wwPDB X-ray Structure Validation Summary Report (i)

Feb 20, 2024 – 12:40 AM EST

PDB ID	:	4M83
Title	:	Ensemble refinement of protein crystal structure (2IYF) of macrolide glycosyltransferases OleD complexed with UDP and Erythromycin A
Authors	:	Wang, F.; Helmich, K.E.; Xu, W.; Singh, S.; Olmos Jr., J.L.; Martinez iii, E.; Bingman, C.A.; Thorson, J.S.; Phillips Jr., G.N.; Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on	:	2013-08-12
Resolution	:	1.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

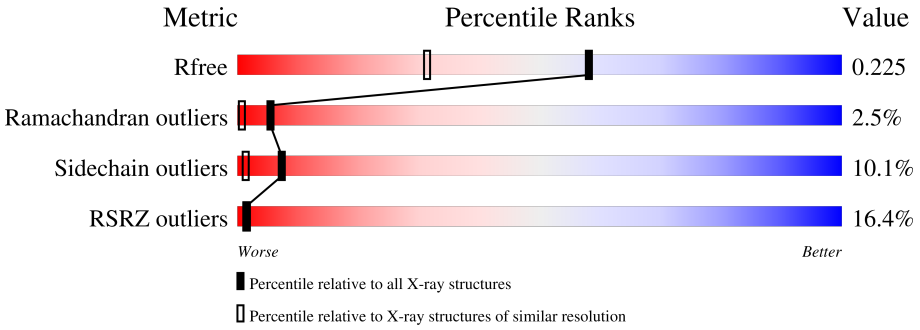
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	1-A	415	15% 84% 10% • 5%
1	1-B	415	16% 87% 8% 5%
1	10-A	415	15% 93% • 5%
1	10-B	415	16% 94% • 5%
1	11-A	415	15% 93% • 5%
1	11-B	415	16% 92% • 5%
1	12-A	415	15% 93% • 5%

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Mol	Chain	Length	Quality of chain
1	12-B	415	16% 91% • 5%
1	13-A	415	15% 93% • 5%
1	13-B	415	16% 93% • 5%
1	14-A	415	15% 92% • 5%
1	14-B	415	16% 93% • 5%
1	15-A	415	15% 91% • 5%
1	15-B	415	16% 91% • 5%
1	16-A	415	15% 93% • 5%
1	16-B	415	16% 93% • 5%
1	17-A	415	15% 93% • 5%
1	17-B	415	16% 93% • 5%
1	18-A	415	15% 92% • 5%
1	18-B	415	16% 94% • 5%
1	19-A	415	15% 92% • 5%
1	19-B	415	16% 93% • 5%
1	2-A	415	15% 93% • 5%
1	2-B	415	16% 92% • 5%
1	20-A	415	15% 92% • 5%
1	20-B	415	16% 92% • 5%
1	3-A	415	15% 92% • 5%
1	3-B	415	16% 93% • 5%
1	4-A	415	15% 92% • 5%
1	4-B	415	16% 93% • 5%
1	5-A	415	15% 91% • 5%
1	5-B	415	16% 92% • 5%

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Mol	Chain	Length	Quality of chain
1	6-A	415	15% 93% 5%
1	6-B	415	16% 92% 5%
1	7-A	415	15% 93% 5%
1	7-B	415	16% 92% 5%
1	8-A	415	15% 93% 5%
1	8-B	415	16% 92% 5%
1	9-A	415	15% 92% 5%
1	9-B	415	16% 93% 5%

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
4	MG	1-B	503[A]	-	-	-	X
4	MG	10-B	503[J]	-	-	-	X
4	MG	11-B	503[K]	-	-	-	X
4	MG	12-B	503[L]	-	-	-	X
4	MG	13-B	503[M]	-	-	-	X
4	MG	14-B	503[N]	-	-	-	X
4	MG	15-B	503[O]	-	-	-	X
4	MG	16-B	503[P]	-	-	-	X
4	MG	17-B	503[Q]	-	-	-	X
4	MG	18-B	503[R]	-	-	-	X
4	MG	19-B	503[S]	-	-	-	X
4	MG	2-B	503[B]	-	-	-	X
4	MG	20-B	503[T]	-	-	-	X
4	MG	3-B	503[C]	-	-	-	X
4	MG	4-B	503[D]	-	-	-	X
4	MG	5-B	503[E]	-	-	-	X
4	MG	6-B	503[F]	-	-	-	X
4	MG	7-B	503[G]	-	-	-	X
4	MG	8-B	503[H]	-	-	-	X
4	MG	9-B	503[I]	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 132758 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 protein called Oleandomycin glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	2-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	3-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	4-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	5-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	6-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	7-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	8-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	9-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	10-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	11-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	12-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	13-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	14-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	15-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	16-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	17-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	18-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	19-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	20-A	393	Total	C	N	O	S	0	393	0
			2978	1886	535	550	7			
1	1-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	2-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	3-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	4-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	5-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	6-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	7-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	8-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	9-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	10-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	11-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	12-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	13-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	14-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	15-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	16-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	17-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			

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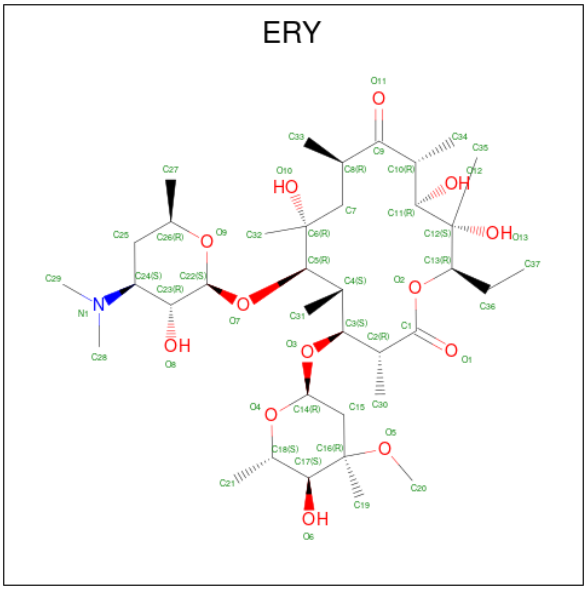
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	18-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	19-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			
1	20-B	394	Total	C	N	O	S	0	394	0
			2996	1902	535	552	7			

- Molecule 2 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	1-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	2-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	3-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	4-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	5-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	6-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	7-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	8-A	1	Total	C	N	O	0	1
			51	37	1	13		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	9-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	10-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	11-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	12-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	13-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	14-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	15-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	16-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	17-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	18-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	19-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	20-A	1	Total	C	N	O	0	1
			51	37	1	13		
2	1-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	2-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	3-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	4-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	5-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	6-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	7-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	8-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	9-B	1	Total	C	N	O	0	1
			51	37	1	13		

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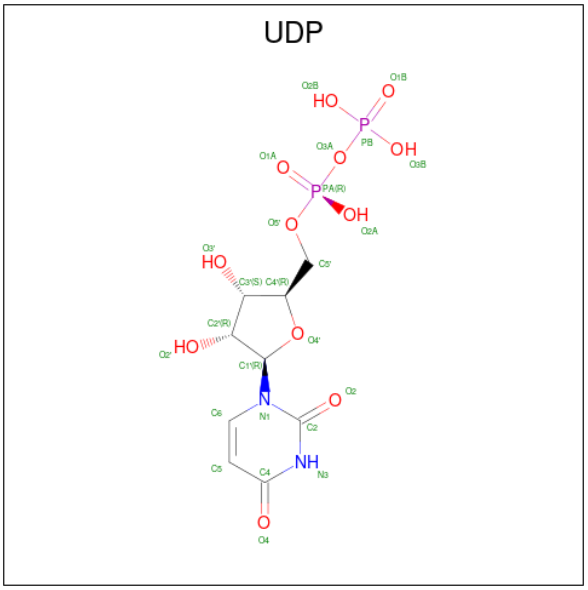
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	10-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	11-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	12-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	13-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	14-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	15-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	16-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	17-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	18-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	19-B	1	Total	C	N	O	0	1
			51	37	1	13		
2	20-B	1	Total	C	N	O	0	1
			51	37	1	13		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	2-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	3-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	4-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	5-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	6-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	7-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	8-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	9-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	10-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	11-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	12-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	13-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	14-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	15-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	16-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	17-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	18-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	19-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	20-A	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	1-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	2-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	3-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	4-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	5-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	6-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	7-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	8-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	9-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	10-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	11-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	12-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	13-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	14-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	15-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	16-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	17-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	18-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	19-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		
3	20-B	1	Total	C	N	O	P	0	1
			25	9	2	12	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-B	1	Total	Mg	0	1
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	2-B	1	Total Mg 1 1	0	1
4	3-B	1	Total Mg 1 1	0	1
4	4-B	1	Total Mg 1 1	0	1
4	5-B	1	Total Mg 1 1	0	1
4	6-B	1	Total Mg 1 1	0	1
4	7-B	1	Total Mg 1 1	0	1
4	8-B	1	Total Mg 1 1	0	1
4	9-B	1	Total Mg 1 1	0	1
4	10-B	1	Total Mg 1 1	0	1
4	11-B	1	Total Mg 1 1	0	1
4	12-B	1	Total Mg 1 1	0	1
4	13-B	1	Total Mg 1 1	0	1
4	14-B	1	Total Mg 1 1	0	1
4	15-B	1	Total Mg 1 1	0	1
4	16-B	1	Total Mg 1 1	0	1
4	17-B	1	Total Mg 1 1	0	1
4	18-B	1	Total Mg 1 1	0	1
4	19-B	1	Total Mg 1 1	0	1
4	20-B	1	Total Mg 1 1	0	1

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-A	271	Total O 271 271	0	271
5	2-A	259	Total O 259 259	0	259
5	3-A	244	Total O 244 244	0	244
5	4-A	267	Total O 267 267	0	267
5	5-A	273	Total O 273 273	0	273
5	6-A	256	Total O 256 256	0	256
5	7-A	271	Total O 271 271	0	271
5	8-A	273	Total O 273 273	0	273
5	9-A	291	Total O 291 291	0	291
5	10-A	243	Total O 243 243	0	243
5	11-A	258	Total O 258 258	0	258
5	12-A	264	Total O 264 264	0	264
5	13-A	281	Total O 281 281	0	281
5	14-A	248	Total O 248 248	0	248
5	15-A	268	Total O 268 268	0	268
5	16-A	253	Total O 253 253	0	253
5	17-A	270	Total O 270 270	0	270
5	18-A	271	Total O 271 271	0	271
5	19-A	249	Total O 249 249	0	249
5	20-A	266	Total O 266 266	0	266
5	1-B	250	Total O 250 250	0	250
5	2-B	242	Total O 242 242	0	242

Continued on next page...

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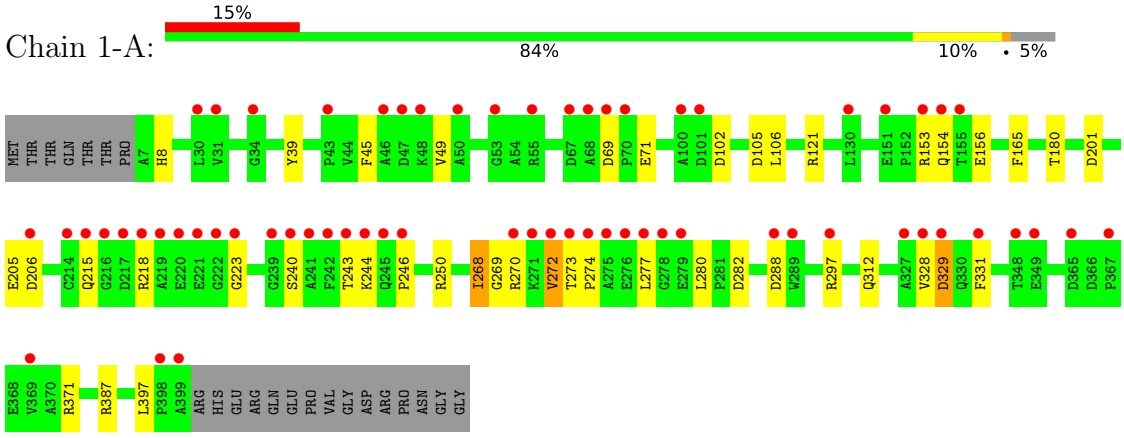
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	3-B	261	Total O 261 261	0	261
5	4-B	250	Total O 250 250	0	250
5	5-B	252	Total O 252 252	0	252
5	6-B	239	Total O 239 239	0	239
5	7-B	256	Total O 256 256	0	256
5	8-B	241	Total O 241 241	0	241
5	9-B	218	Total O 218 218	0	218
5	10-B	256	Total O 256 256	0	256
5	11-B	271	Total O 271 271	0	271
5	12-B	229	Total O 229 229	0	229
5	13-B	261	Total O 261 261	0	261
5	14-B	249	Total O 249 249	0	249
5	15-B	261	Total O 261 261	0	261
5	16-B	240	Total O 240 240	0	240
5	17-B	220	Total O 220 220	0	220
5	18-B	257	Total O 257 257	0	257
5	19-B	245	Total O 245 245	0	245
5	20-B	244	Total O 244 244	0	244

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.

