



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 08:58 pm BST

PDB ID : 4W2G
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with pactamycin (soaked), mRNA and three deacylated tRNAs in the A, P and E sites
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 : 2.55 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

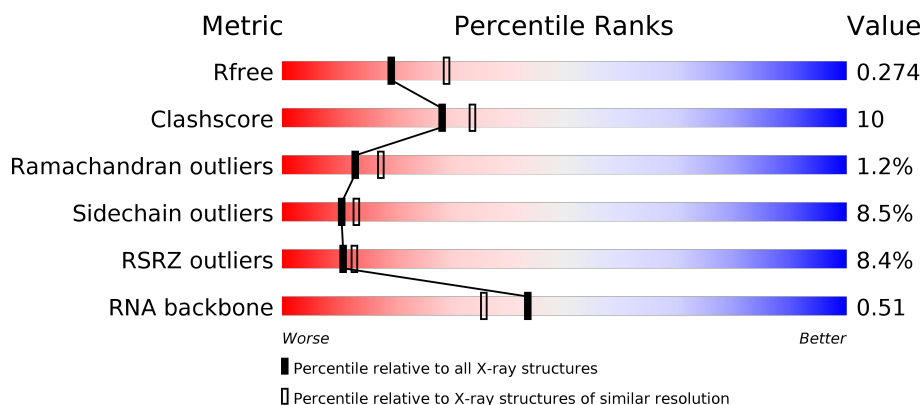
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)
RNA backbone	3102	1026 (2.88-2.20)

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 ≥ 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>4%</div> <div> <div></div> <div>55%</div> <div>32%</div> <div>10%</div> <div>..</div> </div> </div>
1	CA	1521	<div> <div>3%</div> <div> <div></div> <div>50%</div> <div>37%</div> <div>10%</div> <div>..</div> </div> </div>
2	AB	256	<div> <div>17%</div> <div> <div></div> <div>48%</div> <div>36%</div> <div>5%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	CB	256	
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	















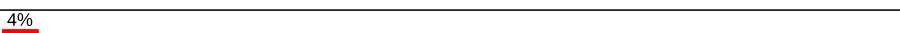




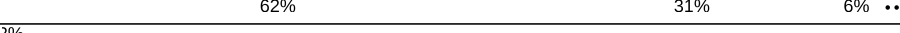





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Mol	Chain	Length	Quality of chain
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	76	
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	77	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













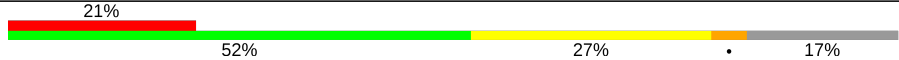
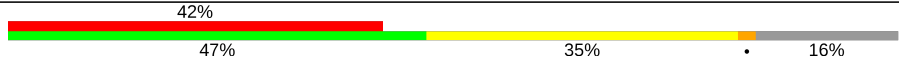
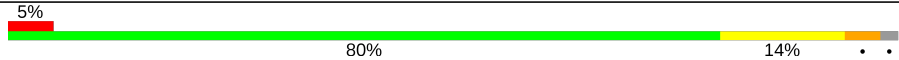
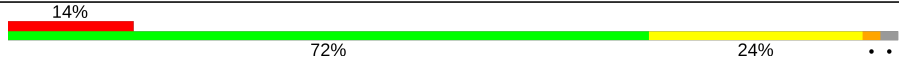
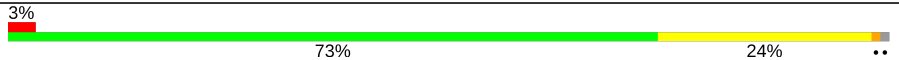
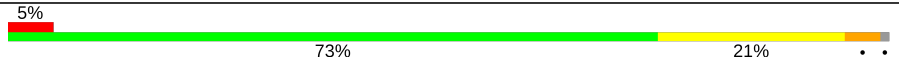
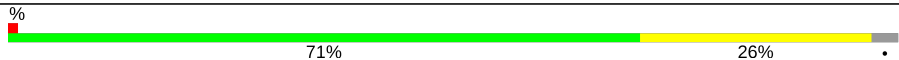
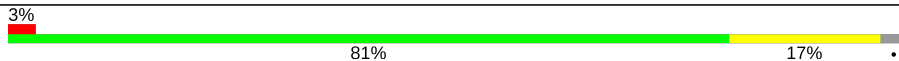

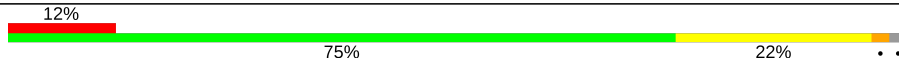
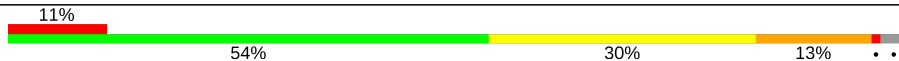
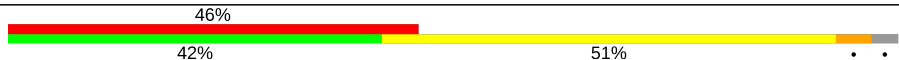

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Mol	Chain	Length	Quality of chain
26	DB	121	
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	118	
38	BS	112	
38	DS	112	

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

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Mol	Chain	Length	Quality of chain
51	D5	60	
52	B6	54	
52	D6	54	
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	
55	B9	37	
55	D9	37	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	5MU	CY	54	-	-	-	X
56	MG	B1	102	-	-	-	X
56	MG	BR	202	-	-	-	X
56	MG	CA	3027	-	-	-	X
56	MG	CX	3006	-	-	-	X
56	MG	DA	3199	-	-	-	X
56	MG	DA	3596	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297273 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1498	Total	C	N	O	P	0	0	0
			32205	14333	5970	10404	1498			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2819	Total	C	N	O	P	0	0	0
			60729	27026	11370	19515	2818			
25	DA	2800	Total	C	N	O	P	0	0	0
			60311	26840	11284	19388	2799			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
50	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	64	Total	C	N	O	S	0	0	0
			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	839	Total	Mg	0	0
			839	839		
56	AK	2	Total	Mg	0	0
			2	2		
56	DQ	4	Total	Mg	0	0
			4	4		
56	D3	1	Total	Mg	0	0
			1	1		
56	DF	5	Total	Mg	0	0
			5	5		
56	CV	1	Total	Mg	0	0
			1	1		
56	B8	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BE	8	Total 8	Mg 8	0	0
56	AW	7	Total 7	Mg 7	0	0
56	DU	2	Total 2	Mg 2	0	0
56	B1	2	Total 2	Mg 2	0	0
56	AN	1	Total 1	Mg 1	0	0
56	BP	3	Total 3	Mg 3	0	0
56	AX	12	Total 12	Mg 12	0	0
56	DN	1	Total 1	Mg 1	0	0
56	CY	1	Total 1	Mg 1	0	0
56	CA	177	Total 177	Mg 177	0	0
56	B5	4	Total 4	Mg 4	0	0
56	BB	23	Total 23	Mg 23	0	0
56	D8	1	Total 1	Mg 1	0	0
56	AE	1	Total 1	Mg 1	0	0
56	DG	1	Total 1	Mg 1	0	0
56	B9	1	Total 1	Mg 1	0	0
56	BF	12	Total 12	Mg 12	0	0
56	AV	1	Total 1	Mg 1	0	0
56	BX	2	Total 2	Mg 2	0	0
56	B2	1	Total 1	Mg 1	0	0
56	AA	230	Total 230	Mg 230	0	0

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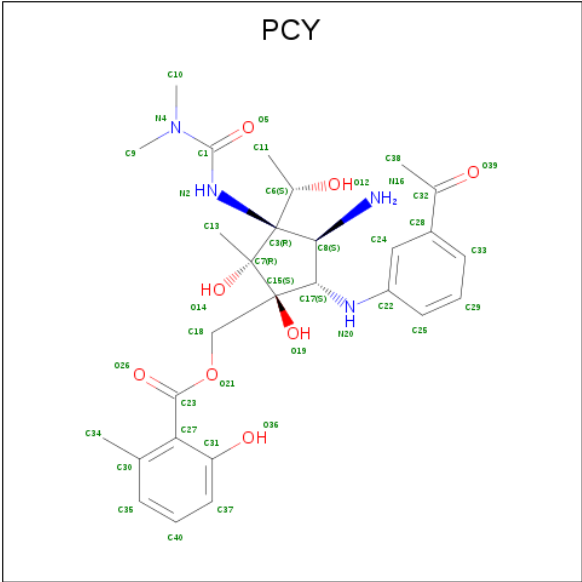
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BQ	5	Total 5	Mg 5	0	0
56	D7	2	Total 2	Mg 2	0	0
56	CX	5	Total 5	Mg 5	0	0
56	DV	3	Total 3	Mg 3	0	0
56	B6	2	Total 2	Mg 2	0	0
56	AM	1	Total 1	Mg 1	0	0
56	BU	9	Total 9	Mg 9	0	0
56	DR	1	Total 1	Mg 1	0	0
56	AD	1	Total 1	Mg 1	0	0
56	BN	5	Total 5	Mg 5	0	0
56	CT	1	Total 1	Mg 1	0	0
56	D0	2	Total 2	Mg 2	0	0
56	BG	3	Total 3	Mg 3	0	0
56	BY	1	Total 1	Mg 1	0	0
56	DE	4	Total 4	Mg 4	0	0
56	B3	3	Total 3	Mg 3	0	0
56	CJ	1	Total 1	Mg 1	0	0
56	BR	5	Total 5	Mg 5	0	0
56	DA	675	Total 675	Mg 675	0	0
56	DW	3	Total 3	Mg 3	0	0
56	B7	2	Total 2	Mg 2	0	0

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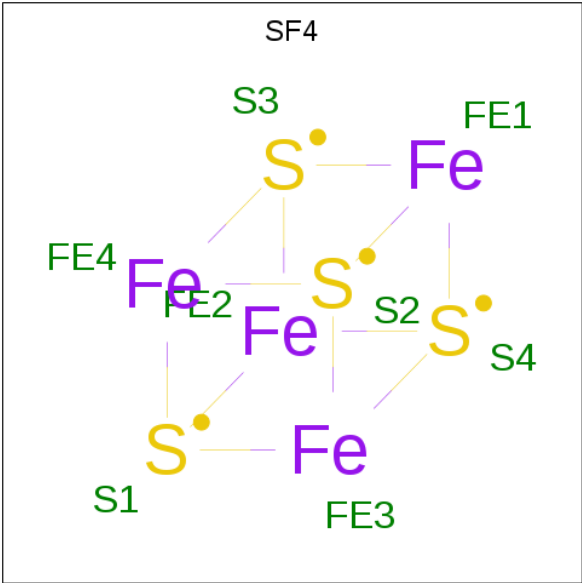
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CF	1	Total 1	Mg 1	0	0
56	BV	5	Total 5	Mg 5	0	0
56	DO	1	Total 1	Mg 1	0	0
56	BO	1	Total 1	Mg 1	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	DY	1	Total 1	Mg 1	0	0
56	CW	2	Total 2	Mg 2	0	0
56	BD	11	Total 11	Mg 11	0	0
56	B0	3	Total 3	Mg 3	0	0
56	CE	2	Total 2	Mg 2	0	0
56	BW	3	Total 3	Mg 3	0	0
56	AY	3	Total 3	Mg 3	0	0
56	DD	7	Total 7	Mg 7	0	0
56	AF	1	Total 1	Mg 1	0	0
56	DB	11	Total 11	Mg 11	0	0

- 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: Fe₄S₄).



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 1	Zn 1	0	0
59	B4	1	Total 1	Zn 1	0	0
59	CN	1	Total 1	Zn 1	0	0
59	BY	1	Total 1	Zn 1	0	0
59	B9	1	Total 1	Zn 1	0	0
59	DY	1	Total 1	Zn 1	0	0
59	D5	1	Total 1	Zn 1	0	0
59	D4	1	Total 1	Zn 1	0	0
59	AN	1	Total 1	Zn 1	0	0
59	D6	1	Total 1	Zn 1	0	0
59	D9	1	Total 1	Zn 1	0	0
59	B6	1	Total 1	Zn 1	0	0

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

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	226	Total 226	O 226	0	0
61	AE	3	Total 3	O 3	0	0
61	AJ	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AL	4	Total 4	O 4	0	0
61	AM	1	Total 1	O 1	0	0
61	AV	4	Total 4	O 4	0	0
61	AW	6	Total 6	O 6	0	0
61	AX	8	Total 8	O 8	0	0
61	AY	3	Total 3	O 3	0	0
61	BA	1411	Total 1411	O 1411	0	0
61	BB	36	Total 36	O 36	0	0
61	BD	16	Total 16	O 16	0	0
61	BE	13	Total 13	O 13	0	0
61	BF	7	Total 7	O 7	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0
61	BN	2	Total 2	O 2	0	0
61	BO	3	Total 3	O 3	0	0
61	BP	17	Total 17	O 17	0	0
61	BQ	2	Total 2	O 2	0	0
61	BR	2	Total 2	O 2	0	0
61	BT	1	Total 1	O 1	0	0
61	BU	6	Total 6	O 6	0	0
61	BV	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BW	4	Total 4	O 4	0	0
61	BX	1	Total 1	O 1	0	0
61	B0	4	Total 4	O 4	0	0
61	B1	2	Total 2	O 2	0	0
61	B3	2	Total 2	O 2	0	0
61	B5	5	Total 5	O 5	0	0
61	B6	1	Total 1	O 1	0	0
61	B7	3	Total 3	O 3	0	0
61	B8	11	Total 11	O 11	0	0
61	CA	173	Total 173	O 173	0	0
61	CJ	2	Total 2	O 2	0	0
61	CL	1	Total 1	O 1	0	0
61	CV	2	Total 2	O 2	0	0
61	CW	1	Total 1	O 1	0	0
61	CX	4	Total 4	O 4	0	0
61	DA	1002	Total 1002	O 1002	0	0
61	DB	10	Total 10	O 10	0	0
61	DD	17	Total 17	O 17	0	0
61	DE	11	Total 11	O 11	0	0
61	DF	5	Total 5	O 5	0	0
61	DN	2	Total 2	O 2	0	0

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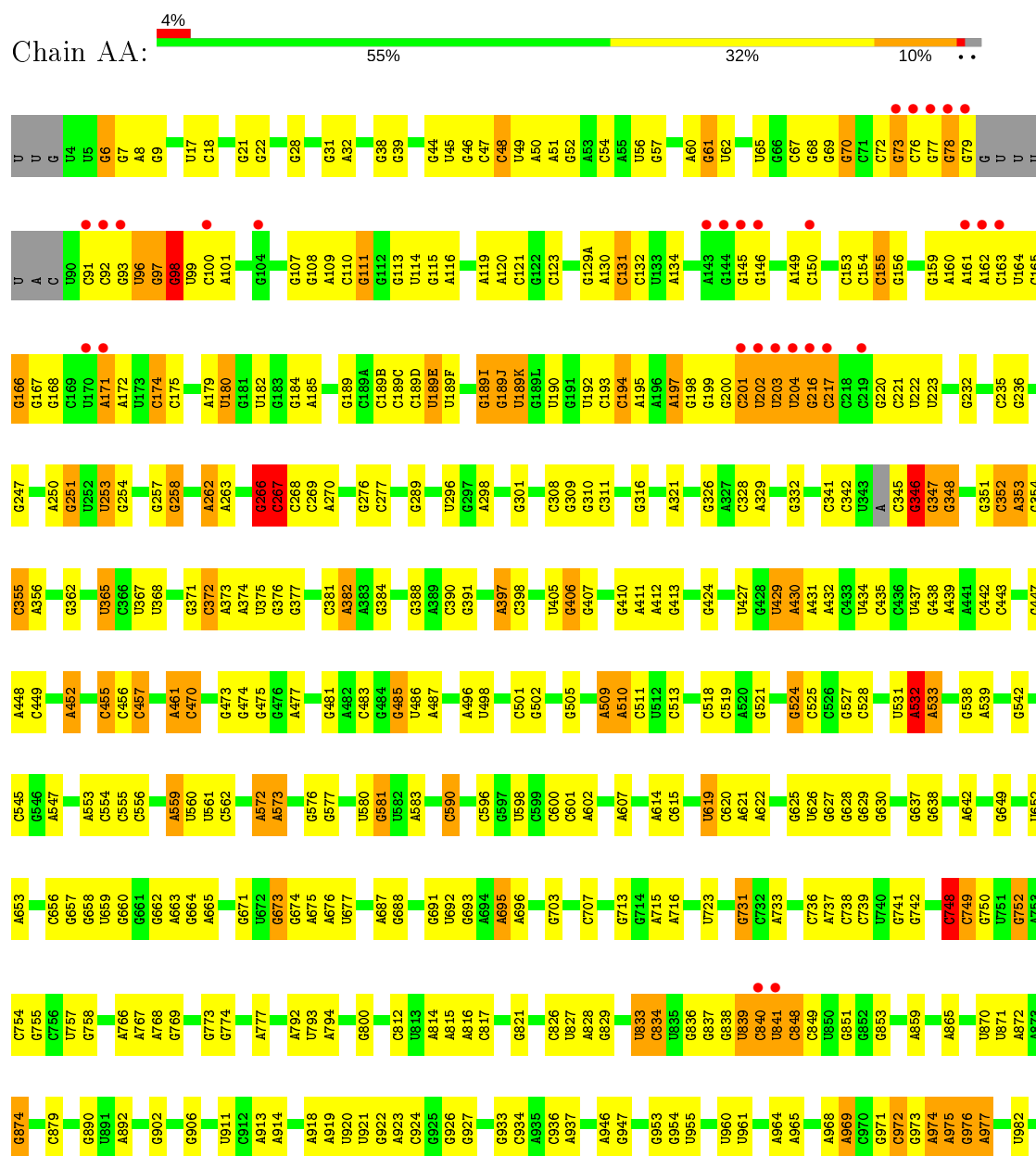
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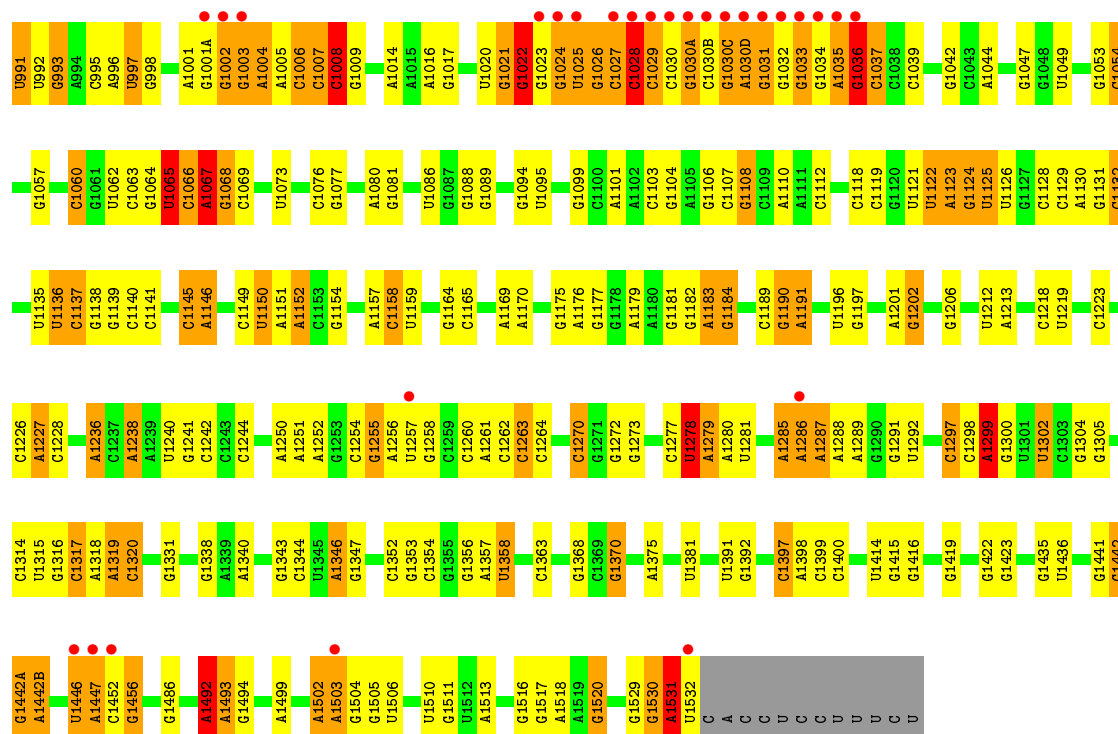
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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			2	2		
61	DP	8	Total	O	0	0
			8	8		
61	DQ	1	Total	O	0	0
			1	1		
61	DR	1	Total	O	0	0
			1	1		
61	DU	2	Total	O	0	0
			2	2		
61	DW	1	Total	O	0	0
			1	1		
61	DY	1	Total	O	0	0
			1	1		
61	D0	5	Total	O	0	0
			5	5		
61	D3	1	Total	O	0	0
			1	1		
61	D7	3	Total	O	0	0
			3	3		
61	D8	4	Total	O	0	0
			4	4		

3 Residue-property plots [i](#)

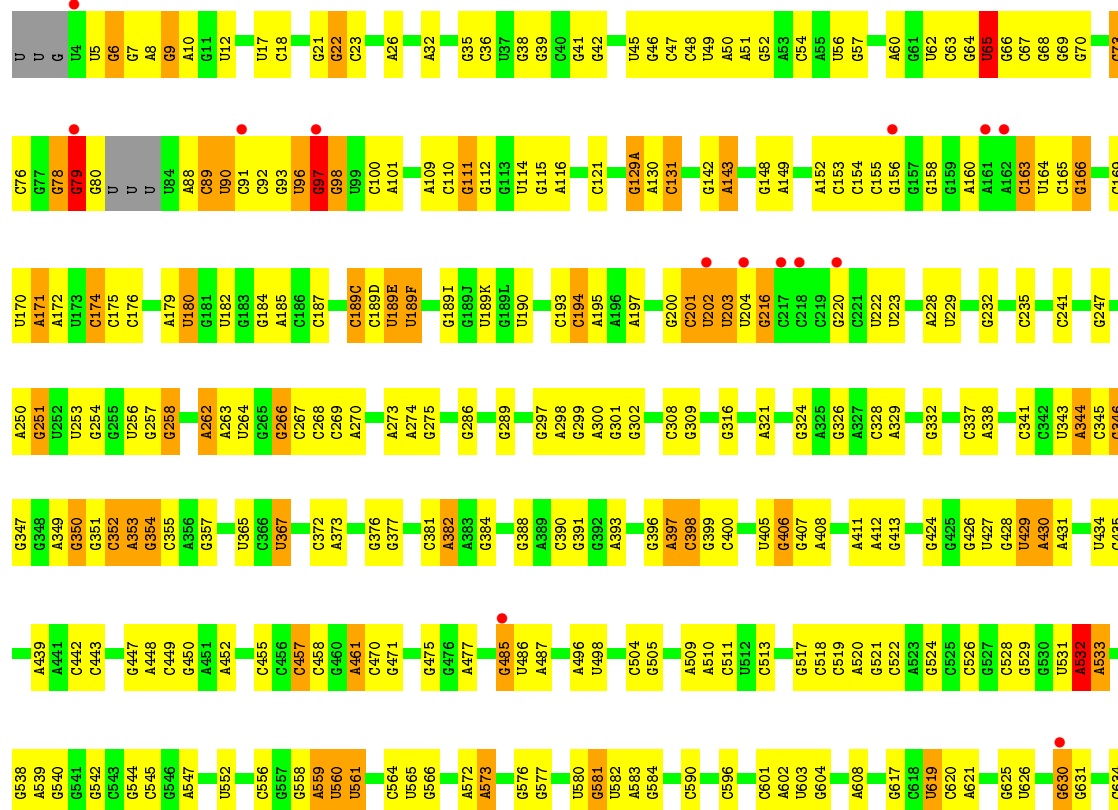
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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





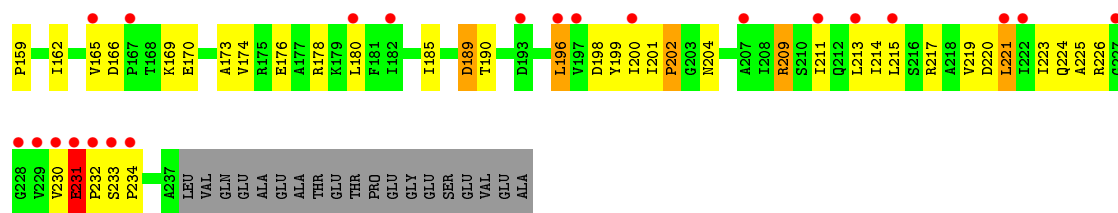
• Molecule 1: 16S Ribosomal RNA



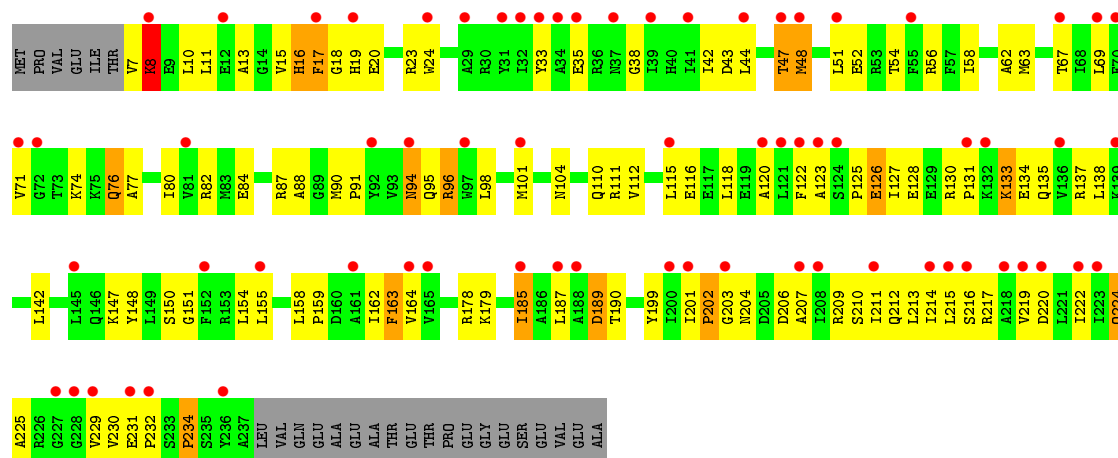


Frequency	Percentage
Daily	48%
Weekly	36%
Monthly	5%
Other	10%
Unlabeled (Red)	17%

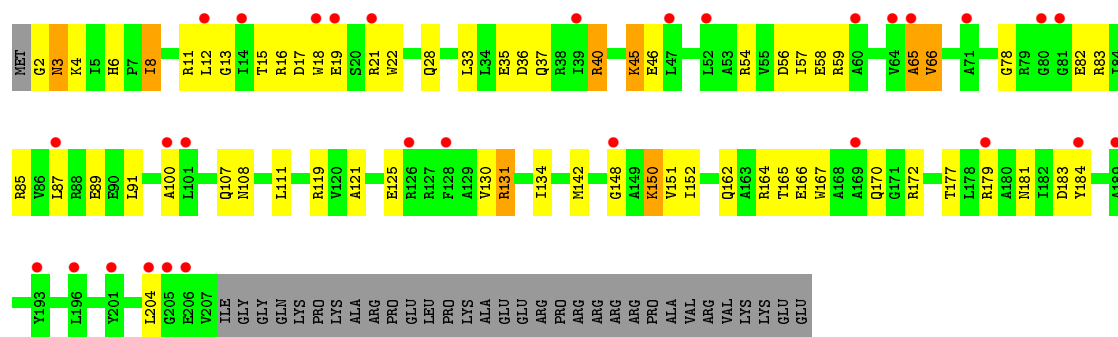




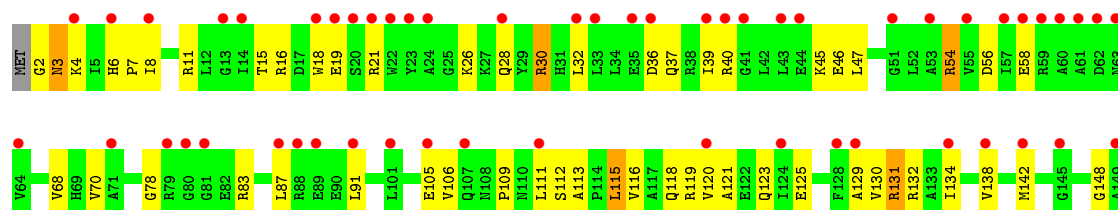
• Molecule 2: 30S Ribosomal Protein S2

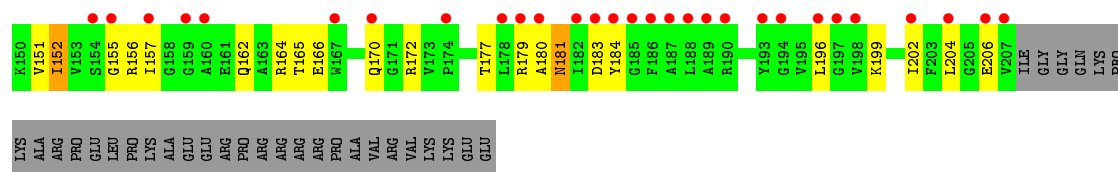


• Molecule 3: 30S Ribosomal Protein S3

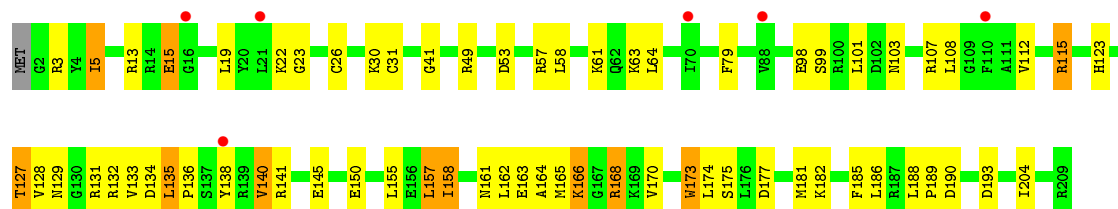


• Molecule 3: 30S Ribosomal Protein S3

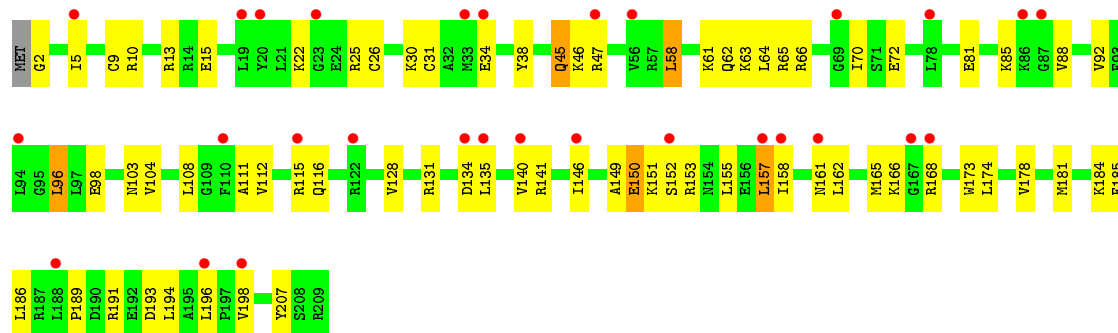




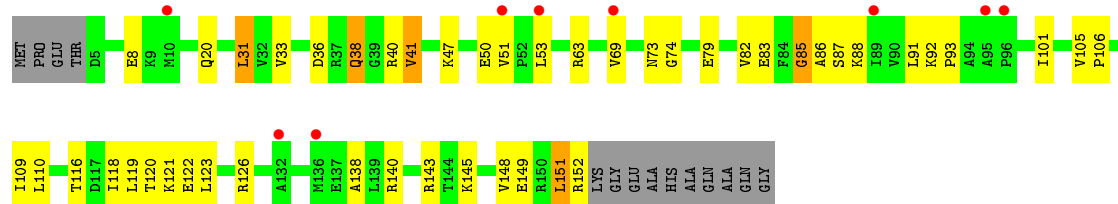
• Molecule 4: 30S Ribosomal Protein S4



• Molecule 4: 30S Ribosomal Protein S4



• Molecule 5: 30S Ribosomal Protein S5

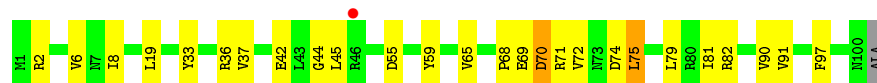
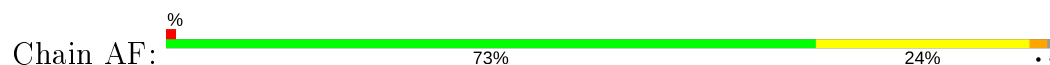


• Molecule 5: 30S Ribosomal Protein S5





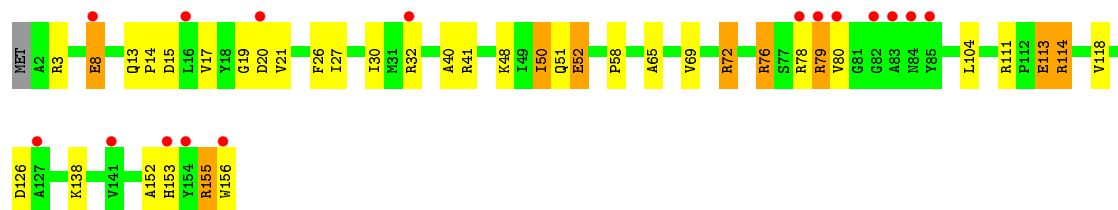
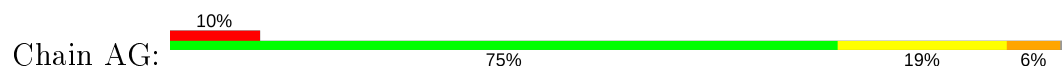
• Molecule 6: 30S Ribosomal Protein S6



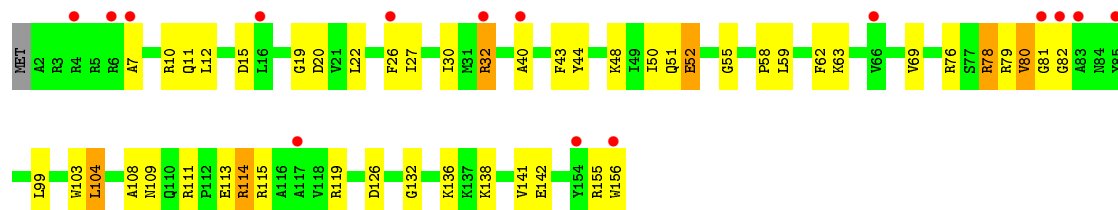
• Molecule 6: 30S Ribosomal Protein S6



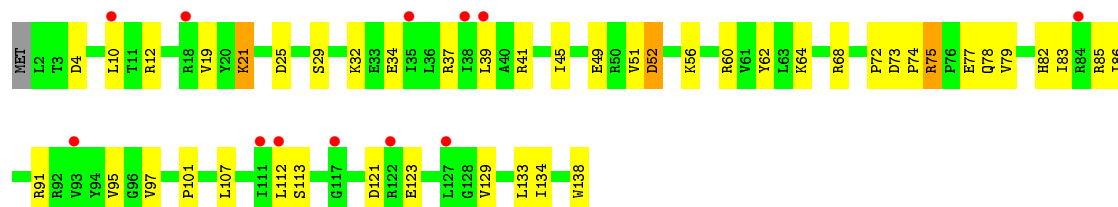
• Molecule 7: 30S Ribosomal Protein S7



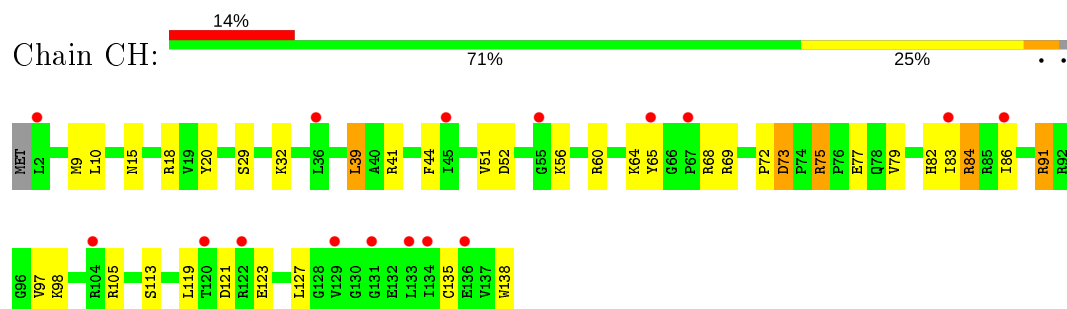
• Molecule 7: 30S Ribosomal Protein S7



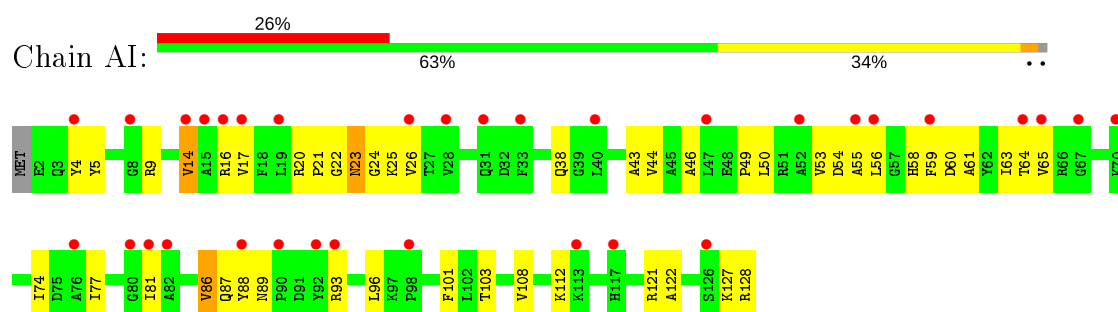
• Molecule 8: 30S Ribosomal Protein S8



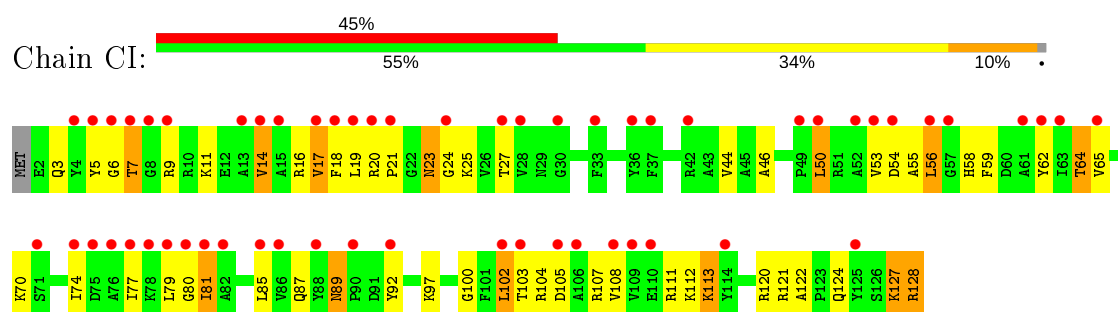
- Molecule 8: 30S Ribosomal Protein S8



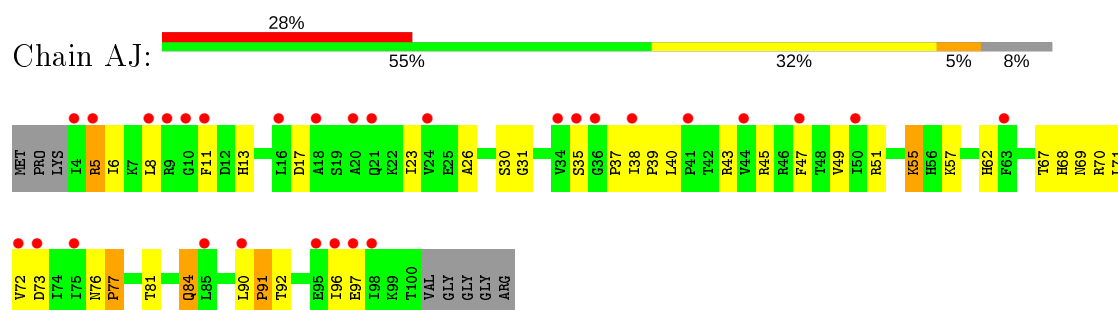
- Molecule 9: 30S Ribosomal Protein S9



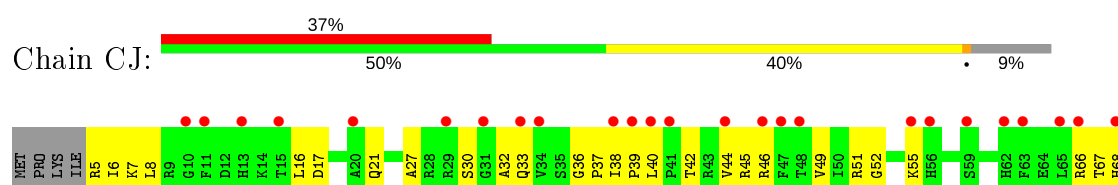
- Molecule 9: 30S Ribosomal Protein S9

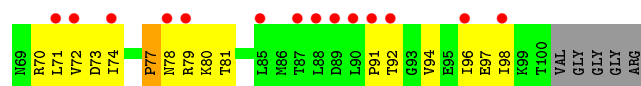


- Molecule 10: 30S Ribosomal Protein S10

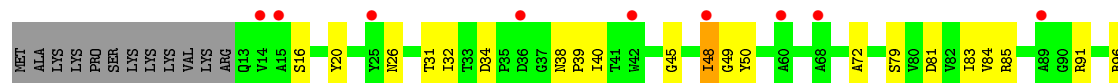


- Molecule 10: 30S Ribosomal Protein S10





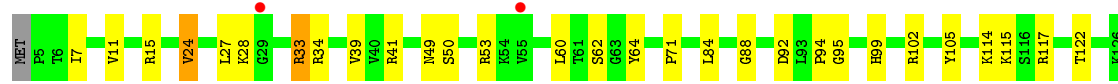
• Molecule 11: 30S Ribosomal Protein S11



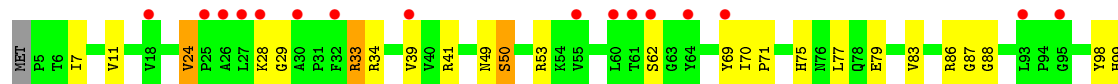
• Molecule 11: 30S Ribosomal Protein S11



