56	MG	DD	304	1/1	0.96	0.08	33,33,33,33	0
56	MG	DA	3105	1/1	0.96	0.10	41,41,41,41	0
56	MG	AA	3018	1/1	0.96	0.15	50,50,50,50	0
56	MG	AA	3137	1/1	0.96	0.11	42,42,42,42	0
56	MG	DA	3525	1/1	0.96	0.12	44,44,44,44	0
56	MG	AA	3088	1/1	0.96	0.10	42,42,42,42	0
56	MG	D3	3001	1/1	0.96	0.42	60,60,60,60	0
56	MG	BA	3104	1/1	0.96	0.25	23,23,23,23	0
56	MG	D0	102	1/1	0.96	0.11	51,51,51,51	0
56	MG	DA	3317	1/1	0.96	0.14	38,38,38,38	0
56	MG	CA	3170	1/1	0.96	0.10	53,53,53,53	0
56	MG	DA	3417	1/1	0.96	0.14	62,62,62,62	0
56	MG	DA	3475	1/1	0.96	0.14	38,38,38,38	0
56	MG	BA	3656	1/1	0.96	0.10	64,64,64,64	0
56	MG	BA	3476	1/1	0.96	0.36	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	3408	1/1	0.96	0.29	51,51,51,51	0
56	MG	BB	201	1/1	0.96	0.12	65,65,65,65	0
56	MG	BA	3023	1/1	0.96	0.22	35,35,35,35	0
56	MG	DA	3531	1/1	0.96	0.17	62,62,62,62	0
56	MG	BA	3339	1/1	0.96	0.19	23,23,23,23	0
56	MG	DA	3186	1/1	0.96	0.15	54,54,54,54	0
56	MG	BA	3445	1/1	0.96	0.26	48,48,48,48	0
56	MG	DA	3371	1/1	0.96	0.16	22,22,22,22	0
56	MG	AA	3117	1/1	0.96	0.19	34,34,34,34	0
56	MG	DA	3618	1/1	0.96	0.17	64,64,64,64	0
56	MG	DA	3121	1/1	0.96	0.15	40,40,40,40	0
56	MG	CA	3153	1/1	0.96	0.11	52,52,52,52	0
56	MG	BA	3403	1/1	0.96	0.13	22,22,22,22	0
56	MG	AA	3190	1/1	0.96	0.13	48,48,48,48	0
56	MG	AA	3061	1/1	0.96	0.23	54,54,54,54	0
56	MG	BA	3134	1/1	0.96	0.17	36,36,36,36	0
56	MG	AA	3075	1/1	0.96	0.23	49,49,49,49	0
56	MG	BA	3753	1/1	0.96	0.12	27,27,27,27	0
56	MG	BY	204	1/1	0.96	0.31	52,52,52,52	0
56	MG	AA	3003	1/1	0.96	0.15	63,63,63,63	0
56	MG	BA	3113	1/1	0.96	0.45	39,39,39,39	0
56	MG	BA	3465	1/1	0.96	0.22	47,47,47,47	0
56	MG	BA	3654	1/1	0.96	0.12	49,49,49,49	0
56	MG	BA	3572	1/1	0.96	0.15	52,52,52,52	0
56	MG	BA	3438	1/1	0.96	0.14	21,21,21,21	0
56	MG	BA	3388	1/1	0.96	0.22	27,27,27,27	0
56	MG	DA	3302	1/1	0.96	0.12	32,32,32,32	0
56	MG	AA	3092	1/1	0.96	0.31	54,54,54,54	0
56	MG	CA	3167	1/1	0.96	0.06	47,47,47,47	0
56	MG	BA	3087	1/1	0.96	0.57	40,40,40,40	0
56	MG	AA	3178	1/1	0.96	0.12	59,59,59,59	0
56	MG	BA	3500	1/1	0.96	0.22	32,32,32,32	0
56	MG	DA	3239	1/1	0.96	0.07	51,51,51,51	0
56	MG	DA	3204	1/1	0.96	0.37	50,50,50,50	0
56	MG	DA	3540	1/1	0.96	0.08	56,56,56,56	0
56	MG	DA	3529	1/1	0.96	0.11	57,57,57,57	0
56	MG	BA	3255	1/1	0.96	0.16	41,41,41,41	0
56	MG	DA	3478	1/1	0.96	0.15	67,67,67,67	0
56	MG	BA	3398	1/1	0.96	0.12	51,51,51,51	0
56	MG	BA	3718	1/1	0.96	0.14	53,53,53,53	0
56	MG	DA	3045	1/1	0.96	0.10	60,60,60,60	0
56	MG	DA	3629	1/1	0.96	0.04	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	3656	1/1	0.96	0.07	57,57,57,57	0
56	MG	DA	3321	1/1	0.96	0.10	30,30,30,30	0