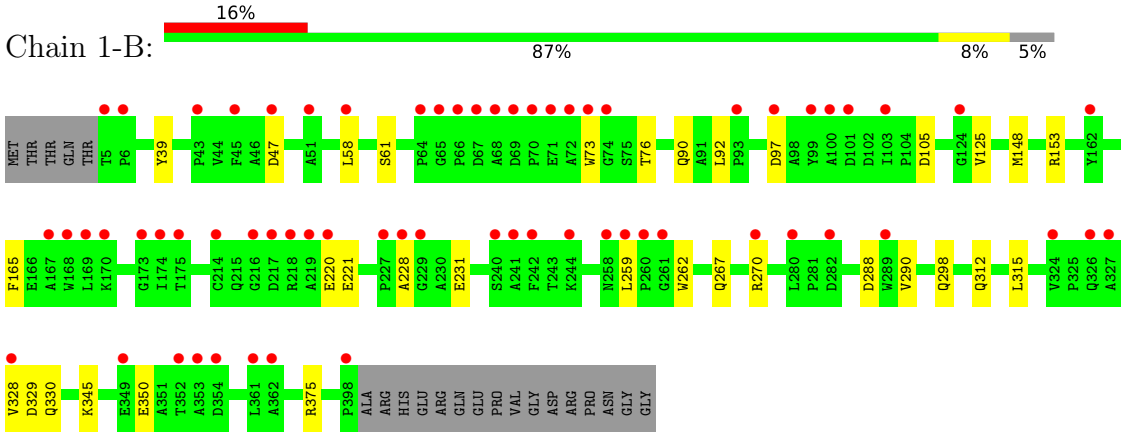
• Molecule 1: Oleandomycin glycosyltransferase

Chain 1-A:



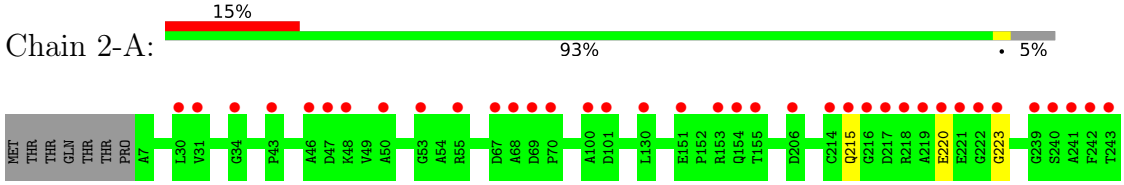
• Molecule 1: Oleandomycin glycosyltransferase

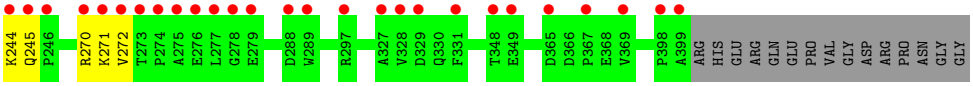
Chain 1-B:



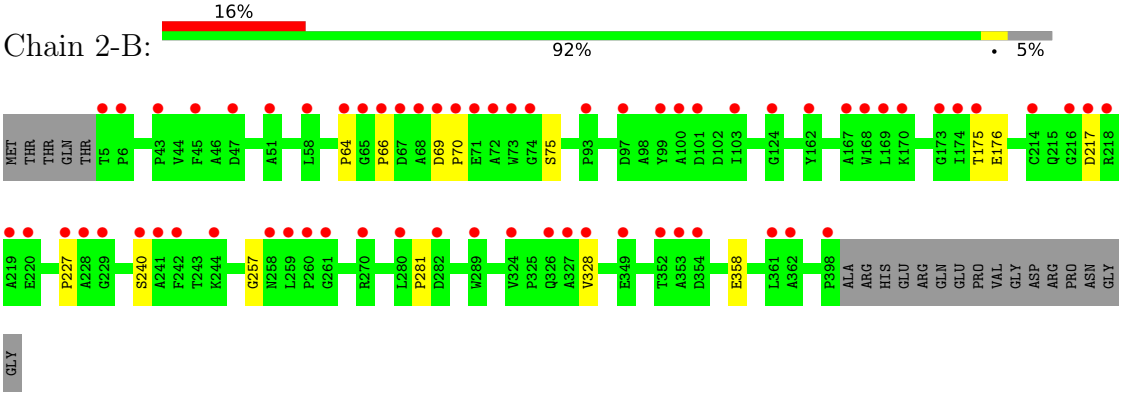
• Molecule 1: Oleandomycin glycosyltransferase

Chain 2-A:

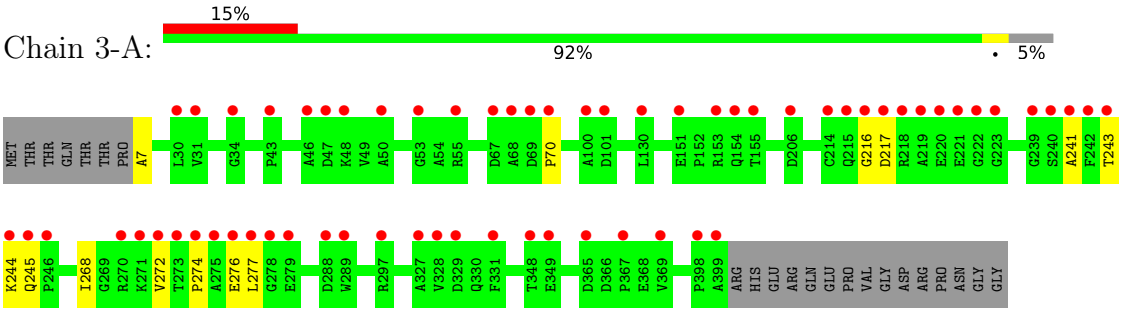




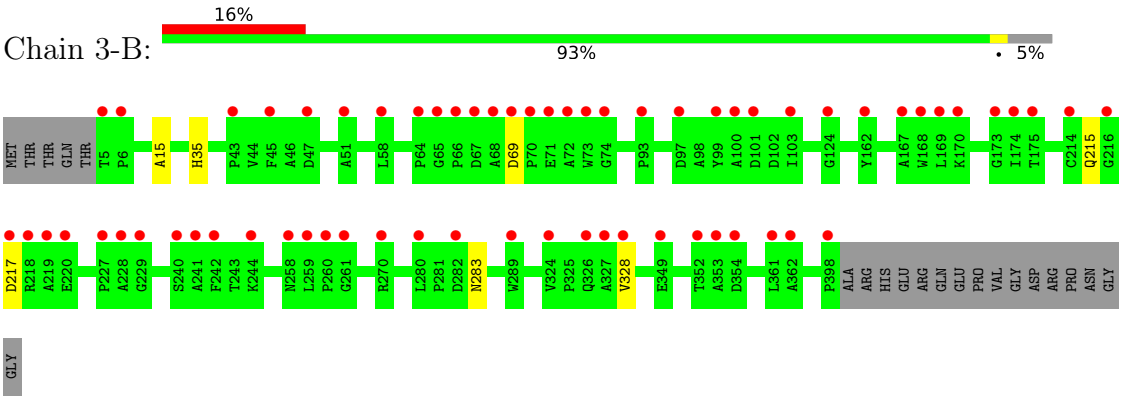
• Molecule 1: Oleandomycin glycosyltransferase



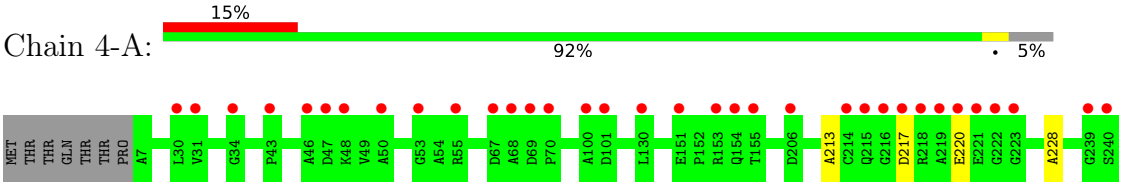
• Molecule 1: Oleandomycin glycosyltransferase

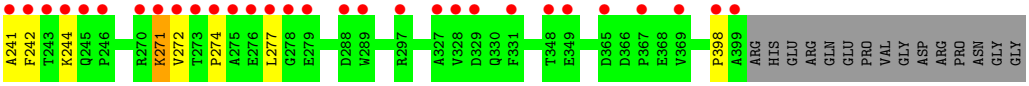


• Molecule 1: Oleandomycin glycosyltransferase



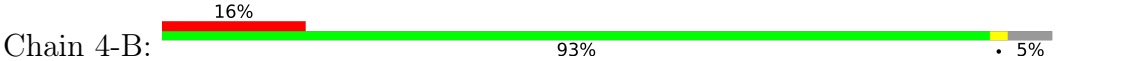
• Molecule 1: Oleandomycin glycosyltransferase

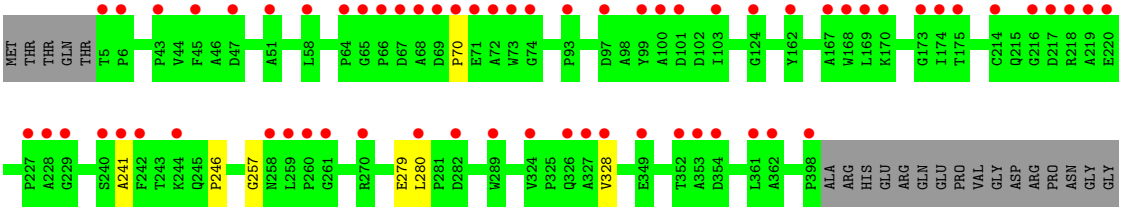




• Molecule 1: Oleandomycin glycosyltransferase

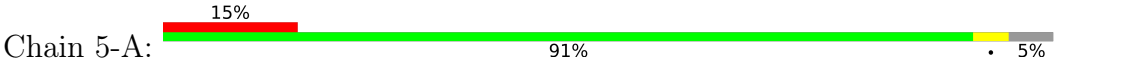
Chain 4-B:

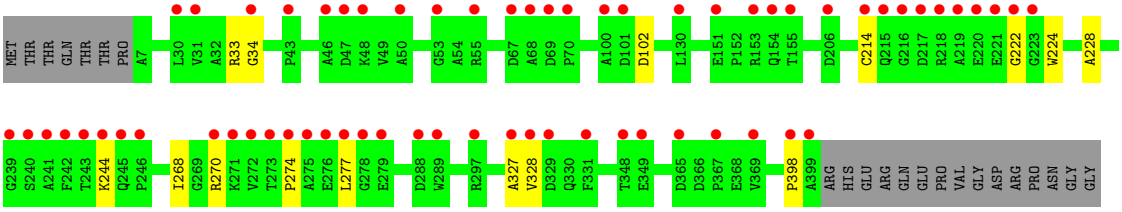




• Molecule 1: Oleandomycin glycosyltransferase

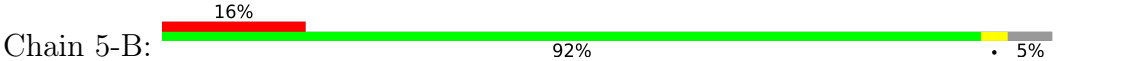
Chain 5-A:

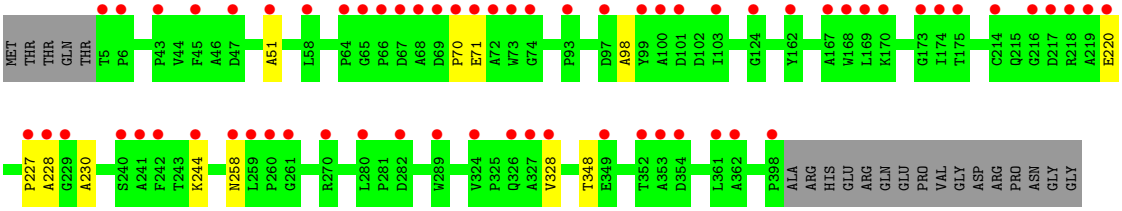




• Molecule 1: Oleandomycin glycosyltransferase

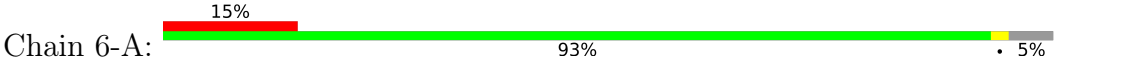
Chain 5-B:

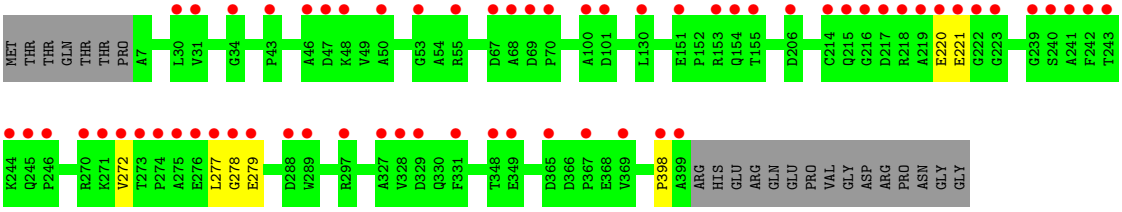




• Molecule 1: Oleandomycin glycosyltransferase

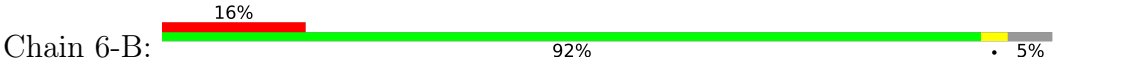
Chain 6-A:

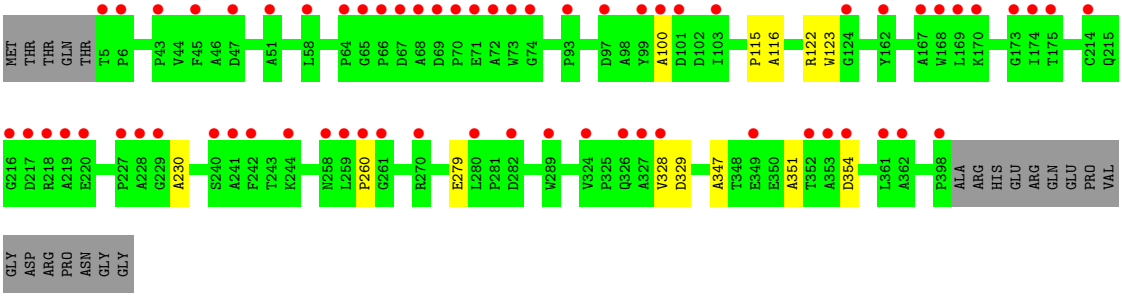




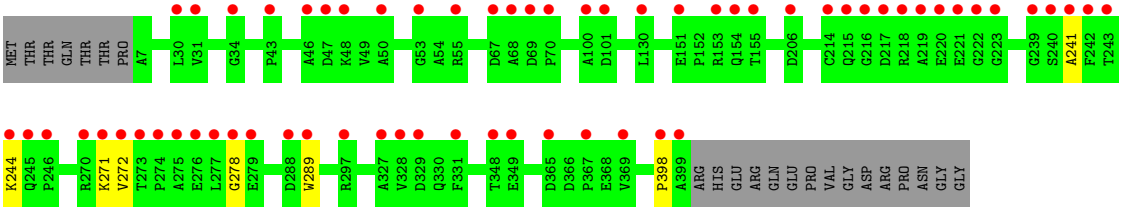
• Molecule 1: Oleandomycin glycosyltransferase

Chain 6-B:

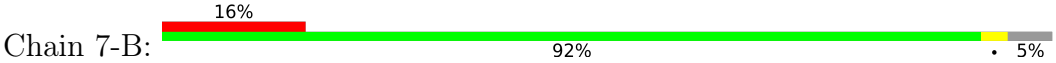


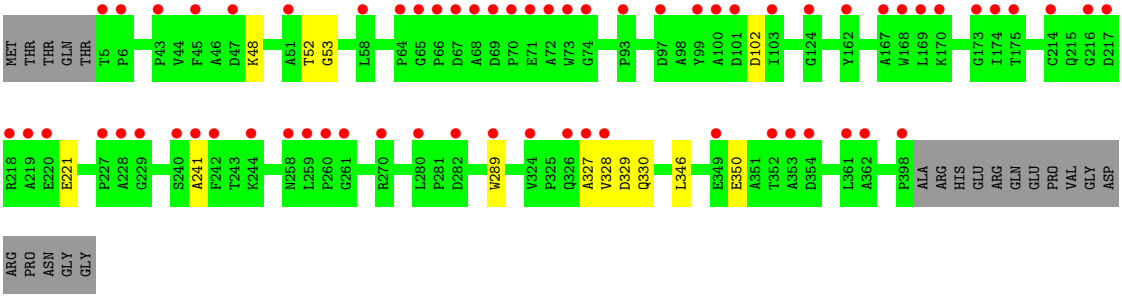


• Molecule 1: Oleandomycin glycosyltransferase

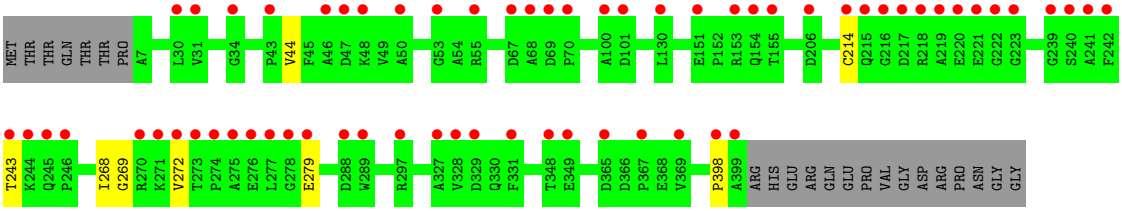


• Molecule 1: Oleandomycin glycosyltransferase

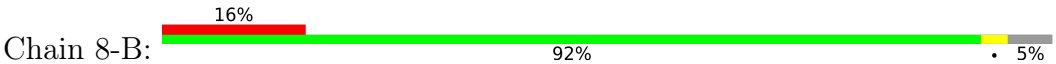


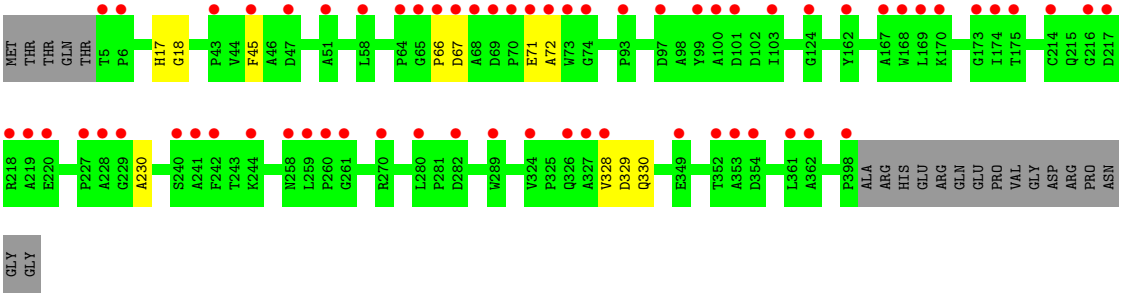


• Molecule 1: Oleandomycin glycosyltransferase

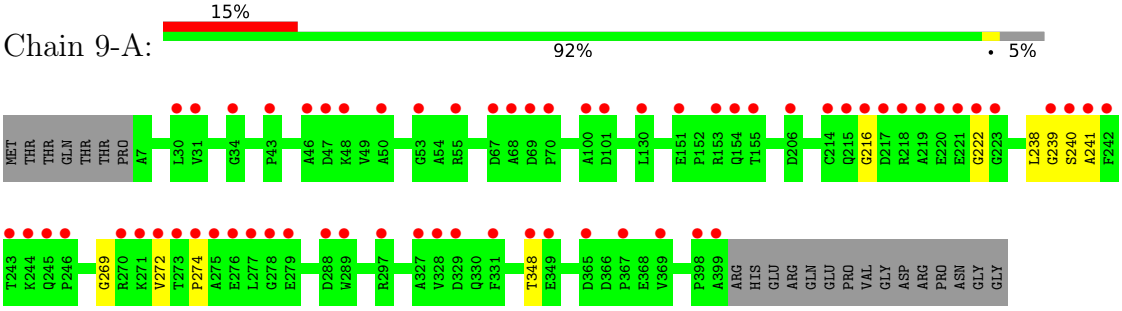


• Molecule 1: Oleandomycin glycosyltransferase

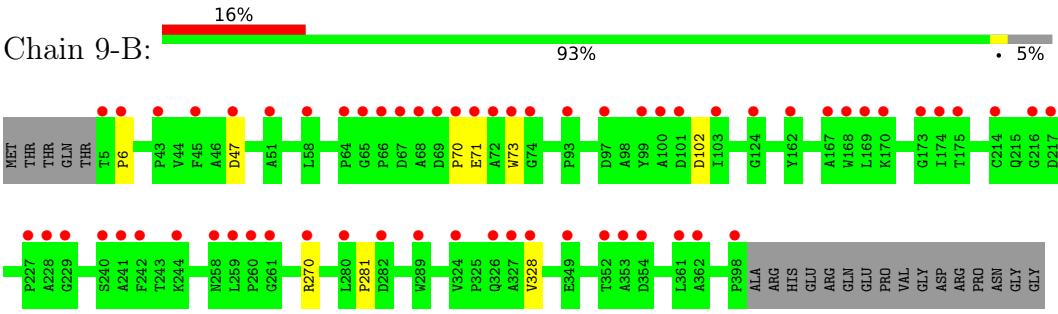




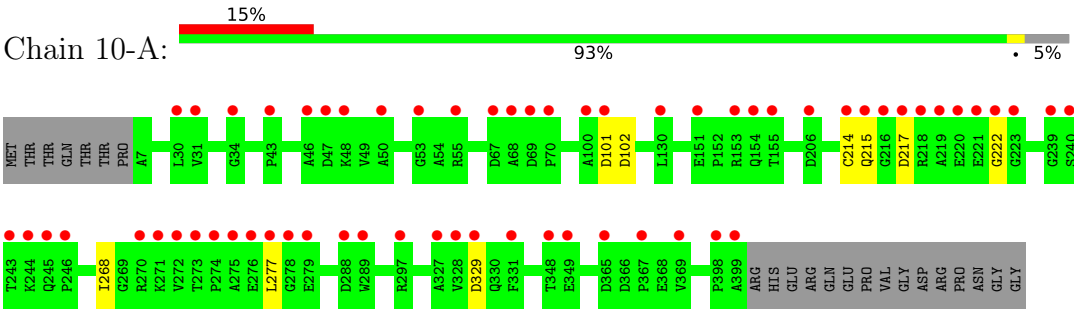
• Molecule 1: Oleandomycin glycosyltransferase



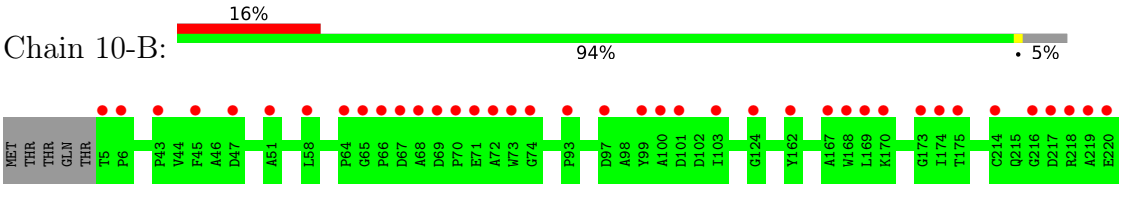
• Molecule 1: Oleandomycin glycosyltransferase

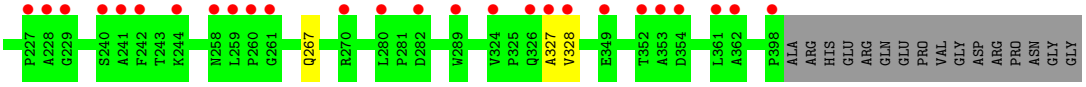


• Molecule 1: Oleandomycin glycosyltransferase



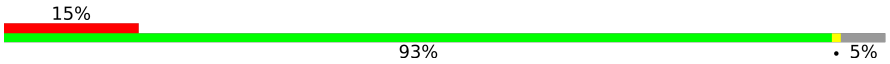
• Molecule 1: Oleandomycin glycosyltransferase

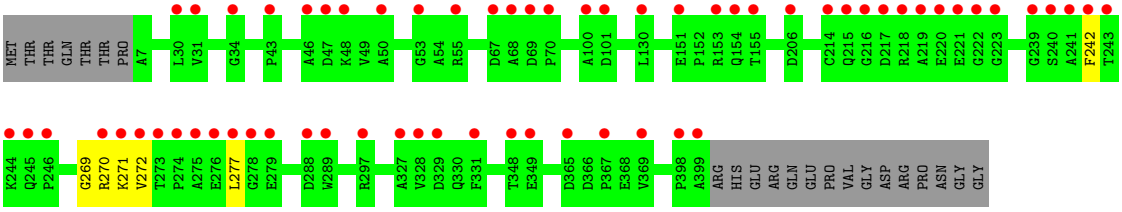




• Molecule 1: Oleandomycin glycosyltransferase

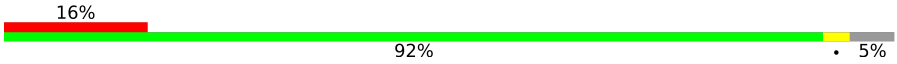
Chain 11-A:

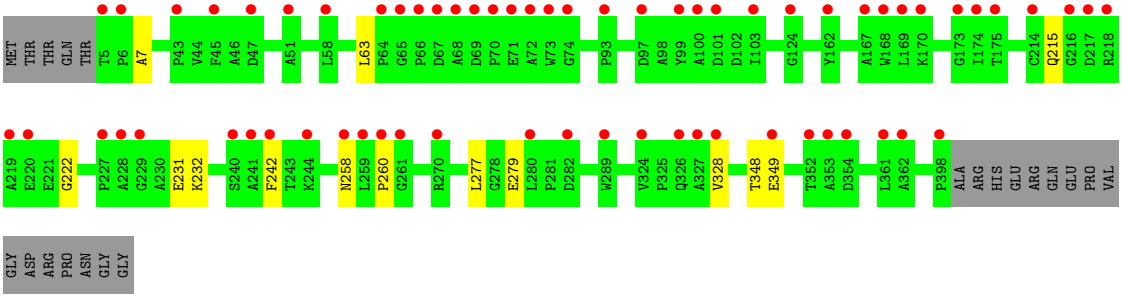




• Molecule 1: Oleandomycin glycosyltransferase

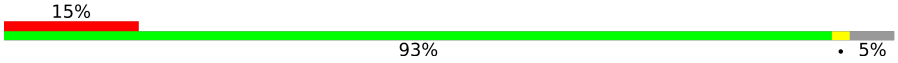
Chain 11-B:

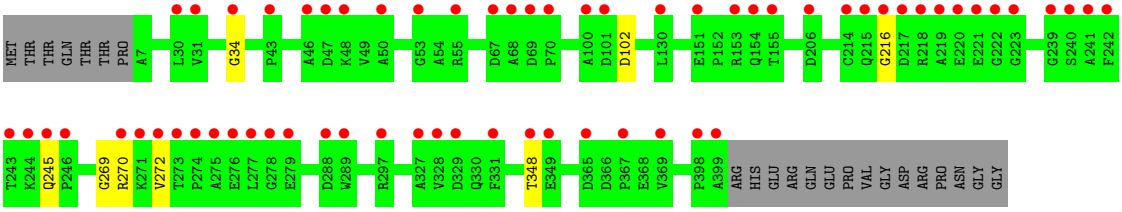




• Molecule 1: Oleandomycin glycosyltransferase

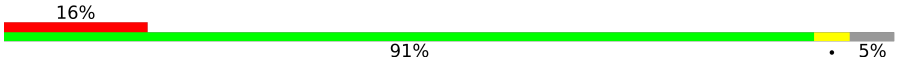
Chain 12-A:

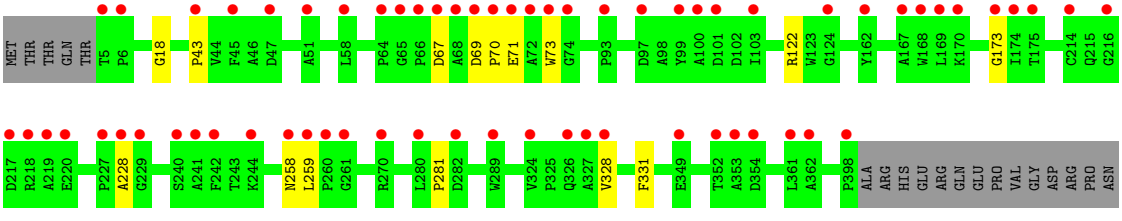




• Molecule 1: Oleandomycin glycosyltransferase

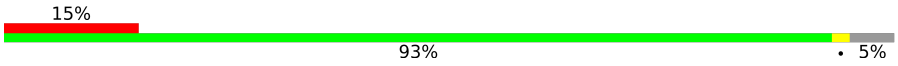
Chain 12-B:

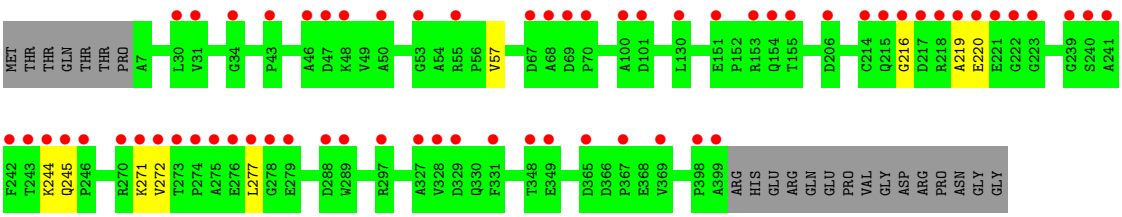




• Molecule 1: Oleandomycin glycosyltransferase

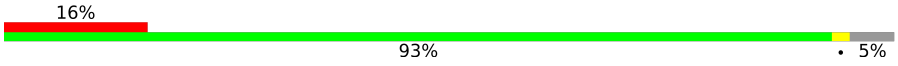
Chain 13-A:

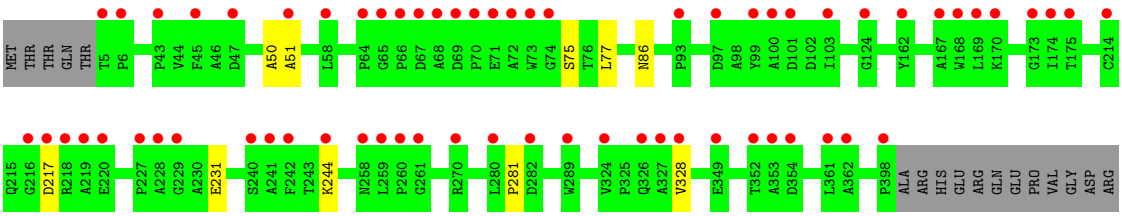




• Molecule 1: Oleandomycin glycosyltransferase

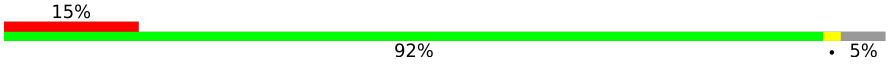
Chain 13-B:

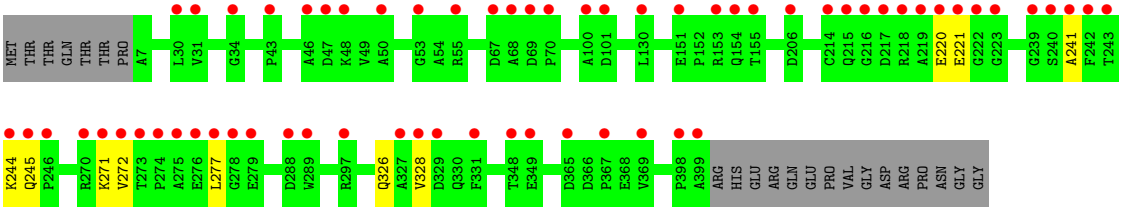




• Molecule 1: Oleandomycin glycosyltransferase

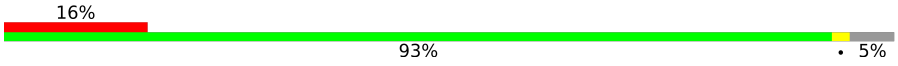
Chain 14-A:

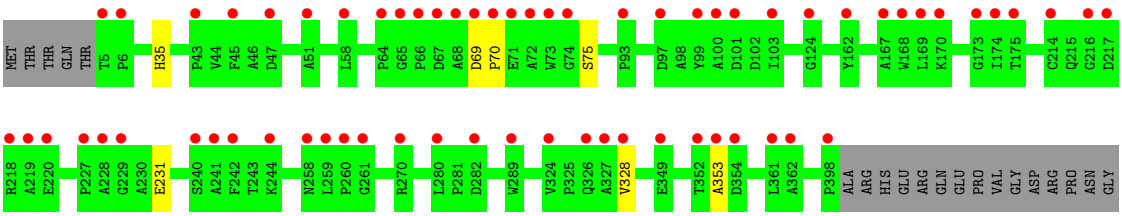




• Molecule 1: Oleandomycin glycosyltransferase

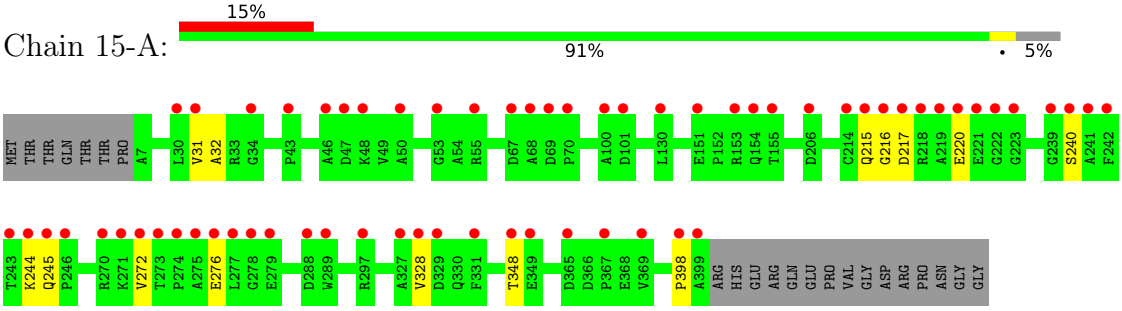
Chain 14-B:





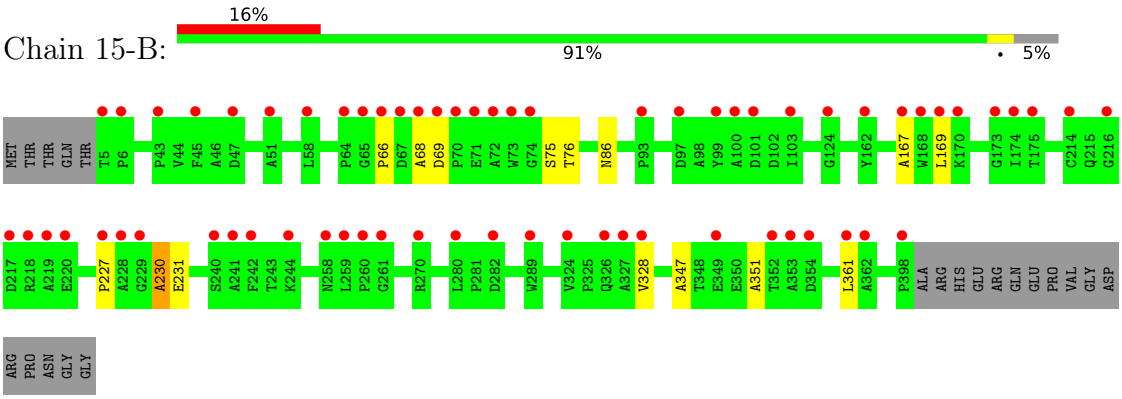
• Molecule 1: Oleandomycin glycosyltransferase

Chain 15-A:



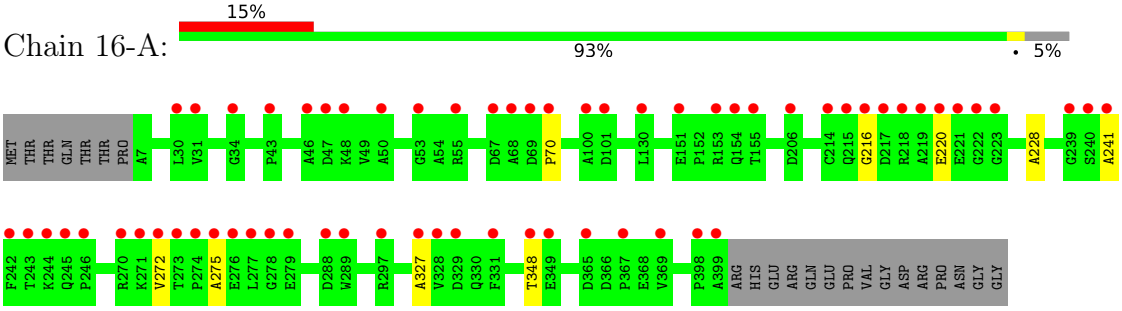
• Molecule 1: Oleandomycin glycosyltransferase

Chain 15-B:



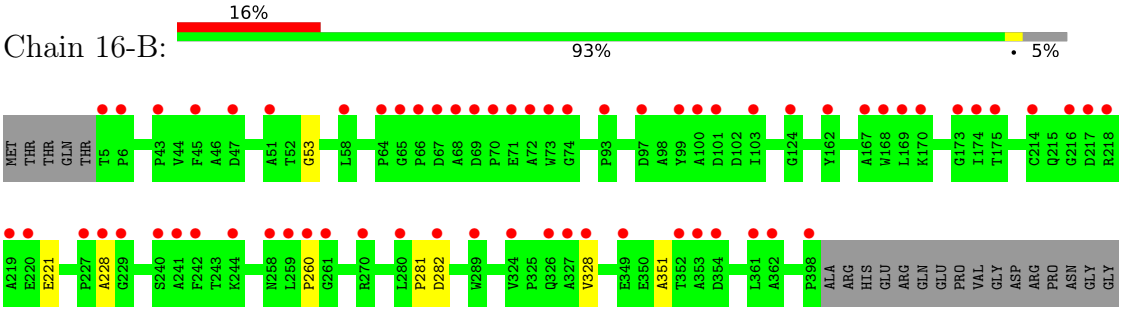
• Molecule 1: Oleandomycin glycosyltransferase

Chain 16-A:



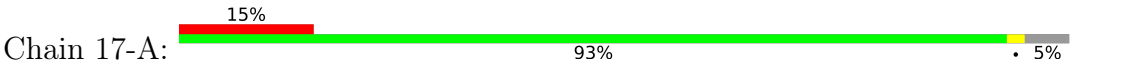
• Molecule 1: Oleandomycin glycosyltransferase

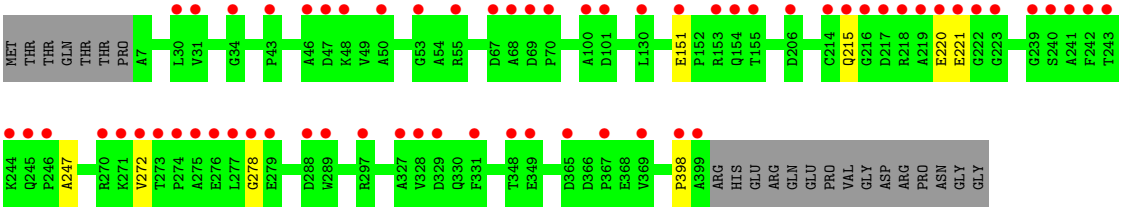
Chain 16-B:



• Molecule 1: Oleandomycin glycosyltransferase

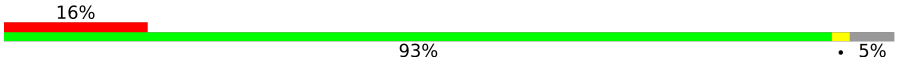
Chain 17-A:

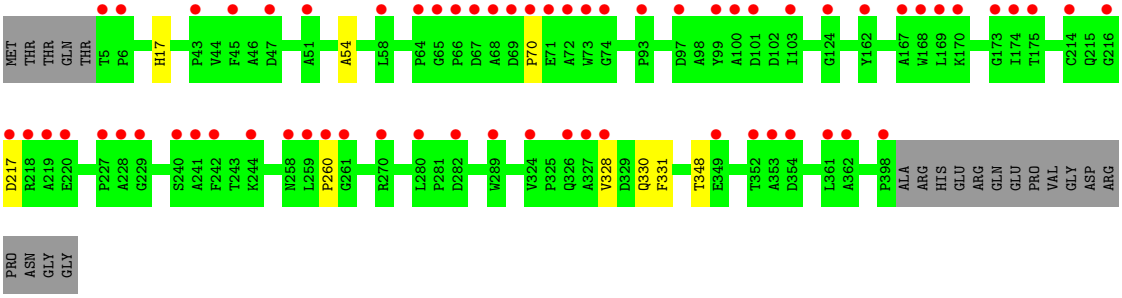




• Molecule 1: Oleandomycin glycosyltransferase

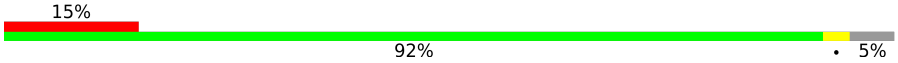
Chain 17-B:

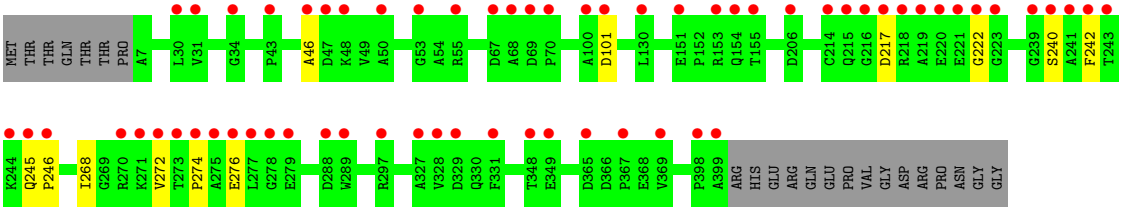




• Molecule 1: Oleandomycin glycosyltransferase

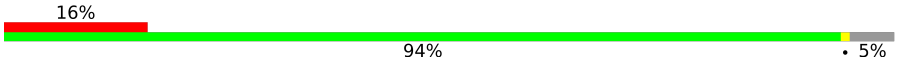
Chain 18-A:

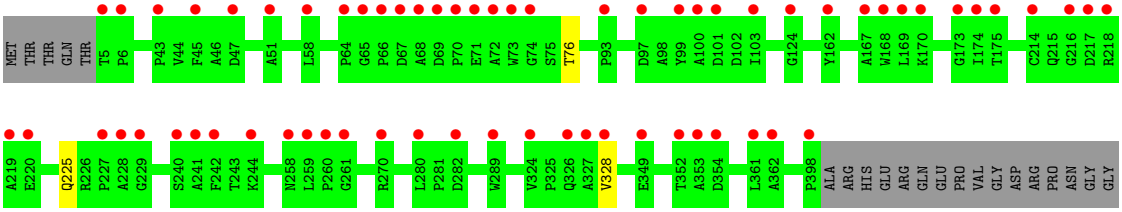




• Molecule 1: Oleandomycin glycosyltransferase

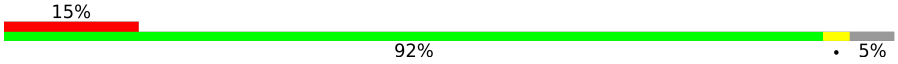
Chain 18-B:

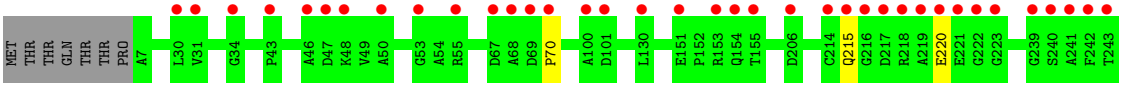


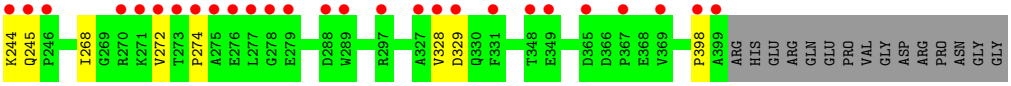


• Molecule 1: Oleandomycin glycosyltransferase

Chain 19-A:

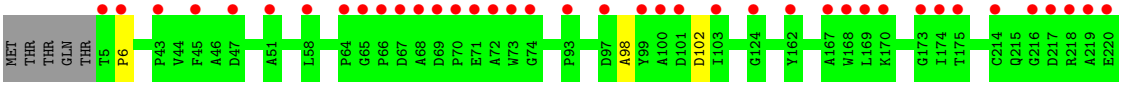


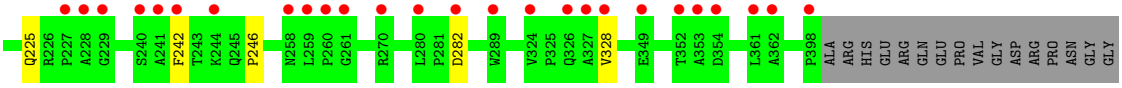




• Molecule 1: Oleandomycin glycosyltransferase

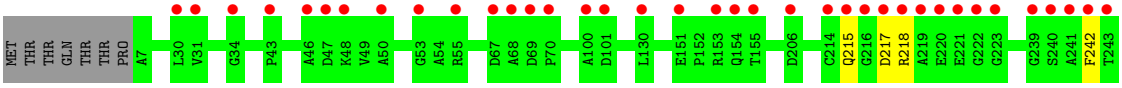
Chain 19-B:





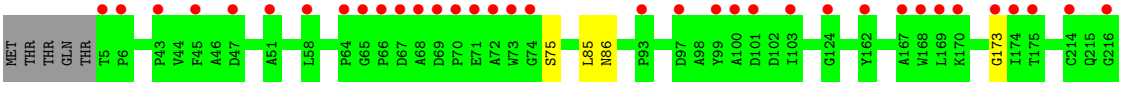
• Molecule 1: Oleandomycin glycosyltransferase

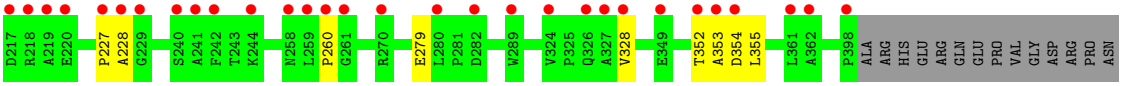
Chain 20-A:



• Molecule 1: Oleandomycin glycosyltransferase

Chain 20-B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.72Å 65.78Å 91.94Å 90.00° 100.42° 90.00°	Depositor
Resolution (Å)	29.03 – 1.70 29.03 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.03-1.70) 99.7 (29.03-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement: dev_1420)	Depositor
R, R_{free}	0.160 , 0.201 0.192 , 0.225	Depositor DCC
R_{free} test set	1992 reflections (2.12%)	wwPDB-VP
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 301.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	132758	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ERY, UDP, MG

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	1-A	0.37	0/3052	0.63	0/4170
1	1-B	0.34	0/3074	0.59	0/4205
All	All	0.35	0/6126	0.61	0/8375

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	3
1	2-A	0	1
1	3-A	0	1
1	4-A	0	1
1	6-B	0	2
1	10-A	0	2
1	13-A	0	2
1	14-A	0	1
1	15-B	0	2
1	19-B	0	1
1	20-A	0	1
All	All	0	17

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	272[A]	VAL	Peptide
1	1-A	274[A]	PRO	Peptide
1	1-A	329[A]	ASP	Peptide
1	2-A	271[B]	LYS	Peptide
1	3-A	7[C]	ALA	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	1-A	2978	0	2900	0	0
1	1-B	2996	0	2919	0	0
1	2-A	2978	0	2900	0	0
1	2-B	2996	0	2919	0	0
1	3-A	2978	0	2900	0	0
1	3-B	2996	0	2919	0	0
1	4-A	2978	0	2900	0	0
1	4-B	2996	0	2919	0	0
1	5-A	2978	0	2900	0	0
1	5-B	2996	0	2919	0	0
1	6-A	2978	0	2900	0	0
1	6-B	2996	0	2919	0	0
1	7-A	2978	0	2900	0	0
1	7-B	2996	0	2919	0	0
1	8-A	2978	0	2900	0	0
1	8-B	2996	0	2919	0	0
1	9-A	2978	0	2900	0	0
1	9-B	2996	0	2917	0	0
1	10-A	2978	0	2900	0	0
1	10-B	2996	0	2919	0	0
1	11-A	2978	0	2900	0	0
1	11-B	2996	0	2919	0	0
1	12-A	2978	0	2900	0	0
1	12-B	2996	0	2919	0	0
1	13-A	2978	0	2900	0	0
1	13-B	2996	0	2919	0	0
1	14-A	2978	0	2900	0	0
1	14-B	2996	0	2919	0	0
1	15-A	2978	0	2900	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	15-B	2996	0	2919	0	0
1	16-A	2978	0	2900	0	0
1	16-B	2996	0	2919	0	0
1	17-A	2978	0	2900	0	0
1	17-B	2996	0	2919	0	0
1	18-A	2978	0	2900	0	0
1	18-B	2996	0	2919	0	0
1	19-A	2978	0	2900	0	0
1	19-B	2996	0	2919	0	0
1	20-A	2978	0	2900	0	0
1	20-B	2996	0	2919	0	0
2	1-A	51	0	67	0	0
2	1-B	51	0	67	0	0
2	2-A	51	0	67	0	0
2	2-B	51	0	67	0	0
2	3-A	51	0	67	0	0
2	3-B	51	0	67	0	0
2	4-A	51	0	67	0	0
2	4-B	51	0	67	0	0
2	5-A	51	0	67	0	0
2	5-B	51	0	67	0	0
2	6-A	51	0	67	0	0
2	6-B	51	0	67	0	0
2	7-A	51	0	67	0	0
2	7-B	51	0	67	0	0
2	8-A	51	0	67	0	0
2	8-B	51	0	67	0	0
2	9-A	51	0	67	0	0
2	9-B	51	0	67	0	0
2	10-A	51	0	67	0	0
2	10-B	51	0	67	0	0
2	11-A	51	0	67	0	0
2	11-B	51	0	67	0	0
2	12-A	51	0	67	0	0
2	12-B	51	0	67	0	0
2	13-A	51	0	67	0	0
2	13-B	51	0	67	0	0
2	14-A	51	0	67	0	0
2	14-B	51	0	67	0	0
2	15-A	51	0	67	0	0
2	15-B	51	0	67	0	0
2	16-A	51	0	67	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	16-B	51	0	67	0	0
2	17-A	51	0	67	0	0
2	17-B	51	0	67	0	0
2	18-A	51	0	67	0	0
2	18-B	51	0	67	0	0
2	19-A	51	0	67	0	0
2	19-B	51	0	67	0	0
2	20-A	51	0	67	0	0
2	20-B	51	0	67	0	0
3	1-A	25	0	11	0	0
3	1-B	25	0	11	0	0
3	2-A	25	0	11	0	0
3	2-B	25	0	11	0	0
3	3-A	25	0	11	0	0
3	3-B	25	0	11	0	0
3	4-A	25	0	11	0	0
3	4-B	25	0	11	0	0
3	5-A	25	0	11	0	0
3	5-B	25	0	11	0	0
3	6-A	25	0	11	0	0
3	6-B	25	0	11	0	0
3	7-A	25	0	11	0	0
3	7-B	25	0	11	0	0
3	8-A	25	0	11	0	0
3	8-B	25	0	11	0	0
3	9-A	25	0	11	0	0
3	9-B	25	0	11	0	0
3	10-A	25	0	11	0	0
3	10-B	25	0	11	0	0
3	11-A	25	0	11	0	0
3	11-B	25	0	11	0	0
3	12-A	25	0	11	0	0
3	12-B	25	0	11	0	0
3	13-A	25	0	11	0	0
3	13-B	25	0	11	0	0
3	14-A	25	0	11	0	0
3	14-B	25	0	11	0	0
3	15-A	25	0	11	0	0
3	15-B	25	0	11	0	0
3	16-A	25	0	11	0	0
3	16-B	25	0	11	0	0
3	17-A	25	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	17-B	25	0	11	0	0
3	18-A	25	0	11	0	0
3	18-B	25	0	11	0	0
3	19-A	25	0	11	0	0
3	19-B	25	0	11	0	0
3	20-A	25	0	11	0	0
3	20-B	25	0	11	0	0
4	1-B	1	0	0	0	0
4	2-B	1	0	0	0	0
4	3-B	1	0	0	0	0
4	4-B	1	0	0	0	0
4	5-B	1	0	0	0	0
4	6-B	1	0	0	0	0
4	7-B	1	0	0	0	0
4	8-B	1	0	0	0	0
4	9-B	1	0	0	0	0
4	10-B	1	0	0	0	0
4	11-B	1	0	0	0	0
4	12-B	1	0	0	0	0
4	13-B	1	0	0	0	0
4	14-B	1	0	0	0	0
4	15-B	1	0	0	0	0
4	16-B	1	0	0	0	0
4	17-B	1	0	0	0	0
4	18-B	1	0	0	0	0
4	19-B	1	0	0	0	0
4	20-B	1	0	0	0	0
5	1-A	271	0	0	0	0
5	1-B	250	0	0	0	0
5	2-A	259	0	0	0	0
5	2-B	242	0	0	0	0
5	3-A	244	0	0	0	0
5	3-B	261	0	0	0	0
5	4-A	267	0	0	0	0
5	4-B	250	0	0	0	0
5	5-A	273	0	0	0	0
5	5-B	252	0	0	0	0
5	6-A	256	0	0	0	0
5	6-B	239	0	0	0	0
5	7-A	271	0	0	0	0
5	7-B	256	0	0	0	0
5	8-A	273	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	8-B	241	0	0	0	0
5	9-A	291	0	0	0	0
5	9-B	218	0	0	0	0
5	10-A	243	0	0	0	0
5	10-B	256	0	0	0	0
5	11-A	258	0	0	0	0
5	11-B	271	0	0	0	0
5	12-A	264	0	0	0	0
5	12-B	229	0	0	0	0
5	13-A	281	0	0	0	0
5	13-B	261	0	0	0	0
5	14-A	248	0	0	0	0
5	14-B	249	0	0	0	0
5	15-A	268	0	0	0	0
5	15-B	261	0	0	0	0
5	16-A	253	0	0	0	0
5	16-B	240	0	0	0	0
5	17-A	270	0	0	0	0
5	17-B	220	0	0	0	0
5	18-A	271	0	0	0	0
5	18-B	257	0	0	0	0
5	19-A	249	0	0	0	0
5	19-B	245	0	0	0	0
5	20-A	266	0	0	0	0
5	20-B	244	0	0	0	0
All	All	132758	0	119498	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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
1	1-A	389/415 (94%)	346 (89%)	31 (8%)	12 (3%)	4 0
1	1-B	392/415 (94%)	362 (92%)	25 (6%)	5 (1%)	12 2
1	2-A	389/415 (94%)	358 (92%)	24 (6%)	7 (2%)	8 1
1	2-B	392/415 (94%)	346 (88%)	32 (8%)	14 (4%)	3 0
1	3-A	389/415 (94%)	354 (91%)	23 (6%)	12 (3%)	4 0
1	3-B	392/415 (94%)	355 (91%)	30 (8%)	7 (2%)	8 1
1	4-A	389/415 (94%)	354 (91%)	23 (6%)	12 (3%)	4 0
1	4-B	392/415 (94%)	361 (92%)	24 (6%)	7 (2%)	8 1
1	5-A	389/415 (94%)	352 (90%)	22 (6%)	15 (4%)	3 0
1	5-B	392/415 (94%)	355 (91%)	25 (6%)	12 (3%)	4 0
1	6-A	389/415 (94%)	365 (94%)	17 (4%)	7 (2%)	8 1
1	6-B	392/415 (94%)	352 (90%)	29 (7%)	11 (3%)	5 0
1	7-A	389/415 (94%)	357 (92%)	25 (6%)	7 (2%)	8 1
1	7-B	392/415 (94%)	360 (92%)	19 (5%)	13 (3%)	4 0
1	8-A	389/415 (94%)	364 (94%)	17 (4%)	8 (2%)	7 1
1	8-B	392/415 (94%)	357 (91%)	24 (6%)	11 (3%)	5 0
1	9-A	389/415 (94%)	363 (93%)	16 (4%)	10 (3%)	5 1
1	9-B	392/415 (94%)	358 (91%)	25 (6%)	9 (2%)	6 1
1	10-A	389/415 (94%)	358 (92%)	24 (6%)	7 (2%)	8 1
1	10-B	392/415 (94%)	376 (96%)	13 (3%)	3 (1%)	19 6
1	11-A	389/415 (94%)	362 (93%)	21 (5%)	6 (2%)	10 2
1	11-B	392/415 (94%)	342 (87%)	36 (9%)	14 (4%)	3 0
1	12-A	389/415 (94%)	358 (92%)	23 (6%)	8 (2%)	7 1
1	12-B	392/415 (94%)	349 (89%)	28 (7%)	15 (4%)	3 0
1	13-A	389/415 (94%)	360 (92%)	22 (6%)	7 (2%)	8 1
1	13-B	392/415 (94%)	353 (90%)	29 (7%)	10 (3%)	5 1
1	14-A	389/415 (94%)	361 (93%)	19 (5%)	9 (2%)	6 1
1	14-B	392/415 (94%)	353 (90%)	32 (8%)	7 (2%)	8 1
1	15-A	389/415 (94%)	357 (92%)	18 (5%)	14 (4%)	3 0
1	15-B	392/415 (94%)	350 (89%)	28 (7%)	14 (4%)	3 0
1	16-A	389/415 (94%)	360 (92%)	20 (5%)	9 (2%)	6 1
1	16-B	392/415 (94%)	355 (91%)	29 (7%)	8 (2%)	7 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	17-A	389/415 (94%)	357 (92%)	24 (6%)	8 (2%)	7 1
1	17-B	392/415 (94%)	348 (89%)	35 (9%)	9 (2%)	6 1
1	18-A	389/415 (94%)	353 (91%)	24 (6%)	12 (3%)	4 0
1	18-B	392/415 (94%)	359 (92%)	30 (8%)	3 (1%)	19 6
1	19-A	389/415 (94%)	361 (93%)	17 (4%)	11 (3%)	5 0
1	19-B	392/415 (94%)	363 (93%)	22 (6%)	7 (2%)	8 1
1	20-A	389/415 (94%)	361 (93%)	17 (4%)	11 (3%)	5 0
1	20-B	392/415 (94%)	363 (93%)	16 (4%)	13 (3%)	4 0
All	All	15620/16600 (94%)	14278 (91%)	958 (6%)	384 (2%)	5 1

5 of 384 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	102[A]	ASP
1	1-A	215[A]	GLN
1	1-A	272[A]	VAL
1	1-A	277[A]	LEU
1	1-A	328[A]	VAL

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
1	1-A	295/326 (90%)	263 (89%)	32 (11%)	6 1
1	1-B	297/326 (91%)	269 (91%)	28 (9%)	8 1
All	All	592/652 (91%)	532 (90%)	60 (10%)	7 1

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	312[A]	GLN
1	1-B	329[A]	ASP