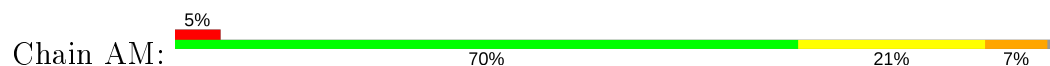
• Molecule 12: 30S Ribosomal Protein S12

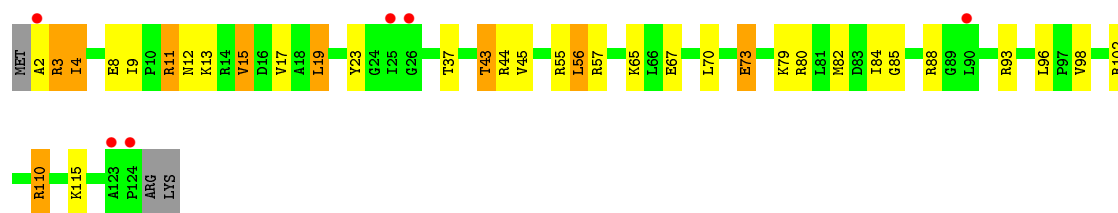


• Molecule 12: 30S Ribosomal Protein S12

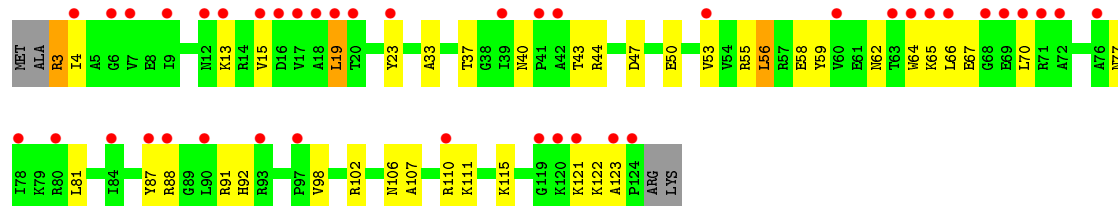


• Molecule 13: 30S Ribosomal Protein S13





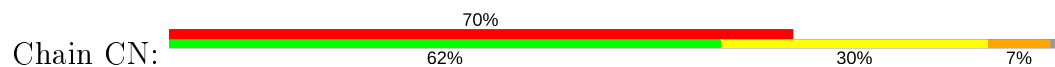
• Molecule 13: 30S Ribosomal Protein S13



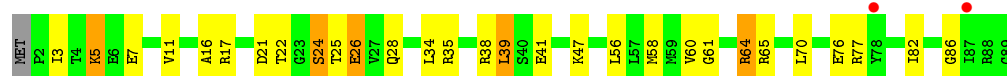
• Molecule 14: 30S Ribosomal Protein S14



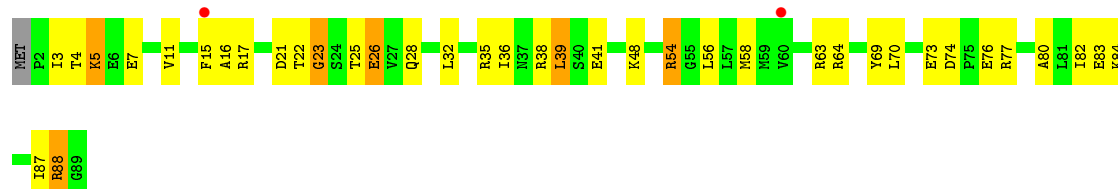
• Molecule 14: 30S Ribosomal Protein S14



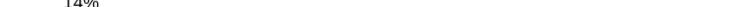
• Molecule 15: 30S Ribosomal Protein S15

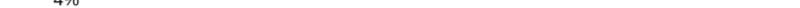


• Molecule 15: 30S Ribosomal Protein S15



Chain AP:

Chain CP: 

Chain AQ: 

Chain CQ:

30% 70% 22% 6%

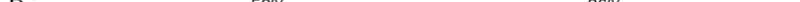
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MET	30%
P2	70%
V5	22%
L6	6%
V9	30%
V10	70%
V11	70%
S12	70%
D13	22%
K14	6%
M15	22%
T18	30%
V19	70%
T20	70%
V21	70%
L22	70%
V23	70%
E24	70%
R25	30%
Q26	22%
P27	70%
P28	70%
H29	70%
P30	70%
L31	70%
V32	70%
G33	30%
I36	30%
K37	22%
Y42	30%
P47	70%
Y51	70%
G54	22%
D55	6%
V56	22%
I59	70%
I60	70%
R63	70%
P64	70%
L65	70%
S66	22%
K69	70%
R70	70%
V73	30%
L74	22%
R75	70%
L76	70%
V77	70%
E78	30%
S79	70%
G80	70%
R81	22%
K82	6%
D83	22%
L84	70%
N94	70%
Y95	70%
E96	70%
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S99	70%
K100	70%
ARG	70%
GLY	70%
GLY	70%
LYS	70%
ALA	70%

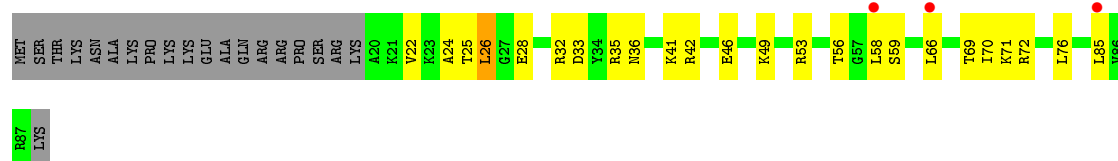
Chain AR:

Category	Value
Green	53%
Yellow	24%
Grey	23%

6%

Category	Value
Green	53%
Yellow	24%
Grey	23%

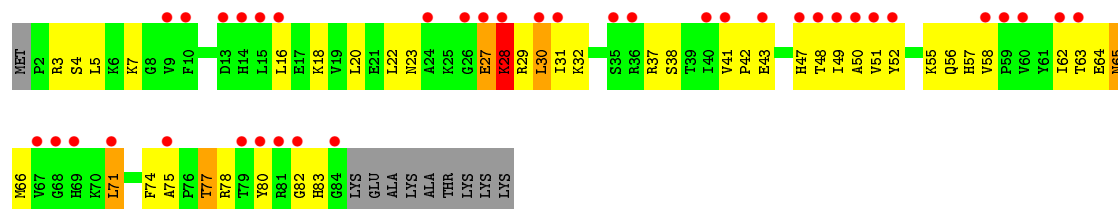
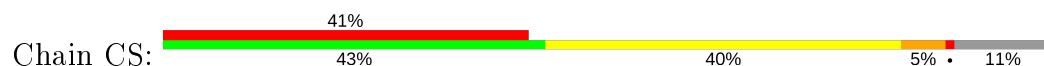
Chain CR: 



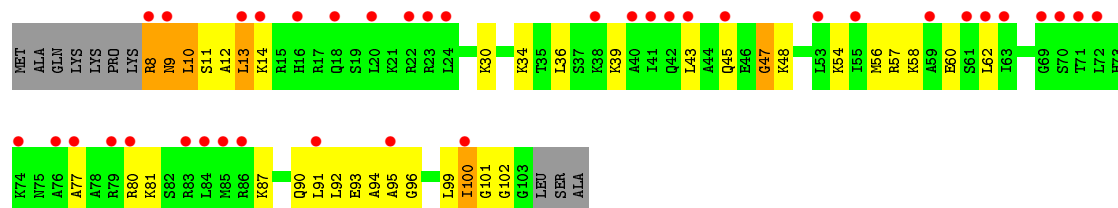
- Molecule 19: 30S Ribosomal Protein S19



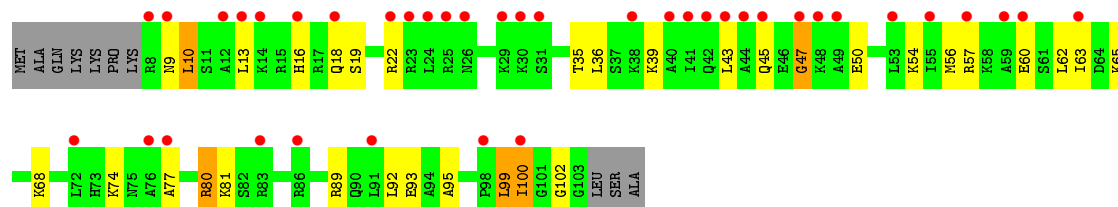
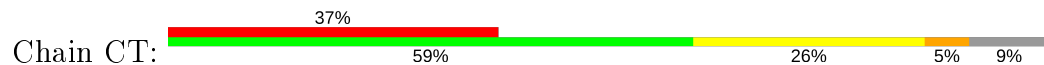
- Molecule 19: 30S Ribosomal Protein S19



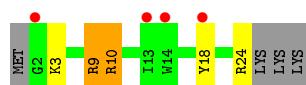
- Molecule 20: 30S Ribosomal Protein S20



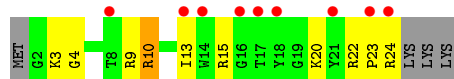
- Molecule 20: 30S Ribosomal Protein S20



- Molecule 21: 30S Ribosomal Protein THX



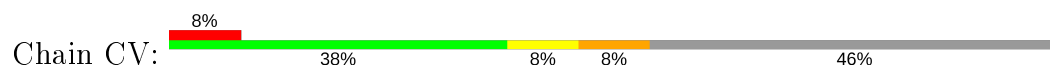
- Molecule 21: 30S Ribosomal Protein THX



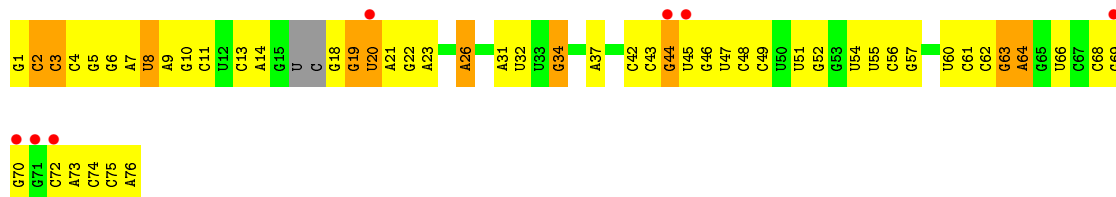
- Molecule 22: mRNA



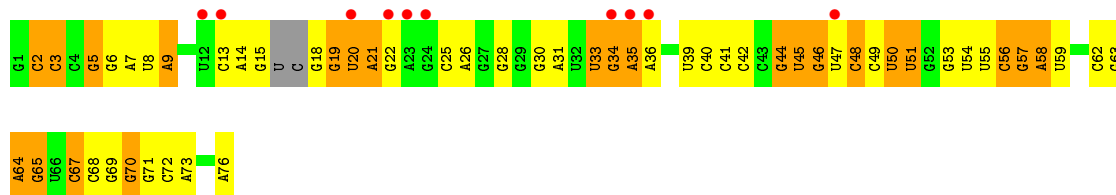
- Molecule 22: mRNA



- Molecule 23: A/P-site tRNA

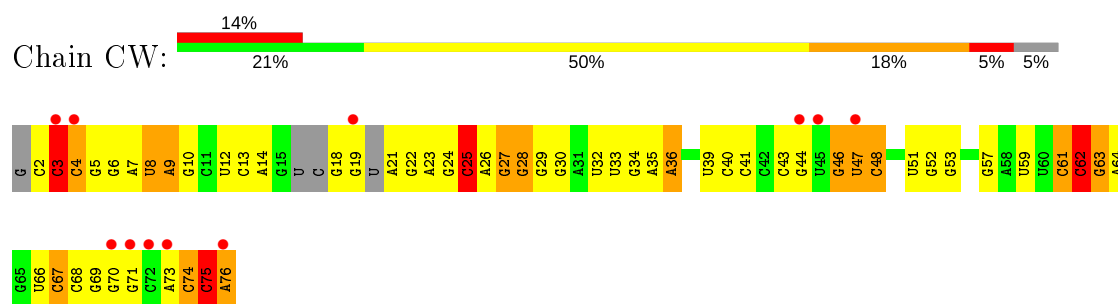


- Molecule 23: A/P-site tRNA

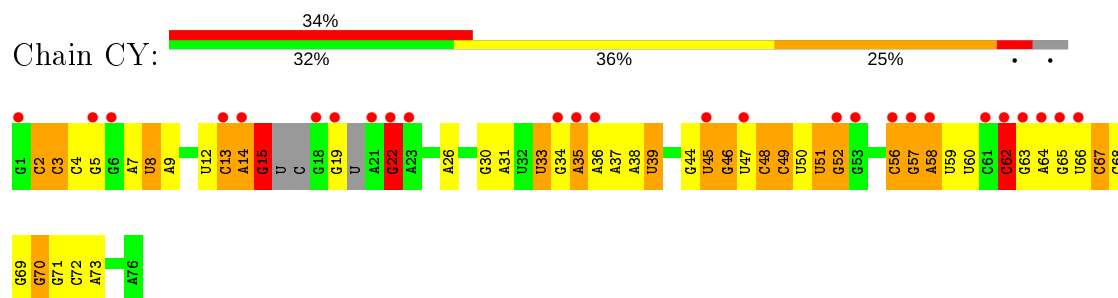


- Molecule 23: A/P-site tRNA

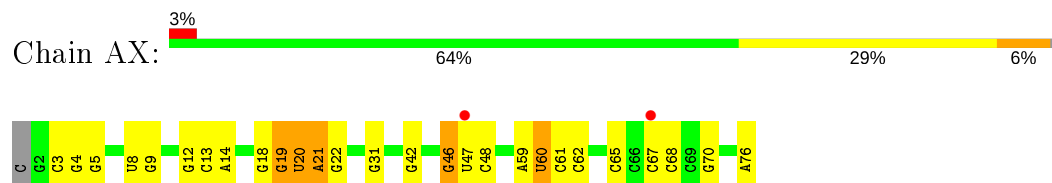




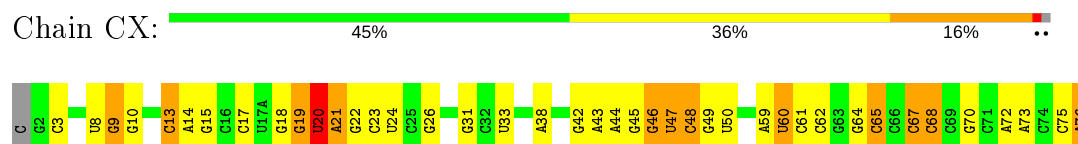
- Molecule 23: A/P-site tRNA



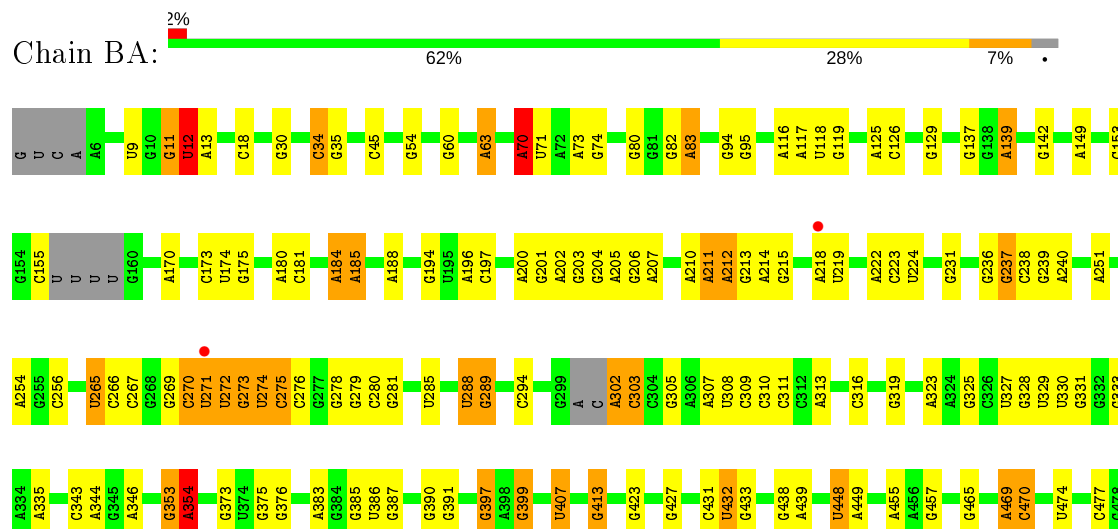
- Molecule 24: E-site tRNA



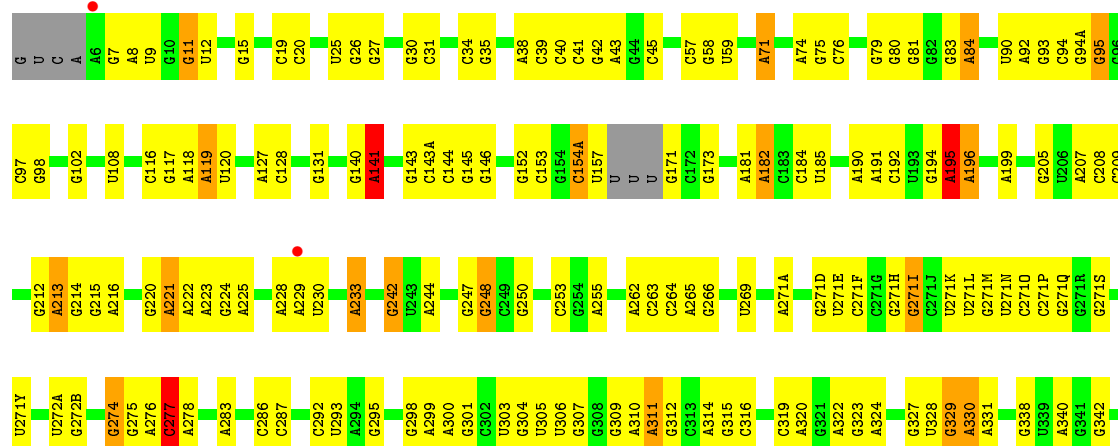
- Molecule 24: E-site tRNA



- Molecule 25: 23S Ribosomal RNA




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G1847	C1733	C1594	G1495	G1236	G1082	A978	A876	G772	A689	G886	A460
G3848	G1734	C1595	A1496	C1246	C1083	U982	B877	G776	A671	C481	C482
G1855	U1735	A1604	G1497	C1249	G1085	G983	C885	G777	G672	U591	A483
G1857	A1736	A1605	U1501	U1250	C1086	A986	U886	G778	A678	G593	G484
G3858	U1740	A1613	G1502	A1255	C1087	U989	U894	G779	A	A594	G489
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A1878	A1745	U1625	G1508	A1258	G1093	G991	C897	U793	G	C597	G493
A1879	G1746	A1632	U1398	C1263	A1094	G992	U898	U794	G	A598	G494
U1882	A1747	G1628	A1405	G1264	G1097	G997	C904	G795	C	U599	G495
C1883	U1748	C1629	A1406	A1265	C1098	A998	U905	G796	C	G600	A496
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G1900	A1767	G1635	C1416	A1272	C	U1003	U910	C801	C	G606	C510
A1911	G1787	G1639	U1418	U1280	A	G1004	A913	C802	C	C610	C511
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A1922	U1793	C1644	A1424	G1285	G	U1006	A925	G822	C	G696	A526
G1928	A1794	A1645	A1425	U1286	C	A1018	G926	G823	C	C697	U529
G1929	G1795	C1646	G1426	A1287	G	G1019	U927	G824	C	G698	A530
C1930	C1796	U1648	G1427	G1288	U	C1020	G928	A829	C	G614	C534
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C1946	C1812	G1670	U1451	G1312	G	A1042	U937	A836	C	U630	U549
A1949	C1813	A1685	U1452	U1313	C	U1043	G938	G839	C	U637	U550
G1951	A1814	C1683	C1453	A1314	C	C1044	C939	A840	C	A551	A551
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U1958	A1816	G1685	G1462	A1318	C	C1058	U941	C844	C	A640	A553
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A1960	A1821	C1687	U1466	A1320	U	U1065	C943	G848	C	G645	G555
U1977	A1822	A1694	G1467	G1324	U	A1066	U945	A851	C	U649	C556
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G1986	C1828	A1699	G1475	U1338	A	G1068	A956	G856	C	A656	G558
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	A1841	G1721	C1483	G1349	U	G1076	C969	A866	C	C665	U577
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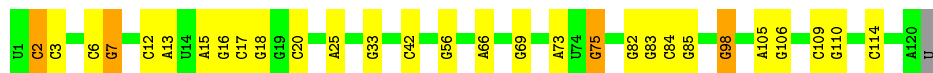


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G1459	G1364	A1274	G1193	G1115	G	G989	G906	G832	U741	U652D	G573	A477	U362
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G1461	G1201	G1278	G1201	G1117	A	G993	C908	U839	A746	G	A575	A479	G370
G1465	G1283	G1283	G1202	G1125	G	C994	A910	C940	U747	G	A576	A480	G380
G1466	A1284	A1284	G1203	A1126	U	C995	A911	C995	G748	C	A577	A481	U380
C1467	G1285	A1204	A1204	A1127	U	A996	C912	G845	G752	C	A578	A482	U383
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A1373	C1207	U1288	C1207	U1130	C	C915	C915	G848	C763	A	G582	A493	G386
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G1473	C1293	C1293	U1211	U1133	A	G1003	A918	U851	A764	C	C588	A503	G400
C1474	G1212	G1212	C1135	U1136	G	C1004	U922	G852	G770	C	C589	U504	A505
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C1387	G1303	G1303	U1142	U1142	C	G1011	G931	U860	A789	A654	G602	C517	C416
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A1494	G1305	G1305	G1227	G1144	A	C1013	A933	G864	C792	A654	A604	G822	G418
A1495	C1308	C1308	G1228	G1144	U	U1014	U937	G865	A784	A654	G604	G823	G419
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A1508	A1239	A1239	U1240	G1156	G	G1022	G946	G880	A800	A654	U614	A	G446
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G1545	G1355	G1355	U1266	C1178	U	A	A973	A896	C816	A654	U614	U569	G570
G1546	U1267	U1267	U1267	C1179	G	G	G974	C897	A819	A654	U614	U569	G570
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					G1112			C903	A829				

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G2819	G2730	C2651	U2449	C2358	A2287	A2169	U2109	C2006	A1786	G1674	U1671	A1566
A2820	G2731	C2652	A2450	C2359	A2288	A2170	G2110	G2012	A1789	A1789	G1685	A1569
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G2830	A2733	G2655	U2457	C2365	U2291	A2172	G2112	A2014	A1791	G1687	U1578	U1578
G2833	A2740	G2659	U2461	C2366	U2292	A2173	U2113	G2018	A1792	C1688	A1579	A1580
G2834	A2741	G2660	U2462	A2369	U2296	C2174	G2114	A2019	U1794	G1689	A1589	A1589
A2835	C2742	G2661	U2463	A2370	U2297	A2175	G2115	G2022	U1795	C1690	C1584	C1584
A2836	G2743	U2555	C2462	A2371	U2298	A2176	G2116	A2023	U1796	G1691	A1587	A1587
A2837	G2744	C2556	U2465	A2372	U2299	C2177	U2117	G2024	U1797	C1692	C1588	C1588
G2838	A2745	G2557	C2466	A2373	U2300	C2178	U2118	G2025	U1798	U1692	C1589	C1589
G2839	A2746	C2558	U2469	C2379	U2301	U2180	G2120	G2026	A1799	U1693	U1590	U1590
G2843	G2751	A2566	C2474	C2383	G2302	C2183	U2121	C2027	A1800	G1694	G1694	G1694
G2844	A2752	G2567	U2475	C2384	G2303	G2184	G2122	G2028	G1801	C1695	C1587	C1587
G2845	A2753	C2568	C2476	C2385	G2304	C2185	G2123	U2029	G1802	G1696	C1588	C1588
G2846	U2754	U2572	A2477	U2390	A2305	C2188	G2124	A2030	A1803	G1697	C1589	C1589
U2847	G2755	A2573	C2478	G2391	G2308	U2189	G2125	A2031	A1804	G1698	U1699	U1699
U2848	A2671	C2574	U2479	A2392	U2312	G2190	A2126	G2032	A1805	G1699	A1700	A1700
U2849	G2672	U2584	C2483	A2393	G2313	G2191	C2127	G2033	G1806	C1699	G1701	G1701
G2854	U2756	U2585	G2484	C2394	C2314	G2192	U2130	A2034	A1807	G1702	G1702	G1702
G2855	G2679	A2590	G2487	G2399	C2316	G2193	U2131	G2041	A1808	G1703	G1703	G1703
A2860	C2681	C2591	A2488	G2400	C2317	G2194	U2132	C2042	G1809	G1704	G1704	G1704
G2867	G2682	G2592	U2489	U2406	G2318	A2198	G2133	C2043	G1810	G1705	G1705	G1705
A2868	U2684	G2593	G2490	U2407	G2319	G2199	A2134	G2046	G1811	U1706	U1706	U1706
G2871	G2685	A2602	C2494	G2410	A2320	U2203	G2135	G2047	G1812	C1707	C1707	C1707
G2872	U2689	G2603	G2495	G2411	A2321	C2205	A2136	C2055	A1813	U1709	U1709	U1709
G2873	C2690	U2605	C2502	G2412	A2322	G2206	C2137	G2056	U1814	C1710	C1710	C1710
A2874	G2691	C2606	A2503	G2413	G2323	G2207	C2138	A2059	U1815	C1711	C1711	C1711
G2875	C2692	G2607	U2504	U2419	G2324	A2208	C2139	A2060	U1816	G1721	G1721	G1721
G2876	A2693	U2609	G2505	G2420	G2325	U2218	C2140	G2061	G1817	A1722	A1722	A1722
G2879	G2694	C2610	U2506	G2421	A2326	A2225	C2141	G2062	U1818	U1739	U1739	U1739
C2880	C2699	U2611	G2507	A2422	G2327	G2238	C2142	G2063	G1819	G1740	G1740	G1740
C2881	G2700	C2612	G2508	U2423	G2328	U2243	U2144	G2064	A1847	A1741	A1741	A1741
A2882	G2701	U2615	U2514	C2424	G2331	U2244	G2145	G2070	A1848	G1742	G1742	G1742
G2886	C2702	C2616	C2515	A2425	G2334	U2245	G2146	C2071	G1849	G1756	G1756	G1756
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U	A2713	U2636	U2522	A2433	U2344	U2271	G2156	G2089	U1856	A1773	A1773	A1773
G	C2801A	G2637	G2523	A2434	U2345	A2272	G2157	G2090	U1857	G1774	G1774	G1774
G	C2802	G2638	G2524	A2435	C2346	A2273	A2158	G2091	A1858	U1775	U1775	U1775
A	C2803	G2639	A2530	A2436	C2347	A2274	G2159	C2092	G1859	U1776	U1776	U1776
A	C2804	G2640	A2531	A2437	C2348	C2275	G2160	C2093	G1860	U1777	U1777	U1777
C	C2805	G2641	G2532	A2438	C2349	C2276	G2161	C2094	G1861	U1778	U1778	U1778
C	G2806	G2642	G2533	A2439	C2350	G2277	G2162	U2098	G1862	U1779	U1779	U1779
C	G2807	G2643	G2534	A2440	C2351	A2278	G2163	G2100	G1863	A1780	A1780	A1780
C	G2808	G2644	G2535	C2441	G2352	G2279	C2164	G2101	G1864	C1781	C1781	C1781
C	U2809	G2645	U2537	C2442	G2353	G2280	G2165	G2102	G1865	G1782	G1782	G1782
C	A2725	G2646	C2538	G2443	G2354	G2281	G2166	C2103	A1866	A1783	A1783	A1783
C	U2726	G2647	C2539	G2444	G2355	C2282	G2167					
C	G2727	G2648	C2540	G2445	C2356		G2168					

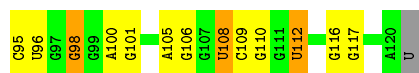
- Molecule 26: 5S Ribosomal RNA

Chain BB:  75% 21%



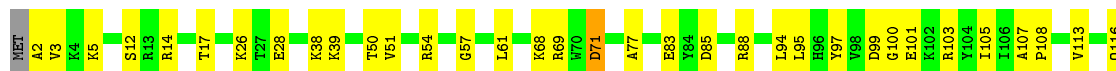
- Molecule 26: 5S Ribosomal RNA

Chain DB:  54% 38% 7%




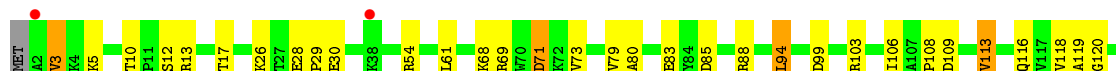
- Molecule 27: 50S Ribosomal Protein L2

Chain BD:  73% 24%



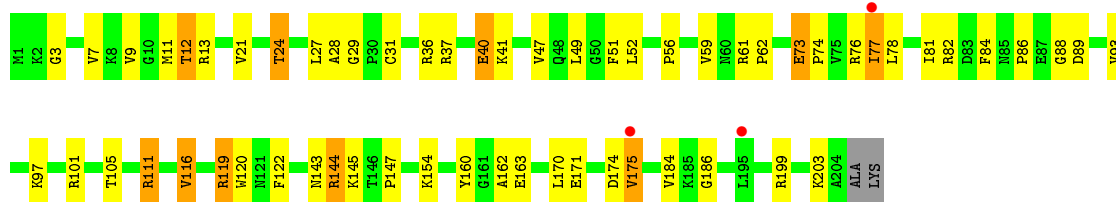
- Molecule 27: 50S Ribosomal Protein L2

Chain DD:  75% 21%

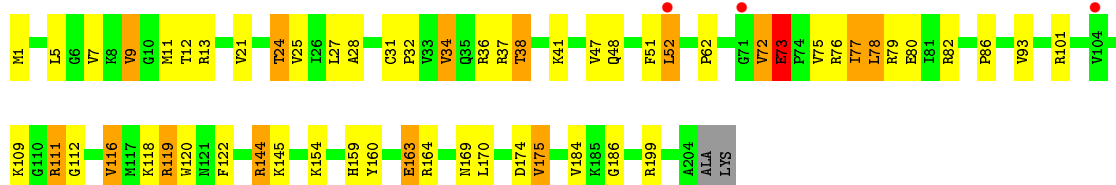
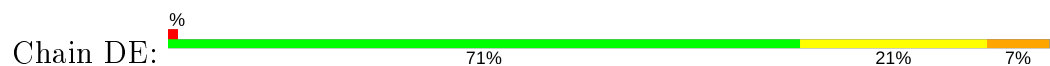


- Molecule 28: 50S Ribosomal Protein L3

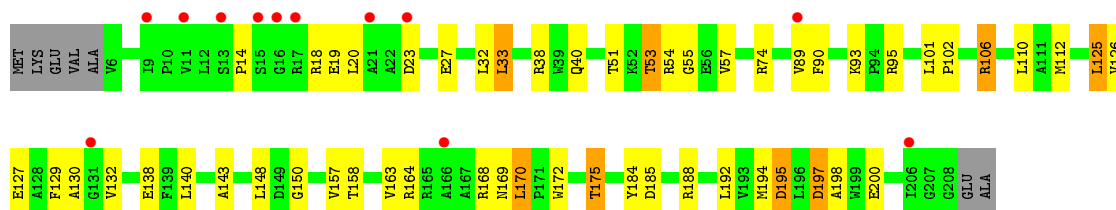
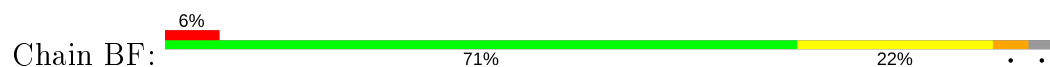
Chain BE:  70% 24% 5%



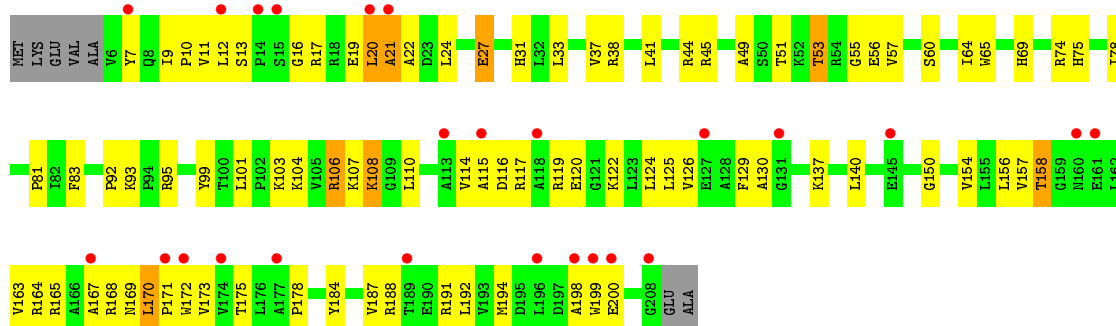
• Molecule 28: 50S Ribosomal Protein L3



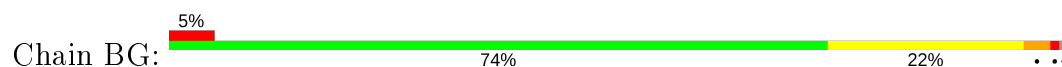
• Molecule 29: 50S Ribosomal Protein L4



• Molecule 29: 50S Ribosomal Protein L4

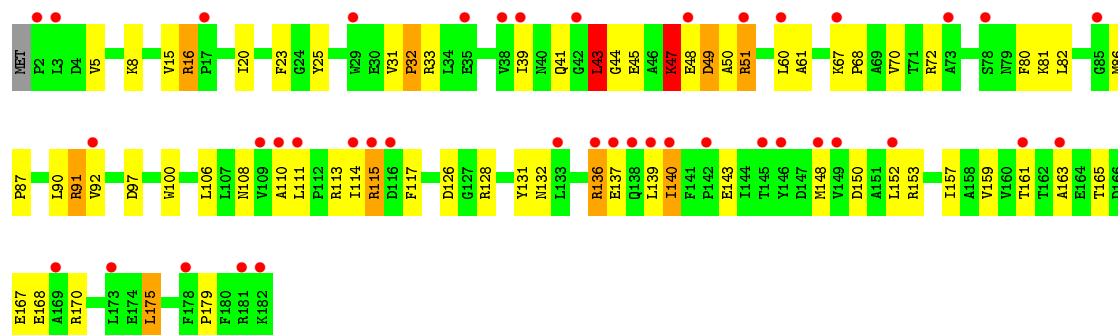


• Molecule 30: 50S Ribosomal Protein L5

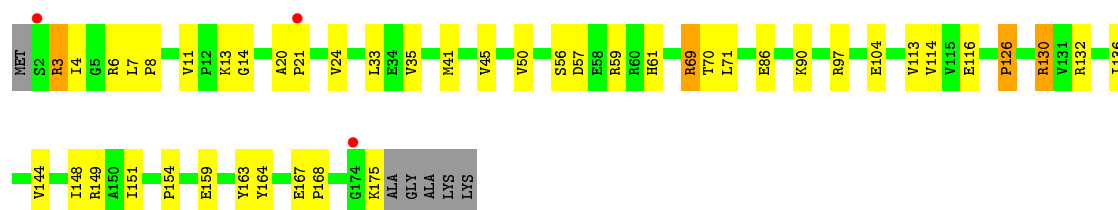
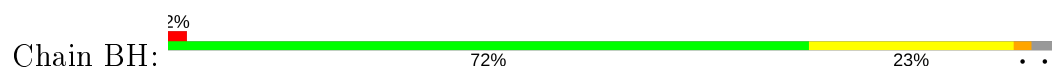




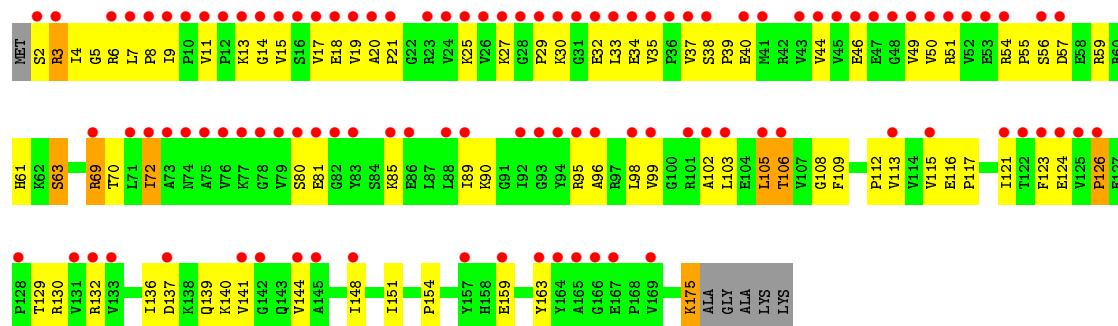
• Molecule 30: 50S Ribosomal Protein L5



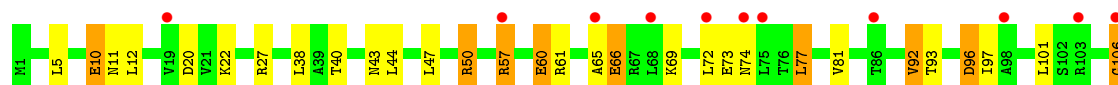
• Molecule 31: 50S Ribosomal Protein L6

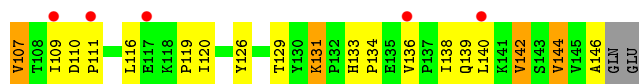


• Molecule 31: 50S Ribosomal Protein L6

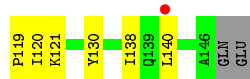
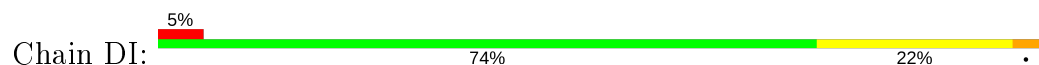


• Molecule 32: 50S Ribosomal Protein L9

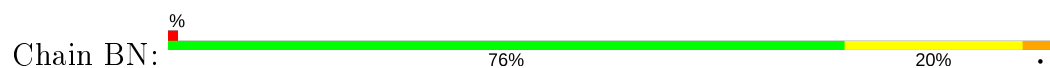




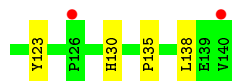
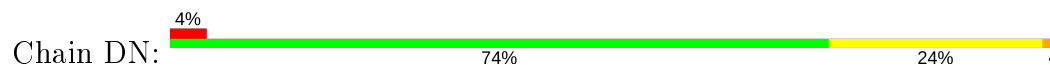
- Molecule 32: 50S Ribosomal Protein L9



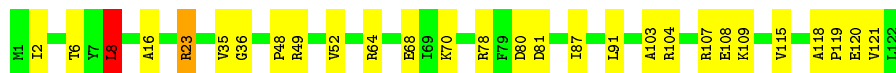
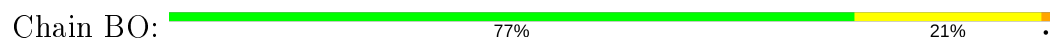
- Molecule 33: 50S Ribosomal Protein L13



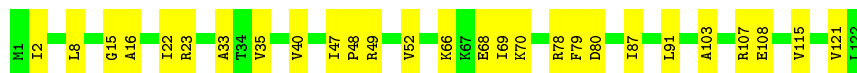
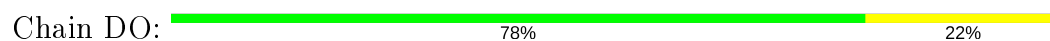
- Molecule 33: 50S Ribosomal Protein L13



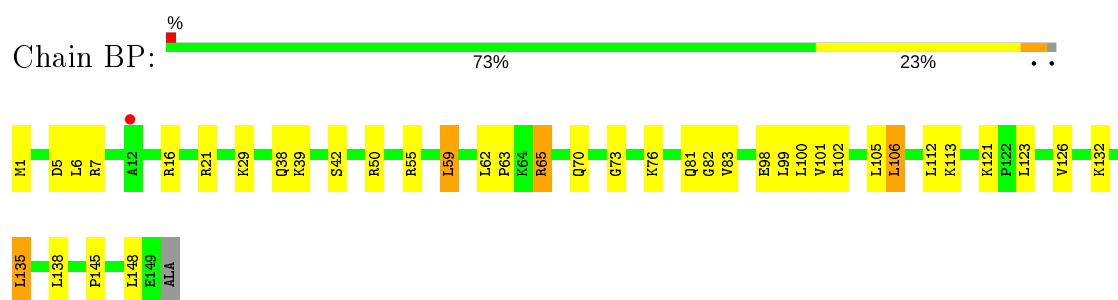
- Molecule 34: 50S Ribosomal Protein L14



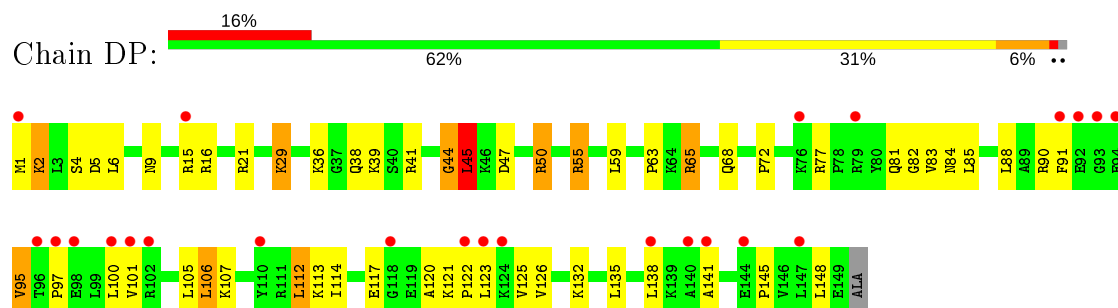
- Molecule 34: 50S Ribosomal Protein L14



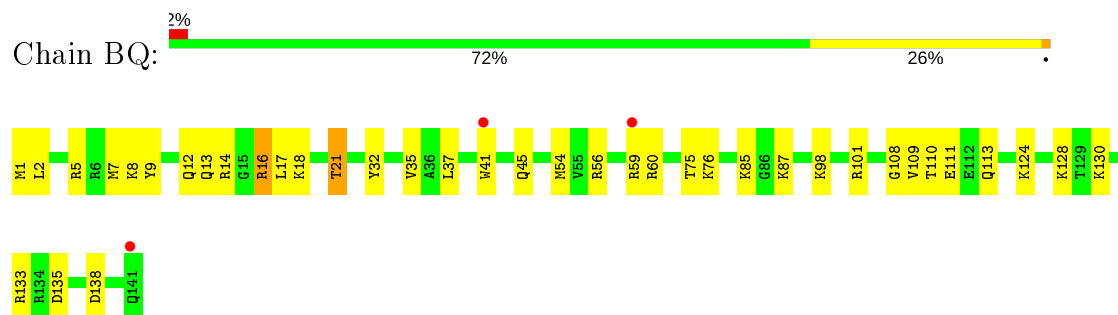
- Molecule 35: 50S Ribosomal Protein L15



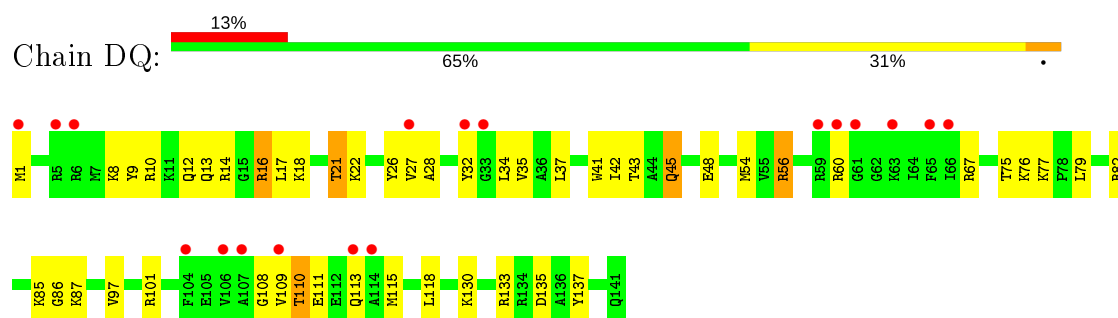
• Molecule 35: 50S Ribosomal Protein L15



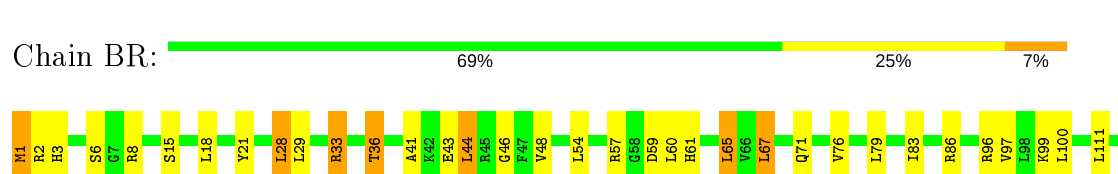
• Molecule 36: 50S Ribosomal Protein L16



• Molecule 36: 50S Ribosomal Protein L16



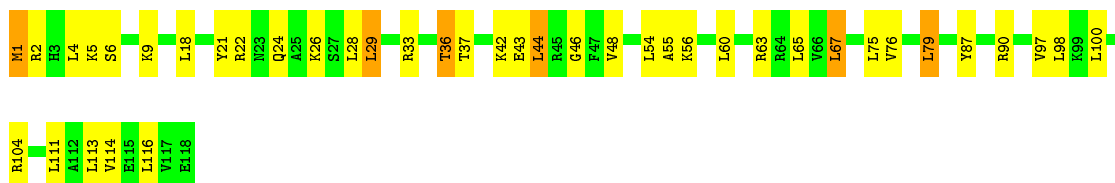
• Molecule 37: 50S Ribosomal Protein L17





• Molecule 37: 50S Ribosomal Protein L17

Chain DR: 65% 30% 5%



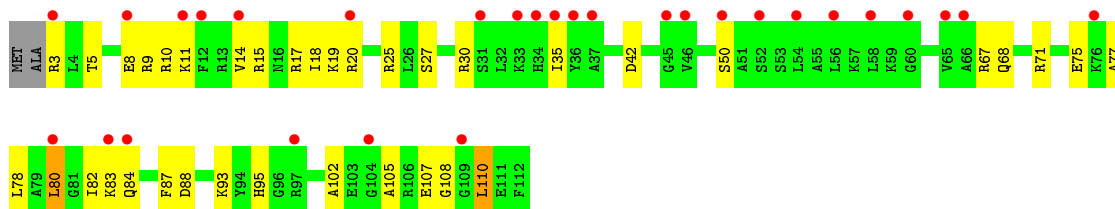
• Molecule 38: 50S Ribosomal Protein L18

Chain BS: % 72% 21% . .