56	MG	BA	3423	1/1	0.96	0.12	31,31,31,31	0
56	MG	AA	3032	1/1	0.96	0.19	59,59,59,59	0
56	MG	DA	3214	1/1	0.96	0.11	51,51,51,51	0
56	MG	BA	3293	1/1	0.96	0.17	40,40,40,40	0
56	MG	DA	3517	1/1	0.96	0.08	57,57,57,57	0
56	MG	BA	3282	1/1	0.96	0.20	41,41,41,41	0
56	MG	DA	3166	1/1	0.96	0.19	35,35,35,35	0
56	MG	BA	3602	1/1	0.96	0.18	32,32,32,32	0
56	MG	BA	3273	1/1	0.96	0.32	41,41,41,41	0
56	MG	CA	3135	1/1	0.96	0.14	63,63,63,63	0
56	MG	CA	3163	1/1	0.96	0.11	78,78,78,78	0
56	MG	BA	3152	1/1	0.96	0.30	42,42,42,42	0
56	MG	CA	3109	1/1	0.96	0.17	41,41,41,41	0
56	MG	BA	3527	1/1	0.96	0.19	27,27,27,27	0
56	MG	AA	3035	1/1	0.96	0.14	26,26,26,26	0
56	MG	BA	3343	1/1	0.96	0.16	30,30,30,30	0
56	MG	DA	3296	1/1	0.96	0.12	35,35,35,35	0
56	MG	CA	3070	1/1	0.96	0.07	49,49,49,49	0
56	MG	DA	3196	1/1	0.96	0.48	45,45,45,45	0
56	MG	DA	3315	1/1	0.96	0.12	44,44,44,44	0
56	MG	BA	3709	1/1	0.96	0.29	28,28,28,28	0
56	MG	BA	3345	1/1	0.96	0.11	28,28,28,28	0
56	MG	DA	3514	1/1	0.96	0.27	45,45,45,45	0
56	MG	BA	3215	1/1	0.96	0.22	47,47,47,47	0
56	MG	DA	3645	1/1	0.96	0.07	38,38,38,38	0
56	MG	BB	213	1/1	0.96	0.23	30,30,30,30	0
56	MG	BA	3409	1/1	0.97	0.21	21,21,21,21	0
56	MG	BA	3486	1/1	0.97	0.13	22,22,22,22	0
56	MG	BA	3173	1/1	0.97	0.54	41,41,41,41	0
56	MG	DQ	3002	1/1	0.97	0.12	41,41,41,41	0
56	MG	BU	202	1/1	0.97	0.14	29,29,29,29	0
56	MG	BP	201	1/1	0.97	0.38	28,28,28,28	0
56	MG	BA	3436	1/1	0.97	0.20	17,17,17,17	0
56	MG	BA	3127	1/1	0.97	0.28	36,36,36,36	0
56	MG	CA	3010	1/1	0.97	0.13	57,57,57,57	0
56	MG	DA	3355	1/1	0.97	0.12	35,35,35,35	0
56	MG	BA	3286	1/1	0.97	0.33	41,41,41,41	0
56	MG	BA	3003	1/1	0.97	0.13	30,30,30,30	0
56	MG	BA	3528	1/1	0.97	0.29	46,46,46,46	0
56	MG	DA	3327	1/1	0.97	0.11	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BD	3309	1/1	0.97	0.14	40,40,40,40	0
56	MG	BA	3458	1/1	0.97	0.14	66,66,66,66	0
56	MG	DA	3306	1/1	0.97	0.28	35,35,35,35	0
56	MG	BA	3354	1/1	0.97	0.17	20,20,20,20	0
56	MG	CA	3133	1/1	0.97	0.11	45,45,45,45	0
56	MG	BA	3542	1/1	0.97	0.17	20,20,20,20	0
56	MG	BA	3676	1/1	0.97	0.17	37,37,37,37	0
56	MG	DA	3234	1/1	0.97	0.18	56,56,56,56	0
56	MG	BA	3749	1/1	0.97	0.11	29,29,29,29	0
56	MG	BA	3726	1/1	0.97	0.09	65,65,65,65	0
56	MG	DA	3021	1/1	0.97	0.45	40,40,40,40	0
56	MG	BA	3608	1/1	0.97	0.15	34,34,34,34	0
56	MG	BA	3788	1/1	0.97	0.13	10,10,10,10	0
56	MG	BA	3508	1/1	0.97	0.09	34,34,34,34	0
56	MG	BE	307	1/1	0.97	0.12	31,31,31,31	0
56	MG	BF	307	1/1	0.97	0.64	40,40,40,40	0
56	MG	CA	3114	1/1	0.97	0.09	52,52,52,52	0
56	MG	DA	3512	1/1	0.97	0.11	48,48,48,48	0
56	MG	CA	3140	1/1	0.97	0.10	75,75,75,75	0
56	MG	BA	3811	1/1	0.97	0.49	41,41,41,41	0
