wwPDB X-ray Structure Validation Summary Report (i)

Apr 4, 2024 – 12:40 PM JST

PDB ID	:	8JWO
Title	:	Crystal structure of AKRtyl-tylosin complex
Authors	:	Lin, S.; Dai, S.; Xiao, Z.
Deposited on	:	2023-06-29
Resolution	:	2.25 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 (i)) were used in the production of this report:

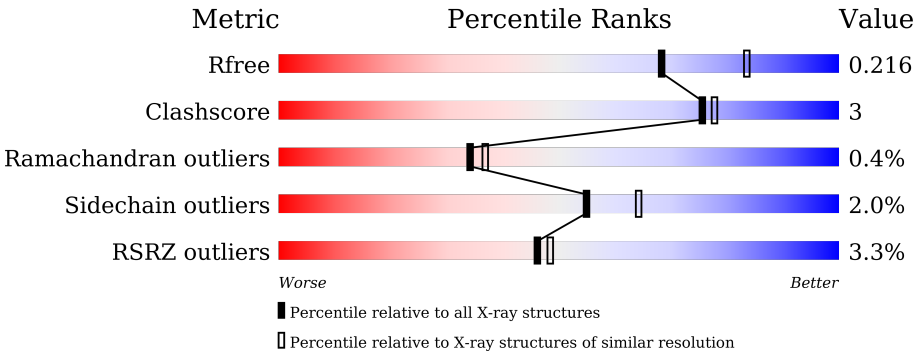
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	A	351	3% 75% 10% • 15%
1	B	351	3% 81% 7% • 11%
1	C	351	4% 77% 8% 15%
1	D	351	5% 83% 5% • 12%
1	E	351	2% 75% 9% 17%
1	F	351	5% 81% 8% 11%

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Mol	Chain	Length	Quality of chain
1	G	351	3% 76% 9% 15%
1	H	351	5% 82% 7% 11%
1	I	351	2% 79% 6% 14%
1	J	351	% 82% 8% 11%
1	K	351	3% 75% 8% 16%
1	L	351	% 83% 5% 11%
1	M	351	4% 75% 9% 15%
1	N	351	2% 82% 7% 10%
1	O	351	2% 80% 7% 13%
1	P	351	2% 83% 8% 9%

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
2	TYK	B	401	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 41183 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 Aldo/keto reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2327	1464	417	440	6			
1	B	314	Total	C	N	O	S	0	0	0
			2438	1535	435	460	8			
1	C	297	Total	C	N	O	S	0	0	0
			2312	1457	416	432	7			
1	D	310	Total	C	N	O	S	0	0	0
			2403	1515	429	451	8			
1	E	292	Total	C	N	O	S	0	0	0
			2275	1434	408	426	7			
1	F	312	Total	C	N	O	S	0	0	0
			2421	1526	432	455	8			
1	G	298	Total	C	N	O	S	0	0	0
			2320	1460	416	437	7			
1	H	313	Total	C	N	O	S	0	0	0
			2430	1531	434	457	8			
1	I	301	Total	C	N	O	S	0	0	0
			2337	1470	419	442	6			
1	J	314	Total	C	N	O	S	0	0	0
			2438	1535	435	460	8			
1	K	296	Total	C	N	O	S	0	0	0
			2302	1450	412	433	7			
1	L	311	Total	C	N	O	S	0	0	0
			2412	1521	431	452	8			
1	M	297	Total	C	N	O	S	0	0	0
			2312	1456	416	433	7			
1	N	315	Total	C	N	O	S	0	0	0
			2446	1542	436	460	8			
1	O	305	Total	C	N	O	S	0	0	0
			2376	1495	424	450	7			
1	P	318	Total	C	N	O	S	0	0	0
			2463	1549	441	465	8			