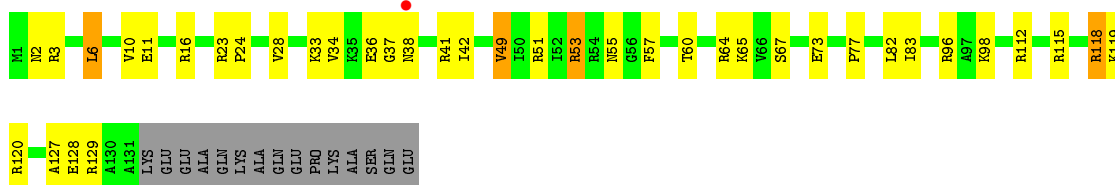
• Molecule 38: 50S Ribosomal Protein L18

Chain DS: 26% 65% 31% . .



• Molecule 39: 50S Ribosomal Protein L19

Chain BT: % 63% 24% . 10%



• Molecule 39: 50S Ribosomal Protein L19

Chain DT: % 58% 31% . 10%





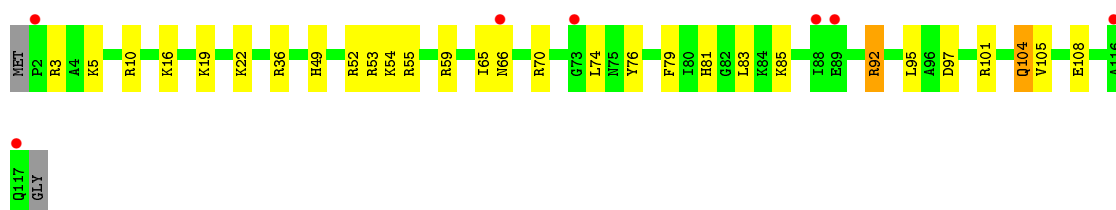
- Molecule 40: 50S Ribosomal Protein L20

Chain BU: 81% 14% ..



- Molecule 40: 50S Ribosomal Protein L20

Chain DU: 6% 74% 23% ..



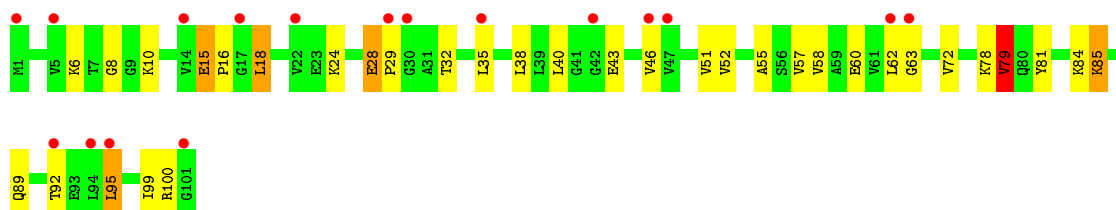
- Molecule 41: 50S Ribosomal Protein L21

Chain BV: 77% 18% 5%



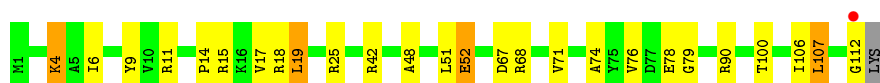
- Molecule 41: 50S Ribosomal Protein L21

Chain DV: 17% 66% 28% 5% ..



- Molecule 42: 50S Ribosomal Protein L22

Chain BW: % 76% 19% ..

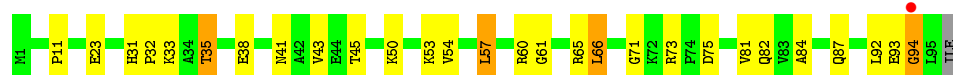


- Molecule 42: 50S Ribosomal Protein L22

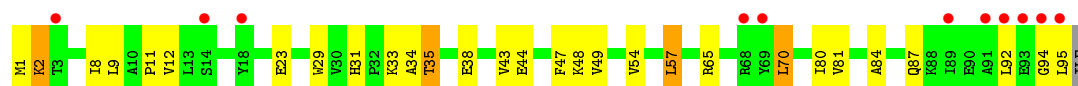
Chain DW: % 76% 20% ..



- Molecule 43: 50S Ribosomal Protein L23



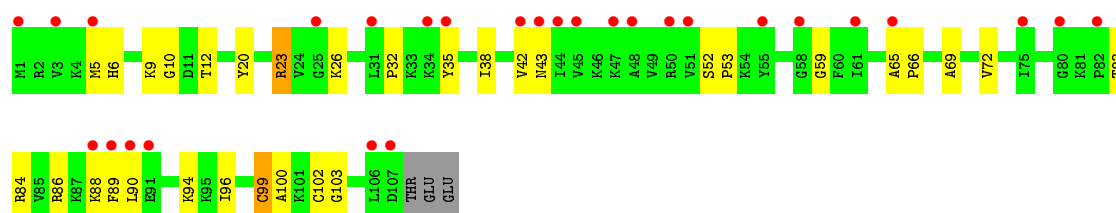
- Molecule 43: 50S Ribosomal Protein L23



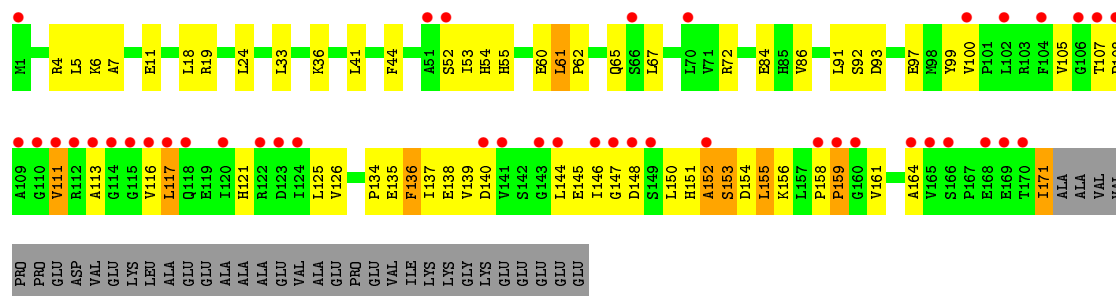
- Molecule 44: 50S Ribosomal Protein L24



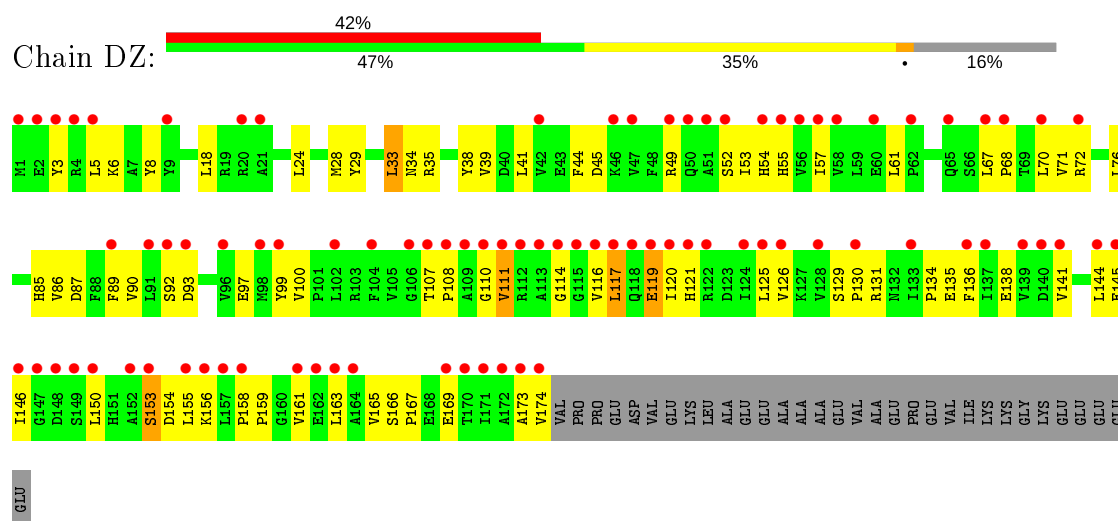
- Molecule 44: 50S Ribosomal Protein L24



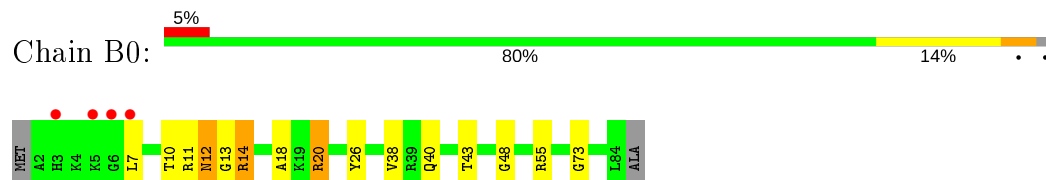
- Molecule 45: 50S Ribosomal Protein L25



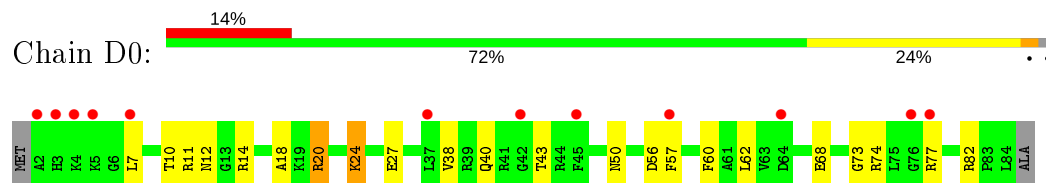
- Molecule 45: 50S Ribosomal Protein L25



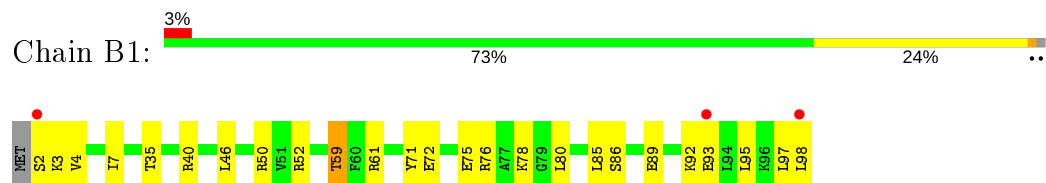
- Molecule 46: 50S Ribosomal Protein L27



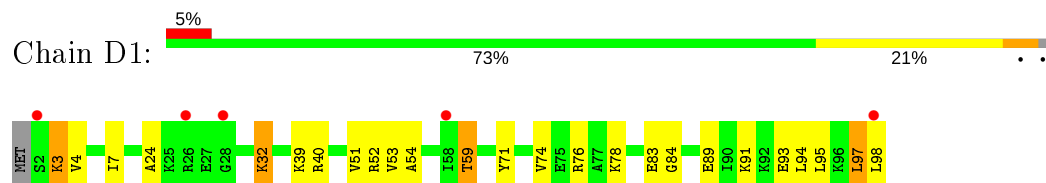
- Molecule 46: 50S Ribosomal Protein L27



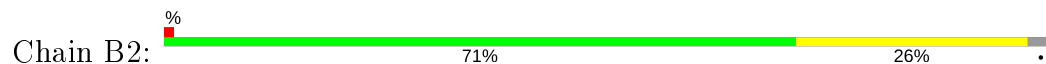
- Molecule 47: 50S Ribosomal Protein L28



- Molecule 47: 50S Ribosomal Protein L28

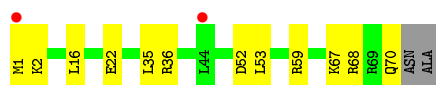
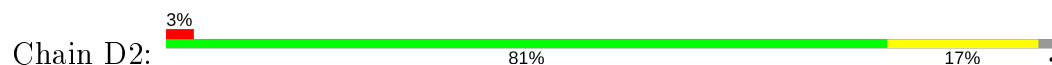


- Molecule 48: 50S Ribosomal Protein L29

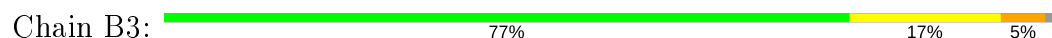




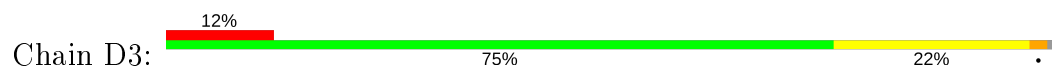
• Molecule 48: 50S Ribosomal Protein L29



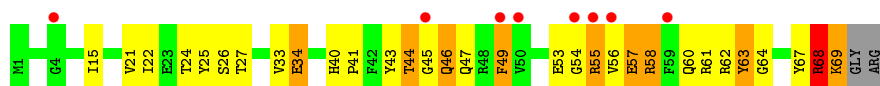
• Molecule 49: 50S Ribosomal Protein L30



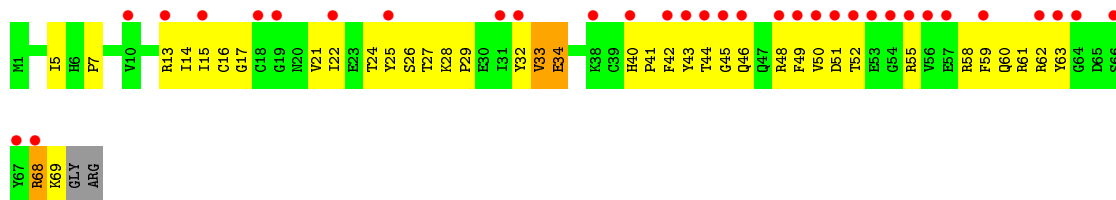
• Molecule 49: 50S Ribosomal Protein L30



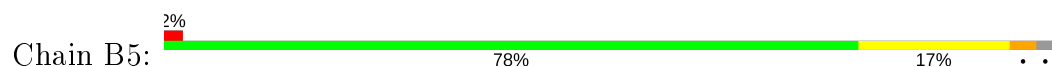
• Molecule 50: 50S Ribosomal Protein L31




• Molecule 50: 50S Ribosomal Protein L31



• Molecule 51: 50S Ribosomal Protein L32



- Molecule 51: 50S Ribosomal Protein L32

Chain D5:  2% 82% 15% ..



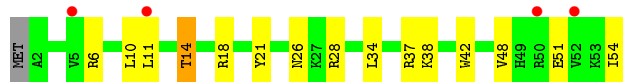
- Molecule 52: 50S Ribosomal Protein L33

Chain B6:  69% 28% ..



- Molecule 52: 50S Ribosomal Protein L33

Chain D6:  7% 70% 26% ..




- Molecule 53: 50S Ribosomal Protein L34

Chain B7:  4% 67% 29% ..



- Molecule 53: 50S Ribosomal Protein L34

Chain D7:  6% 82% 14% ..



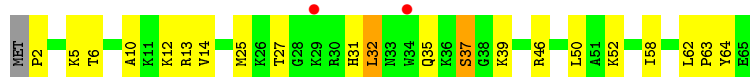
- Molecule 54: 50S Ribosomal Protein L35

Chain B8:  66% 32% ..




- Molecule 54: 50S Ribosomal Protein L35

Chain D8:  3% 66% 29% ..




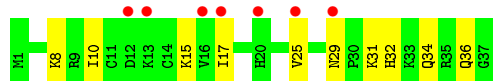
● Molecule 55: 50S Ribosomal Protein L36

Chain B9:  3% 86% 14%



● Molecule 55: 50S Ribosomal Protein L36

Chain D9:  19% 73% 27%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.35Å 449.01Å 621.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.52 – 2.55 145.52 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.0 (145.52-2.55) 99.0 (145.52-2.55)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.225 , 0.273 0.226 , 0.274	Depositor DCC
R_{free} test set	93275 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	297273	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.43	0/36049	0.93	45/56261 (0.1%)
1	CA	0.42	2/36170 (0.0%)	0.95	52/56452 (0.1%)
2	AB	0.31	0/1881	0.62	1/2542 (0.0%)
2	CB	0.32	0/1860	0.59	0/2518
3	AC	0.30	0/1576	0.52	0/2130
3	CC	0.31	0/1566	0.55	0/2119
4	AD	0.32	0/1689	0.53	0/2267
4	CD	0.32	0/1704	0.55	0/2284
5	AE	0.31	0/1145	0.54	0/1543
5	CE	0.33	0/1149	0.59	0/1548
6	AF	0.32	0/819	0.53	0/1111
6	CF	0.30	0/829	0.52	0/1123
7	AG	0.30	0/1250	0.49	0/1679
7	CG	0.30	0/1254	0.50	0/1683
8	AH	0.30	0/1108	0.51	0/1494
8	CH	0.30	0/1108	0.53	0/1494
9	AI	0.32	0/1002	0.56	0/1346
9	CI	0.32	0/997	0.59	0/1343
10	AJ	0.30	0/722	0.56	0/982
10	CJ	0.31	0/727	0.60	0/988
11	AK	0.31	0/844	0.54	0/1145
11	CK	0.30	0/848	0.54	0/1149
12	AL	0.33	0/946	0.53	0/1274
12	CL	0.32	0/946	0.57	0/1274
13	AM	0.30	0/969	0.57	0/1302
13	CM	0.30	0/961	0.53	0/1291
14	AN	0.34	0/501	0.50	0/664
14	CN	0.33	0/501	0.56	0/664
15	AO	0.30	0/739	0.56	0/985
15	CO	0.31	0/739	0.54	0/985
16	AP	0.32	0/697	0.53	0/939
16	CP	0.31	0/693	0.50	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.31	0/836	0.49	0/1117
17	CQ	0.30	0/836	0.52	0/1117
18	AR	0.32	0/560	0.55	0/746
18	CR	0.28	0/560	0.49	0/746
19	AS	0.30	0/667	0.54	0/900
19	CS	0.34	0/661	0.66	0/893
20	AT	0.29	0/730	0.57	0/965
20	CT	0.30	0/729	0.53	0/965
21	AU	0.33	0/203	0.50	0/266
21	CU	0.34	0/203	0.53	0/266
22	AV	0.48	0/310	1.00	0/480
22	CV	0.45	0/310	0.91	2/480 (0.4%)
23	AW	0.48	0/1602	1.06	0/2493
23	AY	0.52	0/1602	1.16	4/2493 (0.2%)
23	CW	0.52	0/1556	1.19	10/2418 (0.4%)
23	CY	0.54	0/1579	1.18	5/2455 (0.2%)
24	AX	0.55	2/1725 (0.1%)	1.16	12/2689 (0.4%)
24	CX	0.56	1/1725 (0.1%)	1.18	18/2689 (0.7%)
25	BA	0.60	6/68013 (0.0%)	1.02	122/106165 (0.1%)
25	DA	0.49	0/67542	0.98	62/105428 (0.1%)
26	BB	0.49	0/2878	0.91	0/4490
26	DB	0.51	0/2878	0.96	1/4490 (0.0%)
27	BD	0.41	0/2186	0.64	1/2944 (0.0%)
27	DD	0.38	0/2186	0.59	1/2944 (0.0%)
28	BE	0.42	0/1592	0.58	0/2149
28	DE	0.36	0/1592	0.58	1/2149 (0.0%)
29	BF	0.40	0/1619	0.58	0/2193
29	DF	0.36	0/1615	0.59	0/2188
30	BG	0.33	0/1450	0.56	1/1959 (0.1%)
30	DG	0.33	0/1449	0.56	0/1958
31	BH	0.34	0/1356	0.52	0/1834
31	DH	0.32	0/1356	0.53	0/1834
32	BI	0.31	0/1100	0.57	0/1501
32	DI	0.29	0/1076	0.56	0/1471
33	BN	0.39	0/1144	0.56	0/1543
33	DN	0.35	0/1144	0.56	0/1543
34	BO	0.42	0/943	0.60	1/1269 (0.1%)
34	DO	0.34	0/943	0.51	0/1269
35	BP	0.38	0/1152	0.59	0/1533
35	DP	0.35	0/1152	0.61	1/1533 (0.1%)
36	BQ	0.41	0/1143	0.55	0/1527
36	DQ	0.36	0/1143	0.55	0/1527
37	BR	0.42	0/982	0.65	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DR	0.31	0/982	0.54	0/1312
38	BS	0.34	0/887	0.59	0/1180
38	DS	0.32	0/880	0.55	0/1172
39	BT	0.39	0/1105	0.60	0/1477
39	DT	0.31	0/1097	0.52	0/1468
40	BU	0.45	0/977	0.62	1/1301 (0.1%)
40	DU	0.32	0/977	0.52	0/1301
41	BV	0.44	0/782	0.61	0/1049
41	DV	0.33	0/782	0.54	0/1049
42	BW	0.44	0/897	0.61	0/1205
42	DW	0.33	0/897	0.53	0/1205
43	BX	0.44	0/764	0.64	1/1025 (0.1%)
43	DX	0.36	0/764	0.57	1/1025 (0.1%)
44	BY	0.42	0/819	0.64	0/1095
44	DY	0.33	0/819	0.52	0/1095
45	BZ	0.35	0/1379	0.60	0/1873
45	DZ	0.33	0/1390	0.56	0/1890
46	B0	0.40	0/662	0.66	1/881 (0.1%)
46	D0	0.33	0/662	0.52	0/881
47	B1	0.40	0/762	0.57	0/1014
47	D1	0.34	0/762	0.56	0/1014
48	B2	0.37	0/590	0.65	0/781
48	D2	0.30	0/590	0.47	0/781
49	B3	0.42	0/474	0.62	0/635
49	D3	0.30	0/469	0.53	0/630
50	B4	0.39	0/571	0.66	0/768
50	D4	0.33	0/545	0.60	0/737
51	B5	0.39	0/469	0.64	0/635
51	D5	0.33	0/469	0.58	0/635
52	B6	0.42	0/460	0.58	0/613
52	D6	0.36	0/456	0.49	0/608
53	B7	0.45	0/426	0.66	0/561
53	D7	0.36	0/426	0.52	0/561
54	B8	0.41	0/519	0.62	0/684
54	D8	0.33	0/525	0.55	0/691
55	B9	0.44	0/310	0.52	0/407
55	D9	0.34	0/310	0.57	0/407
All	All	0.47	11/316672 (0.0%)	0.90	344/474091 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	1
7	AG	0	1
7	CG	0	1
19	CS	0	1
27	DD	0	1
38	BS	0	1
44	BY	0	1
All	All	0	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	354	A	N9-C4	-7.89	1.33	1.37
1	CA	1154	G	C6-N1	-7.66	1.34	1.39
25	BA	1188	A	N9-C4	-7.63	1.33	1.37
25	BA	1067	A	N9-C4	-6.49	1.33	1.37
24	AX	14	A	N7-C5	-6.24	1.35	1.39

The worst 5 of 344 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1154	G	C5-C6-O6	17.34	139.00	128.60
1	CA	1119	C	C2-N3-C4	16.52	128.16	119.90
1	CA	1154	G	N3-C2-N2	14.11	129.78	119.90
1	CA	1119	C	N1-C2-O2	14.07	127.34	118.90
1	CA	1154	G	N1-C6-O6	-11.05	113.27	119.90

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	231	GLU	Peptide
7	AG	78	ARG	Peptide
38	BS	58	LEU	Peptide
44	BY	54	LYS	Peptide
7	CG	78	ARG	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32205	0	16255	434	0
1	CA	32312	0	16307	550	0
2	AB	1846	0	1867	70	0
2	CB	1825	0	1828	90	0
3	AC	1552	0	1546	45	0
3	CC	1542	0	1517	56	0
4	AD	1659	0	1676	53	0
4	CD	1674	0	1714	54	0
5	AE	1129	0	1185	33	0
5	CE	1133	0	1191	30	0
6	AF	806	0	793	18	0
6	CF	816	0	808	17	0
7	AG	1231	0	1238	22	0
7	CG	1235	0	1249	31	0
8	AH	1088	0	1126	32	0
8	CH	1088	0	1126	31	0
9	AI	983	0	986	28	0
9	CI	978	0	966	46	0
10	AJ	709	0	650	32	0
10	CJ	714	0	672	36	0
11	AK	829	0	825	15	0
11	CK	833	0	836	22	0
12	AL	930	0	980	18	0
12	CL	930	0	980	23	0
13	AM	958	0	1002	26	0
13	CM	950	0	988	24	0
14	AN	492	0	529	20	0
14	CN	492	0	529	17	0
15	AO	728	0	760	18	0
15	CO	728	0	760	31	0
16	AP	681	0	697	21	0
16	CP	677	0	686	17	0
17	AQ	823	0	891	16	0
17	CQ	823	0	891	19	0
18	AR	555	0	618	12	0
18	CR	555	0	618	13	0
19	AS	652	0	662	35	0
19	CS	646	0	644	34	0
20	AT	728	0	798	19	0
20	CT	727	0	796	20	0
21	AU	199	0	208	5	0
21	CU	199	0	208	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AV	277	0	140	2	0
22	CV	277	0	140	2	0
23	AW	1588	0	820	30	0
23	AY	1581	0	805	57	0
23	CW	1541	0	784	50	0
23	CY	1561	0	796	46	0
24	AX	1625	0	828	11	0
24	CX	1625	0	828	28	0
25	BA	60729	0	30622	619	0
25	DA	60311	0	30414	867	0
26	BB	2573	0	1306	18	0
26	DB	2573	0	1306	38	0
27	BD	2136	0	2218	52	0
27	DD	2136	0	2218	51	0
28	BE	1559	0	1618	38	0
28	DE	1559	0	1618	41	0
29	BF	1584	0	1625	33	0
29	DF	1580	0	1619	64	0
30	BG	1425	0	1443	23	0
30	DG	1424	0	1434	47	0
31	BH	1330	0	1407	26	0
31	DH	1330	0	1407	61	0
32	BI	1085	0	1114	26	0
32	DI	1061	0	1080	19	0
33	BN	1117	0	1184	15	0
33	DN	1117	0	1184	24	0
34	BO	933	0	996	21	0
34	DO	933	0	996	18	0
35	BP	1135	0	1212	28	0
35	DP	1135	0	1212	50	0
36	BQ	1122	0	1179	23	0
36	DQ	1122	0	1179	38	0
37	BR	968	0	1033	25	0
37	DR	968	0	1033	26	0
38	BS	877	0	938	26	0
38	DS	870	0	923	23	0
39	BT	1091	0	1151	29	0
39	DT	1083	0	1136	30	0
40	BU	959	0	1019	14	0
40	DU	959	0	1019	28	0
41	BV	771	0	830	17	0
41	DV	771	0	830	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BW	886	0	940	15	0
42	DW	886	0	940	13	0
43	BX	750	0	814	23	0
43	DX	750	0	814	22	0
44	BY	806	0	881	21	0
44	DY	806	0	881	20	0
45	BZ	1349	0	1355	41	0
45	DZ	1360	0	1363	63	0
46	B0	653	0	674	16	0
46	D0	653	0	674	24	0
47	B1	755	0	826	17	0
47	D1	755	0	826	15	0
48	B2	588	0	643	9	0
48	D2	588	0	643	8	0
49	B3	469	0	518	8	0
49	D3	464	0	514	9	0
50	B4	558	0	544	34	0
50	D4	532	0	503	25	0
51	B5	455	0	465	11	0
51	D5	455	0	465	8	0
52	B6	453	0	473	7	0
52	D6	449	0	469	8	0
53	B7	418	0	467	11	0
53	D7	418	0	467	6	0
54	B8	511	0	571	18	0
54	D8	517	0	582	21	0
55	B9	307	0	335	4	0
55	D9	307	0	335	8	0
56	AA	230	0	0	0	0
56	AD	1	0	0	0	0
56	AE	1	0	0	0	0
56	AF	1	0	0	0	0
56	AK	2	0	0	0	0
56	AM	1	0	0	0	0
56	AN	1	0	0	0	0
56	AV	1	0	0	0	0
56	AW	7	0	0	0	0
56	AX	12	0	0	0	0
56	AY	3	0	0	0	0
56	B0	3	0	0	0	0
56	B1	2	0	0	0	0
56	B2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B3	3	0	0	0	0
56	B4	1	0	0	0	0
56	B5	4	0	0	0	0
56	B6	2	0	0	0	0
56	B7	2	0	0	0	0
56	B8	3	0	0	0	0
56	B9	1	0	0	0	0
56	BA	839	0	0	0	0
56	BB	23	0	0	0	0
56	BD	11	0	0	0	0
56	BE	8	0	0	0	0
56	BF	12	0	0	0	0
56	BG	3	0	0	0	0
56	BN	5	0	0	0	0
56	BO	1	0	0	0	0
56	BP	3	0	0	0	0
56	BQ	5	0	0	0	0
56	BR	5	0	0	0	0
56	BU	9	0	0	0	0
56	BV	5	0	0	0	0
56	BW	3	0	0	0	0
56	BX	2	0	0	0	0
56	BY	1	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	177	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	CV	1	0	0	0	0
56	CW	2	0	0	0	0
56	CX	5	0	0	0	0
56	CY	1	0	0	0	0
56	D0	2	0	0	0	0
56	D3	1	0	0	0	0
56	D7	2	0	0	0	0
56	D8	1	0	0	0	0
56	DA	675	0	0	0	0
56	DB	11	0	0	0	0
56	DD	7	0	0	0	0
56	DE	4	0	0	0	0
56	DF	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DG	1	0	0	0	0
56	DN	1	0	0	0	0
56	DO	1	0	0	0	0
56	DQ	4	0	0	0	0
56	DR	1	0	0	0	0
56	DU	2	0	0	0	0
56	DV	3	0	0	0	0
56	DW	3	0	0	0	0
56	DY	1	0	0	0	0
57	AA	40	0	37	7	0
57	CA	40	0	37	9	0
58	AD	8	0	0	0	0
58	CD	8	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	226	0	0	17	0
61	AE	3	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	4	0	0	1	0
61	AM	1	0	0	0	0
61	AV	4	0	0	0	0
61	AW	6	0	0	0	0
61	AX	8	0	0	0	0
61	AY	3	0	0	0	0
61	B0	4	0	0	0	0
61	B1	2	0	0	0	0
61	B3	2	0	0	0	0
61	B5	5	0	0	1	0
61	B6	1	0	0	0	0
61	B7	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B8	11	0	0	1	0
61	BA	1411	0	0	69	0
61	BB	36	0	0	1	0
61	BD	16	0	0	2	0
61	BE	13	0	0	2	0
61	BF	7	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BN	2	0	0	0	0
61	BO	3	0	0	0	0
61	BP	17	0	0	1	0
61	BQ	2	0	0	0	0
61	BR	2	0	0	0	0
61	BT	1	0	0	0	0
61	BU	6	0	0	0	0
61	BV	2	0	0	0	0
61	BW	4	0	0	0	0
61	BX	1	0	0	0	0
61	CA	173	0	0	15	0
61	CJ	2	0	0	2	0
61	CL	1	0	0	0	0
61	CV	2	0	0	0	0
61	CW	1	0	0	0	0
61	CX	4	0	0	2	0
61	D0	5	0	0	0	0
61	D3	1	0	0	0	0
61	D7	3	0	0	1	0
61	D8	4	0	0	0	0
61	DA	1002	0	0	68	0
61	DB	10	0	0	0	0
61	DD	17	0	0	1	0
61	DE	11	0	0	0	0
61	DF	5	0	0	0	0
61	DN	2	0	0	0	0
61	DO	2	0	0	0	0
61	DP	8	0	0	1	0
61	DQ	1	0	0	0	0
61	DR	1	0	0	0	0
61	DU	2	0	0	0	0
61	DW	1	0	0	0	0
61	DY	1	0	0	0	0
All	All	297273	0	196306	4649	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 10.

The worst 5 of 4649 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1256:A:H61	1:CA:1278:U:H1'	1.25	1.02
1:CA:999:C:N4	1:CA:1042:G:H1	1.59	1.00
1:AA:1025:U:O2	1:AA:1036:G:O6	1.82	0.98
23:CW:27:G:H1	23:CW:43:C:N4	1.62	0.97
1:CA:1029:C:N4	1:CA:1032:G:C6	2.33	0.97

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	229/256 (90%)	200 (87%)	19 (8%)	10 (4%)	2	1
2	CB	229/256 (90%)	195 (85%)	24 (10%)	10 (4%)	2	1
3	AC	204/239 (85%)	184 (90%)	17 (8%)	3 (2%)	10	14
3	CC	204/239 (85%)	180 (88%)	22 (11%)	2 (1%)	15	22
4	AD	206/209 (99%)	192 (93%)	12 (6%)	2 (1%)	15	22
4	CD	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	29	40
5	AE	146/162 (90%)	134 (92%)	9 (6%)	3 (2%)	7	7
5	CE	146/162 (90%)	138 (94%)	7 (5%)	1 (1%)	22	30
6	AF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
6	CF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
7	AG	153/156 (98%)	143 (94%)	8 (5%)	2 (1%)	12	16
7	CG	153/156 (98%)	140 (92%)	9 (6%)	4 (3%)	5	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
8	CH	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	22	30
9	AI	125/128 (98%)	111 (89%)	11 (9%)	3 (2%)	6	5
9	CI	125/128 (98%)	114 (91%)	8 (6%)	3 (2%)	6	5
10	AJ	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	4	3
10	CJ	94/105 (90%)	81 (86%)	10 (11%)	3 (3%)	4	3
11	AK	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	8	10
11	CK	112/129 (87%)	107 (96%)	3 (3%)	2 (2%)	8	10
12	AL	120/132 (91%)	115 (96%)	5 (4%)	0	100	100
12	CL	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
13	AM	121/126 (96%)	110 (91%)	9 (7%)	2 (2%)	9	11
13	CM	120/126 (95%)	108 (90%)	9 (8%)	3 (2%)	5	5
14	AN	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
14	CN	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	CO	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	6	6
16	AP	80/88 (91%)	78 (98%)	2 (2%)	0	100	100
16	CP	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	12	16
17	AQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	CQ	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	15	22
18	AR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
18	CR	66/88 (75%)	65 (98%)	0	1 (2%)	10	14
19	AS	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
19	CS	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
20	AT	94/106 (89%)	84 (89%)	3 (3%)	7 (7%)	1	0
20	CT	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	2	0
21	AU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
21	CU	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	1
27	BD	273/276 (99%)	257 (94%)	15 (6%)	1 (0%)	34	46
27	DD	273/276 (99%)	258 (94%)	13 (5%)	2 (1%)	22	30
28	BE	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	29	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	DE	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	15	22
29	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	29	40
29	DF	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	15	22
30	BG	179/182 (98%)	167 (93%)	7 (4%)	5 (3%)	5	4
30	DG	179/182 (98%)	165 (92%)	7 (4%)	7 (4%)	3	1
31	BH	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	25	34
31	DH	172/180 (96%)	157 (91%)	13 (8%)	2 (1%)	13	17
32	BI	144/148 (97%)	123 (85%)	16 (11%)	5 (4%)	3	2
32	DI	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	22	30
33	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
33	DN	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	22	30
34	BO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
34	DO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
35	BP	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	22	30
35	DP	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	11	15
36	BQ	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
36	DQ	139/141 (99%)	129 (93%)	8 (6%)	2 (1%)	11	15
37	BR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
37	DR	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
38	BS	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
38	DS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	17	24
39	BT	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	19	27
39	DT	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	19	27
40	BU	114/118 (97%)	114 (100%)	0	0	100	100
40	DU	114/118 (97%)	114 (100%)	0	0	100	100
41	BV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	22
41	DV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	22
42	BW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
42	DW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
43	BX	93/96 (97%)	90 (97%)	1 (1%)	2 (2%)	6	7
43	DX	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	14	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	BY	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
44	DY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
45	BZ	169/206 (82%)	143 (85%)	24 (14%)	2 (1%)	13	17
45	DZ	172/206 (84%)	149 (87%)	22 (13%)	1 (1%)	25	34
46	B0	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	13	17
46	D0	81/85 (95%)	75 (93%)	6 (7%)	0	100	100
47	B1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
47	D1	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
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%)	57 (100%)	0	0	100	100
49	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
50	B4	67/71 (94%)	50 (75%)	11 (16%)	6 (9%)	1	0
50	D4	67/71 (94%)	51 (76%)	12 (18%)	4 (6%)	1	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%)	2 (4%)	0	100	100
52	D6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
53	B7	46/49 (94%)	46 (100%)	0	0	100	100
53	D7	46/49 (94%)	45 (98%)	0	1 (2%)	6	7
54	B8	62/65 (95%)	62 (100%)	0	0	100	100
54	D8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
55	B9	35/37 (95%)	35 (100%)	0	0	100	100
55	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11409/12128 (94%)	10643 (93%)	629 (6%)	137 (1%)	13	17

5 of 137 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL
2	AB	16	HIS
2	AB	17	PHE
2	AB	126	GLU