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Mol	Chain	Res	Type
1	1-B	61[A]	SER
1	1-B	328[A]	VAL
1	1-B	375[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	1-B	94[A]	GLN
1	1-B	197[A]	GLN
1	1-B	312[A]	GLN
1	1-B	263[A]	HIS
1	1-B	177[A]	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 100 ligands modelled in this entry, 20 are monoatomic - leaving 80 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	$\#\|Z\| > 2$
2	ERY	20-B	501[T]	-	53,53,53	1.25	5 (9%)	82,82,82	1.17	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	UDP	14-B	502[N]	-	24,26,26	0.94	0	37,40,40	1.55	5 (13%)
3	UDP	3-A	1401[C]	-	24,26,26	0.92	0	37,40,40	1.47	4 (10%)
3	UDP	8-B	502[H]	-	24,26,26	0.92	0	37,40,40	1.53	6 (16%)
3	UDP	19-A	1401[S]	-	24,26,26	0.91	1 (4%)	37,40,40	1.46	6 (16%)
2	ERY	17-B	501[Q]	-	53,53,53	1.25	5 (9%)	82,82,82	1.25	8 (9%)
2	ERY	20-A	1400[T]	-	53,53,53	1.25	6 (11%)	82,82,82	1.26	10 (12%)
2	ERY	2-A	1400[B]	-	53,53,53	1.23	6 (11%)	82,82,82	1.25	9 (10%)
3	UDP	6-B	502[F]	-	24,26,26	0.95	0	37,40,40	1.57	5 (13%)
2	ERY	10-A	1400[J]	-	53,53,53	1.22	6 (11%)	82,82,82	1.21	8 (9%)
2	ERY	4-B	501[D]	-	53,53,53	1.25	6 (11%)	82,82,82	1.44	10 (12%)
2	ERY	1-B	501[A]	-	53,53,53	1.21	5 (9%)	82,82,82	1.34	11 (13%)
3	UDP	1-A	1401[A]	-	24,26,26	0.98	1 (4%)	37,40,40	1.41	6 (16%)
2	ERY	1-A	1400[A]	-	53,53,53	1.25	6 (11%)	82,82,82	1.26	6 (7%)
2	ERY	3-A	1400[C]	-	53,53,53	1.26	6 (11%)	82,82,82	1.22	8 (9%)
2	ERY	9-B	501[I]	-	53,53,53	1.22	5 (9%)	82,82,82	1.43	11 (13%)
2	ERY	7-B	501[G]	-	53,53,53	1.23	5 (9%)	82,82,82	1.51	9 (10%)
3	UDP	12-B	502[L]	-	24,26,26	0.97	1 (4%)	37,40,40	1.56	6 (16%)
2	ERY	16-A	1400[P]	-	53,53,53	1.26	6 (11%)	82,82,82	1.48	18 (21%)
3	UDP	7-A	1401[G]	-	24,26,26	0.94	0	37,40,40	1.47	5 (13%)
3	UDP	20-B	502[T]	-	24,26,26	0.92	0	37,40,40	1.41	5 (13%)
3	UDP	9-B	502[I]	-	24,26,26	0.93	0	37,40,40	1.46	4 (10%)
3	UDP	2-B	502[B]	-	24,26,26	0.96	1 (4%)	37,40,40	1.45	5 (13%)
3	UDP	17-A	1401[Q]	-	24,26,26	0.94	0	37,40,40	1.36	4 (10%)
2	ERY	8-A	1400[H]	-	53,53,53	1.27	6 (11%)	82,82,82	1.36	9 (10%)
3	UDP	13-A	1401[M]	-	24,26,26	0.92	0	37,40,40	1.33	4 (10%)
2	ERY	13-A	1400[M]	-	53,53,53	1.26	6 (11%)	82,82,82	1.16	6 (7%)
2	ERY	12-A	1400[L]	-	53,53,53	1.22	6 (11%)	82,82,82	1.32	11 (13%)
2	ERY	2-B	501[B]	-	53,53,53	1.18	5 (9%)	82,82,82	1.44	12 (14%)
2	ERY	10-B	501[J]	-	53,53,53	1.27	5 (9%)	82,82,82	1.39	10 (12%)
2	ERY	15-B	501[O]	-	53,53,53	1.24	6 (11%)	82,82,82	1.58	15 (18%)
3	UDP	20-A	1401[T]	-	24,26,26	0.97	1 (4%)	37,40,40	1.49	5 (13%)
2	ERY	16-B	501[P]	-	53,53,53	1.23	4 (7%)	82,82,82	1.36	12 (14%)
2	ERY	9-A	1400[I]	-	53,53,53	1.24	6 (11%)	82,82,82	1.35	10 (12%)
2	ERY	14-A	1400[N]	-	53,53,53	1.21	5 (9%)	82,82,82	1.16	6 (7%)
2	ERY	18-B	501[R]	-	53,53,53	1.23	5 (9%)	82,82,82	1.48	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ERY	12-B	501[L]	-	53,53,53	1.24	4 (7%)	82,82,82	1.44	11 (13%)
2	ERY	5-B	501[E]	-	53,53,53	1.24	5 (9%)	82,82,82	1.36	13 (15%)
3	UDP	5-B	502[E]	-	24,26,26	0.92	1 (4%)	37,40,40	1.56	7 (18%)
3	UDP	9-A	1401[I]	-	24,26,26	0.98	1 (4%)	37,40,40	1.44	6 (16%)
3	UDP	18-A	1401[R]	-	24,26,26	0.91	1 (4%)	37,40,40	1.59	8 (21%)
3	UDP	15-A	1401[O]	-	24,26,26	1.00	1 (4%)	37,40,40	2.05	12 (32%)
2	ERY	14-B	501[N]	-	53,53,53	1.22	4 (7%)	82,82,82	1.60	17 (20%)
3	UDP	14-A	1401[N]	-	24,26,26	0.93	0	37,40,40	1.46	7 (18%)
3	UDP	8-A	1401[H]	-	24,26,26	0.97	0	37,40,40	1.56	5 (13%)
3	UDP	2-A	1401[B]	-	24,26,26	1.02	1 (4%)	37,40,40	1.57	6 (16%)
2	ERY	3-B	501[C]	-	53,53,53	1.23	5 (9%)	82,82,82	1.24	10 (12%)
2	ERY	11-B	501[K]	-	53,53,53	1.27	5 (9%)	82,82,82	1.26	7 (8%)
3	UDP	18-B	502[R]	-	24,26,26	0.95	0	37,40,40	1.49	4 (10%)
3	UDP	11-A	1401[K]	-	24,26,26	0.96	1 (4%)	37,40,40	1.59	6 (16%)
3	UDP	10-A	1401[J]	-	24,26,26	0.92	1 (4%)	37,40,40	1.51	6 (16%)
2	ERY	11-A	1400[K]	-	53,53,53	1.23	6 (11%)	82,82,82	1.34	9 (10%)
2	ERY	19-A	1400[S]	-	53,53,53	1.27	6 (11%)	82,82,82	1.46	13 (15%)
2	ERY	8-B	501[H]	-	53,53,53	1.23	5 (9%)	82,82,82	1.40	9 (10%)
3	UDP	7-B	502[G]	-	24,26,26	0.94	0	37,40,40	1.50	6 (16%)
2	ERY	18-A	1400[R]	-	53,53,53	1.24	6 (11%)	82,82,82	1.26	7 (8%)
3	UDP	4-A	1401[D]	-	24,26,26	0.95	1 (4%)	37,40,40	1.56	7 (18%)
3	UDP	12-A	1401[L]	-	24,26,26	0.93	1 (4%)	37,40,40	1.47	5 (13%)
3	UDP	16-A	1401[P]	-	24,26,26	0.95	0	37,40,40	1.41	4 (10%)
3	UDP	1-B	502[A]	-	24,26,26	0.95	1 (4%)	37,40,40	1.46	4 (10%)
3	UDP	4-B	502[D]	-	24,26,26	0.95	1 (4%)	37,40,40	1.53	5 (13%)
3	UDP	5-A	1401[E]	-	24,26,26	0.93	1 (4%)	37,40,40	1.64	8 (21%)
2	ERY	17-A	1400[Q]	-	53,53,53	1.25	6 (11%)	82,82,82	1.36	9 (10%)
3	UDP	13-B	502[M]	-	24,26,26	0.96	1 (4%)	37,40,40	1.55	6 (16%)
3	UDP	15-B	502[O]	-	24,26,26	0.97	0	37,40,40	1.51	4 (10%)
2	ERY	7-A	1400[G]	-	53,53,53	1.22	6 (11%)	82,82,82	1.28	9 (10%)
3	UDP	10-B	502[J]	-	24,26,26	0.94	0	37,40,40	1.56	6 (16%)
3	UDP	3-B	502[C]	-	24,26,26	0.93	1 (4%)	37,40,40	1.36	5 (13%)
3	UDP	19-B	502[S]	-	24,26,26	0.95	0	37,40,40	1.44	5 (13%)
2	ERY	4-A	1400[D]	-	53,53,53	1.25	5 (9%)	82,82,82	1.20	8 (9%)
3	UDP	6-A	1401[F]	-	24,26,26	1.00	1 (4%)	37,40,40	1.53	5 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ERY	5-A	1400[E]	-	53,53,53	1.23	6 (11%)	82,82,82	1.42	12 (14%)
2	ERY	6-A	1400[F]	-	53,53,53	1.23	6 (11%)	82,82,82	1.32	9 (10%)
2	ERY	19-B	501[S]	-	53,53,53	1.26	5 (9%)	82,82,82	1.36	13 (15%)
2	ERY	6-B	501[F]	-	53,53,53	1.25	4 (7%)	82,82,82	1.71	13 (15%)
3	UDP	17-B	502[Q]	-	24,26,26	0.93	1 (4%)	37,40,40	1.36	4 (10%)
2	ERY	15-A	1400[O]	-	53,53,53	1.28	6 (11%)	82,82,82	1.33	13 (15%)
2	ERY	13-B	501[M]	-	53,53,53	1.21	5 (9%)	82,82,82	1.69	15 (18%)
3	UDP	11-B	502[K]	-	24,26,26	0.93	0	37,40,40	1.49	5 (13%)
3	UDP	16-B	502[P]	-	24,26,26	0.98	1 (4%)	37,40,40	1.69	7 (18%)

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
2	ERY	20-B	501[T]	-	-	0/72/107/107	0/3/3/3
3	UDP	14-B	502[N]	-	-	3/16/32/32	0/2/2/2
3	UDP	3-A	1401[C]	-	-	3/16/32/32	0/2/2/2
3	UDP	8-B	502[H]	-	-	3/16/32/32	0/2/2/2
3	UDP	19-A	1401[S]	-	-	5/16/32/32	0/2/2/2
2	ERY	17-B	501[Q]	-	-	2/72/107/107	0/3/3/3
2	ERY	20-A	1400[T]	-	-	1/72/107/107	0/3/3/3
2	ERY	2-A	1400[B]	-	-	0/72/107/107	0/3/3/3
3	UDP	6-B	502[F]	-	-	2/16/32/32	0/2/2/2
2	ERY	10-A	1400[J]	-	-	1/72/107/107	0/3/3/3
2	ERY	4-B	501[D]	-	-	5/72/107/107	0/3/3/3
2	ERY	1-B	501[A]	-	-	1/72/107/107	0/3/3/3
3	UDP	1-A	1401[A]	-	-	4/16/32/32	0/2/2/2
2	ERY	1-A	1400[A]	-	-	1/72/107/107	0/3/3/3
2	ERY	3-A	1400[C]	-	-	5/72/107/107	0/3/3/3
2	ERY	9-B	501[I]	-	-	3/72/107/107	0/3/3/3
2	ERY	7-B	501[G]	-	-	2/72/107/107	0/3/3/3
3	UDP	12-B	502[L]	-	-	3/16/32/32	0/2/2/2
2	ERY	16-A	1400[P]	-	-	4/72/107/107	0/3/3/3
3	UDP	7-A	1401[G]	-	-	7/16/32/32	0/2/2/2
3	UDP	20-B	502[T]	-	-	3/16/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDP	9-B	502[I]	-	-	3/16/32/32	0/2/2/2
3	UDP	2-B	502[B]	-	-	2/16/32/32	0/2/2/2
3	UDP	17-A	1401[Q]	-	-	2/16/32/32	0/2/2/2
2	ERY	8-A	1400[H]	-	-	2/72/107/107	0/3/3/3
3	UDP	13-A	1401[M]	-	-	3/16/32/32	0/2/2/2
2	ERY	13-A	1400[M]	-	-	1/72/107/107	0/3/3/3
2	ERY	12-A	1400[L]	-	-	0/72/107/107	0/3/3/3
2	ERY	2-B	501[B]	-	-	3/72/107/107	0/3/3/3
2	ERY	10-B	501[J]	-	-	3/72/107/107	0/3/3/3
2	ERY	15-B	501[O]	-	-	2/72/107/107	0/3/3/3
3	UDP	20-A	1401[T]	-	-	3/16/32/32	0/2/2/2
2	ERY	16-B	501[P]	-	-	1/72/107/107	0/3/3/3
2	ERY	9-A	1400[I]	-	-	0/72/107/107	0/3/3/3
2	ERY	14-A	1400[N]	-	-	1/72/107/107	0/3/3/3
2	ERY	18-B	501[R]	-	-	2/72/107/107	0/3/3/3
2	ERY	12-B	501[L]	-	-	1/72/107/107	0/3/3/3
2	ERY	5-B	501[E]	-	-	0/72/107/107	0/3/3/3
3	UDP	5-B	502[E]	-	-	1/16/32/32	0/2/2/2
3	UDP	9-A	1401[I]	-	-	5/16/32/32	0/2/2/2
3	UDP	18-A	1401[R]	-	-	4/16/32/32	0/2/2/2
3	UDP	15-A	1401[O]	-	-	4/16/32/32	0/2/2/2
2	ERY	14-B	501[N]	-	-	5/72/107/107	0/3/3/3
3	UDP	14-A	1401[N]	-	-	4/16/32/32	0/2/2/2
3	UDP	8-A	1401[H]	-	-	2/16/32/32	0/2/2/2
3	UDP	2-A	1401[B]	-	-	5/16/32/32	0/2/2/2
2	ERY	3-B	501[C]	-	-	2/72/107/107	0/3/3/3
2	ERY	11-B	501[K]	-	-	1/72/107/107	0/3/3/3
3	UDP	18-B	502[R]	-	-	3/16/32/32	0/2/2/2
3	UDP	11-A	1401[K]	-	-	4/16/32/32	0/2/2/2
3	UDP	10-A	1401[J]	-	-	6/16/32/32	0/2/2/2
2	ERY	11-A	1400[K]	-	-	1/72/107/107	0/3/3/3
2	ERY	19-A	1400[S]	-	-	3/72/107/107	0/3/3/3
2	ERY	8-B	501[H]	-	-	1/72/107/107	0/3/3/3
3	UDP	7-B	502[G]	-	-	3/16/32/32	0/2/2/2
2	ERY	18-A	1400[R]	-	-	0/72/107/107	0/3/3/3
3	UDP	4-A	1401[D]	-	-	3/16/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDP	12-A	1401[L]	-	-	2/16/32/32	0/2/2/2
3	UDP	16-A	1401[P]	-	-	7/16/32/32	0/2/2/2
3	UDP	1-B	502[A]	-	-	3/16/32/32	0/2/2/2
3	UDP	4-B	502[D]	-	-	1/16/32/32	0/2/2/2
3	UDP	5-A	1401[E]	-	-	6/16/32/32	0/2/2/2
2	ERY	17-A	1400[Q]	-	-	0/72/107/107	0/3/3/3
3	UDP	13-B	502[M]	-	-	4/16/32/32	0/2/2/2
3	UDP	15-B	502[O]	-	-	4/16/32/32	0/2/2/2
2	ERY	7-A	1400[G]	-	-	1/72/107/107	0/3/3/3
3	UDP	10-B	502[J]	-	-	1/16/32/32	0/2/2/2
3	UDP	3-B	502[C]	-	-	4/16/32/32	0/2/2/2
3	UDP	19-B	502[S]	-	-	2/16/32/32	0/2/2/2
2	ERY	4-A	1400[D]	-	-	1/72/107/107	0/3/3/3
3	UDP	6-A	1401[F]	-	-	5/16/32/32	0/2/2/2
2	ERY	5-A	1400[E]	-	-	3/72/107/107	0/3/3/3
2	ERY	6-A	1400[F]	-	-	5/72/107/107	0/3/3/3
2	ERY	19-B	501[S]	-	-	1/72/107/107	0/3/3/3
2	ERY	6-B	501[F]	-	-	8/72/107/107	0/3/3/3
3	UDP	17-B	502[Q]	-	-	3/16/32/32	0/2/2/2
2	ERY	15-A	1400[O]	-	-	3/72/107/107	0/3/3/3
2	ERY	13-B	501[M]	-	-	4/72/107/107	0/3/3/3
3	UDP	11-B	502[K]	-	-	3/16/32/32	0/2/2/2
3	UDP	16-B	502[P]	-	-	6/16/32/32	0/2/2/2

The worst 5 of 238 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	8-B	501[H]	ERY	O2-C1	4.53	1.44	1.34
2	12-B	501[L]	ERY	O2-C1	4.51	1.44	1.34
2	4-B	501[D]	ERY	O2-C1	4.49	1.44	1.34
2	19-B	501[S]	ERY	O2-C1	4.47	1.44	1.34
2	6-B	501[F]	ERY	O2-C1	4.46	1.44	1.34

The worst 5 of 638 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	7-B	501[G]	ERY	O5-C16-C17	7.29	114.61	103.81
2	6-B	501[F]	ERY	O3-C3-C4	-6.10	100.88	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5-A	1400[E]	ERY	O5-C16-C17	5.42	111.84	103.81
2	8-B	501[H]	ERY	O5-C16-C17	5.24	111.57	103.81
3	8-B	502[H]	UDP	C4-N3-C2	-5.20	119.72	126.58

There are no chirality outliers.