There are 320 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A3R7J519
A	-18	GLY	-	expression tag	UNP A0A3R7J519
A	-17	SER	-	expression tag	UNP A0A3R7J519
A	-16	SER	-	expression tag	UNP A0A3R7J519
A	-15	HIS	-	expression tag	UNP A0A3R7J519
A	-14	HIS	-	expression tag	UNP A0A3R7J519
A	-13	HIS	-	expression tag	UNP A0A3R7J519
A	-12	HIS	-	expression tag	UNP A0A3R7J519
A	-11	HIS	-	expression tag	UNP A0A3R7J519
A	-10	HIS	-	expression tag	UNP A0A3R7J519
A	-9	SER	-	expression tag	UNP A0A3R7J519
A	-8	SER	-	expression tag	UNP A0A3R7J519
A	-7	GLY	-	expression tag	UNP A0A3R7J519
A	-6	LEU	-	expression tag	UNP A0A3R7J519
A	-5	VAL	-	expression tag	UNP A0A3R7J519
A	-4	PRO	-	expression tag	UNP A0A3R7J519
A	-3	ARG	-	expression tag	UNP A0A3R7J519
A	-2	GLY	-	expression tag	UNP A0A3R7J519
A	-1	SER	-	expression tag	UNP A0A3R7J519
A	0	HIS	-	expression tag	UNP A0A3R7J519
B	-19	MET	-	initiating methionine	UNP A0A3R7J519
B	-18	GLY	-	expression tag	UNP A0A3R7J519
B	-17	SER	-	expression tag	UNP A0A3R7J519
B	-16	SER	-	expression tag	UNP A0A3R7J519
B	-15	HIS	-	expression tag	UNP A0A3R7J519
B	-14	HIS	-	expression tag	UNP A0A3R7J519
B	-13	HIS	-	expression tag	UNP A0A3R7J519
B	-12	HIS	-	expression tag	UNP A0A3R7J519
B	-11	HIS	-	expression tag	UNP A0A3R7J519
B	-10	HIS	-	expression tag	UNP A0A3R7J519
B	-9	SER	-	expression tag	UNP A0A3R7J519
B	-8	SER	-	expression tag	UNP A0A3R7J519
B	-7	GLY	-	expression tag	UNP A0A3R7J519
B	-6	LEU	-	expression tag	UNP A0A3R7J519
B	-5	VAL	-	expression tag	UNP A0A3R7J519
B	-4	PRO	-	expression tag	UNP A0A3R7J519
B	-3	ARG	-	expression tag	UNP A0A3R7J519
B	-2	GLY	-	expression tag	UNP A0A3R7J519
B	-1	SER	-	expression tag	UNP A0A3R7J519
B	0	HIS	-	expression tag	UNP A0A3R7J519
C	-19	MET	-	initiating methionine	UNP A0A3R7J519
C	-18	GLY	-	expression tag	UNP A0A3R7J519