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%)	169 (88%)	23 (12%)	5	5
2	CB	187/220 (85%)	168 (90%)	19 (10%)	7	8
3	AC	143/188 (76%)	132 (92%)	11 (8%)	13	16
3	CC	140/188 (74%)	127 (91%)	13 (9%)	9	10
4	AD	170/181 (94%)	155 (91%)	15 (9%)	10	12
4	CD	173/181 (96%)	160 (92%)	13 (8%)	13	17
5	AE	113/123 (92%)	106 (94%)	7 (6%)	18	24
5	CE	114/123 (93%)	105 (92%)	9 (8%)	12	15
6	AF	83/90 (92%)	77 (93%)	6 (7%)	14	18
6	CF	85/90 (94%)	81 (95%)	4 (5%)	26	35
7	AG	119/127 (94%)	106 (89%)	13 (11%)	6	6
7	CG	120/127 (94%)	111 (92%)	9 (8%)	13	17
8	AH	114/119 (96%)	107 (94%)	7 (6%)	18	24
8	CH	114/119 (96%)	104 (91%)	10 (9%)	10	12
9	AI	90/99 (91%)	82 (91%)	8 (9%)	9	12
9	CI	89/99 (90%)	73 (82%)	16 (18%)	1	1
10	AJ	66/92 (72%)	62 (94%)	4 (6%)	18	24
10	CJ	69/92 (75%)	66 (96%)	3 (4%)	29	39
11	AK	82/99 (83%)	76 (93%)	6 (7%)	14	18
11	CK	83/99 (84%)	77 (93%)	6 (7%)	14	18
12	AL	97/109 (89%)	93 (96%)	4 (4%)	30	41
12	CL	97/109 (89%)	92 (95%)	5 (5%)	23	30
13	AM	93/101 (92%)	83 (89%)	10 (11%)	6	6
13	CM	92/101 (91%)	83 (90%)	9 (10%)	8	9
14	AN	49/50 (98%)	43 (88%)	6 (12%)	5	4
14	CN	49/50 (98%)	43 (88%)	6 (12%)	5	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	78/80 (98%)	67 (86%)	11 (14%)	3	3
15	CO	78/80 (98%)	70 (90%)	8 (10%)	7	7
16	AP	69/74 (93%)	62 (90%)	7 (10%)	7	8
16	CP	68/74 (92%)	63 (93%)	5 (7%)	13	18
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	39	53
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	17	23
18	AR	59/77 (77%)	56 (95%)	3 (5%)	24	32
18	CR	59/77 (77%)	54 (92%)	5 (8%)	10	13
19	AS	69/80 (86%)	66 (96%)	3 (4%)	29	39
19	CS	67/80 (84%)	57 (85%)	10 (15%)	3	2
20	AT	70/82 (85%)	64 (91%)	6 (9%)	10	13
20	CT	70/82 (85%)	64 (91%)	6 (9%)	10	13
21	AU	18/22 (82%)	16 (89%)	2 (11%)	6	6
21	CU	18/22 (82%)	16 (89%)	2 (11%)	6	6
27	BD	215/218 (99%)	200 (93%)	15 (7%)	15	19
27	DD	215/218 (99%)	202 (94%)	13 (6%)	19	25
28	BE	164/166 (99%)	147 (90%)	17 (10%)	7	7
28	DE	164/166 (99%)	145 (88%)	19 (12%)	5	5
29	BF	160/166 (96%)	142 (89%)	18 (11%)	6	5
29	DF	159/166 (96%)	142 (89%)	17 (11%)	6	7
30	BG	143/156 (92%)	130 (91%)	13 (9%)	9	11
30	DG	142/156 (91%)	128 (90%)	14 (10%)	8	9
31	BH	144/148 (97%)	136 (94%)	8 (6%)	21	28
31	DH	144/148 (97%)	133 (92%)	11 (8%)	13	17
32	BI	110/124 (89%)	92 (84%)	18 (16%)	2	2
32	DI	104/124 (84%)	93 (89%)	11 (11%)	6	7
33	BN	118/119 (99%)	103 (87%)	15 (13%)	4	4
33	DN	118/119 (99%)	107 (91%)	11 (9%)	9	10
34	BO	100/100 (100%)	97 (97%)	3 (3%)	41	55
34	DO	100/100 (100%)	96 (96%)	4 (4%)	31	43
35	BP	115/116 (99%)	107 (93%)	8 (7%)	15	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	DP	115/116 (99%)	103 (90%)	12 (10%)	7	7
36	BQ	111/111 (100%)	97 (87%)	14 (13%)	4	4
36	DQ	111/111 (100%)	101 (91%)	10 (9%)	9	11
37	BR	101/101 (100%)	84 (83%)	17 (17%)	2	2
37	DR	101/101 (100%)	86 (85%)	15 (15%)	3	2
38	BS	87/88 (99%)	78 (90%)	9 (10%)	7	7
38	DS	85/88 (97%)	78 (92%)	7 (8%)	11	14
39	BT	115/127 (91%)	109 (95%)	6 (5%)	23	30
39	DT	113/127 (89%)	106 (94%)	7 (6%)	18	24
40	BU	93/94 (99%)	86 (92%)	7 (8%)	13	17
40	DU	93/94 (99%)	88 (95%)	5 (5%)	22	29
41	BV	80/82 (98%)	72 (90%)	8 (10%)	7	8
41	DV	80/82 (98%)	71 (89%)	9 (11%)	6	5
42	BW	90/92 (98%)	82 (91%)	8 (9%)	9	12
42	DW	90/92 (98%)	84 (93%)	6 (7%)	16	21
43	BX	77/78 (99%)	72 (94%)	5 (6%)	17	23
43	DX	77/78 (99%)	72 (94%)	5 (6%)	17	23
44	BY	85/91 (93%)	80 (94%)	5 (6%)	19	25
44	DY	85/91 (93%)	82 (96%)	3 (4%)	36	49
45	BZ	145/179 (81%)	131 (90%)	14 (10%)	8	9
45	DZ	145/179 (81%)	132 (91%)	13 (9%)	9	11
46	B0	65/67 (97%)	63 (97%)	2 (3%)	40	54
46	D0	65/67 (97%)	63 (97%)	2 (3%)	40	54
47	B1	80/83 (96%)	75 (94%)	5 (6%)	18	23
47	D1	80/83 (96%)	73 (91%)	7 (9%)	10	12
48	B2	65/67 (97%)	61 (94%)	4 (6%)	18	24
48	D2	65/67 (97%)	64 (98%)	1 (2%)	65	77
49	B3	51/52 (98%)	47 (92%)	4 (8%)	12	16
49	D3	50/52 (96%)	45 (90%)	5 (10%)	7	8
50	B4	60/63 (95%)	52 (87%)	8 (13%)	4	3
50	D4	53/63 (84%)	47 (89%)	6 (11%)	6	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	B5	50/52 (96%)	47 (94%)	3 (6%)	19	25
51	D5	50/52 (96%)	45 (90%)	5 (10%)	7	8
52	B6	51/52 (98%)	46 (90%)	5 (10%)	8	9
52	D6	50/52 (96%)	48 (96%)	2 (4%)	31	43
53	B7	41/42 (98%)	38 (93%)	3 (7%)	14	18
53	D7	41/42 (98%)	40 (98%)	1 (2%)	49	64
54	B8	53/55 (96%)	50 (94%)	3 (6%)	20	27
54	D8	54/55 (98%)	51 (94%)	3 (6%)	21	28
55	B9	34/34 (100%)	34 (100%)	0	100	100
55	D9	34/34 (100%)	34 (100%)	0	100	100
All	All	9320/10066 (93%)	8532 (92%)	788 (8%)	10	13

5 of 788 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	BZ	117	LEU
4	CD	150	GLU
41	DV	95	LEU
47	B1	59	THR
2	CB	8	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 122 such sidechains are listed below:

Mol	Chain	Res	Type
43	BX	82	GLN
3	CC	37	GLN
37	DR	13	HIS
44	BY	6	HIS
49	B3	32	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	306 (20%)	21 (1%)
1	CA	1501/1521 (98%)	310 (20%)	23 (1%)
22	AV	12/24 (50%)	3 (25%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	CV	12/24 (50%)	3 (25%)	0
23	AW	71/76 (93%)	30 (42%)	2 (2%)
23	AY	71/76 (93%)	33 (46%)	1 (1%)
23	CW	68/76 (89%)	30 (44%)	3 (4%)
23	CY	69/76 (90%)	28 (40%)	0
24	AX	75/77 (97%)	18 (24%)	1 (1%)
24	CX	75/77 (97%)	19 (25%)	0
25	BA	2811/2915 (96%)	433 (15%)	27 (0%)
25	DA	2791/2915 (95%)	499 (17%)	33 (1%)
26	BB	119/121 (98%)	13 (10%)	0
26	DB	119/121 (98%)	17 (14%)	0
All	All	9289/9620 (96%)	1742 (18%)	111 (1%)

5 of 1742 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G

5 of 111 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2418	U
1	CA	991	U
25	DA	1913	A
25	BA	2701	U
1	CA	509	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PSU	CY	55	23	17,21,22	1.50	3 (17%)	20,30,33	3.01	6 (30%)
23	MIA	AY	37	23	18,24,32	1.15	2 (11%)	18,35,47	1.23	2 (11%)
23	7MG	AW	46	23	22,26,27	1.80	4 (18%)	28,39,42	2.84	9 (32%)
24	5MC	AX	32	24	15,22,23	1.32	1 (6%)	19,32,35	1.40	3 (15%)
24	4SU	AX	8	24	14,21,22	1.46	2 (14%)	15,30,33	2.87	2 (13%)
23	5MU	CY	54	23	15,22,23	1.14	1 (6%)	16,32,35	2.10	1 (6%)
23	MIA	AW	37	23	24,31,32	2.28	3 (12%)	26,44,47	2.40	8 (30%)
24	PSU	AX	55	24	17,21,22	1.69	3 (17%)	20,30,33	3.19	6 (30%)
23	PSU	CY	32	23	17,21,22	1.39	2 (11%)	20,30,33	3.17	6 (30%)
23	7MG	CW	46	23	22,26,27	1.77	3 (13%)	28,39,42	2.75	8 (28%)
23	4SU	AY	8	23	14,21,22	1.20	1 (7%)	15,30,33	1.94	2 (13%)
23	PSU	AW	55	23	17,21,22	1.49	2 (11%)	20,30,33	3.34	6 (30%)
23	5MU	CW	54	23	15,22,23	1.08	1 (6%)	16,32,35	1.97	1 (6%)
23	4SU	CY	8	23	14,21,22	1.28	1 (7%)	15,30,33	1.54	2 (13%)
23	PSU	CY	39	23	17,21,22	1.65	3 (17%)	20,30,33	3.28	7 (35%)
24	5MC	CX	32	24	15,22,23	1.30	1 (6%)	19,32,35	1.53	4 (21%)
24	5MU	AX	54	24,56	15,22,23	1.13	2 (13%)	16,32,35	1.92	2 (12%)
23	PSU	CW	39	23	17,21,22	1.46	3 (17%)	20,30,33	3.52	6 (30%)
23	MIA	CW	37	23	18,24,32	1.07	2 (11%)	18,35,47	1.38	2 (11%)
23	7MG	AY	46	23	22,26,27	1.85	3 (13%)	28,39,42	2.92	10 (35%)
24	PSU	CX	55	24	17,21,22	1.36	2 (11%)	20,30,33	3.09	5 (25%)
23	PSU	AW	39	23	17,21,22	1.53	2 (11%)	20,30,33	3.07	6 (30%)
24	5MU	CX	54	24	15,22,23	1.14	1 (6%)	16,32,35	1.80	1 (6%)
23	4SU	AW	8	23	14,21,22	1.23	1 (7%)	15,30,33	1.73	2 (13%)
23	PSU	CW	32	23	17,21,22	1.43	3 (17%)	20,30,33	3.21	6 (30%)
23	PSU	AY	32	23	17,21,22	1.56	2 (11%)	20,30,33	3.16	6 (30%)
23	PSU	AY	39	23	17,21,22	1.53	3 (17%)	20,30,33	3.61	6 (30%)
23	PSU	CW	55	23	17,21,22	1.42	2 (11%)	20,30,33	3.24	6 (30%)
24	4SU	CX	8	24	14,21,22	1.25	2 (14%)	15,30,33	2.71	2 (13%)
23	5MU	AW	54	23	15,22,23	1.09	2 (13%)	16,32,35	2.25	1 (6%)
23	5MU	AY	54	23	15,22,23	1.07	1 (6%)	16,32,35	2.40	1 (6%)
23	4SU	CW	8	56,23	14,21,22	1.24	1 (7%)	15,30,33	1.57	2 (13%)
23	7MG	CY	46	23	22,26,27	1.80	4 (18%)	28,39,42	2.86	10 (35%)
23	PSU	AW	32	56,23	17,21,22	1.52	3 (17%)	20,30,33	3.33	6 (30%)
23	PSU	AY	55	23	17,21,22	1.44	2 (11%)	20,30,33	3.13	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	MIA	CY	37	23	18,24,32	1.16	2 (11%)	18,35,47	1.28	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	CY	55	23	-	2/7/25/26	0/2/2/2
23	MIA	AY	37	23	-	1/3/25/34	0/3/3/3
23	7MG	AW	46	23	-	3/7/37/38	0/3/3/3
24	5MC	AX	32	24	-	0/5/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/5/25/26	0/2/2/2
23	5MU	CY	54	23	-	1/5/25/26	0/2/2/2
23	MIA	AW	37	23	-	1/11/33/34	0/3/3/3
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
23	PSU	CY	32	23	-	1/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	3/7/37/38	0/3/3/3
23	4SU	AY	8	23	-	1/5/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	5MU	CW	54	23	-	0/5/25/26	0/2/2/2
23	4SU	CY	8	23	-	2/5/25/26	0/2/2/2
23	PSU	CY	39	23	-	2/7/25/26	0/2/2/2
24	5MC	CX	32	24	-	2/5/25/26	0/2/2/2
24	5MU	AX	54	24,56	-	0/5/25/26	0/2/2/2
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
23	MIA	CW	37	23	-	0/3/25/34	0/3/3/3
23	7MG	AY	46	23	-	3/7/37/38	0/3/3/3
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/5/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/5/25/26	0/2/2/2
23	PSU	CW	32	23	-	2/7/25/26	0/2/2/2
23	PSU	AY	32	23	-	0/7/25/26	0/2/2/2
23	PSU	AY	39	23	-	3/7/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/5/25/26	0/2/2/2
23	5MU	AW	54	23	-	0/5/25/26	0/2/2/2
23	5MU	AY	54	23	-	0/5/25/26	0/2/2/2
23	4SU	CW	8	56,23	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	7MG	CY	46	23	-	2/7/37/38	0/3/3/3
23	PSU	AW	32	56,23	-	0/7/25/26	0/2/2/2
23	PSU	AY	55	23	-	1/7/25/26	0/2/2/2
23	MIA	CY	37	23	-	3/3/25/34	0/3/3/3

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C2-S10	-7.27	1.69	1.75
23	AW	37	MIA	C13-C14	7.14	1.52	1.32
23	AY	46	7MG	C5-C4	5.02	1.49	1.39
23	AW	46	7MG	C6-C5	5.02	1.48	1.41
24	AX	55	PSU	C5-C1'	-5.00	1.48	1.52

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	CW	39	PSU	N1-C2-N3	-9.98	120.50	128.43
23	AY	39	PSU	N1-C2-N3	-9.84	120.61	128.43
24	AX	8	4SU	C2-N3-C4	9.74	129.28	115.15
23	AY	46	7MG	N3-C4-N9	9.48	139.09	126.91
23	AW	46	7MG	N3-C4-N9	9.38	138.96	126.91

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	CY	54	5MU	C2'-C1'-N1-C6
23	AW	37	MIA	C12-C13-C14-C16
23	AY	8	4SU	C2'-C1'-N1-C6
23	CY	8	4SU	O4'-C4'-C5'-O5'
23	CY	39	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

19 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AX	8	4SU	2	0
23	AW	37	MIA	1	0
23	CW	46	7MG	5	0

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2152 ligands modelled in this entry, 2148 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	PCY	AA	3231	-	36,42,42	1.68	5 (13%)	41,65,65	1.42	8 (19%)
57	PCY	CA	3178	-	36,42,42	1.63	4 (11%)	41,65,65	1.17	4 (9%)
58	SF4	CD	501	4	0,12,12	0.00	-	-		
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
57	PCY	AA	3231	-	-	5/33/67/67	0/3/3/3
57	PCY	CA	3178	-	-	9/33/67/67	0/3/3/3
58	SF4	CD	501	4	-	-	0/6/5/5
58	SF4	AD	501	4	-	-	0/6/5/5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	CA	3178	PCY	C28-C32	-5.59	1.39	1.49
57	AA	3231	PCY	C28-C32	-5.44	1.39	1.49
57	AA	3231	PCY	C34-C30	-5.24	1.40	1.51
57	CA	3178	PCY	C34-C30	-5.21	1.40	1.51
57	AA	3231	PCY	C27-C23	-4.06	1.40	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	AA	3231	PCY	C18-O21-C23	-4.75	107.00	116.57
57	CA	3178	PCY	C18-O21-C23	-3.62	109.27	116.57
57	AA	3231	PCY	O21-C23-C27	3.01	119.12	112.33
57	AA	3231	PCY	O21-C18-C15	2.78	112.92	107.79
57	AA	3231	PCY	O36-C31-C27	-2.26	116.91	121.14

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

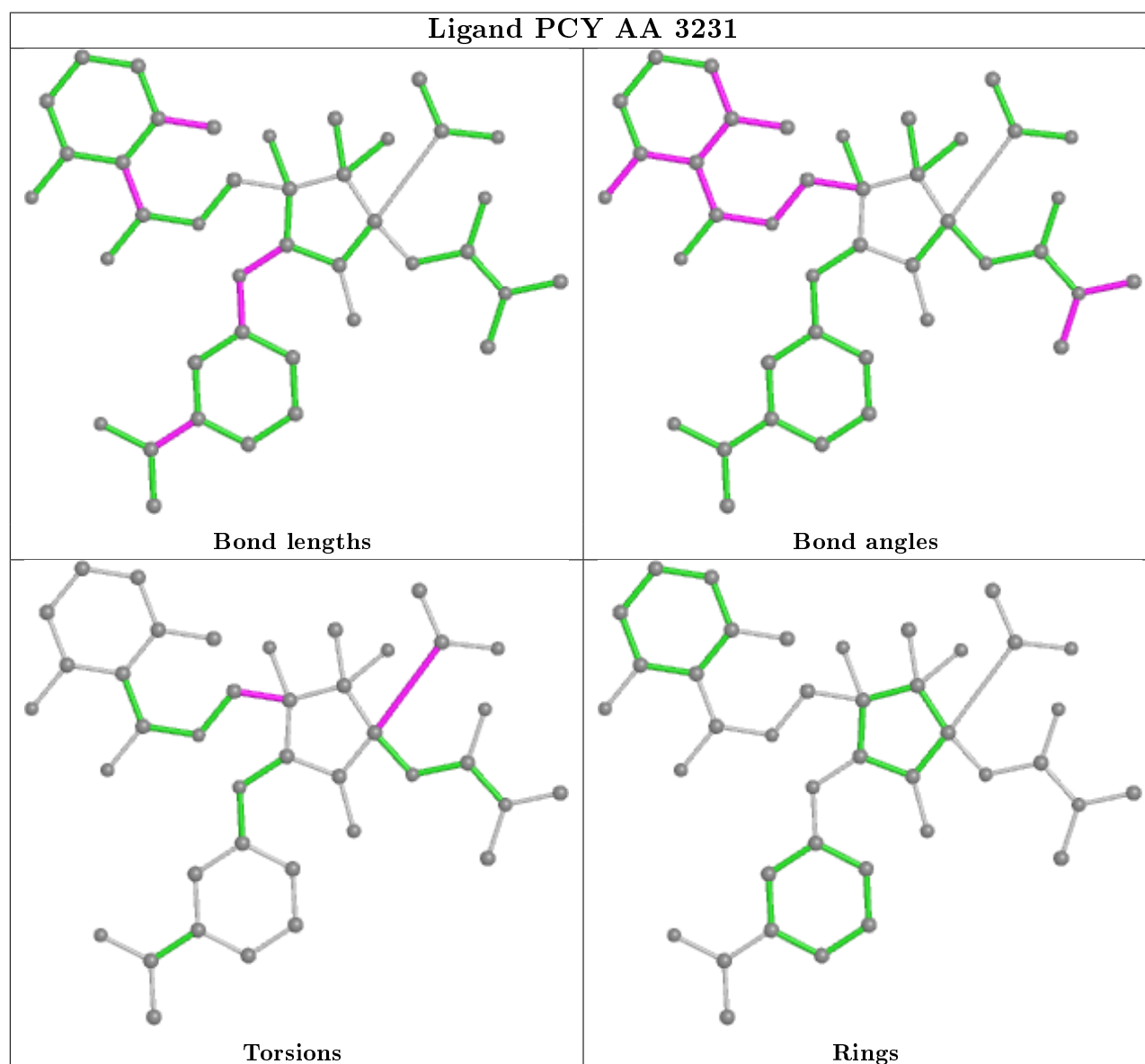
Mol	Chain	Res	Type	Atoms
57	AA	3231	PCY	N2-C3-C6-C11
57	AA	3231	PCY	C7-C3-C6-C11
57	AA	3231	PCY	C7-C15-C18-O21
57	AA	3231	PCY	C17-C15-C18-O21
57	AA	3231	PCY	O19-C15-C18-O21

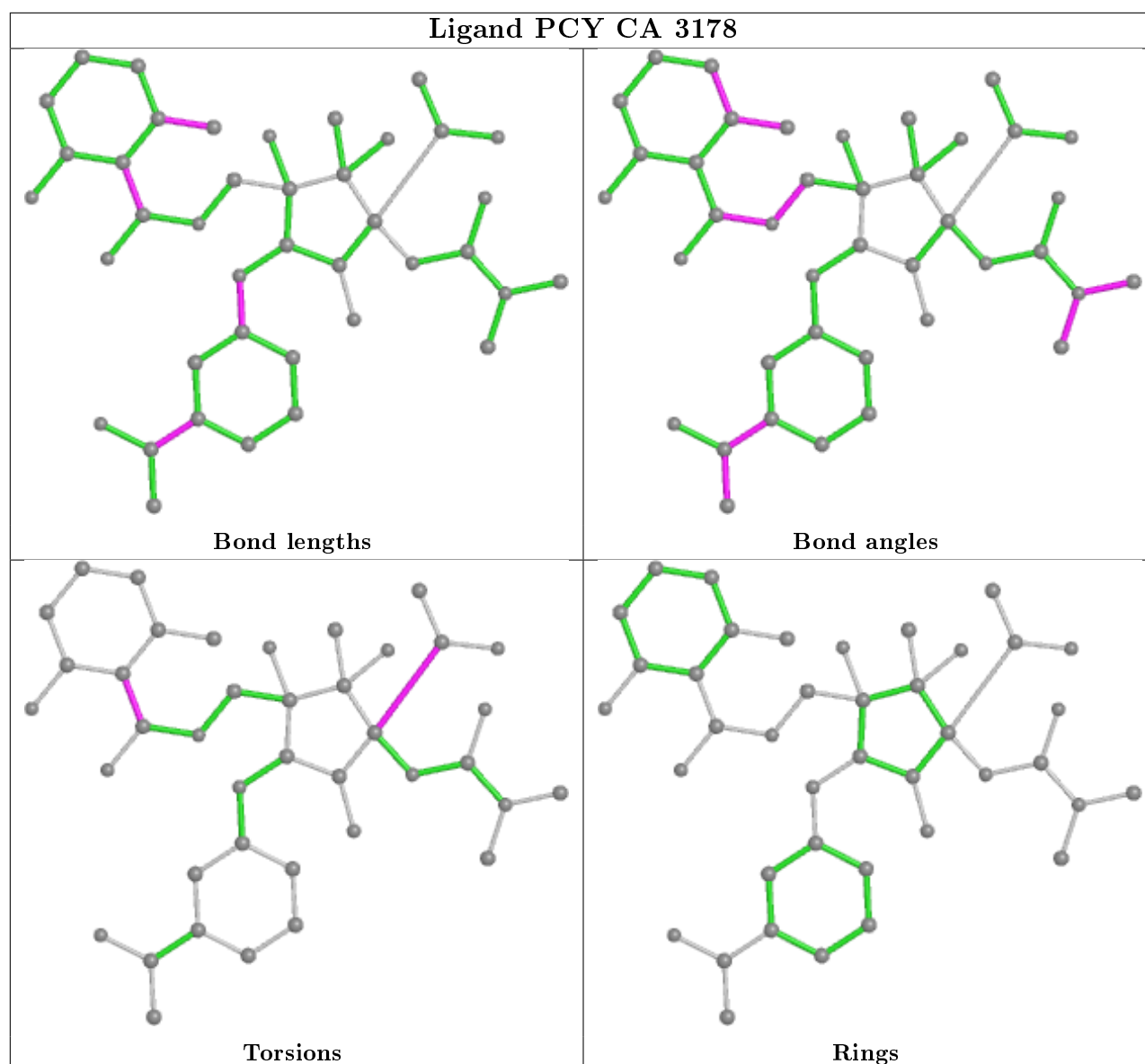
There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	AA	3231	PCY	7	0
57	CA	3178	PCY	9	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1498/1521 (98%)	0.22	56 (3%) 41 48	40, 67, 92, 106	0
1	CA	1503/1521 (98%)	0.11	52 (3%) 44 51	43, 69, 92, 106	0
2	AB	231/256 (90%)	1.20	44 (19%) 1 1	63, 80, 90, 94	0
2	CB	231/256 (90%)	1.47	68 (29%) 0 0	64, 82, 89, 96	0
3	AC	206/239 (86%)	1.09	30 (14%) 2 3	61, 74, 84, 92	0
3	CC	206/239 (86%)	1.76	83 (40%) 0 0	64, 76, 86, 92	0
4	AD	208/209 (99%)	0.47	6 (2%) 51 59	56, 68, 79, 87	0
4	CD	208/209 (99%)	1.06	29 (13%) 2 3	57, 68, 78, 87	0
5	AE	148/162 (91%)	0.78	9 (6%) 21 25	56, 67, 77, 91	0
5	CE	148/162 (91%)	0.89	17 (11%) 4 6	57, 69, 79, 92	0
6	AF	100/101 (99%)	0.40	1 (1%) 82 86	53, 66, 76, 82	0
6	CF	100/101 (99%)	0.30	1 (1%) 82 86	54, 66, 76, 82	0
7	AG	155/156 (99%)	0.86	16 (10%) 6 8	61, 71, 83, 93	0
7	CG	155/156 (99%)	0.94	15 (9%) 7 9	62, 73, 84, 96	0
8	AH	137/138 (99%)	0.81	12 (8%) 10 11	57, 69, 75, 83	0
8	CH	137/138 (99%)	1.05	19 (13%) 2 3	59, 71, 77, 84	0
9	AI	127/128 (99%)	1.50	33 (25%) 0 0	56, 78, 85, 90	0
9	CI	127/128 (99%)	2.04	57 (44%) 0 0	62, 79, 86, 89	0
10	AJ	97/105 (92%)	1.46	29 (29%) 0 0	57, 78, 90, 91	0
10	CJ	96/105 (91%)	1.85	39 (40%) 0 0	60, 80, 91, 93	0
11	AK	114/129 (88%)	0.88	9 (7%) 12 16	47, 67, 80, 83	0
11	CK	114/129 (88%)	0.39	2 (1%) 68 74	47, 67, 79, 83	0
12	AL	122/132 (92%)	0.52	2 (1%) 72 78	42, 56, 69, 75	0
12	CL	122/132 (92%)	0.94	16 (13%) 3 4	45, 58, 71, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	123/126 (97%)	0.57	6 (4%) 29 35	42, 63, 75, 80	0
13	CM	122/126 (96%)	1.59	42 (34%) 0 0	66, 79, 86, 90	0
14	AN	60/61 (98%)	1.13	8 (13%) 3 4	60, 70, 77, 81	0
14	CN	60/61 (98%)	2.77	43 (71%) 0 0	64, 73, 80, 83	0
15	AO	88/89 (98%)	0.34	2 (2%) 60 67	50, 66, 76, 82	0
15	CO	88/89 (98%)	0.56	2 (2%) 60 67	53, 68, 77, 82	0
16	AP	82/88 (93%)	1.03	11 (13%) 3 4	52, 68, 76, 80	0
16	CP	82/88 (93%)	1.08	12 (14%) 2 3	51, 68, 76, 79	0
17	AQ	99/105 (94%)	0.66	4 (4%) 38 45	55, 68, 77, 79	0
17	CQ	99/105 (94%)	1.53	32 (32%) 0 0	57, 69, 77, 80	0
18	AR	68/88 (77%)	0.80	5 (7%) 14 18	58, 66, 76, 80	0
18	CR	68/88 (77%)	0.53	3 (4%) 34 41	59, 68, 77, 80	0
19	AS	83/93 (89%)	0.81	4 (4%) 30 37	63, 73, 81, 91	0
19	CS	83/93 (89%)	1.99	38 (45%) 0 0	66, 76, 84, 92	0
20	AT	96/106 (90%)	1.72	38 (39%) 0 0	57, 68, 80, 86	0
20	CT	96/106 (90%)	1.69	39 (40%) 0 0	58, 68, 82, 87	0
21	AU	23/27 (85%)	1.29	4 (17%) 1 1	63, 66, 72, 75	0
21	CU	23/27 (85%)	1.58	9 (39%) 0 0	65, 68, 74, 77	0
22	AV	13/24 (54%)	0.99	1 (7%) 13 17	52, 64, 82, 98	0
22	CV	13/24 (54%)	0.49	2 (15%) 2 2	56, 67, 85, 99	0
23	AW	67/76 (88%)	1.00	7 (10%) 6 8	47, 84, 97, 104	0
23	AY	67/76 (88%)	1.04	10 (14%) 2 2	38, 97, 101, 104	0
23	CW	65/76 (85%)	0.97	11 (16%) 1 1	68, 91, 102, 104	0
23	CY	66/76 (86%)	1.54	26 (39%) 0 0	43, 97, 101, 104	0
24	AX	72/77 (93%)	0.57	2 (2%) 53 60	39, 68, 85, 93	0
24	CX	72/77 (93%)	-0.04	0 100 100	43, 71, 86, 94	0
25	BA	2819/2915 (96%)	0.43	64 (2%) 60 67	23, 42, 88, 104	0
25	DA	2800/2915 (96%)	-0.09	84 (3%) 50 57	27, 47, 89, 108	0
26	BB	120/121 (99%)	-0.04	0 100 100	35, 56, 70, 86	0
26	DB	120/121 (99%)	-0.03	0 100 100	42, 62, 73, 87	0
27	BD	275/276 (99%)	0.72	3 (1%) 80 85	23, 40, 55, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DD	275/276 (99%)	0.40	3 (1%) 80 85	26, 42, 56, 77	0
28	BE	204/206 (99%)	0.67	3 (1%) 73 79	22, 47, 66, 76	0
28	DE	204/206 (99%)	0.21	3 (1%) 73 79	28, 50, 67, 77	0
29	BF	203/210 (96%)	0.72	12 (5%) 22 26	23, 49, 73, 88	0
29	DF	203/210 (96%)	0.81	25 (12%) 4 5	27, 55, 75, 88	0
30	BG	181/182 (99%)	0.50	10 (5%) 25 30	44, 64, 78, 90	0
30	DG	181/182 (99%)	1.27	41 (22%) 0 0	50, 67, 80, 90	0
31	BH	174/180 (96%)	0.43	3 (1%) 70 76	51, 65, 76, 85	0
31	DH	174/180 (96%)	2.63	106 (60%) 0 0	57, 70, 80, 86	0
32	BI	146/148 (98%)	0.90	16 (10%) 5 7	50, 71, 82, 86	0
32	DI	146/148 (98%)	0.48	8 (5%) 25 30	53, 71, 82, 85	0
33	BN	140/140 (100%)	0.53	1 (0%) 87 90	32, 47, 68, 75	0
33	DN	140/140 (100%)	0.65	6 (4%) 35 42	36, 52, 70, 77	0
34	BO	122/122 (100%)	0.35	0 100 100	25, 38, 59, 65	0
34	DO	122/122 (100%)	0.49	0 100 100	47, 59, 74, 79	0
35	BP	149/150 (99%)	0.46	1 (0%) 87 90	24, 55, 74, 81	0
35	DP	149/150 (99%)	0.87	24 (16%) 1 2	29, 59, 76, 82	0
36	BQ	141/141 (100%)	0.77	3 (2%) 63 70	31, 50, 66, 77	0
36	DQ	141/141 (100%)	0.85	18 (12%) 3 4	38, 54, 69, 80	0
37	BR	118/118 (100%)	0.28	0 100 100	21, 32, 50, 58	0
37	DR	118/118 (100%)	0.24	0 100 100	38, 53, 64, 74	0
38	BS	110/112 (98%)	0.44	1 (0%) 84 88	32, 48, 64, 67	0
38	DS	110/112 (98%)	1.47	29 (26%) 0 0	58, 69, 80, 85	0
39	BT	131/146 (89%)	0.20	1 (0%) 86 89	31, 42, 68, 89	0
39	DT	131/146 (89%)	0.29	1 (0%) 86 89	51, 64, 78, 84	0
40	BU	116/118 (98%)	0.26	0 100 100	17, 28, 47, 65	0
40	DU	116/118 (98%)	0.55	7 (6%) 21 25	40, 62, 76, 82	0
41	BV	101/101 (100%)	0.15	0 100 100	15, 35, 54, 67	0
41	DV	101/101 (100%)	1.02	17 (16%) 1 1	39, 74, 81, 88	0
42	BW	112/113 (99%)	0.32	1 (0%) 84 88	17, 28, 53, 79	0
42	DW	112/113 (99%)	0.55	1 (0%) 84 88	38, 51, 68, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BX	95/96 (98%)	0.32	1 (1%) 80 85	21, 35, 60, 75	0
43	DX	95/96 (98%)	0.99	11 (11%) 4 6	38, 56, 76, 85	0
44	BY	107/110 (97%)	0.20	2 (1%) 66 73	30, 46, 65, 83	0
44	DY	107/110 (97%)	1.34	28 (26%) 0 0	57, 71, 83, 86	0
45	BZ	171/206 (83%)	1.66	43 (25%) 0 0	35, 67, 94, 105	0
45	DZ	174/206 (84%)	2.79	87 (50%) 0 0	65, 83, 97, 103	0
46	B0	83/85 (97%)	0.42	4 (4%) 30 37	20, 36, 57, 76	0
46	D0	83/85 (97%)	1.09	12 (14%) 2 3	44, 64, 74, 79	0
47	B1	97/98 (98%)	0.49	3 (3%) 49 56	24, 45, 70, 73	0
47	D1	97/98 (98%)	0.68	5 (5%) 27 32	37, 56, 75, 86	0
48	B2	70/72 (97%)	0.46	1 (1%) 75 81	30, 45, 58, 78	0
48	D2	70/72 (97%)	0.58	2 (2%) 51 59	53, 66, 78, 82	0
49	B3	59/60 (98%)	0.18	0 100 100	19, 31, 58, 75	0
49	D3	59/60 (98%)	0.85	7 (11%) 4 5	54, 66, 78, 88	0
50	B4	69/71 (97%)	0.60	8 (11%) 4 6	51, 70, 89, 99	0
50	D4	69/71 (97%)	2.02	33 (47%) 0 0	72, 82, 92, 93	0
51	B5	59/60 (98%)	0.36	1 (1%) 70 76	17, 27, 43, 54	0
51	D5	59/60 (98%)	0.38	1 (1%) 70 76	35, 50, 66, 74	0
52	B6	53/54 (98%)	0.18	0 100 100	28, 39, 56, 67	0
52	D6	53/54 (98%)	0.70	4 (7%) 14 17	48, 59, 71, 76	0
53	B7	48/49 (97%)	0.62	2 (4%) 36 42	18, 26, 62, 72	0
53	D7	48/49 (97%)	0.90	3 (6%) 20 23	30, 41, 61, 78	0
54	B8	64/65 (98%)	0.19	0 100 100	19, 31, 40, 63	0
54	D8	64/65 (98%)	0.77	2 (3%) 49 56	44, 54, 65, 71	0
55	B9	37/37 (100%)	0.61	1 (2%) 54 61	26, 47, 63, 70	0
55	D9	37/37 (100%)	1.30	7 (18%) 1 1	45, 57, 68, 75	0
All	All	20900/21748 (96%)	0.58	1766 (8%) 11 13	15, 61, 87, 108	0

The worst 5 of 1766 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	BZ	108	PRO	15.6
45	DZ	116	VAL	13.2