5 of 221 torsion outliers are listed below:

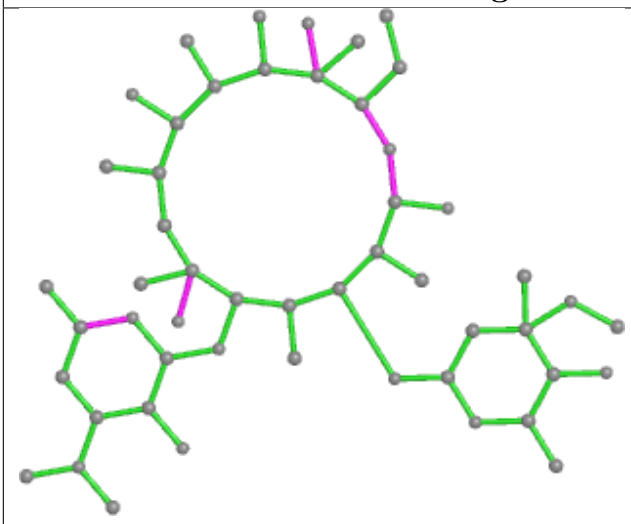
Mol	Chain	Res	Type	Atoms
2	3-A	1400[C]	ERY	C15-C16-O5-C20
2	3-A	1400[C]	ERY	C19-C16-O5-C20
2	16-A	1400[P]	ERY	C12-C13-C36-C37
2	2-B	501[B]	ERY	C12-C13-C36-C37
2	2-B	501[B]	ERY	O2-C13-C36-C37

There are no ring outliers.

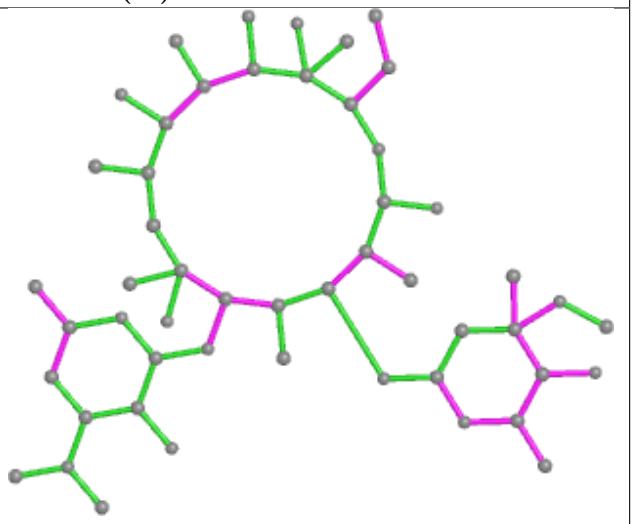
No monomer is involved in short contacts.

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.

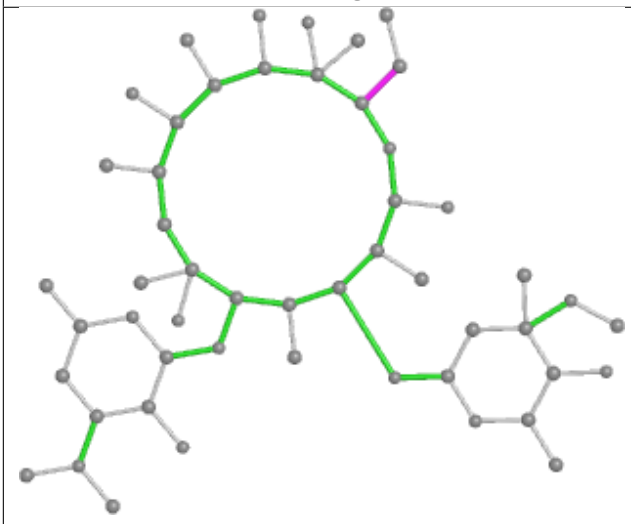
Ligand ERY B 501 (A)



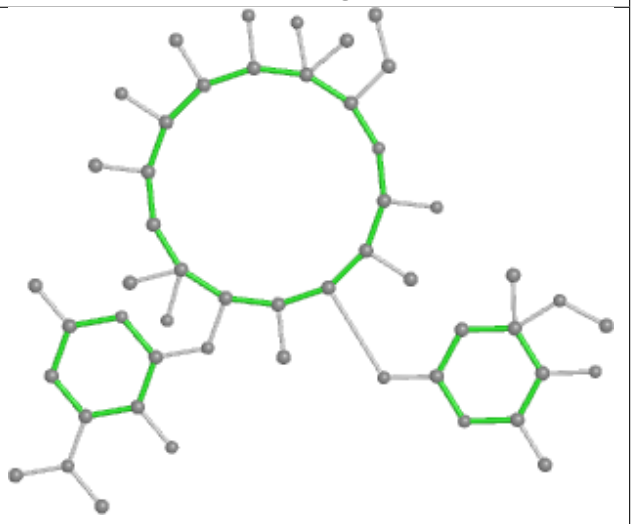
Bond lengths



Bond angles

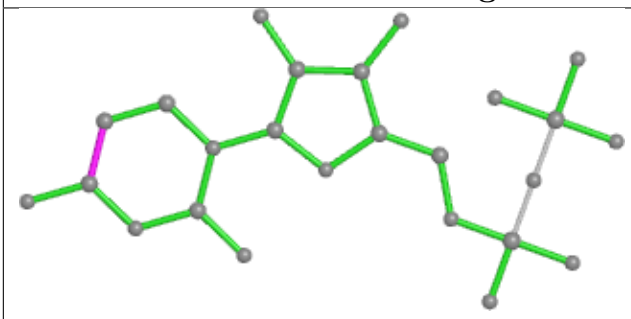


Torsions

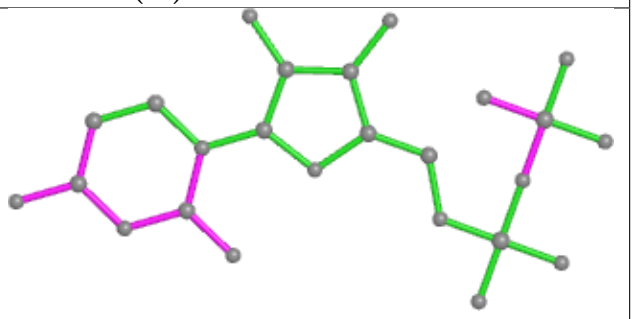


Rings

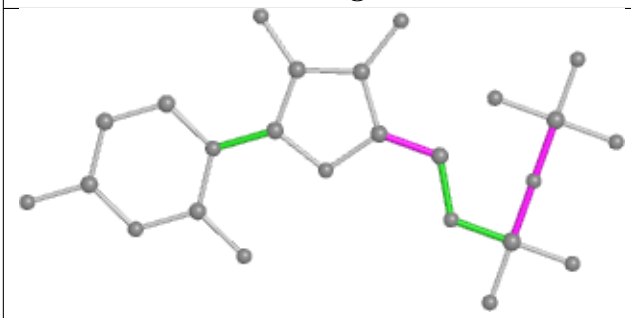
Ligand UDP A 1401 (A)



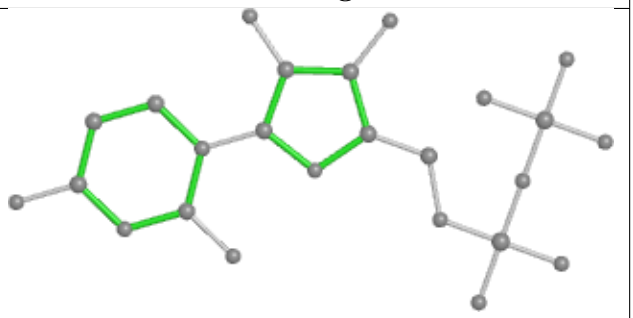
Bond lengths



Bond angles

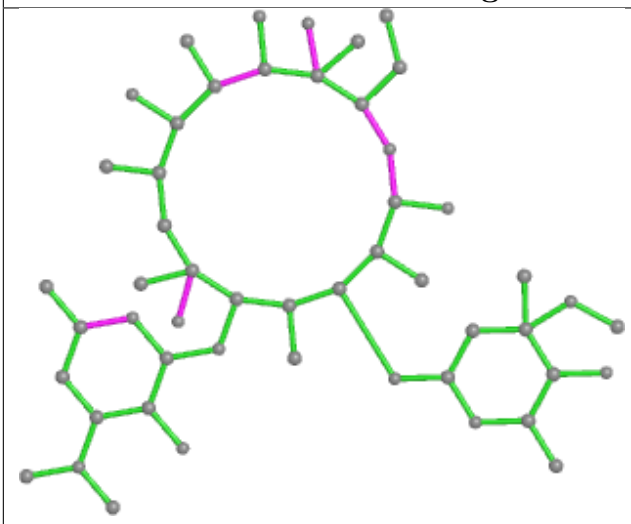


Torsions

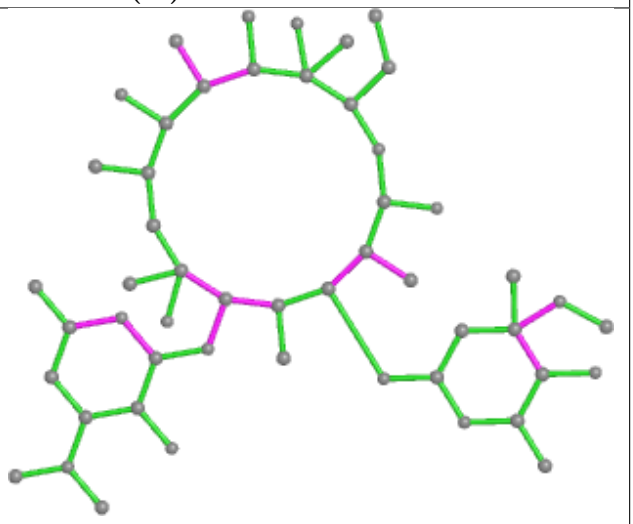


Rings

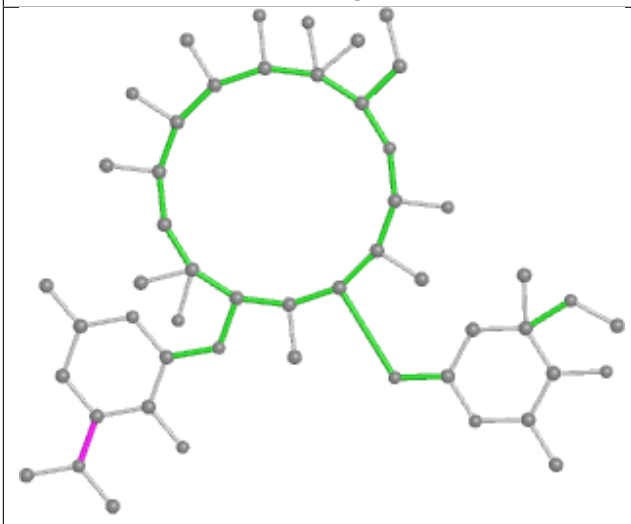
Ligand ERY A 1400 (A)



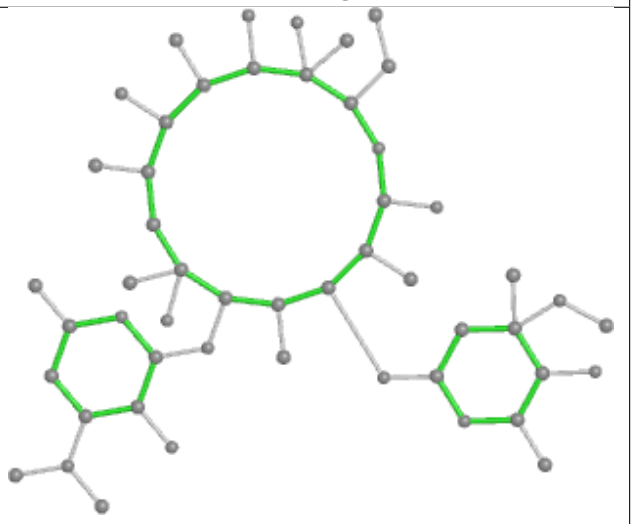
Bond lengths



Bond angles

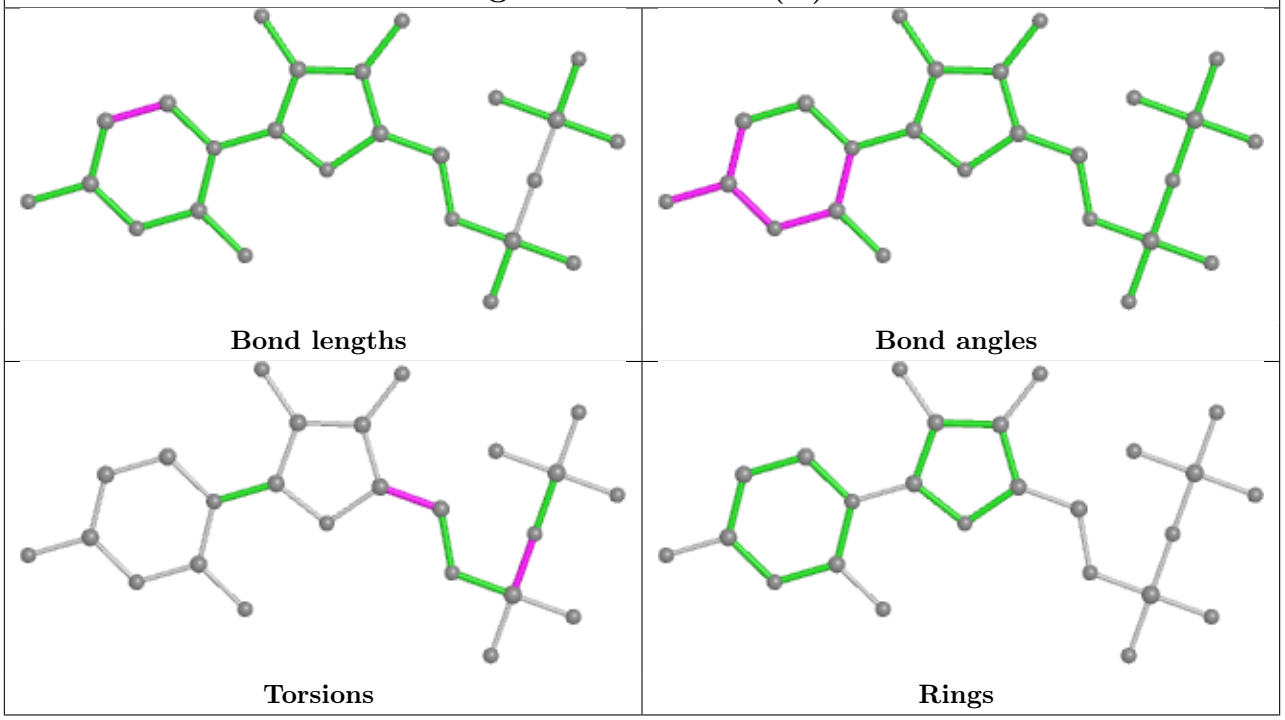


Torsions



Rings

Ligand UDP B 502 (A)