56	MG	DA	3483	1/1	0.97	0.11	32,32,32,32	0
56	MG	CA	3175	1/1	0.97	0.20	46,46,46,46	0
56	MG	BA	3078	1/1	0.97	0.17	15,15,15,15	0
56	MG	DA	3492	1/1	0.97	0.07	44,44,44,44	0
56	MG	BA	3812	1/1	0.97	0.27	31,31,31,31	0
56	MG	DA	3598	1/1	0.97	0.25	30,30,30,30	0
56	MG	DA	3635	1/1	0.97	0.18	47,47,47,47	0
56	MG	BA	3631	1/1	0.97	0.17	49,49,49,49	0
56	MG	BA	3424	1/1	0.97	0.16	55,55,55,55	0
56	MG	BA	3051	1/1	0.97	0.19	18,18,18,18	0
56	MG	BA	3712	1/1	0.97	0.34	29,29,29,29	0
56	MG	DA	3077	1/1	0.97	0.17	47,47,47,47	0
56	MG	CA	3076	1/1	0.97	0.17	35,35,35,35	0
56	MG	DA	3641	1/1	0.97	0.14	49,49,49,49	0
56	MG	BA	3280	1/1	0.97	0.14	32,32,32,32	0
56	MG	BA	3001	1/1	0.97	0.14	31,31,31,31	0
56	MG	BA	3708	1/1	0.97	0.23	36,36,36,36	0
56	MG	DA	3271	1/1	0.97	0.12	51,51,51,51	0
56	MG	AA	3129	1/1	0.97	0.14	70,70,70,70	0
56	MG	DA	3254	1/1	0.97	0.20	35,35,35,35	0
56	MG	CA	3108	1/1	0.97	0.07	52,52,52,52	0
56	MG	BV	202	1/1	0.97	0.33	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	3181	1/1	0.97	0.14	63,63,63,63	0
56	MG	BA	3362	1/1	0.97	0.19	40,40,40,40	0
56	MG	DA	3515	1/1	0.97	0.09	39,39,39,39	0
56	MG	BA	3285	1/1	0.97	0.14	54,54,54,54	0
56	MG	DA	3505	1/1	0.97	0.12	45,45,45,45	0
56	MG	BA	3043	1/1	0.97	0.15	35,35,35,35	0
56	MG	BA	3385	1/1	0.97	0.23	41,41,41,41	0
56	MG	BF	301	1/1	0.97	0.49	32,32,32,32	0
56	MG	BA	3009	1/1	0.97	0.16	25,25,25,25	0
56	MG	DA	3223	1/1	0.97	0.20	41,41,41,41	0
56	MG	BA	3320	1/1	0.97	0.17	55,55,55,55	0
56	MG	DA	3013	1/1	0.97	0.06	32,32,32,32	0
56	MG	DA	3464	1/1	0.97	0.10	24,24,24,24	0
56	MG	BA	3805	1/1	0.97	0.15	30,30,30,30	0
59	ZN	D9	501	1/1	0.97	0.14	65,65,65,65	0
56	MG	DF	304	1/1	0.97	0.88	40,40,40,40	0
56	MG	BA	3632	1/1	0.97	0.24	43,43,43,43	0
56	MG	DA	3055	1/1	0.97	0.07	54,54,54,54	0
56	MG	DA	3348	1/1	0.97	0.11	32,32,32,32	0
56	MG	DA	3188	1/1	0.97	0.07	26,26,26,26	0
56	MG	BA	3487	1/1	0.97	0.21	23,23,23,23	0
56	MG	BA	3390	1/1	0.97	0.21	25,25,25,25	0
56	MG	BA	3769	1/1	0.97	0.10	24,24,24,24	0
56	MG	CA	3157	1/1	0.97	0.09	61,61,61,61	0
56	MG	DD	305	1/1	0.97	0.91	39,39,39,39	0
56	MG	DA	3573	1/1	0.97	0.10	27,27,27,27	0
56	MG	BA	3074	1/1	0.97	0.16	31,31,31,31	0
56	MG	DA	3450	1/1	0.97	0.08	41,41,41,41	0
56	MG	BA	3223	1/1	0.97	0.08	39,39,39,39	0
56	MG	DA	3330	1/1	0.97	0.14	54,54,54,54	0
56	MG	DA	3263	1/1	0.97	0.27	44,44,44,44	0
56	MG	DA	3456	1/1	0.97	0.16	54,54,54,54	0
56	MG	DA	3320	1/1	0.97	0.15	34,34,34,34	0
56	MG	DA	3380	1/1	0.97	0.06	35,35,35,35	0
56	MG	CA	3119	1/1	0.97	0.13	51,51,51,51	0
56	MG	DA	3384	1/1	0.97	0.17	39,39,39,39	0
56	MG	DA	3362	1/1	0.97	0.09	59,59,59,59	0
56	MG	DA	3022	1/1	0.97	0.10	29,29,29,29	0