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Mol	Chain	Res	Type	RSRZ
45	DZ	115	GLY	12.4
45	DZ	107	THR	11.0
45	DZ	114	GLY	11.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	MIA	CY	37	22/30	0.68	0.33	82,93,117,140	0
23	PSU	AY	55	20/21	0.69	0.28	93,99,105,118	0
23	5MU	CY	54	21/22	0.69	0.40	78,92,113,136	0
23	4SU	CY	8	20/21	0.70	0.19	83,99,114,124	0
23	7MG	AY	46	24/25	0.72	0.24	80,94,107,121	0
23	4SU	CW	8	20/21	0.75	0.24	88,94,105,122	0
23	7MG	CY	46	24/25	0.77	0.18	86,95,102,125	0
23	PSU	CY	32	20/21	0.79	0.20	83,92,99,105	0
23	7MG	CW	46	24/25	0.80	0.30	85,98,110,126	0
23	5MU	AY	54	21/22	0.81	0.23	81,91,102,125	0
23	4SU	AY	8	20/21	0.82	0.20	92,98,108,126	0
23	MIA	AY	37	22/30	0.82	0.25	72,87,104,128	0
23	PSU	CW	55	20/21	0.83	0.20	61,83,94,94	0
23	PSU	CY	55	20/21	0.83	0.29	92,98,105,119	0
23	7MG	AW	46	24/25	0.83	0.22	70,83,111,120	0
23	PSU	AY	32	20/21	0.85	0.24	83,91,98,100	0
23	PSU	CY	39	20/21	0.87	0.19	80,88,99,111	0
23	5MU	CW	54	21/22	0.90	0.17	60,72,84,86	0
23	PSU	AY	39	20/21	0.90	0.21	77,86,97,100	0
24	PSU	CX	55	20/21	0.90	0.16	63,69,89,97	0
23	PSU	CW	32	20/21	0.90	0.19	70,85,92,95	0
23	4SU	AW	8	20/21	0.91	0.17	73,85,96,105	0
23	MIA	CW	37	22/30	0.91	0.16	55,66,75,81	0
24	5MU	CX	54	21/22	0.92	0.23	71,80,88,94	0
24	4SU	CX	8	20/21	0.93	0.17	54,78,85,86	0
23	PSU	AW	55	20/21	0.93	0.20	50,70,80,81	0
24	5MU	AX	54	21/22	0.94	0.18	58,65,74,81	0
24	PSU	AX	55	20/21	0.94	0.18	60,67,93,94	0
23	PSU	AW	32	20/21	0.95	0.16	50,60,69,69	0
23	5MU	AW	54	21/22	0.95	0.16	42,58,69,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	5MC	CX	32	21/22	0.95	0.16	66,71,81,83	0
23	PSU	CW	39	20/21	0.96	0.17	63,72,81,82	0
23	PSU	AW	39	20/21	0.96	0.20	49,59,65,65	0
24	4SU	AX	8	20/21	0.96	0.18	51,64,80,88	0
23	MIA	AW	37	29/30	0.96	0.21	40,49,63,75	0
24	5MC	AX	32	21/22	0.97	0.19	48,54,58,72	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3571	1/1	0.29	0.10	66,66,66,66	0
56	MG	DA	3565	1/1	0.51	0.18	70,70,70,70	0
56	MG	CJ	5001	1/1	0.53	0.14	76,76,76,76	0
56	MG	AA	3192	1/1	0.56	0.30	69,69,69,69	0
56	MG	AA	3098	1/1	0.57	0.17	68,68,68,68	0
56	MG	DA	3419	1/1	0.59	0.17	44,44,44,44	0
56	MG	BA	3224	1/1	0.60	0.18	64,64,64,64	0
56	MG	BA	3677	1/1	0.61	0.12	62,62,62,62	0
56	MG	DA	3182	1/1	0.63	0.30	64,64,64,64	0
56	MG	BA	3712	1/1	0.63	0.13	64,64,64,64	0
56	MG	DA	3241	1/1	0.64	0.20	50,50,50,50	0
56	MG	CA	3051	1/1	0.64	0.11	66,66,66,66	0
56	MG	BA	3683	1/1	0.64	0.15	61,61,61,61	0
56	MG	DB	3005	1/1	0.65	0.28	64,64,64,64	0
56	MG	DA	3596	1/1	0.65	0.44	63,63,63,63	0
56	MG	BA	3726	1/1	0.65	0.23	70,70,70,70	0
56	MG	DA	3109	1/1	0.65	0.20	66,66,66,66	0
56	MG	AA	3110	1/1	0.66	0.22	61,61,61,61	0
56	MG	BA	3804	1/1	0.66	0.10	58,58,58,58	0
56	MG	CA	3064	1/1	0.67	0.11	57,57,57,57	0
56	MG	DA	3607	1/1	0.68	0.34	53,53,53,53	0
56	MG	DA	3505	1/1	0.68	0.12	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3051	1/1	0.68	0.20	56,56,56,56	0
56	MG	BR	202	1/1	0.68	0.41	53,53,53,53	0
56	MG	BA	3527	1/1	0.68	0.11	52,52,52,52	0
56	MG	DA	3504	1/1	0.69	0.13	60,60,60,60	0
56	MG	BA	3725	1/1	0.69	0.22	67,67,67,67	0
56	MG	BA	3446	1/1	0.70	0.27	52,52,52,52	0
56	MG	AX	3003	1/1	0.70	0.16	66,66,66,66	0
56	MG	BA	3249	1/1	0.70	0.29	74,74,74,74	0
56	MG	BA	3639	1/1	0.70	0.29	59,59,59,59	0
56	MG	CX	3006	1/1	0.70	0.50	70,70,70,70	0
56	MG	BA	3728	1/1	0.70	0.10	72,72,72,72	0
56	MG	CA	3049	1/1	0.70	0.23	68,68,68,68	0
56	MG	CA	3027	1/1	0.71	0.51	70,70,70,70	0
56	MG	BA	3431	1/1	0.71	0.27	55,55,55,55	0
56	MG	BA	3030	1/1	0.71	0.19	50,50,50,50	0
56	MG	BA	3470	1/1	0.72	0.16	48,48,48,48	0
56	MG	BA	3079	1/1	0.72	0.32	57,57,57,57	0
56	MG	BA	3734	1/1	0.72	0.35	60,60,60,60	0
56	MG	AA	3082	1/1	0.72	0.26	68,68,68,68	0
56	MG	DA	3041	1/1	0.72	0.18	55,55,55,55	0
56	MG	DA	3466	1/1	0.72	0.17	62,62,62,62	0
56	MG	DA	3448	1/1	0.73	0.14	41,41,41,41	0
56	MG	BA	3807	1/1	0.73	0.11	67,67,67,67	0
56	MG	DA	3538	1/1	0.73	0.27	56,56,56,56	0
56	MG	DA	3098	1/1	0.73	0.21	43,43,43,43	0
56	MG	DA	3541	1/1	0.73	0.08	54,54,54,54	0
56	MG	B8	101	1/1	0.73	0.14	42,42,42,42	0
56	MG	DA	3238	1/1	0.73	0.24	61,61,61,61	0
56	MG	AA	3095	1/1	0.73	0.28	68,68,68,68	0
56	MG	AA	3204	1/1	0.73	0.19	71,71,71,71	0
56	MG	AA	3004	1/1	0.73	0.14	67,67,67,67	0
56	MG	BA	3434	1/1	0.74	0.20	34,34,34,34	0
56	MG	DA	3028	1/1	0.74	0.17	70,70,70,70	0
56	MG	BA	3221	1/1	0.74	0.20	54,54,54,54	0
56	MG	BA	3605	1/1	0.74	0.13	61,61,61,61	0
56	MG	BA	3333	1/1	0.74	0.11	61,61,61,61	0
56	MG	DA	3312	1/1	0.74	0.14	52,52,52,52	0
56	MG	BA	3689	1/1	0.75	0.22	57,57,57,57	0
56	MG	BA	3020	1/1	0.75	0.20	61,61,61,61	0
56	MG	DA	3452	1/1	0.75	0.24	61,61,61,61	0
56	MG	DA	3066	1/1	0.75	0.13	65,65,65,65	0
56	MG	DA	3251	1/1	0.75	0.27	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BB	3015	1/1	0.75	0.10	51,51,51,51	0
56	MG	BA	3560	1/1	0.75	0.23	35,35,35,35	0
56	MG	CA	3055	1/1	0.76	0.12	53,53,53,53	0
56	MG	AA	3038	1/1	0.76	0.14	51,51,51,51	0
56	MG	DA	3521	1/1	0.76	0.17	51,51,51,51	0
56	MG	DA	3209	1/1	0.76	0.24	52,52,52,52	0
56	MG	BA	3315	1/1	0.76	0.14	56,56,56,56	0
56	MG	DA	3632	1/1	0.76	0.16	58,58,58,58	0
56	MG	DA	3436	1/1	0.77	0.13	54,54,54,54	0
56	MG	DA	3286	1/1	0.77	0.14	64,64,64,64	0
56	MG	BA	3663	1/1	0.77	0.14	50,50,50,50	0
56	MG	AA	3042	1/1	0.77	0.21	57,57,57,57	0
56	MG	CA	3069	1/1	0.77	0.12	68,68,68,68	0
56	MG	DA	3604	1/1	0.77	0.13	57,57,57,57	0
56	MG	CA	3025	1/1	0.77	0.14	61,61,61,61	0
56	MG	BA	3229	1/1	0.78	0.31	51,51,51,51	0
56	MG	BA	3204	1/1	0.78	0.33	66,66,66,66	0
56	MG	DA	3404	1/1	0.78	0.20	51,51,51,51	0
56	MG	DA	3542	1/1	0.78	0.20	63,63,63,63	0
56	MG	DW	3002	1/1	0.78	0.39	65,65,65,65	0
56	MG	DA	3487	1/1	0.78	0.24	65,65,65,65	0
56	MG	BA	3241	1/1	0.78	0.22	52,52,52,52	0
56	MG	DA	3199	1/1	0.78	0.41	52,52,52,52	0
56	MG	BA	3377	1/1	0.78	0.23	30,30,30,30	0
56	MG	DA	3445	1/1	0.78	0.23	72,72,72,72	0
56	MG	DA	3614	1/1	0.78	0.14	50,50,50,50	0
56	MG	AW	3001	1/1	0.78	0.09	55,55,55,55	0
56	MG	DA	3127	1/1	0.78	0.27	38,38,38,38	0
56	MG	DA	3605	1/1	0.79	0.15	52,52,52,52	0
56	MG	AA	3114	1/1	0.79	0.34	51,51,51,51	0
56	MG	AA	3072	1/1	0.79	0.19	68,68,68,68	0
56	MG	BA	3699	1/1	0.79	0.18	42,42,42,42	0
56	MG	CA	3026	1/1	0.79	0.29	64,64,64,64	0
56	MG	CA	3169	1/1	0.79	0.21	65,65,65,65	0
56	MG	BA	3162	1/1	0.79	0.26	46,46,46,46	0
56	MG	BB	3009	1/1	0.79	0.27	58,58,58,58	0
56	MG	DA	3325	1/1	0.79	0.25	57,57,57,57	0
56	MG	DA	3547	1/1	0.79	0.17	65,65,65,65	0
56	MG	B1	102	1/1	0.79	0.41	68,68,68,68	0
56	MG	BA	3367	1/1	0.79	0.33	53,53,53,53	0
56	MG	DA	3508	1/1	0.79	0.10	59,59,59,59	0
56	MG	BA	3347	1/1	0.79	0.26	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3224	1/1	0.79	0.35	48,48,48,48	0
56	MG	DA	3105	1/1	0.79	0.19	60,60,60,60	0
56	MG	BA	3028	1/1	0.79	0.14	59,59,59,59	0
56	MG	CA	3065	1/1	0.79	0.07	65,65,65,65	0
56	MG	BA	3720	1/1	0.79	0.23	46,46,46,46	0
56	MG	DA	3645	1/1	0.80	0.20	44,44,44,44	0
56	MG	AA	3040	1/1	0.80	0.16	59,59,59,59	0
56	MG	CA	3020	1/1	0.80	0.13	73,73,73,73	0
56	MG	BA	3585	1/1	0.80	0.39	55,55,55,55	0
56	MG	DA	3509	1/1	0.80	0.18	53,53,53,53	0
56	MG	BA	3277	1/1	0.80	0.19	54,54,54,54	0
56	MG	BQ	3005	1/1	0.80	0.30	50,50,50,50	0
56	MG	AA	3091	1/1	0.80	0.10	70,70,70,70	0
56	MG	BA	3095	1/1	0.80	0.30	53,53,53,53	0
56	MG	BA	3583	1/1	0.80	0.12	45,45,45,45	0
56	MG	CA	3061	1/1	0.80	0.22	56,56,56,56	0
56	MG	AW	3002	1/1	0.80	0.17	69,69,69,69	0
56	MG	CA	3034	1/1	0.80	0.13	61,61,61,61	0
56	MG	DA	3170	1/1	0.80	0.09	50,50,50,50	0
56	MG	DA	3513	1/1	0.80	0.17	50,50,50,50	0
56	MG	BA	3595	1/1	0.80	0.21	32,32,32,32	0
56	MG	BA	3070	1/1	0.80	0.26	55,55,55,55	0
56	MG	BA	3516	1/1	0.81	0.22	65,65,65,65	0
56	MG	DA	3309	1/1	0.81	0.14	42,42,42,42	0
56	MG	DA	3213	1/1	0.81	0.23	61,61,61,61	0
56	MG	BA	3831	1/1	0.81	0.95	52,52,52,52	0
56	MG	BA	3409	1/1	0.81	0.23	62,62,62,62	0
56	MG	DA	3037	1/1	0.81	0.16	54,54,54,54	0
56	MG	AA	3062	1/1	0.81	0.14	60,60,60,60	0
56	MG	AA	3153	1/1	0.81	0.18	55,55,55,55	0
56	MG	DA	3121	1/1	0.81	0.28	41,41,41,41	0
56	MG	DA	3540	1/1	0.81	0.18	67,67,67,67	0
56	MG	DA	3566	1/1	0.81	0.17	48,48,48,48	0
56	MG	DA	3115	1/1	0.81	0.18	41,41,41,41	0
56	MG	DA	3393	1/1	0.81	0.10	52,52,52,52	0
56	MG	BB	3011	1/1	0.81	0.06	59,59,59,59	0
56	MG	BA	3472	1/1	0.81	0.23	70,70,70,70	0
56	MG	AA	3087	1/1	0.81	0.34	52,52,52,52	0
56	MG	BA	3022	1/1	0.81	0.26	40,40,40,40	0
56	MG	DA	3468	1/1	0.81	0.20	44,44,44,44	0
56	MG	CA	3070	1/1	0.81	0.14	71,71,71,71	0
56	MG	BA	3317	1/1	0.82	0.19	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3081	1/1	0.82	0.18	58,58,58,58	0
56	MG	BA	3101	1/1	0.82	0.25	60,60,60,60	0
56	MG	BA	3413	1/1	0.82	0.19	41,41,41,41	0
56	MG	DA	3429	1/1	0.82	0.26	40,40,40,40	0
56	MG	AA	3068	1/1	0.82	0.17	60,60,60,60	0
56	MG	BA	3603	1/1	0.82	0.11	54,54,54,54	0
56	MG	CA	3122	1/1	0.82	0.15	70,70,70,70	0
56	MG	DA	3305	1/1	0.82	0.18	28,28,28,28	0
56	MG	DA	3214	1/1	0.82	0.34	47,47,47,47	0
56	MG	AA	3190	1/1	0.82	0.11	65,65,65,65	0
56	MG	BA	3408	1/1	0.82	0.20	55,55,55,55	0
56	MG	DA	3568	1/1	0.82	0.12	54,54,54,54	0
56	MG	BA	3590	1/1	0.82	0.23	32,32,32,32	0
56	MG	AA	3145	1/1	0.82	0.16	58,58,58,58	0
56	MG	AA	3125	1/1	0.82	0.11	71,71,71,71	0
56	MG	DA	3493	1/1	0.82	0.27	58,58,58,58	0
56	MG	BA	3005	1/1	0.82	0.21	51,51,51,51	0
56	MG	BR	203	1/1	0.82	0.20	44,44,44,44	0
56	MG	DA	3583	1/1	0.82	0.25	60,60,60,60	0
56	MG	BB	3008	1/1	0.83	0.30	54,54,54,54	0
56	MG	CX	3002	1/1	0.83	0.20	81,81,81,81	0
56	MG	BA	3289	1/1	0.83	0.26	55,55,55,55	0
56	MG	BA	3064	1/1	0.83	0.36	61,61,61,61	0
56	MG	AA	3170	1/1	0.83	0.13	57,57,57,57	0
56	MG	BA	3659	1/1	0.83	0.27	53,53,53,53	0
56	MG	BA	3442	1/1	0.83	0.11	59,59,59,59	0
56	MG	BA	3295	1/1	0.83	0.26	42,42,42,42	0
56	MG	BA	3553	1/1	0.83	0.16	42,42,42,42	0
56	MG	DA	3078	1/1	0.83	0.11	45,45,45,45	0
56	MG	BA	3002	1/1	0.83	0.37	62,62,62,62	0
56	MG	DA	3620	1/1	0.83	0.17	62,62,62,62	0
56	MG	DA	3234	1/1	0.83	0.19	45,45,45,45	0
56	MG	AA	3073	1/1	0.83	0.24	58,58,58,58	0
56	MG	AA	3175	1/1	0.83	0.20	54,54,54,54	0
56	MG	AA	3085	1/1	0.83	0.15	55,55,55,55	0
56	MG	BA	3705	1/1	0.83	0.17	54,54,54,54	0
56	MG	BQ	3003	1/1	0.83	0.15	54,54,54,54	0
56	MG	DA	3410	1/1	0.83	0.15	62,62,62,62	0
56	MG	CA	3037	1/1	0.83	0.25	55,55,55,55	0
56	MG	BA	3291	1/1	0.83	0.21	71,71,71,71	0
56	MG	CA	3023	1/1	0.83	0.22	55,55,55,55	0
56	MG	BA	3393	1/1	0.83	0.26	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3706	1/1	0.83	0.23	50,50,50,50	0
56	MG	BA	3407	1/1	0.83	0.19	37,37,37,37	0
56	MG	DA	3155	1/1	0.83	0.29	40,40,40,40	0
56	MG	AA	3205	1/1	0.83	0.12	51,51,51,51	0
56	MG	BA	3758	1/1	0.83	0.14	34,34,34,34	0
56	MG	DA	3451	1/1	0.83	0.30	56,56,56,56	0
56	MG	BA	3365	1/1	0.83	0.13	49,49,49,49	0
56	MG	BA	3227	1/1	0.83	0.26	57,57,57,57	0
56	MG	BA	3742	1/1	0.83	0.17	51,51,51,51	0
56	MG	CA	3011	1/1	0.83	0.17	63,63,63,63	0
56	MG	BA	3220	1/1	0.83	0.20	55,55,55,55	0
56	MG	BA	3322	1/1	0.83	0.16	32,32,32,32	0
56	MG	DA	3387	1/1	0.83	0.22	56,56,56,56	0
56	MG	DA	3110	1/1	0.83	0.13	50,50,50,50	0
56	MG	BA	3238	1/1	0.83	0.25	43,43,43,43	0
56	MG	DA	3611	1/1	0.83	0.32	55,55,55,55	0
56	MG	AA	3113	1/1	0.84	0.20	59,59,59,59	0
56	MG	DA	3319	1/1	0.84	0.30	43,43,43,43	0
56	MG	BA	3629	1/1	0.84	0.14	56,56,56,56	0
56	MG	BA	3402	1/1	0.84	0.19	30,30,30,30	0
56	MG	DA	3231	1/1	0.84	0.32	57,57,57,57	0
56	MG	AA	3165	1/1	0.84	0.25	60,60,60,60	0
56	MG	BA	3514	1/1	0.84	0.25	41,41,41,41	0
56	MG	BA	3481	1/1	0.84	0.29	45,45,45,45	0
56	MG	BA	3152	1/1	0.84	0.18	43,43,43,43	0
56	MG	AX	3009	1/1	0.84	0.25	71,71,71,71	0
56	MG	DA	3423	1/1	0.84	0.14	51,51,51,51	0
56	MG	CA	3147	1/1	0.84	0.18	72,72,72,72	0
56	MG	DA	3192	1/1	0.84	0.18	51,51,51,51	0
56	MG	BA	3692	1/1	0.84	0.28	57,57,57,57	0
56	MG	DV	3002	1/1	0.84	0.43	57,57,57,57	0
56	MG	CA	3087	1/1	0.84	0.15	63,63,63,63	0
56	MG	AN	502	1/1	0.84	0.13	52,52,52,52	0
56	MG	DA	3580	1/1	0.84	0.19	64,64,64,64	0
56	MG	BA	3693	1/1	0.84	0.13	70,70,70,70	0
56	MG	CA	3121	1/1	0.84	0.23	75,75,75,75	0
56	MG	DA	3591	1/1	0.84	0.20	56,56,56,56	0
56	MG	BA	3736	1/1	0.84	0.17	56,56,56,56	0
56	MG	CA	3152	1/1	0.84	0.36	79,79,79,79	0
56	MG	BA	3716	1/1	0.84	0.24	54,54,54,54	0
56	MG	BA	3196	1/1	0.84	0.23	51,51,51,51	0
56	MG	BA	3192	1/1	0.84	0.25	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3467	1/1	0.84	0.20	39,39,39,39	0
56	MG	DA	3549	1/1	0.84	0.18	57,57,57,57	0
56	MG	DA	3343	1/1	0.84	0.20	40,40,40,40	0
56	MG	BA	3181	1/1	0.84	0.24	41,41,41,41	0
56	MG	DA	3674	1/1	0.84	0.40	73,73,73,73	0
56	MG	AA	3161	1/1	0.84	0.26	46,46,46,46	0
56	MG	DA	3642	1/1	0.84	0.15	49,49,49,49	0
56	MG	DA	3176	1/1	0.85	0.12	52,52,52,52	0
56	MG	DA	3168	1/1	0.85	0.29	53,53,53,53	0
56	MG	DA	3359	1/1	0.85	0.13	57,57,57,57	0
56	MG	CA	3072	1/1	0.85	0.14	62,62,62,62	0
56	MG	BA	3798	1/1	0.85	0.14	61,61,61,61	0
56	MG	CA	3133	1/1	0.85	0.20	65,65,65,65	0
56	MG	AA	3136	1/1	0.85	0.08	53,53,53,53	0
56	MG	AA	3181	1/1	0.85	0.19	75,75,75,75	0
56	MG	DA	3102	1/1	0.85	0.12	57,57,57,57	0
56	MG	BA	3100	1/1	0.85	0.14	45,45,45,45	0
56	MG	AA	3112	1/1	0.85	0.14	57,57,57,57	0
56	MG	AA	3100	1/1	0.85	0.08	68,68,68,68	0
56	MG	CA	3137	1/1	0.85	0.19	52,52,52,52	0
56	MG	AW	3005	1/1	0.85	0.39	68,68,68,68	0
56	MG	DA	3665	1/1	0.85	0.17	58,58,58,58	0
56	MG	BA	3371	1/1	0.85	0.13	54,54,54,54	0
56	MG	BA	3634	1/1	0.85	0.16	64,64,64,64	0
56	MG	CA	3084	1/1	0.85	0.31	69,69,69,69	0
56	MG	DA	3403	1/1	0.85	0.15	57,57,57,57	0
56	MG	BA	3138	1/1	0.85	0.16	48,48,48,48	0
56	MG	CA	3031	1/1	0.85	0.14	53,53,53,53	0
56	MG	DA	3569	1/1	0.85	0.21	57,57,57,57	0
56	MG	DA	3671	1/1	0.85	0.22	59,59,59,59	0
56	MG	BA	3170	1/1	0.85	0.23	48,48,48,48	0
56	MG	DA	3086	1/1	0.85	0.19	62,62,62,62	0
56	MG	AA	3071	1/1	0.85	0.25	62,62,62,62	0
56	MG	DA	3144	1/1	0.85	0.14	63,63,63,63	0
56	MG	BA	3802	1/1	0.85	0.13	56,56,56,56	0
56	MG	BA	3673	1/1	0.85	0.17	47,47,47,47	0
56	MG	AA	3142	1/1	0.85	0.23	62,62,62,62	0
56	MG	BA	3171	1/1	0.85	0.33	53,53,53,53	0
59	ZN	D4	501	1/1	0.85	0.08	119,119,119,119	0
57	PCY	CA	3178	40/40	0.85	0.35	58,78,89,91	0
56	MG	BA	3225	1/1	0.85	0.35	42,42,42,42	0
56	MG	AA	3226	1/1	0.85	0.26	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3017	1/1	0.85	0.22	50,50,50,50	0
56	MG	AA	3116	1/1	0.85	0.27	61,61,61,61	0
56	MG	DA	3103	1/1	0.85	0.22	50,50,50,50	0
56	MG	AA	3059	1/1	0.85	0.29	59,59,59,59	0
56	MG	AA	3199	1/1	0.85	0.24	59,59,59,59	0
56	MG	CA	3028	1/1	0.86	0.19	60,60,60,60	0
56	MG	BA	3674	1/1	0.86	0.11	47,47,47,47	0
56	MG	DA	3366	1/1	0.86	0.13	50,50,50,50	0
56	MG	CA	3053	1/1	0.86	0.07	74,74,74,74	0
56	MG	DA	3287	1/1	0.86	0.16	47,47,47,47	0
56	MG	CA	3083	1/1	0.86	0.09	58,58,58,58	0
56	MG	AA	3159	1/1	0.86	0.09	59,59,59,59	0
56	MG	CA	3019	1/1	0.86	0.39	58,58,58,58	0
56	MG	BA	3757	1/1	0.86	0.16	25,25,25,25	0
56	MG	DA	3053	1/1	0.86	0.09	45,45,45,45	0
56	MG	BA	3618	1/1	0.86	0.18	63,63,63,63	0
56	MG	BA	3567	1/1	0.86	0.18	50,50,50,50	0
56	MG	CA	3018	1/1	0.86	0.18	45,45,45,45	0
56	MG	BA	3747	1/1	0.86	0.27	42,42,42,42	0
56	MG	DA	3184	1/1	0.86	0.30	49,49,49,49	0
56	MG	DA	3453	1/1	0.86	0.23	45,45,45,45	0
56	MG	DA	3628	1/1	0.86	0.14	56,56,56,56	0
56	MG	CA	3007	1/1	0.86	0.18	69,69,69,69	0
56	MG	BA	3357	1/1	0.86	0.19	46,46,46,46	0
56	MG	DA	3179	1/1	0.86	0.08	46,46,46,46	0
56	MG	BA	3180	1/1	0.86	0.12	58,58,58,58	0
56	MG	DA	3424	1/1	0.86	0.24	63,63,63,63	0
56	MG	DA	3246	1/1	0.86	0.12	39,39,39,39	0
56	MG	BA	3278	1/1	0.86	0.10	55,55,55,55	0
56	MG	BA	3392	1/1	0.86	0.19	46,46,46,46	0
56	MG	DA	3186	1/1	0.86	0.23	40,40,40,40	0
56	MG	BA	3444	1/1	0.86	0.18	48,48,48,48	0
56	MG	BA	3014	1/1	0.86	0.23	33,33,33,33	0
56	MG	BA	3218	1/1	0.86	0.18	44,44,44,44	0
56	MG	BE	307	1/1	0.86	0.20	70,70,70,70	0
56	MG	CA	3005	1/1	0.86	0.10	58,58,58,58	0
56	MG	BA	3203	1/1	0.86	0.15	39,39,39,39	0
56	MG	DA	3397	1/1	0.86	0.17	49,49,49,49	0
56	MG	BA	3748	1/1	0.86	0.17	63,63,63,63	0
56	MG	DA	3002	1/1	0.86	0.17	68,68,68,68	0
56	MG	BA	3197	1/1	0.86	0.31	36,36,36,36	0
56	MG	BA	3311	1/1	0.86	0.20	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3266	1/1	0.86	0.24	64,64,64,64	0
56	MG	DA	3306	1/1	0.86	0.13	42,42,42,42	0
56	MG	CA	3016	1/1	0.86	0.10	61,61,61,61	0
56	MG	DA	3079	1/1	0.86	0.17	48,48,48,48	0
56	MG	DA	3057	1/1	0.86	0.08	47,47,47,47	0
56	MG	BA	3782	1/1	0.86	0.11	51,51,51,51	0
56	MG	AA	3228	1/1	0.86	0.10	68,68,68,68	0
56	MG	BA	3695	1/1	0.86	0.22	48,48,48,48	0
56	MG	BA	3102	1/1	0.86	0.27	54,54,54,54	0
56	MG	AA	3130	1/1	0.86	0.16	43,43,43,43	0
56	MG	CA	3142	1/1	0.86	0.18	61,61,61,61	0
56	MG	DA	3507	1/1	0.86	0.22	60,60,60,60	0
56	MG	DA	3610	1/1	0.86	0.22	48,48,48,48	0
56	MG	BB	3004	1/1	0.86	0.11	47,47,47,47	0
56	MG	DA	3149	1/1	0.86	0.10	48,48,48,48	0
56	MG	AA	3202	1/1	0.86	0.15	57,57,57,57	0
56	MG	BA	3753	1/1	0.86	0.29	44,44,44,44	0
56	MG	BA	3670	1/1	0.86	0.20	47,47,47,47	0
56	MG	DA	3615	1/1	0.86	0.33	47,47,47,47	0
56	MG	DA	3106	1/1	0.86	0.27	61,61,61,61	0
56	MG	CA	3059	1/1	0.86	0.42	67,67,67,67	0
56	MG	BA	3637	1/1	0.86	0.20	59,59,59,59	0
56	MG	AA	3003	1/1	0.86	0.16	66,66,66,66	0
56	MG	BB	3019	1/1	0.86	0.16	49,49,49,49	0
56	MG	BA	3298	1/1	0.86	0.18	68,68,68,68	0
56	MG	CA	3054	1/1	0.86	0.16	71,71,71,71	0
56	MG	AX	3002	1/1	0.86	0.24	53,53,53,53	0
56	MG	DA	3085	1/1	0.86	0.19	52,52,52,52	0
56	MG	DA	3321	1/1	0.86	0.27	35,35,35,35	0
56	MG	BA	3717	1/1	0.86	0.19	58,58,58,58	0
56	MG	BA	3274	1/1	0.86	0.16	49,49,49,49	0
56	MG	BA	3760	1/1	0.86	0.26	68,68,68,68	0
56	MG	BA	3140	1/1	0.86	0.23	46,46,46,46	0
56	MG	DA	3060	1/1	0.86	0.23	47,47,47,47	0
56	MG	BA	3326	1/1	0.87	0.24	38,38,38,38	0
56	MG	DA	3273	1/1	0.87	0.11	45,45,45,45	0
56	MG	DA	3297	1/1	0.87	0.12	66,66,66,66	0
56	MG	BA	3752	1/1	0.87	0.18	19,19,19,19	0
56	MG	AA	3221	1/1	0.87	0.14	49,49,49,49	0
56	MG	BA	3478	1/1	0.87	0.20	59,59,59,59	0
56	MG	BA	3511	1/1	0.87	0.23	54,54,54,54	0
56	MG	DA	3068	1/1	0.87	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3032	1/1	0.87	0.09	75,75,75,75	0
56	MG	BA	3060	1/1	0.87	0.20	56,56,56,56	0
56	MG	BA	3455	1/1	0.87	0.17	39,39,39,39	0
56	MG	DA	3324	1/1	0.87	0.29	39,39,39,39	0
56	MG	DR	5001	1/1	0.87	0.08	58,58,58,58	0
56	MG	DA	3044	1/1	0.87	0.10	58,58,58,58	0
56	MG	BA	3557	1/1	0.87	0.22	56,56,56,56	0
56	MG	BA	3523	1/1	0.87	0.15	64,64,64,64	0
56	MG	AA	3134	1/1	0.87	0.22	69,69,69,69	0
56	MG	BA	3606	1/1	0.87	0.19	34,34,34,34	0
56	MG	DA	3439	1/1	0.87	0.14	50,50,50,50	0
56	MG	BF	307	1/1	0.87	0.23	39,39,39,39	0
56	MG	DA	3235	1/1	0.87	0.28	61,61,61,61	0
56	MG	BA	3668	1/1	0.87	0.18	56,56,56,56	0
56	MG	BA	3604	1/1	0.87	0.28	72,72,72,72	0
56	MG	BA	3290	1/1	0.87	0.30	58,58,58,58	0
56	MG	DA	3567	1/1	0.87	0.16	46,46,46,46	0
56	MG	BA	3594	1/1	0.87	0.23	24,24,24,24	0
56	MG	DA	3272	1/1	0.87	0.16	44,44,44,44	0
56	MG	BA	3186	1/1	0.87	0.19	51,51,51,51	0
56	MG	BA	3512	1/1	0.87	0.28	27,27,27,27	0
56	MG	BA	3586	1/1	0.87	0.16	65,65,65,65	0
56	MG	BA	3059	1/1	0.87	0.11	55,55,55,55	0
56	MG	BA	3638	1/1	0.87	0.26	38,38,38,38	0
56	MG	DB	3003	1/1	0.87	0.15	68,68,68,68	0
56	MG	BA	3313	1/1	0.87	0.15	46,46,46,46	0
56	MG	BA	3769	1/1	0.87	0.17	56,56,56,56	0
56	MG	AX	3010	1/1	0.87	0.10	62,62,62,62	0
56	MG	BA	3729	1/1	0.87	0.11	52,52,52,52	0
56	MG	DA	3480	1/1	0.87	0.14	48,48,48,48	0
56	MG	DD	303	1/1	0.87	0.25	49,49,49,49	0
56	MG	BA	3113	1/1	0.87	0.32	58,58,58,58	0
56	MG	BA	3435	1/1	0.87	0.16	57,57,57,57	0
56	MG	CA	3060	1/1	0.87	0.24	68,68,68,68	0
56	MG	DA	3623	1/1	0.87	0.15	70,70,70,70	0
56	MG	BA	3133	1/1	0.87	0.30	47,47,47,47	0
56	MG	BW	201	1/1	0.87	0.21	46,46,46,46	0
56	MG	BA	3633	1/1	0.87	0.17	45,45,45,45	0
56	MG	CA	3006	1/1	0.87	0.30	53,53,53,53	0
56	MG	BA	3588	1/1	0.87	0.17	47,47,47,47	0
56	MG	B7	102	1/1	0.87	0.24	58,58,58,58	0
56	MG	BA	3655	1/1	0.87	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DB	3010	1/1	0.87	0.17	55,55,55,55	0
56	MG	AA	3198	1/1	0.87	0.39	70,70,70,70	0
56	MG	DA	3657	1/1	0.87	0.10	67,67,67,67	0
56	MG	DA	3096	1/1	0.87	0.22	51,51,51,51	0
56	MG	BA	3477	1/1	0.87	0.20	55,55,55,55	0
56	MG	DA	3032	1/1	0.87	0.15	40,40,40,40	0
56	MG	BA	3779	1/1	0.87	0.12	59,59,59,59	0
56	MG	BA	3424	1/1	0.87	0.25	24,24,24,24	0
56	MG	BA	3564	1/1	0.88	0.18	41,41,41,41	0
56	MG	BZ	3001	1/1	0.88	0.22	52,52,52,52	0
56	MG	DA	3514	1/1	0.88	0.12	41,41,41,41	0
56	MG	DA	3211	1/1	0.88	0.20	48,48,48,48	0
56	MG	BA	3261	1/1	0.88	0.26	44,44,44,44	0
56	MG	B6	102	1/1	0.88	0.32	55,55,55,55	0
56	MG	CA	3090	1/1	0.88	0.17	62,62,62,62	0
56	MG	D8	5001	1/1	0.88	0.23	55,55,55,55	0
56	MG	BA	3275	1/1	0.88	0.13	46,46,46,46	0
56	MG	CA	3111	1/1	0.88	0.21	61,61,61,61	0
56	MG	DD	302	1/1	0.88	0.23	49,49,49,49	0
56	MG	BA	3690	1/1	0.88	0.21	63,63,63,63	0
56	MG	BA	3574	1/1	0.88	0.12	63,63,63,63	0
56	MG	AA	3047	1/1	0.88	0.09	47,47,47,47	0
56	MG	CA	3132	1/1	0.88	0.37	70,70,70,70	0
56	MG	DA	3197	1/1	0.88	0.15	48,48,48,48	0
56	MG	BA	3179	1/1	0.88	0.19	39,39,39,39	0
56	MG	BA	3439	1/1	0.88	0.17	58,58,58,58	0
56	MG	CA	3010	1/1	0.88	0.12	53,53,53,53	0
56	MG	BA	3672	1/1	0.88	0.21	61,61,61,61	0
56	MG	DA	3437	1/1	0.88	0.25	39,39,39,39	0
56	MG	DA	3201	1/1	0.88	0.23	52,52,52,52	0
56	MG	BA	3708	1/1	0.88	0.24	63,63,63,63	0
56	MG	CA	3177	1/1	0.88	0.21	62,62,62,62	0
56	MG	DA	3194	1/1	0.88	0.23	35,35,35,35	0
56	MG	BB	3012	1/1	0.88	0.08	59,59,59,59	0
56	MG	CA	3172	1/1	0.88	0.15	64,64,64,64	0
56	MG	BA	3254	1/1	0.88	0.16	30,30,30,30	0
56	MG	BA	3127	1/1	0.88	0.17	41,41,41,41	0
56	MG	BA	3320	1/1	0.88	0.30	60,60,60,60	0
56	MG	BA	3770	1/1	0.88	0.30	37,37,37,37	0
56	MG	BA	3679	1/1	0.88	0.23	61,61,61,61	0
56	MG	BA	3451	1/1	0.88	0.11	64,64,64,64	0
56	MG	CA	3173	1/1	0.88	0.08	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3457	1/1	0.88	0.24	47,47,47,47	0
56	MG	BA	3312	1/1	0.88	0.18	33,33,33,33	0
56	MG	BA	3112	1/1	0.88	0.34	57,57,57,57	0
56	MG	BQ	3002	1/1	0.88	0.16	37,37,37,37	0
56	MG	DA	3477	1/1	0.88	0.08	55,55,55,55	0
56	MG	CA	3085	1/1	0.88	0.20	71,71,71,71	0
56	MG	BA	3743	1/1	0.88	0.18	21,21,21,21	0
56	MG	DA	3187	1/1	0.88	0.12	56,56,56,56	0
56	MG	AA	3139	1/1	0.88	0.14	58,58,58,58	0
56	MG	CA	3153	1/1	0.88	0.16	61,61,61,61	0
56	MG	DA	3600	1/1	0.88	0.08	53,53,53,53	0
56	MG	AV	101	1/1	0.88	0.28	59,59,59,59	0
56	MG	BA	3524	1/1	0.88	0.13	53,53,53,53	0
56	MG	B4	502	1/1	0.88	0.12	72,72,72,72	0
56	MG	DA	3408	1/1	0.88	0.22	48,48,48,48	0
56	MG	DA	3248	1/1	0.88	0.31	33,33,33,33	0
56	MG	DB	3004	1/1	0.88	0.15	51,51,51,51	0
56	MG	DA	3434	1/1	0.88	0.46	51,51,51,51	0
56	MG	DA	3222	1/1	0.88	0.18	54,54,54,54	0
56	MG	AA	3011	1/1	0.88	0.20	64,64,64,64	0
56	MG	DA	3145	1/1	0.88	0.32	49,49,49,49	0
56	MG	BA	3205	1/1	0.88	0.24	41,41,41,41	0
56	MG	AA	3155	1/1	0.88	0.18	53,53,53,53	0
56	MG	BA	3264	1/1	0.88	0.29	39,39,39,39	0
56	MG	DA	3495	1/1	0.88	0.09	62,62,62,62	0
56	MG	DA	3399	1/1	0.88	0.18	47,47,47,47	0
56	MG	BA	3777	1/1	0.88	0.23	49,49,49,49	0
56	MG	DA	3034	1/1	0.88	0.15	43,43,43,43	0
56	MG	AA	3018	1/1	0.88	0.10	51,51,51,51	0
56	MG	DA	3395	1/1	0.88	0.19	42,42,42,42	0
56	MG	BA	3727	1/1	0.88	0.14	39,39,39,39	0
56	MG	DA	3247	1/1	0.88	0.38	57,57,57,57	0
56	MG	CA	3029	1/1	0.88	0.38	61,61,61,61	0
56	MG	DA	3546	1/1	0.88	0.11	53,53,53,53	0
56	MG	BA	3047	1/1	0.88	0.15	27,27,27,27	0
56	MG	DA	3320	1/1	0.88	0.16	40,40,40,40	0
56	MG	BA	3114	1/1	0.88	0.36	52,52,52,52	0
56	MG	BA	3482	1/1	0.88	0.22	59,59,59,59	0
56	MG	AA	3094	1/1	0.88	0.23	44,44,44,44	0
56	MG	BE	306	1/1	0.88	0.23	25,25,25,25	0
56	MG	DA	3196	1/1	0.88	0.09	53,53,53,53	0
56	MG	BA	3198	1/1	0.88	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3673	1/1	0.89	0.16	61,61,61,61	0
56	MG	BA	3207	1/1	0.89	0.18	38,38,38,38	0
56	MG	DA	3303	1/1	0.89	0.15	42,42,42,42	0
56	MG	CA	3015	1/1	0.89	0.12	58,58,58,58	0
56	MG	BA	3052	1/1	0.89	0.31	43,43,43,43	0
56	MG	CA	3125	1/1	0.89	0.14	64,64,64,64	0
56	MG	DA	3499	1/1	0.89	0.10	60,60,60,60	0
56	MG	BB	3001	1/1	0.89	0.20	50,50,50,50	0
56	MG	DA	3545	1/1	0.89	0.16	37,37,37,37	0
56	MG	BA	3094	1/1	0.89	0.24	43,43,43,43	0
56	MG	BA	3358	1/1	0.89	0.42	64,64,64,64	0
56	MG	BA	3292	1/1	0.89	0.15	42,42,42,42	0
56	MG	AA	3197	1/1	0.89	0.14	56,56,56,56	0
56	MG	BA	3427	1/1	0.89	0.25	32,32,32,32	0
56	MG	BA	3356	1/1	0.89	0.13	55,55,55,55	0
56	MG	BA	3088	1/1	0.89	0.16	50,50,50,50	0
56	MG	DA	3516	1/1	0.89	0.09	59,59,59,59	0
56	MG	AA	3030	1/1	0.89	0.16	57,57,57,57	0
56	MG	CA	3146	1/1	0.89	0.05	69,69,69,69	0
56	MG	DA	3323	1/1	0.89	0.32	53,53,53,53	0
56	MG	DA	3602	1/1	0.89	0.34	51,51,51,51	0
56	MG	CA	3161	1/1	0.89	0.10	70,70,70,70	0
56	MG	BA	3832	1/1	0.89	0.09	37,37,37,37	0
56	MG	DA	3643	1/1	0.89	0.10	60,60,60,60	0
56	MG	BA	3328	1/1	0.89	0.16	60,60,60,60	0
56	MG	BA	3544	1/1	0.89	0.20	35,35,35,35	0
56	MG	BA	3437	1/1	0.89	0.20	28,28,28,28	0
56	MG	DA	3225	1/1	0.89	0.23	54,54,54,54	0
56	MG	B2	3001	1/1	0.89	0.17	45,45,45,45	0
56	MG	BA	3667	1/1	0.89	0.11	52,52,52,52	0
56	MG	DA	3229	1/1	0.89	0.12	55,55,55,55	0
56	MG	CA	3115	1/1	0.89	0.18	62,62,62,62	0
56	MG	DA	3132	1/1	0.89	0.43	41,41,41,41	0
56	MG	BA	3250	1/1	0.89	0.20	40,40,40,40	0
56	MG	AA	3048	1/1	0.89	0.08	51,51,51,51	0
56	MG	DA	3370	1/1	0.89	0.08	46,46,46,46	0
56	MG	BA	3703	1/1	0.89	0.23	48,48,48,48	0
56	MG	BA	3714	1/1	0.89	0.06	47,47,47,47	0
56	MG	B5	102	1/1	0.89	0.18	45,45,45,45	0
56	MG	DA	3587	1/1	0.89	0.09	61,61,61,61	0
56	MG	DA	3470	1/1	0.89	0.16	42,42,42,42	0
56	MG	AA	3051	1/1	0.89	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BE	302	1/1	0.89	0.17	34,34,34,34	0
56	MG	DA	3172	1/1	0.89	0.32	51,51,51,51	0
56	MG	AA	3212	1/1	0.89	0.30	59,59,59,59	0
56	MG	B3	101	1/1	0.89	0.31	48,48,48,48	0
56	MG	BA	3269	1/1	0.89	0.38	53,53,53,53	0
56	MG	BA	3723	1/1	0.89	0.16	47,47,47,47	0
56	MG	BA	3835	1/1	0.89	0.20	46,46,46,46	0
56	MG	DA	3269	1/1	0.89	0.20	32,32,32,32	0
56	MG	BA	3419	1/1	0.89	0.17	39,39,39,39	0
56	MG	BN	3002	1/1	0.89	0.12	46,46,46,46	0
56	MG	AX	3008	1/1	0.89	0.36	57,57,57,57	0
56	MG	BA	3491	1/1	0.89	0.23	47,47,47,47	0
56	MG	CA	3002	1/1	0.89	0.07	51,51,51,51	0
56	MG	AA	3022	1/1	0.89	0.28	55,55,55,55	0
56	MG	DA	3375	1/1	0.89	0.11	40,40,40,40	0
56	MG	AA	3230	1/1	0.89	0.18	68,68,68,68	0
56	MG	BA	3778	1/1	0.89	0.14	35,35,35,35	0
56	MG	DA	3358	1/1	0.89	0.32	45,45,45,45	0
56	MG	BA	3115	1/1	0.89	0.08	67,67,67,67	0
56	MG	BA	3508	1/1	0.89	0.09	54,54,54,54	0
56	MG	BN	3001	1/1	0.89	0.33	51,51,51,51	0
56	MG	BA	3700	1/1	0.89	0.20	54,54,54,54	0
56	MG	DA	3536	1/1	0.89	0.32	54,54,54,54	0
56	MG	BA	3255	1/1	0.89	0.26	58,58,58,58	0
56	MG	BA	3739	1/1	0.89	0.19	46,46,46,46	0
56	MG	DA	3443	1/1	0.89	0.10	51,51,51,51	0
56	MG	DA	3612	1/1	0.89	0.23	56,56,56,56	0
56	MG	BA	3004	1/1	0.89	0.24	36,36,36,36	0
56	MG	DA	3655	1/1	0.89	0.17	57,57,57,57	0
56	MG	AA	3078	1/1	0.89	0.06	48,48,48,48	0
56	MG	DA	3069	1/1	0.89	0.39	53,53,53,53	0
56	MG	DA	3454	1/1	0.89	0.28	54,54,54,54	0
56	MG	BA	3791	1/1	0.89	0.13	47,47,47,47	0
56	MG	AA	3102	1/1	0.89	0.34	51,51,51,51	0
56	MG	DA	3157	1/1	0.89	0.28	44,44,44,44	0
56	MG	DA	3107	1/1	0.89	0.19	49,49,49,49	0
56	MG	DA	3630	1/1	0.89	0.17	49,49,49,49	0
56	MG	BA	3046	1/1	0.89	0.18	43,43,43,43	0
56	MG	CX	3004	1/1	0.89	0.33	54,54,54,54	0
56	MG	DA	3396	1/1	0.89	0.13	45,45,45,45	0
56	MG	BA	3820	1/1	0.89	0.20	45,45,45,45	0
56	MG	DA	3500	1/1	0.89	0.12	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3354	1/1	0.90	0.24	46,46,46,46	0
56	MG	AX	3012	1/1	0.90	0.23	59,59,59,59	0
56	MG	DA	3333	1/1	0.90	0.07	50,50,50,50	0
56	MG	BA	3768	1/1	0.90	0.06	56,56,56,56	0
56	MG	AA	3115	1/1	0.90	0.11	51,51,51,51	0
56	MG	DA	3181	1/1	0.90	0.30	45,45,45,45	0
56	MG	AA	3020	1/1	0.90	0.15	59,59,59,59	0
56	MG	BA	3838	1/1	0.90	0.19	50,50,50,50	0
56	MG	DA	3061	1/1	0.90	0.21	56,56,56,56	0
56	MG	AA	3057	1/1	0.90	0.20	61,61,61,61	0
56	MG	BA	3464	1/1	0.90	0.21	56,56,56,56	0
56	MG	CA	3036	1/1	0.90	0.09	60,60,60,60	0
56	MG	BA	3724	1/1	0.90	0.34	44,44,44,44	0
56	MG	BA	3433	1/1	0.90	0.19	57,57,57,57	0
56	MG	BA	3149	1/1	0.90	0.13	53,53,53,53	0
56	MG	DA	3539	1/1	0.90	0.14	46,46,46,46	0
56	MG	BA	3749	1/1	0.90	0.25	45,45,45,45	0
56	MG	BA	3233	1/1	0.90	0.33	48,48,48,48	0
56	MG	AA	3035	1/1	0.90	0.07	46,46,46,46	0
56	MG	DA	3271	1/1	0.90	0.14	47,47,47,47	0
56	MG	DA	3597	1/1	0.90	0.10	51,51,51,51	0
56	MG	CA	3175	1/1	0.90	0.16	39,39,39,39	0
56	MG	BA	3139	1/1	0.90	0.09	61,61,61,61	0
56	MG	DA	3089	1/1	0.90	0.23	46,46,46,46	0
56	MG	DA	3407	1/1	0.90	0.08	46,46,46,46	0
56	MG	CA	3176	1/1	0.90	0.13	43,43,43,43	0
56	MG	AA	3089	1/1	0.90	0.27	57,57,57,57	0
56	MG	BA	3293	1/1	0.90	0.25	52,52,52,52	0
56	MG	BA	3492	1/1	0.90	0.12	55,55,55,55	0
56	MG	AA	3055	1/1	0.90	0.22	58,58,58,58	0
56	MG	AA	3086	1/1	0.90	0.20	52,52,52,52	0
56	MG	BA	3410	1/1	0.90	0.10	46,46,46,46	0
56	MG	BA	3751	1/1	0.90	0.14	45,45,45,45	0
56	MG	CA	3123	1/1	0.90	0.12	80,80,80,80	0
56	MG	BA	3504	1/1	0.90	0.19	58,58,58,58	0
56	MG	DA	3183	1/1	0.90	0.22	58,58,58,58	0
56	MG	AD	502	1/1	0.90	0.29	56,56,56,56	0
56	MG	BA	3738	1/1	0.90	0.11	58,58,58,58	0
56	MG	BA	3447	1/1	0.90	0.23	26,26,26,26	0
56	MG	DA	3533	1/1	0.90	0.30	53,53,53,53	0
56	MG	BA	3089	1/1	0.90	0.29	45,45,45,45	0
56	MG	DA	3020	1/1	0.90	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3080	1/1	0.90	0.21	47,47,47,47	0
56	MG	BA	3143	1/1	0.90	0.25	42,42,42,42	0
56	MG	DA	3376	1/1	0.90	0.24	54,54,54,54	0
56	MG	BA	3015	1/1	0.90	0.23	47,47,47,47	0
56	MG	BA	3641	1/1	0.90	0.19	49,49,49,49	0
56	MG	DA	3087	1/1	0.90	0.21	49,49,49,49	0
56	MG	CA	3139	1/1	0.90	0.15	61,61,61,61	0
56	MG	CA	3013	1/1	0.90	0.10	63,63,63,63	0
56	MG	DB	3002	1/1	0.90	0.15	56,56,56,56	0
56	MG	BA	3228	1/1	0.90	0.22	50,50,50,50	0
56	MG	BA	3346	1/1	0.90	0.14	32,32,32,32	0
56	MG	DA	3616	1/1	0.90	0.07	45,45,45,45	0
56	MG	DA	3460	1/1	0.90	0.17	65,65,65,65	0
56	MG	DQ	3003	1/1	0.90	0.19	58,58,58,58	0
56	MG	DA	3422	1/1	0.90	0.36	43,43,43,43	0
56	MG	BA	3579	1/1	0.90	0.08	47,47,47,47	0
56	MG	DA	3355	1/1	0.90	0.10	50,50,50,50	0
56	MG	DA	3368	1/1	0.90	0.19	50,50,50,50	0
56	MG	DF	302	1/1	0.90	0.18	43,43,43,43	0
56	MG	CA	3101	1/1	0.90	0.22	54,54,54,54	0
56	MG	DA	3531	1/1	0.90	0.33	54,54,54,54	0
56	MG	BA	3828	1/1	0.90	0.20	37,37,37,37	0
56	MG	AA	3058	1/1	0.90	0.21	57,57,57,57	0
56	MG	DA	3574	1/1	0.90	0.20	51,51,51,51	0
56	MG	CA	3167	1/1	0.90	0.17	48,48,48,48	0
56	MG	DA	3648	1/1	0.90	0.12	60,60,60,60	0
56	MG	BA	3172	1/1	0.90	0.23	45,45,45,45	0
56	MG	CA	3024	1/1	0.90	0.14	63,63,63,63	0
56	MG	DA	3029	1/1	0.90	0.21	51,51,51,51	0
56	MG	BA	3718	1/1	0.90	0.20	46,46,46,46	0
56	MG	AA	3158	1/1	0.90	0.27	59,59,59,59	0
56	MG	DA	3621	1/1	0.90	0.29	45,45,45,45	0
56	MG	BO	5001	1/1	0.90	0.17	55,55,55,55	0
56	MG	BA	3283	1/1	0.90	0.12	36,36,36,36	0
56	MG	DA	3506	1/1	0.90	0.10	48,48,48,48	0
56	MG	BW	202	1/1	0.90	0.31	49,49,49,49	0
56	MG	DA	3093	1/1	0.90	0.10	57,57,57,57	0
56	MG	AA	3169	1/1	0.90	0.19	64,64,64,64	0
56	MG	BA	3566	1/1	0.90	0.23	30,30,30,30	0
56	MG	AA	3185	1/1	0.90	0.26	53,53,53,53	0
56	MG	BA	3787	1/1	0.90	0.22	59,59,59,59	0
56	MG	BA	3273	1/1	0.90	0.29	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3248	1/1	0.90	0.15	45,45,45,45	0
56	MG	CA	3126	1/1	0.90	0.17	72,72,72,72	0
56	MG	BA	3797	1/1	0.90	0.20	52,52,52,52	0
56	MG	BA	3620	1/1	0.90	0.15	47,47,47,47	0
56	MG	CA	3017	1/1	0.90	0.17	49,49,49,49	0
56	MG	BA	3150	1/1	0.90	0.12	48,48,48,48	0
56	MG	AA	3033	1/1	0.90	0.15	57,57,57,57	0
56	MG	DA	3039	1/1	0.90	0.22	56,56,56,56	0
56	MG	AA	3017	1/1	0.90	0.12	62,62,62,62	0
56	MG	BA	3023	1/1	0.90	0.27	55,55,55,55	0
56	MG	BA	3093	1/1	0.90	0.32	38,38,38,38	0
56	MG	CA	3124	1/1	0.90	0.16	79,79,79,79	0
56	MG	CA	3067	1/1	0.90	0.10	79,79,79,79	0
56	MG	DA	3140	1/1	0.90	0.11	34,34,34,34	0
56	MG	DA	3191	1/1	0.90	0.32	44,44,44,44	0
56	MG	BA	3686	1/1	0.90	0.24	30,30,30,30	0
56	MG	CA	3040	1/1	0.90	0.12	58,58,58,58	0
56	MG	BA	3475	1/1	0.90	0.15	53,53,53,53	0
56	MG	AA	3213	1/1	0.90	0.08	69,69,69,69	0
56	MG	BA	3348	1/1	0.90	0.13	54,54,54,54	0
56	MG	DA	3178	1/1	0.90	0.12	54,54,54,54	0
56	MG	DA	3534	1/1	0.90	0.26	74,74,74,74	0
56	MG	DA	3515	1/1	0.90	0.14	57,57,57,57	0
56	MG	DA	3019	1/1	0.90	0.15	57,57,57,57	0
56	MG	DA	3310	1/1	0.90	0.22	55,55,55,55	0
56	MG	DA	3563	1/1	0.90	0.15	42,42,42,42	0
56	MG	BA	3569	1/1	0.90	0.33	57,57,57,57	0
56	MG	DA	3142	1/1	0.90	0.11	45,45,45,45	0
56	MG	DA	3221	1/1	0.90	0.17	49,49,49,49	0
56	MG	DA	3101	1/1	0.90	0.12	53,53,53,53	0
56	MG	AA	3079	1/1	0.90	0.22	47,47,47,47	0
56	MG	BA	3548	1/1	0.90	0.28	48,48,48,48	0
56	MG	CA	3164	1/1	0.90	0.07	54,54,54,54	0
56	MG	DA	3380	1/1	0.90	0.09	55,55,55,55	0
56	MG	BA	3049	1/1	0.90	0.27	37,37,37,37	0
56	MG	DA	3405	1/1	0.90	0.13	52,52,52,52	0
56	MG	DB	3006	1/1	0.90	0.18	62,62,62,62	0
56	MG	BA	3364	1/1	0.90	0.15	42,42,42,42	0
56	MG	CA	3097	1/1	0.91	0.23	57,57,57,57	0
56	MG	AW	3006	1/1	0.91	0.16	50,50,50,50	0
56	MG	CA	3134	1/1	0.91	0.14	70,70,70,70	0
56	MG	AY	3003	1/1	0.91	0.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3606	1/1	0.91	0.22	54,54,54,54	0
56	MG	BA	3438	1/1	0.91	0.19	47,47,47,47	0
56	MG	DB	3011	1/1	0.91	0.09	52,52,52,52	0
56	MG	DA	3649	1/1	0.91	0.07	64,64,64,64	0
56	MG	AA	3183	1/1	0.91	0.14	71,71,71,71	0
56	MG	BA	3526	1/1	0.91	0.09	32,32,32,32	0
56	MG	DA	3072	1/1	0.91	0.09	36,36,36,36	0
56	MG	BP	202	1/1	0.91	0.20	34,34,34,34	0
56	MG	BA	3031	1/1	0.91	0.23	56,56,56,56	0
56	MG	BA	3666	1/1	0.91	0.12	58,58,58,58	0
56	MG	DA	3081	1/1	0.91	0.27	45,45,45,45	0
56	MG	DA	3581	1/1	0.91	0.19	63,63,63,63	0
56	MG	BA	3058	1/1	0.91	0.20	36,36,36,36	0
56	MG	BA	3453	1/1	0.91	0.21	42,42,42,42	0
56	MG	BA	3812	1/1	0.91	0.18	52,52,52,52	0
56	MG	DA	3418	1/1	0.91	0.22	37,37,37,37	0
56	MG	DA	3415	1/1	0.91	0.24	50,50,50,50	0
56	MG	CA	3046	1/1	0.91	0.09	56,56,56,56	0
56	MG	BA	3701	1/1	0.91	0.14	51,51,51,51	0
56	MG	BA	3342	1/1	0.91	0.18	51,51,51,51	0
56	MG	DA	3537	1/1	0.91	0.17	55,55,55,55	0
56	MG	AW	3003	1/1	0.91	0.31	59,59,59,59	0
56	MG	BA	3236	1/1	0.91	0.15	43,43,43,43	0
56	MG	DA	3223	1/1	0.91	0.29	54,54,54,54	0
56	MG	BA	3622	1/1	0.91	0.19	31,31,31,31	0
56	MG	BA	3789	1/1	0.91	0.17	39,39,39,39	0
56	MG	BA	3201	1/1	0.91	0.17	40,40,40,40	0
56	MG	BA	3090	1/1	0.91	0.20	37,37,37,37	0
56	MG	BA	3153	1/1	0.91	0.22	39,39,39,39	0
56	MG	BA	3345	1/1	0.91	0.12	44,44,44,44	0
56	MG	DA	3365	1/1	0.91	0.34	57,57,57,57	0
56	MG	DA	3402	1/1	0.91	0.27	65,65,65,65	0
56	MG	BB	3022	1/1	0.91	0.14	62,62,62,62	0
56	MG	CA	3073	1/1	0.91	0.32	48,48,48,48	0
56	MG	DA	3001	1/1	0.91	0.26	58,58,58,58	0
56	MG	DA	3328	1/1	0.91	0.15	47,47,47,47	0
56	MG	BD	306	1/1	0.91	0.36	22,22,22,22	0
56	MG	DA	3384	1/1	0.91	0.10	52,52,52,52	0
56	MG	AA	3223	1/1	0.91	0.30	59,59,59,59	0
56	MG	AA	3005	1/1	0.91	0.07	53,53,53,53	0
56	MG	AA	3106	1/1	0.91	0.17	51,51,51,51	0
56	MG	CA	3157	1/1	0.91	0.28	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3210	1/1	0.91	0.11	44,44,44,44	0
56	MG	BA	3436	1/1	0.91	0.22	46,46,46,46	0
56	MG	BA	3360	1/1	0.91	0.09	50,50,50,50	0
56	MG	BA	3219	1/1	0.91	0.19	29,29,29,29	0
56	MG	DD	307	1/1	0.91	0.14	56,56,56,56	0
56	MG	AA	3194	1/1	0.91	0.17	58,58,58,58	0
56	MG	AA	3216	1/1	0.91	0.13	72,72,72,72	0
56	MG	BA	3065	1/1	0.91	0.12	37,37,37,37	0
56	MG	BA	3314	1/1	0.91	0.15	47,47,47,47	0
56	MG	AA	3049	1/1	0.91	0.22	52,52,52,52	0
56	MG	BA	3625	1/1	0.91	0.14	57,57,57,57	0
59	ZN	D9	501	1/1	0.91	0.07	63,63,63,63	0
56	MG	BA	3650	1/1	0.91	0.12	57,57,57,57	0
56	MG	BA	3774	1/1	0.91	0.19	43,43,43,43	0
56	MG	AA	3066	1/1	0.91	0.12	44,44,44,44	0
56	MG	BA	3613	1/1	0.91	0.13	45,45,45,45	0
56	MG	AA	3143	1/1	0.91	0.16	73,73,73,73	0
56	MG	CA	3086	1/1	0.91	0.12	61,61,61,61	0
56	MG	DA	3026	1/1	0.91	0.14	42,42,42,42	0
56	MG	DA	3351	1/1	0.91	0.12	39,39,39,39	0
56	MG	BA	3144	1/1	0.91	0.09	43,43,43,43	0
56	MG	BA	3503	1/1	0.91	0.23	58,58,58,58	0
56	MG	AA	3189	1/1	0.91	0.17	59,59,59,59	0
56	MG	BA	3763	1/1	0.91	0.27	34,34,34,34	0
56	MG	BA	3537	1/1	0.91	0.13	49,49,49,49	0
56	MG	AA	3021	1/1	0.91	0.17	45,45,45,45	0
56	MG	BA	3341	1/1	0.91	0.16	57,57,57,57	0
56	MG	DA	3131	1/1	0.91	0.15	52,52,52,52	0
56	MG	BG	203	1/1	0.91	0.07	36,36,36,36	0
56	MG	BE	305	1/1	0.91	0.22	59,59,59,59	0
56	MG	DA	3432	1/1	0.91	0.15	56,56,56,56	0
56	MG	BA	3441	1/1	0.91	0.27	46,46,46,46	0
56	MG	BA	3568	1/1	0.91	0.25	52,52,52,52	0
56	MG	BB	3003	1/1	0.91	0.12	40,40,40,40	0
56	MG	BA	3124	1/1	0.91	0.20	38,38,38,38	0
56	MG	BA	3240	1/1	0.91	0.26	45,45,45,45	0
56	MG	BA	3592	1/1	0.91	0.14	29,29,29,29	0
56	MG	DA	3595	1/1	0.91	0.18	61,61,61,61	0
56	MG	BA	3016	1/1	0.91	0.20	44,44,44,44	0
56	MG	DA	3497	1/1	0.91	0.32	51,51,51,51	0
56	MG	DA	3589	1/1	0.91	0.15	63,63,63,63	0
56	MG	BA	3251	1/1	0.91	0.32	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3406	1/1	0.91	0.15	40,40,40,40	0
56	MG	BA	3762	1/1	0.91	0.38	40,40,40,40	0
56	MG	BA	3414	1/1	0.91	0.22	29,29,29,29	0
56	MG	BA	3062	1/1	0.91	0.25	57,57,57,57	0
56	MG	BA	3707	1/1	0.91	0.14	66,66,66,66	0
56	MG	CA	3043	1/1	0.91	0.26	54,54,54,54	0
56	MG	DA	3638	1/1	0.91	0.25	60,60,60,60	0
56	MG	BA	3815	1/1	0.91	0.28	50,50,50,50	0
56	MG	DA	3293	1/1	0.91	0.11	60,60,60,60	0
56	MG	BA	3096	1/1	0.91	0.30	41,41,41,41	0
56	MG	AA	3015	1/1	0.91	0.17	60,60,60,60	0
56	MG	AA	3103	1/1	0.91	0.14	59,59,59,59	0
56	MG	BA	3352	1/1	0.91	0.26	29,29,29,29	0
56	MG	DA	3236	1/1	0.91	0.13	48,48,48,48	0
56	MG	DA	3318	1/1	0.91	0.18	42,42,42,42	0
56	MG	BA	3429	1/1	0.91	0.24	47,47,47,47	0
56	MG	BA	3756	1/1	0.91	0.21	27,27,27,27	0
56	MG	BA	3581	1/1	0.91	0.11	38,38,38,38	0
56	MG	BA	3445	1/1	0.91	0.20	32,32,32,32	0
56	MG	AA	3156	1/1	0.91	0.14	52,52,52,52	0
56	MG	CW	3001	1/1	0.91	0.32	63,63,63,63	0
56	MG	DA	3650	1/1	0.91	0.27	44,44,44,44	0
56	MG	CA	3099	1/1	0.91	0.11	62,62,62,62	0
59	ZN	CN	501	1/1	0.91	0.04	92,92,92,92	0
56	MG	BA	3702	1/1	0.91	0.07	51,51,51,51	0
56	MG	DA	3585	1/1	0.91	0.10	51,51,51,51	0
56	MG	BA	3307	1/1	0.91	0.17	37,37,37,37	0
56	MG	BA	3280	1/1	0.91	0.24	49,49,49,49	0
56	MG	BA	3500	1/1	0.91	0.18	26,26,26,26	0
56	MG	BA	3387	1/1	0.91	0.06	65,65,65,65	0
56	MG	DA	3119	1/1	0.92	0.20	62,62,62,62	0
56	MG	DA	3548	1/1	0.92	0.17	65,65,65,65	0
56	MG	B9	502	1/1	0.92	0.10	57,57,57,57	0
56	MG	AA	3050	1/1	0.92	0.10	70,70,70,70	0
56	MG	BA	3151	1/1	0.92	0.28	42,42,42,42	0
56	MG	CA	3104	1/1	0.92	0.11	64,64,64,64	0
56	MG	BA	3232	1/1	0.92	0.14	37,37,37,37	0
56	MG	BF	305	1/1	0.92	0.26	47,47,47,47	0
56	MG	BA	3411	1/1	0.92	0.13	36,36,36,36	0
56	MG	BA	3593	1/1	0.92	0.14	42,42,42,42	0
56	MG	BA	3428	1/1	0.92	0.30	38,38,38,38	0
56	MG	B5	103	1/1	0.92	0.18	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3114	1/1	0.92	0.20	56,56,56,56	0
56	MG	BA	3375	1/1	0.92	0.15	35,35,35,35	0
56	MG	BA	3396	1/1	0.92	0.22	55,55,55,55	0
56	MG	CA	3074	1/1	0.92	0.39	55,55,55,55	0
56	MG	AA	3210	1/1	0.92	0.19	69,69,69,69	0
56	MG	DA	3661	1/1	0.92	0.20	42,42,42,42	0
56	MG	CA	3143	1/1	0.92	0.15	62,62,62,62	0
56	MG	AX	3005	1/1	0.92	0.15	44,44,44,44	0
56	MG	BA	3837	1/1	0.92	0.20	40,40,40,40	0
56	MG	BA	3522	1/1	0.92	0.28	36,36,36,36	0
56	MG	DA	3618	1/1	0.92	0.26	54,54,54,54	0
56	MG	CA	3092	1/1	0.92	0.15	44,44,44,44	0
56	MG	CA	3119	1/1	0.92	0.26	58,58,58,58	0
56	MG	DA	3167	1/1	0.92	0.25	47,47,47,47	0
56	MG	DA	3367	1/1	0.92	0.08	51,51,51,51	0
56	MG	CA	3170	1/1	0.92	0.12	64,64,64,64	0
56	MG	BA	3131	1/1	0.92	0.18	38,38,38,38	0
56	MG	BA	3484	1/1	0.92	0.29	36,36,36,36	0
56	MG	B1	101	1/1	0.92	0.38	44,44,44,44	0
56	MG	BA	3520	1/1	0.92	0.32	47,47,47,47	0
57	PCY	AA	3231	40/40	0.92	0.33	45,69,81,87	0
56	MG	BA	3099	1/1	0.92	0.16	50,50,50,50	0
56	MG	BA	3765	1/1	0.92	0.17	33,33,33,33	0
56	MG	DA	3025	1/1	0.92	0.16	44,44,44,44	0
56	MG	DA	3122	1/1	0.92	0.22	36,36,36,36	0
56	MG	BA	3061	1/1	0.92	0.17	40,40,40,40	0
60	K	CX	3001	1/1	0.92	0.17	74,74,74,74	0
56	MG	DA	3220	1/1	0.92	0.19	46,46,46,46	0
56	MG	DA	3441	1/1	0.92	0.09	43,43,43,43	0
56	MG	AA	3120	1/1	0.92	0.16	59,59,59,59	0
56	MG	DA	3526	1/1	0.92	0.22	47,47,47,47	0
56	MG	DA	3208	1/1	0.92	0.10	59,59,59,59	0
56	MG	DE	304	1/1	0.92	0.22	47,47,47,47	0
56	MG	DA	3491	1/1	0.92	0.17	45,45,45,45	0
56	MG	DA	3556	1/1	0.92	0.19	64,64,64,64	0
56	MG	DA	3147	1/1	0.92	0.09	44,44,44,44	0
56	MG	BA	3063	1/1	0.92	0.17	47,47,47,47	0
56	MG	BA	3651	1/1	0.92	0.19	56,56,56,56	0
56	MG	DA	3043	1/1	0.92	0.17	48,48,48,48	0
56	MG	DA	3138	1/1	0.92	0.41	59,59,59,59	0
56	MG	BA	3825	1/1	0.92	0.18	65,65,65,65	0
56	MG	AA	3215	1/1	0.92	0.19	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3083	1/1	0.92	0.29	47,47,47,47	0
56	MG	BA	3623	1/1	0.92	0.13	52,52,52,52	0
56	MG	DA	3391	1/1	0.92	0.09	44,44,44,44	0
56	MG	CA	3082	1/1	0.92	0.13	63,63,63,63	0
56	MG	BA	3582	1/1	0.92	0.16	44,44,44,44	0
56	MG	BA	3117	1/1	0.92	0.23	42,42,42,42	0
56	MG	DA	3523	1/1	0.92	0.14	57,57,57,57	0
56	MG	DA	3663	1/1	0.92	0.25	60,60,60,60	0
56	MG	BA	3449	1/1	0.92	0.29	60,60,60,60	0
56	MG	B3	102	1/1	0.92	0.11	35,35,35,35	0
56	MG	AA	3127	1/1	0.92	0.18	48,48,48,48	0
56	MG	BA	3194	1/1	0.92	0.20	37,37,37,37	0
56	MG	DA	3483	1/1	0.92	0.38	48,48,48,48	0
56	MG	AA	3138	1/1	0.92	0.17	34,34,34,34	0
56	MG	BA	3253	1/1	0.92	0.21	40,40,40,40	0
56	MG	DA	3390	1/1	0.92	0.07	54,54,54,54	0
56	MG	AA	3150	1/1	0.92	0.44	55,55,55,55	0
56	MG	DA	3485	1/1	0.92	0.11	44,44,44,44	0
56	MG	BA	3001	1/1	0.92	0.20	43,43,43,43	0
56	MG	DA	3094	1/1	0.92	0.19	52,52,52,52	0
56	MG	BA	3376	1/1	0.92	0.11	34,34,34,34	0
56	MG	DA	3250	1/1	0.92	0.13	61,61,61,61	0
56	MG	BA	3681	1/1	0.92	0.22	53,53,53,53	0
56	MG	BA	3354	1/1	0.92	0.17	31,31,31,31	0
56	MG	BA	3259	1/1	0.92	0.40	52,52,52,52	0
56	MG	BA	3237	1/1	0.92	0.14	36,36,36,36	0
56	MG	BA	3284	1/1	0.92	0.26	51,51,51,51	0
56	MG	AA	3016	1/1	0.92	0.16	46,46,46,46	0
56	MG	DA	3635	1/1	0.92	0.15	52,52,52,52	0
56	MG	AA	3144	1/1	0.92	0.12	50,50,50,50	0
56	MG	AA	3174	1/1	0.92	0.13	60,60,60,60	0
56	MG	DA	3027	1/1	0.92	0.21	53,53,53,53	0
56	MG	DA	3672	1/1	0.92	0.28	52,52,52,52	0
56	MG	DA	3239	1/1	0.92	0.20	54,54,54,54	0
56	MG	AA	3061	1/1	0.92	0.08	54,54,54,54	0
56	MG	DA	3204	1/1	0.92	0.31	51,51,51,51	0
56	MG	CA	3148	1/1	0.92	0.11	67,67,67,67	0
56	MG	CA	3159	1/1	0.92	0.13	57,57,57,57	0
56	MG	CA	3162	1/1	0.92	0.14	67,67,67,67	0
56	MG	BA	3601	1/1	0.92	0.16	42,42,42,42	0
56	MG	DA	3335	1/1	0.92	0.19	32,32,32,32	0
56	MG	BA	3669	1/1	0.92	0.13	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3209	1/1	0.92	0.30	51,51,51,51	0
56	MG	DA	3667	1/1	0.92	0.96	73,73,73,73	0
56	MG	BA	3597	1/1	0.92	0.20	44,44,44,44	0
56	MG	DF	301	1/1	0.92	0.15	47,47,47,47	0
56	MG	CA	3021	1/1	0.92	0.13	42,42,42,42	0
56	MG	DA	3394	1/1	0.92	0.14	49,49,49,49	0
56	MG	DA	3586	1/1	0.92	0.09	44,44,44,44	0
56	MG	BA	3740	1/1	0.92	0.21	51,51,51,51	0
56	MG	BA	3394	1/1	0.92	0.21	52,52,52,52	0
56	MG	BA	3305	1/1	0.92	0.12	33,33,33,33	0
56	MG	BA	3542	1/1	0.92	0.16	48,48,48,48	0
56	MG	BA	3182	1/1	0.92	0.31	41,41,41,41	0
56	MG	CA	3004	1/1	0.92	0.07	71,71,71,71	0
56	MG	AA	3101	1/1	0.92	0.17	54,54,54,54	0
56	MG	CA	3128	1/1	0.92	0.10	63,63,63,63	0
56	MG	DA	3636	1/1	0.92	0.24	56,56,56,56	0
56	MG	AA	3044	1/1	0.92	0.32	71,71,71,71	0
56	MG	AA	3023	1/1	0.92	0.15	37,37,37,37	0
56	MG	DA	3195	1/1	0.92	0.19	57,57,57,57	0
56	MG	BA	3351	1/1	0.92	0.17	34,34,34,34	0
56	MG	DA	3502	1/1	0.92	0.20	64,64,64,64	0
56	MG	BA	3158	1/1	0.92	0.19	44,44,44,44	0
56	MG	AA	3081	1/1	0.92	0.26	58,58,58,58	0
56	MG	BA	3344	1/1	0.92	0.14	37,37,37,37	0
56	MG	AA	3148	1/1	0.92	0.15	63,63,63,63	0
56	MG	DA	3190	1/1	0.92	0.26	45,45,45,45	0
59	ZN	DY	501	1/1	0.92	0.09	106,106,106,106	0
56	MG	DA	3295	1/1	0.92	0.17	58,58,58,58	0
56	MG	CA	3151	1/1	0.92	0.08	65,65,65,65	0
56	MG	BA	3509	1/1	0.92	0.25	39,39,39,39	0
56	MG	AA	3109	1/1	0.92	0.32	64,64,64,64	0
56	MG	DA	3378	1/1	0.92	0.13	45,45,45,45	0
56	MG	BA	3271	1/1	0.92	0.11	26,26,26,26	0
56	MG	BA	3808	1/1	0.92	0.14	34,34,34,34	0
56	MG	BA	3287	1/1	0.92	0.29	54,54,54,54	0
56	MG	BB	3020	1/1	0.92	0.16	54,54,54,54	0
56	MG	CA	3098	1/1	0.92	0.22	43,43,43,43	0
56	MG	AX	3004	1/1	0.92	0.21	70,70,70,70	0
56	MG	DA	3503	1/1	0.92	0.14	37,37,37,37	0
56	MG	DA	3288	1/1	0.92	0.16	61,61,61,61	0
56	MG	DA	3203	1/1	0.92	0.28	37,37,37,37	0
56	MG	BA	3294	1/1	0.92	0.20	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3130	1/1	0.92	0.26	48,48,48,48	0
56	MG	CA	3117	1/1	0.92	0.10	48,48,48,48	0
56	MG	DA	3401	1/1	0.92	0.29	36,36,36,36	0
56	MG	BA	3626	1/1	0.92	0.18	49,49,49,49	0
56	MG	BA	3617	1/1	0.92	0.13	64,64,64,64	0
56	MG	BB	3018	1/1	0.92	0.15	77,77,77,77	0
56	MG	BA	3530	1/1	0.92	0.20	51,51,51,51	0
56	MG	DA	3111	1/1	0.92	0.14	33,33,33,33	0
56	MG	DA	3300	1/1	0.92	0.26	60,60,60,60	0
56	MG	BA	3019	1/1	0.92	0.32	42,42,42,42	0
56	MG	AA	3045	1/1	0.92	0.32	59,59,59,59	0
56	MG	BA	3270	1/1	0.92	0.24	57,57,57,57	0
56	MG	AA	3067	1/1	0.92	0.09	59,59,59,59	0
56	MG	DA	3133	1/1	0.92	0.29	40,40,40,40	0
56	MG	DA	3338	1/1	0.93	0.19	40,40,40,40	0
56	MG	DA	3033	1/1	0.93	0.22	31,31,31,31	0
56	MG	BA	3474	1/1	0.93	0.09	61,61,61,61	0
56	MG	BA	3636	1/1	0.93	0.10	53,53,53,53	0
56	MG	BA	3529	1/1	0.93	0.16	33,33,33,33	0
56	MG	DA	3212	1/1	0.93	0.29	44,44,44,44	0
56	MG	AA	3171	1/1	0.93	0.10	48,48,48,48	0
56	MG	BA	3721	1/1	0.93	0.18	47,47,47,47	0
56	MG	BA	3007	1/1	0.93	0.24	51,51,51,51	0
56	MG	DA	3150	1/1	0.93	0.06	41,41,41,41	0
56	MG	BA	3773	1/1	0.93	0.22	49,49,49,49	0
56	MG	AA	3222	1/1	0.93	0.24	67,67,67,67	0
56	MG	DA	3137	1/1	0.93	0.13	54,54,54,54	0
56	MG	BA	3370	1/1	0.93	0.12	60,60,60,60	0
56	MG	DA	3498	1/1	0.93	0.09	57,57,57,57	0
56	MG	BA	3412	1/1	0.93	0.20	41,41,41,41	0
56	MG	DA	3259	1/1	0.93	0.12	34,34,34,34	0
56	MG	BA	3786	1/1	0.93	0.10	37,37,37,37	0
56	MG	DA	3256	1/1	0.93	0.12	47,47,47,47	0
56	MG	CA	3003	1/1	0.93	0.24	58,58,58,58	0
56	MG	CA	3032	1/1	0.93	0.23	52,52,52,52	0
56	MG	BA	3136	1/1	0.93	0.12	58,58,58,58	0
56	MG	AA	3090	1/1	0.93	0.35	53,53,53,53	0
56	MG	BA	3252	1/1	0.93	0.24	45,45,45,45	0
56	MG	DA	3075	1/1	0.93	0.12	39,39,39,39	0
56	MG	AA	3083	1/1	0.93	0.15	52,52,52,52	0
56	MG	DA	3092	1/1	0.93	0.26	48,48,48,48	0
56	MG	BA	3805	1/1	0.93	0.16	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3648	1/1	0.93	0.37	53,53,53,53	0
56	MG	DA	3572	1/1	0.93	0.26	28,28,28,28	0
56	MG	DA	3550	1/1	0.93	0.08	51,51,51,51	0
56	MG	BA	3310	1/1	0.93	0.20	57,57,57,57	0
56	MG	CA	3109	1/1	0.93	0.24	68,68,68,68	0
56	MG	BA	3576	1/1	0.93	0.17	48,48,48,48	0
56	MG	BA	3422	1/1	0.93	0.18	32,32,32,32	0
56	MG	BA	3337	1/1	0.93	0.17	35,35,35,35	0
56	MG	DA	3146	1/1	0.93	0.27	46,46,46,46	0
56	MG	BA	3704	1/1	0.93	0.23	55,55,55,55	0
56	MG	BF	311	1/1	0.93	0.18	43,43,43,43	0
56	MG	DA	3090	1/1	0.93	0.21	45,45,45,45	0
56	MG	BA	3423	1/1	0.93	0.18	23,23,23,23	0
56	MG	DA	3180	1/1	0.93	0.14	51,51,51,51	0
56	MG	DA	3461	1/1	0.93	0.13	56,56,56,56	0
56	MG	BD	301	1/1	0.93	0.21	49,49,49,49	0
56	MG	AY	3002	1/1	0.93	0.12	68,68,68,68	0
56	MG	BA	3810	1/1	0.93	0.25	50,50,50,50	0
56	MG	DA	3609	1/1	0.93	0.16	60,60,60,60	0
56	MG	AA	3077	1/1	0.93	0.14	49,49,49,49	0
56	MG	B6	101	1/1	0.93	0.18	48,48,48,48	0
56	MG	DA	3304	1/1	0.93	0.12	40,40,40,40	0
56	MG	BA	3754	1/1	0.93	0.17	60,60,60,60	0
56	MG	CA	3076	1/1	0.93	0.19	56,56,56,56	0
56	MG	AA	3208	1/1	0.93	0.16	45,45,45,45	0
56	MG	AA	3140	1/1	0.93	0.11	71,71,71,71	0
56	MG	AA	3111	1/1	0.93	0.18	52,52,52,52	0
56	MG	BA	3145	1/1	0.93	0.26	32,32,32,32	0
56	MG	DE	302	1/1	0.93	0.20	39,39,39,39	0
56	MG	DA	3551	1/1	0.93	0.16	55,55,55,55	0
56	MG	BA	3619	1/1	0.93	0.40	51,51,51,51	0
56	MG	BA	3033	1/1	0.93	0.26	33,33,33,33	0
56	MG	BX	101	1/1	0.93	0.26	65,65,65,65	0
56	MG	BB	3005	1/1	0.93	0.19	64,64,64,64	0
56	MG	BA	3081	1/1	0.93	0.19	49,49,49,49	0
56	MG	D0	102	1/1	0.93	0.17	62,62,62,62	0
56	MG	BA	3116	1/1	0.93	0.15	29,29,29,29	0
56	MG	BA	3711	1/1	0.93	0.26	45,45,45,45	0
56	MG	AA	3218	1/1	0.93	0.25	53,53,53,53	0
56	MG	DA	3046	1/1	0.93	0.37	57,57,57,57	0
56	MG	DA	3255	1/1	0.93	0.05	59,59,59,59	0
56	MG	BA	3628	1/1	0.93	0.17	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3002	1/1	0.93	0.08	62,62,62,62	0
56	MG	BA	3260	1/1	0.93	0.56	57,57,57,57	0
56	MG	BA	3244	1/1	0.93	0.10	63,63,63,63	0
56	MG	BA	3156	1/1	0.93	0.23	41,41,41,41	0
56	MG	BA	3304	1/1	0.93	0.20	39,39,39,39	0
56	MG	CA	3154	1/1	0.93	0.17	62,62,62,62	0
56	MG	AA	3054	1/1	0.93	0.43	52,52,52,52	0
56	MG	AA	3008	1/1	0.93	0.15	54,54,54,54	0
56	MG	BA	3199	1/1	0.93	0.09	53,53,53,53	0