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	expression tag	UNP A0A3R7J519
C	-16	SER	-	expression tag	UNP A0A3R7J519
C	-15	HIS	-	expression tag	UNP A0A3R7J519
C	-14	HIS	-	expression tag	UNP A0A3R7J519
C	-13	HIS	-	expression tag	UNP A0A3R7J519
C	-12	HIS	-	expression tag	UNP A0A3R7J519
C	-11	HIS	-	expression tag	UNP A0A3R7J519
C	-10	HIS	-	expression tag	UNP A0A3R7J519
C	-9	SER	-	expression tag	UNP A0A3R7J519
C	-8	SER	-	expression tag	UNP A0A3R7J519
C	-7	GLY	-	expression tag	UNP A0A3R7J519
C	-6	LEU	-	expression tag	UNP A0A3R7J519
C	-5	VAL	-	expression tag	UNP A0A3R7J519
C	-4	PRO	-	expression tag	UNP A0A3R7J519
C	-3	ARG	-	expression tag	UNP A0A3R7J519
C	-2	GLY	-	expression tag	UNP A0A3R7J519
C	-1	SER	-	expression tag	UNP A0A3R7J519
C	0	HIS	-	expression tag	UNP A0A3R7J519
D	-19	MET	-	initiating methionine	UNP A0A3R7J519
D	-18	GLY	-	expression tag	UNP A0A3R7J519
D	-17	SER	-	expression tag	UNP A0A3R7J519
D	-16	SER	-	expression tag	UNP A0A3R7J519
D	-15	HIS	-	expression tag	UNP A0A3R7J519
D	-14	HIS	-	expression tag	UNP A0A3R7J519
D	-13	HIS	-	expression tag	UNP A0A3R7J519
D	-12	HIS	-	expression tag	UNP A0A3R7J519
D	-11	HIS	-	expression tag	UNP A0A3R7J519
D	-10	HIS	-	expression tag	UNP A0A3R7J519
D	-9	SER	-	expression tag	UNP A0A3R7J519
D	-8	SER	-	expression tag	UNP A0A3R7J519
D	-7	GLY	-	expression tag	UNP A0A3R7J519
D	-6	LEU	-	expression tag	UNP A0A3R7J519
D	-5	VAL	-	expression tag	UNP A0A3R7J519
D	-4	PRO	-	expression tag	UNP A0A3R7J519
D	-3	ARG	-	expression tag	UNP A0A3R7J519
D	-2	GLY	-	expression tag	UNP A0A3R7J519
D	-1	SER	-	expression tag	UNP A0A3R7J519
D	0	HIS	-	expression tag	UNP A0A3R7J519
E	-19	MET	-	initiating methionine	UNP A0A3R7J519
E	-18	GLY	-	expression tag	UNP A0A3R7J519
E	-17	SER	-	expression tag	UNP A0A3R7J519
E	-16	SER	-	expression tag	UNP A0A3R7J519

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	HIS	-	expression tag	UNP A0A3R7J519
E	-14	HIS	-	expression tag	UNP A0A3R7J519
E	-13	HIS	-	expression tag	UNP A0A3R7J519
E	-12	HIS	-	expression tag	UNP A0A3R7J519
E	-11	HIS	-	expression tag	UNP A0A3R7J519
E	-10	HIS	-	expression tag	UNP A0A3R7J519
E	-9	SER	-	expression tag	UNP A0A3R7J519
E	-8	SER	-	expression tag	UNP A0A3R7J519
E	-7	GLY	-	expression tag	UNP A0A3R7J519
E	-6	LEU	-	expression tag	UNP A0A3R7J519
E	-5	VAL	-	expression tag	UNP A0A3R7J519
E	-4	PRO	-	expression tag	UNP A0A3R7J519
E	-3	ARG	-	expression tag	UNP A0A3R7J519
E	-2	GLY	-	expression tag	UNP A0A3R7J519
E	-1	SER	-	expression tag	UNP A0A3R7J519
E	0	HIS	-	expression tag	UNP A0A3R7J519
F	-19	MET	-	initiating methionine	UNP A0A3R7J519
F	-18	GLY	-	expression tag	UNP A0A3R7J519
F	-17	SER	-	expression tag	UNP A0A3R7J519
F	-16	SER	-	expression tag	UNP A0A3R7J519
F	-15	HIS	-	expression tag	UNP A0A3R7J519
F	-14	HIS	-	expression tag	UNP A0A3R7J519
F	-13	HIS	-	expression tag	UNP A0A3R7J519
F	-12	HIS	-	expression tag	UNP A0A3R7J519
F	-11	HIS	-	expression tag	UNP A0A3R7J519
F	-10	HIS	-	expression tag	UNP A0A3R7J519
F	-9	SER	-	expression tag	UNP A0A3R7J519
F	-8	SER	-	expression tag	UNP A0A3R7J519
F	-7	GLY	-	expression tag	UNP A0A3R7J519
F	-6	LEU	-	expression tag	UNP A0A3R7J519
F	-5	VAL	-	expression tag	UNP A0A3R7J519
F	-4	PRO	-	expression tag	UNP A0A3R7J519
F	-3	ARG	-	expression tag	UNP A0A3R7J519
F	-2	GLY	-	expression tag	UNP A0A3R7J519
F	-1	SER	-	expression tag	UNP A0A3R7J519
F	0	HIS	-	expression tag	UNP A0A3R7J519
G	-19	MET	-	initiating methionine	UNP A0A3R7J519
G	-18	GLY	-	expression tag	UNP A0A3R7J519
G	-17	SER	-	expression tag	UNP A0A3R7J519
G	-16	SER	-	expression tag	UNP A0A3R7J519
G	-15	HIS	-	expression tag	UNP A0A3R7J519
G	-14	HIS	-	expression tag	UNP A0A3R7J519

