wwPDB X-ray Structure Validation Summary Report (i)

Dec 18, 2023 – 05:29 PM EST

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.; Kusochek, 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

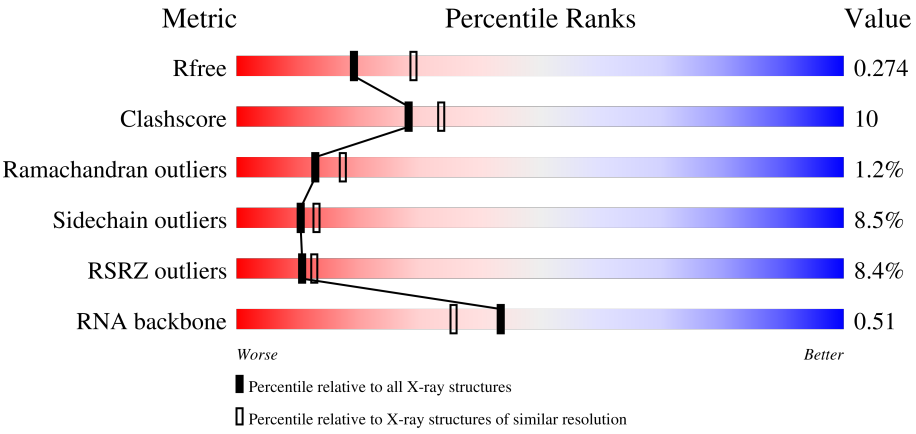
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

1 Overall quality at a glance (i)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1521	4% 55% 32% 10%

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Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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Mol	Chain	Length	Quality of chain
1	CA	1521	3% 50% 37% 10%
2	AB	256	17% 48% 36% 5% 10%
2	CB	256	27% 47% 37% 6% 10%
3	AC	239	13% 59% 24% 14%
3	CC	239	35% 54% 29% 14%
4	AD	209	3% 68% 26% 5%
4	CD	209	14% 65% 32%
5	AE	162	6% 62% 26% 9%
5	CE	162	10% 65% 23% 9%
6	AF	101	% 73% 24%
6	CF	101	% 72% 26%
7	AG	156	10% 75% 19% 6%
7	CG	156	10% 68% 28%
8	AH	138	9% 67% 30%
8	CH	138	14% 71% 25%
9	AI	128	26% 62% 34%
9	CI	128	45% 55% 34% 10%
10	AJ	105	28% 55% 32% 5% 8%
10	CJ	105	37% 50% 40% 9%
11	AK	129	7% 67% 19% 12%
11	CK	129	2% 61% 24% 12%
12	AL	132	2% 70% 20% 8%
12	CL	132	12% 67% 23% 8%
13	AM	126	5% 70% 21% 7%
13	CM	126	33% 65% 29%

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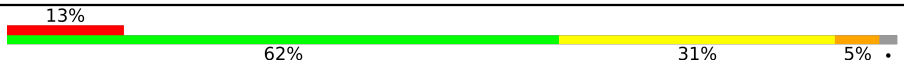
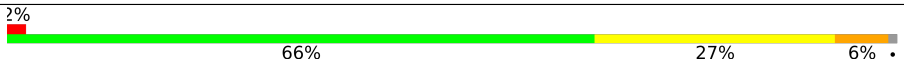
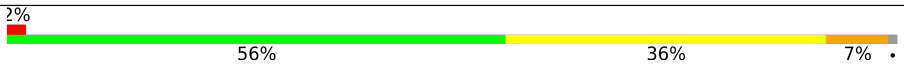
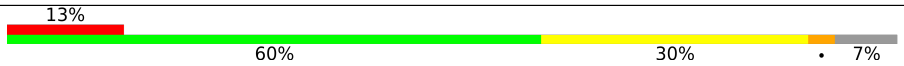
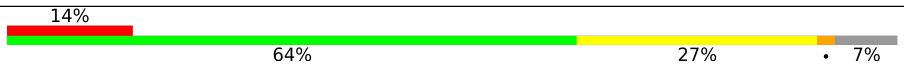
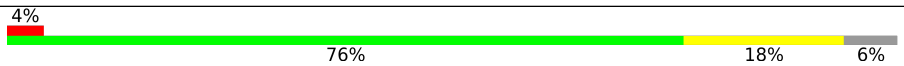
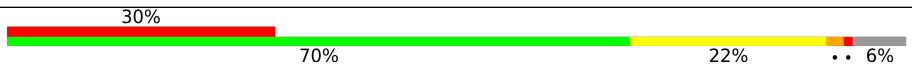
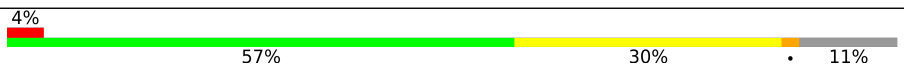
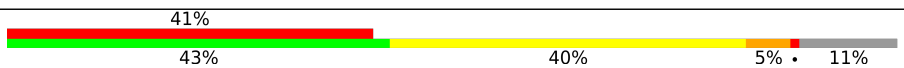
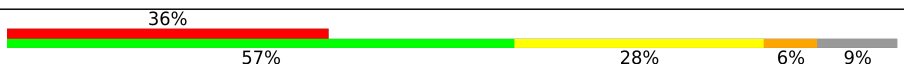
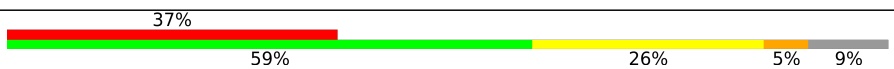
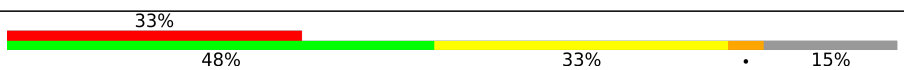
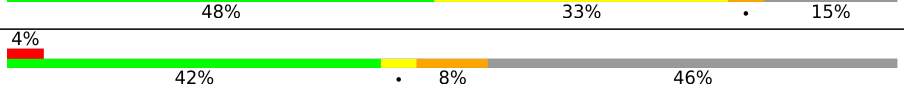
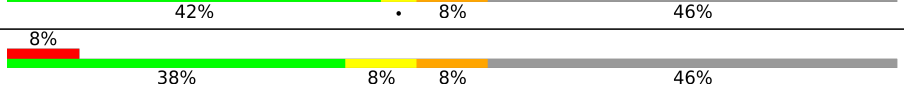
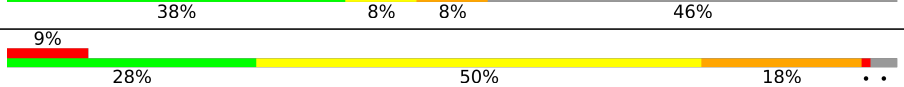
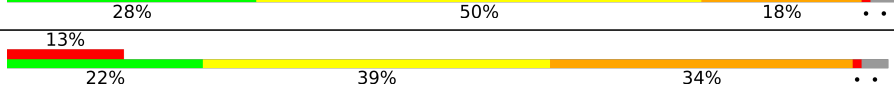
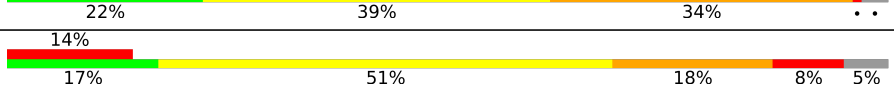
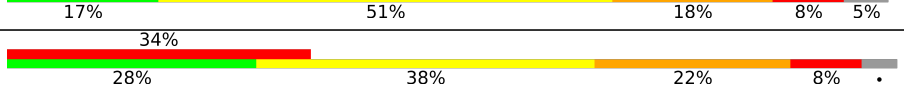
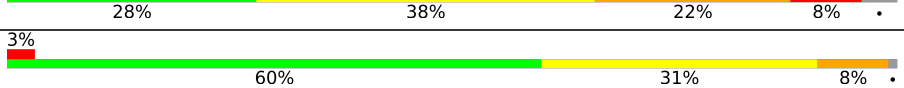
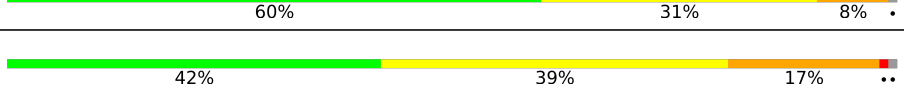
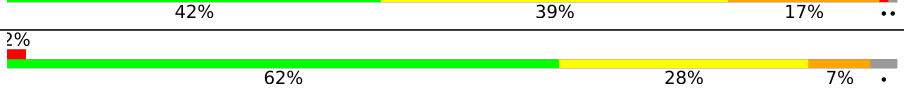
Mol	Chain	Length	Quality of chain
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	76	
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	77	
24	CX	77	
25	BA	2915	

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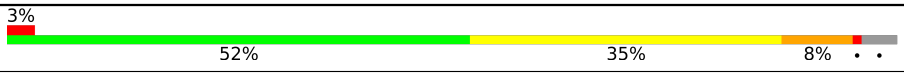
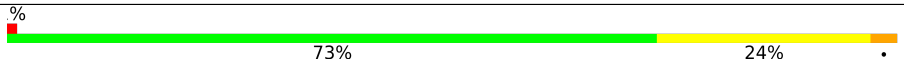
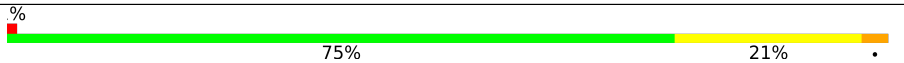
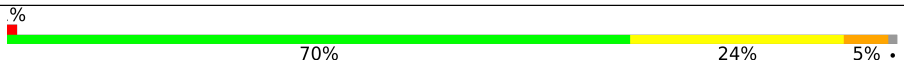
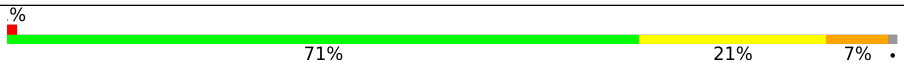
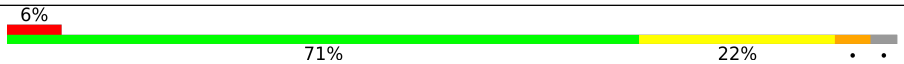
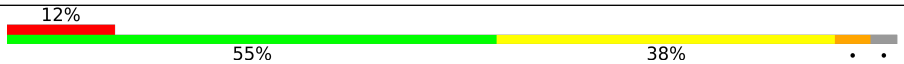
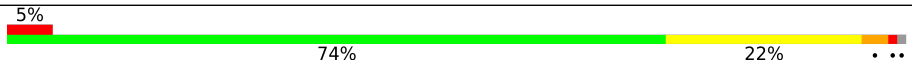
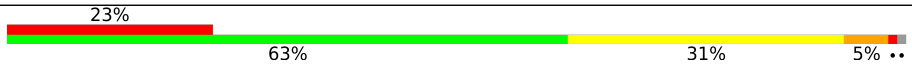
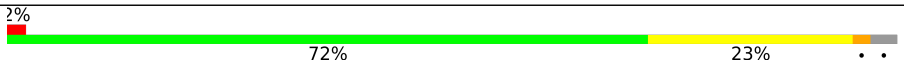
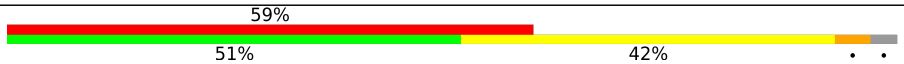
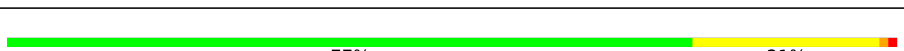
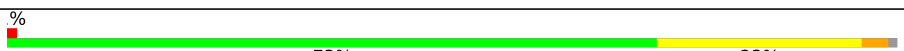
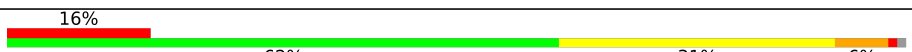
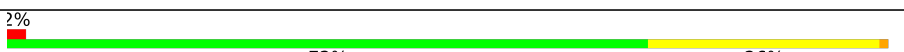
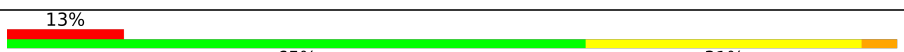
Mol	Chain	Length	Quality of chain
25	DA	2915	
26	BB	121	
26	DB	121	
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BN	140	
33	DN	140	
34	BO	122	
34	DO	122	
35	BP	150	
35	DP	150	
36	BQ	141	
36	DQ	141	
37	BR	118	
37	DR	118	

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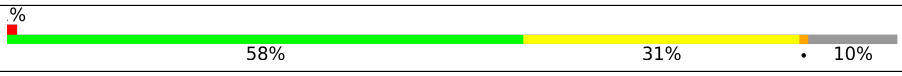
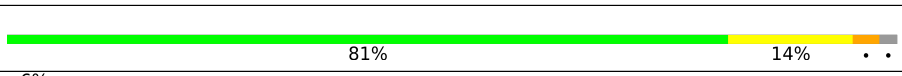
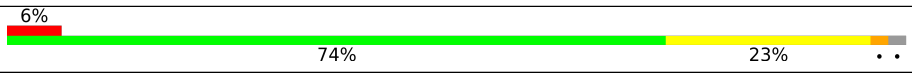
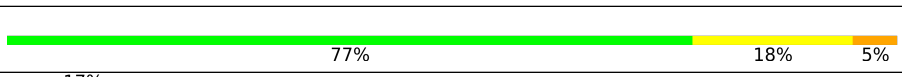
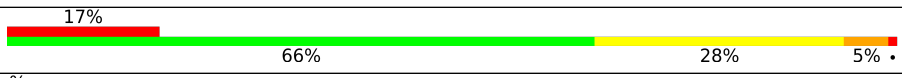
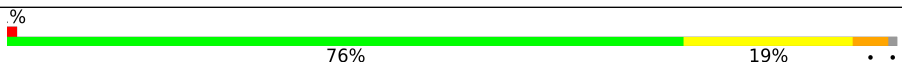
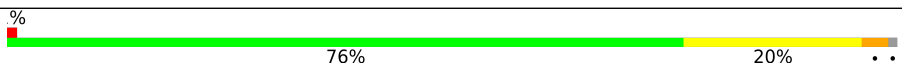
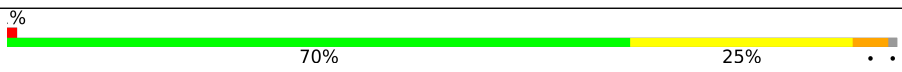
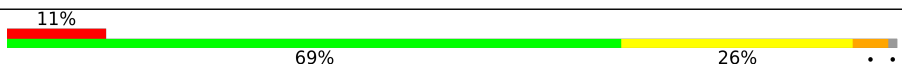
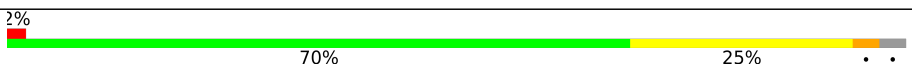
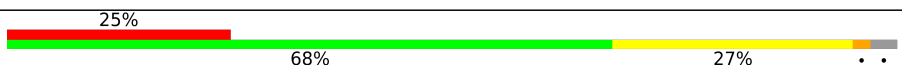
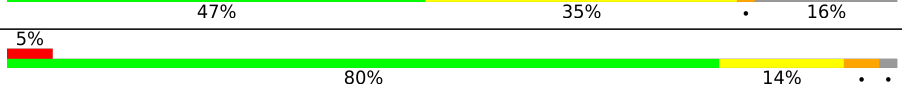
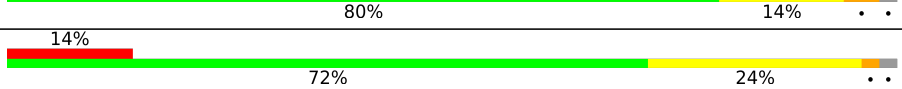
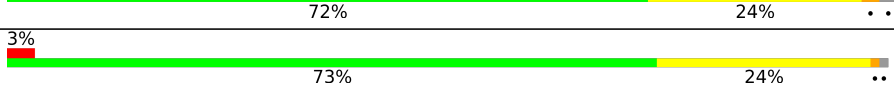
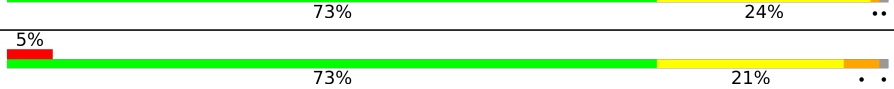
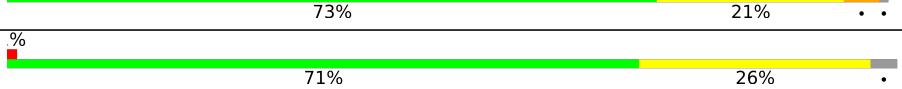
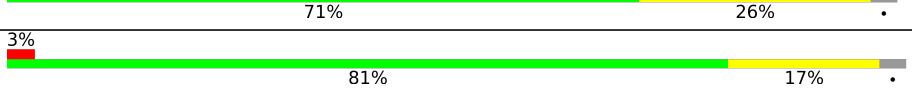
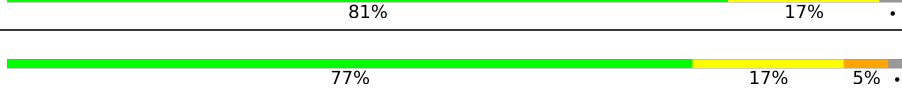
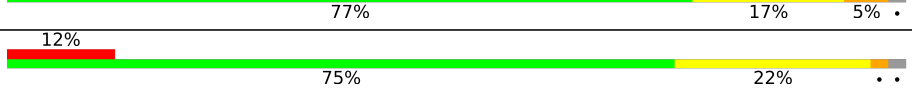
Mol	Chain	Length	Quality of chain
38	BS	112	
38	DS	112	
39	BT	146	
39	DT	146	
40	BU	118	
40	DU	118	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	96	
43	DX	96	
44	BY	110	
44	DY	110	
45	BZ	206	
45	DZ	206	
46	B0	85	
46	D0	85	
47	B1	98	
47	D1	98	
48	B2	72	
48	D2	72	
49	B3	60	
49	D3	60	
50	B4	71	

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Mol	Chain	Length	Quality of chain
50	D4	71	46% 42% 51%
51	B5	60	2% 78% 17%
51	D5	60	2% 82% 15%
52	B6	54	69% 28%
52	D6	54	7% 70% 26%
53	B7	49	4% 67% 29%
53	D7	49	6% 82% 14%
54	B8	65	66% 32%
54	D8	65	3% 66% 29%
55	B9	37	3% 86% 14%
55	D9	37	19% 73% 27%

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 (i)

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 714	C 445	N 138	O 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 829	C 516	N 155	O 155	S 3	0	0	0
11	CK	114	Total 833	C 519	N 156	O 155	S 3	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total 728	C 456	N 144	O 126	S 2	0	0	0
15	CO	88	Total 728	C 456	N 144	O 126	S 2	0	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	AA	230	Total	Mg	0	0
			230	230		
56	AD	1	Total	Mg	0	0
			1	1		
56	AE	1	Total	Mg	0	0
			1	1		
56	AF	1	Total	Mg	0	0
			1	1		
56	AK	2	Total	Mg	0	0
			2	2		
56	AM	1	Total	Mg	0	0
			1	1		
56	AN	1	Total	Mg	0	0
			1	1		
56	AV	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AW	7	Total Mg 7 7	0	0
56	AX	12	Total Mg 12 12	0	0
56	AY	3	Total Mg 3 3	0	0
56	BA	839	Total Mg 839 839	0	0
56	BB	23	Total Mg 23 23	0	0
56	BD	11	Total Mg 11 11	0	0
56	BE	8	Total Mg 8 8	0	0
56	BF	12	Total Mg 12 12	0	0
56	BG	3	Total Mg 3 3	0	0
56	BN	5	Total Mg 5 5	0	0
56	BO	1	Total Mg 1 1	0	0
56	BP	3	Total Mg 3 3	0	0
56	BQ	5	Total Mg 5 5	0	0
56	BR	5	Total Mg 5 5	0	0
56	BU	9	Total Mg 9 9	0	0
56	BV	5	Total Mg 5 5	0	0
56	BW	3	Total Mg 3 3	0	0
56	BX	2	Total Mg 2 2	0	0
56	BY	1	Total Mg 1 1	0	0
56	BZ	1	Total Mg 1 1	0	0
56	B0	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	B1	2	Total Mg 2 2	0	0
56	B2	1	Total Mg 1 1	0	0
56	B3	3	Total Mg 3 3	0	0
56	B4	1	Total Mg 1 1	0	0
56	B5	4	Total Mg 4 4	0	0
56	B6	2	Total Mg 2 2	0	0
56	B7	2	Total Mg 2 2	0	0
56	B8	3	Total Mg 3 3	0	0
56	B9	1	Total Mg 1 1	0	0
56	CA	177	Total Mg 177 177	0	0
56	CE	2	Total Mg 2 2	0	0
56	CF	1	Total Mg 1 1	0	0
56	CJ	1	Total Mg 1 1	0	0
56	CT	1	Total Mg 1 1	0	0
56	CV	1	Total Mg 1 1	0	0
56	CW	2	Total Mg 2 2	0	0
56	CX	5	Total Mg 5 5	0	0
56	CY	1	Total Mg 1 1	0	0
56	DA	675	Total Mg 675 675	0	0
56	DB	11	Total Mg 11 11	0	0
56	DD	7	Total Mg 7 7	0	0

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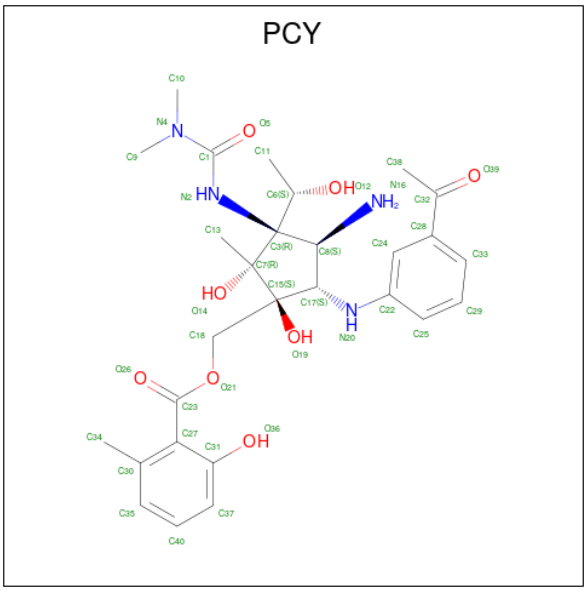
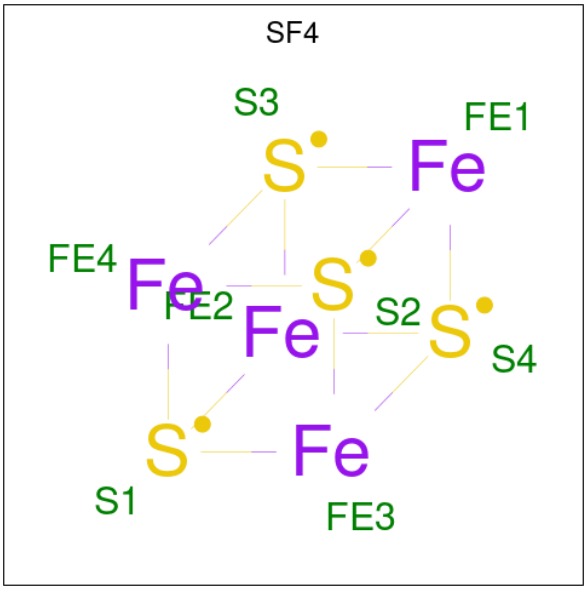
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	DE	4	Total Mg 4 4	0	0
56	DF	5	Total Mg 5 5	0	0
56	DG	1	Total Mg 1 1	0	0
56	DN	1	Total Mg 1 1	0	0
56	DO	1	Total Mg 1 1	0	0
56	DQ	4	Total Mg 4 4	0	0
56	DR	1	Total Mg 1 1	0	0
56	DU	2	Total Mg 2 2	0	0
56	DV	3	Total Mg 3 3	0	0
56	DW	3	Total Mg 3 3	0	0
56	DY	1	Total Mg 1 1	0	0
56	D0	2	Total Mg 2 2	0	0
56	D3	1	Total Mg 1 1	0	0
56	D7	2	Total Mg 2 2	0	0
56	D8	1	Total Mg 1 1	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 40 28 4 8	0	0
57	CA	1	Total C N O 40 28 4 8	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AN	1	Total Zn 1 1	0	0
59	BY	1	Total Zn 1 1	0	0
59	B4	1	Total Zn 1 1	0	0
59	B5	1	Total Zn 1 1	0	0
59	B6	1	Total Zn 1 1	0	0
59	B9	1	Total Zn 1 1	0	0
59	CN	1	Total Zn 1 1	0	0
59	DY	1	Total Zn 1 1	0	0
59	D4	1	Total Zn 1 1	0	0
59	D5	1	Total Zn 1 1	0	0
59	D6	1	Total Zn 1 1	0	0
59	D9	1	Total Zn 1 1	0	0

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

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

- Molecule 61 is water.

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

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

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

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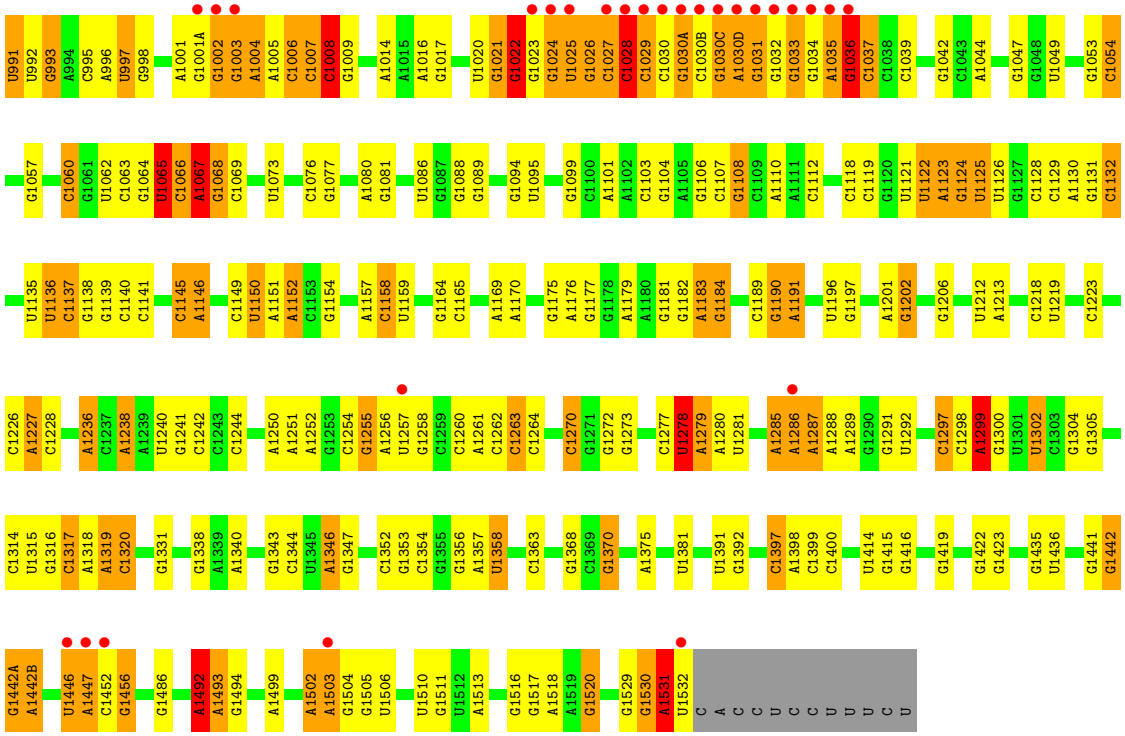
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	DO	2	Total O 2 2	0	0
61	DP	8	Total O 8 8	0	0
61	DQ	1	Total O 1 1	0	0
61	DR	1	Total O 1 1	0	0
61	DU	2	Total O 2 2	0	0
61	DW	1	Total O 1 1	0	0
61	DY	1	Total O 1 1	0	0
61	D0	5	Total O 5 5	0	0
61	D3	1	Total O 1 1	0	0
61	D7	3	Total O 3 3	0	0
61	D8	4	Total O 4 4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

3 Residue-property plots (i)

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

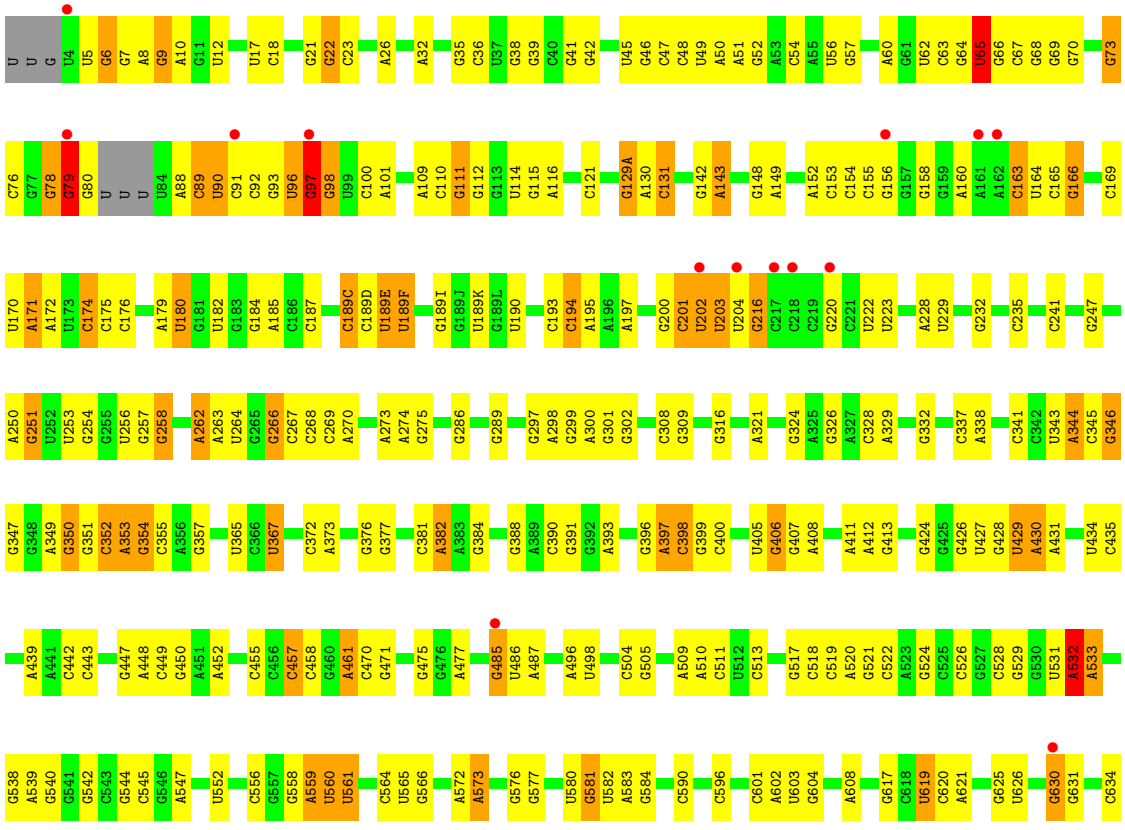
- Molecule 1: 16S Ribosomal RNA

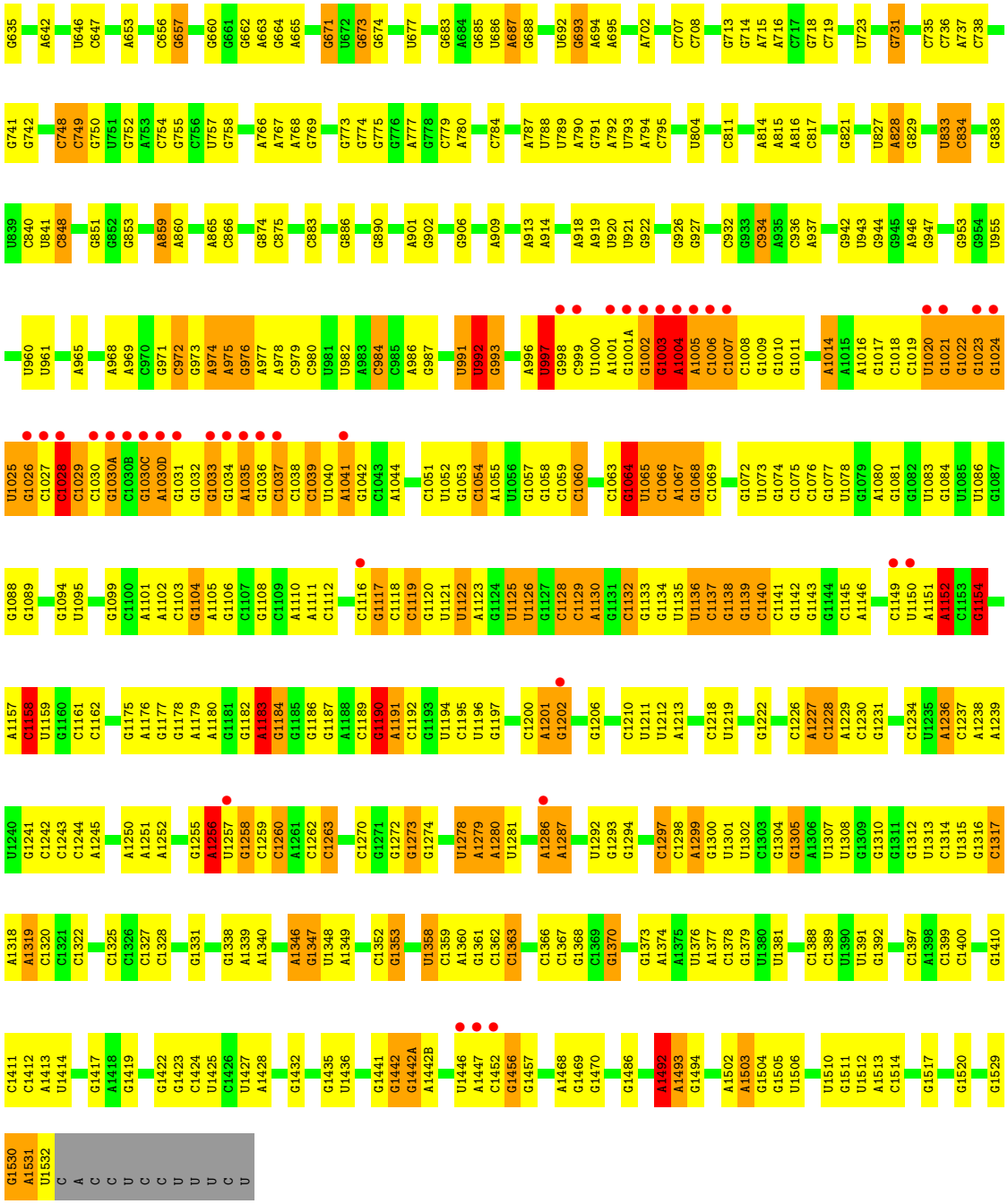
Chain AA: 



• Molecule 1: 16S Ribosomal RNA

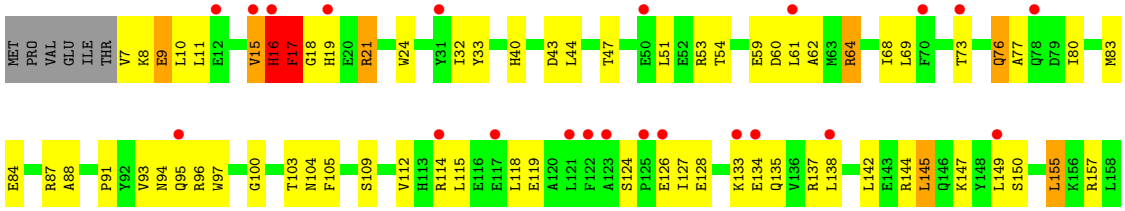
Chain CA:

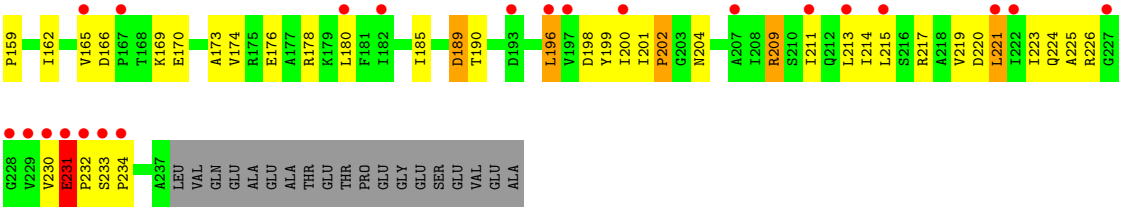




• Molecule 2: 30S Ribosomal Protein S2

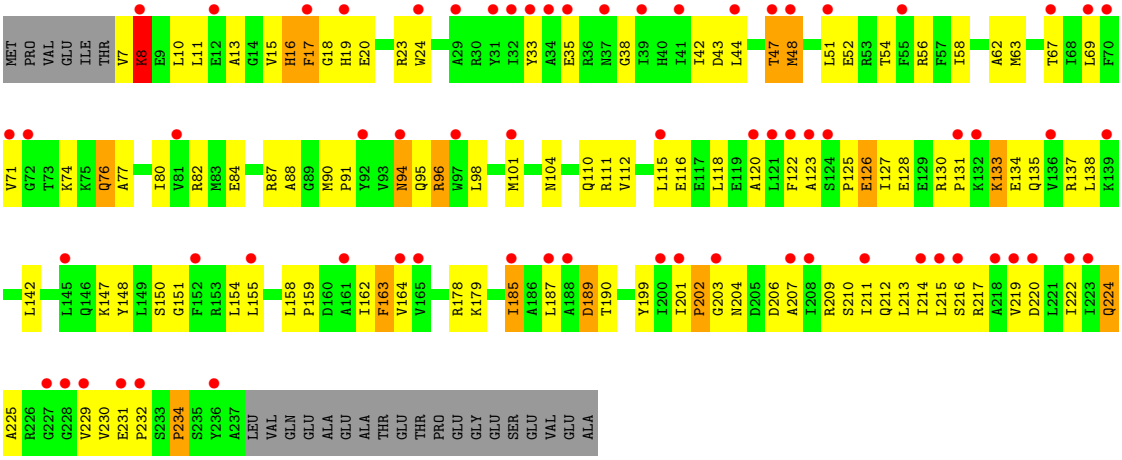
Chain AB:





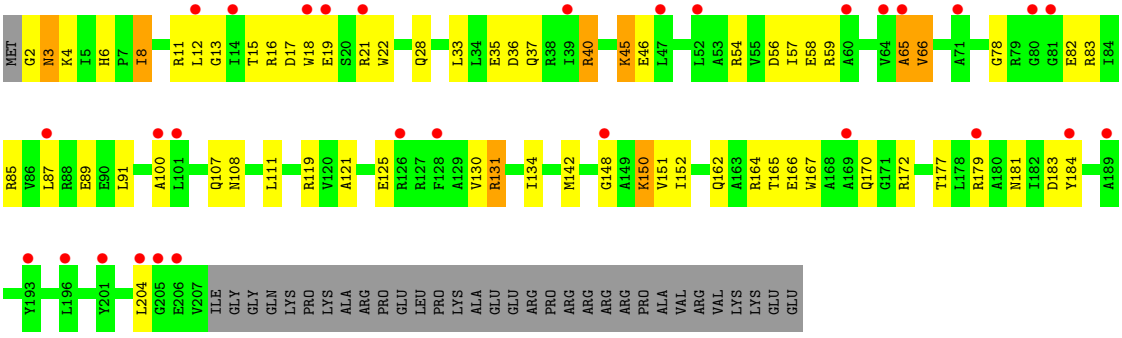
• Molecule 2: 30S Ribosomal Protein S2

Chain CB:



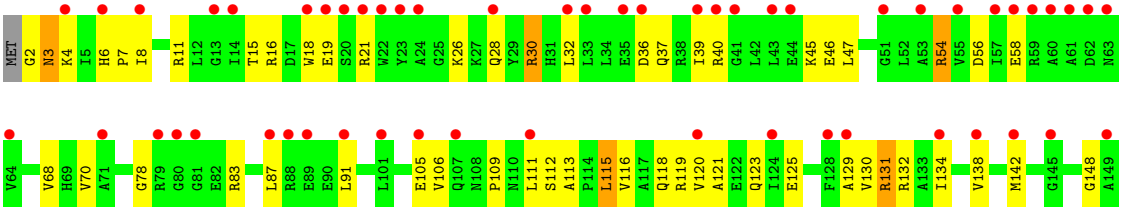
• Molecule 3: 30S Ribosomal Protein S3

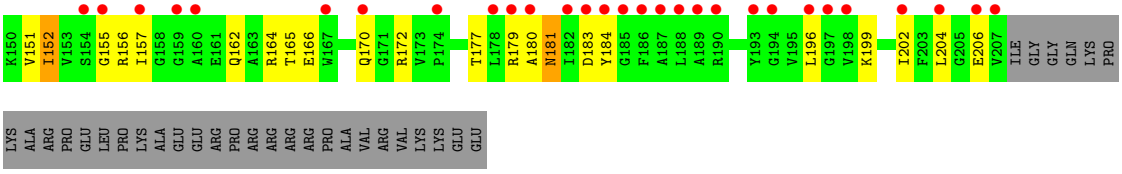
Chain AC:



• Molecule 3: 30S Ribosomal Protein S3

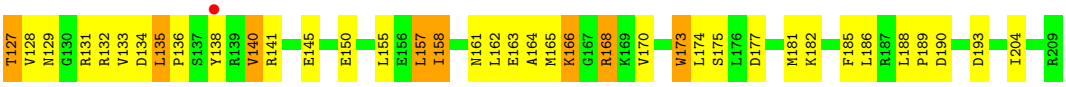
Chain CC:





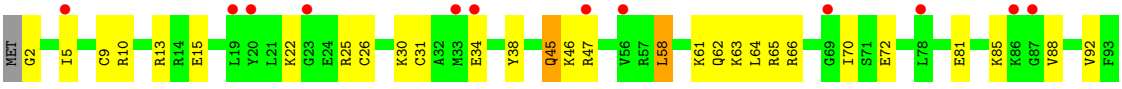
• Molecule 4: 30S Ribosomal Protein S4

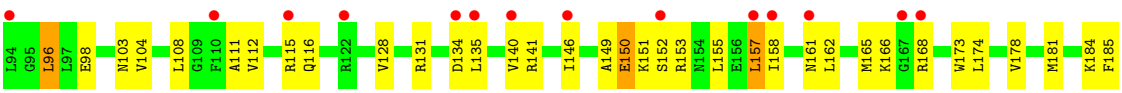
Chain AD:

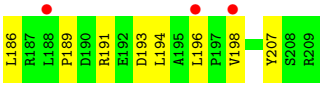


• Molecule 4: 30S Ribosomal Protein S4

Chain CD:

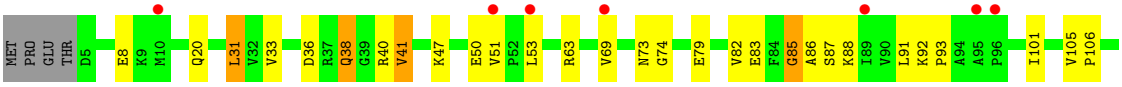


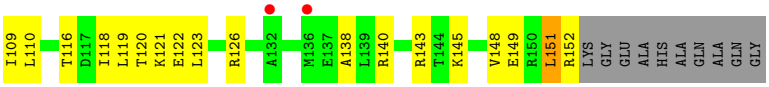




• Molecule 5: 30S Ribosomal Protein S5

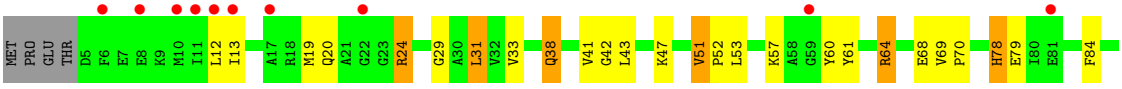
Chain AE:





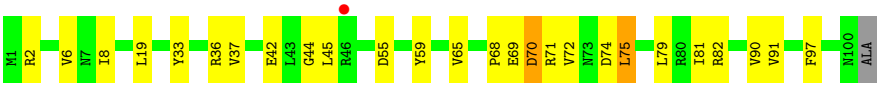
• Molecule 5: 30S Ribosomal Protein S5

Chain CE:



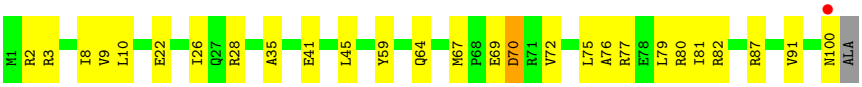
• Molecule 6: 30S Ribosomal Protein S6

Chain AF:



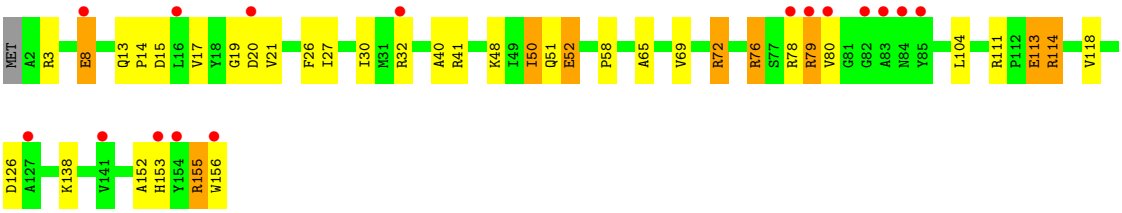
• Molecule 6: 30S Ribosomal Protein S6

Chain CF:



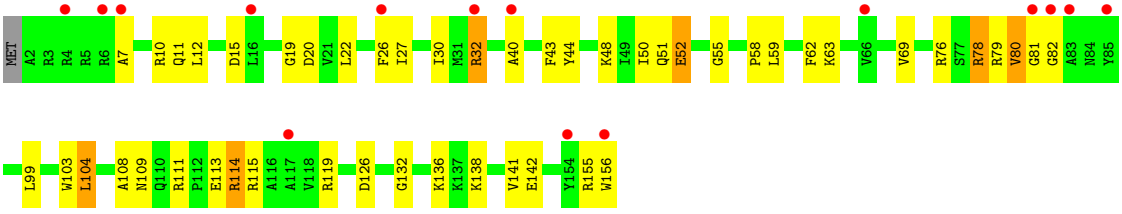
• Molecule 7: 30S Ribosomal Protein S7

Chain AG:



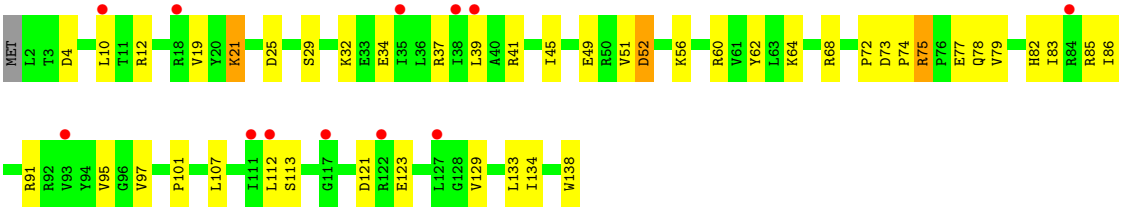
• Molecule 7: 30S Ribosomal Protein S7

Chain CG:



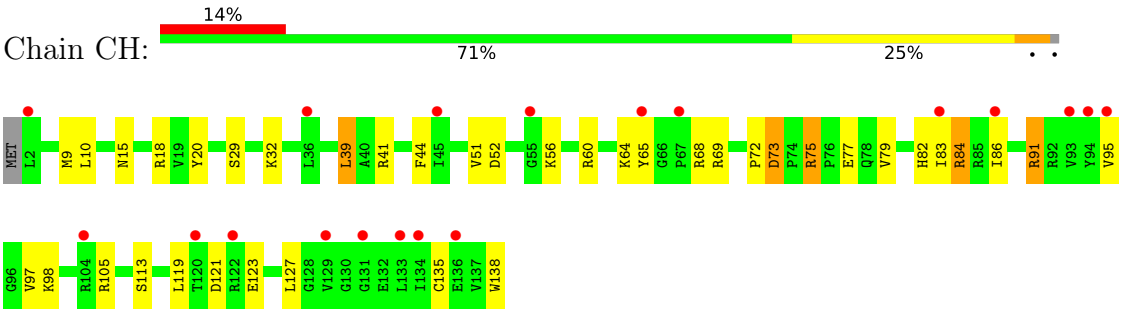
• Molecule 8: 30S Ribosomal Protein S8

Chain AH:



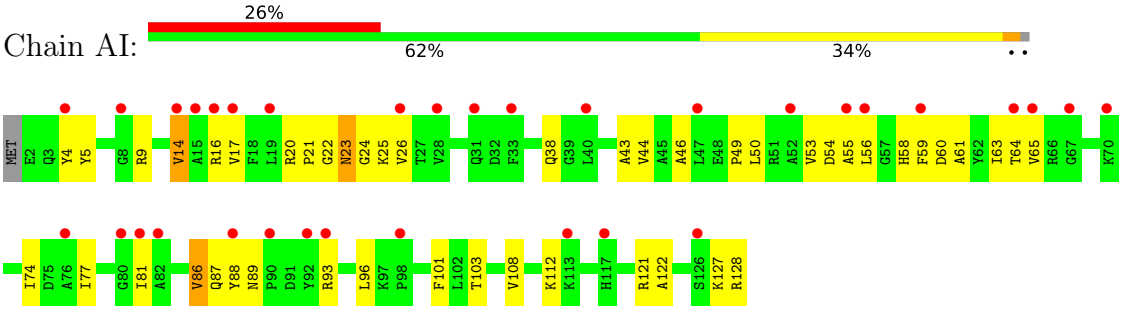
• Molecule 8: 30S Ribosomal Protein S8

Chain CH:



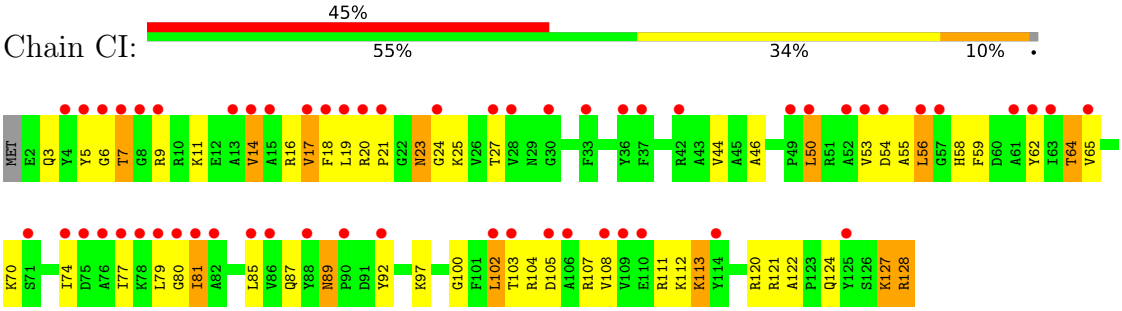
• Molecule 9: 30S Ribosomal Protein S9

Chain AI:



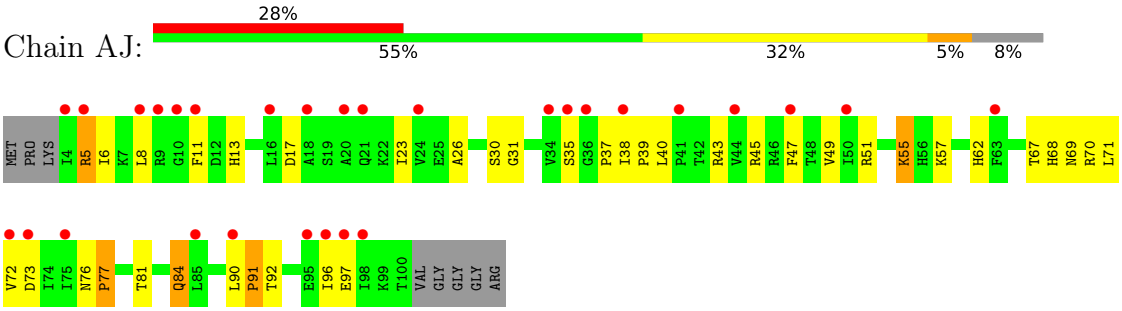
• Molecule 9: 30S Ribosomal Protein S9

Chain CI:



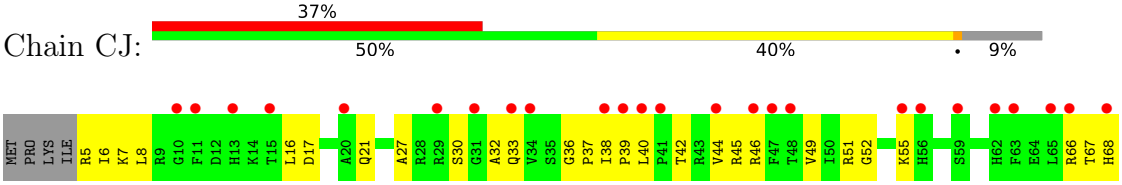
• Molecule 10: 30S Ribosomal Protein S10

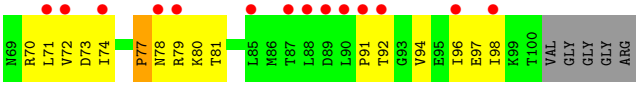
Chain AJ:



• Molecule 10: 30S Ribosomal Protein S10

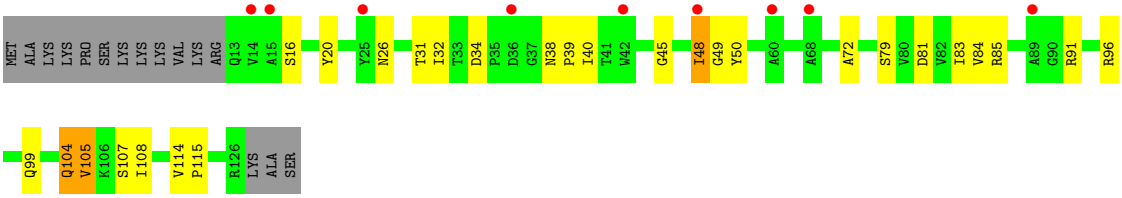
Chain CJ:





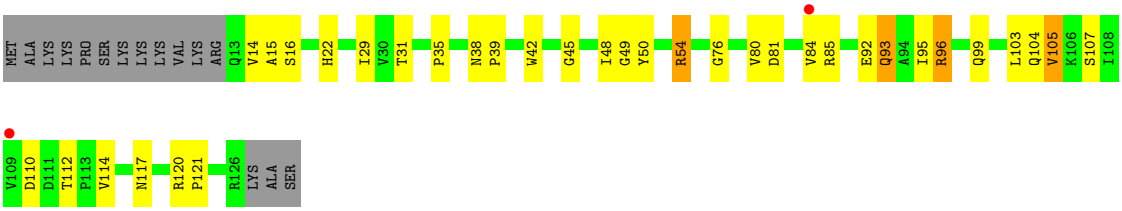
• Molecule 11: 30S Ribosomal Protein S11

Chain AK:



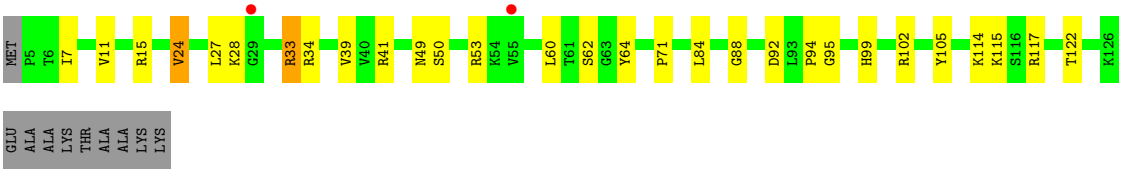
• Molecule 11: 30S Ribosomal Protein S11

Chain CK:



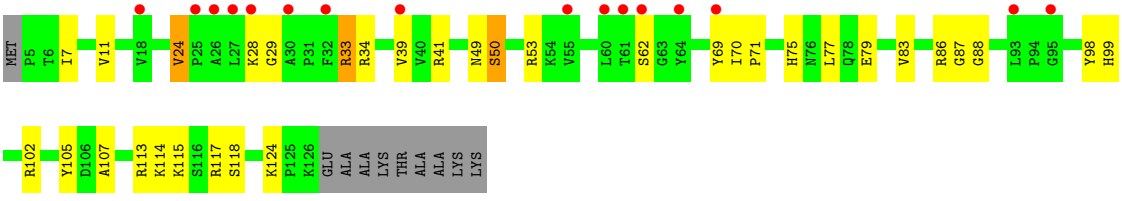
• Molecule 12: 30S Ribosomal Protein S12

Chain AL:



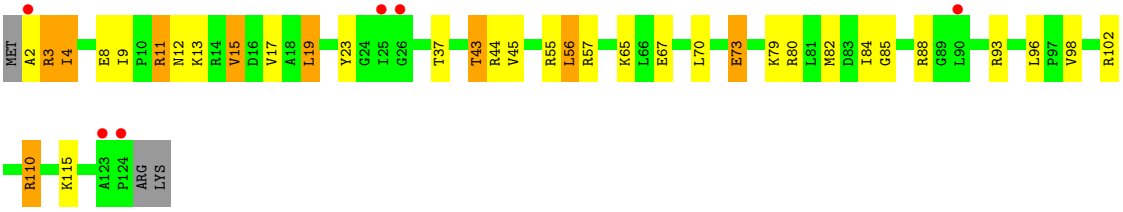
• Molecule 12: 30S Ribosomal Protein S12

Chain CL:



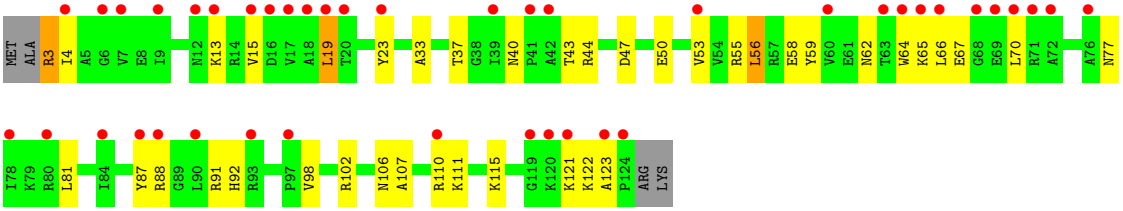
• Molecule 13: 30S Ribosomal Protein S13

Chain AM:



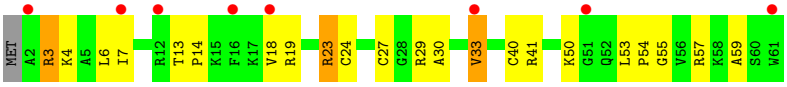
• Molecule 13: 30S Ribosomal Protein S13

Chain CM:



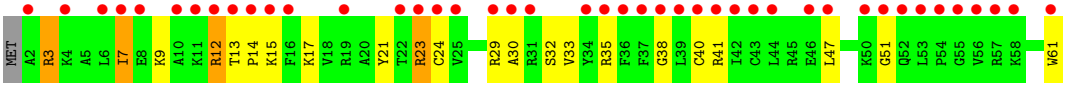
• Molecule 14: 30S Ribosomal Protein S14

Chain AN:



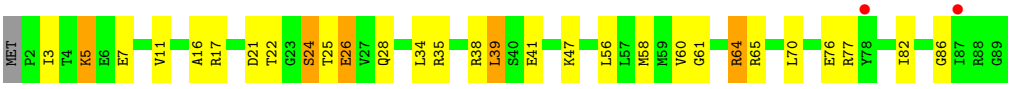
• Molecule 14: 30S Ribosomal Protein S14

Chain CN:



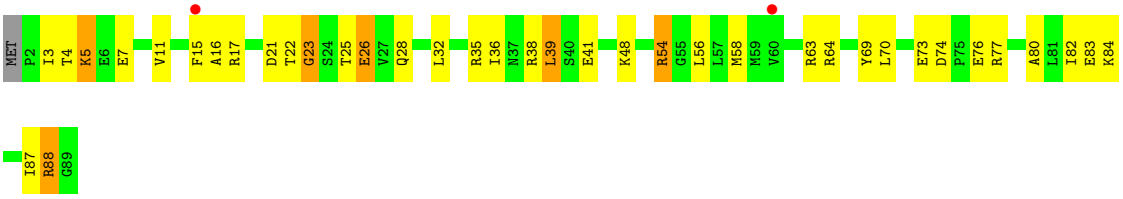
• Molecule 15: 30S Ribosomal Protein S15

Chain AO:



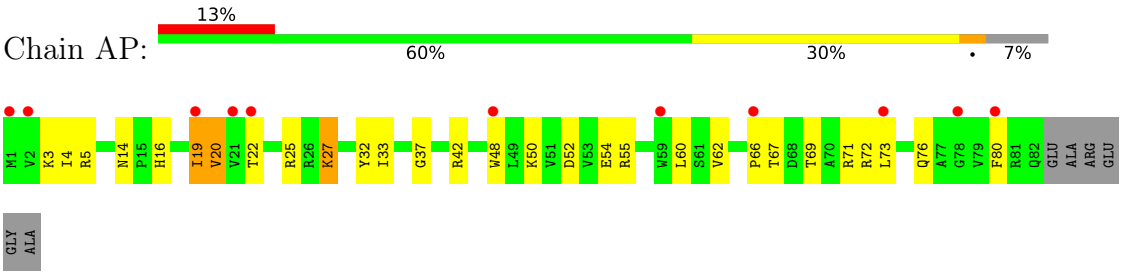
• Molecule 15: 30S Ribosomal Protein S15

Chain CO:



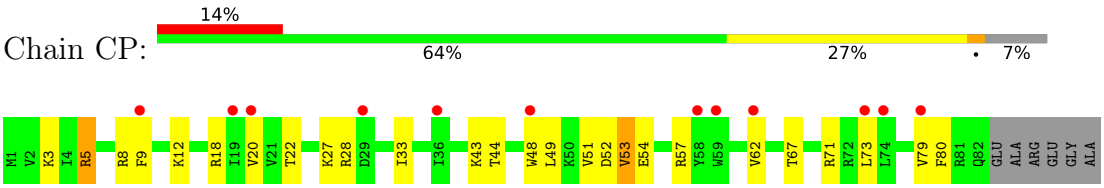
• Molecule 16: 30S Ribosomal Protein S16

Chain AP:



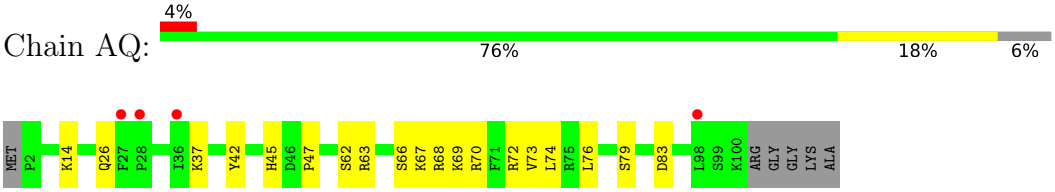
• Molecule 16: 30S Ribosomal Protein S16

Chain CP:



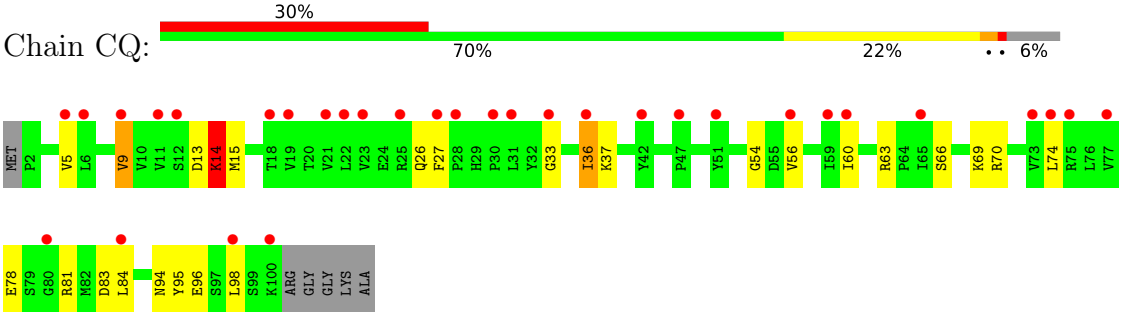
• Molecule 17: 30S Ribosomal Protein S17

Chain AQ:



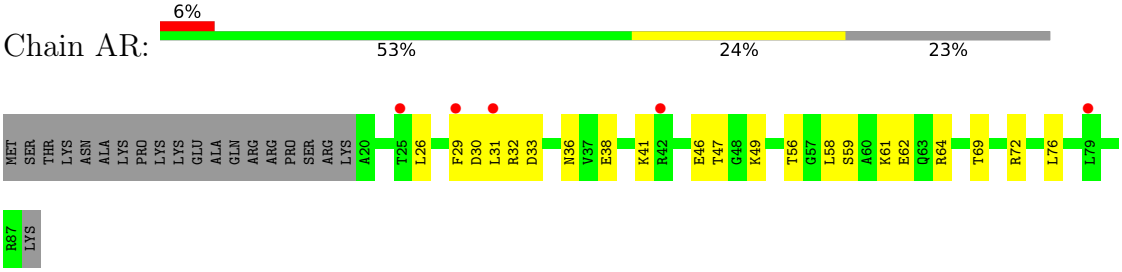
• Molecule 17: 30S Ribosomal Protein S17

Chain CQ:



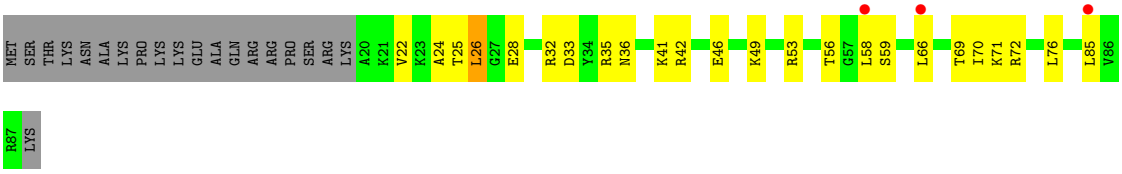
• Molecule 18: 30S Ribosomal Protein S18

Chain AR:



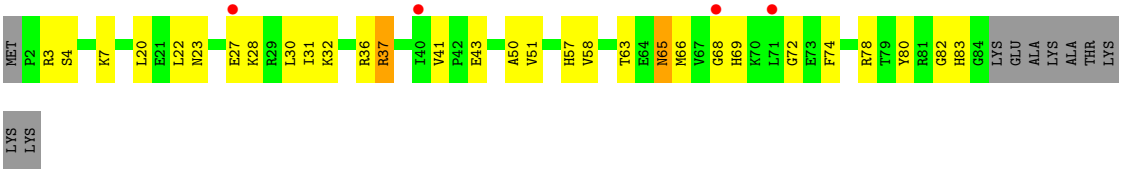
• Molecule 18: 30S Ribosomal Protein S18

Chain CR:



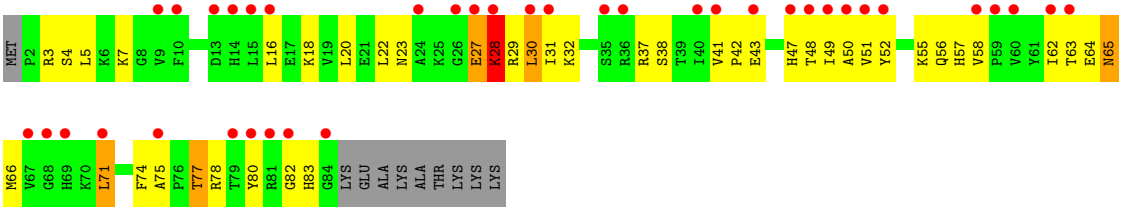
• Molecule 19: 30S Ribosomal Protein S19

Chain AS:



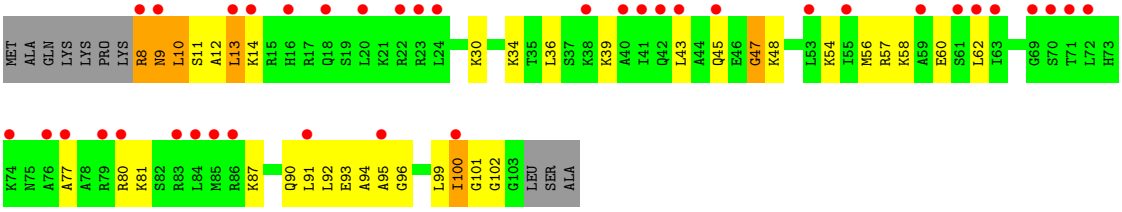
• Molecule 19: 30S Ribosomal Protein S19

Chain CS:



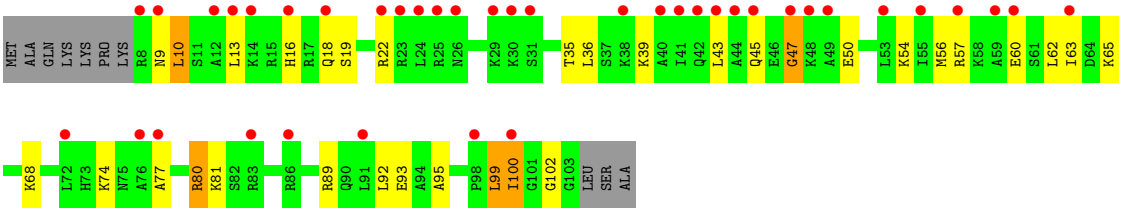
• Molecule 20: 30S Ribosomal Protein S20

Chain AT:



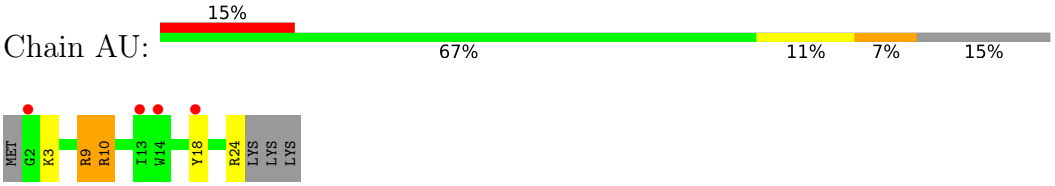
• Molecule 20: 30S Ribosomal Protein S20

Chain CT:



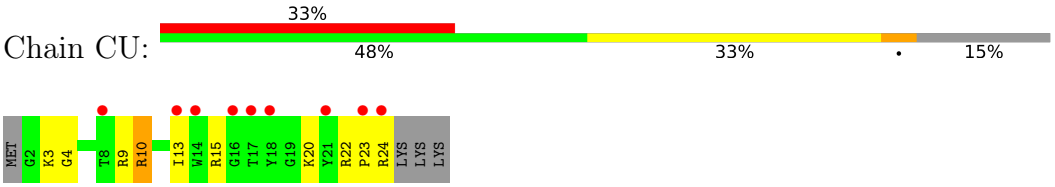
• Molecule 21: 30S Ribosomal Protein THX

Chain AU:



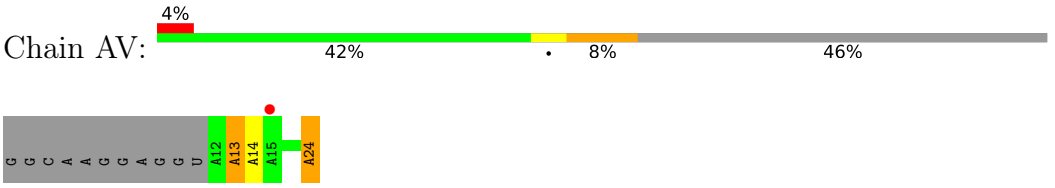
• Molecule 21: 30S Ribosomal Protein THX

Chain CU:



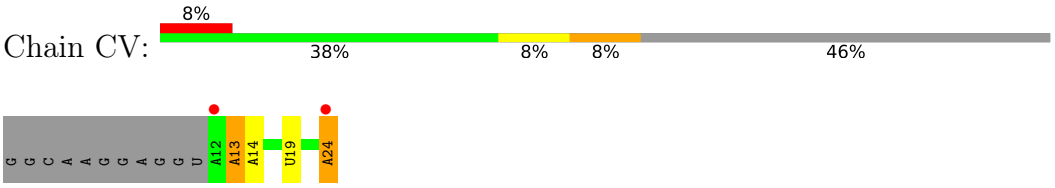
• Molecule 22: mRNA

Chain AV:



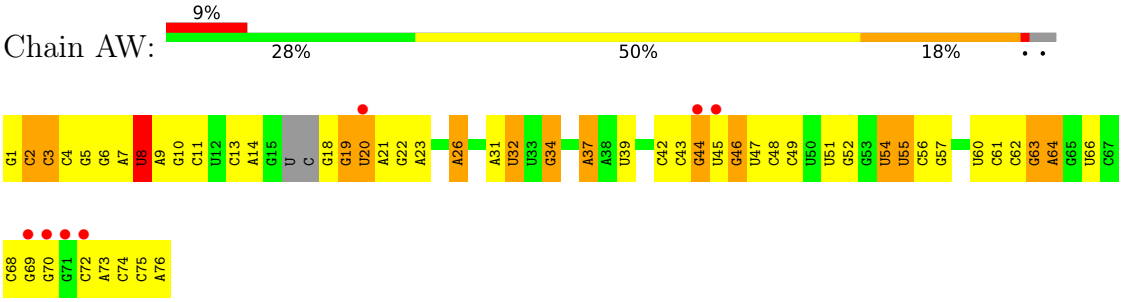
• Molecule 22: mRNA

Chain CV:



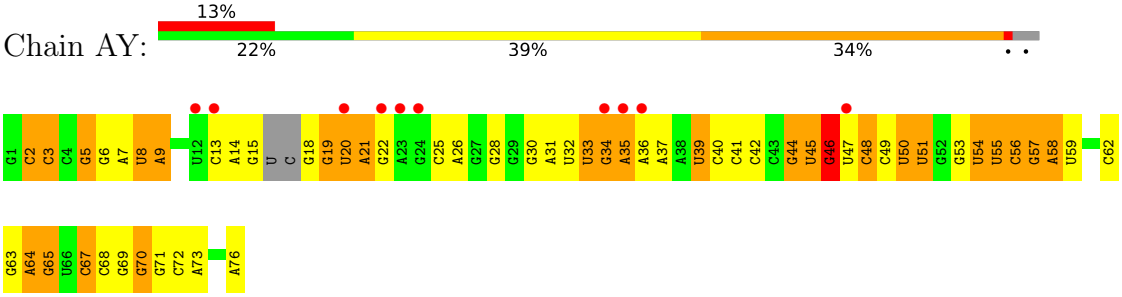
• Molecule 23: A/P-site tRNA

Chain AW:



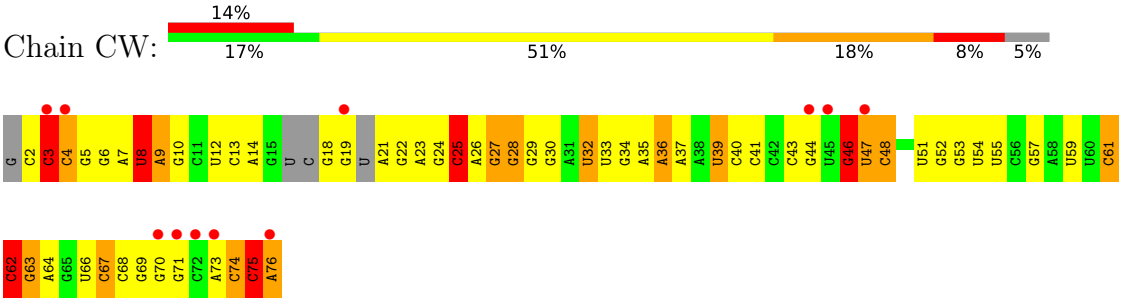
• Molecule 23: A/P-site tRNA

Chain AY:



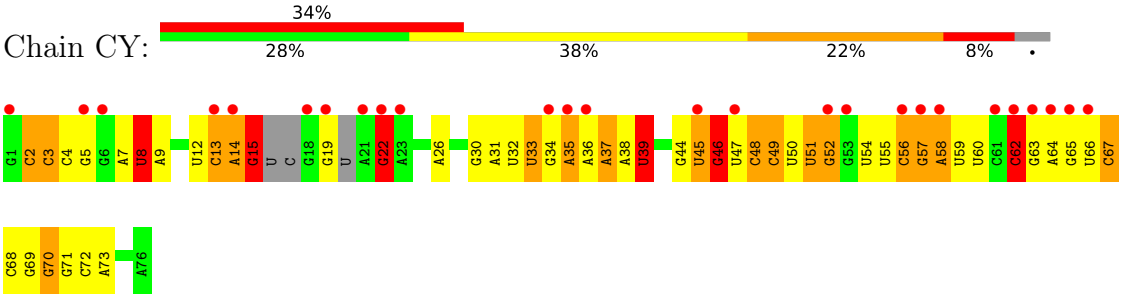
• Molecule 23: A/P-site tRNA

Chain CW:



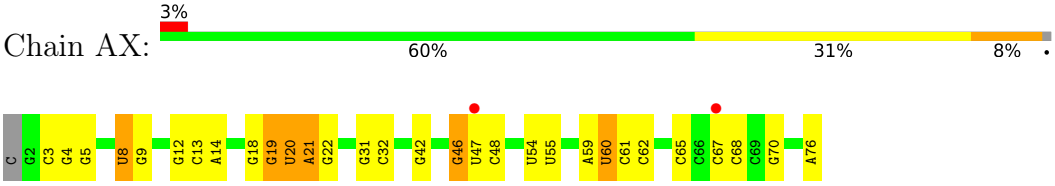
• Molecule 23: A/P-site tRNA

Chain CY:



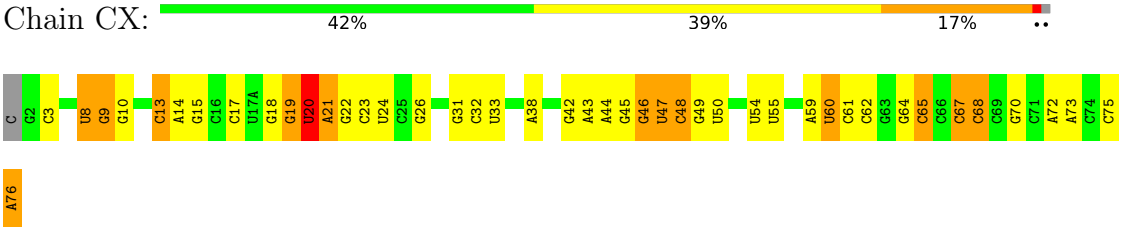
• Molecule 24: E-site tRNA

Chain AX:



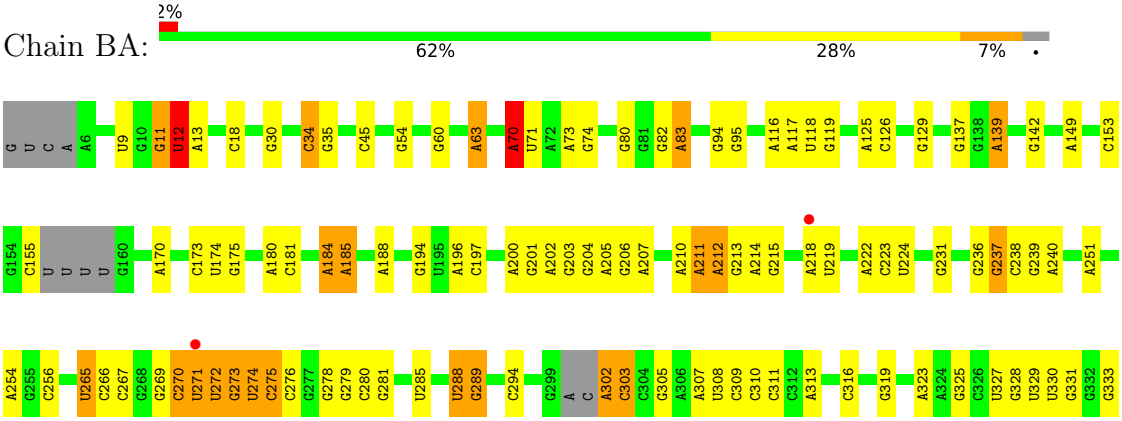
• Molecule 24: E-site tRNA

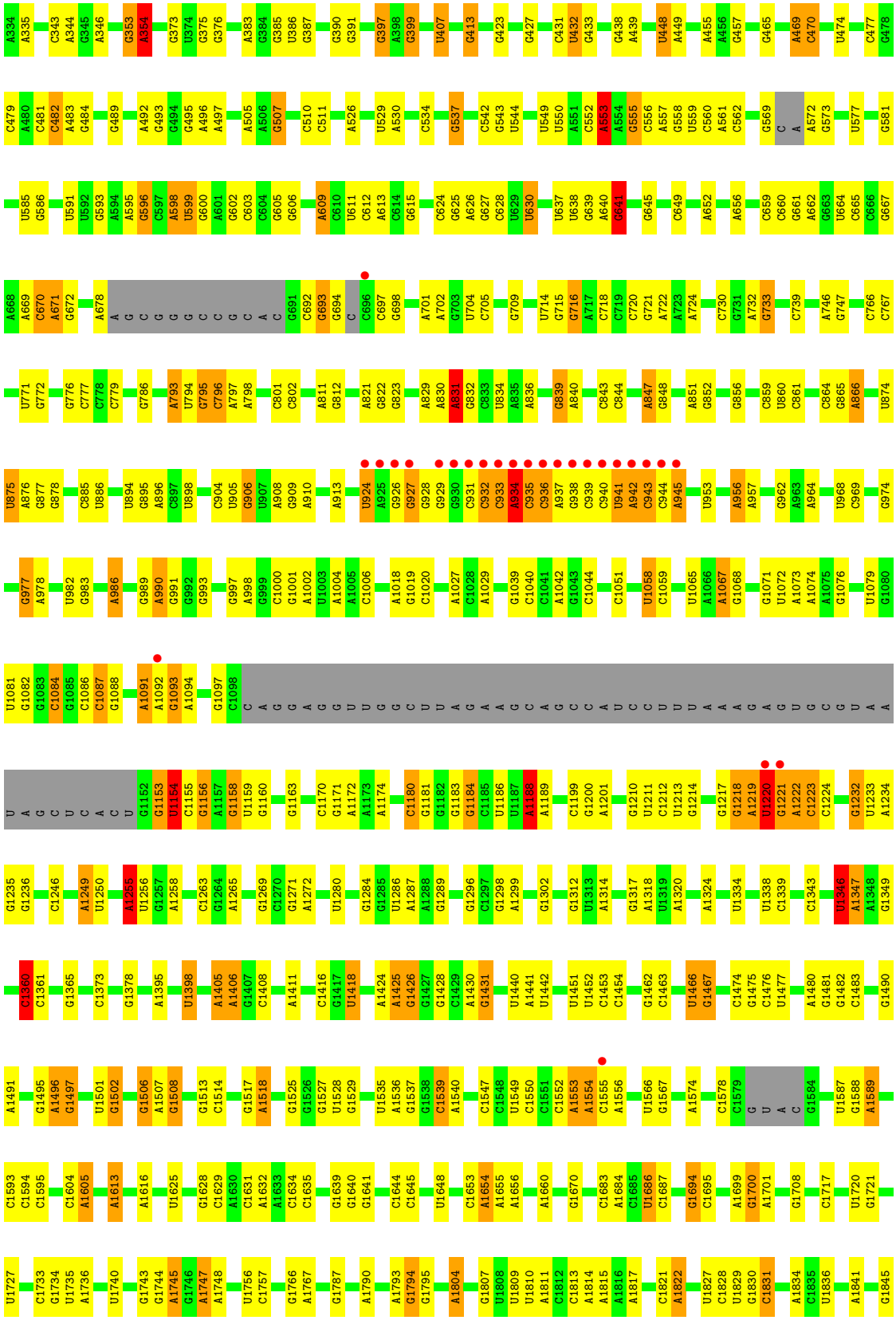
Chain CX:

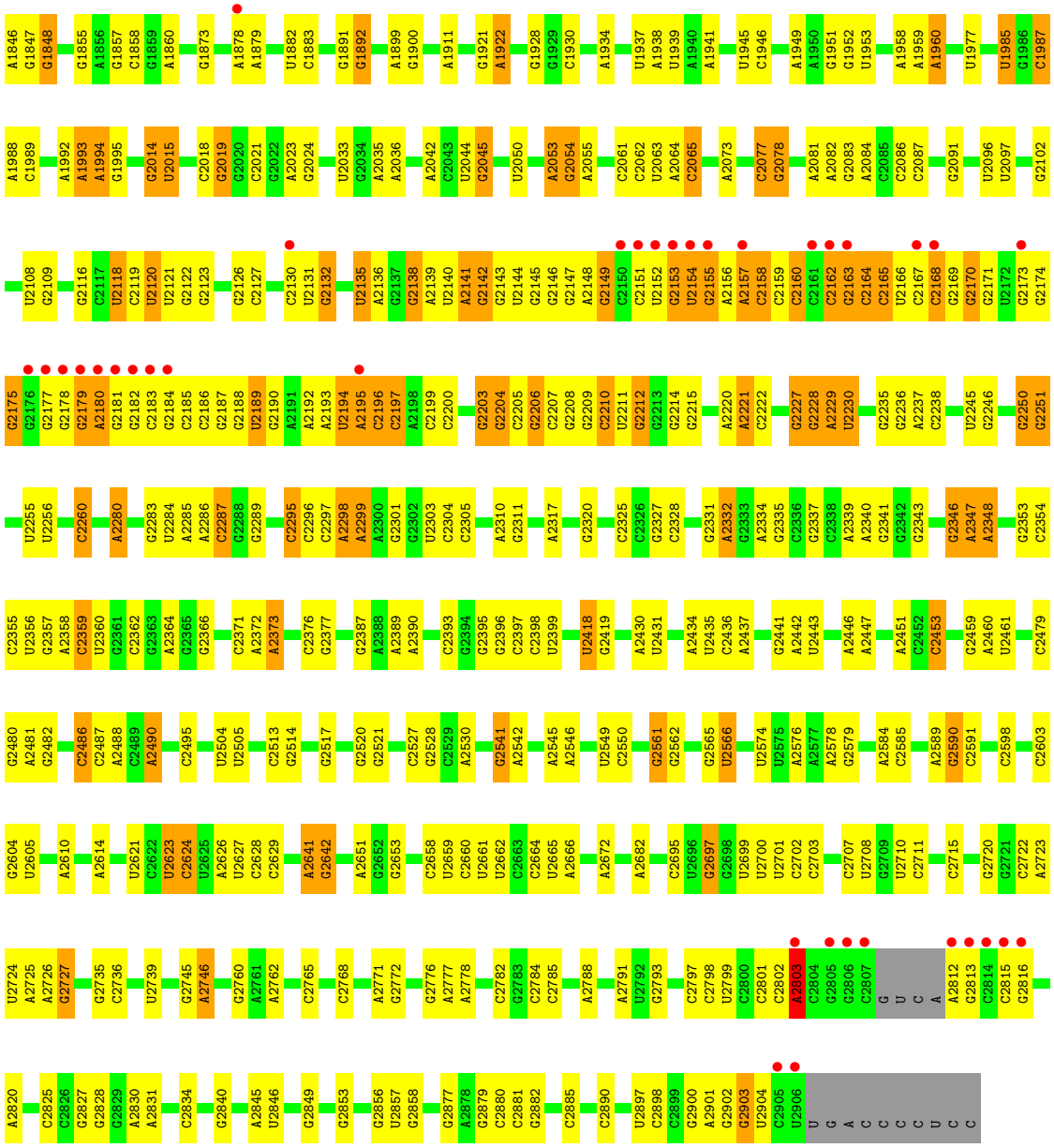


• Molecule 25: 23S Ribosomal RNA

Chain BA:

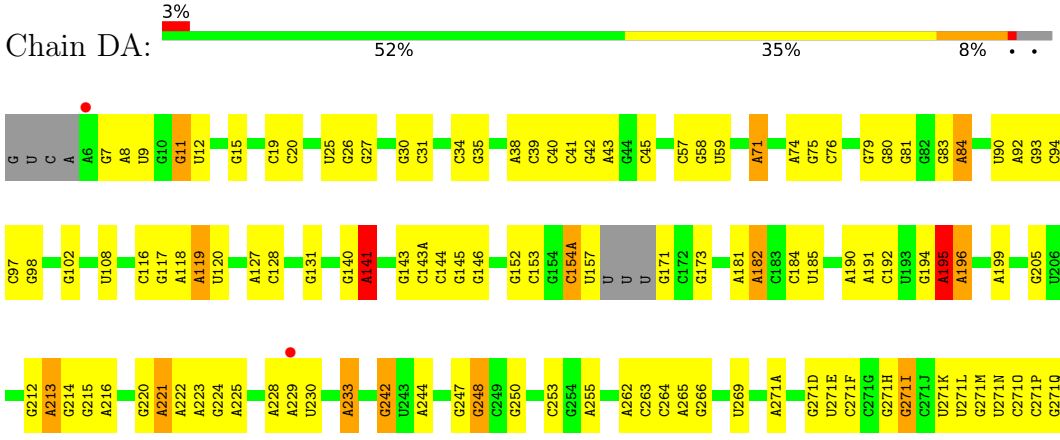


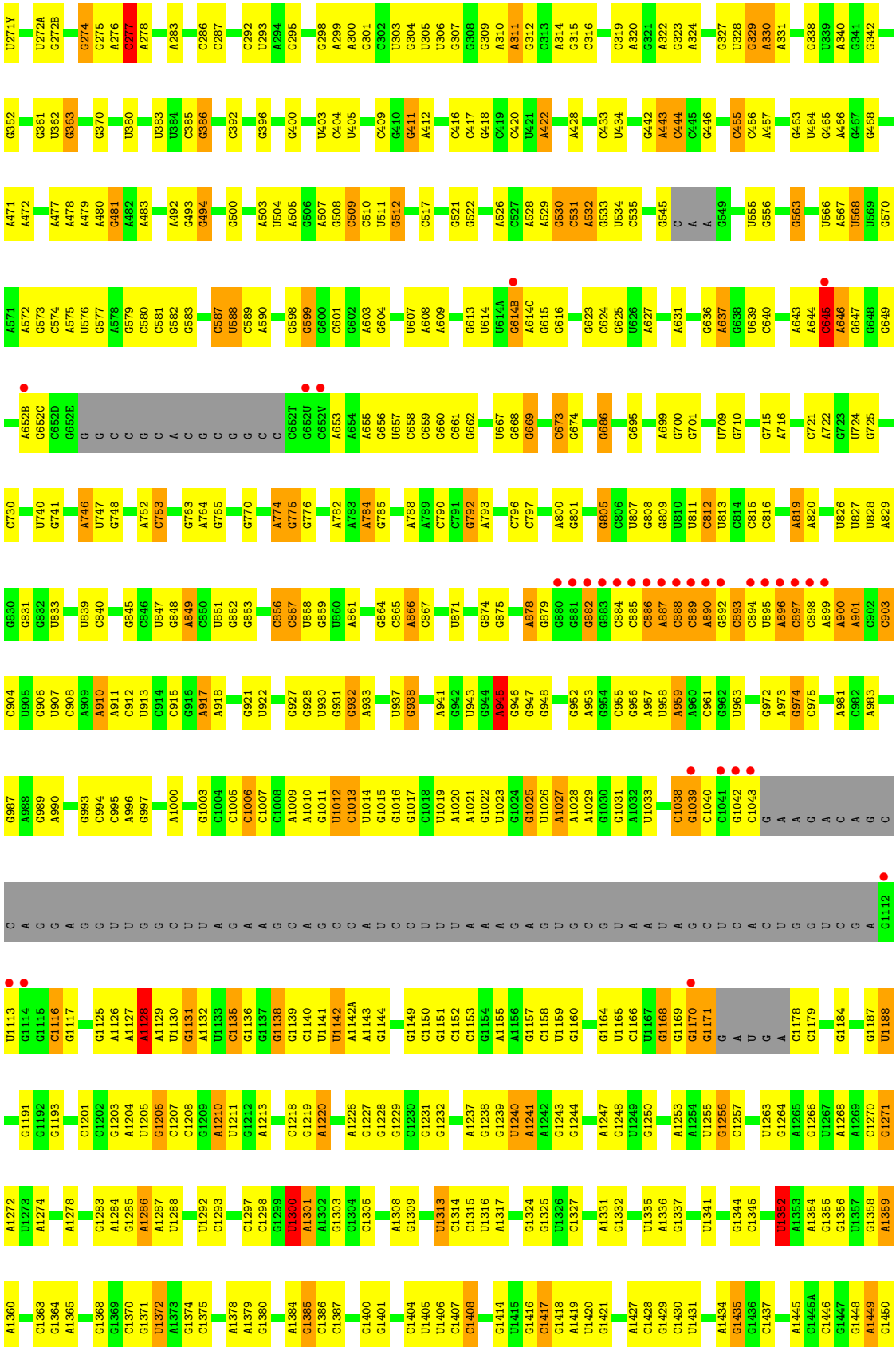


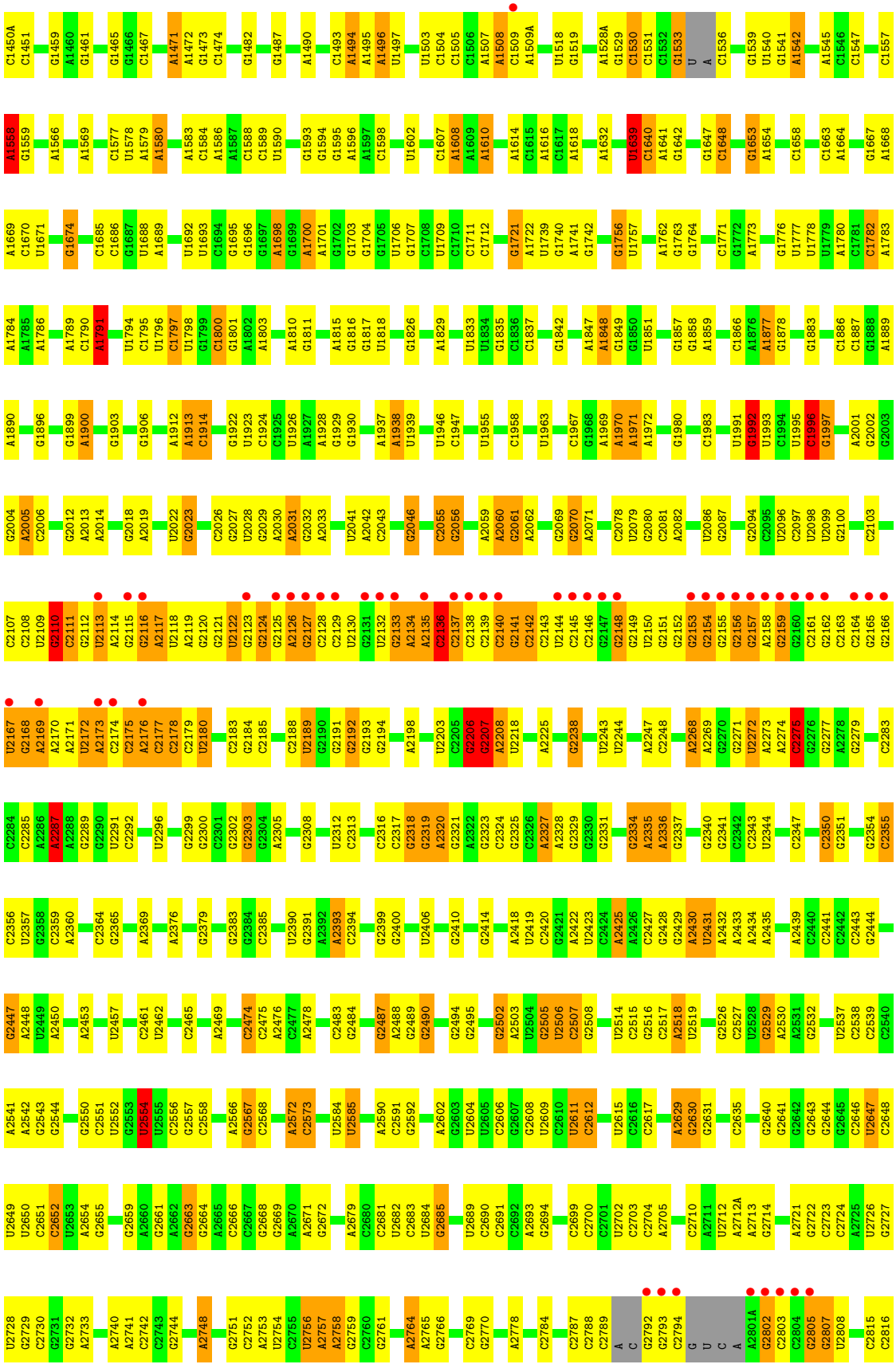


• Molecule 25: 23S Ribosomal RNA

Chain DA:



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A1558 G1559 A1566 A1569 C1577 U1578 A1579 A1580 A1583 C1584 A1586 A1587 C1588 C1589 U1590 G1593 G1594 G1595 A1596 A1597 C1598 U1602 C1607 A1608 A1609 A1610 A1614 C1615 A1616 C1617 A1618 A1632 U1639 C1640 A1641 G1642 G1647 C1648 G1653 A1654 C1658 C1663 A1664 G1667 A1668
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C2107 C2108 U2109 C2110 C2111 C2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 C2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166
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U2649 U2650 C2651 C2652 U2653 A2654 G2655 G2659 A2660 G2661 A2662 G2663 G2664 A2665 C2666 C2667 G2668 G2669 A2670 A2671 G2672 A2679 C2680 C2681 U2682 C2683 U2684 G2685 U2689 C2690 C2691 C2692 A2693 G2694 C2699 C2700 C2701 U2702 C2703 C2704 A2705 C2710 A2711 U2712 A2712A A2713 G2714 A2721 G2722 C2723 C2724 A2725 U2726 G2727
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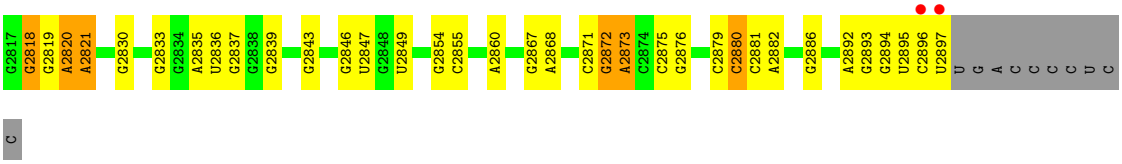
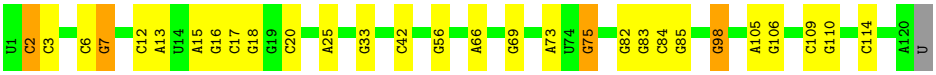


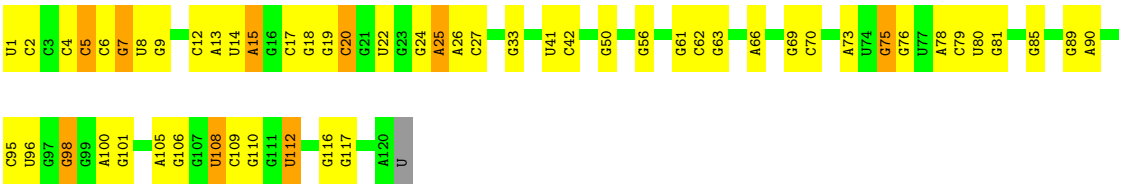
• Molecule 26: 5S Ribosomal RNA

Chain BB:



• Molecule 26: 5S Ribosomal RNA

Chain DB:

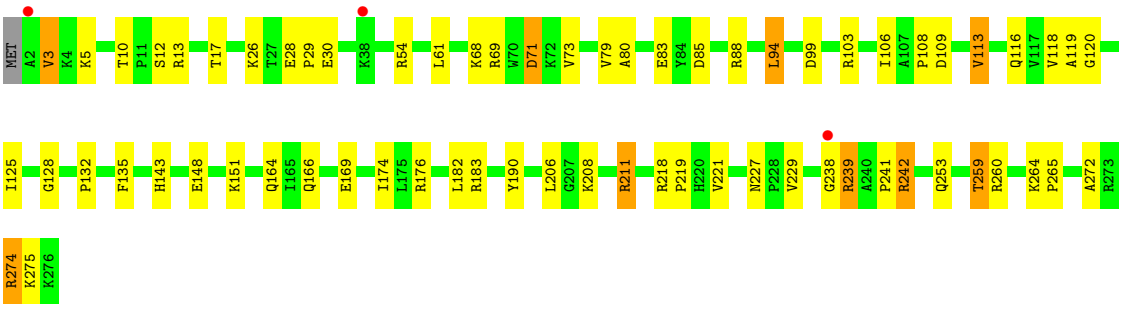


• Molecule 27: 50S Ribosomal Protein L2

Chain BD:

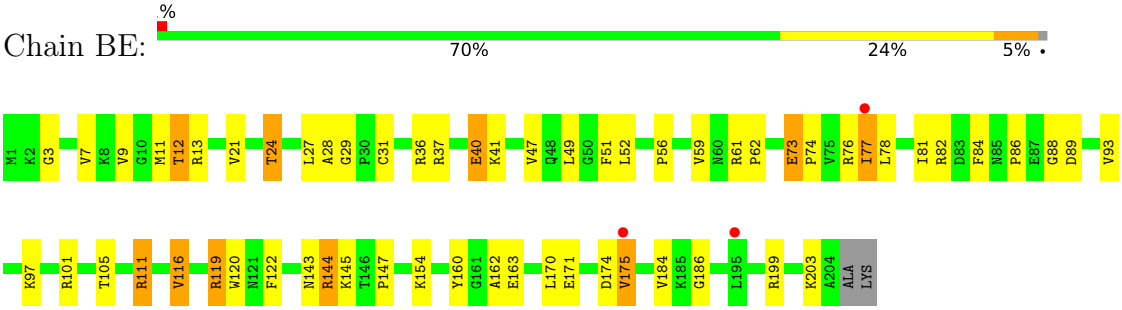
• Molecule 27: 50S Ribosomal Protein L2

Chain DD:



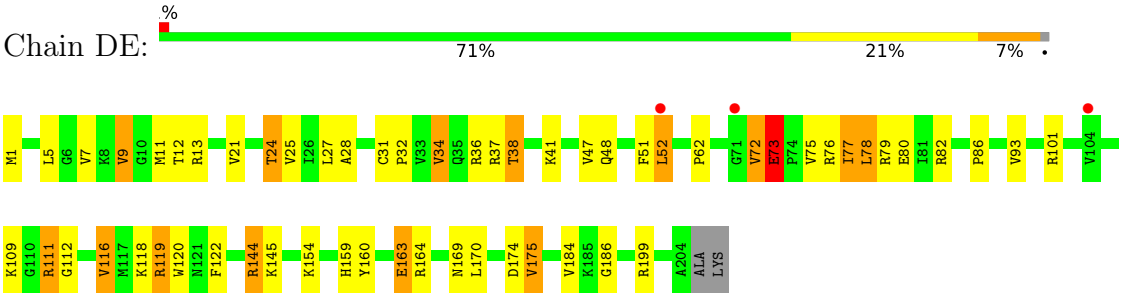
• Molecule 28: 50S Ribosomal Protein L3

Chain BE:



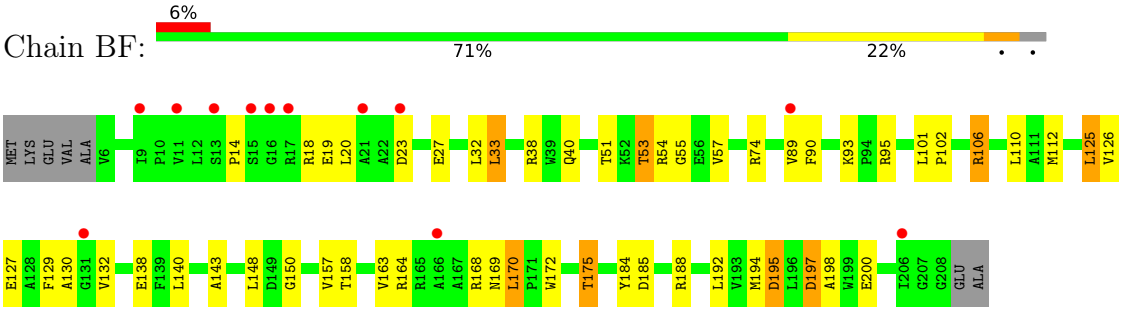
• Molecule 28: 50S Ribosomal Protein L3

Chain DE:



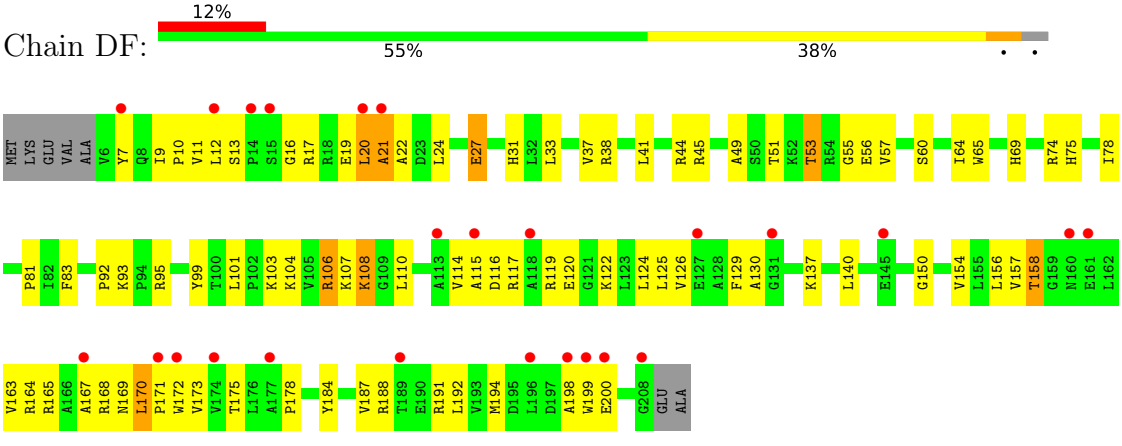
• Molecule 29: 50S Ribosomal Protein L4

Chain BF:



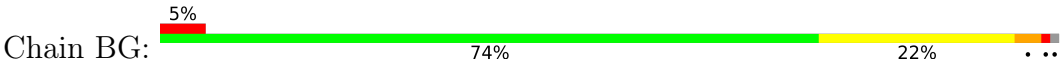
• Molecule 29: 50S Ribosomal Protein L4

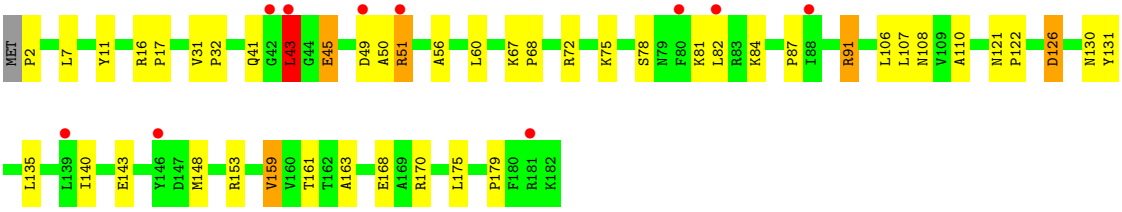
Chain DF:



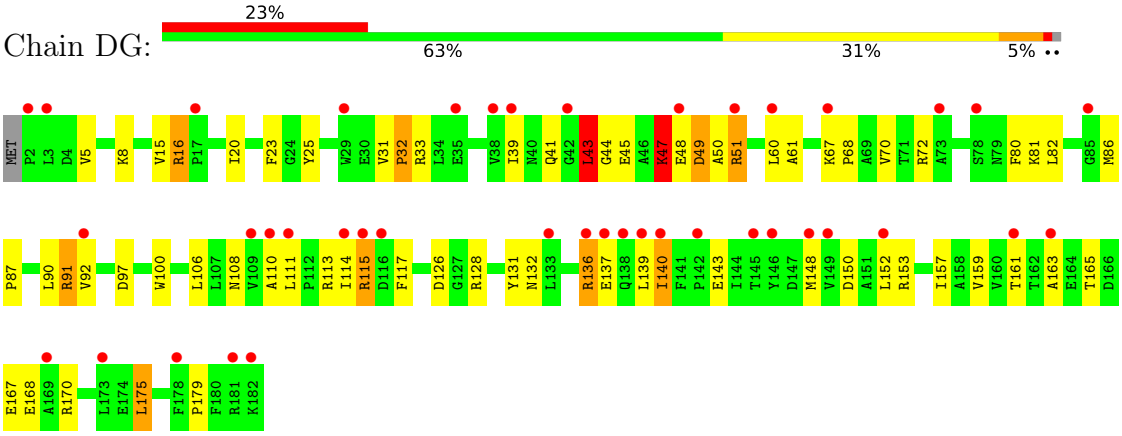
• Molecule 30: 50S Ribosomal Protein L5

Chain BG:

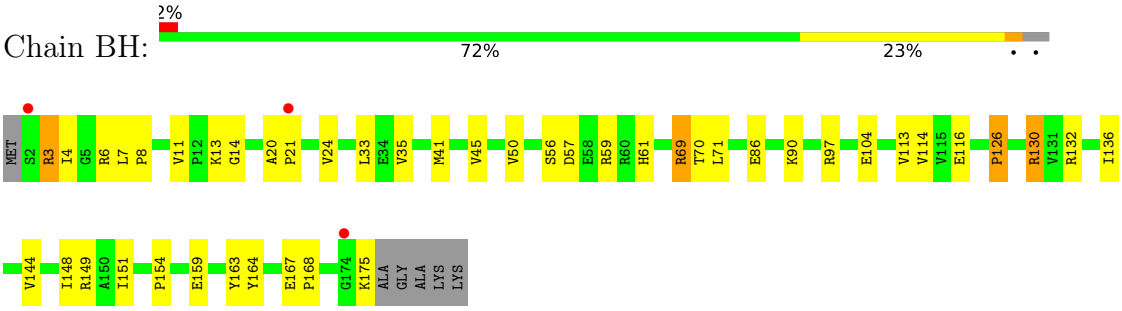




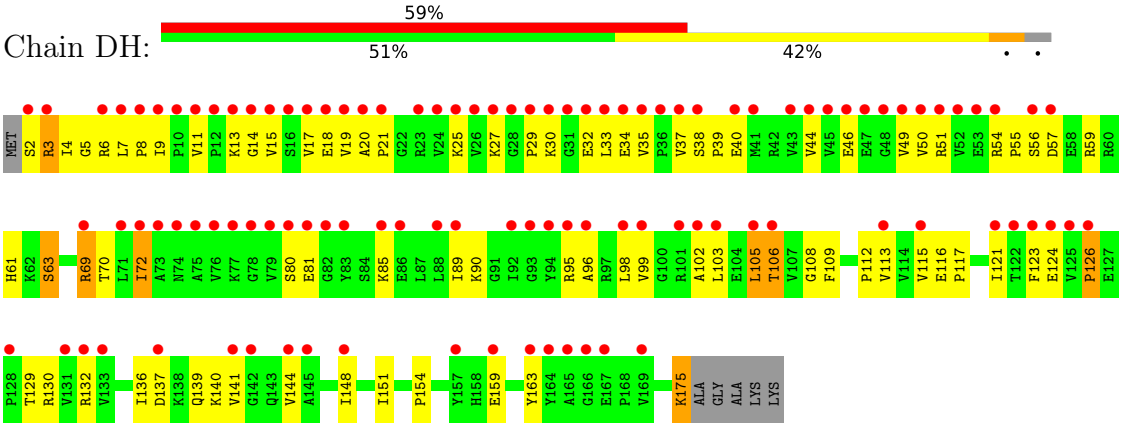
• Molecule 30: 50S Ribosomal Protein L5



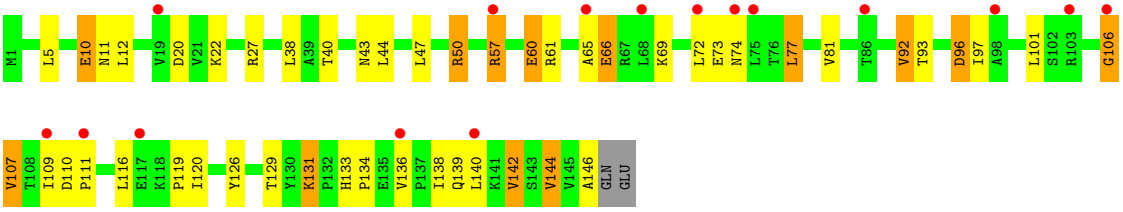
• Molecule 31: 50S Ribosomal Protein L6



• Molecule 31: 50S Ribosomal Protein L6

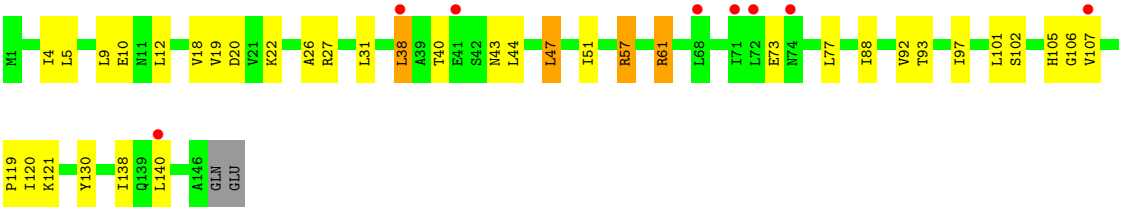


• Molecule 32: 50S Ribosomal Protein L9



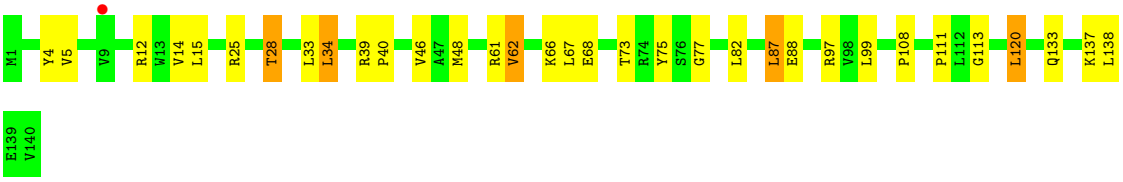
• Molecule 32: 50S Ribosomal Protein L9

Chain DI:



• Molecule 33: 50S Ribosomal Protein L13

Chain BN:

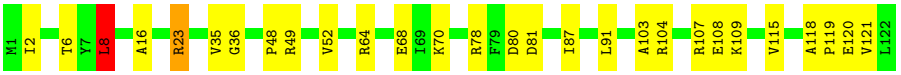


• Molecule 33: 50S Ribosomal Protein L13

Chain DN:

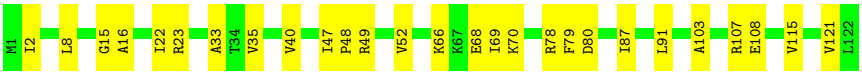
• Molecule 34: 50S Ribosomal Protein L14

Chain BO:



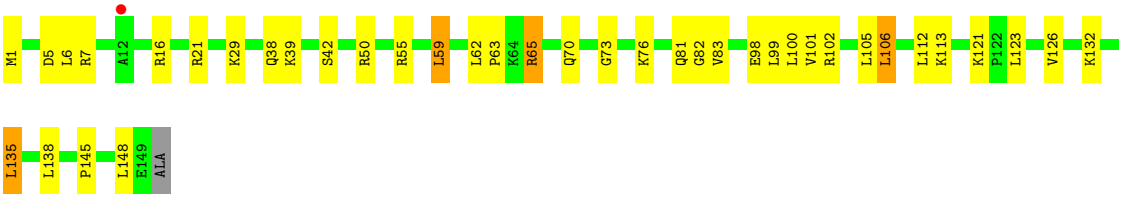
• Molecule 34: 50S Ribosomal Protein L14

Chain DO:



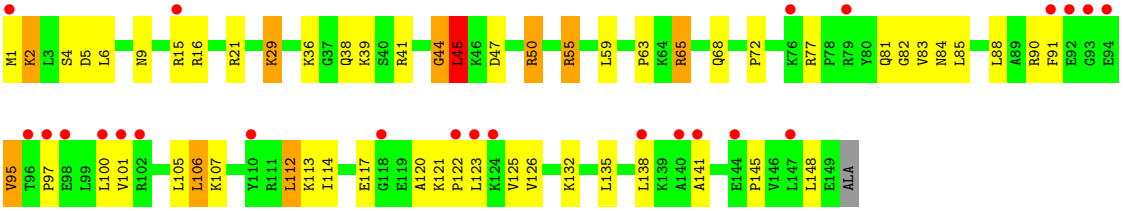
• Molecule 35: 50S Ribosomal Protein L15

Chain BP:



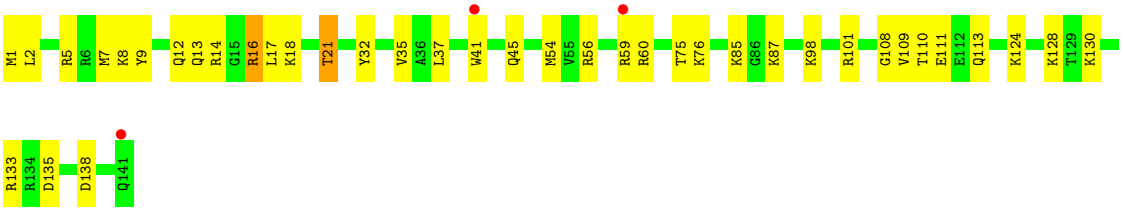
• Molecule 35: 50S Ribosomal Protein L15

Chain DP:



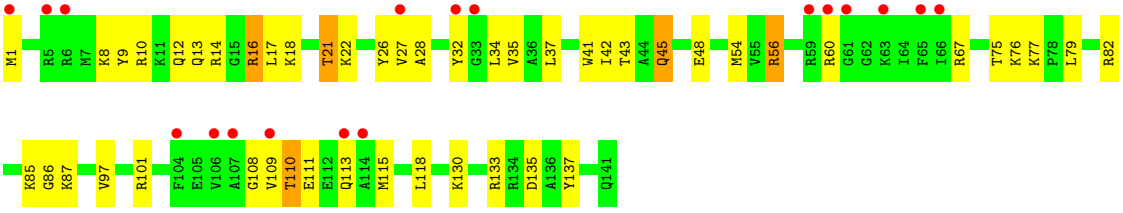
• Molecule 36: 50S Ribosomal Protein L16

Chain BQ:



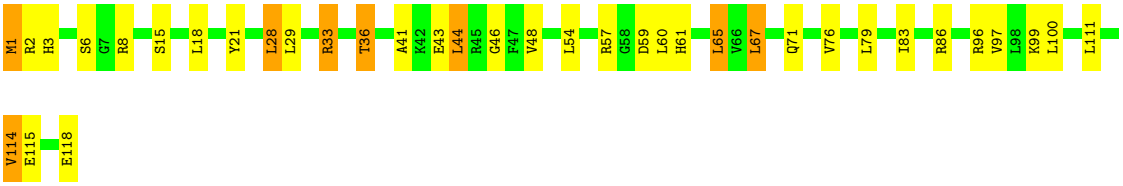
• Molecule 36: 50S Ribosomal Protein L16

Chain DQ:



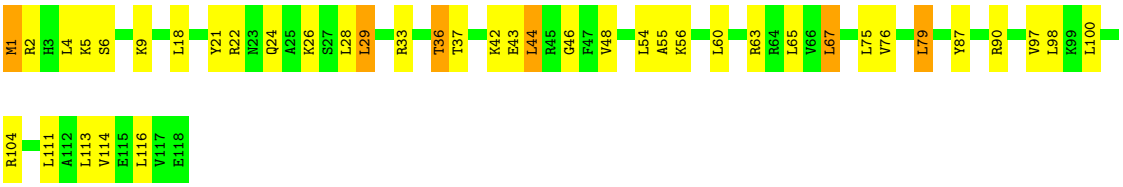
• Molecule 37: 50S Ribosomal Protein L17

Chain BR:



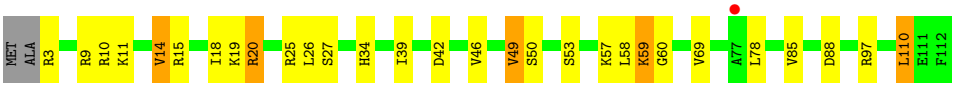
• Molecule 37: 50S Ribosomal Protein L17

Chain DR:



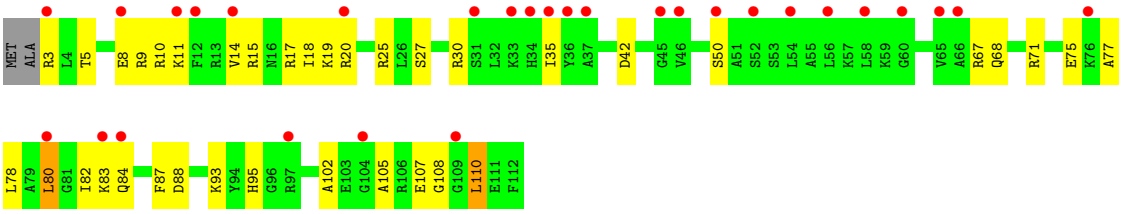
• Molecule 38: 50S Ribosomal Protein L18

Chain BS:



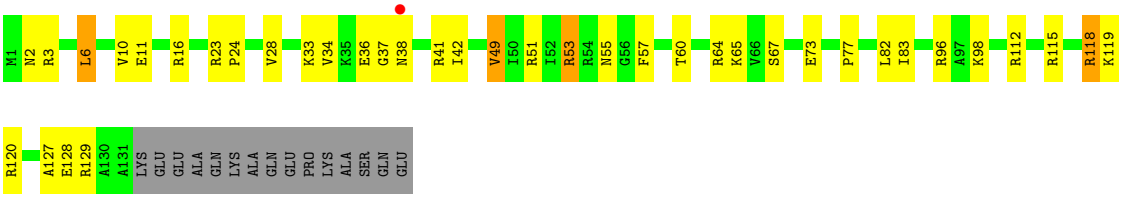
• Molecule 38: 50S Ribosomal Protein L18

Chain DS:



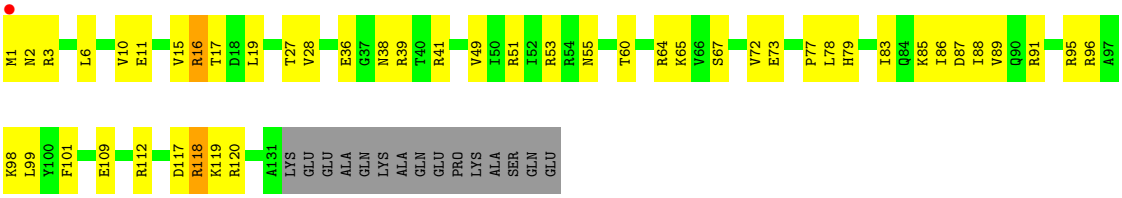
• Molecule 39: 50S Ribosomal Protein L19

Chain BT:



• Molecule 39: 50S Ribosomal Protein L19

Chain DT:

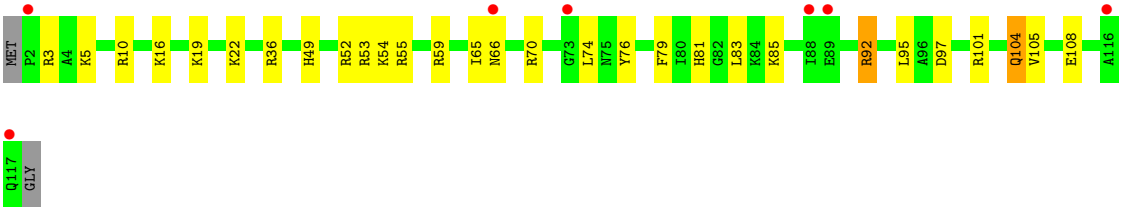


• Molecule 40: 50S Ribosomal Protein L20

Chain BU:

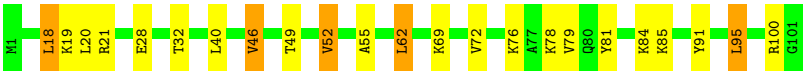
• Molecule 40: 50S Ribosomal Protein L20

Chain DU:



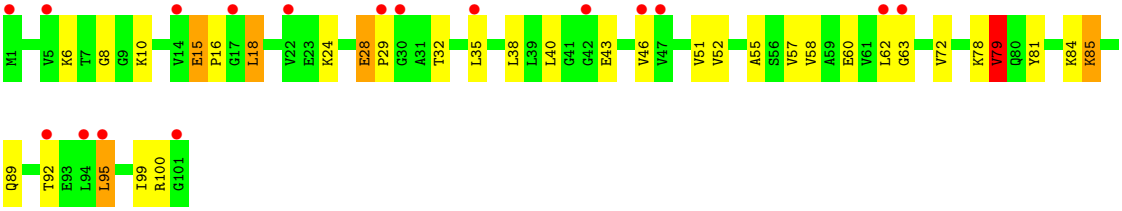
• Molecule 41: 50S Ribosomal Protein L21

Chain BV:



• Molecule 41: 50S Ribosomal Protein L21

Chain DV:

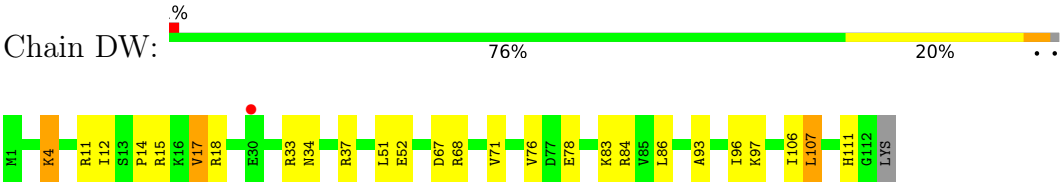


• Molecule 42: 50S Ribosomal Protein L22

Chain BW:

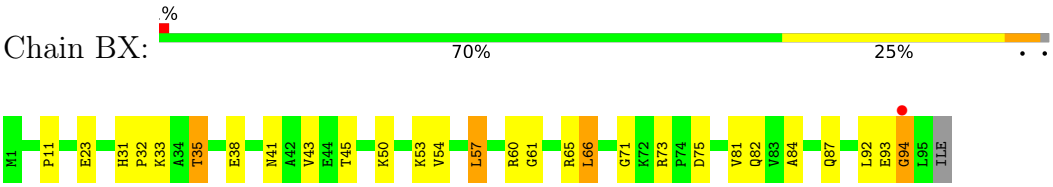
• Molecule 42: 50S Ribosomal Protein L22

Chain DW:



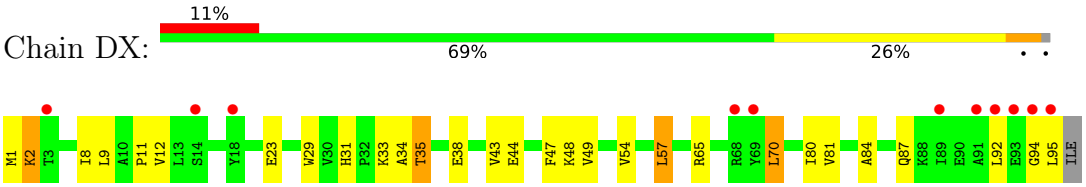
• Molecule 43: 50S Ribosomal Protein L23

Chain BX:



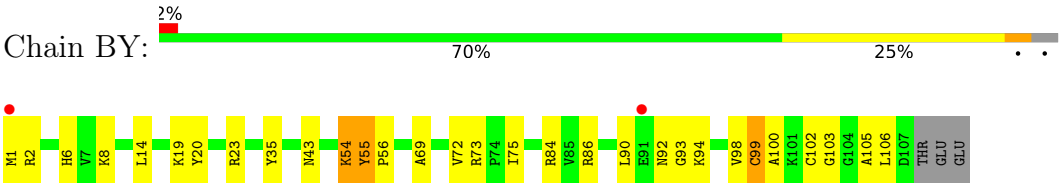
• Molecule 43: 50S Ribosomal Protein L23

Chain DX:



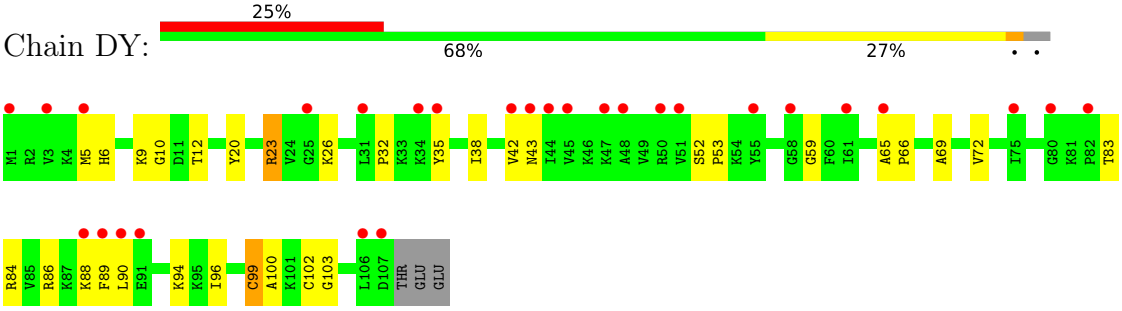
• Molecule 44: 50S Ribosomal Protein L24

Chain BY:



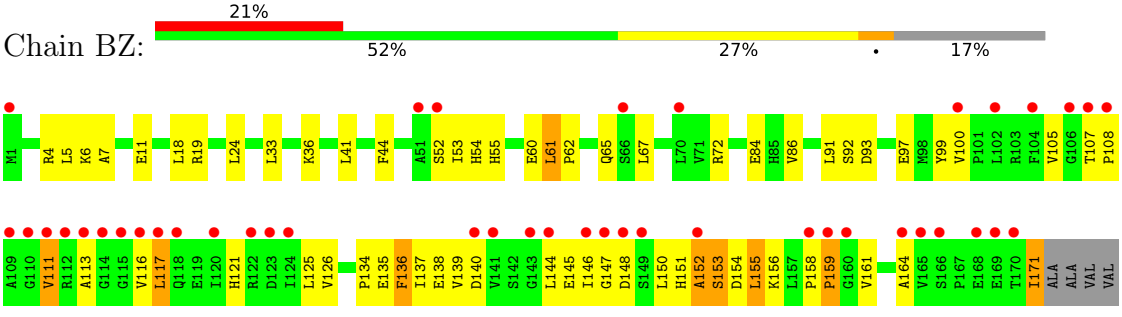
• Molecule 44: 50S Ribosomal Protein L24

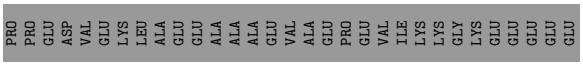
Chain DY:



• Molecule 45: 50S Ribosomal Protein L25

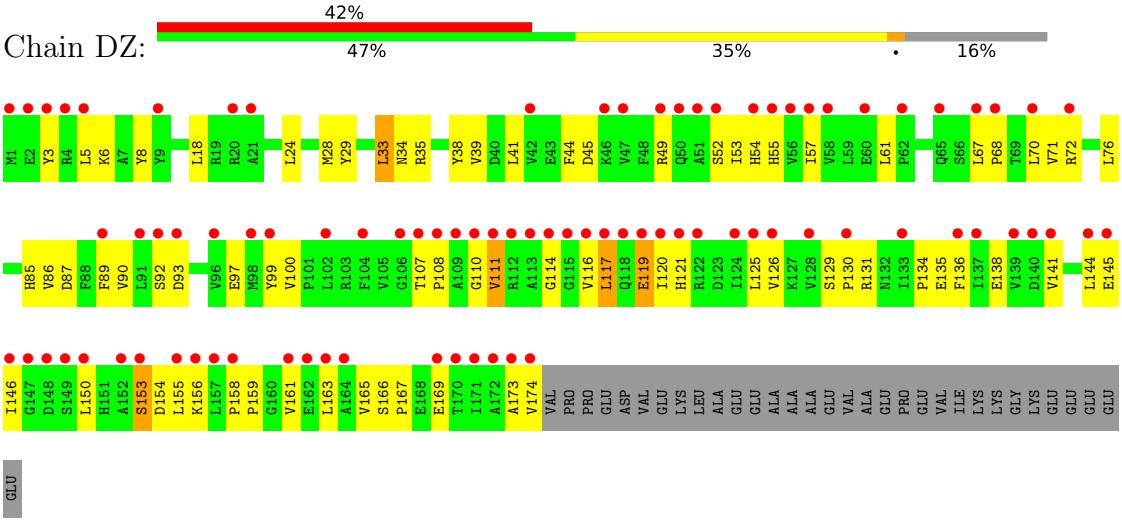
Chain BZ:





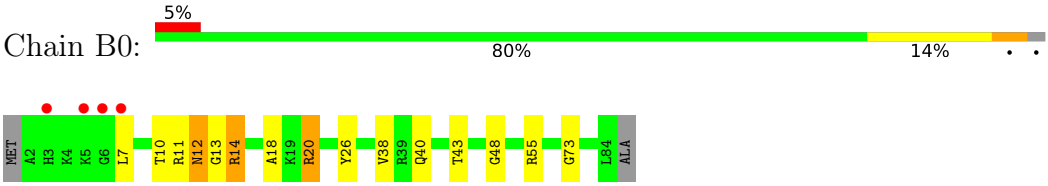
• Molecule 45: 50S Ribosomal Protein L25

Chain DZ:



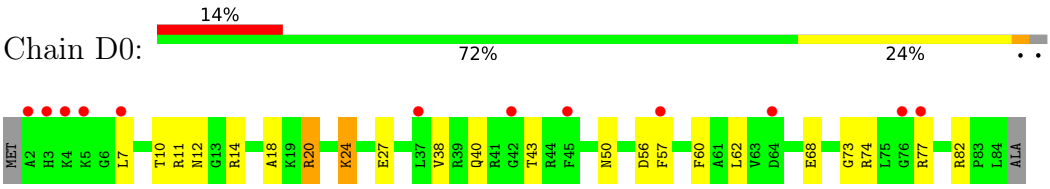
• Molecule 46: 50S Ribosomal Protein L27

Chain B0:



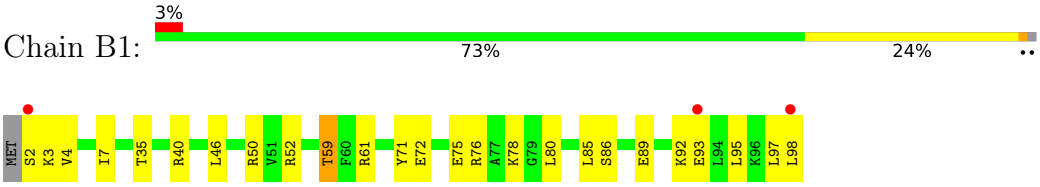
• Molecule 46: 50S Ribosomal Protein L27

Chain D0:



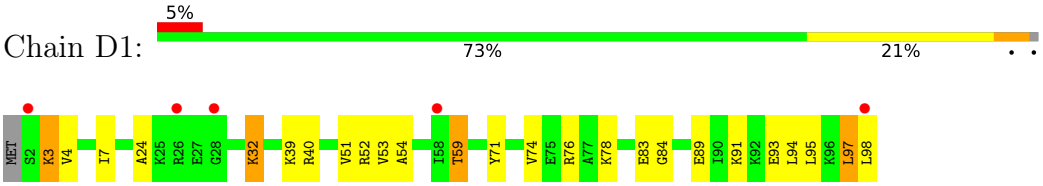
• Molecule 47: 50S Ribosomal Protein L28

Chain B1:



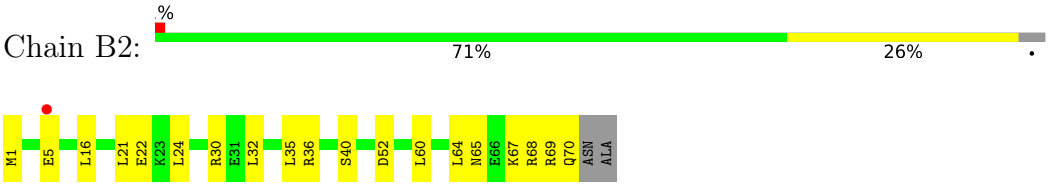
• Molecule 47: 50S Ribosomal Protein L28

Chain D1:



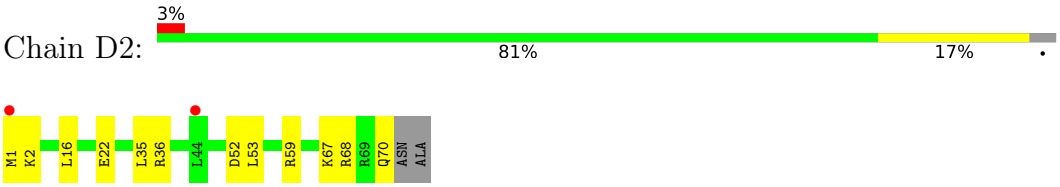
• Molecule 48: 50S Ribosomal Protein L29

Chain B2:



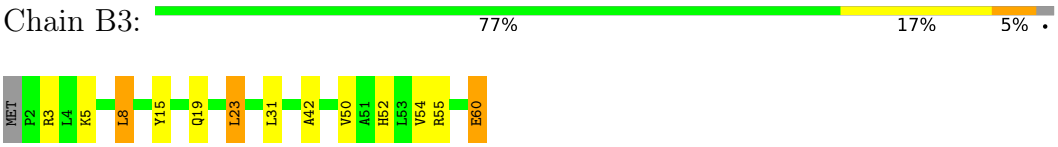
• Molecule 48: 50S Ribosomal Protein L29

Chain D2:



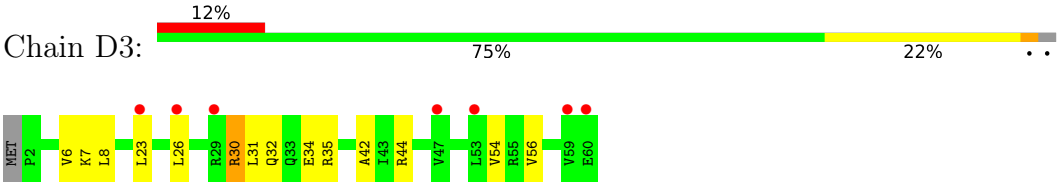
• Molecule 49: 50S Ribosomal Protein L30

Chain B3:



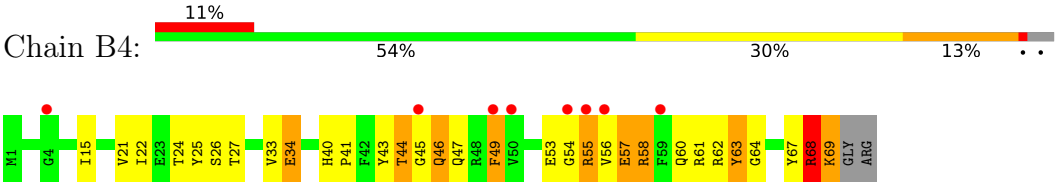
• Molecule 49: 50S Ribosomal Protein L30

Chain D3:



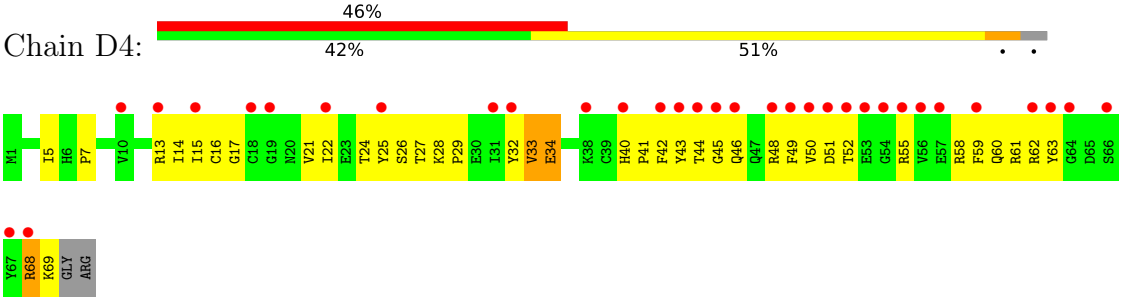
• Molecule 50: 50S Ribosomal Protein L31

Chain B4:



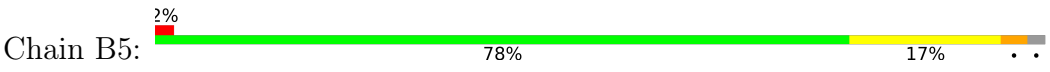
• Molecule 50: 50S Ribosomal Protein L31

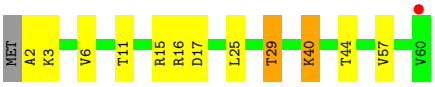
Chain D4:



• Molecule 51: 50S Ribosomal Protein L32

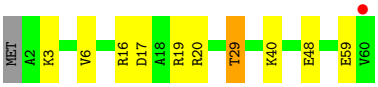
Chain B5:





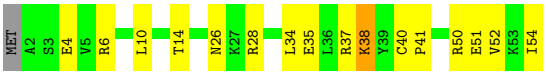
• Molecule 51: 50S Ribosomal Protein L32

Chain D5:



• Molecule 52: 50S Ribosomal Protein L33

Chain B6:

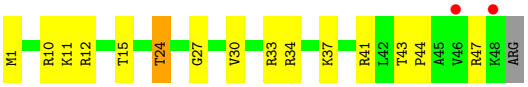


• Molecule 52: 50S Ribosomal Protein L33

Chain D6:

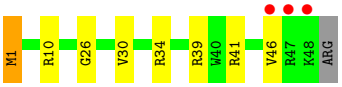
• Molecule 53: 50S Ribosomal Protein L34

Chain B7:



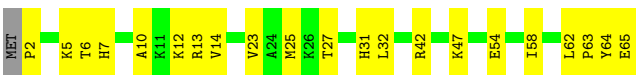
• Molecule 53: 50S Ribosomal Protein L34

Chain D7:



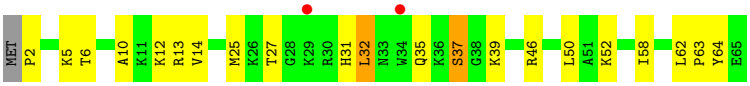
• Molecule 54: 50S Ribosomal Protein L35

Chain B8:



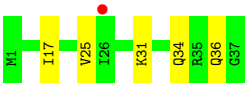
• Molecule 54: 50S Ribosomal Protein L35

Chain D8:



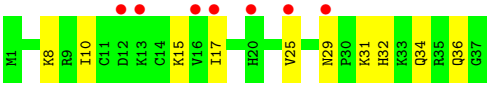
• Molecule 55: 50S Ribosomal Protein L36

Chain B9:



• Molecule 55: 50S Ribosomal Protein L36

Chain D9:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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(^{o})	Ideal(^{o})
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 (i)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	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 (i)

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
7	CG	52	GLU
27	DD	221	VAL
8	CH	127	LEU
7	CG	51	GLN
14	CN	23	ARG

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

Mol	Chain	Res	Type
45	BZ	34	ASN
36	DQ	45	GLN
3	CC	136	GLN
35	DP	38	GLN
43	DX	31	HIS

5.3.3 RNA (i)

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
1	CA	532	A
25	DA	2756	U
1	CA	1212	U
25	DA	2689	U
25	DA	1558	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	39	23	18,21,22	1.44	3 (16%)	22,30,33	1.81	3 (13%)
23	MIA	CY	37	23	18,24,32	1.16	2 (11%)	18,35,47	1.28	2 (11%)
23	PSU	CY	55	23	18,21,22	1.38	2 (11%)	22,30,33	1.95	3 (13%)
24	5MU	AX	54	56,24	19,22,23	1.44	6 (31%)	28,32,35	2.03	6 (21%)
24	5MC	AX	32	24	18,22,23	1.01	2 (11%)	26,32,35	1.25	2 (7%)
24	PSU	AX	55	24	18,21,22	1.34	2 (11%)	22,30,33	1.83	3 (13%)
23	4SU	CW	8	56,23	18,21,22	1.61	4 (22%)	26,30,33	1.95	4 (15%)
24	5MU	CX	54	24	19,22,23	1.38	6 (31%)	28,32,35	2.08	8 (28%)
23	PSU	AY	39	23	18,21,22	1.48	3 (16%)	22,30,33	1.57	4 (18%)
23	PSU	CW	55	23	18,21,22	1.38	2 (11%)	22,30,33	1.94	3 (13%)
24	PSU	CX	55	24	18,21,22	1.34	2 (11%)	22,30,33	1.84	4 (18%)
23	PSU	AW	55	23	18,21,22	1.38	2 (11%)	22,30,33	1.89	3 (13%)
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	1.34	3 (13%)	29,39,42	2.52	7 (24%)
24	4SU	AX	8	24	18,21,22	2.19	6 (33%)	26,30,33	1.71	6 (23%)
23	7MG	AY	46	23	22,26,27	1.40	4 (18%)	29,39,42	2.50	7 (24%)
24	4SU	CX	8	24	18,21,22	1.88	4 (22%)	26,30,33	1.31	3 (11%)
23	PSU	AW	39	23	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
23	PSU	CY	32	23	18,21,22	1.34	2 (11%)	22,30,33	1.76	3 (13%)
23	7MG	CW	46	23	22,26,27	1.34	4 (18%)	29,39,42	2.54	6 (20%)
23	4SU	AW	8	23	18,21,22	1.72	5 (27%)	26,30,33	1.79	6 (23%)
23	5MU	CY	54	23	19,22,23	1.50	5 (26%)	28,32,35	1.93	9 (32%)
24	5MC	CX	32	24	18,22,23	1.04	2 (11%)	26,32,35	1.27	3 (11%)
23	PSU	CW	39	23	18,21,22	1.39	2 (11%)	22,30,33	1.53	3 (13%)
23	PSU	AW	32	56,23	18,21,22	1.37	3 (16%)	22,30,33	1.70	3 (13%)
23	7MG	CY	46	23	22,26,27	1.40	4 (18%)	29,39,42	2.52	7 (24%)
23	PSU	AY	55	23	18,21,22	1.26	2 (11%)	22,30,33	1.91	6 (27%)
23	5MU	AW	54	23	19,22,23	1.46	5 (26%)	28,32,35	1.69	5 (17%)
23	MIA	CW	37	23	18,24,32	1.07	2 (11%)	18,35,47	1.38	2 (11%)
23	MIA	AW	37	23	24,31,32	2.28	3 (12%)	26,44,47	2.40	8 (30%)
23	5MU	AY	54	23	19,22,23	1.47	4 (21%)	28,32,35	1.61	6 (21%)
23	PSU	CW	32	23	18,21,22	1.35	3 (16%)	22,30,33	1.86	4 (18%)
23	PSU	AY	32	23	18,21,22	1.32	2 (11%)	22,30,33	1.90	3 (13%)
23	4SU	CY	8	23	18,21,22	1.66	4 (22%)	26,30,33	2.20	4 (15%)
23	5MU	CW	54	23	19,22,23	1.33	5 (26%)	28,32,35	1.95	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	4SU	AY	8	23	18,21,22	1.72	7 (38%)	26,30,33	1.54	5 (19%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	AY	32	23	-	0/7/25/26	0/2/2/2
23	4SU	CY	8	23	-	2/7/25/26	0/2/2/2
23	5MU	CW	54	23	-	0/7/25/26	0/2/2/2
23	4SU	AY	8	23	-	1/7/25/26	0/2/2/2

The worst 5 of 121 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
24	AX	8	4SU	C4-N3	-5.67	1.31	1.37
23	CY	8	4SU	C4-S4	-4.45	1.60	1.68
24	CX	8	4SU	C4-N3	-4.30	1.33	1.37

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AY	46	7MG	N9-C4-N3	9.11	139.09	125.47
23	AW	46	7MG	N9-C4-N3	9.02	138.96	125.47
23	CW	46	7MG	N9-C4-N3	8.82	138.66	125.47
23	CY	46	7MG	N9-C4-N3	8.63	138.38	125.47
23	AW	37	MIA	C12-C13-C14	-7.69	112.17	127.14

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	AW	37	MIA	C12-C13-C14-C16
23	AY	39	PSU	C3'-C4'-C5'-O5'
23	AY	46	7MG	C4'-C5'-O5'-P
23	CW	32	PSU	C2'-C1'-C5-C4
23	CW	32	PSU	C2'-C1'-C5-C6

There are no ring outliers.

19 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	CY	39	PSU	2	0
23	CY	37	MIA	1	0
23	CW	8	4SU	1	0
23	AW	55	PSU	1	0

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
58	SF4	AD	501	4	0,12,12	-	-	-		
57	PCY	CA	3178	-	36,42,42	1.63	4 (11%)	41,65,65	1.17	4 (9%)
57	PCY	AA	3231	-	36,42,42	1.68	5 (13%)	41,65,65	1.42	8 (19%)
58	SF4	CD	501	4	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	AD	501	4	-	-	0/6/5/5
57	PCY	CA	3178	-	-	9/33/67/67	0/3/3/3
57	PCY	AA	3231	-	-	5/33/67/67	0/3/3/3
58	SF4	CD	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(^{o})	Ideal(^{o})
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

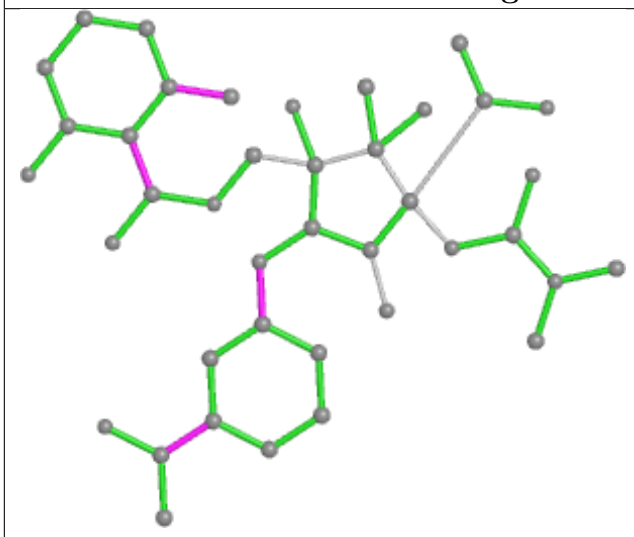
There are no ring outliers.

2 monomers are involved in 16 short contacts:

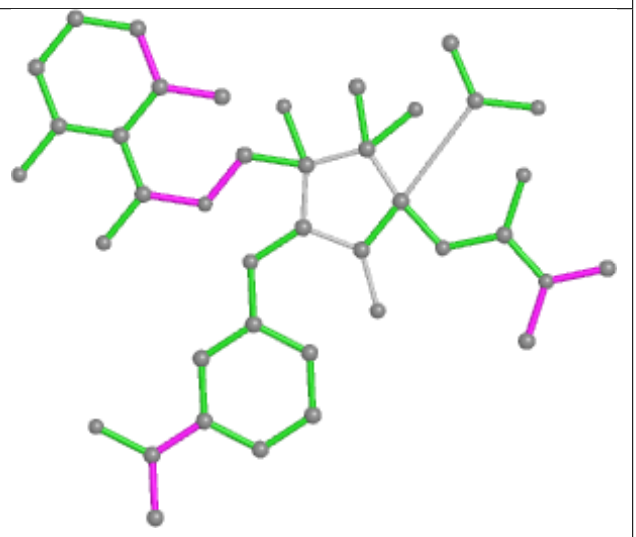
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	CA	3178	PCY	9	0
57	AA	3231	PCY	7	0

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 then 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.