56	MG	BA	3493	1/1	0.93	0.13	46,46,46,46	0
56	MG	DA	3420	1/1	0.93	0.16	46,46,46,46	0
56	MG	DA	3578	1/1	0.93	0.10	55,55,55,55	0
56	MG	DA	3233	1/1	0.93	0.25	43,43,43,43	0
56	MG	DA	3135	1/1	0.93	0.11	50,50,50,50	0
56	MG	DA	3030	1/1	0.93	0.28	40,40,40,40	0
56	MG	DA	3561	1/1	0.93	0.22	48,48,48,48	0
56	MG	BA	3685	1/1	0.93	0.17	59,59,59,59	0
56	MG	DA	3442	1/1	0.93	0.15	44,44,44,44	0
56	MG	BA	3554	1/1	0.93	0.21	37,37,37,37	0
56	MG	BA	3578	1/1	0.93	0.25	47,47,47,47	0
56	MG	BA	3097	1/1	0.93	0.17	52,52,52,52	0
56	MG	DA	3383	1/1	0.93	0.24	37,37,37,37	0
56	MG	BA	3732	1/1	0.93	0.26	40,40,40,40	0
56	MG	AA	3024	1/1	0.93	0.15	58,58,58,58	0
56	MG	DA	3205	1/1	0.93	0.21	47,47,47,47	0
56	MG	CA	3038	1/1	0.93	0.19	46,46,46,46	0
56	MG	BA	3741	1/1	0.93	0.11	28,28,28,28	0
56	MG	BA	3366	1/1	0.93	0.17	45,45,45,45	0
56	MG	BA	3279	1/1	0.93	0.22	43,43,43,43	0
56	MG	BA	3323	1/1	0.93	0.22	39,39,39,39	0
56	MG	DA	3562	1/1	0.93	0.34	58,58,58,58	0
56	MG	BA	3374	1/1	0.93	0.08	37,37,37,37	0
56	MG	DA	3518	1/1	0.93	0.18	50,50,50,50	0
56	MG	BB	3002	1/1	0.93	0.18	52,52,52,52	0
56	MG	AA	3056	1/1	0.93	0.19	46,46,46,46	0
56	MG	BA	3430	1/1	0.93	0.33	32,32,32,32	0
56	MG	DA	3095	1/1	0.93	0.27	47,47,47,47	0
56	MG	DA	3070	1/1	0.93	0.23	48,48,48,48	0
56	MG	BA	3819	1/1	0.93	0.24	32,32,32,32	0
56	MG	BA	3106	1/1	0.93	0.47	50,50,50,50	0
56	MG	BA	3426	1/1	0.93	0.21	22,22,22,22	0
56	MG	DA	3613	1/1	0.93	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3616	1/1	0.93	0.12	53,53,53,53	0
56	MG	BA	3698	1/1	0.93	0.13	48,48,48,48	0
56	MG	DU	3002	1/1	0.93	0.22	50,50,50,50	0
56	MG	BA	3235	1/1	0.93	0.16	37,37,37,37	0
56	MG	DA	3409	1/1	0.93	0.09	47,47,47,47	0
56	MG	DA	3369	1/1	0.93	0.05	61,61,61,61	0
56	MG	CA	3120	1/1	0.93	0.12	64,64,64,64	0
56	MG	DA	3675	1/1	0.93	0.28	44,44,44,44	0
56	MG	BA	3719	1/1	0.93	0.13	42,42,42,42	0
56	MG	AA	3166	1/1	0.93	0.13	65,65,65,65	0
56	MG	BA	3302	1/1	0.93	0.16	35,35,35,35	0
56	MG	DA	3557	1/1	0.93	0.23	34,34,34,34	0
56	MG	AX	3006	1/1	0.93	0.18	74,74,74,74	0
56	MG	DA	3559	1/1	0.93	0.18	48,48,48,48	0
56	MG	BA	3164	1/1	0.93	0.28	43,43,43,43	0
56	MG	AA	3135	1/1	0.93	0.10	65,65,65,65	0
56	MG	DA	3577	1/1	0.93	0.14	49,49,49,49	0
56	MG	BA	3125	1/1	0.93	0.14	42,42,42,42	0
56	MG	DA	3263	1/1	0.93	0.10	61,61,61,61	0
56	MG	BW	203	1/1	0.93	0.23	34,34,34,34	0
56	MG	BA	3645	1/1	0.93	0.18	32,32,32,32	0
56	MG	DA	3474	1/1	0.93	0.07	53,53,53,53	0
56	MG	BA	3329	1/1	0.93	0.19	29,29,29,29	0
56	MG	BA	3839	1/1	0.93	0.12	38,38,38,38	0
56	MG	AA	3026	1/1	0.93	0.22	53,53,53,53	0
56	MG	AA	3105	1/1	0.93	0.20	49,49,49,49	0
56	MG	DA	3139	1/1	0.93	0.10	40,40,40,40	0
56	MG	BA	3120	1/1	0.93	0.23	32,32,32,32	0
56	MG	BA	3092	1/1	0.93	0.26	41,41,41,41	0
56	MG	CE	202	1/1	0.93	0.05	66,66,66,66	0
56	MG	DA	3374	1/1	0.93	0.18	37,37,37,37	0
56	MG	BA	3818	1/1	0.93	0.26	32,32,32,32	0
56	MG	BA	3766	1/1	0.93	0.19	31,31,31,31	0
56	MG	BA	3519	1/1	0.93	0.12	44,44,44,44	0
56	MG	BN	3005	1/1	0.93	0.39	51,51,51,51	0
56	MG	BA	3803	1/1	0.93	0.09	47,47,47,47	0
56	MG	BA	3658	1/1	0.94	0.23	45,45,45,45	0
56	MG	BA	3327	1/1	0.94	0.25	25,25,25,25	0
56	MG	BA	3286	1/1	0.94	0.32	46,46,46,46	0
56	MG	BA	3105	1/1	0.94	0.45	69,69,69,69	0
56	MG	AA	3152	1/1	0.94	0.13	45,45,45,45	0
56	MG	BA	3359	1/1	0.94	0.14	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3105	1/1	0.94	0.14	49,49,49,49	0
56	MG	AA	3184	1/1	0.94	0.12	55,55,55,55	0
56	MG	BA	3034	1/1	0.94	0.21	28,28,28,28	0
56	MG	DA	3031	1/1	0.94	0.41	51,51,51,51	0
56	MG	DA	3243	1/1	0.94	0.17	54,54,54,54	0
56	MG	BA	3454	1/1	0.94	0.15	31,31,31,31	0
56	MG	DA	3283	1/1	0.94	0.25	46,46,46,46	0
56	MG	AA	3053	1/1	0.94	0.37	49,49,49,49	0
56	MG	AA	3029	1/1	0.94	0.28	53,53,53,53	0
56	MG	BU	208	1/1	0.94	0.13	41,41,41,41	0
56	MG	BA	3175	1/1	0.94	0.21	35,35,35,35	0
56	MG	CA	3014	1/1	0.94	0.14	47,47,47,47	0
56	MG	DA	3159	1/1	0.94	0.30	41,41,41,41	0
56	MG	D7	101	1/1	0.94	0.19	39,39,39,39	0
56	MG	CA	3068	1/1	0.94	0.40	55,55,55,55	0
56	MG	BA	3267	1/1	0.94	0.14	37,37,37,37	0
56	MG	AA	3043	1/1	0.94	0.27	26,26,26,26	0
56	MG	AA	3064	1/1	0.94	0.13	61,61,61,61	0
56	MG	DA	3511	1/1	0.94	0.11	45,45,45,45	0
56	MG	DA	3242	1/1	0.94	0.07	43,43,43,43	0
56	MG	AW	3004	1/1	0.94	0.12	51,51,51,51	0
56	MG	BA	3361	1/1	0.94	0.16	35,35,35,35	0
56	MG	CA	3094	1/1	0.94	0.18	72,72,72,72	0
56	MG	DA	3048	1/1	0.94	0.15	45,45,45,45	0
56	MG	DA	3152	1/1	0.94	0.25	42,42,42,42	0
56	MG	CX	3005	1/1	0.94	0.45	58,58,58,58	0
56	MG	BA	3296	1/1	0.94	0.19	31,31,31,31	0
56	MG	D0	101	1/1	0.94	0.08	56,56,56,56	0
56	MG	BA	3533	1/1	0.94	0.23	50,50,50,50	0
56	MG	CA	3052	1/1	0.94	0.09	65,65,65,65	0
56	MG	DA	3282	1/1	0.94	0.10	42,42,42,42	0
56	MG	BA	3750	1/1	0.94	0.21	49,49,49,49	0
56	MG	DA	3065	1/1	0.94	0.08	56,56,56,56	0
56	MG	DA	3659	1/1	0.94	0.48	67,67,67,67	0
56	MG	BA	3814	1/1	0.94	0.28	26,26,26,26	0
56	MG	BA	3276	1/1	0.94	0.29	41,41,41,41	0
56	MG	BA	3137	1/1	0.94	0.24	45,45,45,45	0
56	MG	CA	3035	1/1	0.94	0.10	60,60,60,60	0
56	MG	AA	3129	1/1	0.94	0.08	73,73,73,73	0
56	MG	BA	3021	1/1	0.94	0.17	60,60,60,60	0
56	MG	AA	3188	1/1	0.94	0.16	56,56,56,56	0
56	MG	BA	3570	1/1	0.94	0.35	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3603	1/1	0.94	0.14	52,52,52,52	0
56	MG	AA	3052	1/1	0.94	0.32	68,68,68,68	0
56	MG	AA	3099	1/1	0.94	0.25	63,63,63,63	0
56	MG	BA	3098	1/1	0.94	0.35	26,26,26,26	0
56	MG	BA	3223	1/1	0.94	0.16	29,29,29,29	0
56	MG	DA	3270	1/1	0.94	0.22	49,49,49,49	0
56	MG	BA	3680	1/1	0.94	0.15	52,52,52,52	0
56	MG	AA	3096	1/1	0.94	0.27	48,48,48,48	0
56	MG	BA	3456	1/1	0.94	0.39	41,41,41,41	0
56	MG	BA	3662	1/1	0.94	0.32	50,50,50,50	0
56	MG	BB	3010	1/1	0.94	0.11	48,48,48,48	0
56	MG	BA	3502	1/1	0.94	0.31	45,45,45,45	0
56	MG	AA	3206	1/1	0.94	0.17	47,47,47,47	0
56	MG	DA	3564	1/1	0.94	0.31	53,53,53,53	0
56	MG	BV	203	1/1	0.94	0.24	32,32,32,32	0
56	MG	DA	3156	1/1	0.94	0.12	43,43,43,43	0
56	MG	DA	3641	1/1	0.94	0.09	44,44,44,44	0
56	MG	AA	3119	1/1	0.94	0.10	58,58,58,58	0
56	MG	BA	3213	1/1	0.94	0.09	45,45,45,45	0
56	MG	BA	3745	1/1	0.94	0.17	30,30,30,30	0
56	MG	AA	3092	1/1	0.94	0.20	39,39,39,39	0
56	MG	CA	3012	1/1	0.94	0.20	68,68,68,68	0
56	MG	BA	3008	1/1	0.94	0.22	27,27,27,27	0
56	MG	DA	3100	1/1	0.94	0.24	36,36,36,36	0
56	MG	DA	3467	1/1	0.94	0.31	43,43,43,43	0
56	MG	AA	3147	1/1	0.94	0.11	55,55,55,55	0
56	MG	AA	3173	1/1	0.94	0.11	47,47,47,47	0
56	MG	AA	3162	1/1	0.94	0.28	59,59,59,59	0
56	MG	AA	3176	1/1	0.94	0.09	54,54,54,54	0
56	MG	DA	3631	1/1	0.94	0.13	56,56,56,56	0
56	MG	BA	3691	1/1	0.94	0.25	38,38,38,38	0
56	MG	BA	3505	1/1	0.94	0.12	54,54,54,54	0
56	MG	BF	306	1/1	0.94	0.31	40,40,40,40	0
56	MG	CA	3171	1/1	0.94	0.19	63,63,63,63	0
56	MG	BA	3575	1/1	0.94	0.09	64,64,64,64	0
56	MG	CA	3113	1/1	0.94	0.11	55,55,55,55	0
56	MG	DA	3440	1/1	0.94	0.18	39,39,39,39	0
56	MG	DA	3014	1/1	0.94	0.14	50,50,50,50	0
56	MG	AA	3028	1/1	0.94	0.38	56,56,56,56	0
56	MG	DA	3216	1/1	0.94	0.29	46,46,46,46	0
56	MG	DA	3478	1/1	0.94	0.18	47,47,47,47	0
56	MG	BA	3788	1/1	0.94	0.17	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3260	1/1	0.94	0.13	41,41,41,41	0
56	MG	DA	3342	1/1	0.94	0.10	56,56,56,56	0
56	MG	AA	3041	1/1	0.94	0.26	52,52,52,52	0
56	MG	BA	3425	1/1	0.94	0.27	29,29,29,29	0
56	MG	BA	3602	1/1	0.94	0.17	46,46,46,46	0
56	MG	BA	3379	1/1	0.94	0.18	45,45,45,45	0
56	MG	AA	3084	1/1	0.94	0.17	49,49,49,49	0
56	MG	B0	101	1/1	0.94	0.20	39,39,39,39	0
56	MG	BF	310	1/1	0.94	0.25	38,38,38,38	0
56	MG	BA	3381	1/1	0.94	0.14	43,43,43,43	0
56	MG	AA	3093	1/1	0.94	0.14	50,50,50,50	0
56	MG	AX	3007	1/1	0.94	0.24	72,72,72,72	0
56	MG	BA	3550	1/1	0.94	0.20	34,34,34,34	0
56	MG	DD	305	1/1	0.94	0.24	38,38,38,38	0
56	MG	BA	3543	1/1	0.94	0.25	26,26,26,26	0
56	MG	BA	3281	1/1	0.94	0.17	49,49,49,49	0
56	MG	DA	3054	1/1	0.94	0.15	43,43,43,43	0
56	MG	DA	3160	1/1	0.94	0.20	59,59,59,59	0
56	MG	BA	3132	1/1	0.94	0.21	42,42,42,42	0
56	MG	DA	3206	1/1	0.94	0.10	39,39,39,39	0
56	MG	CA	3129	1/1	0.94	0.19	61,61,61,61	0
56	MG	BA	3457	1/1	0.94	0.21	44,44,44,44	0
56	MG	DA	3647	1/1	0.94	0.22	47,47,47,47	0
56	MG	CF	3001	1/1	0.94	0.26	38,38,38,38	0
56	MG	BA	3190	1/1	0.94	0.16	45,45,45,45	0
56	MG	AA	3107	1/1	0.94	0.25	51,51,51,51	0
56	MG	AA	3128	1/1	0.94	0.17	41,41,41,41	0
56	MG	DA	3640	1/1	0.94	0.14	52,52,52,52	0
56	MG	BA	3501	1/1	0.94	0.18	20,20,20,20	0
56	MG	DA	3162	1/1	0.94	0.34	43,43,43,43	0
56	MG	DA	3141	1/1	0.94	0.21	56,56,56,56	0
56	MG	DA	3598	1/1	0.94	0.11	63,63,63,63	0
56	MG	DA	3331	1/1	0.94	0.25	39,39,39,39	0
56	MG	DA	3592	1/1	0.94	0.17	52,52,52,52	0
56	MG	BA	3420	1/1	0.94	0.19	22,22,22,22	0
56	MG	BA	3257	1/1	0.94	0.21	41,41,41,41	0
56	MG	BA	3214	1/1	0.94	0.20	49,49,49,49	0
56	MG	AA	3036	1/1	0.94	0.12	52,52,52,52	0
56	MG	CA	3033	1/1	0.94	0.15	56,56,56,56	0
56	MG	DA	3669	1/1	0.94	0.22	49,49,49,49	0
56	MG	BA	3110	1/1	0.94	0.26	41,41,41,41	0
56	MG	BA	3676	1/1	0.94	0.28	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3527	1/1	0.94	0.17	53,53,53,53	0
56	MG	BA	3200	1/1	0.94	0.28	56,56,56,56	0
56	MG	DA	3005	1/1	0.94	0.20	58,58,58,58	0
56	MG	BB	3013	1/1	0.94	0.14	42,42,42,42	0
56	MG	BA	3665	1/1	0.94	0.29	49,49,49,49	0
56	MG	DA	3097	1/1	0.94	0.21	43,43,43,43	0
56	MG	BA	3141	1/1	0.94	0.23	38,38,38,38	0
56	MG	BU	201	1/1	0.94	0.14	39,39,39,39	0
56	MG	BA	3416	1/1	0.94	0.17	21,21,21,21	0
56	MG	BE	304	1/1	0.94	0.26	40,40,40,40	0
56	MG	CA	3095	1/1	0.94	0.10	61,61,61,61	0
56	MG	DA	3377	1/1	0.94	0.07	42,42,42,42	0
56	MG	DE	303	1/1	0.94	0.26	44,44,44,44	0
56	MG	DA	3664	1/1	0.94	0.08	38,38,38,38	0
56	MG	CT	3001	1/1	0.94	0.07	47,47,47,47	0
56	MG	DA	3398	1/1	0.94	0.18	57,57,57,57	0
56	MG	BA	3316	1/1	0.94	0.25	23,23,23,23	0
56	MG	AA	3031	1/1	0.94	0.09	44,44,44,44	0
56	MG	DA	3626	1/1	0.94	0.06	54,54,54,54	0
56	MG	BA	3256	1/1	0.94	0.32	49,49,49,49	0
56	MG	BD	308	1/1	0.94	0.28	39,39,39,39	0
56	MG	BA	3528	1/1	0.94	0.11	43,43,43,43	0
56	MG	AA	3118	1/1	0.94	0.20	53,53,53,53	0
56	MG	BX	102	1/1	0.94	0.31	41,41,41,41	0
56	MG	BA	3761	1/1	0.94	0.19	54,54,54,54	0
56	MG	BA	3448	1/1	0.94	0.22	28,28,28,28	0
56	MG	CA	3118	1/1	0.94	0.18	47,47,47,47	0
56	MG	AA	3027	1/1	0.94	0.24	54,54,54,54	0
56	MG	BA	3011	1/1	0.94	0.20	40,40,40,40	0
56	MG	CA	3071	1/1	0.94	0.09	50,50,50,50	0
56	MG	AA	3039	1/1	0.94	0.15	61,61,61,61	0
56	MG	BA	3378	1/1	0.94	0.10	34,34,34,34	0
56	MG	B5	105	1/1	0.94	0.10	49,49,49,49	0
56	MG	DA	3535	1/1	0.94	0.35	54,54,54,54	0
56	MG	DA	3458	1/1	0.94	0.11	42,42,42,42	0
56	MG	BA	3790	1/1	0.94	0.21	32,32,32,32	0
56	MG	DW	3001	1/1	0.94	0.23	43,43,43,43	0
56	MG	AA	3097	1/1	0.94	0.13	50,50,50,50	0
56	MG	CA	3080	1/1	0.94	0.28	52,52,52,52	0
56	MG	BA	3688	1/1	0.94	0.20	45,45,45,45	0
56	MG	BA	3055	1/1	0.94	0.23	31,31,31,31	0
56	MG	BA	3531	1/1	0.94	0.39	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3399	1/1	0.94	0.16	25,25,25,25	0
56	MG	DA	3117	1/1	0.94	0.28	60,60,60,60	0
56	MG	AA	3126	1/1	0.94	0.17	46,46,46,46	0
56	MG	BA	3614	1/1	0.94	0.15	26,26,26,26	0
56	MG	BA	3306	1/1	0.94	0.18	31,31,31,31	0
56	MG	AA	3187	1/1	0.94	0.12	62,62,62,62	0
56	MG	BA	3661	1/1	0.94	0.09	53,53,53,53	0
56	MG	AA	3211	1/1	0.94	0.09	59,59,59,59	0
56	MG	DA	3035	1/1	0.94	0.24	38,38,38,38	0
56	MG	DA	3274	1/1	0.94	0.22	33,33,33,33	0
56	MG	BA	3506	1/1	0.94	0.26	51,51,51,51	0
56	MG	BR	201	1/1	0.94	0.17	44,44,44,44	0
56	MG	BY	502	1/1	0.94	0.13	50,50,50,50	0
56	MG	BA	3469	1/1	0.94	0.31	37,37,37,37	0
56	MG	DA	3449	1/1	0.94	0.19	47,47,47,47	0
56	MG	DA	3258	1/1	0.94	0.18	59,59,59,59	0
56	MG	BA	3183	1/1	0.94	0.22	40,40,40,40	0
56	MG	BA	3545	1/1	0.94	0.25	41,41,41,41	0
56	MG	DA	3348	1/1	0.94	0.27	38,38,38,38	0
56	MG	BA	3350	1/1	0.94	0.24	27,27,27,27	0
56	MG	DA	3633	1/1	0.94	0.14	61,61,61,61	0
56	MG	DA	3296	1/1	0.94	0.18	48,48,48,48	0
56	MG	DA	3278	1/1	0.94	0.21	53,53,53,53	0
56	MG	BA	3559	1/1	0.94	0.20	30,30,30,30	0
56	MG	CA	3030	1/1	0.94	0.08	59,59,59,59	0
56	MG	BA	3829	1/1	0.94	0.34	45,45,45,45	0
56	MG	DA	3073	1/1	0.94	0.17	54,54,54,54	0
56	MG	DA	3059	1/1	0.94	0.45	53,53,53,53	0
56	MG	BA	3300	1/1	0.94	0.18	22,22,22,22	0
56	MG	CA	3001	1/1	0.94	0.25	73,73,73,73	0
56	MG	BA	3654	1/1	0.94	0.15	55,55,55,55	0
56	MG	BA	3382	1/1	0.94	0.21	55,55,55,55	0
56	MG	CA	3063	1/1	0.94	0.14	59,59,59,59	0
56	MG	DA	3311	1/1	0.94	0.18	42,42,42,42	0
56	MG	DA	3484	1/1	0.94	0.05	45,45,45,45	0
56	MG	DA	3381	1/1	0.94	0.11	60,60,60,60	0
56	MG	DA	3652	1/1	0.94	0.12	49,49,49,49	0
56	MG	CA	3168	1/1	0.94	0.19	72,72,72,72	0
56	MG	CA	3041	1/1	0.94	0.16	58,58,58,58	0
56	MG	BA	3404	1/1	0.95	0.18	36,36,36,36	0
56	MG	BA	3406	1/1	0.95	0.19	32,32,32,32	0
56	MG	AA	3046	1/1	0.95	0.16	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3077	1/1	0.95	0.20	34,34,34,34	0
56	MG	DA	3464	1/1	0.95	0.11	44,44,44,44	0
56	MG	DA	3074	1/1	0.95	0.22	50,50,50,50	0
56	MG	BA	3109	1/1	0.95	0.28	42,42,42,42	0
56	MG	BA	3206	1/1	0.95	0.21	29,29,29,29	0
56	MG	DA	3279	1/1	0.95	0.07	48,48,48,48	0
56	MG	DA	3639	1/1	0.95	0.14	64,64,64,64	0
56	MG	AA	3141	1/1	0.95	0.10	55,55,55,55	0
56	MG	DA	3285	1/1	0.95	0.20	28,28,28,28	0
56	MG	AA	3010	1/1	0.95	0.14	59,59,59,59	0
56	MG	AA	3075	1/1	0.95	0.22	33,33,33,33	0
56	MG	BA	3066	1/1	0.95	0.39	51,51,51,51	0
56	MG	BA	3722	1/1	0.95	0.13	50,50,50,50	0
56	MG	DA	3008	1/1	0.95	0.21	33,33,33,33	0
56	MG	BA	3202	1/1	0.95	0.13	46,46,46,46	0
56	MG	BA	3587	1/1	0.95	0.20	44,44,44,44	0
56	MG	BA	3483	1/1	0.95	0.28	38,38,38,38	0
56	MG	CA	3103	1/1	0.95	0.10	75,75,75,75	0
56	MG	DA	3099	1/1	0.95	0.09	60,60,60,60	0
56	MG	DA	3007	1/1	0.95	0.39	54,54,54,54	0
56	MG	BA	3558	1/1	0.95	0.19	29,29,29,29	0
56	MG	BG	202	1/1	0.95	0.07	46,46,46,46	0
56	MG	AA	3149	1/1	0.95	0.21	41,41,41,41	0
56	MG	CA	3145	1/1	0.95	0.13	63,63,63,63	0
56	MG	BA	3485	1/1	0.95	0.23	46,46,46,46	0
56	MG	DA	3529	1/1	0.95	0.10	41,41,41,41	0
56	MG	DA	3601	1/1	0.95	0.19	54,54,54,54	0
56	MG	DA	3174	1/1	0.95	0.17	48,48,48,48	0
56	MG	DA	3134	1/1	0.95	0.13	49,49,49,49	0
56	MG	BA	3173	1/1	0.95	0.30	36,36,36,36	0
56	MG	CA	3022	1/1	0.95	0.10	53,53,53,53	0
56	MG	BA	3709	1/1	0.95	0.29	44,44,44,44	0
56	MG	BA	3631	1/1	0.95	0.14	43,43,43,43	0
56	MG	CA	3100	1/1	0.95	0.23	62,62,62,62	0
56	MG	DA	3372	1/1	0.95	0.15	47,47,47,47	0
56	MG	AK	201	1/1	0.95	0.14	61,61,61,61	0
56	MG	BA	3827	1/1	0.95	0.20	30,30,30,30	0
56	MG	CA	3149	1/1	0.95	0.27	65,65,65,65	0
56	MG	DA	3185	1/1	0.95	0.24	54,54,54,54	0
56	MG	CW	3002	1/1	0.95	0.16	74,74,74,74	0
56	MG	DA	3126	1/1	0.95	0.15	44,44,44,44	0
56	MG	BA	3135	1/1	0.95	0.21	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3347	1/1	0.95	0.16	44,44,44,44	0
56	MG	BV	204	1/1	0.95	0.21	50,50,50,50	0
56	MG	BA	3532	1/1	0.95	0.27	49,49,49,49	0
56	MG	BU	205	1/1	0.95	0.22	38,38,38,38	0
56	MG	DA	3021	1/1	0.95	0.30	48,48,48,48	0
56	MG	DA	3337	1/1	0.95	0.09	43,43,43,43	0
56	MG	BA	3517	1/1	0.95	0.12	51,51,51,51	0
56	MG	BA	3794	1/1	0.95	0.20	33,33,33,33	0
56	MG	DA	3076	1/1	0.95	0.22	43,43,43,43	0
56	MG	DA	3244	1/1	0.95	0.13	48,48,48,48	0
56	MG	BA	3126	1/1	0.95	0.26	43,43,43,43	0
56	MG	CA	3160	1/1	0.95	0.16	65,65,65,65	0
56	MG	AA	3108	1/1	0.95	0.20	55,55,55,55	0
56	MG	DA	3245	1/1	0.95	0.10	62,62,62,62	0
56	MG	DA	3013	1/1	0.95	0.17	40,40,40,40	0
56	MG	BA	3834	1/1	0.95	0.13	35,35,35,35	0
56	MG	BA	3539	1/1	0.95	0.21	23,23,23,23	0
56	MG	AA	3207	1/1	0.95	0.14	68,68,68,68	0
56	MG	DA	3617	1/1	0.95	0.36	53,53,53,53	0
56	MG	BF	304	1/1	0.95	0.15	32,32,32,32	0
56	MG	DA	3426	1/1	0.95	0.17	41,41,41,41	0
56	MG	BA	3563	1/1	0.95	0.08	60,60,60,60	0
56	MG	BA	3243	1/1	0.95	0.18	44,44,44,44	0
56	MG	CA	3140	1/1	0.95	0.16	79,79,79,79	0
56	MG	BQ	3004	1/1	0.95	0.24	35,35,35,35	0
56	MG	BA	3191	1/1	0.95	0.26	40,40,40,40	0
56	MG	BA	3134	1/1	0.95	0.15	35,35,35,35	0
56	MG	CA	3107	1/1	0.95	0.10	66,66,66,66	0
56	MG	CA	3150	1/1	0.95	0.16	62,62,62,62	0
56	MG	AA	3132	1/1	0.95	0.13	22,22,22,22	0
56	MG	DA	3360	1/1	0.95	0.16	51,51,51,51	0
56	MG	DA	3077	1/1	0.95	0.18	43,43,43,43	0
56	MG	DA	3265	1/1	0.95	0.31	52,52,52,52	0
56	MG	DA	3163	1/1	0.95	0.27	49,49,49,49	0
56	MG	BA	3536	1/1	0.95	0.18	48,48,48,48	0
56	MG	AA	3191	1/1	0.95	0.24	48,48,48,48	0
56	MG	AA	3220	1/1	0.95	0.07	64,64,64,64	0
56	MG	DA	3357	1/1	0.95	0.14	44,44,44,44	0
56	MG	AA	3014	1/1	0.95	0.12	69,69,69,69	0
56	MG	DA	3575	1/1	0.95	0.10	47,47,47,47	0
56	MG	BA	3432	1/1	0.95	0.10	52,52,52,52	0
56	MG	DA	3125	1/1	0.95	0.26	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3494	1/1	0.95	0.13	57,57,57,57	0
56	MG	DA	3327	1/1	0.95	0.19	59,59,59,59	0
56	MG	DA	3417	1/1	0.95	0.22	33,33,33,33	0
56	MG	DA	3226	1/1	0.95	0.15	54,54,54,54	0
56	MG	AA	3009	1/1	0.95	0.26	46,46,46,46	0
56	MG	AA	3034	1/1	0.95	0.26	48,48,48,48	0
56	MG	BA	3580	1/1	0.95	0.22	42,42,42,42	0
56	MG	DA	3593	1/1	0.95	0.24	39,39,39,39	0
56	MG	BA	3463	1/1	0.95	0.20	37,37,37,37	0
56	MG	BA	3486	1/1	0.95	0.23	48,48,48,48	0
56	MG	DA	3488	1/1	0.95	0.13	37,37,37,37	0
56	MG	AA	3012	1/1	0.95	0.23	33,33,33,33	0
56	MG	BU	206	1/1	0.95	0.34	43,43,43,43	0
56	MG	DA	3462	1/1	0.95	0.28	43,43,43,43	0
56	MG	AA	3163	1/1	0.95	0.15	37,37,37,37	0
56	MG	BA	3216	1/1	0.95	0.21	34,34,34,34	0
56	MG	AA	3124	1/1	0.95	0.20	53,53,53,53	0
56	MG	BA	3362	1/1	0.95	0.25	19,19,19,19	0
56	MG	BA	3598	1/1	0.95	0.15	47,47,47,47	0
56	MG	BA	3608	1/1	0.95	0.21	60,60,60,60	0
56	MG	BA	3800	1/1	0.95	0.15	39,39,39,39	0
56	MG	DF	303	1/1	0.95	0.07	46,46,46,46	0
56	MG	BA	3343	1/1	0.95	0.18	33,33,33,33	0
56	MG	BA	3339	1/1	0.95	0.15	40,40,40,40	0
56	MG	BA	3309	1/1	0.95	0.07	55,55,55,55	0
56	MG	DA	3584	1/1	0.95	0.40	58,58,58,58	0
56	MG	BA	3611	1/1	0.95	0.13	42,42,42,42	0
56	MG	BA	3187	1/1	0.95	0.16	36,36,36,36	0
56	MG	BB	3021	1/1	0.95	0.13	54,54,54,54	0
56	MG	DE	301	1/1	0.95	0.29	45,45,45,45	0
56	MG	BA	3652	1/1	0.95	0.13	46,46,46,46	0
56	MG	BA	3230	1/1	0.95	0.14	62,62,62,62	0
56	MG	DA	3154	1/1	0.95	0.32	52,52,52,52	0
56	MG	CA	3136	1/1	0.95	0.18	65,65,65,65	0
56	MG	DA	3553	1/1	0.95	0.14	54,54,54,54	0
56	MG	BA	3268	1/1	0.95	0.28	58,58,58,58	0
56	MG	DA	3326	1/1	0.95	0.18	46,46,46,46	0
56	MG	DA	3400	1/1	0.95	0.34	39,39,39,39	0
56	MG	BA	3169	1/1	0.95	0.25	47,47,47,47	0
56	MG	DA	3123	1/1	0.95	0.12	47,47,47,47	0
56	MG	DA	3353	1/1	0.95	0.14	37,37,37,37	0
56	MG	DA	3634	1/1	0.95	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3687	1/1	0.95	0.23	36,36,36,36	0
56	MG	BA	3037	1/1	0.95	0.16	37,37,37,37	0
56	MG	BA	3792	1/1	0.95	0.16	32,32,32,32	0
56	MG	BA	3647	1/1	0.95	0.16	45,45,45,45	0
56	MG	DA	3067	1/1	0.95	0.25	49,49,49,49	0
56	MG	BA	3388	1/1	0.95	0.13	52,52,52,52	0
56	MG	DV	3001	1/1	0.95	0.35	71,71,71,71	0
56	MG	DA	3188	1/1	0.95	0.38	50,50,50,50	0
56	MG	DA	3496	1/1	0.95	0.06	48,48,48,48	0
56	MG	DA	3148	1/1	0.95	0.23	29,29,29,29	0
56	MG	CA	3112	1/1	0.95	0.15	59,59,59,59	0
56	MG	DA	3475	1/1	0.95	0.13	42,42,42,42	0
56	MG	BA	3799	1/1	0.95	0.22	47,47,47,47	0
56	MG	BA	3833	1/1	0.95	0.20	43,43,43,43	0
56	MG	BA	3262	1/1	0.95	0.31	47,47,47,47	0
56	MG	DA	3052	1/1	0.95	0.12	38,38,38,38	0
56	MG	DA	3330	1/1	0.95	0.17	46,46,46,46	0
56	MG	DA	3267	1/1	0.95	0.26	38,38,38,38	0
56	MG	DA	3058	1/1	0.95	0.21	46,46,46,46	0
56	MG	BA	3177	1/1	0.95	0.30	44,44,44,44	0
56	MG	DA	3302	1/1	0.95	0.12	33,33,33,33	0
56	MG	CV	3001	1/1	0.95	0.19	58,58,58,58	0
56	MG	BA	3488	1/1	0.95	0.10	50,50,50,50	0
56	MG	BA	3671	1/1	0.95	0.14	45,45,45,45	0
56	MG	BA	3796	1/1	0.95	0.13	40,40,40,40	0
56	MG	DA	3268	1/1	0.95	0.04	60,60,60,60	0
56	MG	DA	3489	1/1	0.95	0.16	37,37,37,37	0
56	MG	BF	301	1/1	0.95	0.26	38,38,38,38	0
56	MG	DA	3084	1/1	0.95	0.27	27,27,27,27	0
56	MG	DA	3555	1/1	0.95	0.08	54,54,54,54	0
56	MG	DA	3264	1/1	0.95	0.13	31,31,31,31	0
56	MG	BA	3577	1/1	0.95	0.19	60,60,60,60	0
56	MG	DA	3130	1/1	0.95	0.25	47,47,47,47	0
56	MG	CA	3165	1/1	0.95	0.08	56,56,56,56	0
56	MG	BA	3471	1/1	0.95	0.06	45,45,45,45	0
56	MG	BA	3222	1/1	0.95	0.36	27,27,27,27	0
56	MG	DB	3007	1/1	0.95	0.09	59,59,59,59	0
56	MG	DA	3232	1/1	0.95	0.28	53,53,53,53	0
56	MG	DA	3040	1/1	0.95	0.11	53,53,53,53	0
56	MG	BA	3263	1/1	0.95	0.18	32,32,32,32	0
56	MG	BA	3635	1/1	0.95	0.28	62,62,62,62	0
56	MG	AA	3069	1/1	0.95	0.21	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3082	1/1	0.95	0.22	34,34,34,34	0
59	ZN	B4	501	1/1	0.95	0.12	73,73,73,73	0
56	MG	DB	3008	1/1	0.95	0.14	68,68,68,68	0
56	MG	BA	3499	1/1	0.95	0.24	33,33,33,33	0
56	MG	DA	3202	1/1	0.95	0.33	50,50,50,50	0
56	MG	CA	3075	1/1	0.95	0.10	44,44,44,44	0
56	MG	DA	3379	1/1	0.95	0.20	59,59,59,59	0
56	MG	DA	3414	1/1	0.95	0.16	41,41,41,41	0
56	MG	BA	3324	1/1	0.95	0.17	34,34,34,34	0
56	MG	BA	3401	1/1	0.95	0.14	48,48,48,48	0
56	MG	AA	3074	1/1	0.95	0.17	47,47,47,47	0
56	MG	BA	3600	1/1	0.95	0.10	56,56,56,56	0
56	MG	CA	3056	1/1	0.95	0.23	60,60,60,60	0
56	MG	BA	3715	1/1	0.95	0.24	53,53,53,53	0
56	MG	BA	3642	1/1	0.95	0.09	37,37,37,37	0
56	MG	AA	3019	1/1	0.95	0.15	48,48,48,48	0
56	MG	DA	3083	1/1	0.95	0.18	51,51,51,51	0
56	MG	AA	3219	1/1	0.95	0.21	65,65,65,65	0
56	MG	BA	3783	1/1	0.95	0.19	53,53,53,53	0
56	MG	BA	3584	1/1	0.95	0.24	27,27,27,27	0
56	MG	DA	3169	1/1	0.95	0.13	49,49,49,49	0
56	MG	BA	3385	1/1	0.95	0.15	39,39,39,39	0
56	MG	AA	3180	1/1	0.95	0.14	57,57,57,57	0
56	MG	DA	3525	1/1	0.95	0.17	41,41,41,41	0
56	MG	BA	3696	1/1	0.95	0.16	33,33,33,33	0
56	MG	DA	3625	1/1	0.95	0.20	53,53,53,53	0
56	MG	AK	202	1/1	0.95	0.26	38,38,38,38	0
56	MG	DA	3413	1/1	0.95	0.20	36,36,36,36	0
56	MG	BA	3403	1/1	0.95	0.28	31,31,31,31	0
56	MG	DA	3240	1/1	0.95	0.17	51,51,51,51	0
56	MG	BA	3067	1/1	0.95	0.23	49,49,49,49	0
56	MG	DA	3042	1/1	0.95	0.15	41,41,41,41	0
56	MG	BA	3051	1/1	0.95	0.23	25,25,25,25	0
56	MG	DA	3362	1/1	0.95	0.22	43,43,43,43	0
56	MG	DA	3063	1/1	0.95	0.14	46,46,46,46	0
56	MG	BA	3380	1/1	0.95	0.12	60,60,60,60	0
56	MG	BD	310	1/1	0.95	0.15	31,31,31,31	0
56	MG	AA	3178	1/1	0.95	0.12	54,54,54,54	0
56	MG	DA	3023	1/1	0.95	0.14	30,30,30,30	0
56	MG	BA	3318	1/1	0.95	0.27	37,37,37,37	0
56	MG	BA	3163	1/1	0.95	0.22	45,45,45,45	0
56	MG	BA	3480	1/1	0.95	0.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DN	5001	1/1	0.95	0.07	62,62,62,62	0
56	MG	BP	203	1/1	0.95	0.12	32,32,32,32	0
56	MG	BA	3390	1/1	0.95	0.21	52,52,52,52	0
56	MG	BF	302	1/1	0.96	0.22	39,39,39,39	0
56	MG	CY	3001	1/1	0.96	0.27	58,58,58,58	0
56	MG	BA	3417	1/1	0.96	0.22	33,33,33,33	0
56	MG	BA	3573	1/1	0.96	0.09	32,32,32,32	0
56	MG	BA	3386	1/1	0.96	0.22	42,42,42,42	0
56	MG	BA	3538	1/1	0.96	0.20	45,45,45,45	0
56	MG	DA	3576	1/1	0.96	0.16	37,37,37,37	0
56	MG	CA	3079	1/1	0.96	0.15	54,54,54,54	0
56	MG	BQ	3001	1/1	0.96	0.23	40,40,40,40	0
56	MG	AA	3182	1/1	0.96	0.20	52,52,52,52	0
56	MG	DA	3519	1/1	0.96	0.17	24,24,24,24	0
56	MG	DA	3416	1/1	0.96	0.34	40,40,40,40	0
56	MG	AA	3122	1/1	0.96	0.19	60,60,60,60	0
56	MG	CX	3003	1/1	0.96	0.38	50,50,50,50	0
56	MG	BA	3245	1/1	0.96	0.28	29,29,29,29	0
56	MG	BE	303	1/1	0.96	0.16	27,27,27,27	0
56	MG	BA	3349	1/1	0.96	0.19	34,34,34,34	0
56	MG	DA	3512	1/1	0.96	0.22	46,46,46,46	0
56	MG	DA	3177	1/1	0.96	0.17	54,54,54,54	0
56	MG	AX	3013	1/1	0.96	0.30	39,39,39,39	0
56	MG	BA	3146	1/1	0.96	0.19	42,42,42,42	0
56	MG	DA	3332	1/1	0.96	0.20	41,41,41,41	0
56	MG	DA	3450	1/1	0.96	0.16	36,36,36,36	0
56	MG	DF	305	1/1	0.96	0.17	43,43,43,43	0
56	MG	DA	3364	1/1	0.96	0.14	38,38,38,38	0
56	MG	BA	3247	1/1	0.96	0.30	28,28,28,28	0
56	MG	CA	3057	1/1	0.96	0.17	58,58,58,58	0
56	MG	B5	101	1/1	0.96	0.14	31,31,31,31	0
56	MG	DA	3431	1/1	0.96	0.17	25,25,25,25	0
56	MG	BA	3189	1/1	0.96	0.16	30,30,30,30	0
56	MG	BA	3468	1/1	0.96	0.23	49,49,49,49	0
56	MG	DA	3277	1/1	0.96	0.10	56,56,56,56	0
56	MG	BA	3085	1/1	0.96	0.13	31,31,31,31	0
56	MG	BA	3242	1/1	0.96	0.33	42,42,42,42	0
56	MG	DA	3080	1/1	0.96	0.22	45,45,45,45	0
56	MG	DA	3579	1/1	0.96	0.07	55,55,55,55	0
56	MG	AA	3060	1/1	0.96	0.21	59,59,59,59	0
56	MG	DA	3666	1/1	0.96	0.22	41,41,41,41	0
56	MG	DA	3490	1/1	0.96	0.18	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3552	1/1	0.96	0.26	34,34,34,34	0
56	MG	BA	3258	1/1	0.96	0.28	41,41,41,41	0
56	MG	BA	3040	1/1	0.96	0.14	47,47,47,47	0
56	MG	DW	3003	1/1	0.96	0.34	47,47,47,47	0
56	MG	BA	3325	1/1	0.96	0.28	56,56,56,56	0
56	MG	BA	3612	1/1	0.96	0.10	62,62,62,62	0
56	MG	DA	3492	1/1	0.96	0.12	47,47,47,47	0
56	MG	DA	3373	1/1	0.96	0.10	31,31,31,31	0
56	MG	BA	3184	1/1	0.96	0.12	30,30,30,30	0
56	MG	DA	3262	1/1	0.96	0.12	43,43,43,43	0
59	ZN	D6	501	1/1	0.96	0.11	73,73,73,73	0
56	MG	CA	3110	1/1	0.96	0.11	48,48,48,48	0
56	MG	AA	3006	1/1	0.96	0.14	37,37,37,37	0
56	MG	BA	3389	1/1	0.96	0.28	37,37,37,37	0
56	MG	BA	3498	1/1	0.96	0.07	54,54,54,54	0
56	MG	BF	312	1/1	0.96	0.14	47,47,47,47	0
56	MG	DA	3088	1/1	0.96	0.18	42,42,42,42	0
56	MG	BA	3459	1/1	0.96	0.17	48,48,48,48	0
56	MG	BA	3521	1/1	0.96	0.13	36,36,36,36	0
56	MG	BA	3159	1/1	0.96	0.22	30,30,30,30	0
56	MG	BA	3027	1/1	0.96	0.20	42,42,42,42	0
56	MG	BA	3297	1/1	0.96	0.55	55,55,55,55	0
56	MG	BD	311	1/1	0.96	0.21	51,51,51,51	0
56	MG	BA	3660	1/1	0.96	0.18	51,51,51,51	0
56	MG	AA	3121	1/1	0.96	0.15	66,66,66,66	0
56	MG	CA	3096	1/1	0.96	0.15	61,61,61,61	0
56	MG	DA	3315	1/1	0.96	0.17	41,41,41,41	0
56	MG	BA	3398	1/1	0.96	0.20	42,42,42,42	0
56	MG	DV	3003	1/1	0.96	0.12	52,52,52,52	0
56	MG	DA	3411	1/1	0.96	0.17	46,46,46,46	0
56	MG	BA	3038	1/1	0.96	0.30	47,47,47,47	0
56	MG	DA	3463	1/1	0.96	0.15	37,37,37,37	0
56	MG	BA	3075	1/1	0.96	0.20	27,27,27,27	0
56	MG	AA	3133	1/1	0.96	0.23	30,30,30,30	0
56	MG	DA	3230	1/1	0.96	0.15	33,33,33,33	0
56	MG	BA	3299	1/1	0.96	0.15	32,32,32,32	0
56	MG	BA	3068	1/1	0.96	0.26	51,51,51,51	0
56	MG	B0	102	1/1	0.96	0.12	68,68,68,68	0
56	MG	AX	3011	1/1	0.96	0.16	50,50,50,50	0
56	MG	BA	3308	1/1	0.96	0.21	39,39,39,39	0
56	MG	BA	3025	1/1	0.96	0.15	38,38,38,38	0
56	MG	BA	3643	1/1	0.96	0.20	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3397	1/1	0.96	0.23	53,53,53,53	0
56	MG	DA	3128	1/1	0.96	0.07	45,45,45,45	0
56	MG	BA	3746	1/1	0.96	0.33	25,25,25,25	0
56	MG	DA	3266	1/1	0.96	0.10	47,47,47,47	0
56	MG	DA	3129	1/1	0.96	0.12	45,45,45,45	0
56	MG	DA	3558	1/1	0.96	0.25	34,34,34,34	0
56	MG	BA	3515	1/1	0.96	0.21	20,20,20,20	0
56	MG	BA	3176	1/1	0.96	0.29	55,55,55,55	0
56	MG	CA	3116	1/1	0.96	0.06	55,55,55,55	0
56	MG	BA	3452	1/1	0.96	0.30	27,27,27,27	0
56	MG	DA	3198	1/1	0.96	0.08	51,51,51,51	0
56	MG	BA	3596	1/1	0.96	0.32	45,45,45,45	0
56	MG	BA	3084	1/1	0.96	0.18	45,45,45,45	0
56	MG	BA	3784	1/1	0.96	0.22	52,52,52,52	0
56	MG	CA	3048	1/1	0.96	0.27	52,52,52,52	0
56	MG	AA	3168	1/1	0.96	0.08	62,62,62,62	0
56	MG	AA	3104	1/1	0.96	0.20	50,50,50,50	0
56	MG	CA	3009	1/1	0.96	0.22	50,50,50,50	0
56	MG	CA	3174	1/1	0.96	0.25	46,46,46,46	0
56	MG	DA	3217	1/1	0.96	0.14	50,50,50,50	0
56	MG	DA	3486	1/1	0.96	0.22	44,44,44,44	0
56	MG	BP	201	1/1	0.96	0.39	41,41,41,41	0
56	MG	DA	3522	1/1	0.96	0.29	25,25,25,25	0
56	MG	BA	3239	1/1	0.96	0.15	31,31,31,31	0
56	MG	BA	3461	1/1	0.96	0.19	31,31,31,31	0
56	MG	BA	3764	1/1	0.96	0.12	58,58,58,58	0
56	MG	BA	3826	1/1	0.96	0.22	33,33,33,33	0
56	MG	CA	3135	1/1	0.96	0.11	53,53,53,53	0
56	MG	BA	3630	1/1	0.96	0.08	30,30,30,30	0
56	MG	BA	3338	1/1	0.96	0.16	41,41,41,41	0
56	MG	CA	3062	1/1	0.96	0.23	44,44,44,44	0
56	MG	DA	3136	1/1	0.96	0.22	44,44,44,44	0
56	MG	DA	3590	1/1	0.96	0.19	60,60,60,60	0
56	MG	DA	3298	1/1	0.96	0.17	33,33,33,33	0
56	MG	BD	305	1/1	0.96	0.14	37,37,37,37	0
56	MG	BA	3147	1/1	0.96	0.13	30,30,30,30	0
56	MG	DB	3001	1/1	0.96	0.04	73,73,73,73	0
56	MG	CA	3102	1/1	0.96	0.09	54,54,54,54	0
56	MG	BA	3161	1/1	0.96	0.23	37,37,37,37	0
56	MG	BA	3555	1/1	0.96	0.29	33,33,33,33	0
56	MG	DA	3341	1/1	0.96	0.21	31,31,31,31	0
56	MG	DA	3166	1/1	0.96	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3299	1/1	0.96	0.24	43,43,43,43	0
56	MG	DA	3481	1/1	0.96	0.18	30,30,30,30	0
56	MG	BA	3209	1/1	0.96	0.12	41,41,41,41	0
56	MG	AA	3217	1/1	0.96	0.16	55,55,55,55	0
56	MG	BA	3627	1/1	0.96	0.17	45,45,45,45	0
56	MG	BA	3148	1/1	0.96	0.27	15,15,15,15	0
56	MG	BA	3785	1/1	0.96	0.16	41,41,41,41	0
56	MG	DA	3472	1/1	0.96	0.06	33,33,33,33	0
56	MG	DA	3662	1/1	0.96	0.09	27,27,27,27	0
56	MG	DA	3386	1/1	0.96	0.17	48,48,48,48	0
56	MG	AA	3025	1/1	0.96	0.12	43,43,43,43	0
56	MG	BA	3301	1/1	0.96	0.14	26,26,26,26	0
56	MG	CE	201	1/1	0.96	0.19	50,50,50,50	0
56	MG	BA	3540	1/1	0.96	0.17	44,44,44,44	0
56	MG	DA	3412	1/1	0.96	0.16	63,63,63,63	0
56	MG	BA	3285	1/1	0.96	0.37	49,49,49,49	0
56	MG	CA	3141	1/1	0.96	0.17	49,49,49,49	0
56	MG	AA	3203	1/1	0.96	0.34	57,57,57,57	0
56	MG	DA	3629	1/1	0.96	0.22	52,52,52,52	0
56	MG	BA	3082	1/1	0.96	0.11	59,59,59,59	0
56	MG	DA	3627	1/1	0.96	0.04	48,48,48,48	0
56	MG	DA	3257	1/1	0.96	0.20	34,34,34,34	0
56	MG	DA	3471	1/1	0.96	0.15	50,50,50,50	0
56	MG	CA	3155	1/1	0.96	0.14	50,50,50,50	0
56	MG	BA	3507	1/1	0.96	0.12	39,39,39,39	0
56	MG	BA	3733	1/1	0.96	0.26	41,41,41,41	0
56	MG	DA	3016	1/1	0.96	0.12	53,53,53,53	0
56	MG	DA	3010	1/1	0.96	0.07	43,43,43,43	0
56	MG	DA	3164	1/1	0.96	0.26	33,33,33,33	0
56	MG	CA	3156	1/1	0.96	0.10	68,68,68,68	0
56	MG	BA	3490	1/1	0.96	0.22	44,44,44,44	0
56	MG	DB	3009	1/1	0.96	0.19	47,47,47,47	0
56	MG	DA	3307	1/1	0.96	0.08	45,45,45,45	0
56	MG	DA	3352	1/1	0.96	0.15	35,35,35,35	0
56	MG	BA	3684	1/1	0.96	0.20	49,49,49,49	0
56	MG	DA	3062	1/1	0.96	0.18	53,53,53,53	0
56	MG	BA	3006	1/1	0.96	0.15	52,52,52,52	0
56	MG	AA	3177	1/1	0.96	0.14	57,57,57,57	0
56	MG	BA	3208	1/1	0.96	0.32	48,48,48,48	0
56	MG	BA	3473	1/1	0.96	0.28	57,57,57,57	0
56	MG	AM	201	1/1	0.96	0.05	50,50,50,50	0
56	MG	DA	3658	1/1	0.96	0.39	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3517	1/1	0.96	0.10	47,47,47,47	0
56	MG	BB	3014	1/1	0.96	0.14	69,69,69,69	0
56	MG	CA	3130	1/1	0.96	0.12	60,60,60,60	0
56	MG	BA	3541	1/1	0.96	0.14	29,29,29,29	0
56	MG	DA	3151	1/1	0.96	0.26	44,44,44,44	0
56	MG	BA	3562	1/1	0.96	0.18	35,35,35,35	0
56	MG	DA	3091	1/1	0.96	0.18	43,43,43,43	0
56	MG	DF	304	1/1	0.96	0.22	39,39,39,39	0
56	MG	BA	3073	1/1	0.96	0.17	41,41,41,41	0
56	MG	BE	308	1/1	0.96	0.17	21,21,21,21	0
56	MG	BA	3534	1/1	0.96	0.30	31,31,31,31	0
56	MG	DA	3455	1/1	0.96	0.18	27,27,27,27	0
56	MG	AA	3001	1/1	0.96	0.18	34,34,34,34	0
56	MG	BA	3103	1/1	0.96	0.33	48,48,48,48	0
56	MG	DA	3004	1/1	0.96	0.19	42,42,42,42	0
56	MG	DA	3421	1/1	0.96	0.21	53,53,53,53	0
56	MG	DA	3494	1/1	0.96	0.18	30,30,30,30	0
56	MG	B3	103	1/1	0.96	0.07	45,45,45,45	0
56	MG	DA	3049	1/1	0.96	0.22	24,24,24,24	0
56	MG	BA	3167	1/1	0.96	0.19	50,50,50,50	0
56	MG	DA	3289	1/1	0.96	0.36	42,42,42,42	0
56	MG	AE	3001	1/1	0.96	0.06	66,66,66,66	0
56	MG	DA	3193	1/1	0.96	0.33	40,40,40,40	0
56	MG	BA	3215	1/1	0.96	0.30	45,45,45,45	0
56	MG	DA	3276	1/1	0.96	0.08	33,33,33,33	0
56	MG	DA	3501	1/1	0.96	0.15	59,59,59,59	0
56	MG	BA	3710	1/1	0.96	0.19	28,28,28,28	0
56	MG	DA	3284	1/1	0.96	0.18	40,40,40,40	0
56	MG	DA	3153	1/1	0.96	0.15	44,44,44,44	0
56	MG	AY	3001	1/1	0.96	0.31	70,70,70,70	0
56	MG	CA	3163	1/1	0.96	0.17	53,53,53,53	0
56	MG	AA	3007	1/1	0.96	0.26	65,65,65,65	0
56	MG	BA	3755	1/1	0.96	0.19	52,52,52,52	0
56	MG	BA	3086	1/1	0.96	0.28	41,41,41,41	0
56	MG	CA	3166	1/1	0.96	0.13	66,66,66,66	0
56	MG	DA	3594	1/1	0.96	0.07	44,44,44,44	0
56	MG	CA	3093	1/1	0.96	0.17	34,34,34,34	0
56	MG	BA	3744	1/1	0.96	0.13	20,20,20,20	0
56	MG	DA	3143	1/1	0.96	0.23	50,50,50,50	0
56	MG	BA	3713	1/1	0.96	0.23	54,54,54,54	0
56	MG	AA	3146	1/1	0.96	0.11	53,53,53,53	0
56	MG	DA	3349	1/1	0.96	0.11	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3196	1/1	0.97	0.13	32,32,32,32	0
56	MG	BA	3154	1/1	0.97	0.28	29,29,29,29	0
56	MG	DA	3543	1/1	0.97	0.23	55,55,55,55	0
56	MG	BA	3450	1/1	0.97	0.28	34,34,34,34	0
56	MG	DA	3336	1/1	0.97	0.09	47,47,47,47	0
56	MG	AW	3007	1/1	0.97	0.05	64,64,64,64	0
56	MG	BA	3816	1/1	0.97	0.19	21,21,21,21	0
56	MG	BA	3336	1/1	0.97	0.13	35,35,35,35	0
56	MG	BA	3384	1/1	0.97	0.23	30,30,30,30	0
56	MG	DA	3124	1/1	0.97	0.19	34,34,34,34	0
56	MG	BA	3767	1/1	0.97	0.11	29,29,29,29	0
56	MG	AA	3167	1/1	0.97	0.21	47,47,47,47	0
56	MG	BA	3168	1/1	0.97	0.19	27,27,27,27	0
56	MG	BA	3123	1/1	0.97	0.16	35,35,35,35	0
56	MG	BA	3072	1/1	0.97	0.14	30,30,30,30	0
56	MG	BA	3303	1/1	0.97	0.17	35,35,35,35	0
56	MG	BA	3546	1/1	0.97	0.26	30,30,30,30	0
56	MG	DA	3275	1/1	0.97	0.09	52,52,52,52	0
56	MG	BA	3551	1/1	0.97	0.19	33,33,33,33	0
56	MG	DA	3346	1/1	0.97	0.15	35,35,35,35	0
56	MG	BA	3565	1/1	0.97	0.24	42,42,42,42	0
56	MG	DY	502	1/1	0.97	0.12	52,52,52,52	0
56	MG	AA	3160	1/1	0.97	0.14	57,57,57,57	0
56	MG	DA	3654	1/1	0.97	0.11	55,55,55,55	0
56	MG	DA	3599	1/1	0.97	0.24	38,38,38,38	0
56	MG	BA	3111	1/1	0.97	0.23	47,47,47,47	0
56	MG	DQ	3002	1/1	0.97	0.17	42,42,42,42	0
56	MG	BA	3465	1/1	0.97	0.19	42,42,42,42	0
56	MG	BA	3048	1/1	0.97	0.25	28,28,28,28	0
56	MG	DA	3253	1/1	0.97	0.22	38,38,38,38	0
56	MG	BA	3443	1/1	0.97	0.12	25,25,25,25	0
56	MG	BA	3624	1/1	0.97	0.18	29,29,29,29	0
56	MG	DA	3189	1/1	0.97	0.25	48,48,48,48	0
56	MG	BA	3076	1/1	0.97	0.29	23,23,23,23	0
56	MG	AA	3076	1/1	0.97	0.17	55,55,55,55	0
56	MG	AA	3070	1/1	0.97	0.23	49,49,49,49	0
56	MG	BR	204	1/1	0.97	0.36	42,42,42,42	0
56	MG	BA	3029	1/1	0.97	0.31	46,46,46,46	0
56	MG	DA	3644	1/1	0.97	0.49	55,55,55,55	0
56	MG	BA	3561	1/1	0.97	0.15	27,27,27,27	0
56	MG	BA	3811	1/1	0.97	0.31	38,38,38,38	0
56	MG	DA	3651	1/1	0.97	0.16	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3428	1/1	0.97	0.10	61,61,61,61	0
56	MG	BA	3822	1/1	0.97	0.20	21,21,21,21	0
56	MG	DA	3344	1/1	0.97	0.09	44,44,44,44	0
56	MG	DQ	3001	1/1	0.97	0.11	48,48,48,48	0
56	MG	BA	3615	1/1	0.97	0.28	35,35,35,35	0
56	MG	DA	3314	1/1	0.97	0.18	33,33,33,33	0
56	MG	DA	3249	1/1	0.97	0.27	41,41,41,41	0
56	MG	BA	3012	1/1	0.97	0.21	26,26,26,26	0
56	MG	DA	3047	1/1	0.97	0.21	49,49,49,49	0
56	MG	BA	3656	1/1	0.97	0.18	45,45,45,45	0
56	MG	DA	3660	1/1	0.97	0.19	40,40,40,40	0
56	MG	BA	3775	1/1	0.97	0.17	43,43,43,43	0
56	MG	DA	3114	1/1	0.97	0.13	28,28,28,28	0
56	MG	DA	3624	1/1	0.97	0.07	47,47,47,47	0
56	MG	DA	3427	1/1	0.97	0.08	38,38,38,38	0
56	MG	D7	102	1/1	0.97	0.22	43,43,43,43	0
56	MG	BA	3026	1/1	0.97	0.14	19,19,19,19	0
56	MG	DA	3552	1/1	0.97	0.07	43,43,43,43	0
56	MG	BD	302	1/1	0.97	0.16	23,23,23,23	0
56	MG	BA	3036	1/1	0.97	0.18	26,26,26,26	0
56	MG	BA	3118	1/1	0.97	0.34	38,38,38,38	0
56	MG	CA	3131	1/1	0.97	0.18	55,55,55,55	0
56	MG	DA	3118	1/1	0.97	0.25	52,52,52,52	0
56	MG	BA	3607	1/1	0.97	0.26	40,40,40,40	0
56	MG	BA	3335	1/1	0.97	0.17	50,50,50,50	0
56	MG	B8	103	1/1	0.97	0.22	48,48,48,48	0
56	MG	BA	3054	1/1	0.97	0.17	30,30,30,30	0
56	MG	DA	3371	1/1	0.97	0.17	55,55,55,55	0
56	MG	DA	3582	1/1	0.97	0.11	39,39,39,39	0
56	MG	AA	3227	1/1	0.97	0.18	48,48,48,48	0
56	MG	DA	3200	1/1	0.97	0.35	43,43,43,43	0
56	MG	DA	3290	1/1	0.97	0.17	44,44,44,44	0
56	MG	DA	3045	1/1	0.97	0.12	47,47,47,47	0
56	MG	BA	3044	1/1	0.97	0.25	49,49,49,49	0
56	MG	AA	3179	1/1	0.97	0.35	79,79,79,79	0
56	MG	DA	3120	1/1	0.97	0.19	45,45,45,45	0
56	MG	BA	3556	1/1	0.97	0.11	45,45,45,45	0
56	MG	DA	3340	1/1	0.97	0.21	42,42,42,42	0
56	MG	BA	3653	1/1	0.97	0.28	49,49,49,49	0
56	MG	DA	3108	1/1	0.97	0.22	30,30,30,30	0
56	MG	DA	3385	1/1	0.97	0.14	55,55,55,55	0
56	MG	BA	3372	1/1	0.97	0.22	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3122	1/1	0.97	0.18	26,26,26,26	0
56	MG	DD	301	1/1	0.97	0.37	39,39,39,39	0
56	MG	DA	3012	1/1	0.97	0.18	39,39,39,39	0
56	MG	DA	3425	1/1	0.97	0.07	45,45,45,45	0
56	MG	CA	3008	1/1	0.97	0.12	50,50,50,50	0
56	MG	BB	3023	1/1	0.97	0.11	46,46,46,46	0
56	MG	DG	3001	1/1	0.97	0.04	56,56,56,56	0
56	MG	BA	3535	1/1	0.97	0.25	18,18,18,18	0
56	MG	AA	3088	1/1	0.97	0.30	56,56,56,56	0
56	MG	B8	102	1/1	0.97	0.08	50,50,50,50	0
56	MG	BA	3795	1/1	0.97	0.16	53,53,53,53	0
56	MG	BA	3497	1/1	0.97	0.21	41,41,41,41	0
56	MG	BA	3009	1/1	0.97	0.17	25,25,25,25	0
56	MG	DA	3207	1/1	0.97	0.29	57,57,57,57	0
56	MG	BA	3042	1/1	0.97	0.18	40,40,40,40	0
56	MG	DU	3001	1/1	0.97	0.25	50,50,50,50	0
56	MG	AA	3214	1/1	0.97	0.15	44,44,44,44	0
56	MG	DA	3571	1/1	0.97	0.16	57,57,57,57	0
56	MG	DA	3071	1/1	0.97	0.37	44,44,44,44	0
56	MG	BA	3069	1/1	0.97	0.14	31,31,31,31	0
56	MG	AA	3164	1/1	0.97	0.24	50,50,50,50	0
56	MG	DA	3009	1/1	0.97	0.19	38,38,38,38	0
56	MG	AA	3037	1/1	0.97	0.24	44,44,44,44	0
56	MG	BA	3217	1/1	0.97	0.21	20,20,20,20	0
56	MG	BA	3824	1/1	0.97	0.12	43,43,43,43	0
56	MG	BA	3395	1/1	0.97	0.19	44,44,44,44	0
56	MG	BA	3043	1/1	0.97	0.30	39,39,39,39	0
56	MG	BA	3678	1/1	0.97	0.22	58,58,58,58	0
56	MG	BB	3006	1/1	0.97	0.14	38,38,38,38	0
56	MG	BA	3547	1/1	0.97	0.19	41,41,41,41	0
56	MG	CA	3158	1/1	0.97	0.19	53,53,53,53	0
56	MG	DA	3479	1/1	0.97	0.17	50,50,50,50	0
56	MG	DA	3573	1/1	0.97	0.31	46,46,46,46	0
56	MG	DA	3024	1/1	0.97	0.44	40,40,40,40	0
56	MG	CA	3078	1/1	0.97	0.16	48,48,48,48	0
56	MG	BD	304	1/1	0.97	0.20	48,48,48,48	0
56	MG	DA	3006	1/1	0.97	0.15	43,43,43,43	0
56	MG	BA	3391	1/1	0.97	0.14	41,41,41,41	0
56	MG	DA	3175	1/1	0.97	0.08	53,53,53,53	0
56	MG	BA	3644	1/1	0.97	0.10	36,36,36,36	0
56	MG	DA	3668	1/1	0.97	0.15	79,79,79,79	0
56	MG	BA	3737	1/1	0.97	0.11	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3793	1/1	0.97	0.20	38,38,38,38	0
56	MG	BA	3195	1/1	0.97	0.27	50,50,50,50	0
56	MG	CA	3045	1/1	0.97	0.36	58,58,58,58	0
56	MG	AA	3172	1/1	0.97	0.16	47,47,47,47	0
56	MG	DA	3322	1/1	0.97	0.29	43,43,43,43	0
56	MG	CA	3108	1/1	0.97	0.14	51,51,51,51	0
56	MG	CA	3089	1/1	0.97	0.07	58,58,58,58	0
56	MG	DA	3459	1/1	0.97	0.07	57,57,57,57	0
56	MG	DA	3456	1/1	0.97	0.20	49,49,49,49	0
56	MG	BA	3518	1/1	0.97	0.20	43,43,43,43	0
56	MG	BA	3010	1/1	0.97	0.13	29,29,29,29	0
56	MG	BA	3332	1/1	0.97	0.17	30,30,30,30	0
56	MG	BA	3024	1/1	0.97	0.27	22,22,22,22	0
56	MG	BA	3776	1/1	0.97	0.14	49,49,49,49	0
56	MG	BA	3121	1/1	0.97	0.36	41,41,41,41	0
56	MG	BA	3373	1/1	0.97	0.18	38,38,38,38	0
56	MG	BA	3421	1/1	0.97	0.22	33,33,33,33	0
56	MG	DA	3530	1/1	0.97	0.23	55,55,55,55	0
56	MG	BA	3013	1/1	0.97	0.28	34,34,34,34	0
56	MG	AA	3200	1/1	0.97	0.22	45,45,45,45	0
56	MG	DA	3334	1/1	0.97	0.17	32,32,32,32	0
56	MG	DA	3345	1/1	0.97	0.18	35,35,35,35	0
56	MG	B0	103	1/1	0.97	0.06	54,54,54,54	0
56	MG	BA	3340	1/1	0.97	0.13	45,45,45,45	0
56	MG	BA	3155	1/1	0.97	0.12	54,54,54,54	0
56	MG	BA	3415	1/1	0.97	0.20	29,29,29,29	0
56	MG	DA	3055	1/1	0.97	0.24	36,36,36,36	0
56	MG	DA	3435	1/1	0.97	0.16	44,44,44,44	0
56	MG	BA	3836	1/1	0.97	0.29	45,45,45,45	0
56	MG	BA	3489	1/1	0.97	0.11	44,44,44,44	0
56	MG	BA	3610	1/1	0.97	0.16	64,64,64,64	0
56	MG	BA	3363	1/1	0.97	0.19	50,50,50,50	0
56	MG	AA	3013	1/1	0.97	0.07	51,51,51,51	0
56	MG	BA	3108	1/1	0.97	0.19	24,24,24,24	0
56	MG	DA	3113	1/1	0.97	0.29	44,44,44,44	0
56	MG	DA	3520	1/1	0.97	0.05	48,48,48,48	0
56	MG	DA	3003	1/1	0.97	0.26	20,20,20,20	0
56	MG	BA	3211	1/1	0.97	0.28	36,36,36,36	0
56	MG	BA	3178	1/1	0.97	0.25	38,38,38,38	0
56	MG	BA	3513	1/1	0.97	0.15	34,34,34,34	0
56	MG	DA	3313	1/1	0.97	0.20	23,23,23,23	0
56	MG	BA	3035	1/1	0.97	0.14	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3319	1/1	0.97	0.29	20,20,20,20	0
56	MG	BA	3549	1/1	0.97	0.19	37,37,37,37	0
56	MG	BA	3495	1/1	0.97	0.24	34,34,34,34	0
56	MG	DA	3446	1/1	0.97	0.32	47,47,47,47	0
56	MG	BA	3056	1/1	0.97	0.28	33,33,33,33	0
56	MG	BA	3032	1/1	0.97	0.21	38,38,38,38	0
56	MG	DA	3447	1/1	0.97	0.27	35,35,35,35	0
56	MG	BB	3007	1/1	0.97	0.09	36,36,36,36	0
56	MG	DA	3317	1/1	0.97	0.15	55,55,55,55	0
56	MG	DA	3237	1/1	0.97	0.07	51,51,51,51	0
56	MG	BA	3781	1/1	0.97	0.21	52,52,52,52	0
56	MG	BA	3166	1/1	0.97	0.22	40,40,40,40	0
56	MG	DA	3022	1/1	0.97	0.21	40,40,40,40	0
56	MG	DA	3622	1/1	0.97	0.18	53,53,53,53	0
56	MG	DA	3570	1/1	0.97	0.10	49,49,49,49	0
56	MG	DA	3528	1/1	0.97	0.09	57,57,57,57	0
56	MG	AA	3123	1/1	0.97	0.17	57,57,57,57	0
56	MG	DA	3308	1/1	0.97	0.16	45,45,45,45	0
56	MG	BA	3525	1/1	0.97	0.18	52,52,52,52	0
56	MG	BE	301	1/1	0.97	0.20	23,23,23,23	0
56	MG	AA	3063	1/1	0.97	0.07	63,63,63,63	0
56	MG	BA	3087	1/1	0.97	0.12	37,37,37,37	0
56	MG	DA	3056	1/1	0.97	0.25	44,44,44,44	0
56	MG	BA	3806	1/1	0.97	0.17	51,51,51,51	0
56	MG	BA	3074	1/1	0.97	0.24	32,32,32,32	0
56	MG	AA	3117	1/1	0.97	0.16	48,48,48,48	0
56	MG	DA	3532	1/1	0.97	0.14	57,57,57,57	0
56	MG	BA	3823	1/1	0.97	0.08	53,53,53,53	0
56	MG	BA	3331	1/1	0.97	0.14	32,32,32,32	0
56	MG	BG	201	1/1	0.97	0.09	57,57,57,57	0
56	MG	BA	3119	1/1	0.97	0.19	36,36,36,36	0
56	MG	DA	3469	1/1	0.97	0.13	54,54,54,54	0
56	MG	DA	3392	1/1	0.97	0.15	36,36,36,36	0
56	MG	BA	3234	1/1	0.97	0.25	48,48,48,48	0
60	K	AX	3001	1/1	0.97	0.22	57,57,57,57	0
56	MG	CA	3050	1/1	0.97	0.14	60,60,60,60	0
56	MG	BR	205	1/1	0.97	0.15	29,29,29,29	0
56	MG	CA	3042	1/1	0.97	0.12	58,58,58,58	0
56	MG	DA	3588	1/1	0.97	0.16	39,39,39,39	0
56	MG	BA	3165	1/1	0.97	0.26	40,40,40,40	0
56	MG	DA	3382	1/1	0.97	0.12	44,44,44,44	0
56	MG	BA	3694	1/1	0.97	0.23	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3510	1/1	0.97	0.24	50,50,50,50	0
56	MG	AA	3201	1/1	0.97	0.07	59,59,59,59	0
56	MG	DA	3038	1/1	0.97	0.43	47,47,47,47	0
56	MG	CA	3127	1/1	0.97	0.17	44,44,44,44	0
56	MG	BA	3591	1/1	0.97	0.21	23,23,23,23	0
56	MG	AA	3195	1/1	0.98	0.15	59,59,59,59	0
56	MG	AA	3154	1/1	0.98	0.14	59,59,59,59	0
56	MG	BA	3632	1/1	0.98	0.17	55,55,55,55	0
56	MG	DA	3482	1/1	0.98	0.17	50,50,50,50	0
58	SF4	CD	501	8/8	0.98	0.10	54,64,76,87	0
56	MG	BA	3405	1/1	0.98	0.18	33,33,33,33	0
56	MG	DA	3158	1/1	0.98	0.26	40,40,40,40	0
56	MG	DA	3292	1/1	0.98	0.12	37,37,37,37	0
56	MG	AA	3131	1/1	0.98	0.32	63,63,63,63	0
56	MG	BA	3107	1/1	0.98	0.19	20,20,20,20	0
56	MG	B7	101	1/1	0.98	0.14	33,33,33,33	0
56	MG	BA	3174	1/1	0.98	0.16	34,34,34,34	0
56	MG	BA	3288	1/1	0.98	0.38	40,40,40,40	0
56	MG	CA	3044	1/1	0.98	0.23	55,55,55,55	0
56	MG	BA	3080	1/1	0.98	0.10	24,24,24,24	0
56	MG	DA	3524	1/1	0.98	0.06	38,38,38,38	0
56	MG	BA	3649	1/1	0.98	0.10	43,43,43,43	0
56	MG	DA	3171	1/1	0.98	0.28	38,38,38,38	0
56	MG	DA	3670	1/1	0.98	0.13	38,38,38,38	0
56	MG	DO	5001	1/1	0.98	0.16	51,51,51,51	0
56	MG	AA	3151	1/1	0.98	0.16	41,41,41,41	0
56	MG	BA	3185	1/1	0.98	0.20	32,32,32,32	0
56	MG	DA	3560	1/1	0.98	0.19	34,34,34,34	0
56	MG	DA	3165	1/1	0.98	0.29	33,33,33,33	0
56	MG	BA	3780	1/1	0.98	0.12	41,41,41,41	0
56	MG	BA	3018	1/1	0.98	0.25	34,34,34,34	0
56	MG	BA	3226	1/1	0.98	0.24	41,41,41,41	0
56	MG	BA	3466	1/1	0.98	0.17	28,28,28,28	0
56	MG	BN	3004	1/1	0.98	0.20	50,50,50,50	0
56	MG	DA	3363	1/1	0.98	0.38	54,54,54,54	0
56	MG	DA	3015	1/1	0.98	0.26	31,31,31,31	0
56	MG	BA	3193	1/1	0.98	0.28	57,57,57,57	0
56	MG	BN	3003	1/1	0.98	0.15	38,38,38,38	0
56	MG	DA	3361	1/1	0.98	0.36	55,55,55,55	0
56	MG	BF	309	1/1	0.98	0.16	30,30,30,30	0
56	MG	DA	3227	1/1	0.98	0.21	38,38,38,38	0
56	MG	CA	3047	1/1	0.98	0.24	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3329	1/1	0.98	0.21	29,29,29,29	0
56	MG	BA	3675	1/1	0.98	0.17	37,37,37,37	0
56	MG	DA	3161	1/1	0.98	0.20	49,49,49,49	0
56	MG	DA	3215	1/1	0.98	0.20	37,37,37,37	0
56	MG	DA	3653	1/1	0.98	0.15	58,58,58,58	0
56	MG	CA	3039	1/1	0.98	0.23	50,50,50,50	0
56	MG	BA	3282	1/1	0.98	0.30	24,24,24,24	0
56	MG	BA	3487	1/1	0.98	0.24	25,25,25,25	0
56	MG	BA	3730	1/1	0.98	0.13	27,27,27,27	0
56	MG	BA	3160	1/1	0.98	0.17	32,32,32,32	0
56	MG	BA	3353	1/1	0.98	0.10	49,49,49,49	0
56	MG	BA	3091	1/1	0.98	0.32	38,38,38,38	0
56	MG	DA	3430	1/1	0.98	0.21	28,28,28,28	0
59	ZN	BY	501	1/1	0.98	0.11	58,58,58,58	0
56	MG	DA	3112	1/1	0.98	0.26	42,42,42,42	0
56	MG	BA	3078	1/1	0.98	0.19	17,17,17,17	0
56	MG	DA	3252	1/1	0.98	0.20	29,29,29,29	0
56	MG	BA	3418	1/1	0.98	0.16	32,32,32,32	0
56	MG	BA	3813	1/1	0.98	0.19	4,4,4,4	0
56	MG	BA	3476	1/1	0.98	0.21	24,24,24,24	0
56	MG	CA	3138	1/1	0.98	0.14	59,59,59,59	0
56	MG	CA	3058	1/1	0.98	0.14	70,70,70,70	0
56	MG	BA	3369	1/1	0.98	0.17	55,55,55,55	0
56	MG	BU	207	1/1	0.98	0.14	29,29,29,29	0
56	MG	BA	3265	1/1	0.98	0.27	29,29,29,29	0
56	MG	BA	3821	1/1	0.98	0.17	50,50,50,50	0
56	MG	BA	3104	1/1	0.98	0.19	27,27,27,27	0
56	MG	BA	3817	1/1	0.98	0.17	47,47,47,47	0
56	MG	DA	3294	1/1	0.98	0.26	42,42,42,42	0
56	MG	BA	3646	1/1	0.98	0.19	38,38,38,38	0
56	MG	DA	3473	1/1	0.98	0.06	49,49,49,49	0
56	MG	AF	3001	1/1	0.98	0.26	40,40,40,40	0
56	MG	DA	3389	1/1	0.98	0.06	53,53,53,53	0
56	MG	BD	303	1/1	0.98	0.15	44,44,44,44	0
56	MG	DA	3316	1/1	0.98	0.06	44,44,44,44	0
56	MG	DA	3116	1/1	0.98	0.10	57,57,57,57	0
56	MG	BA	3142	1/1	0.98	0.14	34,34,34,34	0
56	MG	DA	3064	1/1	0.98	0.10	64,64,64,64	0
56	MG	AA	3224	1/1	0.98	0.15	33,33,33,33	0
59	ZN	AN	501	1/1	0.98	0.12	58,58,58,58	0
56	MG	BA	3041	1/1	0.98	0.25	18,18,18,18	0
56	MG	BA	3479	1/1	0.98	0.14	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3510	1/1	0.98	0.08	48,48,48,48	0
56	MG	BF	308	1/1	0.98	0.11	36,36,36,36	0
56	MG	BA	3640	1/1	0.98	0.19	39,39,39,39	0
56	MG	DA	3388	1/1	0.98	0.14	35,35,35,35	0
56	MG	AA	3193	1/1	0.98	0.09	43,43,43,43	0
56	MG	BA	3664	1/1	0.98	0.14	43,43,43,43	0
59	ZN	B9	501	1/1	0.98	0.17	49,49,49,49	0
56	MG	BF	303	1/1	0.98	0.22	42,42,42,42	0
56	MG	BA	3772	1/1	0.98	0.17	31,31,31,31	0
56	MG	BA	3771	1/1	0.98	0.20	41,41,41,41	0
56	MG	BA	3830	1/1	0.98	0.18	21,21,21,21	0
56	MG	BD	309	1/1	0.98	0.20	37,37,37,37	0
56	MG	DA	3646	1/1	0.98	0.08	49,49,49,49	0
56	MG	DA	3608	1/1	0.98	0.13	53,53,53,53	0
56	MG	DA	3291	1/1	0.98	0.18	42,42,42,42	0
56	MG	BA	3809	1/1	0.98	0.14	29,29,29,29	0
56	MG	BA	3801	1/1	0.98	0.10	53,53,53,53	0
56	MG	CA	3106	1/1	0.98	0.16	50,50,50,50	0
56	MG	BA	3157	1/1	0.98	0.17	36,36,36,36	0
56	MG	AA	3229	1/1	0.98	0.35	62,62,62,62	0
56	MG	BA	3330	1/1	0.98	0.17	29,29,29,29	0
56	MG	DD	304	1/1	0.98	0.39	31,31,31,31	0
56	MG	BA	3383	1/1	0.98	0.23	24,24,24,24	0
56	MG	DA	3444	1/1	0.98	0.18	30,30,30,30	0
56	MG	DA	3433	1/1	0.98	0.20	61,61,61,61	0
56	MG	BA	3657	1/1	0.98	0.20	47,47,47,47	0
56	MG	BU	204	1/1	0.98	0.21	38,38,38,38	0
56	MG	BA	3735	1/1	0.98	0.14	35,35,35,35	0
56	MG	DA	3554	1/1	0.98	0.18	23,23,23,23	0
56	MG	DA	3637	1/1	0.98	0.06	44,44,44,44	0
56	MG	AA	3065	1/1	0.98	0.17	58,58,58,58	0
56	MG	BU	202	1/1	0.98	0.22	40,40,40,40	0
56	MG	DA	3011	1/1	0.98	0.09	40,40,40,40	0
56	MG	DA	3219	1/1	0.98	0.27	54,54,54,54	0
56	MG	DA	3104	1/1	0.98	0.15	46,46,46,46	0
56	MG	DA	3173	1/1	0.98	0.17	30,30,30,30	0
56	MG	BA	3057	1/1	0.98	0.20	53,53,53,53	0
56	MG	BA	3496	1/1	0.98	0.24	39,39,39,39	0
56	MG	DQ	3004	1/1	0.98	0.16	51,51,51,51	0
56	MG	BB	3017	1/1	0.98	0.20	33,33,33,33	0
56	MG	DA	3261	1/1	0.98	0.07	44,44,44,44	0
56	MG	DA	3356	1/1	0.98	0.26	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3476	1/1	0.98	0.24	45,45,45,45	0
56	MG	D3	3001	1/1	0.98	0.16	58,58,58,58	0
56	MG	DA	3281	1/1	0.98	0.23	33,33,33,33	0
56	MG	BA	3212	1/1	0.98	0.20	42,42,42,42	0
56	MG	CA	3066	1/1	0.98	0.14	66,66,66,66	0
56	MG	CA	3091	1/1	0.98	0.15	48,48,48,48	0
56	MG	BA	3210	1/1	0.98	0.20	31,31,31,31	0
56	MG	BA	3599	1/1	0.98	0.20	23,23,23,23	0
56	MG	DA	3465	1/1	0.98	0.07	55,55,55,55	0
56	MG	BA	3589	1/1	0.98	0.18	17,17,17,17	0
56	MG	BA	3045	1/1	0.98	0.20	42,42,42,42	0
56	MG	DA	3339	1/1	0.98	0.10	52,52,52,52	0
56	MG	BA	3128	1/1	0.98	0.24	27,27,27,27	0
56	MG	DA	3301	1/1	0.98	0.23	48,48,48,48	0
56	MG	BA	3572	1/1	0.98	0.27	63,63,63,63	0
56	MG	BA	3321	1/1	0.98	0.08	54,54,54,54	0
56	MG	BA	3460	1/1	0.98	0.23	35,35,35,35	0
59	ZN	B6	103	1/1	0.98	0.13	29,29,29,29	0
56	MG	DA	3544	1/1	0.98	0.14	37,37,37,37	0
56	MG	CA	3144	1/1	0.98	0.18	59,59,59,59	0
56	MG	BA	3246	1/1	0.99	0.10	27,27,27,27	0
56	MG	DA	3619	1/1	0.99	0.03	58,58,58,58	0
56	MG	DA	3017	1/1	0.99	0.21	28,28,28,28	0
59	ZN	D5	501	1/1	0.99	0.15	53,53,53,53	0
56	MG	BA	3368	1/1	0.99	0.19	12,12,12,12	0
56	MG	CA	3088	1/1	0.99	0.41	53,53,53,53	0
56	MG	BA	3050	1/1	0.99	0.17	31,31,31,31	0
56	MG	AA	3225	1/1	0.99	0.11	26,26,26,26	0
56	MG	BA	3697	1/1	0.99	0.12	35,35,35,35	0
56	MG	DA	3280	1/1	0.99	0.14	43,43,43,43	0
56	MG	BA	3053	1/1	0.99	0.27	22,22,22,22	0
56	MG	BA	3731	1/1	0.99	0.12	23,23,23,23	0
58	SF4	AD	501	8/8	0.99	0.14	56,62,64,76	0
56	MG	BA	3334	1/1	0.99	0.25	30,30,30,30	0
56	MG	BA	3355	1/1	0.99	0.15	24,24,24,24	0
56	MG	BA	3039	1/1	0.99	0.28	47,47,47,47	0
56	MG	DA	3350	1/1	0.99	0.30	29,29,29,29	0
56	MG	BA	3231	1/1	0.99	0.24	37,37,37,37	0
56	MG	BD	307	1/1	0.99	0.21	35,35,35,35	0
56	MG	DA	3036	1/1	0.99	0.15	29,29,29,29	0
56	MG	DA	3050	1/1	0.99	0.23	40,40,40,40	0
56	MG	BV	202	1/1	0.99	0.13	26,26,26,26	0