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	HIS	-	expression tag	UNP A0A3R7J519
G	-12	HIS	-	expression tag	UNP A0A3R7J519
G	-11	HIS	-	expression tag	UNP A0A3R7J519
G	-10	HIS	-	expression tag	UNP A0A3R7J519
G	-9	SER	-	expression tag	UNP A0A3R7J519
G	-8	SER	-	expression tag	UNP A0A3R7J519
G	-7	GLY	-	expression tag	UNP A0A3R7J519
G	-6	LEU	-	expression tag	UNP A0A3R7J519
G	-5	VAL	-	expression tag	UNP A0A3R7J519
G	-4	PRO	-	expression tag	UNP A0A3R7J519
G	-3	ARG	-	expression tag	UNP A0A3R7J519
G	-2	GLY	-	expression tag	UNP A0A3R7J519
G	-1	SER	-	expression tag	UNP A0A3R7J519
G	0	HIS	-	expression tag	UNP A0A3R7J519
H	-19	MET	-	initiating methionine	UNP A0A3R7J519
H	-18	GLY	-	expression tag	UNP A0A3R7J519
H	-17	SER	-	expression tag	UNP A0A3R7J519
H	-16	SER	-	expression tag	UNP A0A3R7J519
H	-15	HIS	-	expression tag	UNP A0A3R7J519
H	-14	HIS	-	expression tag	UNP A0A3R7J519
H	-13	HIS	-	expression tag	UNP A0A3R7J519
H	-12	HIS	-	expression tag	UNP A0A3R7J519
H	-11	HIS	-	expression tag	UNP A0A3R7J519
H	-10	HIS	-	expression tag	UNP A0A3R7J519
H	-9	SER	-	expression tag	UNP A0A3R7J519
H	-8	SER	-	expression tag	UNP A0A3R7J519
H	-7	GLY	-	expression tag	UNP A0A3R7J519
H	-6	LEU	-	expression tag	UNP A0A3R7J519
H	-5	VAL	-	expression tag	UNP A0A3R7J519
H	-4	PRO	-	expression tag	UNP A0A3R7J519
H	-3	ARG	-	expression tag	UNP A0A3R7J519
H	-2	GLY	-	expression tag	UNP A0A3R7J519
H	-1	SER	-	expression tag	UNP A0A3R7J519
H	0	HIS	-	expression tag	UNP A0A3R7J519
I	-19	MET	-	initiating methionine	UNP A0A3R7J519
I	-18	GLY	-	expression tag	UNP A0A3R7J519
I	-17	SER	-	expression tag	UNP A0A3R7J519
I	-16	SER	-	expression tag	UNP A0A3R7J519
I	-15	HIS	-	expression tag	UNP A0A3R7J519
I	-14	HIS	-	expression tag	UNP A0A3R7J519
I	-13	HIS	-	expression tag	UNP A0A3R7J519
I	-12	HIS	-	expression tag	UNP A0A3R7J519