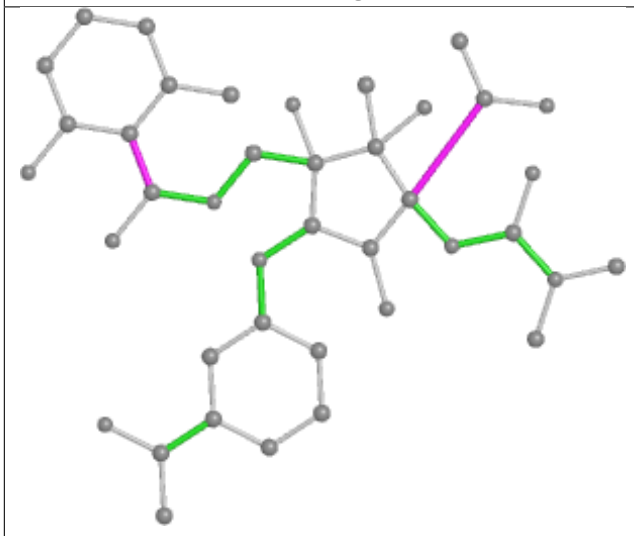
Ligand PCY CA 3178



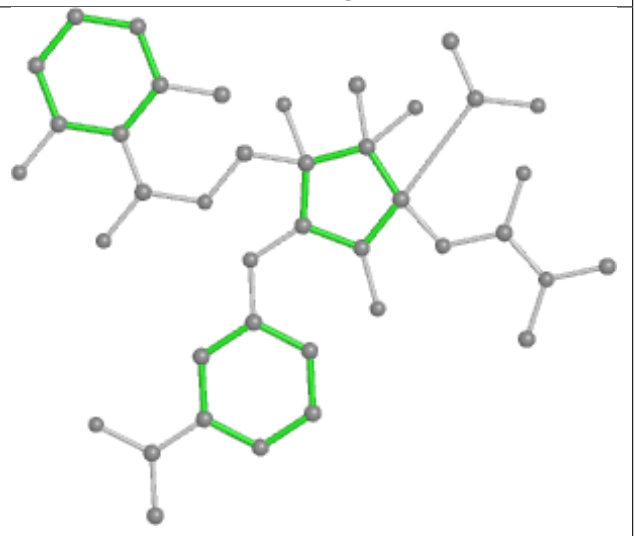
Bond lengths



Bond angles

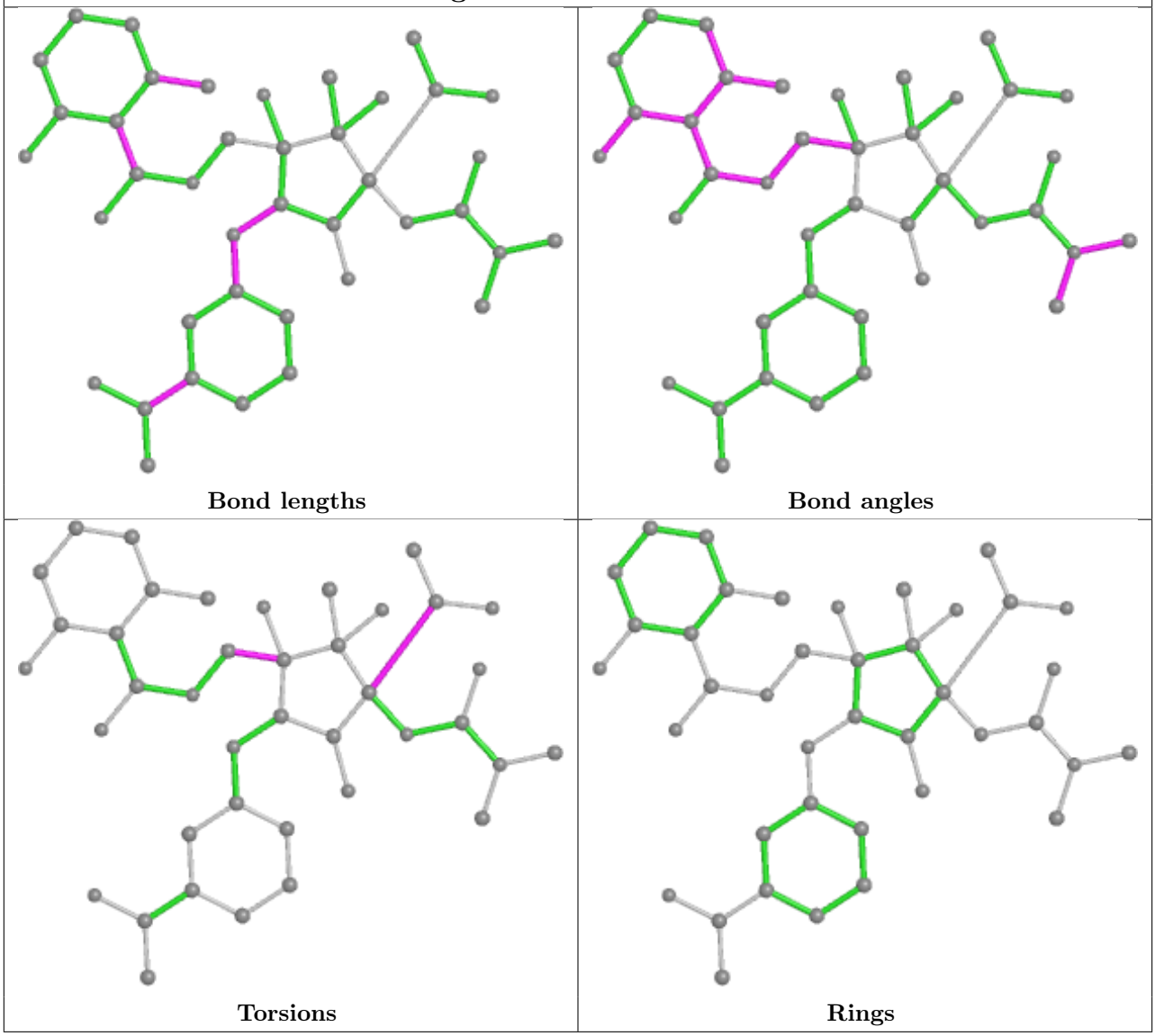


Torsions



Rings

Ligand PCY AA 3231



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	58, 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, 66, 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, 76	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, 95^{th} 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	7MG	AW	46	24/25	0.83	0.22	70,83,111,120	0
23	PSU	CY	55	20/21	0.83	0.29	92,98,105,119	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
24	PSU	CX	55	20/21	0.90	0.16	63,69,89,97	0
23	PSU	AY	39	20/21	0.90	0.21	77,86,97,100	0
23	5MU	CW	54	21/22	0.90	0.17	60,72,84,86	0
23	PSU	CW	32	20/21	0.90	0.19	70,85,92,95	0
23	MIA	CW	37	22/30	0.91	0.16	55,66,75,81	0
23	4SU	AW	8	20/21	0.91	0.17	73,85,96,105	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	PSU	AX	55	20/21	0.94	0.18	60,67,93,94	0
24	5MU	AX	54	21/22	0.94	0.18	58,65,74,81	0
23	5MU	AW	54	21/22	0.95	0.16	42,58,69,76	0
23	PSU	AW	32	20/21	0.95	0.16	50,60,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	5MC	CX	32	21/22	0.95	0.16	66,71,81,83	0
24	4SU	AX	8	20/21	0.96	0.18	51,64,80,88	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
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 monosaccharides 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(Å^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	BA	3712	1/1	0.63	0.13	64,64,64,64	0
56	MG	DA	3182	1/1	0.63	0.30	64,64,64,64	0
56	MG	DA	3241	1/1	0.64	0.20	50,50,50,50	0
56	MG	BA	3683	1/1	0.64	0.15	61,61,61,61	0
56	MG	CA	3051	1/1	0.64	0.11	66,66,66,66	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	DA	3596	1/1	0.65	0.44	63,63,63,63	0
56	MG	DB	3005	1/1	0.65	0.28	64,64,64,64	0
56	MG	BA	3804	1/1	0.66	0.10	58,58,58,58	0
56	MG	AA	3110	1/1	0.66	0.22	61,61,61,61	0
56	MG	CA	3064	1/1	0.67	0.11	57,57,57,57	0
56	MG	DA	3505	1/1	0.68	0.12	66,66,66,66	0
56	MG	BA	3527	1/1	0.68	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3051	1/1	0.68	0.20	56,56,56,56	0
56	MG	DA	3607	1/1	0.68	0.34	53,53,53,53	0
56	MG	BR	202	1/1	0.68	0.41	53,53,53,53	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	BA	3728	1/1	0.70	0.10	72,72,72,72	0
56	MG	CX	3006	1/1	0.70	0.50	70,70,70,70	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	CA	3049	1/1	0.70	0.23	68,68,68,68	0
56	MG	BA	3639	1/1	0.70	0.29	59,59,59,59	0
56	MG	BA	3431	1/1	0.71	0.27	55,55,55,55	0
56	MG	CA	3027	1/1	0.71	0.51	70,70,70,70	0
56	MG	BA	3030	1/1	0.71	0.19	50,50,50,50	0
56	MG	AA	3082	1/1	0.72	0.26	68,68,68,68	0
56	MG	BA	3079	1/1	0.72	0.32	57,57,57,57	0
56	MG	BA	3470	1/1	0.72	0.16	48,48,48,48	0
56	MG	BA	3734	1/1	0.72	0.35	60,60,60,60	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	3098	1/1	0.73	0.21	43,43,43,43	0
56	MG	AA	3004	1/1	0.73	0.14	67,67,67,67	0
56	MG	DA	3538	1/1	0.73	0.27	56,56,56,56	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	3204	1/1	0.73	0.19	71,71,71,71	0
56	MG	AA	3095	1/1	0.73	0.28	68,68,68,68	0
56	MG	DA	3312	1/1	0.74	0.14	52,52,52,52	0
56	MG	BA	3221	1/1	0.74	0.20	54,54,54,54	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	3333	1/1	0.74	0.11	61,61,61,61	0
56	MG	BA	3605	1/1	0.74	0.13	61,61,61,61	0
56	MG	DA	3251	1/1	0.75	0.27	51,51,51,51	0
56	MG	BB	3015	1/1	0.75	0.10	51,51,51,51	0
56	MG	BA	3020	1/1	0.75	0.20	61,61,61,61	0
56	MG	BA	3689	1/1	0.75	0.22	57,57,57,57	0
56	MG	DA	3452	1/1	0.75	0.24	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3560	1/1	0.75	0.23	35,35,35,35	0
56	MG	DA	3066	1/1	0.75	0.13	65,65,65,65	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	CA	3055	1/1	0.76	0.12	53,53,53,53	0
56	MG	DA	3521	1/1	0.76	0.17	51,51,51,51	0
56	MG	DA	3632	1/1	0.76	0.16	58,58,58,58	0
56	MG	AA	3038	1/1	0.76	0.14	51,51,51,51	0
56	MG	CA	3025	1/1	0.77	0.14	61,61,61,61	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	DA	3604	1/1	0.77	0.13	57,57,57,57	0
56	MG	AA	3042	1/1	0.77	0.21	57,57,57,57	0
56	MG	DA	3436	1/1	0.77	0.13	54,54,54,54	0
56	MG	CA	3069	1/1	0.77	0.12	68,68,68,68	0
56	MG	BA	3229	1/1	0.78	0.31	51,51,51,51	0
56	MG	DA	3404	1/1	0.78	0.20	51,51,51,51	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	3542	1/1	0.78	0.20	63,63,63,63	0
56	MG	DA	3445	1/1	0.78	0.23	72,72,72,72	0
56	MG	BA	3241	1/1	0.78	0.22	52,52,52,52	0
56	MG	AW	3001	1/1	0.78	0.09	55,55,55,55	0
56	MG	BA	3204	1/1	0.78	0.33	66,66,66,66	0
56	MG	DA	3614	1/1	0.78	0.14	50,50,50,50	0
56	MG	DA	3487	1/1	0.78	0.24	65,65,65,65	0
56	MG	DA	3127	1/1	0.78	0.27	38,38,38,38	0
56	MG	DW	3002	1/1	0.78	0.39	65,65,65,65	0
56	MG	BB	3009	1/1	0.79	0.27	58,58,58,58	0
56	MG	CA	3065	1/1	0.79	0.07	65,65,65,65	0
56	MG	AA	3072	1/1	0.79	0.19	68,68,68,68	0
56	MG	DA	3224	1/1	0.79	0.35	48,48,48,48	0
56	MG	DA	3508	1/1	0.79	0.10	59,59,59,59	0
56	MG	CA	3169	1/1	0.79	0.21	65,65,65,65	0
56	MG	BA	3720	1/1	0.79	0.23	46,46,46,46	0
56	MG	B1	102	1/1	0.79	0.41	68,68,68,68	0
56	MG	BA	3162	1/1	0.79	0.26	46,46,46,46	0
56	MG	DA	3547	1/1	0.79	0.17	65,65,65,65	0
56	MG	BA	3347	1/1	0.79	0.26	48,48,48,48	0
56	MG	DA	3325	1/1	0.79	0.25	57,57,57,57	0
56	MG	CA	3026	1/1	0.79	0.29	64,64,64,64	0
56	MG	DA	3605	1/1	0.79	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3367	1/1	0.79	0.33	53,53,53,53	0
56	MG	BA	3028	1/1	0.79	0.14	59,59,59,59	0
56	MG	DA	3105	1/1	0.79	0.19	60,60,60,60	0
56	MG	AA	3114	1/1	0.79	0.34	51,51,51,51	0
56	MG	BA	3699	1/1	0.79	0.18	42,42,42,42	0
56	MG	DA	3509	1/1	0.80	0.18	53,53,53,53	0
56	MG	DA	3513	1/1	0.80	0.17	50,50,50,50	0
56	MG	CA	3034	1/1	0.80	0.13	61,61,61,61	0
56	MG	BA	3277	1/1	0.80	0.19	54,54,54,54	0
56	MG	BA	3583	1/1	0.80	0.12	45,45,45,45	0
56	MG	BA	3585	1/1	0.80	0.39	55,55,55,55	0
56	MG	CA	3061	1/1	0.80	0.22	56,56,56,56	0
56	MG	BQ	3005	1/1	0.80	0.30	50,50,50,50	0
56	MG	DA	3170	1/1	0.80	0.09	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	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	3095	1/1	0.80	0.30	53,53,53,53	0
56	MG	DA	3645	1/1	0.80	0.20	44,44,44,44	0
56	MG	AW	3002	1/1	0.80	0.17	69,69,69,69	0
56	MG	AA	3091	1/1	0.80	0.10	70,70,70,70	0
56	MG	BA	3409	1/1	0.81	0.23	62,62,62,62	0
56	MG	DA	3309	1/1	0.81	0.14	42,42,42,42	0
56	MG	CA	3070	1/1	0.81	0.14	71,71,71,71	0
56	MG	DA	3115	1/1	0.81	0.18	41,41,41,41	0
56	MG	DA	3540	1/1	0.81	0.18	67,67,67,67	0
56	MG	DA	3393	1/1	0.81	0.10	52,52,52,52	0
56	MG	DA	3121	1/1	0.81	0.28	41,41,41,41	0
56	MG	BB	3011	1/1	0.81	0.06	59,59,59,59	0
56	MG	AA	3153	1/1	0.81	0.18	55,55,55,55	0
56	MG	DA	3566	1/1	0.81	0.17	48,48,48,48	0
56	MG	BA	3022	1/1	0.81	0.26	40,40,40,40	0
56	MG	AA	3087	1/1	0.81	0.34	52,52,52,52	0
56	MG	DA	3037	1/1	0.81	0.16	54,54,54,54	0
56	MG	DA	3213	1/1	0.81	0.23	61,61,61,61	0
56	MG	DA	3468	1/1	0.81	0.20	44,44,44,44	0
56	MG	AA	3062	1/1	0.81	0.14	60,60,60,60	0
56	MG	BA	3472	1/1	0.81	0.23	70,70,70,70	0
56	MG	BA	3516	1/1	0.81	0.22	65,65,65,65	0
56	MG	BA	3831	1/1	0.81	0.95	52,52,52,52	0
56	MG	BA	3101	1/1	0.82	0.25	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3081	1/1	0.82	0.18	58,58,58,58	0
56	MG	CA	3122	1/1	0.82	0.15	70,70,70,70	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	3429	1/1	0.82	0.26	40,40,40,40	0
56	MG	AA	3125	1/1	0.82	0.11	71,71,71,71	0
56	MG	BA	3413	1/1	0.82	0.19	41,41,41,41	0
56	MG	BA	3005	1/1	0.82	0.21	51,51,51,51	0
56	MG	DA	3568	1/1	0.82	0.12	54,54,54,54	0
56	MG	DA	3583	1/1	0.82	0.25	60,60,60,60	0
56	MG	DA	3214	1/1	0.82	0.34	47,47,47,47	0
56	MG	BA	3317	1/1	0.82	0.19	64,64,64,64	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	DA	3493	1/1	0.82	0.27	58,58,58,58	0
56	MG	BR	203	1/1	0.82	0.20	44,44,44,44	0
56	MG	BA	3603	1/1	0.82	0.11	54,54,54,54	0
56	MG	DA	3305	1/1	0.82	0.18	28,28,28,28	0
56	MG	AA	3068	1/1	0.82	0.17	60,60,60,60	0
56	MG	BB	3008	1/1	0.83	0.30	54,54,54,54	0
56	MG	DA	3410	1/1	0.83	0.15	62,62,62,62	0
56	MG	CX	3002	1/1	0.83	0.20	81,81,81,81	0
56	MG	AA	3170	1/1	0.83	0.13	57,57,57,57	0
56	MG	BA	3393	1/1	0.83	0.26	54,54,54,54	0
56	MG	BA	3407	1/1	0.83	0.19	37,37,37,37	0
56	MG	BQ	3003	1/1	0.83	0.15	54,54,54,54	0
56	MG	DA	3451	1/1	0.83	0.30	56,56,56,56	0
56	MG	BA	3238	1/1	0.83	0.25	43,43,43,43	0
56	MG	AA	3205	1/1	0.83	0.12	51,51,51,51	0
56	MG	DA	3078	1/1	0.83	0.11	45,45,45,45	0
56	MG	BA	3659	1/1	0.83	0.27	53,53,53,53	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	DA	3110	1/1	0.83	0.13	50,50,50,50	0
56	MG	CA	3011	1/1	0.83	0.17	63,63,63,63	0
56	MG	BA	3289	1/1	0.83	0.26	55,55,55,55	0
56	MG	CA	3023	1/1	0.83	0.22	55,55,55,55	0
56	MG	DA	3155	1/1	0.83	0.29	40,40,40,40	0
56	MG	BA	3442	1/1	0.83	0.11	59,59,59,59	0
56	MG	BA	3291	1/1	0.83	0.21	71,71,71,71	0
56	MG	BA	3705	1/1	0.83	0.17	54,54,54,54	0
56	MG	BA	3706	1/1	0.83	0.23	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3037	1/1	0.83	0.25	55,55,55,55	0
56	MG	BA	3295	1/1	0.83	0.26	42,42,42,42	0
56	MG	AA	3073	1/1	0.83	0.24	58,58,58,58	0
56	MG	DA	3234	1/1	0.83	0.19	45,45,45,45	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	BA	3553	1/1	0.83	0.16	42,42,42,42	0
56	MG	BA	3064	1/1	0.83	0.36	61,61,61,61	0
56	MG	BA	3742	1/1	0.83	0.17	51,51,51,51	0
56	MG	DA	3611	1/1	0.83	0.32	55,55,55,55	0
56	MG	BA	3758	1/1	0.83	0.14	34,34,34,34	0
56	MG	DA	3620	1/1	0.83	0.17	62,62,62,62	0
56	MG	BA	3002	1/1	0.83	0.37	62,62,62,62	0
56	MG	BA	3365	1/1	0.83	0.13	49,49,49,49	0
56	MG	DA	3387	1/1	0.83	0.22	56,56,56,56	0
56	MG	BA	3227	1/1	0.83	0.26	57,57,57,57	0
56	MG	DA	3231	1/1	0.84	0.32	57,57,57,57	0
56	MG	BA	3514	1/1	0.84	0.25	41,41,41,41	0
56	MG	BA	3152	1/1	0.84	0.18	43,43,43,43	0
56	MG	AA	3113	1/1	0.84	0.20	59,59,59,59	0
56	MG	BA	3181	1/1	0.84	0.24	41,41,41,41	0
56	MG	BA	3192	1/1	0.84	0.25	48,48,48,48	0
56	MG	BA	3692	1/1	0.84	0.28	57,57,57,57	0
56	MG	BA	3693	1/1	0.84	0.13	70,70,70,70	0
56	MG	BA	3196	1/1	0.84	0.23	51,51,51,51	0
56	MG	DA	3319	1/1	0.84	0.30	43,43,43,43	0
56	MG	AA	3161	1/1	0.84	0.26	46,46,46,46	0
56	MG	DA	3343	1/1	0.84	0.20	40,40,40,40	0
56	MG	DA	3549	1/1	0.84	0.18	57,57,57,57	0
56	MG	AA	3165	1/1	0.84	0.25	60,60,60,60	0
56	MG	AX	3009	1/1	0.84	0.25	71,71,71,71	0
56	MG	BA	3716	1/1	0.84	0.24	54,54,54,54	0
56	MG	DA	3580	1/1	0.84	0.19	64,64,64,64	0
56	MG	BA	3467	1/1	0.84	0.20	39,39,39,39	0
56	MG	DA	3591	1/1	0.84	0.20	56,56,56,56	0
56	MG	AN	502	1/1	0.84	0.13	52,52,52,52	0
56	MG	DA	3423	1/1	0.84	0.14	51,51,51,51	0
56	MG	CA	3087	1/1	0.84	0.15	63,63,63,63	0
56	MG	CA	3121	1/1	0.84	0.23	75,75,75,75	0
56	MG	BA	3402	1/1	0.84	0.19	30,30,30,30	0
56	MG	DA	3192	1/1	0.84	0.18	51,51,51,51	0
56	MG	CA	3147	1/1	0.84	0.18	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3152	1/1	0.84	0.36	79,79,79,79	0
56	MG	DA	3642	1/1	0.84	0.15	49,49,49,49	0
56	MG	BA	3629	1/1	0.84	0.14	56,56,56,56	0
56	MG	DA	3674	1/1	0.84	0.40	73,73,73,73	0
56	MG	BA	3481	1/1	0.84	0.29	45,45,45,45	0
56	MG	DV	3002	1/1	0.84	0.43	57,57,57,57	0
56	MG	BA	3736	1/1	0.84	0.17	56,56,56,56	0
56	MG	DA	3176	1/1	0.85	0.12	52,52,52,52	0
56	MG	CA	3084	1/1	0.85	0.31	69,69,69,69	0
56	MG	AW	3005	1/1	0.85	0.39	68,68,68,68	0
56	MG	AA	3181	1/1	0.85	0.19	75,75,75,75	0
56	MG	BA	3100	1/1	0.85	0.14	45,45,45,45	0
56	MG	CA	3133	1/1	0.85	0.20	65,65,65,65	0
56	MG	CA	3137	1/1	0.85	0.19	52,52,52,52	0
56	MG	AA	3142	1/1	0.85	0.23	62,62,62,62	0
56	MG	BA	3138	1/1	0.85	0.16	48,48,48,48	0
56	MG	AA	3112	1/1	0.85	0.14	57,57,57,57	0
56	MG	AA	3199	1/1	0.85	0.24	59,59,59,59	0
56	MG	BA	3170	1/1	0.85	0.23	48,48,48,48	0
56	MG	BA	3171	1/1	0.85	0.33	53,53,53,53	0
56	MG	BA	3634	1/1	0.85	0.16	64,64,64,64	0
56	MG	BA	3017	1/1	0.85	0.22	50,50,50,50	0
56	MG	CA	3031	1/1	0.85	0.14	53,53,53,53	0
56	MG	AA	3071	1/1	0.85	0.25	62,62,62,62	0
56	MG	BA	3798	1/1	0.85	0.14	61,61,61,61	0
56	MG	DA	3569	1/1	0.85	0.21	57,57,57,57	0
56	MG	BA	3802	1/1	0.85	0.13	56,56,56,56	0
56	MG	DA	3086	1/1	0.85	0.19	62,62,62,62	0
56	MG	DA	3359	1/1	0.85	0.13	57,57,57,57	0
56	MG	AA	3100	1/1	0.85	0.08	68,68,68,68	0
56	MG	DA	3102	1/1	0.85	0.12	57,57,57,57	0
56	MG	DA	3403	1/1	0.85	0.15	57,57,57,57	0
56	MG	DA	3103	1/1	0.85	0.22	50,50,50,50	0
56	MG	BA	3673	1/1	0.85	0.17	47,47,47,47	0
56	MG	AA	3226	1/1	0.85	0.26	58,58,58,58	0
56	MG	AA	3116	1/1	0.85	0.27	61,61,61,61	0
56	MG	AA	3059	1/1	0.85	0.29	59,59,59,59	0
56	MG	AA	3136	1/1	0.85	0.08	53,53,53,53	0
56	MG	BA	3371	1/1	0.85	0.13	54,54,54,54	0
56	MG	DA	3665	1/1	0.85	0.17	58,58,58,58	0
56	MG	DA	3671	1/1	0.85	0.22	59,59,59,59	0
56	MG	DA	3144	1/1	0.85	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3072	1/1	0.85	0.14	62,62,62,62	0
56	MG	DA	3168	1/1	0.85	0.29	53,53,53,53	0
56	MG	BA	3225	1/1	0.85	0.35	42,42,42,42	0
57	PCY	CA	3178	40/40	0.85	0.35	58,78,89,91	0
59	ZN	D4	501	1/1	0.85	0.08	119,119,119,119	0
56	MG	CA	3083	1/1	0.86	0.09	58,58,58,58	0
56	MG	DA	3306	1/1	0.86	0.13	42,42,42,42	0
56	MG	BA	3298	1/1	0.86	0.18	68,68,68,68	0
56	MG	BA	3637	1/1	0.86	0.20	59,59,59,59	0
56	MG	BA	3311	1/1	0.86	0.20	37,37,37,37	0
56	MG	DA	3321	1/1	0.86	0.27	35,35,35,35	0
56	MG	BA	3444	1/1	0.86	0.18	48,48,48,48	0
56	MG	BA	3140	1/1	0.86	0.23	46,46,46,46	0
56	MG	BB	3004	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	3142	1/1	0.86	0.18	61,61,61,61	0
56	MG	BA	3670	1/1	0.86	0.20	47,47,47,47	0
56	MG	DA	3397	1/1	0.86	0.17	49,49,49,49	0
56	MG	AA	3003	1/1	0.86	0.16	66,66,66,66	0
56	MG	BA	3674	1/1	0.86	0.11	47,47,47,47	0
56	MG	BA	3014	1/1	0.86	0.23	33,33,33,33	0
56	MG	BB	3019	1/1	0.86	0.16	49,49,49,49	0
56	MG	BE	307	1/1	0.86	0.20	70,70,70,70	0
56	MG	DA	3424	1/1	0.86	0.24	63,63,63,63	0
56	MG	DA	3002	1/1	0.86	0.17	68,68,68,68	0
56	MG	AA	3130	1/1	0.86	0.16	43,43,43,43	0
56	MG	AX	3002	1/1	0.86	0.24	53,53,53,53	0
56	MG	BA	3357	1/1	0.86	0.19	46,46,46,46	0
56	MG	BA	3180	1/1	0.86	0.12	58,58,58,58	0
56	MG	DA	3053	1/1	0.86	0.09	45,45,45,45	0
56	MG	DA	3453	1/1	0.86	0.23	45,45,45,45	0
56	MG	DA	3057	1/1	0.86	0.08	47,47,47,47	0
56	MG	DA	3060	1/1	0.86	0.23	47,47,47,47	0
56	MG	BA	3695	1/1	0.86	0.22	48,48,48,48	0
56	MG	AA	3228	1/1	0.86	0.10	68,68,68,68	0
56	MG	DA	3079	1/1	0.86	0.17	48,48,48,48	0
56	MG	DA	3085	1/1	0.86	0.19	52,52,52,52	0
56	MG	DA	3507	1/1	0.86	0.22	60,60,60,60	0
56	MG	CA	3005	1/1	0.86	0.10	58,58,58,58	0
56	MG	CA	3007	1/1	0.86	0.18	69,69,69,69	0
56	MG	AA	3202	1/1	0.86	0.15	57,57,57,57	0
56	MG	CA	3016	1/1	0.86	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3018	1/1	0.86	0.18	45,45,45,45	0
56	MG	DA	3106	1/1	0.86	0.27	61,61,61,61	0
56	MG	CA	3019	1/1	0.86	0.39	58,58,58,58	0
56	MG	BA	3102	1/1	0.86	0.27	54,54,54,54	0
56	MG	BA	3567	1/1	0.86	0.18	50,50,50,50	0
56	MG	BA	3392	1/1	0.86	0.19	46,46,46,46	0
56	MG	BA	3717	1/1	0.86	0.19	58,58,58,58	0
56	MG	BA	3266	1/1	0.86	0.24	64,64,64,64	0
56	MG	DA	3149	1/1	0.86	0.10	48,48,48,48	0
56	MG	CA	3028	1/1	0.86	0.19	60,60,60,60	0
56	MG	BA	3274	1/1	0.86	0.16	49,49,49,49	0
56	MG	BA	3197	1/1	0.86	0.31	36,36,36,36	0
56	MG	BA	3278	1/1	0.86	0.10	55,55,55,55	0
56	MG	DA	3179	1/1	0.86	0.08	46,46,46,46	0
56	MG	BA	3203	1/1	0.86	0.15	39,39,39,39	0
56	MG	DA	3184	1/1	0.86	0.30	49,49,49,49	0
56	MG	DA	3186	1/1	0.86	0.23	40,40,40,40	0
56	MG	DA	3610	1/1	0.86	0.22	48,48,48,48	0
56	MG	AA	3159	1/1	0.86	0.09	59,59,59,59	0
56	MG	CA	3053	1/1	0.86	0.07	74,74,74,74	0
56	MG	DA	3615	1/1	0.86	0.33	47,47,47,47	0
56	MG	CA	3054	1/1	0.86	0.16	71,71,71,71	0
56	MG	DA	3628	1/1	0.86	0.14	56,56,56,56	0
56	MG	BA	3618	1/1	0.86	0.18	63,63,63,63	0
56	MG	CA	3059	1/1	0.86	0.42	67,67,67,67	0
56	MG	BA	3747	1/1	0.86	0.27	42,42,42,42	0
56	MG	BA	3748	1/1	0.86	0.17	63,63,63,63	0
56	MG	BA	3753	1/1	0.86	0.29	44,44,44,44	0
56	MG	BA	3757	1/1	0.86	0.16	25,25,25,25	0
56	MG	BA	3218	1/1	0.86	0.18	44,44,44,44	0
56	MG	DA	3246	1/1	0.86	0.12	39,39,39,39	0
56	MG	BA	3760	1/1	0.86	0.26	68,68,68,68	0
56	MG	BA	3782	1/1	0.86	0.11	51,51,51,51	0
56	MG	DA	3287	1/1	0.86	0.16	47,47,47,47	0
56	MG	BA	3113	1/1	0.87	0.32	58,58,58,58	0
56	MG	BA	3186	1/1	0.87	0.19	51,51,51,51	0
56	MG	BA	3435	1/1	0.87	0.16	57,57,57,57	0
56	MG	BF	307	1/1	0.87	0.23	39,39,39,39	0
56	MG	BA	3290	1/1	0.87	0.30	58,58,58,58	0
56	MG	BA	3586	1/1	0.87	0.16	65,65,65,65	0
56	MG	BA	3588	1/1	0.87	0.17	47,47,47,47	0
56	MG	DA	3480	1/1	0.87	0.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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	3594	1/1	0.87	0.23	24,24,24,24	0
56	MG	B7	102	1/1	0.87	0.24	58,58,58,58	0
56	MG	AA	3134	1/1	0.87	0.22	69,69,69,69	0
56	MG	BA	3455	1/1	0.87	0.17	39,39,39,39	0
56	MG	CA	3006	1/1	0.87	0.30	53,53,53,53	0
56	MG	BA	3604	1/1	0.87	0.28	72,72,72,72	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	3235	1/1	0.87	0.28	61,61,61,61	0
56	MG	BA	3606	1/1	0.87	0.19	34,34,34,34	0
56	MG	DA	3032	1/1	0.87	0.15	40,40,40,40	0
56	MG	AA	3198	1/1	0.87	0.39	70,70,70,70	0
56	MG	BA	3313	1/1	0.87	0.15	46,46,46,46	0
56	MG	DA	3272	1/1	0.87	0.16	44,44,44,44	0
56	MG	DA	3273	1/1	0.87	0.11	45,45,45,45	0
56	MG	DA	3567	1/1	0.87	0.16	46,46,46,46	0
56	MG	DA	3044	1/1	0.87	0.10	58,58,58,58	0
56	MG	BA	3633	1/1	0.87	0.17	45,45,45,45	0
56	MG	DA	3297	1/1	0.87	0.12	66,66,66,66	0
56	MG	BA	3477	1/1	0.87	0.20	55,55,55,55	0
56	MG	BA	3752	1/1	0.87	0.18	19,19,19,19	0
56	MG	BA	3478	1/1	0.87	0.20	59,59,59,59	0
56	MG	BA	3638	1/1	0.87	0.26	38,38,38,38	0
56	MG	DA	3068	1/1	0.87	0.17	58,58,58,58	0
56	MG	AA	3032	1/1	0.87	0.09	75,75,75,75	0
56	MG	DA	3324	1/1	0.87	0.29	39,39,39,39	0
56	MG	BA	3655	1/1	0.87	0.12	50,50,50,50	0
56	MG	BA	3769	1/1	0.87	0.17	56,56,56,56	0
56	MG	BA	3779	1/1	0.87	0.12	59,59,59,59	0
56	MG	DA	3096	1/1	0.87	0.22	51,51,51,51	0
56	MG	DA	3623	1/1	0.87	0.15	70,70,70,70	0
56	MG	BA	3511	1/1	0.87	0.23	54,54,54,54	0
56	MG	BA	3512	1/1	0.87	0.28	27,27,27,27	0
56	MG	BA	3668	1/1	0.87	0.18	56,56,56,56	0
56	MG	AA	3221	1/1	0.87	0.14	49,49,49,49	0
56	MG	DA	3657	1/1	0.87	0.10	67,67,67,67	0
56	MG	BA	3059	1/1	0.87	0.11	55,55,55,55	0
56	MG	CA	3060	1/1	0.87	0.24	68,68,68,68	0
56	MG	BA	3523	1/1	0.87	0.15	64,64,64,64	0
56	MG	DB	3003	1/1	0.87	0.15	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3326	1/1	0.87	0.24	38,38,38,38	0
56	MG	DB	3010	1/1	0.87	0.17	55,55,55,55	0
56	MG	DD	303	1/1	0.87	0.25	49,49,49,49	0
56	MG	DR	5001	1/1	0.87	0.08	58,58,58,58	0
56	MG	BA	3060	1/1	0.87	0.20	56,56,56,56	0
56	MG	BA	3557	1/1	0.87	0.22	56,56,56,56	0
56	MG	BA	3424	1/1	0.87	0.25	24,24,24,24	0
56	MG	DA	3439	1/1	0.87	0.14	50,50,50,50	0
56	MG	BB	3012	1/1	0.88	0.08	59,59,59,59	0
56	MG	AV	101	1/1	0.88	0.28	59,59,59,59	0
56	MG	BA	3205	1/1	0.88	0.24	41,41,41,41	0
56	MG	BE	306	1/1	0.88	0.23	25,25,25,25	0
56	MG	AA	3155	1/1	0.88	0.18	53,53,53,53	0
56	MG	DA	3434	1/1	0.88	0.46	51,51,51,51	0
56	MG	BA	3482	1/1	0.88	0.22	59,59,59,59	0
56	MG	DA	3437	1/1	0.88	0.25	39,39,39,39	0
56	MG	BQ	3002	1/1	0.88	0.16	37,37,37,37	0
56	MG	BA	3047	1/1	0.88	0.15	27,27,27,27	0
56	MG	DA	3145	1/1	0.88	0.32	49,49,49,49	0
56	MG	AA	3094	1/1	0.88	0.23	44,44,44,44	0
56	MG	BA	3727	1/1	0.88	0.14	39,39,39,39	0
56	MG	CA	3085	1/1	0.88	0.20	71,71,71,71	0
56	MG	DA	3457	1/1	0.88	0.24	47,47,47,47	0
56	MG	BA	3179	1/1	0.88	0.19	39,39,39,39	0
56	MG	CA	3090	1/1	0.88	0.17	62,62,62,62	0
56	MG	DA	3477	1/1	0.88	0.08	55,55,55,55	0
56	MG	CA	3111	1/1	0.88	0.21	61,61,61,61	0
56	MG	BA	3112	1/1	0.88	0.34	57,57,57,57	0
56	MG	BZ	3001	1/1	0.88	0.22	52,52,52,52	0
56	MG	DA	3495	1/1	0.88	0.09	62,62,62,62	0
56	MG	CA	3132	1/1	0.88	0.37	70,70,70,70	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	DA	3194	1/1	0.88	0.23	35,35,35,35	0
56	MG	DA	3196	1/1	0.88	0.09	53,53,53,53	0
56	MG	DA	3197	1/1	0.88	0.15	48,48,48,48	0
56	MG	DA	3514	1/1	0.88	0.12	41,41,41,41	0
56	MG	B4	502	1/1	0.88	0.12	72,72,72,72	0
56	MG	DA	3201	1/1	0.88	0.23	52,52,52,52	0
56	MG	B6	102	1/1	0.88	0.32	55,55,55,55	0
56	MG	DA	3211	1/1	0.88	0.20	48,48,48,48	0
56	MG	BA	3524	1/1	0.88	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3546	1/1	0.88	0.11	53,53,53,53	0
56	MG	BA	3312	1/1	0.88	0.18	33,33,33,33	0
56	MG	DA	3222	1/1	0.88	0.18	54,54,54,54	0
56	MG	CA	3153	1/1	0.88	0.16	61,61,61,61	0
56	MG	BA	3743	1/1	0.88	0.18	21,21,21,21	0
56	MG	CA	3172	1/1	0.88	0.15	64,64,64,64	0
56	MG	CA	3173	1/1	0.88	0.08	69,69,69,69	0
56	MG	CA	3177	1/1	0.88	0.21	62,62,62,62	0
56	MG	BA	3114	1/1	0.88	0.36	52,52,52,52	0
56	MG	BA	3127	1/1	0.88	0.17	41,41,41,41	0
56	MG	DA	3247	1/1	0.88	0.38	57,57,57,57	0
56	MG	DA	3248	1/1	0.88	0.31	33,33,33,33	0
56	MG	DA	3600	1/1	0.88	0.08	53,53,53,53	0
56	MG	CA	3010	1/1	0.88	0.12	53,53,53,53	0
56	MG	AA	3018	1/1	0.88	0.10	51,51,51,51	0
56	MG	BA	3564	1/1	0.88	0.18	41,41,41,41	0
56	MG	BA	3672	1/1	0.88	0.21	61,61,61,61	0
56	MG	DA	3034	1/1	0.88	0.15	43,43,43,43	0
56	MG	BA	3320	1/1	0.88	0.30	60,60,60,60	0
56	MG	BA	3439	1/1	0.88	0.17	58,58,58,58	0
56	MG	BA	3574	1/1	0.88	0.12	63,63,63,63	0
56	MG	BA	3770	1/1	0.88	0.30	37,37,37,37	0
56	MG	BA	3777	1/1	0.88	0.23	49,49,49,49	0
56	MG	BA	3679	1/1	0.88	0.23	61,61,61,61	0
56	MG	DA	3320	1/1	0.88	0.16	40,40,40,40	0
56	MG	AA	3047	1/1	0.88	0.09	47,47,47,47	0
56	MG	CA	3029	1/1	0.88	0.38	61,61,61,61	0
56	MG	BA	3254	1/1	0.88	0.16	30,30,30,30	0
56	MG	BA	3690	1/1	0.88	0.21	63,63,63,63	0
56	MG	BA	3261	1/1	0.88	0.26	44,44,44,44	0
56	MG	BA	3451	1/1	0.88	0.11	64,64,64,64	0
56	MG	DB	3004	1/1	0.88	0.15	51,51,51,51	0
56	MG	BA	3264	1/1	0.88	0.29	39,39,39,39	0
56	MG	BA	3198	1/1	0.88	0.17	55,55,55,55	0
56	MG	DD	302	1/1	0.88	0.23	49,49,49,49	0
56	MG	DA	3395	1/1	0.88	0.19	42,42,42,42	0
56	MG	AA	3011	1/1	0.88	0.20	64,64,64,64	0
56	MG	DA	3399	1/1	0.88	0.18	47,47,47,47	0
56	MG	BA	3275	1/1	0.88	0.13	46,46,46,46	0
56	MG	D8	5001	1/1	0.88	0.23	55,55,55,55	0
56	MG	BA	3708	1/1	0.88	0.24	63,63,63,63	0
56	MG	DA	3408	1/1	0.88	0.22	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3172	1/1	0.89	0.32	51,51,51,51	0
56	MG	CA	3115	1/1	0.89	0.18	62,62,62,62	0
56	MG	DA	3443	1/1	0.89	0.10	51,51,51,51	0
56	MG	BA	3292	1/1	0.89	0.15	42,42,42,42	0
56	MG	BA	3739	1/1	0.89	0.19	46,46,46,46	0
56	MG	CA	3125	1/1	0.89	0.14	64,64,64,64	0
56	MG	BA	3094	1/1	0.89	0.24	43,43,43,43	0
56	MG	B2	3001	1/1	0.89	0.17	45,45,45,45	0
56	MG	DA	3454	1/1	0.89	0.28	54,54,54,54	0
56	MG	B3	101	1/1	0.89	0.31	48,48,48,48	0
56	MG	AA	3048	1/1	0.89	0.08	51,51,51,51	0
56	MG	CA	3146	1/1	0.89	0.05	69,69,69,69	0
56	MG	DA	3470	1/1	0.89	0.16	42,42,42,42	0
56	MG	B5	102	1/1	0.89	0.18	45,45,45,45	0
56	MG	BA	3667	1/1	0.89	0.11	52,52,52,52	0
56	MG	AA	3212	1/1	0.89	0.30	59,59,59,59	0
56	MG	CA	3161	1/1	0.89	0.10	70,70,70,70	0
56	MG	BA	3544	1/1	0.89	0.20	35,35,35,35	0
56	MG	DA	3499	1/1	0.89	0.10	60,60,60,60	0
56	MG	DA	3500	1/1	0.89	0.12	45,45,45,45	0
56	MG	CA	3002	1/1	0.89	0.07	51,51,51,51	0
56	MG	BA	3419	1/1	0.89	0.17	39,39,39,39	0
56	MG	AA	3051	1/1	0.89	0.17	62,62,62,62	0
56	MG	BA	3427	1/1	0.89	0.25	32,32,32,32	0
56	MG	DA	3225	1/1	0.89	0.23	54,54,54,54	0
56	MG	DA	3229	1/1	0.89	0.12	55,55,55,55	0
56	MG	AA	3197	1/1	0.89	0.14	56,56,56,56	0
56	MG	DA	3516	1/1	0.89	0.09	59,59,59,59	0
56	MG	CX	3004	1/1	0.89	0.33	54,54,54,54	0
56	MG	DA	3536	1/1	0.89	0.32	54,54,54,54	0
56	MG	AX	3008	1/1	0.89	0.36	57,57,57,57	0
56	MG	CA	3015	1/1	0.89	0.12	58,58,58,58	0
56	MG	BA	3250	1/1	0.89	0.20	40,40,40,40	0
56	MG	BA	3437	1/1	0.89	0.20	28,28,28,28	0
56	MG	DA	3545	1/1	0.89	0.16	37,37,37,37	0
56	MG	BA	3778	1/1	0.89	0.14	35,35,35,35	0
56	MG	BA	3046	1/1	0.89	0.18	43,43,43,43	0
56	MG	BA	3255	1/1	0.89	0.26	58,58,58,58	0
56	MG	DA	3269	1/1	0.89	0.20	32,32,32,32	0
56	MG	BA	3791	1/1	0.89	0.13	47,47,47,47	0
56	MG	AA	3030	1/1	0.89	0.16	57,57,57,57	0
56	MG	BA	3328	1/1	0.89	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3115	1/1	0.89	0.08	67,67,67,67	0
56	MG	BA	3700	1/1	0.89	0.20	54,54,54,54	0
56	MG	DA	3303	1/1	0.89	0.15	42,42,42,42	0
56	MG	DA	3587	1/1	0.89	0.09	61,61,61,61	0
56	MG	BA	3820	1/1	0.89	0.20	45,45,45,45	0
56	MG	BA	3703	1/1	0.89	0.23	48,48,48,48	0
56	MG	DA	3069	1/1	0.89	0.39	53,53,53,53	0
56	MG	DA	3602	1/1	0.89	0.34	51,51,51,51	0
56	MG	BA	3832	1/1	0.89	0.09	37,37,37,37	0
56	MG	BA	3835	1/1	0.89	0.20	46,46,46,46	0
56	MG	BB	3001	1/1	0.89	0.20	50,50,50,50	0
56	MG	BA	3052	1/1	0.89	0.31	43,43,43,43	0
56	MG	DA	3323	1/1	0.89	0.32	53,53,53,53	0
56	MG	DA	3612	1/1	0.89	0.23	56,56,56,56	0
56	MG	BA	3356	1/1	0.89	0.13	55,55,55,55	0
56	MG	BA	3269	1/1	0.89	0.38	53,53,53,53	0
56	MG	BA	3358	1/1	0.89	0.42	64,64,64,64	0
56	MG	DA	3358	1/1	0.89	0.32	45,45,45,45	0
56	MG	BA	3714	1/1	0.89	0.06	47,47,47,47	0
56	MG	DA	3630	1/1	0.89	0.17	49,49,49,49	0
56	MG	AA	3230	1/1	0.89	0.18	68,68,68,68	0
56	MG	DA	3370	1/1	0.89	0.08	46,46,46,46	0
56	MG	DA	3643	1/1	0.89	0.10	60,60,60,60	0
56	MG	DA	3375	1/1	0.89	0.11	40,40,40,40	0
56	MG	DA	3655	1/1	0.89	0.17	57,57,57,57	0
56	MG	AA	3102	1/1	0.89	0.34	51,51,51,51	0
56	MG	DA	3107	1/1	0.89	0.19	49,49,49,49	0
56	MG	BE	302	1/1	0.89	0.17	34,34,34,34	0
56	MG	DA	3673	1/1	0.89	0.16	61,61,61,61	0
56	MG	DA	3396	1/1	0.89	0.13	45,45,45,45	0
56	MG	BA	3207	1/1	0.89	0.18	38,38,38,38	0
56	MG	BA	3723	1/1	0.89	0.16	47,47,47,47	0
56	MG	BA	3004	1/1	0.89	0.24	36,36,36,36	0
56	MG	BN	3001	1/1	0.89	0.33	51,51,51,51	0
56	MG	DA	3132	1/1	0.89	0.43	41,41,41,41	0
56	MG	BN	3002	1/1	0.89	0.12	46,46,46,46	0
56	MG	BA	3491	1/1	0.89	0.23	47,47,47,47	0
56	MG	BA	3508	1/1	0.89	0.09	54,54,54,54	0
56	MG	AA	3022	1/1	0.89	0.28	55,55,55,55	0
56	MG	DA	3157	1/1	0.89	0.28	44,44,44,44	0
56	MG	AA	3078	1/1	0.89	0.06	48,48,48,48	0
56	MG	BA	3088	1/1	0.89	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3376	1/1	0.90	0.24	54,54,54,54	0
56	MG	DA	3380	1/1	0.90	0.09	55,55,55,55	0
56	MG	BA	3751	1/1	0.90	0.14	45,45,45,45	0
56	MG	AA	3017	1/1	0.90	0.12	62,62,62,62	0
56	MG	DA	3061	1/1	0.90	0.21	56,56,56,56	0
56	MG	CA	3017	1/1	0.90	0.17	49,49,49,49	0
56	MG	BA	3620	1/1	0.90	0.15	47,47,47,47	0
56	MG	AA	3055	1/1	0.90	0.22	58,58,58,58	0
56	MG	BA	3447	1/1	0.90	0.23	26,26,26,26	0
56	MG	AD	502	1/1	0.90	0.29	56,56,56,56	0
56	MG	DA	3405	1/1	0.90	0.13	52,52,52,52	0
56	MG	DA	3407	1/1	0.90	0.08	46,46,46,46	0
56	MG	CA	3024	1/1	0.90	0.14	63,63,63,63	0
56	MG	BA	3768	1/1	0.90	0.06	56,56,56,56	0
56	MG	DA	3087	1/1	0.90	0.21	49,49,49,49	0
56	MG	DA	3422	1/1	0.90	0.36	43,43,43,43	0
56	MG	DA	3089	1/1	0.90	0.23	46,46,46,46	0
56	MG	DA	3093	1/1	0.90	0.10	57,57,57,57	0
56	MG	BA	3023	1/1	0.90	0.27	55,55,55,55	0
56	MG	BA	3464	1/1	0.90	0.21	56,56,56,56	0
56	MG	DA	3101	1/1	0.90	0.12	53,53,53,53	0
56	MG	AA	3057	1/1	0.90	0.20	61,61,61,61	0
56	MG	BA	3641	1/1	0.90	0.19	49,49,49,49	0
56	MG	AA	3185	1/1	0.90	0.26	53,53,53,53	0
56	MG	AA	3058	1/1	0.90	0.21	57,57,57,57	0
56	MG	CA	3036	1/1	0.90	0.09	60,60,60,60	0
56	MG	BA	3787	1/1	0.90	0.22	59,59,59,59	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	BA	3797	1/1	0.90	0.20	52,52,52,52	0
56	MG	BA	3228	1/1	0.90	0.22	50,50,50,50	0
56	MG	DA	3460	1/1	0.90	0.17	65,65,65,65	0
56	MG	BA	3139	1/1	0.90	0.09	61,61,61,61	0
56	MG	DA	3140	1/1	0.90	0.11	34,34,34,34	0
56	MG	DA	3142	1/1	0.90	0.11	45,45,45,45	0
56	MG	BA	3233	1/1	0.90	0.33	48,48,48,48	0
56	MG	BA	3346	1/1	0.90	0.14	32,32,32,32	0
56	MG	AA	3079	1/1	0.90	0.22	47,47,47,47	0
56	MG	BA	3828	1/1	0.90	0.20	37,37,37,37	0
56	MG	BA	3492	1/1	0.90	0.12	55,55,55,55	0
56	MG	BA	3504	1/1	0.90	0.19	58,58,58,58	0
56	MG	CA	3067	1/1	0.90	0.10	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3348	1/1	0.90	0.13	54,54,54,54	0
56	MG	BA	3838	1/1	0.90	0.19	50,50,50,50	0
56	MG	DA	3506	1/1	0.90	0.10	48,48,48,48	0
56	MG	DA	3178	1/1	0.90	0.12	54,54,54,54	0
56	MG	BA	3143	1/1	0.90	0.25	42,42,42,42	0
56	MG	DA	3181	1/1	0.90	0.30	45,45,45,45	0
56	MG	BA	3686	1/1	0.90	0.24	30,30,30,30	0
56	MG	DA	3183	1/1	0.90	0.22	58,58,58,58	0
56	MG	DA	3515	1/1	0.90	0.14	57,57,57,57	0
56	MG	BA	3248	1/1	0.90	0.15	45,45,45,45	0
56	MG	BA	3149	1/1	0.90	0.13	53,53,53,53	0
56	MG	DA	3531	1/1	0.90	0.33	54,54,54,54	0
56	MG	DA	3533	1/1	0.90	0.30	53,53,53,53	0
56	MG	DA	3534	1/1	0.90	0.26	74,74,74,74	0
56	MG	BA	3364	1/1	0.90	0.15	42,42,42,42	0
56	MG	DA	3191	1/1	0.90	0.32	44,44,44,44	0
56	MG	DA	3539	1/1	0.90	0.14	46,46,46,46	0
56	MG	BA	3150	1/1	0.90	0.12	48,48,48,48	0
56	MG	BA	3049	1/1	0.90	0.27	37,37,37,37	0
56	MG	CA	3101	1/1	0.90	0.22	54,54,54,54	0
56	MG	AA	3080	1/1	0.90	0.21	47,47,47,47	0
56	MG	AA	3033	1/1	0.90	0.15	57,57,57,57	0
56	MG	BA	3548	1/1	0.90	0.28	48,48,48,48	0
56	MG	AA	3035	1/1	0.90	0.07	46,46,46,46	0
56	MG	DA	3563	1/1	0.90	0.15	42,42,42,42	0
56	MG	CA	3123	1/1	0.90	0.12	80,80,80,80	0
56	MG	CA	3124	1/1	0.90	0.16	79,79,79,79	0
56	MG	BA	3172	1/1	0.90	0.23	45,45,45,45	0
56	MG	DA	3221	1/1	0.90	0.17	49,49,49,49	0
56	MG	CA	3126	1/1	0.90	0.17	72,72,72,72	0
56	MG	DA	3574	1/1	0.90	0.20	51,51,51,51	0
56	MG	AA	3086	1/1	0.90	0.20	52,52,52,52	0
56	MG	BA	3273	1/1	0.90	0.29	53,53,53,53	0
56	MG	BO	5001	1/1	0.90	0.17	55,55,55,55	0
56	MG	CA	3139	1/1	0.90	0.15	61,61,61,61	0
56	MG	BA	3566	1/1	0.90	0.23	30,30,30,30	0
56	MG	DA	3597	1/1	0.90	0.10	51,51,51,51	0
56	MG	AA	3158	1/1	0.90	0.27	59,59,59,59	0
56	MG	BA	3569	1/1	0.90	0.33	57,57,57,57	0
56	MG	BA	3718	1/1	0.90	0.20	46,46,46,46	0
56	MG	AA	3020	1/1	0.90	0.15	59,59,59,59	0
56	MG	BA	3410	1/1	0.90	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3164	1/1	0.90	0.07	54,54,54,54	0
56	MG	CA	3167	1/1	0.90	0.17	48,48,48,48	0
56	MG	BW	202	1/1	0.90	0.31	49,49,49,49	0
56	MG	DA	3271	1/1	0.90	0.14	47,47,47,47	0
56	MG	BA	3724	1/1	0.90	0.34	44,44,44,44	0
56	MG	DA	3616	1/1	0.90	0.07	45,45,45,45	0
56	MG	BA	3579	1/1	0.90	0.08	47,47,47,47	0
56	MG	DA	3621	1/1	0.90	0.29	45,45,45,45	0
56	MG	CA	3175	1/1	0.90	0.16	39,39,39,39	0
56	MG	CA	3176	1/1	0.90	0.13	43,43,43,43	0
56	MG	AX	3012	1/1	0.90	0.23	59,59,59,59	0
56	MG	BA	3089	1/1	0.90	0.29	45,45,45,45	0
56	MG	BA	3283	1/1	0.90	0.12	36,36,36,36	0
56	MG	BA	3093	1/1	0.90	0.32	38,38,38,38	0
56	MG	AA	3115	1/1	0.90	0.11	51,51,51,51	0
56	MG	DA	3648	1/1	0.90	0.12	60,60,60,60	0
56	MG	DA	3310	1/1	0.90	0.22	55,55,55,55	0
56	MG	BA	3433	1/1	0.90	0.19	57,57,57,57	0
56	MG	DA	3019	1/1	0.90	0.15	57,57,57,57	0
56	MG	DA	3020	1/1	0.90	0.14	50,50,50,50	0
56	MG	BA	3738	1/1	0.90	0.11	58,58,58,58	0
56	MG	DA	3029	1/1	0.90	0.21	51,51,51,51	0
56	MG	DB	3002	1/1	0.90	0.15	56,56,56,56	0
56	MG	AA	3213	1/1	0.90	0.08	69,69,69,69	0
56	MG	AA	3089	1/1	0.90	0.27	57,57,57,57	0
56	MG	DA	3333	1/1	0.90	0.07	50,50,50,50	0
56	MG	DB	3006	1/1	0.90	0.18	62,62,62,62	0
56	MG	BA	3293	1/1	0.90	0.25	52,52,52,52	0
56	MG	DA	3354	1/1	0.90	0.24	46,46,46,46	0
56	MG	DA	3355	1/1	0.90	0.10	50,50,50,50	0
56	MG	DF	302	1/1	0.90	0.18	43,43,43,43	0
56	MG	DQ	3003	1/1	0.90	0.19	58,58,58,58	0
56	MG	DA	3039	1/1	0.90	0.22	56,56,56,56	0
56	MG	AA	3169	1/1	0.90	0.19	64,64,64,64	0
56	MG	BA	3015	1/1	0.90	0.23	47,47,47,47	0
56	MG	DA	3368	1/1	0.90	0.19	50,50,50,50	0
56	MG	BA	3749	1/1	0.90	0.25	45,45,45,45	0
56	MG	CA	3013	1/1	0.90	0.10	63,63,63,63	0
56	MG	DA	3432	1/1	0.91	0.15	56,56,56,56	0
56	MG	AW	3003	1/1	0.91	0.31	59,59,59,59	0
56	MG	BB	3003	1/1	0.91	0.12	40,40,40,40	0
56	MG	AA	3021	1/1	0.91	0.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AW	3006	1/1	0.91	0.16	50,50,50,50	0
56	MG	CA	3086	1/1	0.91	0.12	61,61,61,61	0
56	MG	BA	3387	1/1	0.91	0.06	65,65,65,65	0
56	MG	AA	3183	1/1	0.91	0.14	71,71,71,71	0
56	MG	CA	3097	1/1	0.91	0.23	57,57,57,57	0
56	MG	CA	3099	1/1	0.91	0.11	62,62,62,62	0
56	MG	BA	3526	1/1	0.91	0.09	32,32,32,32	0
56	MG	BA	3201	1/1	0.91	0.17	40,40,40,40	0
56	MG	BA	3537	1/1	0.91	0.13	49,49,49,49	0
56	MG	BB	3022	1/1	0.91	0.14	62,62,62,62	0
56	MG	BD	306	1/1	0.91	0.36	22,22,22,22	0
56	MG	BA	3701	1/1	0.91	0.14	51,51,51,51	0
56	MG	BE	305	1/1	0.91	0.22	59,59,59,59	0
56	MG	BA	3702	1/1	0.91	0.07	51,51,51,51	0
56	MG	BA	3031	1/1	0.91	0.23	56,56,56,56	0
56	MG	BA	3280	1/1	0.91	0.24	49,49,49,49	0
56	MG	BG	203	1/1	0.91	0.07	36,36,36,36	0
56	MG	CA	3134	1/1	0.91	0.14	70,70,70,70	0
56	MG	DA	3497	1/1	0.91	0.32	51,51,51,51	0
56	MG	AA	3156	1/1	0.91	0.14	52,52,52,52	0
56	MG	BA	3707	1/1	0.91	0.14	66,66,66,66	0
56	MG	AA	3216	1/1	0.91	0.13	72,72,72,72	0
56	MG	BP	202	1/1	0.91	0.20	34,34,34,34	0
56	MG	DA	3210	1/1	0.91	0.11	44,44,44,44	0
56	MG	BA	3124	1/1	0.91	0.20	38,38,38,38	0
56	MG	AA	3189	1/1	0.91	0.17	59,59,59,59	0
56	MG	BA	3414	1/1	0.91	0.22	29,29,29,29	0
56	MG	CA	3157	1/1	0.91	0.28	64,64,64,64	0
56	MG	BA	3219	1/1	0.91	0.19	29,29,29,29	0
56	MG	DA	3223	1/1	0.91	0.29	54,54,54,54	0
56	MG	BA	3568	1/1	0.91	0.25	52,52,52,52	0
56	MG	AA	3223	1/1	0.91	0.30	59,59,59,59	0
56	MG	BA	3058	1/1	0.91	0.20	36,36,36,36	0
56	MG	BA	3429	1/1	0.91	0.24	47,47,47,47	0
56	MG	AA	3066	1/1	0.91	0.12	44,44,44,44	0
56	MG	BA	3581	1/1	0.91	0.11	38,38,38,38	0
56	MG	DA	3537	1/1	0.91	0.17	55,55,55,55	0
56	MG	DA	3236	1/1	0.91	0.13	48,48,48,48	0
56	MG	BA	3307	1/1	0.91	0.17	37,37,37,37	0
56	MG	AY	3003	1/1	0.91	0.14	48,48,48,48	0
56	MG	BA	3062	1/1	0.91	0.25	57,57,57,57	0
56	MG	CW	3001	1/1	0.91	0.32	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3436	1/1	0.91	0.22	46,46,46,46	0
56	MG	BA	3144	1/1	0.91	0.09	43,43,43,43	0
56	MG	BA	3592	1/1	0.91	0.14	29,29,29,29	0
56	MG	DA	3001	1/1	0.91	0.26	58,58,58,58	0
56	MG	BA	3438	1/1	0.91	0.19	47,47,47,47	0
56	MG	BA	3314	1/1	0.91	0.15	47,47,47,47	0
56	MG	BA	3441	1/1	0.91	0.27	46,46,46,46	0
56	MG	DA	3026	1/1	0.91	0.14	42,42,42,42	0
56	MG	DA	3293	1/1	0.91	0.11	60,60,60,60	0
56	MG	AA	3015	1/1	0.91	0.17	60,60,60,60	0
56	MG	BA	3065	1/1	0.91	0.12	37,37,37,37	0
56	MG	BA	3445	1/1	0.91	0.20	32,32,32,32	0
56	MG	DA	3581	1/1	0.91	0.19	63,63,63,63	0
56	MG	BA	3613	1/1	0.91	0.13	45,45,45,45	0
56	MG	DA	3585	1/1	0.91	0.10	51,51,51,51	0
56	MG	BA	3236	1/1	0.91	0.15	43,43,43,43	0
56	MG	DA	3589	1/1	0.91	0.15	63,63,63,63	0
56	MG	AA	3194	1/1	0.91	0.17	58,58,58,58	0
56	MG	DA	3595	1/1	0.91	0.18	61,61,61,61	0
56	MG	BA	3756	1/1	0.91	0.21	27,27,27,27	0
56	MG	DA	3318	1/1	0.91	0.18	42,42,42,42	0
56	MG	BA	3622	1/1	0.91	0.19	31,31,31,31	0
56	MG	BA	3625	1/1	0.91	0.14	57,57,57,57	0
56	MG	BA	3240	1/1	0.91	0.26	45,45,45,45	0
56	MG	BA	3762	1/1	0.91	0.38	40,40,40,40	0
56	MG	DA	3606	1/1	0.91	0.22	54,54,54,54	0
56	MG	BA	3763	1/1	0.91	0.27	34,34,34,34	0
56	MG	BA	3453	1/1	0.91	0.21	42,42,42,42	0
56	MG	DA	3328	1/1	0.91	0.15	47,47,47,47	0
56	MG	BA	3153	1/1	0.91	0.22	39,39,39,39	0
56	MG	AA	3049	1/1	0.91	0.22	52,52,52,52	0
56	MG	DA	3351	1/1	0.91	0.12	39,39,39,39	0
56	MG	BA	3774	1/1	0.91	0.19	43,43,43,43	0
56	MG	DA	3072	1/1	0.91	0.09	36,36,36,36	0
56	MG	BA	3341	1/1	0.91	0.16	57,57,57,57	0
56	MG	BA	3342	1/1	0.91	0.18	51,51,51,51	0
56	MG	DA	3365	1/1	0.91	0.34	57,57,57,57	0
56	MG	DA	3081	1/1	0.91	0.27	45,45,45,45	0
56	MG	BA	3345	1/1	0.91	0.12	44,44,44,44	0
56	MG	DA	3638	1/1	0.91	0.25	60,60,60,60	0
56	MG	BA	3650	1/1	0.91	0.12	57,57,57,57	0
56	MG	AA	3005	1/1	0.91	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3789	1/1	0.91	0.17	39,39,39,39	0
56	MG	CA	3043	1/1	0.91	0.26	54,54,54,54	0
56	MG	DA	3649	1/1	0.91	0.07	64,64,64,64	0
56	MG	DA	3650	1/1	0.91	0.27	44,44,44,44	0
56	MG	DA	3384	1/1	0.91	0.10	52,52,52,52	0
56	MG	CA	3046	1/1	0.91	0.09	56,56,56,56	0
56	MG	AA	3143	1/1	0.91	0.16	73,73,73,73	0
56	MG	BA	3251	1/1	0.91	0.32	52,52,52,52	0
56	MG	BA	3666	1/1	0.91	0.12	58,58,58,58	0
56	MG	BA	3352	1/1	0.91	0.26	29,29,29,29	0
56	MG	BA	3090	1/1	0.91	0.20	37,37,37,37	0
56	MG	DA	3402	1/1	0.91	0.27	65,65,65,65	0
56	MG	BA	3016	1/1	0.91	0.20	44,44,44,44	0
56	MG	BA	3812	1/1	0.91	0.18	52,52,52,52	0
56	MG	BA	3815	1/1	0.91	0.28	50,50,50,50	0
56	MG	DA	3406	1/1	0.91	0.15	40,40,40,40	0
56	MG	DB	3011	1/1	0.91	0.09	52,52,52,52	0
56	MG	AA	3103	1/1	0.91	0.14	59,59,59,59	0
56	MG	BA	3500	1/1	0.91	0.18	26,26,26,26	0
56	MG	DD	307	1/1	0.91	0.14	56,56,56,56	0
56	MG	BA	3503	1/1	0.91	0.23	58,58,58,58	0
56	MG	DA	3415	1/1	0.91	0.24	50,50,50,50	0
56	MG	DA	3418	1/1	0.91	0.22	37,37,37,37	0
56	MG	BA	3360	1/1	0.91	0.09	50,50,50,50	0
56	MG	DA	3131	1/1	0.91	0.15	52,52,52,52	0
56	MG	AA	3106	1/1	0.91	0.17	51,51,51,51	0
56	MG	BA	3096	1/1	0.91	0.30	41,41,41,41	0
59	ZN	CN	501	1/1	0.91	0.04	92,92,92,92	0
56	MG	CA	3073	1/1	0.91	0.32	48,48,48,48	0
59	ZN	D9	501	1/1	0.91	0.07	63,63,63,63	0
56	MG	BA	3375	1/1	0.92	0.15	35,35,35,35	0
56	MG	BA	3376	1/1	0.92	0.11	34,34,34,34	0
56	MG	BA	3837	1/1	0.92	0.20	40,40,40,40	0
56	MG	BA	3681	1/1	0.92	0.22	53,53,53,53	0
56	MG	AA	3044	1/1	0.92	0.32	71,71,71,71	0
56	MG	DA	3111	1/1	0.92	0.14	33,33,33,33	0
56	MG	BA	3520	1/1	0.92	0.32	47,47,47,47	0
56	MG	DA	3119	1/1	0.92	0.20	62,62,62,62	0
56	MG	BA	3522	1/1	0.92	0.28	36,36,36,36	0
56	MG	DA	3122	1/1	0.92	0.22	36,36,36,36	0
56	MG	CA	3074	1/1	0.92	0.39	55,55,55,55	0
56	MG	BA	3099	1/1	0.92	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3082	1/1	0.92	0.13	63,63,63,63	0
56	MG	DA	3133	1/1	0.92	0.29	40,40,40,40	0
56	MG	DA	3138	1/1	0.92	0.41	59,59,59,59	0
56	MG	BA	3194	1/1	0.92	0.20	37,37,37,37	0
56	MG	DA	3441	1/1	0.92	0.09	43,43,43,43	0
56	MG	AA	3101	1/1	0.92	0.17	54,54,54,54	0
56	MG	BA	3394	1/1	0.92	0.21	52,52,52,52	0
56	MG	BA	3530	1/1	0.92	0.20	51,51,51,51	0
56	MG	DA	3147	1/1	0.92	0.09	44,44,44,44	0
56	MG	BB	3018	1/1	0.92	0.15	77,77,77,77	0
56	MG	BA	3396	1/1	0.92	0.22	55,55,55,55	0
56	MG	CA	3092	1/1	0.92	0.15	44,44,44,44	0
56	MG	DA	3167	1/1	0.92	0.25	47,47,47,47	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	BA	3542	1/1	0.92	0.16	48,48,48,48	0
56	MG	AA	3120	1/1	0.92	0.16	59,59,59,59	0
56	MG	CA	3104	1/1	0.92	0.11	64,64,64,64	0
56	MG	AA	3050	1/1	0.92	0.10	70,70,70,70	0
56	MG	DA	3483	1/1	0.92	0.38	48,48,48,48	0
56	MG	DA	3485	1/1	0.92	0.11	44,44,44,44	0
56	MG	CA	3114	1/1	0.92	0.20	56,56,56,56	0
56	MG	DA	3491	1/1	0.92	0.17	45,45,45,45	0
56	MG	AA	3127	1/1	0.92	0.18	48,48,48,48	0
56	MG	CA	3117	1/1	0.92	0.10	48,48,48,48	0
56	MG	CA	3119	1/1	0.92	0.26	58,58,58,58	0
56	MG	BA	3284	1/1	0.92	0.26	51,51,51,51	0
56	MG	BA	3287	1/1	0.92	0.29	54,54,54,54	0
56	MG	DA	3502	1/1	0.92	0.20	64,64,64,64	0
56	MG	DA	3503	1/1	0.92	0.14	37,37,37,37	0
56	MG	DA	3190	1/1	0.92	0.26	45,45,45,45	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	AA	3061	1/1	0.92	0.08	54,54,54,54	0
56	MG	DA	3195	1/1	0.92	0.19	57,57,57,57	0
56	MG	AA	3045	1/1	0.92	0.32	59,59,59,59	0
56	MG	CA	3128	1/1	0.92	0.10	63,63,63,63	0
56	MG	AA	3209	1/1	0.92	0.30	51,51,51,51	0
56	MG	BA	3117	1/1	0.92	0.23	42,42,42,42	0
56	MG	DA	3203	1/1	0.92	0.28	37,37,37,37	0
56	MG	DA	3204	1/1	0.92	0.31	51,51,51,51	0
56	MG	DA	3523	1/1	0.92	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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	AX	3004	1/1	0.92	0.21	70,70,70,70	0
56	MG	BA	3428	1/1	0.92	0.30	38,38,38,38	0
56	MG	BA	3294	1/1	0.92	0.20	45,45,45,45	0
56	MG	AX	3005	1/1	0.92	0.15	44,44,44,44	0
56	MG	CA	3143	1/1	0.92	0.15	62,62,62,62	0
56	MG	DA	3220	1/1	0.92	0.19	46,46,46,46	0
56	MG	BA	3582	1/1	0.92	0.16	44,44,44,44	0
56	MG	BA	3130	1/1	0.92	0.26	48,48,48,48	0
56	MG	CA	3148	1/1	0.92	0.11	67,67,67,67	0
56	MG	CA	3151	1/1	0.92	0.08	65,65,65,65	0
56	MG	BA	3305	1/1	0.92	0.12	33,33,33,33	0
56	MG	BA	3131	1/1	0.92	0.18	38,38,38,38	0
56	MG	DA	3548	1/1	0.92	0.17	65,65,65,65	0
56	MG	AA	3210	1/1	0.92	0.19	69,69,69,69	0
56	MG	DA	3556	1/1	0.92	0.19	64,64,64,64	0
56	MG	CA	3159	1/1	0.92	0.13	57,57,57,57	0
56	MG	B1	101	1/1	0.92	0.38	44,44,44,44	0
56	MG	CA	3162	1/1	0.92	0.14	67,67,67,67	0
56	MG	AA	3109	1/1	0.92	0.32	64,64,64,64	0
56	MG	DA	3239	1/1	0.92	0.20	54,54,54,54	0
56	MG	AA	3138	1/1	0.92	0.17	34,34,34,34	0
56	MG	BA	3593	1/1	0.92	0.14	42,42,42,42	0
56	MG	CA	3170	1/1	0.92	0.12	64,64,64,64	0
56	MG	B3	102	1/1	0.92	0.11	35,35,35,35	0
56	MG	DA	3250	1/1	0.92	0.13	61,61,61,61	0
56	MG	BA	3061	1/1	0.92	0.17	40,40,40,40	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	B5	103	1/1	0.92	0.18	44,44,44,44	0
56	MG	AA	3215	1/1	0.92	0.19	57,57,57,57	0
56	MG	BA	3597	1/1	0.92	0.20	44,44,44,44	0
56	MG	BA	3601	1/1	0.92	0.16	42,42,42,42	0
56	MG	B9	502	1/1	0.92	0.10	57,57,57,57	0
56	MG	DA	3288	1/1	0.92	0.16	61,61,61,61	0
56	MG	BA	3232	1/1	0.92	0.14	37,37,37,37	0
56	MG	DA	3295	1/1	0.92	0.17	58,58,58,58	0
56	MG	CA	3004	1/1	0.92	0.07	71,71,71,71	0
56	MG	DA	3300	1/1	0.92	0.26	60,60,60,60	0
56	MG	BA	3063	1/1	0.92	0.17	47,47,47,47	0
56	MG	AA	3174	1/1	0.92	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3237	1/1	0.92	0.14	36,36,36,36	0
56	MG	BA	3001	1/1	0.92	0.20	43,43,43,43	0
56	MG	DA	3025	1/1	0.92	0.16	44,44,44,44	0
56	MG	BA	3617	1/1	0.92	0.13	64,64,64,64	0
56	MG	DA	3027	1/1	0.92	0.21	53,53,53,53	0
56	MG	DA	3618	1/1	0.92	0.26	54,54,54,54	0
56	MG	BA	3449	1/1	0.92	0.29	60,60,60,60	0
56	MG	BA	3151	1/1	0.92	0.28	42,42,42,42	0
56	MG	AA	3023	1/1	0.92	0.15	37,37,37,37	0
56	MG	BA	3623	1/1	0.92	0.13	52,52,52,52	0
56	MG	AA	3067	1/1	0.92	0.09	59,59,59,59	0
56	MG	BA	3765	1/1	0.92	0.17	33,33,33,33	0
56	MG	DA	3635	1/1	0.92	0.15	52,52,52,52	0
56	MG	DA	3636	1/1	0.92	0.24	56,56,56,56	0
56	MG	BA	3626	1/1	0.92	0.18	49,49,49,49	0
56	MG	DA	3043	1/1	0.92	0.17	48,48,48,48	0
56	MG	DA	3335	1/1	0.92	0.19	32,32,32,32	0
56	MG	CA	3021	1/1	0.92	0.13	42,42,42,42	0
56	MG	BA	3344	1/1	0.92	0.14	37,37,37,37	0
56	MG	BA	3158	1/1	0.92	0.19	44,44,44,44	0
56	MG	BA	3083	1/1	0.92	0.29	47,47,47,47	0
56	MG	AA	3081	1/1	0.92	0.26	58,58,58,58	0
56	MG	BA	3253	1/1	0.92	0.21	40,40,40,40	0
56	MG	DA	3661	1/1	0.92	0.20	42,42,42,42	0
56	MG	DA	3663	1/1	0.92	0.25	60,60,60,60	0
56	MG	BA	3351	1/1	0.92	0.17	34,34,34,34	0
56	MG	DA	3667	1/1	0.92	0.96	73,73,73,73	0
56	MG	AA	3144	1/1	0.92	0.12	50,50,50,50	0
56	MG	DA	3672	1/1	0.92	0.28	52,52,52,52	0
56	MG	DA	3367	1/1	0.92	0.08	51,51,51,51	0
56	MG	BA	3354	1/1	0.92	0.17	31,31,31,31	0
56	MG	BA	3651	1/1	0.92	0.19	56,56,56,56	0
56	MG	AA	3016	1/1	0.92	0.16	46,46,46,46	0
56	MG	BA	3484	1/1	0.92	0.29	36,36,36,36	0
56	MG	DA	3378	1/1	0.92	0.13	45,45,45,45	0
56	MG	BA	3259	1/1	0.92	0.40	52,52,52,52	0
56	MG	AA	3148	1/1	0.92	0.15	63,63,63,63	0
56	MG	AA	3150	1/1	0.92	0.44	55,55,55,55	0
56	MG	DA	3390	1/1	0.92	0.07	54,54,54,54	0
56	MG	DA	3391	1/1	0.92	0.09	44,44,44,44	0
56	MG	BA	3019	1/1	0.92	0.32	42,42,42,42	0
56	MG	DE	304	1/1	0.92	0.22	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DF	301	1/1	0.92	0.15	47,47,47,47	0
56	MG	DA	3394	1/1	0.92	0.14	49,49,49,49	0
56	MG	BA	3808	1/1	0.92	0.14	34,34,34,34	0
56	MG	BA	3669	1/1	0.92	0.13	42,42,42,42	0
56	MG	DA	3094	1/1	0.92	0.19	52,52,52,52	0
56	MG	BA	3182	1/1	0.92	0.31	41,41,41,41	0
56	MG	DA	3401	1/1	0.92	0.29	36,36,36,36	0
57	PCY	AA	3231	40/40	0.92	0.33	45,69,81,87	0
56	MG	BA	3270	1/1	0.92	0.24	57,57,57,57	0
56	MG	BA	3825	1/1	0.92	0.18	65,65,65,65	0
59	ZN	DY	501	1/1	0.92	0.09	106,106,106,106	0
56	MG	BA	3509	1/1	0.92	0.25	39,39,39,39	0
56	MG	BA	3271	1/1	0.92	0.11	26,26,26,26	0
60	K	CX	3001	1/1	0.92	0.17	74,74,74,74	0
56	MG	AA	3218	1/1	0.93	0.25	53,53,53,53	0
56	MG	BA	3493	1/1	0.93	0.13	46,46,46,46	0
56	MG	AX	3006	1/1	0.93	0.18	74,74,74,74	0
56	MG	DA	3461	1/1	0.93	0.13	56,56,56,56	0
56	MG	CA	3154	1/1	0.93	0.17	62,62,62,62	0
56	MG	BA	3628	1/1	0.93	0.17	30,30,30,30	0
56	MG	AA	3135	1/1	0.93	0.10	65,65,65,65	0
56	MG	DA	3474	1/1	0.93	0.07	53,53,53,53	0
56	MG	BA	3033	1/1	0.93	0.26	33,33,33,33	0
56	MG	B6	101	1/1	0.93	0.18	48,48,48,48	0
56	MG	BA	3754	1/1	0.93	0.17	60,60,60,60	0
56	MG	DA	3205	1/1	0.93	0.21	47,47,47,47	0
56	MG	BA	3235	1/1	0.93	0.16	37,37,37,37	0
56	MG	BA	3636	1/1	0.93	0.10	53,53,53,53	0
56	MG	BA	3156	1/1	0.93	0.23	41,41,41,41	0
56	MG	BA	3302	1/1	0.93	0.16	35,35,35,35	0
56	MG	DA	3212	1/1	0.93	0.29	44,44,44,44	0
56	MG	DA	3498	1/1	0.93	0.09	57,57,57,57	0
56	MG	CA	3003	1/1	0.93	0.24	58,58,58,58	0
56	MG	BA	3304	1/1	0.93	0.20	39,39,39,39	0
56	MG	BA	3097	1/1	0.93	0.17	52,52,52,52	0
56	MG	BA	3645	1/1	0.93	0.18	32,32,32,32	0
56	MG	CE	202	1/1	0.93	0.05	66,66,66,66	0
56	MG	BA	3766	1/1	0.93	0.19	31,31,31,31	0
56	MG	BA	3648	1/1	0.93	0.37	53,53,53,53	0
56	MG	AA	3222	1/1	0.93	0.24	67,67,67,67	0
56	MG	BA	3519	1/1	0.93	0.12	44,44,44,44	0
56	MG	BA	3773	1/1	0.93	0.22	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3233	1/1	0.93	0.25	43,43,43,43	0
56	MG	BA	3310	1/1	0.93	0.20	57,57,57,57	0
56	MG	BA	3164	1/1	0.93	0.28	43,43,43,43	0
56	MG	BA	3412	1/1	0.93	0.20	41,41,41,41	0
56	MG	DA	3518	1/1	0.93	0.18	50,50,50,50	0
56	MG	AA	3111	1/1	0.93	0.18	52,52,52,52	0
56	MG	BA	3244	1/1	0.93	0.10	63,63,63,63	0
56	MG	BA	3786	1/1	0.93	0.10	37,37,37,37	0
56	MG	AA	3054	1/1	0.93	0.43	52,52,52,52	0
56	MG	BA	3529	1/1	0.93	0.16	33,33,33,33	0
56	MG	BA	3422	1/1	0.93	0.18	32,32,32,32	0
56	MG	DA	3030	1/1	0.93	0.28	40,40,40,40	0
56	MG	BA	3423	1/1	0.93	0.18	23,23,23,23	0
56	MG	DA	3255	1/1	0.93	0.05	59,59,59,59	0
56	MG	DA	3256	1/1	0.93	0.12	47,47,47,47	0
56	MG	DA	3259	1/1	0.93	0.12	34,34,34,34	0
56	MG	DA	3263	1/1	0.93	0.10	61,61,61,61	0
56	MG	DA	3033	1/1	0.93	0.22	31,31,31,31	0
56	MG	AY	3002	1/1	0.93	0.12	68,68,68,68	0
56	MG	BA	3426	1/1	0.93	0.21	22,22,22,22	0
56	MG	BA	3803	1/1	0.93	0.09	47,47,47,47	0
56	MG	BA	3106	1/1	0.93	0.47	50,50,50,50	0
56	MG	CA	3032	1/1	0.93	0.23	52,52,52,52	0
56	MG	DA	3550	1/1	0.93	0.08	51,51,51,51	0
56	MG	DA	3551	1/1	0.93	0.16	55,55,55,55	0
56	MG	BA	3805	1/1	0.93	0.16	21,21,21,21	0
56	MG	DA	3557	1/1	0.93	0.23	34,34,34,34	0
56	MG	DA	3559	1/1	0.93	0.18	48,48,48,48	0
56	MG	DA	3561	1/1	0.93	0.22	48,48,48,48	0
56	MG	DA	3562	1/1	0.93	0.34	58,58,58,58	0
56	MG	DA	3046	1/1	0.93	0.37	57,57,57,57	0
56	MG	AA	3083	1/1	0.93	0.15	52,52,52,52	0
56	MG	BA	3554	1/1	0.93	0.21	37,37,37,37	0
56	MG	CA	3038	1/1	0.93	0.19	46,46,46,46	0
56	MG	BA	3810	1/1	0.93	0.25	50,50,50,50	0
56	MG	DA	3304	1/1	0.93	0.12	40,40,40,40	0
56	MG	DA	3572	1/1	0.93	0.26	28,28,28,28	0
56	MG	BA	3252	1/1	0.93	0.24	45,45,45,45	0
56	MG	DA	3577	1/1	0.93	0.14	49,49,49,49	0
56	MG	DA	3578	1/1	0.93	0.10	55,55,55,55	0
56	MG	BA	3685	1/1	0.93	0.17	59,59,59,59	0
56	MG	BA	3818	1/1	0.93	0.26	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3819	1/1	0.93	0.24	32,32,32,32	0
56	MG	DA	3070	1/1	0.93	0.23	48,48,48,48	0
56	MG	BA	3430	1/1	0.93	0.33	32,32,32,32	0
56	MG	DA	3075	1/1	0.93	0.12	39,39,39,39	0
56	MG	BA	3323	1/1	0.93	0.22	39,39,39,39	0
56	MG	AA	3140	1/1	0.93	0.11	71,71,71,71	0
56	MG	AA	3166	1/1	0.93	0.13	65,65,65,65	0
56	MG	BA	3329	1/1	0.93	0.19	29,29,29,29	0
56	MG	AA	3024	1/1	0.93	0.15	58,58,58,58	0
56	MG	BA	3698	1/1	0.93	0.13	48,48,48,48	0
56	MG	BA	3337	1/1	0.93	0.17	35,35,35,35	0
56	MG	DA	3090	1/1	0.93	0.21	45,45,45,45	0
56	MG	DA	3338	1/1	0.93	0.19	40,40,40,40	0
56	MG	DA	3092	1/1	0.93	0.26	48,48,48,48	0
56	MG	BA	3839	1/1	0.93	0.12	38,38,38,38	0
56	MG	DA	3609	1/1	0.93	0.16	60,60,60,60	0
56	MG	BA	3116	1/1	0.93	0.15	29,29,29,29	0
56	MG	DA	3095	1/1	0.93	0.27	47,47,47,47	0
56	MG	BB	3002	1/1	0.93	0.18	52,52,52,52	0
56	MG	DA	3613	1/1	0.93	0.14	50,50,50,50	0
56	MG	BA	3576	1/1	0.93	0.17	48,48,48,48	0
56	MG	BA	3578	1/1	0.93	0.25	47,47,47,47	0
56	MG	BB	3005	1/1	0.93	0.19	64,64,64,64	0
56	MG	CA	3076	1/1	0.93	0.19	56,56,56,56	0
56	MG	BA	3260	1/1	0.93	0.56	57,57,57,57	0
56	MG	DA	3369	1/1	0.93	0.05	61,61,61,61	0