56	MG	DA	3359	1/1	0.97	0.12	39,39,39,39	0
56	MG	BA	3364	1/1	0.97	0.26	29,29,29,29	0
56	MG	DA	3207	1/1	0.97	0.22	36,36,36,36	0
56	MG	DA	3577	1/1	0.97	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	BA	3688	1/1	0.97	0.12	16,16,16,16	0
56	MG	BA	3334	1/1	0.97	0.17	26,26,26,26	0
56	MG	BA	3665	1/1	0.97	0.20	40,40,40,40	0
56	MG	AA	3118	1/1	0.97	0.08	39,39,39,39	0
56	MG	CA	3060	1/1	0.97	0.09	47,47,47,47	0
56	MG	DA	3133	1/1	0.97	0.12	52,52,52,52	0
56	MG	BA	3289	1/1	0.97	0.42	35,35,35,35	0
56	MG	AA	3108	1/1	0.97	0.15	58,58,58,58	0
56	MG	DA	3261	1/1	0.97	0.21	36,36,36,36	0
56	MG	BA	3208	1/1	0.97	0.17	19,19,19,19	0
56	MG	BA	3005	1/1	0.97	0.18	33,33,33,33	0
56	MG	BA	3291	1/1	0.97	0.11	50,50,50,50	0
56	MG	BA	3415	1/1	0.97	0.18	34,34,34,34	0
56	MG	BA	3758	1/1	0.97	0.15	44,44,44,44	0
56	MG	DA	3215	1/1	0.97	0.06	49,49,49,49	0
56	MG	BA	3140	1/1	0.97	0.25	34,34,34,34	0
56	MG	DA	3047	1/1	0.97	0.09	39,39,39,39	0
56	MG	BA	3428	1/1	0.97	0.26	36,36,36,36	0
56	MG	DA	3394	1/1	0.97	0.15	40,40,40,40	0
56	MG	BA	3032	1/1	0.97	0.42	42,42,42,42	0
56	MG	BA	3623	1/1	0.97	0.10	33,33,33,33	0
56	MG	BA	3448	1/1	0.97	0.22	23,23,23,23	0
56	MG	CA	3118	1/1	0.97	0.09	60,60,60,60	0
56	MG	BA	3183	1/1	0.97	0.17	35,35,35,35	0
56	MG	DA	3414	1/1	0.97	0.07	38,38,38,38	0
56	MG	DB	3007	1/1	0.97	0.17	42,42,42,42	0
56	MG	DA	3669	1/1	0.97	0.38	38,38,38,38	0
56	MG	DA	3231	1/1	0.97	0.27	38,38,38,38	0
56	MG	BA	3332	1/1	0.97	0.21	36,36,36,36	0
56	MG	AA	3093	1/1	0.97	0.14	51,51,51,51	0
56	MG	BY	202	1/1	0.97	0.17	48,48,48,48	0
56	MG	BA	3546	1/1	0.97	0.14	38,38,38,38	0
56	MG	DA	3349	1/1	0.97	0.15	31,31,31,31	0
56	MG	BW	203	1/1	0.97	0.30	37,37,37,37	0
56	MG	BA	3115	1/1	0.97	0.24	33,33,33,33	0
56	MG	BA	3226	1/1	0.97	0.28	25,25,25,25	0
56	MG	AX	3005	1/1	0.97	0.10	64,64,64,64	0
56	MG	DA	3066	1/1	0.97	0.17	47,47,47,47	0
56	MG	BA	3421	1/1	0.97	0.19	48,48,48,48	0
56	MG	DA	3217	1/1	0.97	0.22	34,34,34,34	0
56	MG	CE	202	1/1	0.97	0.07	74,74,74,74	0
56	MG	AA	3027	1/1	0.97	0.11	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	3653	1/1	0.97	0.15	39,39,39,39	0
56	MG	DA	3390	1/1	0.97	0.11	19,19,19,19	0
56	MG	BA	3661	1/1	0.97	0.11	48,48,48,48	0
56	MG	DA	3145	1/1	0.97	0.09	38,38,38,38	0
56	MG	BA	3372	1/1	0.97	0.15	56,56,56,56	0
56	MG	BA	3519	1/1	0.97	0.25	53,53,53,53	0
56	MG	BV	201	1/1	0.97	0.41	27,27,27,27	0
56	MG	BA	3472	1/1	0.97	0.17	38,38,38,38	0
56	MG	CA	3141	1/1	0.97	0.17	53,53,53,53	0
56	MG	DA	3040	1/1	0.97	0.58	58,58,58,58	0
56	MG	BA	3180	1/1	0.97	0.32	46,46,46,46	0
56	MG	DA	3448	1/1	0.97	0.18	45,45,45,45	0
56	MG	DA	3523	1/1	0.97	0.28	52,52,52,52	0
56	MG	AA	3101	1/1	0.97	0.17	49,49,49,49	0