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	HIS	-	expression tag	UNP A0A3R7J519
I	-10	HIS	-	expression tag	UNP A0A3R7J519
I	-9	SER	-	expression tag	UNP A0A3R7J519
I	-8	SER	-	expression tag	UNP A0A3R7J519
I	-7	GLY	-	expression tag	UNP A0A3R7J519
I	-6	LEU	-	expression tag	UNP A0A3R7J519
I	-5	VAL	-	expression tag	UNP A0A3R7J519
I	-4	PRO	-	expression tag	UNP A0A3R7J519
I	-3	ARG	-	expression tag	UNP A0A3R7J519
I	-2	GLY	-	expression tag	UNP A0A3R7J519
I	-1	SER	-	expression tag	UNP A0A3R7J519
I	0	HIS	-	expression tag	UNP A0A3R7J519
J	-19	MET	-	initiating methionine	UNP A0A3R7J519
J	-18	GLY	-	expression tag	UNP A0A3R7J519
J	-17	SER	-	expression tag	UNP A0A3R7J519
J	-16	SER	-	expression tag	UNP A0A3R7J519
J	-15	HIS	-	expression tag	UNP A0A3R7J519
J	-14	HIS	-	expression tag	UNP A0A3R7J519
J	-13	HIS	-	expression tag	UNP A0A3R7J519
J	-12	HIS	-	expression tag	UNP A0A3R7J519
J	-11	HIS	-	expression tag	UNP A0A3R7J519
J	-10	HIS	-	expression tag	UNP A0A3R7J519
J	-9	SER	-	expression tag	UNP A0A3R7J519
J	-8	SER	-	expression tag	UNP A0A3R7J519
J	-7	GLY	-	expression tag	UNP A0A3R7J519
J	-6	LEU	-	expression tag	UNP A0A3R7J519
J	-5	VAL	-	expression tag	UNP A0A3R7J519
J	-4	PRO	-	expression tag	UNP A0A3R7J519
J	-3	ARG	-	expression tag	UNP A0A3R7J519
J	-2	GLY	-	expression tag	UNP A0A3R7J519
J	-1	SER	-	expression tag	UNP A0A3R7J519
J	0	HIS	-	expression tag	UNP A0A3R7J519
K	-19	MET	-	initiating methionine	UNP A0A3R7J519
K	-18	GLY	-	expression tag	UNP A0A3R7J519
K	-17	SER	-	expression tag	UNP A0A3R7J519
K	-16	SER	-	expression tag	UNP A0A3R7J519
K	-15	HIS	-	expression tag	UNP A0A3R7J519
K	-14	HIS	-	expression tag	UNP A0A3R7J519
K	-13	HIS	-	expression tag	UNP A0A3R7J519
K	-12	HIS	-	expression tag	UNP A0A3R7J519
K	-11	HIS	-	expression tag	UNP A0A3R7J519
K	-10	HIS	-	expression tag	UNP A0A3R7J519

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-9	SER	-	expression tag	UNP A0A3R7J519
K	-8	SER	-	expression tag	UNP A0A3R7J519
K	-7	GLY	-	expression tag	UNP A0A3R7J519
K	-6	LEU	-	expression tag	UNP A0A3R7J519
K	-5	VAL	-	expression tag	UNP A0A3R7J519
K	-4	PRO	-	expression tag	UNP A0A3R7J519
K	-3	ARG	-	expression tag	UNP A0A3R7J519
K	-2	GLY	-	expression tag	UNP A0A3R7J519
K	-1	SER	-	expression tag	UNP A0A3R7J519
K	0	HIS	-	expression tag	UNP A0A3R7J519
L	-19	MET	-	initiating methionine	UNP A0A3R7J519
L	-18	GLY	-	expression tag	UNP A0A3R7J519
L	-17	SER	-	expression tag	UNP A0A3R7J519
L	-16	SER	-	expression tag	UNP A0A3R7J519
L	-15	HIS	-	expression tag	UNP A0A3R7J519
L	-14	HIS	-	expression tag	UNP A0A3R7J519
L	-13	HIS	-	expression tag	UNP A0A3R7J519
L	-12	HIS	-	expression tag	UNP A0A3R7J519
L	-11	HIS	-	expression tag	UNP A0A3R7J519
L	-10	HIS	-	expression tag	UNP A0A3R7J519
L	-9	SER	-	expression tag	UNP A0A3R7J519
L	-8	SER	-	expression tag	UNP A0A3R7J519
L	-7	GLY	-	expression tag	UNP A0A3R7J519
L	-6	LEU	-	expression tag	UNP A0A3R7J519
L	-5	VAL	-	expression tag	UNP A0A3R7J519
L	-4	PRO	-	expression tag	UNP A0A3R7J519
L	-3	ARG	-	expression tag	UNP A0A3R7J519
L	-2	GLY	-	expression tag	UNP A0A3R7J519
L	-1	SER	-	expression tag	UNP A0A3R7J519
L	0	HIS	-	expression tag	UNP A0A3R7J519
M	-19	MET	-	initiating methionine	UNP A0A3R7J519
M	-18	GLY	-	expression tag	UNP A0A3R7J519
M	-17	SER	-	expression tag	UNP A0A3R7J519
M	-16	SER	-	expression tag	UNP A0A3R7J519
M	-15	HIS	-	expression tag	UNP A0A3R7J519
M	-14	HIS	-	expression tag	UNP A0A3R7J519
M	-13	HIS	-	expression tag	UNP A0A3R7J519
M	-12	HIS	-	expression tag	UNP A0A3R7J519
M	-11	HIS	-	expression tag	UNP A0A3R7J519
M	-10	HIS	-	expression tag	UNP A0A3R7J519
M	-9	SER	-	expression tag	UNP A0A3R7J519
M	-8	SER	-	expression tag	UNP A0A3R7J519