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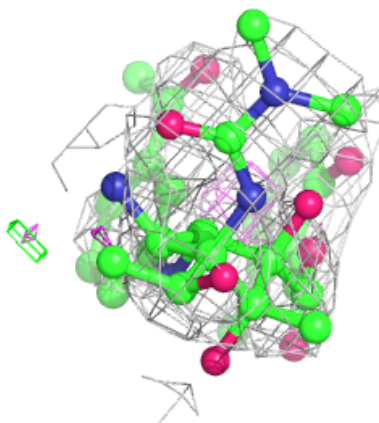
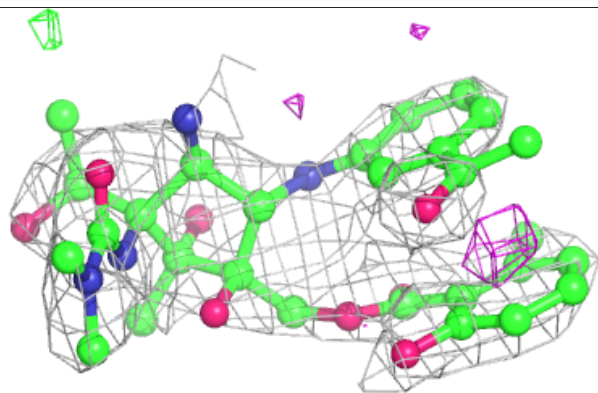
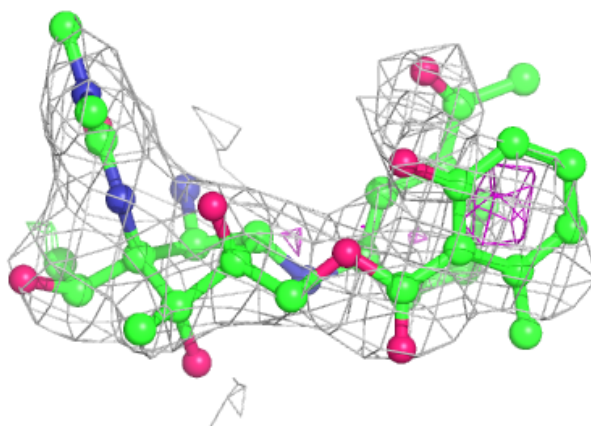
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	3186	1/1	0.99	0.16	52,52,52,52	0
56	MG	BA	3458	1/1	0.99	0.25	19,19,19,19	0
56	MG	BA	3759	1/1	0.99	0.15	9,9,9,9	0
56	MG	DA	3254	1/1	0.99	0.25	21,21,21,21	0
56	MG	BU	209	1/1	0.99	0.19	27,27,27,27	0
56	MG	BA	3621	1/1	0.99	0.23	52,52,52,52	0
56	MG	BA	3682	1/1	0.99	0.13	50,50,50,50	0
56	MG	DA	3018	1/1	0.99	0.18	41,41,41,41	0
56	MG	AA	3137	1/1	0.99	0.19	42,42,42,42	0
56	MG	BB	3016	1/1	0.99	0.16	43,43,43,43	0
56	MG	BA	3071	1/1	0.99	0.33	42,42,42,42	0
56	MG	DA	3218	1/1	0.99	0.16	47,47,47,47	0
56	MG	CA	3077	1/1	0.99	0.06	48,48,48,48	0
56	MG	BA	3609	1/1	0.99	0.26	20,20,20,20	0
56	MG	BA	3003	1/1	0.99	0.26	20,20,20,20	0
56	MG	BA	3462	1/1	0.99	0.13	11,11,11,11	0
56	MG	BV	205	1/1	0.99	0.12	32,32,32,32	0
56	MG	BU	203	1/1	0.99	0.14	31,31,31,31	0
56	MG	BA	3400	1/1	0.99	0.17	25,25,25,25	0
56	MG	DA	3228	1/1	0.99	0.05	42,42,42,42	0
56	MG	BA	3188	1/1	0.99	0.24	19,19,19,19	0
56	MG	BA	3129	1/1	0.99	0.22	36,36,36,36	0
56	MG	DD	306	1/1	0.99	0.26	44,44,44,44	0
56	MG	BA	3440	1/1	0.99	0.27	29,29,29,29	0
56	MG	AA	3157	1/1	0.99	0.19	46,46,46,46	0
56	MG	DA	3656	1/1	0.99	0.17	62,62,62,62	0
56	MG	BV	201	1/1	0.99	0.22	29,29,29,29	0
56	MG	DA	3438	1/1	0.99	0.10	60,60,60,60	0
56	MG	BA	3272	1/1	1.00	0.28	11,11,11,11	0
59	ZN	B5	104	1/1	1.00	0.15	38,38,38,38	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.