56	MG	BA	3511	1/1	0.97	0.22	43,43,43,43	0
56	MG	DA	3088	1/1	0.97	0.10	30,30,30,30	0
56	MG	DA	3065	1/1	0.97	0.08	41,41,41,41	0
56	MG	B3	3001	1/1	0.97	0.20	38,38,38,38	0
56	MG	BA	3331	1/1	0.97	0.16	38,38,38,38	0
56	MG	DA	3558	1/1	0.97	0.04	43,43,43,43	0
56	MG	DA	3094	1/1	0.97	0.15	52,52,52,52	0
56	MG	DA	3671	1/1	0.97	0.24	37,37,37,37	0
56	MG	BA	3118	1/1	0.97	0.55	37,37,37,37	0
56	MG	BA	3181	1/1	0.97	0.20	26,26,26,26	0
56	MG	BA	3187	1/1	0.97	0.22	48,48,48,48	0
56	MG	BA	3685	1/1	0.97	0.14	51,51,51,51	0
56	MG	DA	3368	1/1	0.97	0.14	24,24,24,24	0
56	MG	BA	3300	1/1	0.97	0.30	28,28,28,28	0
56	MG	BA	3352	1/1	0.97	0.17	45,45,45,45	0
56	MG	DA	3029	1/1	0.97	0.26	36,36,36,36	0
56	MG	BA	3038	1/1	0.97	0.39	40,40,40,40	0
56	MG	BA	3201	1/1	0.97	0.39	41,41,41,41	0
56	MG	DA	3155	1/1	0.97	0.21	38,38,38,38	0
56	MG	BA	3485	1/1	0.97	0.14	55,55,55,55	0
56	MG	BA	3298	1/1	0.97	0.20	49,49,49,49	0
56	MG	BA	3800	1/1	0.97	0.09	41,41,41,41	0
56	MG	DA	3328	1/1	0.97	0.16	41,41,41,41	0
56	MG	AA	3033	1/1	0.97	0.23	58,58,58,58	0
56	MG	BA	3496	1/1	0.97	0.06	59,59,59,59	0
56	MG	DA	3487	1/1	0.97	0.16	37,37,37,37	0
56	MG	DA	3216	1/1	0.97	0.11	41,41,41,41	0
56	MG	BA	3024	1/1	0.98	0.41	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	3035	1/1	0.98	0.48	42,42,42,42	0
56	MG	BA	3328	1/1	0.98	0.15	11,11,11,11	0
56	MG	BA	3095	1/1	0.98	0.14	30,30,30,30	0
56	MG	BA	3543	1/1	0.98	0.23	23,23,23,23	0
56	MG	CA	3038	1/1	0.98	0.09	63,63,63,63	0
56	MG	AA	3111	1/1	0.98	0.14	61,61,61,61	0
56	MG	DA	3353	1/1	0.98	0.14	42,42,42,42	0
56	MG	DA	3373	1/1	0.98	0.09	39,39,39,39	0
56	MG	BA	3507	1/1	0.98	0.22	35,35,35,35	0
56	MG	BA	3451	1/1	0.98	0.15	31,31,31,31	0
56	MG	BA	3530	1/1	0.98	0.20	25,25,25,25	0
56	MG	DU	3001	1/1	0.98	0.56	55,55,55,55	0
56	MG	BA	3391	1/1	0.98	0.17	26,26,26,26	0
56	MG	BA	3245	1/1	0.98	0.15	61,61,61,61	0
56	MG	DA	3477	1/1	0.98	0.08	30,30,30,30	0
56	MG	BA	3046	1/1	0.98	0.16	34,34,34,34	0
56	MG	DA	3329	1/1	0.98	0.12	47,47,47,47	0
56	MG	DA	3009	1/1	0.98	0.15	29,29,29,29	0
56	MG	BA	3552	1/1	0.98	0.16	46,46,46,46	0
56	MG	DA	3205	1/1	0.98	0.21	34,34,34,34	0
56	MG	DA	3323	1/1	0.98	0.15	29,29,29,29	0
56	MG	DE	301	1/1	0.98	0.26	35,35,35,35	0
56	MG	DA	3506	1/1	0.98	0.11	40,40,40,40	0
56	MG	BE	303	1/1	0.98	0.59	32,32,32,32	0
56	MG	DA	3561	1/1	0.98	0.40	58,58,58,58	0
56	MG	DA	3027	1/1	0.98	0.47	42,42,42,42	0
56	MG	AA	3063	1/1	0.98	0.09	42,42,42,42	0
56	MG	BA	3802	1/1	0.98	0.27	23,23,23,23	0
56	MG	BA	3792	1/1	0.98	0.13	52,52,52,52	0
56	MG	DA	3334	1/1	0.98	0.10	45,45,45,45	0
56	MG	BA	3278	1/1	0.98	0.37	30,30,30,30	0
56	MG	DA	3117	1/1	0.98	0.35	42,42,42,42	0