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-7	GLY	-	expression tag	UNP A0A3R7J519
M	-6	LEU	-	expression tag	UNP A0A3R7J519
M	-5	VAL	-	expression tag	UNP A0A3R7J519
M	-4	PRO	-	expression tag	UNP A0A3R7J519
M	-3	ARG	-	expression tag	UNP A0A3R7J519
M	-2	GLY	-	expression tag	UNP A0A3R7J519
M	-1	SER	-	expression tag	UNP A0A3R7J519
M	0	HIS	-	expression tag	UNP A0A3R7J519
N	-19	MET	-	initiating methionine	UNP A0A3R7J519
N	-18	GLY	-	expression tag	UNP A0A3R7J519
N	-17	SER	-	expression tag	UNP A0A3R7J519
N	-16	SER	-	expression tag	UNP A0A3R7J519
N	-15	HIS	-	expression tag	UNP A0A3R7J519
N	-14	HIS	-	expression tag	UNP A0A3R7J519
N	-13	HIS	-	expression tag	UNP A0A3R7J519
N	-12	HIS	-	expression tag	UNP A0A3R7J519
N	-11	HIS	-	expression tag	UNP A0A3R7J519
N	-10	HIS	-	expression tag	UNP A0A3R7J519
N	-9	SER	-	expression tag	UNP A0A3R7J519
N	-8	SER	-	expression tag	UNP A0A3R7J519
N	-7	GLY	-	expression tag	UNP A0A3R7J519
N	-6	LEU	-	expression tag	UNP A0A3R7J519
N	-5	VAL	-	expression tag	UNP A0A3R7J519
N	-4	PRO	-	expression tag	UNP A0A3R7J519
N	-3	ARG	-	expression tag	UNP A0A3R7J519
N	-2	GLY	-	expression tag	UNP A0A3R7J519
N	-1	SER	-	expression tag	UNP A0A3R7J519
N	0	HIS	-	expression tag	UNP A0A3R7J519
O	-19	MET	-	initiating methionine	UNP A0A3R7J519
O	-18	GLY	-	expression tag	UNP A0A3R7J519
O	-17	SER	-	expression tag	UNP A0A3R7J519
O	-16	SER	-	expression tag	UNP A0A3R7J519
O	-15	HIS	-	expression tag	UNP A0A3R7J519
O	-14	HIS	-	expression tag	UNP A0A3R7J519
O	-13	HIS	-	expression tag	UNP A0A3R7J519
O	-12	HIS	-	expression tag	UNP A0A3R7J519
O	-11	HIS	-	expression tag	UNP A0A3R7J519
O	-10	HIS	-	expression tag	UNP A0A3R7J519
O	-9	SER	-	expression tag	UNP A0A3R7J519
O	-8	SER	-	expression tag	UNP A0A3R7J519
O	-7	GLY	-	expression tag	UNP A0A3R7J519
O	-6	LEU	-	expression tag	UNP A0A3R7J519