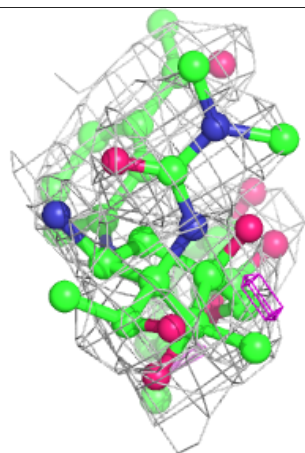
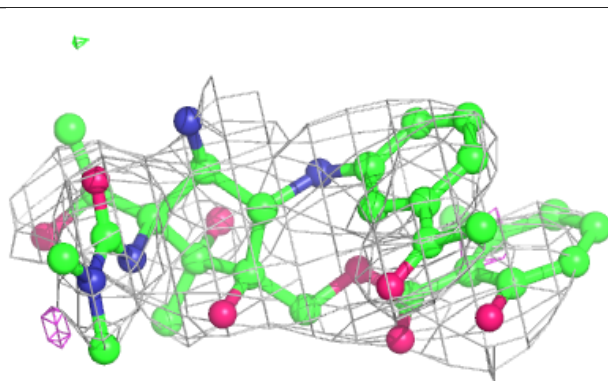
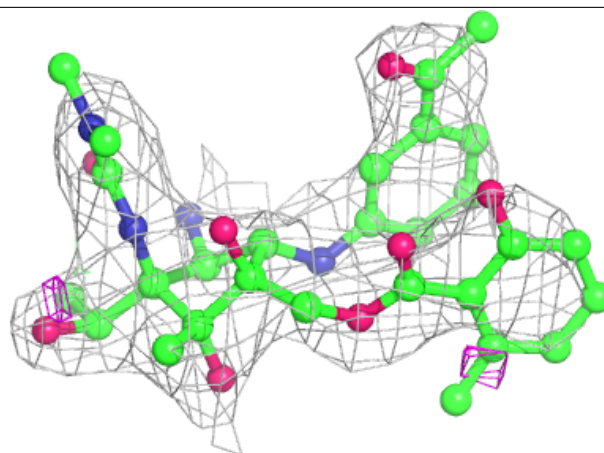
Electron density around PCY CA 3178:

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



Electron density around PCY AA 3231:

$2mF_o - DF_c$ (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.