56	MG	DA	3498	1/1	0.98	0.08	44,44,44,44	0
56	MG	BA	3070	1/1	0.98	0.21	39,39,39,39	0
56	MG	BA	3625	1/1	0.98	0.08	31,31,31,31	0
56	MG	BA	3069	1/1	0.98	0.19	39,39,39,39	0
56	MG	DA	3637	1/1	0.98	0.11	70,70,70,70	0
56	MG	DA	3542	1/1	0.98	0.10	58,58,58,58	0
56	MG	AA	3051	1/1	0.98	0.17	60,60,60,60	0
56	MG	BN	3001	1/1	0.98	0.72	52,52,52,52	0
56	MG	CA	3130	1/1	0.98	0.16	51,51,51,51	0
56	MG	BA	3209	1/1	0.98	0.17	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	AA	3110	1/1	0.98	0.14	46,46,46,46	0
56	MG	BU	209	1/1	0.98	0.38	27,27,27,27	0
56	MG	BB	212	1/1	0.98	0.19	42,42,42,42	0
56	MG	CA	3037	1/1	0.98	0.19	46,46,46,46	0
56	MG	BA	3333	1/1	0.98	0.11	23,23,23,23	0
56	MG	AA	3028	1/1	0.98	0.17	49,49,49,49	0
56	MG	DA	3004	1/1	0.98	0.12	25,25,25,25	0
56	MG	BA	3782	1/1	0.98	0.42	30,30,30,30	0
59	ZN	B9	501	1/1	0.98	0.18	49,49,49,49	0
59	ZN	B5	104	1/1	0.98	0.20	82,82,82,82	0
56	MG	DA	3250	1/1	0.98	0.21	40,40,40,40	0
56	MG	BA	3734	1/1	0.98	0.16	18,18,18,18	0
56	MG	BA	3085	1/1	0.98	0.27	23,23,23,23	0
56	MG	BA	3341	1/1	0.98	0.11	43,43,43,43	0
56	MG	BA	3042	1/1	0.98	0.15	41,41,41,41	0
56	MG	DA	3154	1/1	0.98	0.20	52,52,52,52	0
56	MG	DA	3654	1/1	0.98	0.06	50,50,50,50	0
56	MG	BP	202	1/1	0.98	0.13	27,27,27,27	0
56	MG	BA	3191	1/1	0.98	0.12	43,43,43,43	0
56	MG	CA	3031	1/1	0.98	0.10	59,59,59,59	0
56	MG	BQ	203	1/1	0.98	0.32	36,36,36,36	0
56	MG	BA	3329	1/1	0.98	0.19	24,24,24,24	0
56	MG	BA	3473	1/1	0.98	0.14	52,52,52,52	0
56	MG	BA	3371	1/1	0.98	0.10	40,40,40,40	0
56	MG	DA	3636	1/1	0.98	0.11	52,52,52,52	0
56	MG	DA	3232	1/1	0.98	0.08	45,45,45,45	0
56	MG	DA	3346	1/1	0.98	0.12	48,48,48,48	0
56	MG	AA	3159	1/1	0.98	0.07	59,59,59,59	0
56	MG	BA	3234	1/1	0.98	0.31	32,32,32,32	0
56	MG	DA	3461	1/1	0.98	0.23	57,57,57,57	0
56	MG	CA	3034	1/1	0.98	0.13	51,51,51,51	0
56	MG	B7	102	1/1	0.98	0.23	28,28,28,28	0
56	MG	BA	3645	1/1	0.98	0.07	50,50,50,50	0
56	MG	CA	3046	1/1	0.98	0.10	50,50,50,50	0
56	MG	BN	3004	1/1	0.98	0.59	61,61,61,61	0
56	MG	BA	3730	1/1	0.98	0.20	13,13,13,13	0
56	MG	BR	203	1/1	0.98	0.30	34,34,34,34	0
56	MG	CA	3162	1/1	0.98	0.09	42,42,42,42	0
56	MG	BU	207	1/1	0.98	0.43	29,29,29,29	0
56	MG	AA	3132	1/1	0.98	0.14	36,36,36,36	0
56	MG	BA	3742	1/1	0.98	0.28	21,21,21,21	0
58	SF4	CD	501	8/8	0.98	0.16	64,77,89,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3077	1/1	0.98	0.37	29,29,29,29	0
56	MG	BA	3170	1/1	0.98	0.18	52,52,52,52	0
56	MG	CA	3101	1/1	0.98	0.11	54,54,54,54	0
56	MG	DA	3137	1/1	0.98	0.23	43,43,43,43	0
56	MG	AA	3085	1/1	0.98	0.17	66,66,66,66	0
56	MG	BA	3184	1/1	0.98	0.23	37,37,37,37	0
56	MG	BA	3784	1/1	0.98	0.17	23,23,23,23	0