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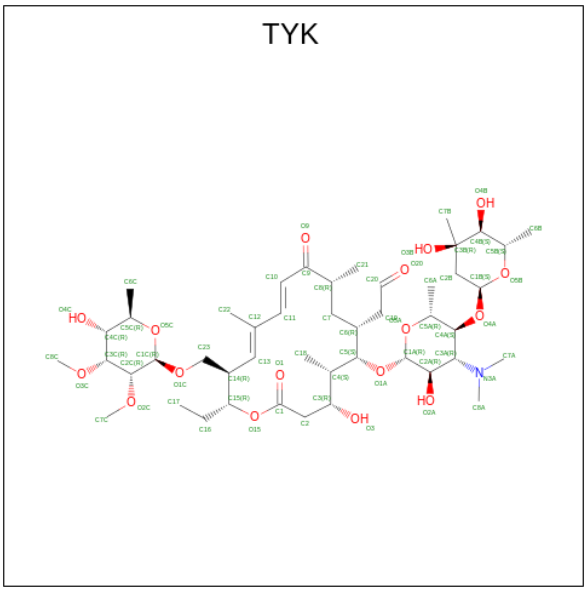
Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	VAL	-	expression tag	UNP A0A3R7J519
O	-4	PRO	-	expression tag	UNP A0A3R7J519
O	-3	ARG	-	expression tag	UNP A0A3R7J519
O	-2	GLY	-	expression tag	UNP A0A3R7J519
O	-1	SER	-	expression tag	UNP A0A3R7J519
O	0	HIS	-	expression tag	UNP A0A3R7J519
P	-19	MET	-	initiating methionine	UNP A0A3R7J519
P	-18	GLY	-	expression tag	UNP A0A3R7J519
P	-17	SER	-	expression tag	UNP A0A3R7J519
P	-16	SER	-	expression tag	UNP A0A3R7J519
P	-15	HIS	-	expression tag	UNP A0A3R7J519
P	-14	HIS	-	expression tag	UNP A0A3R7J519
P	-13	HIS	-	expression tag	UNP A0A3R7J519
P	-12	HIS	-	expression tag	UNP A0A3R7J519
P	-11	HIS	-	expression tag	UNP A0A3R7J519
P	-10	HIS	-	expression tag	UNP A0A3R7J519
P	-9	SER	-	expression tag	UNP A0A3R7J519
P	-8	SER	-	expression tag	UNP A0A3R7J519
P	-7	GLY	-	expression tag	UNP A0A3R7J519
P	-6	LEU	-	expression tag	UNP A0A3R7J519
P	-5	VAL	-	expression tag	UNP A0A3R7J519
P	-4	PRO	-	expression tag	UNP A0A3R7J519
P	-3	ARG	-	expression tag	UNP A0A3R7J519
P	-2	GLY	-	expression tag	UNP A0A3R7J519
P	-1	SER	-	expression tag	UNP A0A3R7J519
P	0	HIS	-	expression tag	UNP A0A3R7J519

- Molecule 2 is TYLOSIN (three-letter code: TYK) (formula: $C_{46}H_{77}NO_{17}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			64	46	1	17		
2	B	1	Total	C	N	O	0	0
			64	46	1	17		
2	C	1	Total	C	N	O	0	0
			64	46	1	17		
2	D	1	Total	C	N	O	0	0
			64	46	1	17		
2	E	1	Total	C	N	O	0	0
			64	46	1	17		
2	F	1	Total	C	N	O	0	0
			64	46	1	17		
2	G	1	Total	C	N	O	0	0
			64	46	1	17		
2	H	1	Total	C	N	O	0	0
			64	46	1	17		
2	I	1	Total	C	N	O	0	0
			64	46	1	17		
2	J	1	Total	C	N	O	0	0
			64	46	1	17		
2	K	1	Total	C	N	O	0	0
			64	46	1	17		
2	L	1	Total	C	N	O	0	0
			64	46	1	17		
2	M	1	Total	C	N	O	0	0
			64	46	1	17		
2	N	1	Total	C	N	O	0	0
			64	46	1	17		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	O	1	Total C N O 64 46 1 17	0	0
2	P	1	Total C N O 64 46 1 17	0	0

- Molecule 3 is water.