56	MG	BA	3704	1/1	0.93	0.23	55,55,55,55	0
56	MG	DA	3374	1/1	0.93	0.18	37,37,37,37	0
56	MG	AA	3077	1/1	0.93	0.14	49,49,49,49	0
56	MG	BA	3120	1/1	0.93	0.23	32,32,32,32	0
56	MG	BA	3007	1/1	0.93	0.24	51,51,51,51	0
56	MG	BA	3125	1/1	0.93	0.14	42,42,42,42	0
56	MG	DA	3383	1/1	0.93	0.24	37,37,37,37	0
56	MG	BA	3711	1/1	0.93	0.26	45,45,45,45	0
56	MG	BA	3199	1/1	0.93	0.09	53,53,53,53	0
56	MG	AA	3171	1/1	0.93	0.10	48,48,48,48	0
56	MG	BD	301	1/1	0.93	0.21	49,49,49,49	0
56	MG	AA	3208	1/1	0.93	0.16	45,45,45,45	0
56	MG	AA	3056	1/1	0.93	0.19	46,46,46,46	0
56	MG	AA	3026	1/1	0.93	0.22	53,53,53,53	0
56	MG	BA	3719	1/1	0.93	0.13	42,42,42,42	0
56	MG	DA	3135	1/1	0.93	0.11	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3137	1/1	0.93	0.13	54,54,54,54	0
56	MG	CA	3109	1/1	0.93	0.24	68,68,68,68	0
56	MG	DA	3139	1/1	0.93	0.10	40,40,40,40	0
56	MG	BA	3136	1/1	0.93	0.12	58,58,58,58	0
56	MG	BA	3721	1/1	0.93	0.18	47,47,47,47	0
56	MG	BA	3081	1/1	0.93	0.19	49,49,49,49	0
56	MG	BF	311	1/1	0.93	0.18	43,43,43,43	0
56	MG	DA	3675	1/1	0.93	0.28	44,44,44,44	0
56	MG	DA	3146	1/1	0.93	0.27	46,46,46,46	0
56	MG	BA	3279	1/1	0.93	0.22	43,43,43,43	0
56	MG	DA	3409	1/1	0.93	0.09	47,47,47,47	0
56	MG	CA	3120	1/1	0.93	0.12	64,64,64,64	0
56	MG	DA	3150	1/1	0.93	0.06	41,41,41,41	0
56	MG	AA	3105	1/1	0.93	0.20	49,49,49,49	0
56	MG	AA	3090	1/1	0.93	0.35	53,53,53,53	0
56	MG	DA	3420	1/1	0.93	0.16	46,46,46,46	0
56	MG	BN	3005	1/1	0.93	0.39	51,51,51,51	0
56	MG	BA	3474	1/1	0.93	0.09	61,61,61,61	0
56	MG	DE	302	1/1	0.93	0.20	39,39,39,39	0
56	MG	BA	3366	1/1	0.93	0.17	45,45,45,45	0
56	MG	AA	3008	1/1	0.93	0.15	54,54,54,54	0
56	MG	BA	3732	1/1	0.93	0.26	40,40,40,40	0
56	MG	BA	3370	1/1	0.93	0.12	60,60,60,60	0
56	MG	BA	3616	1/1	0.93	0.12	53,53,53,53	0
56	MG	DU	3002	1/1	0.93	0.22	50,50,50,50	0
56	MG	DA	3180	1/1	0.93	0.14	51,51,51,51	0
56	MG	AA	3002	1/1	0.93	0.08	62,62,62,62	0
56	MG	D0	102	1/1	0.93	0.17	62,62,62,62	0
56	MG	BA	3374	1/1	0.93	0.08	37,37,37,37	0
56	MG	DA	3442	1/1	0.93	0.15	44,44,44,44	0
56	MG	BA	3619	1/1	0.93	0.40	51,51,51,51	0
56	MG	BW	203	1/1	0.93	0.23	34,34,34,34	0
56	MG	BX	101	1/1	0.93	0.26	65,65,65,65	0
56	MG	BA	3741	1/1	0.93	0.11	28,28,28,28	0
56	MG	BA	3145	1/1	0.93	0.26	32,32,32,32	0
56	MG	BA	3092	1/1	0.93	0.26	41,41,41,41	0
56	MG	BA	3132	1/1	0.94	0.21	42,42,42,42	0
56	MG	DA	3073	1/1	0.94	0.17	54,54,54,54	0
56	MG	AW	3004	1/1	0.94	0.12	51,51,51,51	0
56	MG	BA	3602	1/1	0.94	0.17	46,46,46,46	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3055	1/1	0.94	0.23	31,31,31,31	0
56	MG	BA	3761	1/1	0.94	0.19	54,54,54,54	0
56	MG	BA	3137	1/1	0.94	0.24	45,45,45,45	0
56	MG	AA	3188	1/1	0.94	0.16	56,56,56,56	0
56	MG	AA	3107	1/1	0.94	0.25	51,51,51,51	0
56	MG	BA	3614	1/1	0.94	0.15	26,26,26,26	0
56	MG	AA	3031	1/1	0.94	0.09	44,44,44,44	0
56	MG	BA	3327	1/1	0.94	0.25	25,25,25,25	0
56	MG	BA	3141	1/1	0.94	0.23	38,38,38,38	0
56	MG	CA	3030	1/1	0.94	0.08	59,59,59,59	0
56	MG	BA	3448	1/1	0.94	0.22	28,28,28,28	0
56	MG	DA	3097	1/1	0.94	0.21	43,43,43,43	0
56	MG	AA	3039	1/1	0.94	0.15	61,61,61,61	0
56	MG	DA	3100	1/1	0.94	0.24	36,36,36,36	0
56	MG	CA	3033	1/1	0.94	0.15	56,56,56,56	0
56	MG	AA	3028	1/1	0.94	0.38	56,56,56,56	0
56	MG	CA	3035	1/1	0.94	0.10	60,60,60,60	0
56	MG	AA	3092	1/1	0.94	0.20	39,39,39,39	0
56	MG	BA	3454	1/1	0.94	0.15	31,31,31,31	0
56	MG	AA	3147	1/1	0.94	0.11	55,55,55,55	0
56	MG	BA	3456	1/1	0.94	0.39	41,41,41,41	0
56	MG	CA	3041	1/1	0.94	0.16	58,58,58,58	0
56	MG	BA	3457	1/1	0.94	0.21	44,44,44,44	0
56	MG	DA	3440	1/1	0.94	0.18	39,39,39,39	0
56	MG	BA	3788	1/1	0.94	0.17	41,41,41,41	0
56	MG	DA	3117	1/1	0.94	0.28	60,60,60,60	0
56	MG	AX	3007	1/1	0.94	0.24	72,72,72,72	0
56	MG	BA	3790	1/1	0.94	0.21	32,32,32,32	0
56	MG	CA	3052	1/1	0.94	0.09	65,65,65,65	0
56	MG	DA	3449	1/1	0.94	0.19	47,47,47,47	0
56	MG	AA	3093	1/1	0.94	0.14	50,50,50,50	0
56	MG	BA	3469	1/1	0.94	0.31	37,37,37,37	0
56	MG	AA	3041	1/1	0.94	0.26	52,52,52,52	0
56	MG	AA	3152	1/1	0.94	0.13	45,45,45,45	0
56	MG	AA	3029	1/1	0.94	0.28	53,53,53,53	0
56	MG	DA	3458	1/1	0.94	0.11	42,42,42,42	0
56	MG	AA	3206	1/1	0.94	0.17	47,47,47,47	0
56	MG	CA	3063	1/1	0.94	0.14	59,59,59,59	0
56	MG	BA	3350	1/1	0.94	0.24	27,27,27,27	0
56	MG	DA	3467	1/1	0.94	0.31	43,43,43,43	0
56	MG	AA	3096	1/1	0.94	0.27	48,48,48,48	0
56	MG	DA	3141	1/1	0.94	0.21	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3256	1/1	0.94	0.32	49,49,49,49	0
56	MG	CA	3068	1/1	0.94	0.40	55,55,55,55	0
56	MG	DA	3478	1/1	0.94	0.18	47,47,47,47	0
56	MG	BA	3257	1/1	0.94	0.21	41,41,41,41	0
56	MG	BA	3654	1/1	0.94	0.15	55,55,55,55	0
56	MG	DA	3484	1/1	0.94	0.05	45,45,45,45	0
56	MG	CA	3071	1/1	0.94	0.09	50,50,50,50	0
56	MG	BA	3814	1/1	0.94	0.28	26,26,26,26	0
56	MG	AA	3118	1/1	0.94	0.20	53,53,53,53	0
56	MG	DA	3152	1/1	0.94	0.25	42,42,42,42	0
56	MG	BA	3658	1/1	0.94	0.23	45,45,45,45	0
56	MG	DA	3156	1/1	0.94	0.12	43,43,43,43	0
56	MG	AA	3119	1/1	0.94	0.10	58,58,58,58	0
56	MG	DA	3159	1/1	0.94	0.30	41,41,41,41	0
56	MG	DA	3160	1/1	0.94	0.20	59,59,59,59	0
56	MG	DA	3162	1/1	0.94	0.34	43,43,43,43	0
56	MG	CA	3080	1/1	0.94	0.28	52,52,52,52	0
56	MG	BA	3661	1/1	0.94	0.09	53,53,53,53	0
56	MG	BA	3662	1/1	0.94	0.32	50,50,50,50	0
56	MG	AA	3211	1/1	0.94	0.09	59,59,59,59	0
56	MG	BA	3829	1/1	0.94	0.34	45,45,45,45	0
56	MG	BA	3665	1/1	0.94	0.29	49,49,49,49	0
56	MG	BA	3359	1/1	0.94	0.14	46,46,46,46	0
56	MG	DA	3511	1/1	0.94	0.11	45,45,45,45	0
56	MG	AA	3097	1/1	0.94	0.13	50,50,50,50	0
56	MG	BA	3501	1/1	0.94	0.18	20,20,20,20	0
56	MG	BA	3502	1/1	0.94	0.31	45,45,45,45	0
56	MG	CA	3094	1/1	0.94	0.18	72,72,72,72	0
56	MG	CA	3095	1/1	0.94	0.10	61,61,61,61	0
56	MG	BA	3361	1/1	0.94	0.16	35,35,35,35	0
56	MG	BA	3175	1/1	0.94	0.21	35,35,35,35	0
56	MG	BA	3505	1/1	0.94	0.12	54,54,54,54	0
56	MG	DA	3527	1/1	0.94	0.17	53,53,53,53	0
56	MG	BA	3506	1/1	0.94	0.26	51,51,51,51	0
56	MG	BA	3676	1/1	0.94	0.28	53,53,53,53	0
56	MG	CA	3105	1/1	0.94	0.14	49,49,49,49	0
56	MG	DA	3535	1/1	0.94	0.35	54,54,54,54	0
56	MG	BA	3267	1/1	0.94	0.14	37,37,37,37	0
56	MG	AA	3064	1/1	0.94	0.13	61,61,61,61	0
56	MG	CA	3113	1/1	0.94	0.11	55,55,55,55	0
56	MG	BA	3680	1/1	0.94	0.15	52,52,52,52	0
56	MG	BB	3010	1/1	0.94	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3008	1/1	0.94	0.22	27,27,27,27	0
56	MG	CA	3118	1/1	0.94	0.18	47,47,47,47	0
56	MG	BA	3011	1/1	0.94	0.20	40,40,40,40	0
56	MG	DA	3206	1/1	0.94	0.10	39,39,39,39	0
56	MG	BB	3013	1/1	0.94	0.14	42,42,42,42	0
56	MG	BA	3098	1/1	0.94	0.35	26,26,26,26	0
56	MG	BA	3183	1/1	0.94	0.22	40,40,40,40	0
56	MG	BA	3688	1/1	0.94	0.20	45,45,45,45	0
56	MG	AA	3162	1/1	0.94	0.28	59,59,59,59	0
56	MG	BA	3276	1/1	0.94	0.29	41,41,41,41	0
56	MG	BA	3691	1/1	0.94	0.25	38,38,38,38	0
56	MG	DA	3216	1/1	0.94	0.29	46,46,46,46	0
56	MG	BA	3190	1/1	0.94	0.16	45,45,45,45	0
56	MG	CA	3129	1/1	0.94	0.19	61,61,61,61	0
56	MG	BD	308	1/1	0.94	0.28	39,39,39,39	0
56	MG	DA	3564	1/1	0.94	0.31	53,53,53,53	0
56	MG	BA	3378	1/1	0.94	0.10	34,34,34,34	0
56	MG	BE	304	1/1	0.94	0.26	40,40,40,40	0
56	MG	BA	3379	1/1	0.94	0.18	45,45,45,45	0
56	MG	BA	3381	1/1	0.94	0.14	43,43,43,43	0
56	MG	BA	3382	1/1	0.94	0.21	55,55,55,55	0
56	MG	BA	3528	1/1	0.94	0.11	43,43,43,43	0
56	MG	BF	306	1/1	0.94	0.31	40,40,40,40	0
56	MG	AA	3126	1/1	0.94	0.17	46,46,46,46	0
56	MG	BF	310	1/1	0.94	0.25	38,38,38,38	0
56	MG	AA	3099	1/1	0.94	0.25	63,63,63,63	0
56	MG	BA	3531	1/1	0.94	0.39	61,61,61,61	0
56	MG	BA	3533	1/1	0.94	0.23	50,50,50,50	0
56	MG	DA	3242	1/1	0.94	0.07	43,43,43,43	0
56	MG	DA	3243	1/1	0.94	0.17	54,54,54,54	0
56	MG	AA	3128	1/1	0.94	0.17	41,41,41,41	0
56	MG	BA	3281	1/1	0.94	0.17	49,49,49,49	0
56	MG	BA	3543	1/1	0.94	0.25	26,26,26,26	0
56	MG	DA	3592	1/1	0.94	0.17	52,52,52,52	0
56	MG	BA	3105	1/1	0.94	0.45	69,69,69,69	0
56	MG	BA	3545	1/1	0.94	0.25	41,41,41,41	0
56	MG	BA	3399	1/1	0.94	0.16	25,25,25,25	0
56	MG	DA	3598	1/1	0.94	0.11	63,63,63,63	0
56	MG	BA	3550	1/1	0.94	0.20	34,34,34,34	0
56	MG	DA	3258	1/1	0.94	0.18	59,59,59,59	0
56	MG	DA	3603	1/1	0.94	0.14	52,52,52,52	0
56	MG	CA	3168	1/1	0.94	0.19	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3260	1/1	0.94	0.13	41,41,41,41	0
56	MG	BR	201	1/1	0.94	0.17	44,44,44,44	0
56	MG	AA	3129	1/1	0.94	0.08	73,73,73,73	0
56	MG	DA	3270	1/1	0.94	0.22	49,49,49,49	0
56	MG	CA	3171	1/1	0.94	0.19	63,63,63,63	0
56	MG	BA	3286	1/1	0.94	0.32	46,46,46,46	0
56	MG	BU	201	1/1	0.94	0.14	39,39,39,39	0
56	MG	DA	3274	1/1	0.94	0.22	33,33,33,33	0
56	MG	DA	3278	1/1	0.94	0.21	53,53,53,53	0
56	MG	DA	3282	1/1	0.94	0.10	42,42,42,42	0
56	MG	DA	3283	1/1	0.94	0.25	46,46,46,46	0
56	MG	BU	208	1/1	0.94	0.13	41,41,41,41	0
56	MG	BV	203	1/1	0.94	0.24	32,32,32,32	0
56	MG	BA	3110	1/1	0.94	0.26	41,41,41,41	0
56	MG	BA	3559	1/1	0.94	0.20	30,30,30,30	0
56	MG	DA	3626	1/1	0.94	0.06	54,54,54,54	0
56	MG	CF	3001	1/1	0.94	0.26	38,38,38,38	0
56	MG	DA	3296	1/1	0.94	0.18	48,48,48,48	0
56	MG	DA	3631	1/1	0.94	0.13	56,56,56,56	0
56	MG	BA	3200	1/1	0.94	0.28	56,56,56,56	0
56	MG	DA	3633	1/1	0.94	0.14	61,61,61,61	0
56	MG	CT	3001	1/1	0.94	0.07	47,47,47,47	0
56	MG	AA	3052	1/1	0.94	0.32	68,68,68,68	0
56	MG	BX	102	1/1	0.94	0.31	41,41,41,41	0
56	MG	DA	3640	1/1	0.94	0.14	52,52,52,52	0
56	MG	DA	3641	1/1	0.94	0.09	44,44,44,44	0
56	MG	BY	502	1/1	0.94	0.13	50,50,50,50	0
56	MG	CX	3005	1/1	0.94	0.45	58,58,58,58	0
56	MG	BA	3021	1/1	0.94	0.17	60,60,60,60	0
56	MG	DA	3647	1/1	0.94	0.22	47,47,47,47	0
56	MG	B0	101	1/1	0.94	0.20	39,39,39,39	0
56	MG	DA	3311	1/1	0.94	0.18	42,42,42,42	0
56	MG	AA	3173	1/1	0.94	0.11	47,47,47,47	0
56	MG	DA	3652	1/1	0.94	0.12	49,49,49,49	0
56	MG	DA	3005	1/1	0.94	0.20	58,58,58,58	0
56	MG	DA	3014	1/1	0.94	0.14	50,50,50,50	0
56	MG	DA	3659	1/1	0.94	0.48	67,67,67,67	0
56	MG	AA	3053	1/1	0.94	0.37	49,49,49,49	0
56	MG	AA	3084	1/1	0.94	0.17	49,49,49,49	0
56	MG	DA	3664	1/1	0.94	0.08	38,38,38,38	0
56	MG	BA	3570	1/1	0.94	0.35	30,30,30,30	0
56	MG	BA	3416	1/1	0.94	0.17	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3669	1/1	0.94	0.22	49,49,49,49	0
56	MG	BA	3213	1/1	0.94	0.09	45,45,45,45	0
56	MG	BA	3575	1/1	0.94	0.09	64,64,64,64	0
56	MG	DA	3331	1/1	0.94	0.25	39,39,39,39	0
56	MG	BA	3420	1/1	0.94	0.19	22,22,22,22	0
56	MG	B5	105	1/1	0.94	0.10	49,49,49,49	0
56	MG	DA	3031	1/1	0.94	0.41	51,51,51,51	0
56	MG	DA	3342	1/1	0.94	0.10	56,56,56,56	0
56	MG	BA	3296	1/1	0.94	0.19	31,31,31,31	0
56	MG	DA	3348	1/1	0.94	0.27	38,38,38,38	0
56	MG	BA	3214	1/1	0.94	0.20	49,49,49,49	0
56	MG	BA	3300	1/1	0.94	0.18	22,22,22,22	0
56	MG	DA	3035	1/1	0.94	0.24	38,38,38,38	0
56	MG	BA	3425	1/1	0.94	0.27	29,29,29,29	0
56	MG	AA	3176	1/1	0.94	0.09	54,54,54,54	0
56	MG	DD	305	1/1	0.94	0.24	38,38,38,38	0
56	MG	CA	3001	1/1	0.94	0.25	73,73,73,73	0
56	MG	AA	3043	1/1	0.94	0.27	26,26,26,26	0
56	MG	DE	303	1/1	0.94	0.26	44,44,44,44	0
56	MG	AA	3027	1/1	0.94	0.24	54,54,54,54	0
56	MG	BA	3745	1/1	0.94	0.17	30,30,30,30	0
56	MG	DA	3048	1/1	0.94	0.15	45,45,45,45	0
56	MG	BA	3306	1/1	0.94	0.18	31,31,31,31	0
56	MG	BA	3034	1/1	0.94	0.21	28,28,28,28	0
56	MG	DA	3054	1/1	0.94	0.15	43,43,43,43	0
56	MG	BA	3223	1/1	0.94	0.16	29,29,29,29	0
56	MG	DW	3001	1/1	0.94	0.23	43,43,43,43	0
56	MG	DA	3377	1/1	0.94	0.07	42,42,42,42	0
56	MG	D0	101	1/1	0.94	0.08	56,56,56,56	0
56	MG	DA	3059	1/1	0.94	0.45	53,53,53,53	0
56	MG	D7	101	1/1	0.94	0.19	39,39,39,39	0
56	MG	BA	3750	1/1	0.94	0.21	49,49,49,49	0
56	MG	DA	3381	1/1	0.94	0.11	60,60,60,60	0
56	MG	AA	3184	1/1	0.94	0.12	55,55,55,55	0
56	MG	DA	3065	1/1	0.94	0.08	56,56,56,56	0
56	MG	CA	3012	1/1	0.94	0.20	68,68,68,68	0
56	MG	AA	3036	1/1	0.94	0.12	52,52,52,52	0
56	MG	CA	3014	1/1	0.94	0.14	47,47,47,47	0
56	MG	AA	3187	1/1	0.94	0.12	62,62,62,62	0
56	MG	DA	3426	1/1	0.95	0.17	41,41,41,41	0
56	MG	DA	3154	1/1	0.95	0.32	52,52,52,52	0
56	MG	BA	3318	1/1	0.95	0.27	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3136	1/1	0.95	0.18	65,65,65,65	0
56	MG	BA	3631	1/1	0.95	0.14	43,43,43,43	0
56	MG	AA	3034	1/1	0.95	0.26	48,48,48,48	0
56	MG	CA	3140	1/1	0.95	0.16	79,79,79,79	0
56	MG	AA	3219	1/1	0.95	0.21	65,65,65,65	0
56	MG	DA	3163	1/1	0.95	0.27	49,49,49,49	0
56	MG	BA	3635	1/1	0.95	0.28	62,62,62,62	0
56	MG	CA	3145	1/1	0.95	0.13	63,63,63,63	0
56	MG	DA	3169	1/1	0.95	0.13	49,49,49,49	0
56	MG	AA	3220	1/1	0.95	0.07	64,64,64,64	0
56	MG	BA	3324	1/1	0.95	0.17	34,34,34,34	0
56	MG	DA	3174	1/1	0.95	0.17	48,48,48,48	0
56	MG	BA	3262	1/1	0.95	0.31	47,47,47,47	0
56	MG	CA	3149	1/1	0.95	0.27	65,65,65,65	0
56	MG	CA	3150	1/1	0.95	0.16	62,62,62,62	0
56	MG	BA	3517	1/1	0.95	0.12	51,51,51,51	0
56	MG	BA	3263	1/1	0.95	0.18	32,32,32,32	0
56	MG	BA	3642	1/1	0.95	0.09	37,37,37,37	0
56	MG	AA	3191	1/1	0.95	0.24	48,48,48,48	0
56	MG	DA	3462	1/1	0.95	0.28	43,43,43,43	0
56	MG	DA	3464	1/1	0.95	0.11	44,44,44,44	0
56	MG	BA	3647	1/1	0.95	0.16	45,45,45,45	0
56	MG	DA	3185	1/1	0.95	0.24	54,54,54,54	0
56	MG	BA	3202	1/1	0.95	0.13	46,46,46,46	0
56	MG	CA	3160	1/1	0.95	0.16	65,65,65,65	0
56	MG	DA	3188	1/1	0.95	0.38	50,50,50,50	0
56	MG	DA	3475	1/1	0.95	0.13	42,42,42,42	0
56	MG	AA	3014	1/1	0.95	0.12	69,69,69,69	0
56	MG	BA	3268	1/1	0.95	0.28	58,58,58,58	0
56	MG	BA	3652	1/1	0.95	0.13	46,46,46,46	0
56	MG	CA	3165	1/1	0.95	0.08	56,56,56,56	0
56	MG	BA	3339	1/1	0.95	0.15	40,40,40,40	0
56	MG	BA	3037	1/1	0.95	0.16	37,37,37,37	0
56	MG	AA	3019	1/1	0.95	0.15	48,48,48,48	0
56	MG	DA	3488	1/1	0.95	0.13	37,37,37,37	0
56	MG	DA	3489	1/1	0.95	0.16	37,37,37,37	0
56	MG	BA	3783	1/1	0.95	0.19	53,53,53,53	0
56	MG	BA	3343	1/1	0.95	0.18	33,33,33,33	0
56	MG	DA	3202	1/1	0.95	0.33	50,50,50,50	0
56	MG	DA	3496	1/1	0.95	0.06	48,48,48,48	0
56	MG	BA	3206	1/1	0.95	0.21	29,29,29,29	0
56	MG	AA	3010	1/1	0.95	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3532	1/1	0.95	0.27	49,49,49,49	0
56	MG	AA	3069	1/1	0.95	0.21	67,67,67,67	0
56	MG	BA	3536	1/1	0.95	0.18	48,48,48,48	0
56	MG	BA	3792	1/1	0.95	0.16	32,32,32,32	0
56	MG	BA	3794	1/1	0.95	0.20	33,33,33,33	0
56	MG	BA	3796	1/1	0.95	0.13	40,40,40,40	0
56	MG	BA	3051	1/1	0.95	0.23	25,25,25,25	0
56	MG	CV	3001	1/1	0.95	0.19	58,58,58,58	0
56	MG	BA	3539	1/1	0.95	0.21	23,23,23,23	0
56	MG	CW	3002	1/1	0.95	0.16	74,74,74,74	0
56	MG	BA	3799	1/1	0.95	0.22	47,47,47,47	0
56	MG	BA	3800	1/1	0.95	0.15	39,39,39,39	0
56	MG	BA	3432	1/1	0.95	0.10	52,52,52,52	0
56	MG	BA	3216	1/1	0.95	0.21	34,34,34,34	0
56	MG	BA	3671	1/1	0.95	0.14	45,45,45,45	0
56	MG	AA	3149	1/1	0.95	0.21	41,41,41,41	0
56	MG	DA	3226	1/1	0.95	0.15	54,54,54,54	0
56	MG	CA	3022	1/1	0.95	0.10	53,53,53,53	0
56	MG	DA	3525	1/1	0.95	0.17	41,41,41,41	0
56	MG	DA	3007	1/1	0.95	0.39	54,54,54,54	0
56	MG	DA	3232	1/1	0.95	0.28	53,53,53,53	0
56	MG	DA	3529	1/1	0.95	0.10	41,41,41,41	0
56	MG	DA	3008	1/1	0.95	0.21	33,33,33,33	0
56	MG	DA	3013	1/1	0.95	0.17	40,40,40,40	0
56	MG	AA	3132	1/1	0.95	0.13	22,22,22,22	0
56	MG	AK	201	1/1	0.95	0.14	61,61,61,61	0
56	MG	AK	202	1/1	0.95	0.26	38,38,38,38	0
56	MG	DA	3021	1/1	0.95	0.30	48,48,48,48	0
56	MG	DA	3240	1/1	0.95	0.17	51,51,51,51	0
56	MG	DA	3023	1/1	0.95	0.14	30,30,30,30	0
56	MG	BA	3222	1/1	0.95	0.36	27,27,27,27	0
56	MG	BA	3109	1/1	0.95	0.28	42,42,42,42	0
56	MG	DA	3244	1/1	0.95	0.13	48,48,48,48	0
56	MG	DA	3245	1/1	0.95	0.10	62,62,62,62	0
56	MG	AA	3009	1/1	0.95	0.26	46,46,46,46	0
56	MG	BA	3558	1/1	0.95	0.19	29,29,29,29	0
56	MG	AA	3046	1/1	0.95	0.16	56,56,56,56	0
56	MG	BA	3163	1/1	0.95	0.22	45,45,45,45	0
56	MG	BA	3563	1/1	0.95	0.08	60,60,60,60	0
56	MG	BA	3827	1/1	0.95	0.20	30,30,30,30	0
56	MG	DA	3553	1/1	0.95	0.14	54,54,54,54	0
56	MG	DA	3555	1/1	0.95	0.08	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3687	1/1	0.95	0.23	36,36,36,36	0
56	MG	AA	3178	1/1	0.95	0.12	54,54,54,54	0
56	MG	BA	3362	1/1	0.95	0.25	19,19,19,19	0
56	MG	BA	3169	1/1	0.95	0.25	47,47,47,47	0
56	MG	BA	3833	1/1	0.95	0.20	43,43,43,43	0
56	MG	DA	3264	1/1	0.95	0.13	31,31,31,31	0
56	MG	DA	3265	1/1	0.95	0.31	52,52,52,52	0
56	MG	DA	3267	1/1	0.95	0.26	38,38,38,38	0
56	MG	DA	3268	1/1	0.95	0.04	60,60,60,60	0
56	MG	DA	3040	1/1	0.95	0.11	53,53,53,53	0
56	MG	BA	3834	1/1	0.95	0.13	35,35,35,35	0
56	MG	DA	3042	1/1	0.95	0.15	41,41,41,41	0
56	MG	BA	3230	1/1	0.95	0.14	62,62,62,62	0
56	MG	AA	3207	1/1	0.95	0.14	68,68,68,68	0
56	MG	DA	3575	1/1	0.95	0.10	47,47,47,47	0
56	MG	AA	3180	1/1	0.95	0.14	57,57,57,57	0
56	MG	AA	3012	1/1	0.95	0.23	33,33,33,33	0
56	MG	DA	3279	1/1	0.95	0.07	48,48,48,48	0
56	MG	BA	3696	1/1	0.95	0.16	33,33,33,33	0
56	MG	DA	3052	1/1	0.95	0.12	38,38,38,38	0
56	MG	DA	3584	1/1	0.95	0.40	58,58,58,58	0
56	MG	DA	3285	1/1	0.95	0.20	28,28,28,28	0
56	MG	BA	3173	1/1	0.95	0.30	36,36,36,36	0
56	MG	BA	3066	1/1	0.95	0.39	51,51,51,51	0
56	MG	BA	3177	1/1	0.95	0.30	44,44,44,44	0
56	MG	DA	3058	1/1	0.95	0.21	46,46,46,46	0
56	MG	BA	3577	1/1	0.95	0.19	60,60,60,60	0
56	MG	DA	3593	1/1	0.95	0.24	39,39,39,39	0
56	MG	CA	3056	1/1	0.95	0.23	60,60,60,60	0
56	MG	BA	3067	1/1	0.95	0.23	49,49,49,49	0
56	MG	DA	3063	1/1	0.95	0.14	46,46,46,46	0
56	MG	DA	3302	1/1	0.95	0.12	33,33,33,33	0
56	MG	BA	3463	1/1	0.95	0.20	37,37,37,37	0
56	MG	DA	3601	1/1	0.95	0.19	54,54,54,54	0
56	MG	BA	3580	1/1	0.95	0.22	42,42,42,42	0
56	MG	DA	3067	1/1	0.95	0.25	49,49,49,49	0
56	MG	AA	3074	1/1	0.95	0.17	47,47,47,47	0
56	MG	BA	3243	1/1	0.95	0.18	44,44,44,44	0
56	MG	BA	3077	1/1	0.95	0.20	34,34,34,34	0
56	MG	BA	3584	1/1	0.95	0.24	27,27,27,27	0
56	MG	BA	3709	1/1	0.95	0.29	44,44,44,44	0
56	MG	DA	3074	1/1	0.95	0.22	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3380	1/1	0.95	0.12	60,60,60,60	0
56	MG	DA	3076	1/1	0.95	0.22	43,43,43,43	0
56	MG	DA	3077	1/1	0.95	0.18	43,43,43,43	0
56	MG	BA	3471	1/1	0.95	0.06	45,45,45,45	0
56	MG	BB	3021	1/1	0.95	0.13	54,54,54,54	0
56	MG	BA	3587	1/1	0.95	0.20	44,44,44,44	0
56	MG	DA	3617	1/1	0.95	0.36	53,53,53,53	0
56	MG	DA	3326	1/1	0.95	0.18	46,46,46,46	0
56	MG	DA	3327	1/1	0.95	0.19	59,59,59,59	0
56	MG	DA	3082	1/1	0.95	0.22	34,34,34,34	0
56	MG	DA	3330	1/1	0.95	0.17	46,46,46,46	0
56	MG	DA	3625	1/1	0.95	0.20	53,53,53,53	0
56	MG	DA	3083	1/1	0.95	0.18	51,51,51,51	0
56	MG	DA	3084	1/1	0.95	0.27	27,27,27,27	0
56	MG	BA	3715	1/1	0.95	0.24	53,53,53,53	0
56	MG	DA	3337	1/1	0.95	0.09	43,43,43,43	0
56	MG	BA	3126	1/1	0.95	0.26	43,43,43,43	0
56	MG	CA	3075	1/1	0.95	0.10	44,44,44,44	0
56	MG	DA	3634	1/1	0.95	0.14	53,53,53,53	0
56	MG	AA	3108	1/1	0.95	0.20	55,55,55,55	0
56	MG	DA	3347	1/1	0.95	0.16	44,44,44,44	0
56	MG	BD	310	1/1	0.95	0.15	31,31,31,31	0
56	MG	DA	3639	1/1	0.95	0.14	64,64,64,64	0
56	MG	BA	3385	1/1	0.95	0.15	39,39,39,39	0
56	MG	DA	3353	1/1	0.95	0.14	37,37,37,37	0
56	MG	BA	3309	1/1	0.95	0.07	55,55,55,55	0
56	MG	BA	3388	1/1	0.95	0.13	52,52,52,52	0
56	MG	DA	3357	1/1	0.95	0.14	44,44,44,44	0
56	MG	BA	3480	1/1	0.95	0.15	56,56,56,56	0
56	MG	BA	3722	1/1	0.95	0.13	50,50,50,50	0
56	MG	DA	3360	1/1	0.95	0.16	51,51,51,51	0
56	MG	DA	3362	1/1	0.95	0.22	43,43,43,43	0
56	MG	BF	301	1/1	0.95	0.26	38,38,38,38	0
56	MG	BF	304	1/1	0.95	0.15	32,32,32,32	0
56	MG	DA	3099	1/1	0.95	0.09	60,60,60,60	0
56	MG	BA	3390	1/1	0.95	0.21	52,52,52,52	0
56	MG	BA	3598	1/1	0.95	0.15	47,47,47,47	0
56	MG	BA	3600	1/1	0.95	0.10	56,56,56,56	0
56	MG	DA	3372	1/1	0.95	0.15	47,47,47,47	0
56	MG	AA	3124	1/1	0.95	0.20	53,53,53,53	0
56	MG	BA	3483	1/1	0.95	0.28	38,38,38,38	0
56	MG	BG	202	1/1	0.95	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3187	1/1	0.95	0.16	36,36,36,36	0
56	MG	CA	3100	1/1	0.95	0.23	62,62,62,62	0
56	MG	DA	3379	1/1	0.95	0.20	59,59,59,59	0
56	MG	BA	3485	1/1	0.95	0.23	46,46,46,46	0
56	MG	CA	3103	1/1	0.95	0.10	75,75,75,75	0
56	MG	BA	3486	1/1	0.95	0.23	48,48,48,48	0
56	MG	BA	3488	1/1	0.95	0.10	50,50,50,50	0
56	MG	CA	3107	1/1	0.95	0.10	66,66,66,66	0
56	MG	BA	3608	1/1	0.95	0.21	60,60,60,60	0
56	MG	BA	3611	1/1	0.95	0.13	42,42,42,42	0
56	MG	DB	3007	1/1	0.95	0.09	59,59,59,59	0
56	MG	DB	3008	1/1	0.95	0.14	68,68,68,68	0
56	MG	DA	3123	1/1	0.95	0.12	47,47,47,47	0
56	MG	DA	3125	1/1	0.95	0.26	45,45,45,45	0
56	MG	DA	3126	1/1	0.95	0.15	44,44,44,44	0
56	MG	CA	3112	1/1	0.95	0.15	59,59,59,59	0
56	MG	DA	3130	1/1	0.95	0.25	47,47,47,47	0
56	MG	BP	203	1/1	0.95	0.12	32,32,32,32	0
56	MG	DE	301	1/1	0.95	0.29	45,45,45,45	0
56	MG	AA	3141	1/1	0.95	0.10	55,55,55,55	0
56	MG	DA	3400	1/1	0.95	0.34	39,39,39,39	0
56	MG	BA	3191	1/1	0.95	0.26	40,40,40,40	0
56	MG	DA	3134	1/1	0.95	0.13	49,49,49,49	0
56	MG	BQ	3004	1/1	0.95	0.24	35,35,35,35	0
56	MG	DF	303	1/1	0.95	0.07	46,46,46,46	0
56	MG	DN	5001	1/1	0.95	0.07	62,62,62,62	0
56	MG	AA	3075	1/1	0.95	0.22	33,33,33,33	0
56	MG	BA	3494	1/1	0.95	0.13	57,57,57,57	0
56	MG	BA	3499	1/1	0.95	0.24	33,33,33,33	0
56	MG	DV	3001	1/1	0.95	0.35	71,71,71,71	0
56	MG	BA	3401	1/1	0.95	0.14	48,48,48,48	0
56	MG	AA	3163	1/1	0.95	0.15	37,37,37,37	0
56	MG	BU	205	1/1	0.95	0.22	38,38,38,38	0
56	MG	BU	206	1/1	0.95	0.34	43,43,43,43	0
56	MG	DA	3413	1/1	0.95	0.20	36,36,36,36	0
56	MG	DA	3414	1/1	0.95	0.16	41,41,41,41	0
56	MG	BA	3403	1/1	0.95	0.28	31,31,31,31	0
56	MG	DA	3417	1/1	0.95	0.22	33,33,33,33	0
56	MG	BA	3404	1/1	0.95	0.18	36,36,36,36	0
59	ZN	B4	501	1/1	0.95	0.12	73,73,73,73	0
56	MG	BV	204	1/1	0.95	0.21	50,50,50,50	0
56	MG	DA	3148	1/1	0.95	0.23	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3406	1/1	0.95	0.19	32,32,32,32	0
56	MG	BA	3134	1/1	0.95	0.15	35,35,35,35	0
56	MG	BA	3135	1/1	0.95	0.21	35,35,35,35	0
56	MG	CA	3102	1/1	0.96	0.09	54,54,54,54	0
56	MG	DA	3486	1/1	0.96	0.22	44,44,44,44	0
56	MG	BA	3555	1/1	0.96	0.29	33,33,33,33	0
56	MG	BA	3247	1/1	0.96	0.30	28,28,28,28	0
56	MG	BA	3189	1/1	0.96	0.16	30,30,30,30	0
56	MG	DA	3490	1/1	0.96	0.18	39,39,39,39	0
56	MG	DA	3257	1/1	0.96	0.20	34,34,34,34	0
56	MG	DA	3492	1/1	0.96	0.12	47,47,47,47	0
56	MG	BA	3459	1/1	0.96	0.17	48,48,48,48	0
56	MG	DA	3494	1/1	0.96	0.18	30,30,30,30	0
56	MG	BA	3461	1/1	0.96	0.19	31,31,31,31	0
56	MG	CA	3110	1/1	0.96	0.11	48,48,48,48	0
56	MG	DA	3262	1/1	0.96	0.12	43,43,43,43	0
56	MG	DA	3080	1/1	0.96	0.22	45,45,45,45	0
56	MG	BA	3562	1/1	0.96	0.18	35,35,35,35	0
56	MG	BA	3308	1/1	0.96	0.21	39,39,39,39	0
56	MG	DA	3501	1/1	0.96	0.15	59,59,59,59	0
56	MG	DA	3266	1/1	0.96	0.10	47,47,47,47	0
56	MG	BA	3040	1/1	0.96	0.14	47,47,47,47	0
56	MG	BA	3784	1/1	0.96	0.22	52,52,52,52	0
56	MG	BA	3785	1/1	0.96	0.16	41,41,41,41	0
56	MG	CA	3116	1/1	0.96	0.06	55,55,55,55	0
56	MG	BA	3386	1/1	0.96	0.22	42,42,42,42	0
56	MG	DA	3088	1/1	0.96	0.18	42,42,42,42	0
56	MG	BA	3468	1/1	0.96	0.23	49,49,49,49	0
56	MG	AA	3122	1/1	0.96	0.19	60,60,60,60	0
56	MG	DA	3512	1/1	0.96	0.22	46,46,46,46	0
56	MG	DA	3276	1/1	0.96	0.08	33,33,33,33	0
56	MG	DA	3277	1/1	0.96	0.10	56,56,56,56	0
56	MG	DA	3091	1/1	0.96	0.18	43,43,43,43	0
56	MG	B0	102	1/1	0.96	0.12	68,68,68,68	0
56	MG	DA	3517	1/1	0.96	0.10	47,47,47,47	0
56	MG	AA	3133	1/1	0.96	0.23	30,30,30,30	0
56	MG	DA	3519	1/1	0.96	0.17	24,24,24,24	0
56	MG	BA	3389	1/1	0.96	0.28	37,37,37,37	0
56	MG	DA	3522	1/1	0.96	0.29	25,25,25,25	0
56	MG	DA	3284	1/1	0.96	0.18	40,40,40,40	0
56	MG	BA	3006	1/1	0.96	0.15	52,52,52,52	0
56	MG	BA	3573	1/1	0.96	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3473	1/1	0.96	0.28	57,57,57,57	0
56	MG	B3	103	1/1	0.96	0.07	45,45,45,45	0
56	MG	DA	3289	1/1	0.96	0.36	42,42,42,42	0
56	MG	AA	3001	1/1	0.96	0.18	34,34,34,34	0
56	MG	B5	101	1/1	0.96	0.14	31,31,31,31	0
56	MG	CA	3130	1/1	0.96	0.12	60,60,60,60	0
56	MG	BA	3684	1/1	0.96	0.20	49,49,49,49	0
56	MG	DA	3298	1/1	0.96	0.17	33,33,33,33	0
56	MG	DA	3299	1/1	0.96	0.24	43,43,43,43	0
56	MG	AA	3025	1/1	0.96	0.12	43,43,43,43	0
56	MG	AA	3146	1/1	0.96	0.11	53,53,53,53	0
56	MG	CA	3135	1/1	0.96	0.11	53,53,53,53	0
56	MG	AA	3104	1/1	0.96	0.20	50,50,50,50	0
56	MG	BA	3397	1/1	0.96	0.23	53,53,53,53	0
56	MG	BA	3398	1/1	0.96	0.20	42,42,42,42	0
56	MG	DA	3307	1/1	0.96	0.08	45,45,45,45	0
56	MG	AA	3006	1/1	0.96	0.14	37,37,37,37	0
56	MG	CA	3141	1/1	0.96	0.17	49,49,49,49	0
56	MG	BA	3258	1/1	0.96	0.28	41,41,41,41	0
56	MG	BA	3146	1/1	0.96	0.19	42,42,42,42	0
56	MG	DA	3315	1/1	0.96	0.17	41,41,41,41	0
56	MG	BA	3147	1/1	0.96	0.13	30,30,30,30	0
56	MG	BA	3148	1/1	0.96	0.27	15,15,15,15	0
56	MG	AA	3177	1/1	0.96	0.14	57,57,57,57	0
56	MG	DA	3558	1/1	0.96	0.25	34,34,34,34	0
56	MG	BA	3490	1/1	0.96	0.22	44,44,44,44	0
56	MG	BA	3325	1/1	0.96	0.28	56,56,56,56	0
56	MG	AE	3001	1/1	0.96	0.06	66,66,66,66	0
56	MG	DA	3128	1/1	0.96	0.07	45,45,45,45	0
56	MG	DA	3129	1/1	0.96	0.12	45,45,45,45	0
56	MG	CA	3009	1/1	0.96	0.22	50,50,50,50	0
56	MG	BA	3103	1/1	0.96	0.33	48,48,48,48	0
56	MG	AA	3060	1/1	0.96	0.21	59,59,59,59	0
56	MG	BA	3498	1/1	0.96	0.07	54,54,54,54	0
56	MG	DA	3332	1/1	0.96	0.20	41,41,41,41	0
56	MG	CA	3155	1/1	0.96	0.14	50,50,50,50	0
56	MG	CA	3156	1/1	0.96	0.10	68,68,68,68	0
56	MG	DA	3136	1/1	0.96	0.22	44,44,44,44	0
56	MG	DA	3576	1/1	0.96	0.16	37,37,37,37	0
56	MG	BA	3826	1/1	0.96	0.22	33,33,33,33	0
56	MG	DA	3341	1/1	0.96	0.21	31,31,31,31	0
56	MG	DA	3579	1/1	0.96	0.07	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3208	1/1	0.96	0.32	48,48,48,48	0
56	MG	BA	3596	1/1	0.96	0.32	45,45,45,45	0
56	MG	BA	3209	1/1	0.96	0.12	41,41,41,41	0
56	MG	AA	3007	1/1	0.96	0.26	65,65,65,65	0
56	MG	DA	3349	1/1	0.96	0.11	44,44,44,44	0
56	MG	CA	3163	1/1	0.96	0.17	53,53,53,53	0
56	MG	DA	3352	1/1	0.96	0.15	35,35,35,35	0
56	MG	DA	3143	1/1	0.96	0.23	50,50,50,50	0
56	MG	DA	3590	1/1	0.96	0.19	60,60,60,60	0
56	MG	BA	3338	1/1	0.96	0.16	41,41,41,41	0
56	MG	AM	201	1/1	0.96	0.05	50,50,50,50	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	BA	3710	1/1	0.96	0.19	28,28,28,28	0
56	MG	BA	3417	1/1	0.96	0.22	33,33,33,33	0
56	MG	BA	3215	1/1	0.96	0.30	45,45,45,45	0
56	MG	BA	3713	1/1	0.96	0.23	54,54,54,54	0
56	MG	DA	3364	1/1	0.96	0.14	38,38,38,38	0
56	MG	DA	3151	1/1	0.96	0.26	44,44,44,44	0
56	MG	AX	3011	1/1	0.96	0.16	50,50,50,50	0
56	MG	DA	3153	1/1	0.96	0.15	44,44,44,44	0
56	MG	BA	3507	1/1	0.96	0.12	39,39,39,39	0
56	MG	BA	3159	1/1	0.96	0.22	30,30,30,30	0
56	MG	CA	3174	1/1	0.96	0.25	46,46,46,46	0
56	MG	BA	3161	1/1	0.96	0.23	37,37,37,37	0
56	MG	DA	3373	1/1	0.96	0.10	31,31,31,31	0
56	MG	AA	3121	1/1	0.96	0.15	66,66,66,66	0
56	MG	BA	3612	1/1	0.96	0.10	62,62,62,62	0
56	MG	CE	201	1/1	0.96	0.19	50,50,50,50	0
56	MG	BA	3025	1/1	0.96	0.15	38,38,38,38	0
56	MG	DA	3164	1/1	0.96	0.26	33,33,33,33	0
56	MG	DA	3166	1/1	0.96	0.17	46,46,46,46	0
56	MG	BA	3068	1/1	0.96	0.26	51,51,51,51	0
56	MG	BA	3515	1/1	0.96	0.21	20,20,20,20	0
56	MG	BA	3167	1/1	0.96	0.19	50,50,50,50	0
56	MG	BA	3349	1/1	0.96	0.19	34,34,34,34	0
56	MG	DA	3386	1/1	0.96	0.17	48,48,48,48	0
56	MG	BA	3027	1/1	0.96	0.20	42,42,42,42	0
56	MG	BB	3014	1/1	0.96	0.14	69,69,69,69	0
56	MG	BA	3073	1/1	0.96	0.17	41,41,41,41	0
56	MG	DA	3627	1/1	0.96	0.04	48,48,48,48	0
56	MG	DA	3177	1/1	0.96	0.17	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3629	1/1	0.96	0.22	52,52,52,52	0
56	MG	CX	3003	1/1	0.96	0.38	50,50,50,50	0
56	MG	BA	3521	1/1	0.96	0.13	36,36,36,36	0
56	MG	BA	3075	1/1	0.96	0.20	27,27,27,27	0
56	MG	AX	3013	1/1	0.96	0.30	39,39,39,39	0
56	MG	CY	3001	1/1	0.96	0.27	58,58,58,58	0
56	MG	BA	3285	1/1	0.96	0.37	49,49,49,49	0
56	MG	BA	3733	1/1	0.96	0.26	41,41,41,41	0
56	MG	DA	3004	1/1	0.96	0.19	42,42,42,42	0
56	MG	CA	3048	1/1	0.96	0.27	52,52,52,52	0
56	MG	BA	3627	1/1	0.96	0.17	45,45,45,45	0
56	MG	BD	305	1/1	0.96	0.14	37,37,37,37	0
56	MG	DA	3010	1/1	0.96	0.07	43,43,43,43	0
56	MG	AY	3001	1/1	0.96	0.31	70,70,70,70	0
56	MG	AA	3182	1/1	0.96	0.20	52,52,52,52	0
56	MG	DA	3193	1/1	0.96	0.33	40,40,40,40	0
56	MG	DA	3016	1/1	0.96	0.12	53,53,53,53	0
56	MG	BA	3630	1/1	0.96	0.08	30,30,30,30	0
56	MG	DA	3411	1/1	0.96	0.17	46,46,46,46	0
56	MG	DA	3412	1/1	0.96	0.16	63,63,63,63	0
56	MG	BD	311	1/1	0.96	0.21	51,51,51,51	0
56	MG	BA	3176	1/1	0.96	0.29	55,55,55,55	0
56	MG	DA	3658	1/1	0.96	0.39	37,37,37,37	0
56	MG	DA	3198	1/1	0.96	0.08	51,51,51,51	0
56	MG	DA	3416	1/1	0.96	0.34	40,40,40,40	0
56	MG	DA	3662	1/1	0.96	0.09	27,27,27,27	0
56	MG	CA	3057	1/1	0.96	0.17	58,58,58,58	0
56	MG	BE	303	1/1	0.96	0.16	27,27,27,27	0
56	MG	BA	3082	1/1	0.96	0.11	59,59,59,59	0
56	MG	DA	3666	1/1	0.96	0.22	41,41,41,41	0
56	MG	AA	3217	1/1	0.96	0.16	55,55,55,55	0
56	MG	DA	3421	1/1	0.96	0.21	53,53,53,53	0
56	MG	CA	3062	1/1	0.96	0.23	44,44,44,44	0
56	MG	BA	3084	1/1	0.96	0.18	45,45,45,45	0
56	MG	BA	3744	1/1	0.96	0.13	20,20,20,20	0
56	MG	BE	308	1/1	0.96	0.17	21,21,21,21	0
56	MG	BA	3085	1/1	0.96	0.13	31,31,31,31	0
56	MG	DB	3001	1/1	0.96	0.04	73,73,73,73	0
56	MG	DA	3431	1/1	0.96	0.17	25,25,25,25	0
56	MG	BF	302	1/1	0.96	0.22	39,39,39,39	0
56	MG	BA	3746	1/1	0.96	0.33	25,25,25,25	0
56	MG	BA	3086	1/1	0.96	0.28	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3534	1/1	0.96	0.30	31,31,31,31	0
56	MG	BA	3239	1/1	0.96	0.15	31,31,31,31	0
56	MG	AA	3168	1/1	0.96	0.08	62,62,62,62	0
56	MG	DB	3009	1/1	0.96	0.19	47,47,47,47	0
56	MG	DA	3217	1/1	0.96	0.14	50,50,50,50	0
56	MG	BA	3538	1/1	0.96	0.20	45,45,45,45	0
56	MG	BF	312	1/1	0.96	0.14	47,47,47,47	0
56	MG	BA	3643	1/1	0.96	0.20	30,30,30,30	0
56	MG	CA	3079	1/1	0.96	0.15	54,54,54,54	0
56	MG	BA	3297	1/1	0.96	0.55	55,55,55,55	0
56	MG	DA	3450	1/1	0.96	0.16	36,36,36,36	0
56	MG	BA	3540	1/1	0.96	0.17	44,44,44,44	0
56	MG	DA	3049	1/1	0.96	0.22	24,24,24,24	0
56	MG	BA	3755	1/1	0.96	0.19	52,52,52,52	0
56	MG	DA	3230	1/1	0.96	0.15	33,33,33,33	0
56	MG	DA	3455	1/1	0.96	0.18	27,27,27,27	0
56	MG	BA	3541	1/1	0.96	0.14	29,29,29,29	0
56	MG	DF	304	1/1	0.96	0.22	39,39,39,39	0
56	MG	DF	305	1/1	0.96	0.17	43,43,43,43	0
56	MG	BA	3184	1/1	0.96	0.12	30,30,30,30	0
56	MG	BP	201	1/1	0.96	0.39	41,41,41,41	0
56	MG	BA	3299	1/1	0.96	0.15	32,32,32,32	0
56	MG	BA	3242	1/1	0.96	0.33	42,42,42,42	0
56	MG	DA	3463	1/1	0.96	0.15	37,37,37,37	0
56	MG	BQ	3001	1/1	0.96	0.23	40,40,40,40	0
56	MG	DV	3003	1/1	0.96	0.12	52,52,52,52	0
56	MG	BA	3301	1/1	0.96	0.14	26,26,26,26	0
56	MG	CA	3093	1/1	0.96	0.17	34,34,34,34	0
56	MG	DW	3003	1/1	0.96	0.34	47,47,47,47	0
56	MG	DA	3062	1/1	0.96	0.18	53,53,53,53	0
56	MG	BA	3452	1/1	0.96	0.30	27,27,27,27	0
56	MG	DA	3471	1/1	0.96	0.15	50,50,50,50	0
56	MG	DA	3472	1/1	0.96	0.06	33,33,33,33	0
56	MG	AA	3203	1/1	0.96	0.34	57,57,57,57	0
56	MG	CA	3096	1/1	0.96	0.15	61,61,61,61	0
56	MG	BA	3764	1/1	0.96	0.12	58,58,58,58	0
56	MG	BA	3552	1/1	0.96	0.26	34,34,34,34	0
56	MG	BA	3660	1/1	0.96	0.18	51,51,51,51	0
56	MG	DA	3481	1/1	0.96	0.18	30,30,30,30	0
59	ZN	D6	501	1/1	0.96	0.11	73,73,73,73	0
56	MG	BA	3038	1/1	0.96	0.30	47,47,47,47	0
56	MG	BA	3245	1/1	0.96	0.28	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3120	1/1	0.97	0.19	45,45,45,45	0
56	MG	BA	3816	1/1	0.97	0.19	21,21,21,21	0
56	MG	BA	3331	1/1	0.97	0.14	32,32,32,32	0
56	MG	BA	3495	1/1	0.97	0.24	34,34,34,34	0
56	MG	DA	3124	1/1	0.97	0.19	34,34,34,34	0
56	MG	DA	3510	1/1	0.97	0.24	50,50,50,50	0
56	MG	CA	3008	1/1	0.97	0.12	50,50,50,50	0
56	MG	BA	3497	1/1	0.97	0.21	41,41,41,41	0
56	MG	DA	3308	1/1	0.97	0.16	45,45,45,45	0
56	MG	BA	3822	1/1	0.97	0.20	21,21,21,21	0
56	MG	BA	3823	1/1	0.97	0.08	53,53,53,53	0
56	MG	BA	3824	1/1	0.97	0.12	43,43,43,43	0
56	MG	CA	3158	1/1	0.97	0.19	53,53,53,53	0
56	MG	DA	3313	1/1	0.97	0.20	23,23,23,23	0
56	MG	DA	3314	1/1	0.97	0.18	33,33,33,33	0
56	MG	DA	3520	1/1	0.97	0.05	48,48,48,48	0
56	MG	BA	3332	1/1	0.97	0.17	30,30,30,30	0
56	MG	DA	3317	1/1	0.97	0.15	55,55,55,55	0
56	MG	BA	3591	1/1	0.97	0.21	23,23,23,23	0
56	MG	BA	3044	1/1	0.97	0.25	49,49,49,49	0
56	MG	BA	3335	1/1	0.97	0.17	50,50,50,50	0
56	MG	BA	3336	1/1	0.97	0.13	35,35,35,35	0
56	MG	DA	3528	1/1	0.97	0.09	57,57,57,57	0
56	MG	DA	3322	1/1	0.97	0.29	43,43,43,43	0
56	MG	DA	3530	1/1	0.97	0.23	55,55,55,55	0
56	MG	BA	3010	1/1	0.97	0.13	29,29,29,29	0
56	MG	DA	3532	1/1	0.97	0.14	57,57,57,57	0
56	MG	BA	3415	1/1	0.97	0.20	29,29,29,29	0
56	MG	AA	3164	1/1	0.97	0.24	50,50,50,50	0
56	MG	BA	3048	1/1	0.97	0.25	28,28,28,28	0
56	MG	BA	3340	1/1	0.97	0.13	45,45,45,45	0
56	MG	BA	3836	1/1	0.97	0.29	45,45,45,45	0
56	MG	BA	3012	1/1	0.97	0.21	26,26,26,26	0
56	MG	BA	3421	1/1	0.97	0.22	33,33,33,33	0
56	MG	BA	3013	1/1	0.97	0.28	34,34,34,34	0
56	MG	BA	3211	1/1	0.97	0.28	36,36,36,36	0
56	MG	DA	3334	1/1	0.97	0.17	32,32,32,32	0
56	MG	DA	3543	1/1	0.97	0.23	55,55,55,55	0
56	MG	AA	3037	1/1	0.97	0.24	44,44,44,44	0
56	MG	DA	3336	1/1	0.97	0.09	47,47,47,47	0
56	MG	BA	3513	1/1	0.97	0.15	34,34,34,34	0
56	MG	BA	3607	1/1	0.97	0.26	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3340	1/1	0.97	0.21	42,42,42,42	0
56	MG	BA	3054	1/1	0.97	0.17	30,30,30,30	0
56	MG	BB	3006	1/1	0.97	0.14	38,38,38,38	0
56	MG	DA	3552	1/1	0.97	0.07	43,43,43,43	0
56	MG	BB	3007	1/1	0.97	0.09	36,36,36,36	0
56	MG	DA	3344	1/1	0.97	0.09	44,44,44,44	0
56	MG	DA	3345	1/1	0.97	0.18	35,35,35,35	0
56	MG	DA	3346	1/1	0.97	0.15	35,35,35,35	0
56	MG	BA	3610	1/1	0.97	0.16	64,64,64,64	0
56	MG	AA	3088	1/1	0.97	0.30	56,56,56,56	0
56	MG	BA	3056	1/1	0.97	0.28	33,33,33,33	0
56	MG	BA	3217	1/1	0.97	0.21	20,20,20,20	0
56	MG	BA	3518	1/1	0.97	0.20	43,43,43,43	0
56	MG	BA	3615	1/1	0.97	0.28	35,35,35,35	0
56	MG	BA	3154	1/1	0.97	0.28	29,29,29,29	0
56	MG	CA	3042	1/1	0.97	0.12	58,58,58,58	0
56	MG	BA	3155	1/1	0.97	0.12	54,54,54,54	0
56	MG	CA	3045	1/1	0.97	0.36	58,58,58,58	0
56	MG	AA	3179	1/1	0.97	0.35	79,79,79,79	0
56	MG	DA	3570	1/1	0.97	0.10	49,49,49,49	0
56	MG	DA	3571	1/1	0.97	0.16	57,57,57,57	0
56	MG	AA	3196	1/1	0.97	0.13	32,32,32,32	0
56	MG	DA	3573	1/1	0.97	0.31	46,46,46,46	0
56	MG	AA	3167	1/1	0.97	0.21	47,47,47,47	0
56	MG	CA	3050	1/1	0.97	0.14	60,60,60,60	0
56	MG	DA	3003	1/1	0.97	0.26	20,20,20,20	0
56	MG	AA	3214	1/1	0.97	0.15	44,44,44,44	0
56	MG	BA	3525	1/1	0.97	0.18	52,52,52,52	0
56	MG	DA	3006	1/1	0.97	0.15	43,43,43,43	0
56	MG	DA	3175	1/1	0.97	0.08	53,53,53,53	0
56	MG	BB	3023	1/1	0.97	0.11	46,46,46,46	0
56	MG	DA	3582	1/1	0.97	0.11	39,39,39,39	0
56	MG	DA	3371	1/1	0.97	0.17	55,55,55,55	0
56	MG	BA	3624	1/1	0.97	0.18	29,29,29,29	0
56	MG	DA	3009	1/1	0.97	0.19	38,38,38,38	0
56	MG	BD	302	1/1	0.97	0.16	23,23,23,23	0
56	MG	DA	3012	1/1	0.97	0.18	39,39,39,39	0
56	MG	DA	3588	1/1	0.97	0.16	39,39,39,39	0
56	MG	BD	304	1/1	0.97	0.20	48,48,48,48	0
56	MG	BA	3108	1/1	0.97	0.19	24,24,24,24	0
56	MG	BA	3737	1/1	0.97	0.11	36,36,36,36	0
56	MG	AA	3013	1/1	0.97	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3070	1/1	0.97	0.23	49,49,49,49	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	DA	3022	1/1	0.97	0.21	40,40,40,40	0
56	MG	BE	301	1/1	0.97	0.20	23,23,23,23	0
56	MG	DA	3385	1/1	0.97	0.14	55,55,55,55	0
56	MG	DA	3599	1/1	0.97	0.24	38,38,38,38	0
56	MG	DA	3189	1/1	0.97	0.25	48,48,48,48	0
56	MG	DA	3024	1/1	0.97	0.44	40,40,40,40	0
56	MG	BA	3166	1/1	0.97	0.22	40,40,40,40	0
56	MG	BA	3111	1/1	0.97	0.23	47,47,47,47	0
56	MG	DA	3392	1/1	0.97	0.15	36,36,36,36	0
56	MG	BA	3363	1/1	0.97	0.19	50,50,50,50	0
56	MG	BA	3443	1/1	0.97	0.12	25,25,25,25	0
56	MG	BA	3168	1/1	0.97	0.19	27,27,27,27	0
56	MG	BA	3535	1/1	0.97	0.25	18,18,18,18	0
56	MG	AA	3200	1/1	0.97	0.22	45,45,45,45	0
56	MG	BA	3234	1/1	0.97	0.25	48,48,48,48	0
56	MG	BA	3024	1/1	0.97	0.27	22,22,22,22	0
56	MG	DA	3200	1/1	0.97	0.35	43,43,43,43	0
56	MG	AA	3201	1/1	0.97	0.07	59,59,59,59	0
56	MG	BA	3026	1/1	0.97	0.14	19,19,19,19	0
56	MG	BA	3450	1/1	0.97	0.28	34,34,34,34	0
56	MG	DA	3038	1/1	0.97	0.43	47,47,47,47	0
56	MG	CA	3078	1/1	0.97	0.16	48,48,48,48	0
56	MG	BA	3372	1/1	0.97	0.22	24,24,24,24	0
56	MG	DA	3207	1/1	0.97	0.29	57,57,57,57	0
56	MG	DA	3622	1/1	0.97	0.18	53,53,53,53	0
56	MG	BA	3644	1/1	0.97	0.10	36,36,36,36	0
56	MG	DA	3624	1/1	0.97	0.07	47,47,47,47	0
56	MG	BA	3373	1/1	0.97	0.18	38,38,38,38	0
56	MG	AA	3063	1/1	0.97	0.07	63,63,63,63	0
56	MG	BG	201	1/1	0.97	0.09	57,57,57,57	0
56	MG	DA	3045	1/1	0.97	0.12	47,47,47,47	0
56	MG	BA	3069	1/1	0.97	0.14	31,31,31,31	0
56	MG	DA	3047	1/1	0.97	0.21	49,49,49,49	0
56	MG	BA	3546	1/1	0.97	0.26	30,30,30,30	0
56	MG	BA	3547	1/1	0.97	0.19	41,41,41,41	0
56	MG	BA	3118	1/1	0.97	0.34	38,38,38,38	0
56	MG	CA	3089	1/1	0.97	0.07	58,58,58,58	0
56	MG	BA	3653	1/1	0.97	0.28	49,49,49,49	0
56	MG	BA	3549	1/1	0.97	0.19	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3055	1/1	0.97	0.24	36,36,36,36	0
56	MG	DA	3056	1/1	0.97	0.25	44,44,44,44	0
56	MG	BA	3303	1/1	0.97	0.17	35,35,35,35	0
56	MG	BA	3656	1/1	0.97	0.18	45,45,45,45	0
56	MG	DA	3425	1/1	0.97	0.07	45,45,45,45	0
56	MG	BA	3551	1/1	0.97	0.19	33,33,33,33	0
56	MG	DA	3644	1/1	0.97	0.49	55,55,55,55	0
56	MG	DA	3427	1/1	0.97	0.08	38,38,38,38	0
56	MG	DA	3428	1/1	0.97	0.10	61,61,61,61	0
56	MG	BA	3767	1/1	0.97	0.11	29,29,29,29	0
56	MG	BA	3119	1/1	0.97	0.19	36,36,36,36	0
56	MG	BA	3178	1/1	0.97	0.25	38,38,38,38	0
56	MG	DA	3651	1/1	0.97	0.16	47,47,47,47	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	3435	1/1	0.97	0.16	44,44,44,44	0
56	MG	BA	3121	1/1	0.97	0.36	41,41,41,41	0
56	MG	BA	3556	1/1	0.97	0.11	45,45,45,45	0
56	MG	DA	3237	1/1	0.97	0.07	51,51,51,51	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	BA	3776	1/1	0.97	0.14	49,49,49,49	0
56	MG	BR	204	1/1	0.97	0.36	42,42,42,42	0
56	MG	BR	205	1/1	0.97	0.15	29,29,29,29	0
56	MG	DA	3071	1/1	0.97	0.37	44,44,44,44	0
56	MG	DA	3446	1/1	0.97	0.32	47,47,47,47	0
56	MG	DA	3447	1/1	0.97	0.27	35,35,35,35	0
56	MG	DA	3668	1/1	0.97	0.15	79,79,79,79	0
56	MG	BA	3122	1/1	0.97	0.18	26,26,26,26	0
56	MG	CA	3108	1/1	0.97	0.14	51,51,51,51	0
56	MG	BA	3465	1/1	0.97	0.19	42,42,42,42	0
56	MG	BA	3384	1/1	0.97	0.23	30,30,30,30	0
56	MG	BA	3781	1/1	0.97	0.21	52,52,52,52	0
56	MG	BA	3123	1/1	0.97	0.16	35,35,35,35	0
56	MG	DA	3249	1/1	0.97	0.27	41,41,41,41	0
56	MG	BA	3561	1/1	0.97	0.15	27,27,27,27	0
56	MG	DA	3456	1/1	0.97	0.20	49,49,49,49	0
56	MG	BA	3072	1/1	0.97	0.14	30,30,30,30	0
56	MG	DA	3253	1/1	0.97	0.22	38,38,38,38	0
56	MG	DA	3459	1/1	0.97	0.07	57,57,57,57	0
56	MG	BA	3029	1/1	0.97	0.31	46,46,46,46	0
56	MG	BA	3074	1/1	0.97	0.24	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3565	1/1	0.97	0.24	42,42,42,42	0
56	MG	AA	3172	1/1	0.97	0.16	47,47,47,47	0
56	MG	BA	3076	1/1	0.97	0.29	23,23,23,23	0
56	MG	DD	301	1/1	0.97	0.37	39,39,39,39	0
56	MG	BA	3391	1/1	0.97	0.14	41,41,41,41	0
56	MG	BA	3678	1/1	0.97	0.22	58,58,58,58	0
56	MG	AA	3123	1/1	0.97	0.17	57,57,57,57	0
56	MG	DA	3469	1/1	0.97	0.13	54,54,54,54	0
56	MG	B0	103	1/1	0.97	0.06	54,54,54,54	0
56	MG	BA	3793	1/1	0.97	0.20	38,38,38,38	0
56	MG	BA	3032	1/1	0.97	0.21	38,38,38,38	0
56	MG	BA	3795	1/1	0.97	0.16	53,53,53,53	0
56	MG	CA	3127	1/1	0.97	0.17	44,44,44,44	0
56	MG	AW	3007	1/1	0.97	0.05	64,64,64,64	0
56	MG	BA	3395	1/1	0.97	0.19	44,44,44,44	0
56	MG	DA	3479	1/1	0.97	0.17	50,50,50,50	0
56	MG	AA	3076	1/1	0.97	0.17	55,55,55,55	0
56	MG	DG	3001	1/1	0.97	0.04	56,56,56,56	0
56	MG	CA	3131	1/1	0.97	0.18	55,55,55,55	0
56	MG	DQ	3001	1/1	0.97	0.11	48,48,48,48	0
56	MG	DQ	3002	1/1	0.97	0.17	42,42,42,42	0
56	MG	BA	3319	1/1	0.97	0.29	20,20,20,20	0
56	MG	BA	3195	1/1	0.97	0.27	50,50,50,50	0
56	MG	DU	3001	1/1	0.97	0.25	50,50,50,50	0
56	MG	DA	3275	1/1	0.97	0.09	52,52,52,52	0
56	MG	BA	3035	1/1	0.97	0.14	31,31,31,31	0
56	MG	BA	3036	1/1	0.97	0.18	26,26,26,26	0
56	MG	AA	3117	1/1	0.97	0.16	48,48,48,48	0
56	MG	AA	3227	1/1	0.97	0.18	48,48,48,48	0
56	MG	BA	3806	1/1	0.97	0.17	51,51,51,51	0
56	MG	BA	3489	1/1	0.97	0.11	44,44,44,44	0
56	MG	DY	502	1/1	0.97	0.12	52,52,52,52	0
56	MG	BA	3087	1/1	0.97	0.12	37,37,37,37	0
56	MG	B8	102	1/1	0.97	0.08	50,50,50,50	0
56	MG	DA	3108	1/1	0.97	0.22	30,30,30,30	0
56	MG	D7	102	1/1	0.97	0.22	43,43,43,43	0
56	MG	B8	103	1/1	0.97	0.22	48,48,48,48	0
56	MG	BA	3009	1/1	0.97	0.17	25,25,25,25	0
56	MG	BA	3811	1/1	0.97	0.31	38,38,38,38	0
56	MG	DA	3290	1/1	0.97	0.17	44,44,44,44	0
56	MG	DA	3113	1/1	0.97	0.29	44,44,44,44	0
56	MG	DA	3114	1/1	0.97	0.13	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	BA	3694	1/1	0.97	0.23	27,27,27,27	0
56	MG	BA	3042	1/1	0.97	0.18	40,40,40,40	0
56	MG	DA	3118	1/1	0.97	0.25	52,52,52,52	0
60	K	AX	3001	1/1	0.97	0.22	57,57,57,57	0
56	MG	BA	3043	1/1	0.97	0.30	39,39,39,39	0
56	MG	BA	3466	1/1	0.98	0.17	28,28,28,28	0
56	MG	CA	3138	1/1	0.98	0.14	59,59,59,59	0
56	MG	BA	3282	1/1	0.98	0.30	24,24,24,24	0
56	MG	DA	3473	1/1	0.98	0.06	49,49,49,49	0
56	MG	AA	3195	1/1	0.98	0.15	59,59,59,59	0
56	MG	BA	3780	1/1	0.98	0.12	41,41,41,41	0
56	MG	DA	3476	1/1	0.98	0.24	45,45,45,45	0
56	MG	BA	3091	1/1	0.98	0.32	38,38,38,38	0
56	MG	BA	3128	1/1	0.98	0.24	27,27,27,27	0
56	MG	DA	3356	1/1	0.98	0.26	20,20,20,20	0
56	MG	CA	3144	1/1	0.98	0.18	59,59,59,59	0
56	MG	DA	3608	1/1	0.98	0.13	53,53,53,53	0
56	MG	BA	3664	1/1	0.98	0.14	43,43,43,43	0
56	MG	DA	3482	1/1	0.98	0.17	50,50,50,50	0
56	MG	AA	3065	1/1	0.98	0.17	58,58,58,58	0
56	MG	CA	3058	1/1	0.98	0.14	70,70,70,70	0
56	MG	DA	3361	1/1	0.98	0.36	55,55,55,55	0
56	MG	BA	3226	1/1	0.98	0.24	41,41,41,41	0
56	MG	DA	3363	1/1	0.98	0.38	54,54,54,54	0
56	MG	BA	3353	1/1	0.98	0.10	49,49,49,49	0
56	MG	BA	3288	1/1	0.98	0.38	40,40,40,40	0
56	MG	AA	3229	1/1	0.98	0.35	62,62,62,62	0
56	MG	BB	3017	1/1	0.98	0.20	33,33,33,33	0
56	MG	BA	3476	1/1	0.98	0.21	24,24,24,24	0
56	MG	DA	3252	1/1	0.98	0.20	29,29,29,29	0
56	MG	BA	3321	1/1	0.98	0.08	54,54,54,54	0
56	MG	CA	3066	1/1	0.98	0.14	66,66,66,66	0
56	MG	BA	3174	1/1	0.98	0.16	34,34,34,34	0
56	MG	BA	3730	1/1	0.98	0.13	27,27,27,27	0
56	MG	BA	3479	1/1	0.98	0.14	37,37,37,37	0
56	MG	BA	3078	1/1	0.98	0.19	17,17,17,17	0
56	MG	BA	3675	1/1	0.98	0.17	37,37,37,37	0
56	MG	DA	3261	1/1	0.98	0.07	44,44,44,44	0
56	MG	BA	3735	1/1	0.98	0.14	35,35,35,35	0
56	MG	DA	3064	1/1	0.98	0.10	64,64,64,64	0
56	MG	DA	3158	1/1	0.98	0.26	40,40,40,40	0
56	MG	BD	303	1/1	0.98	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	AA	3131	1/1	0.98	0.32	63,63,63,63	0
56	MG	DA	3161	1/1	0.98	0.20	49,49,49,49	0
56	MG	DA	3637	1/1	0.98	0.06	44,44,44,44	0
56	MG	BA	3572	1/1	0.98	0.27	63,63,63,63	0
56	MG	BA	3080	1/1	0.98	0.10	24,24,24,24	0
56	MG	AA	3154	1/1	0.98	0.14	59,59,59,59	0
56	MG	DA	3165	1/1	0.98	0.29	33,33,33,33	0
56	MG	DA	3388	1/1	0.98	0.14	35,35,35,35	0
56	MG	DA	3389	1/1	0.98	0.06	53,53,53,53	0
56	MG	B7	101	1/1	0.98	0.14	33,33,33,33	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	BA	3801	1/1	0.98	0.10	53,53,53,53	0
56	MG	BA	3018	1/1	0.98	0.25	34,34,34,34	0
56	MG	BA	3157	1/1	0.98	0.17	36,36,36,36	0
56	MG	DA	3171	1/1	0.98	0.28	38,38,38,38	0
56	MG	BA	3265	1/1	0.98	0.27	29,29,29,29	0
56	MG	DA	3173	1/1	0.98	0.17	30,30,30,30	0
56	MG	DA	3653	1/1	0.98	0.15	58,58,58,58	0
56	MG	DA	3281	1/1	0.98	0.23	33,33,33,33	0
56	MG	BA	3487	1/1	0.98	0.24	25,25,25,25	0
56	MG	DA	3524	1/1	0.98	0.06	38,38,38,38	0
56	MG	BA	3330	1/1	0.98	0.17	29,29,29,29	0
56	MG	BA	3405	1/1	0.98	0.18	33,33,33,33	0
56	MG	AA	3193	1/1	0.98	0.09	43,43,43,43	0
56	MG	BA	3809	1/1	0.98	0.14	29,29,29,29	0
56	MG	CA	3091	1/1	0.98	0.15	48,48,48,48	0
56	MG	BA	3632	1/1	0.98	0.17	55,55,55,55	0
56	MG	BA	3369	1/1	0.98	0.17	55,55,55,55	0
56	MG	BA	3041	1/1	0.98	0.25	18,18,18,18	0
56	MG	DA	3291	1/1	0.98	0.18	42,42,42,42	0
56	MG	DA	3292	1/1	0.98	0.12	37,37,37,37	0
56	MG	BF	303	1/1	0.98	0.22	42,42,42,42	0
56	MG	DA	3294	1/1	0.98	0.26	42,42,42,42	0
56	MG	DA	3670	1/1	0.98	0.13	38,38,38,38	0
56	MG	BA	3813	1/1	0.98	0.19	4,4,4,4	0
56	MG	BA	3160	1/1	0.98	0.17	32,32,32,32	0
56	MG	BA	3210	1/1	0.98	0.20	31,31,31,31	0
56	MG	AF	3001	1/1	0.98	0.26	40,40,40,40	0
56	MG	BF	308	1/1	0.98	0.11	36,36,36,36	0
56	MG	BF	309	1/1	0.98	0.16	30,30,30,30	0
56	MG	DA	3301	1/1	0.98	0.23	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3544	1/1	0.98	0.14	37,37,37,37	0
56	MG	BA	3817	1/1	0.98	0.17	47,47,47,47	0
56	MG	BA	3496	1/1	0.98	0.24	39,39,39,39	0
56	MG	BA	3212	1/1	0.98	0.20	42,42,42,42	0
56	MG	BA	3640	1/1	0.98	0.19	39,39,39,39	0
56	MG	CA	3106	1/1	0.98	0.16	50,50,50,50	0
56	MG	BA	3821	1/1	0.98	0.17	50,50,50,50	0
56	MG	BA	3589	1/1	0.98	0.18	17,17,17,17	0
56	MG	BA	3185	1/1	0.98	0.20	32,32,32,32	0
56	MG	BA	3057	1/1	0.98	0.20	53,53,53,53	0
56	MG	DA	3554	1/1	0.98	0.18	23,23,23,23	0
56	MG	BN	3003	1/1	0.98	0.15	38,38,38,38	0
56	MG	DD	304	1/1	0.98	0.39	31,31,31,31	0
56	MG	BN	3004	1/1	0.98	0.20	50,50,50,50	0
56	MG	DA	3430	1/1	0.98	0.21	28,28,28,28	0
56	MG	AA	3224	1/1	0.98	0.15	33,33,33,33	0
56	MG	DA	3104	1/1	0.98	0.15	46,46,46,46	0
56	MG	DA	3560	1/1	0.98	0.19	34,34,34,34	0
56	MG	DA	3433	1/1	0.98	0.20	61,61,61,61	0
56	MG	BA	3142	1/1	0.98	0.14	34,34,34,34	0
56	MG	DA	3316	1/1	0.98	0.06	44,44,44,44	0
56	MG	DA	3011	1/1	0.98	0.09	40,40,40,40	0
56	MG	BA	3646	1/1	0.98	0.19	38,38,38,38	0
56	MG	BA	3104	1/1	0.98	0.19	27,27,27,27	0
56	MG	BA	3418	1/1	0.98	0.16	32,32,32,32	0
56	MG	DA	3015	1/1	0.98	0.26	31,31,31,31	0
56	MG	DO	5001	1/1	0.98	0.16	51,51,51,51	0
56	MG	BA	3830	1/1	0.98	0.18	21,21,21,21	0
56	MG	DA	3112	1/1	0.98	0.26	42,42,42,42	0
56	MG	DA	3444	1/1	0.98	0.18	30,30,30,30	0
56	MG	DQ	3004	1/1	0.98	0.16	51,51,51,51	0
56	MG	BA	3649	1/1	0.98	0.10	43,43,43,43	0
56	MG	AA	3151	1/1	0.98	0.16	41,41,41,41	0
56	MG	BA	3460	1/1	0.98	0.23	35,35,35,35	0
56	MG	DA	3116	1/1	0.98	0.10	57,57,57,57	0
56	MG	DA	3215	1/1	0.98	0.20	37,37,37,37	0
56	MG	DA	3329	1/1	0.98	0.21	29,29,29,29	0
56	MG	BA	3045	1/1	0.98	0.20	42,42,42,42	0
56	MG	BA	3599	1/1	0.98	0.20	23,23,23,23	0
56	MG	DA	3219	1/1	0.98	0.27	54,54,54,54	0
56	MG	BA	3193	1/1	0.98	0.28	57,57,57,57	0
56	MG	BA	3771	1/1	0.98	0.20	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	CA	3039	1/1	0.98	0.23	50,50,50,50	0
56	MG	D3	3001	1/1	0.98	0.16	58,58,58,58	0
56	MG	BA	3772	1/1	0.98	0.17	31,31,31,31	0
56	MG	BA	3383	1/1	0.98	0.23	24,24,24,24	0
56	MG	BA	3107	1/1	0.98	0.19	20,20,20,20	0
56	MG	DA	3339	1/1	0.98	0.10	52,52,52,52	0
56	MG	BU	202	1/1	0.98	0.22	40,40,40,40	0
58	SF4	CD	501	8/8	0.98	0.10	54,64,76,87	0
59	ZN	AN	501	1/1	0.98	0.12	58,58,58,58	0
59	ZN	BY	501	1/1	0.98	0.11	58,58,58,58	0
56	MG	DA	3227	1/1	0.98	0.21	38,38,38,38	0
59	ZN	B6	103	1/1	0.98	0.13	29,29,29,29	0
59	ZN	B9	501	1/1	0.98	0.17	49,49,49,49	0
56	MG	CA	3044	1/1	0.98	0.23	55,55,55,55	0
56	MG	BU	204	1/1	0.98	0.21	38,38,38,38	0
56	MG	DA	3465	1/1	0.98	0.07	55,55,55,55	0
56	MG	BA	3657	1/1	0.98	0.20	47,47,47,47	0
56	MG	CA	3047	1/1	0.98	0.24	35,35,35,35	0
56	MG	BA	3510	1/1	0.98	0.08	48,48,48,48	0
56	MG	BU	207	1/1	0.98	0.14	29,29,29,29	0
56	MG	BA	3355	1/1	0.99	0.15	24,24,24,24	0
56	MG	BA	3759	1/1	0.99	0.15	9,9,9,9	0
56	MG	DA	3050	1/1	0.99	0.23	40,40,40,40	0
56	MG	BA	3129	1/1	0.99	0.22	36,36,36,36	0
56	MG	BA	3458	1/1	0.99	0.25	19,19,19,19	0
56	MG	BU	209	1/1	0.99	0.19	27,27,27,27	0
56	MG	BV	201	1/1	0.99	0.22	29,29,29,29	0
56	MG	BV	202	1/1	0.99	0.13	26,26,26,26	0
56	MG	DA	3017	1/1	0.99	0.21	28,28,28,28	0
56	MG	DA	3254	1/1	0.99	0.25	21,21,21,21	0
56	MG	DA	3018	1/1	0.99	0.18	41,41,41,41	0
56	MG	DA	3656	1/1	0.99	0.17	62,62,62,62	0
56	MG	BA	3440	1/1	0.99	0.27	29,29,29,29	0
56	MG	BA	3621	1/1	0.99	0.23	52,52,52,52	0
56	MG	BV	205	1/1	0.99	0.12	32,32,32,32	0
56	MG	BD	307	1/1	0.99	0.21	35,35,35,35	0
56	MG	DA	3218	1/1	0.99	0.16	47,47,47,47	0
56	MG	BA	3050	1/1	0.99	0.17	31,31,31,31	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	DA	3438	1/1	0.99	0.10	60,60,60,60	0
56	MG	DA	3619	1/1	0.99	0.03	58,58,58,58	0