56	MG	DA	3081	1/1	0.98	0.17	48,48,48,48	0
56	MG	DA	3351	1/1	0.98	0.12	32,32,32,32	0
56	MG	CA	3137	1/1	0.98	0.15	50,50,50,50	0
56	MG	DA	3289	1/1	0.98	0.07	39,39,39,39	0
56	MG	BA	3195	1/1	0.98	0.33	52,52,52,52	0
56	MG	BA	3526	1/1	0.98	0.20	35,35,35,35	0
56	MG	BA	3145	1/1	0.98	0.25	41,41,41,41	0
56	MG	DA	3407	1/1	0.98	0.07	28,28,28,28	0
59	ZN	BY	203	1/1	0.98	0.19	54,54,54,54	0
56	MG	CA	3094	1/1	0.98	0.20	68,68,68,68	0
56	MG	BA	3630	1/1	0.98	0.20	43,43,43,43	0
56	MG	BA	3644	1/1	0.98	0.24	50,50,50,50	0
56	MG	DA	3530	1/1	0.98	0.19	47,47,47,47	0
56	MG	BU	203	1/1	0.98	0.21	27,27,27,27	0
56	MG	DA	3127	1/1	0.98	0.17	36,36,36,36	0
56	MG	DA	3403	1/1	0.98	0.15	56,56,56,56	0
56	MG	DA	3470	1/1	0.98	0.15	31,31,31,31	0
56	MG	DA	3139	1/1	0.98	0.12	41,41,41,41	0
56	MG	BA	3004	1/1	0.98	0.15	26,26,26,26	0
56	MG	DA	3048	1/1	0.98	0.17	51,51,51,51	0
56	MG	BA	3167	1/1	0.98	0.33	43,43,43,43	0
56	MG	AA	3115	1/1	0.98	0.24	45,45,45,45	0
56	MG	BA	3309	1/1	0.98	0.06	50,50,50,50	0
56	MG	BA	3147	1/1	0.98	0.12	41,41,41,41	0
56	MG	CA	3028	1/1	0.98	0.11	55,55,55,55	0
56	MG	DA	3552	1/1	0.98	0.12	36,36,36,36	0
56	MG	CA	3110	1/1	0.98	0.13	48,48,48,48	0
56	MG	DA	3174	1/1	0.98	0.07	50,50,50,50	0
56	MG	DA	3546	1/1	0.98	0.07	47,47,47,47	0
56	MG	BA	3620	1/1	0.98	0.19	62,62,62,62	0
56	MG	BA	3581	1/1	0.98	0.09	37,37,37,37	0
56	MG	DA	3532	1/1	0.98	0.12	61,61,61,61	0
56	MG	AA	3135	1/1	0.98	0.08	60,60,60,60	0
56	MG	CA	3172	1/1	0.98	0.07	50,50,50,50	0
56	MG	DA	3474	1/1	0.98	0.06	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3164	1/1	0.98	0.44	35,35,35,35	0
58	SF4	AD	501	8/8	0.98	0.18	62,74,91,95	0
56	MG	DA	3167	1/1	0.98	0.14	38,38,38,38	0
56	MG	BA	3400	1/1	0.98	0.12	34,34,34,34	0
56	MG	BA	3306	1/1	0.98	0.21	18,18,18,18	0
56	MG	BA	3463	1/1	0.98	0.13	10,10,10,10	0
56	MG	AA	3053	1/1	0.98	0.11	46,46,46,46	0
56	MG	BA	3491	1/1	0.98	0.19	45,45,45,45	0
56	MG	BA	3573	1/1	0.98	0.17	24,24,24,24	0
56	MG	DA	3646	1/1	0.98	0.11	54,54,54,54	0
56	MG	BW	204	1/1	0.98	0.39	31,31,31,31	0
56	MG	BA	3619	1/1	0.98	0.12	33,33,33,33	0
56	MG	BA	3349	1/1	0.98	0.21	49,49,49,49	0
56	MG	BA	3142	1/1	0.98	0.32	29,29,29,29	0
56	MG	BA	3011	1/1	0.98	0.10	33,33,33,33	0
56	MG	DA	3462	1/1	0.98	0.09	31,31,31,31	0
56	MG	BA	3413	1/1	0.98	0.16	27,27,27,27	0
56	MG	DA	3595	1/1	0.98	0.07	39,39,39,39	0
56	MG	DA	3432	1/1	0.98	0.10	37,37,37,37	0
56	MG	DA	3476	1/1	0.98	0.24	53,53,53,53	0
56	MG	AA	3183	1/1	0.98	0.08	73,73,73,73	0
56	MG	BB	203	1/1	0.98	0.26	44,44,44,44	0
56	MG	DA	3157	1/1	0.98	0.09	42,42,42,42	0
56	MG	BA	3727	1/1	0.98	0.19	34,34,34,34	0
56	MG	DA	3519	1/1	0.98	0.14	32,32,32,32	0