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	1-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	1-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	2-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	2-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	3-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	3-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	4-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	4-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	5-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	5-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	6-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	6-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	7-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	7-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	8-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	8-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	9-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	9-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	10-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	10-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	11-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	11-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	12-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	12-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	13-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	13-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	14-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	14-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	15-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	15-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	16-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	16-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	17-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	17-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	18-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	18-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	19-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	19-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
1	20-A	393/415 (94%)	0.96	64 (16%)	1	1	9, 11, 13, 15	393 (100%)
1	20-B	394/415 (94%)	0.92	65 (16%)	1	1	10, 11, 12, 14	394 (100%)
All	All	15740/16600 (94%)	0.94	2580 (16%)	1	1	9, 11, 13, 15	15740 (100%)

The worst 5 of 2580 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	272[A]	VAL	26.7
1	2-A	272[B]	VAL	26.7
1	3-A	272[C]	VAL	26.7
1	4-A	272[D]	VAL	26.7
1	5-A	272[E]	VAL	26.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 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
4	MG	1-B	503[A]	1/1	0.77	0.43	11,11,11,11	1
4	MG	2-B	503[B]	1/1	0.77	0.43	11,11,11,11	1
4	MG	3-B	503[C]	1/1	0.77	0.43	10,10,10,10	1
4	MG	4-B	503[D]	1/1	0.77	0.43	10,10,10,10	1
4	MG	5-B	503[E]	1/1	0.77	0.43	11,11,11,11	1
4	MG	6-B	503[F]	1/1	0.77	0.43	10,10,10,10	1
4	MG	7-B	503[G]	1/1	0.77	0.43	11,11,11,11	1
4	MG	8-B	503[H]	1/1	0.77	0.43	10,10,10,10	1
4	MG	9-B	503[I]	1/1	0.77	0.43	10,10,10,10	1
4	MG	10-B	503[J]	1/1	0.77	0.43	10,10,10,10	1
4	MG	11-B	503[K]	1/1	0.77	0.43	11,11,11,11	1
4	MG	12-B	503[L]	1/1	0.77	0.43	11,11,11,11	1
4	MG	13-B	503[M]	1/1	0.77	0.43	11,11,11,11	1
4	MG	14-B	503[N]	1/1	0.77	0.43	11,11,11,11	1
4	MG	15-B	503[O]	1/1	0.77	0.43	11,11,11,11	1
4	MG	16-B	503[P]	1/1	0.77	0.43	11,11,11,11	1
4	MG	17-B	503[Q]	1/1	0.77	0.43	11,11,11,11	1
4	MG	18-B	503[R]	1/1	0.77	0.43	11,11,11,11	1
4	MG	19-B	503[S]	1/1	0.77	0.43	11,11,11,11	1
4	MG	20-B	503[T]	1/1	0.77	0.43	10,10,10,10	1
2	ERY	1-B	501[A]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	2-B	501[B]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	3-B	501[C]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	4-B	501[D]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	5-B	501[E]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	6-B	501[F]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	7-B	501[G]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	8-B	501[H]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	9-B	501[I]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	10-B	501[J]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	11-B	501[K]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	12-B	501[L]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	13-B	501[M]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	14-B	501[N]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	15-B	501[O]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	16-B	501[P]	51/51	0.89	0.13	10,10,10,10	51

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ERY	17-B	501[Q]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	18-B	501[R]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	19-B	501[S]	51/51	0.89	0.13	10,10,10,10	51
2	ERY	20-B	501[T]	51/51	0.89	0.13	10,10,10,10	51
3	UDP	1-B	502[A]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	2-B	502[B]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	3-B	502[C]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	4-B	502[D]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	5-B	502[E]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	6-B	502[F]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	7-B	502[G]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	8-B	502[H]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	9-B	502[I]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	10-B	502[J]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	11-B	502[K]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	12-B	502[L]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	13-B	502[M]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	14-B	502[N]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	15-B	502[O]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	16-B	502[P]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	17-B	502[Q]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	18-B	502[R]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	19-B	502[S]	25/25	0.94	0.13	11,11,12,12	25
3	UDP	20-B	502[T]	25/25	0.94	0.13	11,11,12,12	25
2	ERY	1-A	1400[A]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	2-A	1400[B]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	3-A	1400[C]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	4-A	1400[D]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	5-A	1400[E]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	6-A	1400[F]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	7-A	1400[G]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	8-A	1400[H]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	9-A	1400[I]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	10-A	1400[J]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	11-A	1400[K]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	12-A	1400[L]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	13-A	1400[M]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	14-A	1400[N]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	15-A	1400[O]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	16-A	1400[P]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	17-A	1400[Q]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	18-A	1400[R]	51/51	0.95	0.08	10,10,11,11	51

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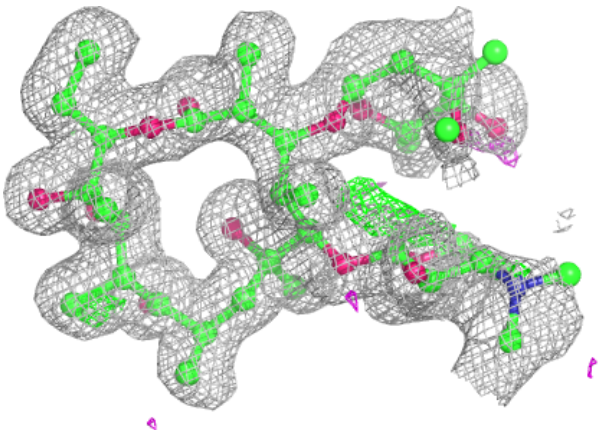
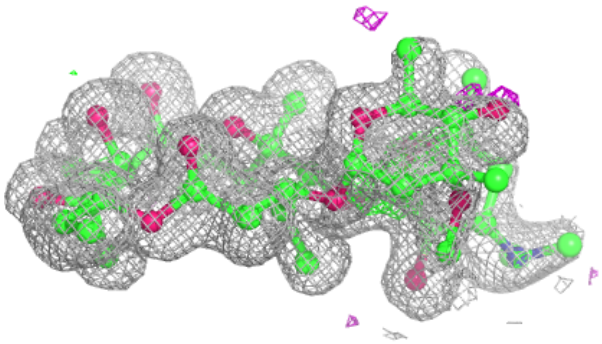
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ERY	19-A	1400[S]	51/51	0.95	0.08	10,10,11,11	51
2	ERY	20-A	1400[T]	51/51	0.95	0.08	10,10,11,11	51
3	UDP	1-A	1401[A]	25/25	0.97	0.17	11,12,12,13	25
3	UDP	2-A	1401[B]	25/25	0.97	0.17	11,12,12,13	25
3	UDP	3-A	1401[C]	25/25	0.97	0.17	11,12,12,13	25
3	UDP	4-A	1401[D]	25/25	0.97	0.17	11,12,12,12	25
3	UDP	5-A	1401[E]	25/25	0.97	0.17	11,12,12,12	25
3	UDP	6-A	1401[F]	25/25	0.97	0.17	11,12,12,13	25
3	UDP	7-A	1401[G]	25/25	0.97	0.17	12,12,12,13	25
3	UDP	8-A	1401[H]	25/25	0.97	0.17	11,12,12,13	25
3	UDP	9-A	1401[I]	25/25	0.97	0.17	11,12,12,13	25
3	UDP	10-A	1401[J]	25/25	0.97	0.17	11,12,12,13	25
3	UDP	11-A	1401[K]	25/25	0.97	0.17	11,12,12,12	25
3	UDP	12-A	1401[L]	25/25	0.97	0.17	11,12,12,13	25
3	UDP	13-A	1401[M]	25/25	0.97	0.17	11,12,12,13	25
3	UDP	14-A	1401[N]	25/25	0.97	0.17	11,12,12,13	25
3	UDP	15-A	1401[O]	25/25	0.97	0.17	12,12,13,13	25
3	UDP	16-A	1401[P]	25/25	0.97	0.17	11,12,12,13	25
3	UDP	17-A	1401[Q]	25/25	0.97	0.17	11,12,12,13	25
3	UDP	18-A	1401[R]	25/25	0.97	0.17	11,12,12,12	25
3	UDP	19-A	1401[S]	25/25	0.97	0.17	11,12,12,13	25
3	UDP	20-A	1401[T]	25/25	0.97	0.17	11,12,12,12	25

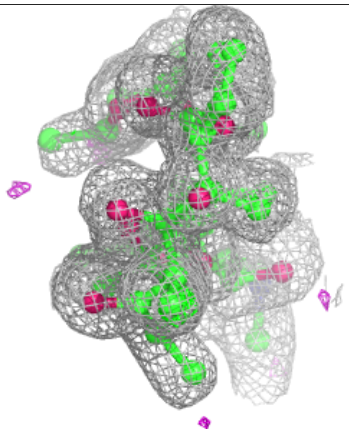
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ERY B 501 (A):

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

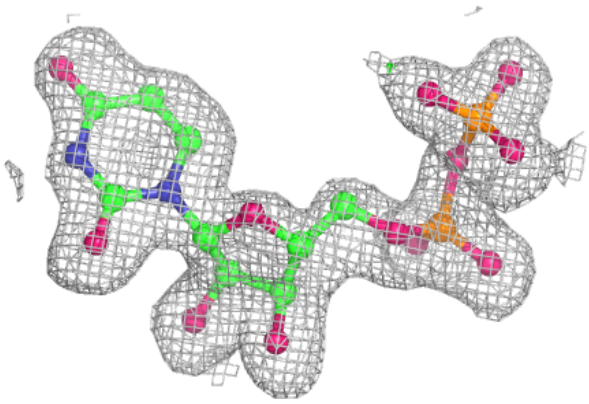


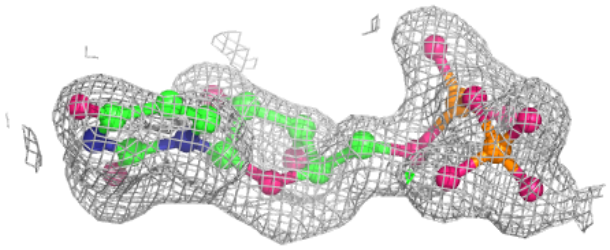


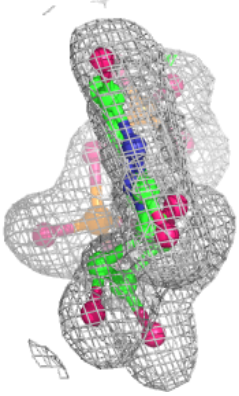


Electron density around UDP B 502 (A):

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

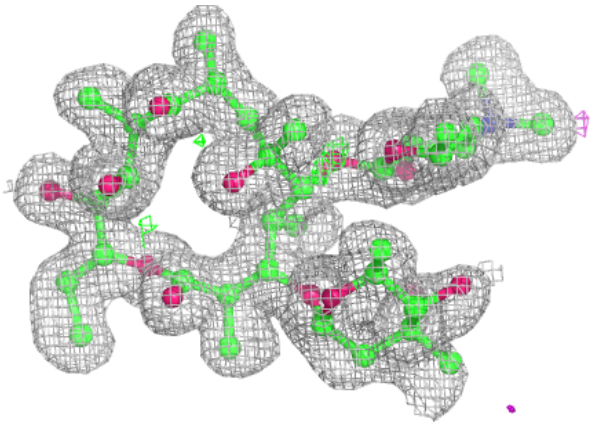


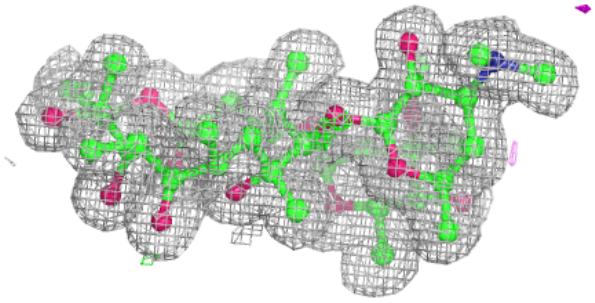


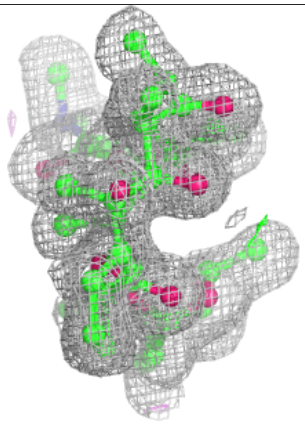


Electron density around ERY A 1400 (A):

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

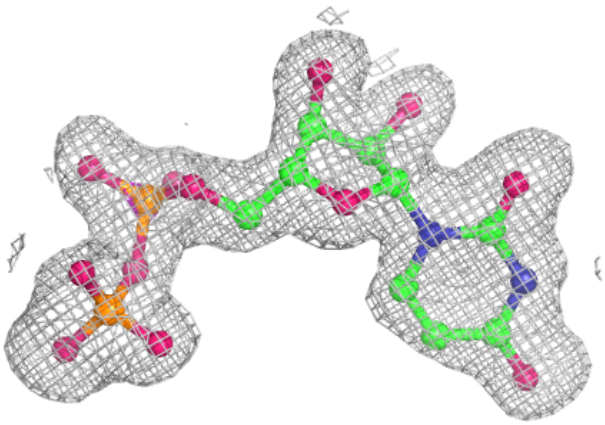


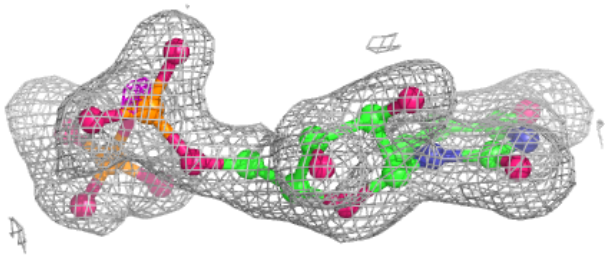


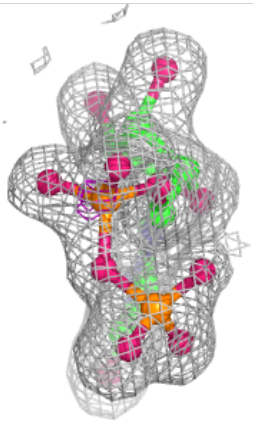


Electron density around UDP A 1401 (A):

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







6.5 Other polymers (i)

There are no such residues in this entry.