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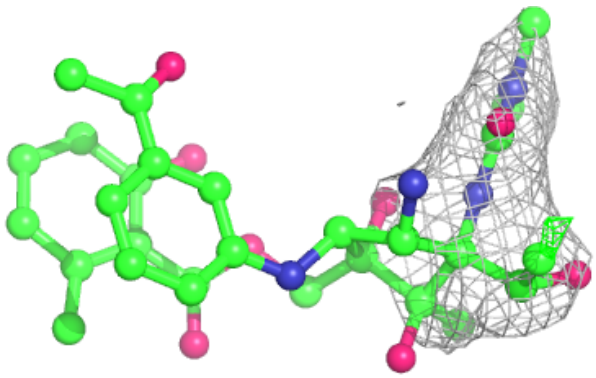
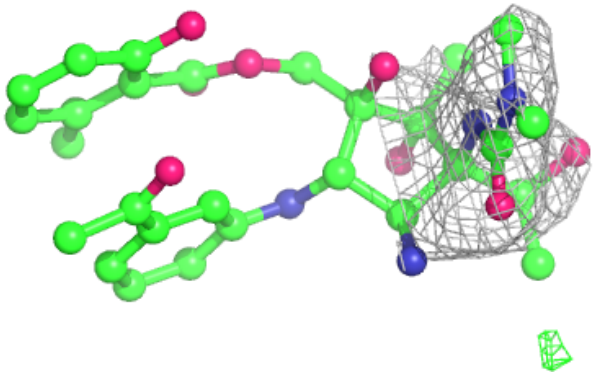
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	DA	3350	1/1	0.99	0.30	29,29,29,29	0
56	MG	BA	3039	1/1	0.99	0.28	47,47,47,47	0
56	MG	BA	3053	1/1	0.99	0.27	22,22,22,22	0
56	MG	CA	3077	1/1	0.99	0.06	48,48,48,48	0
56	MG	AA	3137	1/1	0.99	0.19	42,42,42,42	0
56	MG	BA	3071	1/1	0.99	0.33	42,42,42,42	0
56	MG	BA	3334	1/1	0.99	0.25	30,30,30,30	0
56	MG	DA	3228	1/1	0.99	0.05	42,42,42,42	0
56	MG	BA	3697	1/1	0.99	0.12	35,35,35,35	0
56	MG	AA	3157	1/1	0.99	0.19	46,46,46,46	0
56	MG	BA	3609	1/1	0.99	0.26	20,20,20,20	0
56	MG	BA	3231	1/1	0.99	0.24	37,37,37,37	0
56	MG	DA	3036	1/1	0.99	0.15	29,29,29,29	0
58	SF4	AD	501	8/8	0.99	0.14	56,62,64,76	0
56	MG	AA	3225	1/1	0.99	0.11	26,26,26,26	0
56	MG	BB	3016	1/1	0.99	0.16	43,43,43,43	0
56	MG	BA	3188	1/1	0.99	0.24	19,19,19,19	0
56	MG	CA	3088	1/1	0.99	0.41	53,53,53,53	0
56	MG	DA	3280	1/1	0.99	0.14	43,43,43,43	0
56	MG	BA	3400	1/1	0.99	0.17	25,25,25,25	0
56	MG	BA	3368	1/1	0.99	0.19	12,12,12,12	0
56	MG	BA	3246	1/1	0.99	0.10	27,27,27,27	0
56	MG	BA	3682	1/1	0.99	0.13	50,50,50,50	0
59	ZN	D5	501	1/1	0.99	0.15	53,53,53,53	0
56	MG	BA	3731	1/1	0.99	0.12	23,23,23,23	0
56	MG	BU	203	1/1	0.99	0.14	31,31,31,31	0
56	MG	AA	3186	1/1	0.99	0.16	52,52,52,52	0
56	MG	DD	306	1/1	0.99	0.26	44,44,44,44	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