56	MG	BA	3336	1/1	0.98	0.16	50,50,50,50	0
56	MG	DA	3526	1/1	0.99	0.29	28,28,28,28	0
56	MG	BA	3036	1/1	0.99	0.18	19,19,19,19	0
56	MG	BA	3037	1/1	0.99	0.54	29,29,29,29	0
56	MG	BA	3729	1/1	0.99	0.12	27,27,27,27	0
56	MG	BA	3407	1/1	0.99	0.17	40,40,40,40	0
56	MG	BA	3155	1/1	0.99	0.45	30,30,30,30	0
56	MG	AA	3186	1/1	0.99	0.13	42,42,42,42	0
56	MG	BA	3084	1/1	0.99	0.25	33,33,33,33	0
56	MG	DA	3120	1/1	0.99	0.15	34,34,34,34	0
56	MG	BA	3513	1/1	0.99	0.10	43,43,43,43	0
56	MG	BA	3560	1/1	0.99	0.21	38,38,38,38	0
56	MG	DA	3471	1/1	0.99	0.18	54,54,54,54	0
56	MG	BD	3302	1/1	0.99	0.41	46,46,46,46	0
56	MG	BA	3470	1/1	0.99	0.17	37,37,37,37	0
56	MG	BA	3356	1/1	0.99	0.25	52,52,52,52	0
56	MG	DA	3336	1/1	0.99	0.09	39,39,39,39	0

*Continued on next page...*

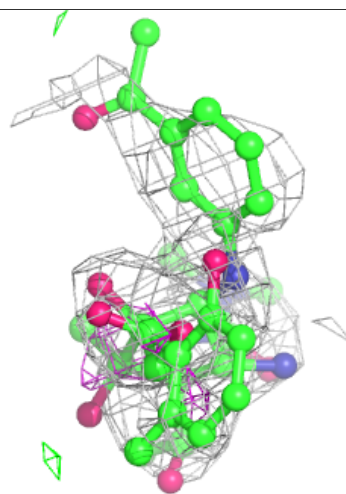
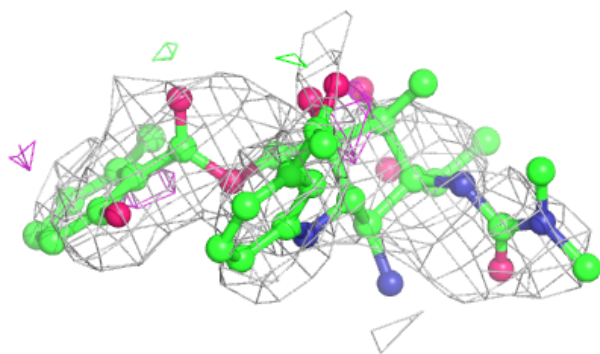
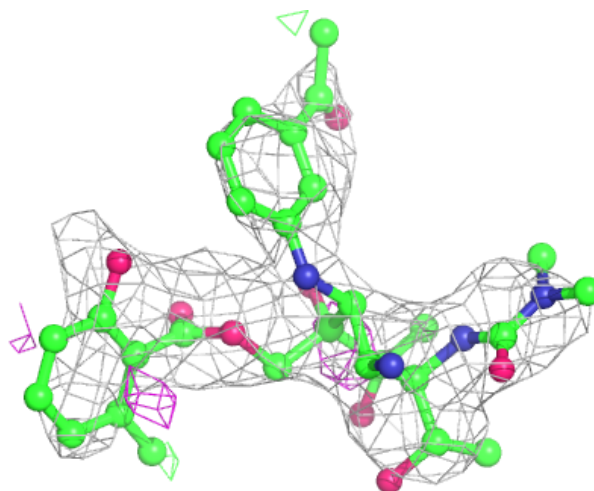
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
59	ZN	B6	103	1/1	0.99	0.16	62,62,62,62	0
56	MG	CA	3095	1/1	0.99	0.04	56,56,56,56	0
56	MG	BA	3098	1/1	0.99	0.26	38,38,38,38	0
56	MG	BA	3680	1/1	0.99	0.07	53,53,53,53	0
56	MG	DA	3601	1/1	0.99	0.10	26,26,26,26	0
56	MG	BA	3374	1/1	0.99	0.13	21,21,21,21	0
56	MG	BA	3557	1/1	0.99	0.11	37,37,37,37	0
56	MG	AA	3136	1/1	0.99	0.20	62,62,62,62	0
56	MG	DA	3005	1/1	0.99	0.20	26,26,26,26	0
56	MG	CA	3035	1/1	0.99	0.13	52,52,52,52	0
59	ZN	D6	501	1/1	0.99	0.20	66,66,66,66	0
56	MG	BD	3305	1/1	0.99	0.27	31,31,31,31	0
56	MG	BA	3675	1/1	0.99	0.23	29,29,29,29	0
56	MG	DA	3112	1/1	0.99	0.15	37,37,37,37	0
56	MG	BA	3601	1/1	0.99	0.14	49,49,49,49	0
56	MG	BB	214	1/1	0.99	0.20	53,53,53,53	0
56	MG	DA	3084	1/1	0.99	0.31	47,47,47,47	0
56	MG	DA	3136	1/1	0.99	0.18	43,43,43,43	0
56	MG	BA	3052	1/1	0.99	0.20	23,23,23,23	0
56	MG	BA	3481	1/1	0.99	0.18	44,44,44,44	0
56	MG	BA	3535	1/1	0.99	0.21	31,31,31,31	0
56	MG	CA	3161	1/1	0.99	0.05	51,51,51,51	0
56	MG	AA	3060	1/1	0.99	0.10	52,52,52,52	0
56	MG	BA	3441	1/1	0.99	0.17	32,32,32,32	0
56	MG	DA	3246	1/1	0.99	0.13	31,31,31,31	0
56	MG	AA	3077	1/1	0.99	0.22	54,54,54,54	0
56	MG	BA	3516	1/1	0.99	0.19	28,28,28,28	0
56	MG	BA	3794	1/1	0.99	0.14	29,29,29,29	0
56	MG	DA	3550	1/1	0.99	0.15	22,22,22,22	0
56	MG	BA	3488	1/1	0.99	0.19	16,16,16,16	0
59	ZN	D5	501	1/1	1.00	0.20	52,52,52,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

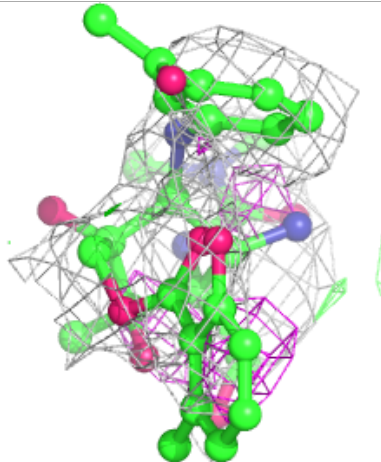
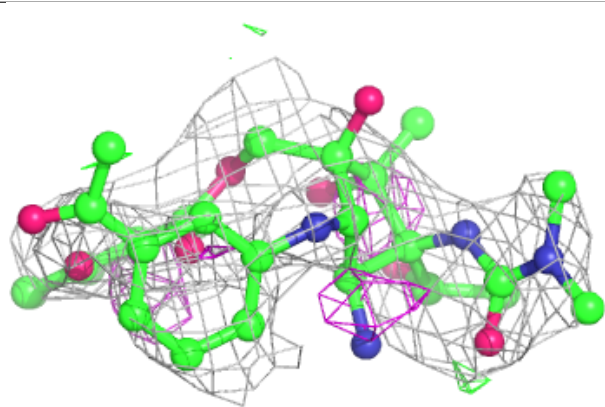
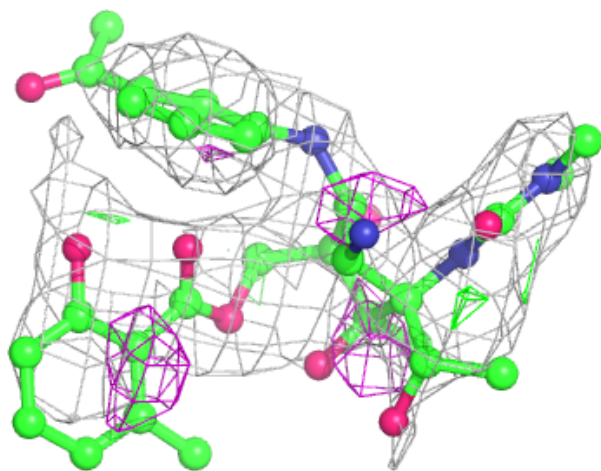
**Electron density around PCY CA 3176:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around PCY AA 3191:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.