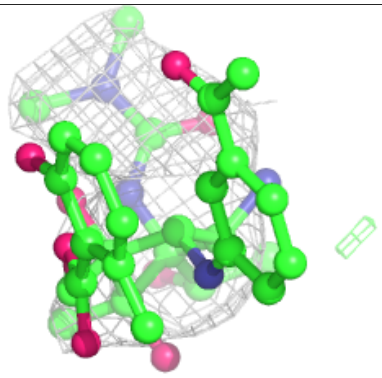
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

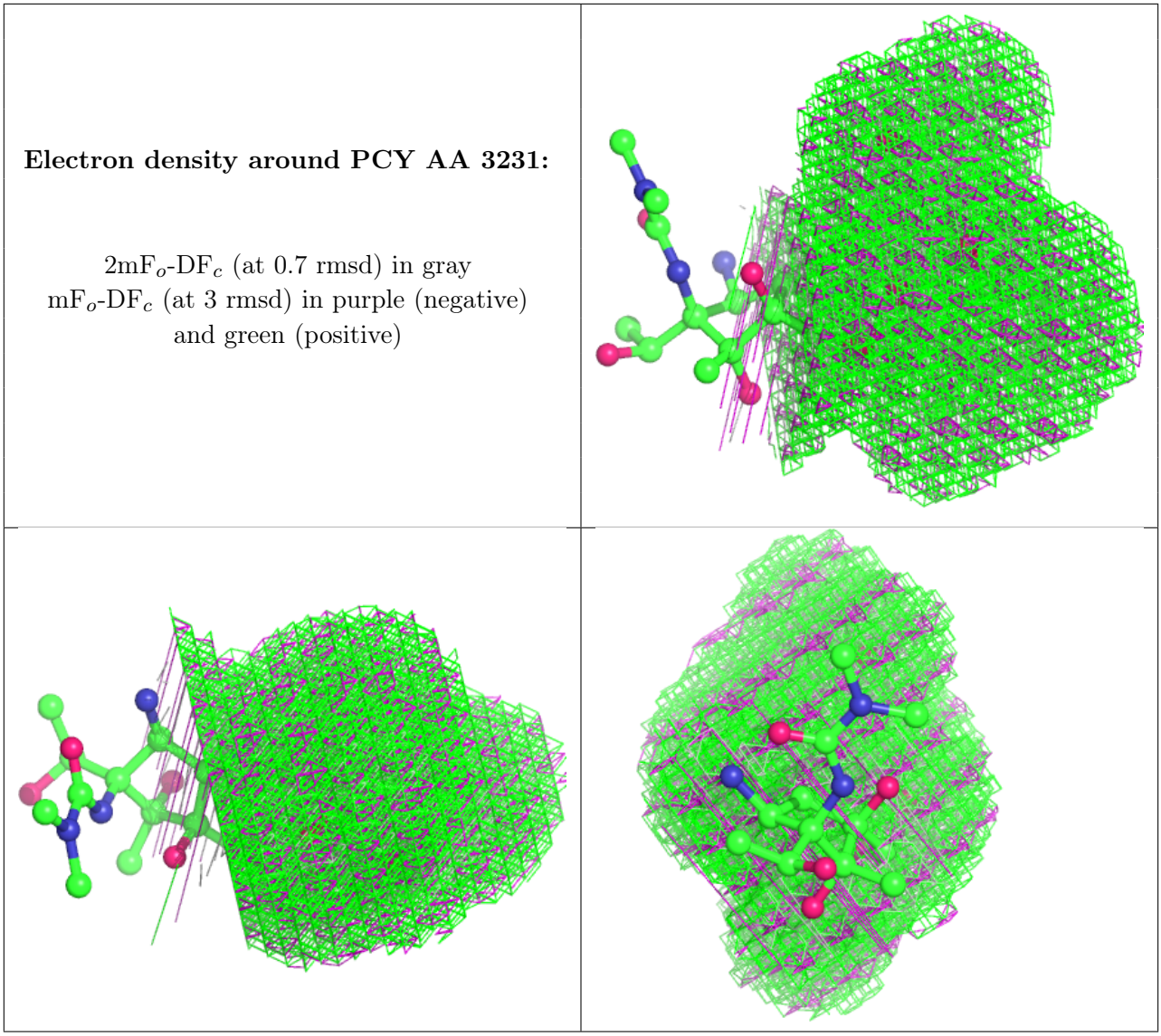






Electron density around PCY AA 3231:

$2mF_o$-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

There are no such residues in this entry.