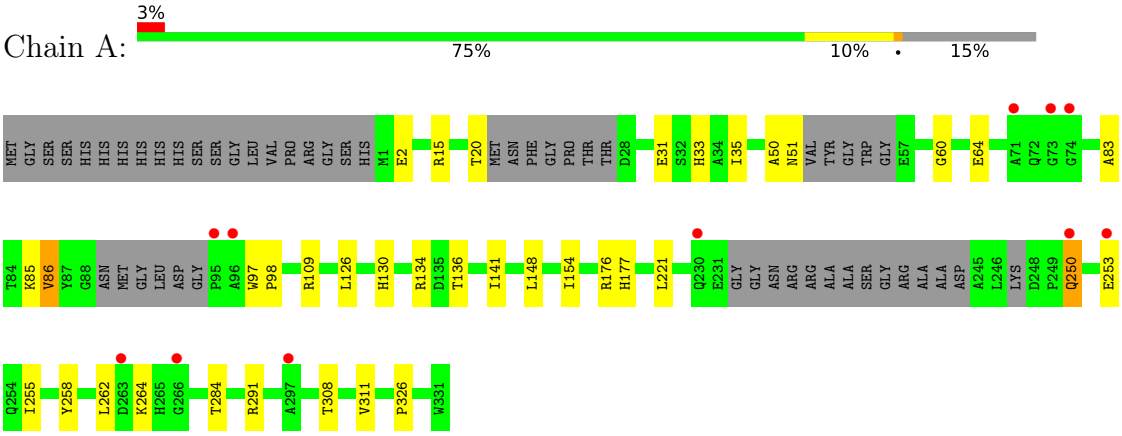
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	110	Total O 110 110	0	0
3	B	144	Total O 144 144	0	0
3	C	112	Total O 112 112	0	0
3	D	128	Total O 128 128	0	0
3	E	104	Total O 104 104	0	0
3	F	118	Total O 118 118	0	0
3	G	109	Total O 109 109	0	0
3	H	126	Total O 126 126	0	0
3	I	137	Total O 137 137	0	0
3	J	163	Total O 163 163	0	0
3	K	121	Total O 121 121	0	0
3	L	183	Total O 183 183	0	0
3	M	117	Total O 117 117	0	0
3	N	169	Total O 169 169	0	0
3	O	132	Total O 132 132	0	0
3	P	174	Total O 174 174	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.

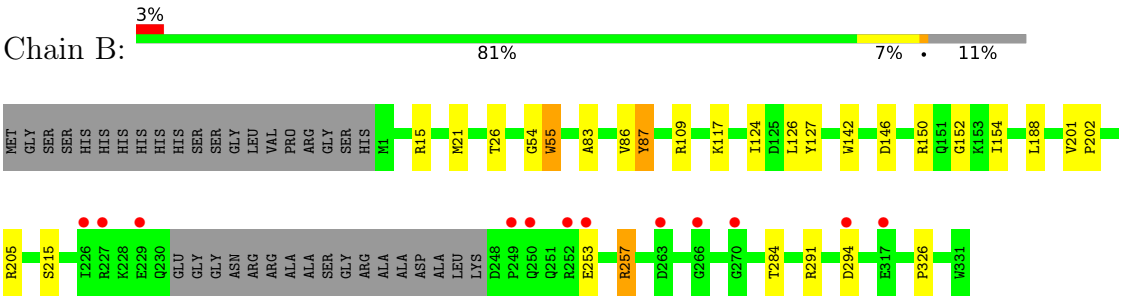
• Molecule 1: Aldo/keto reductase

Chain A:



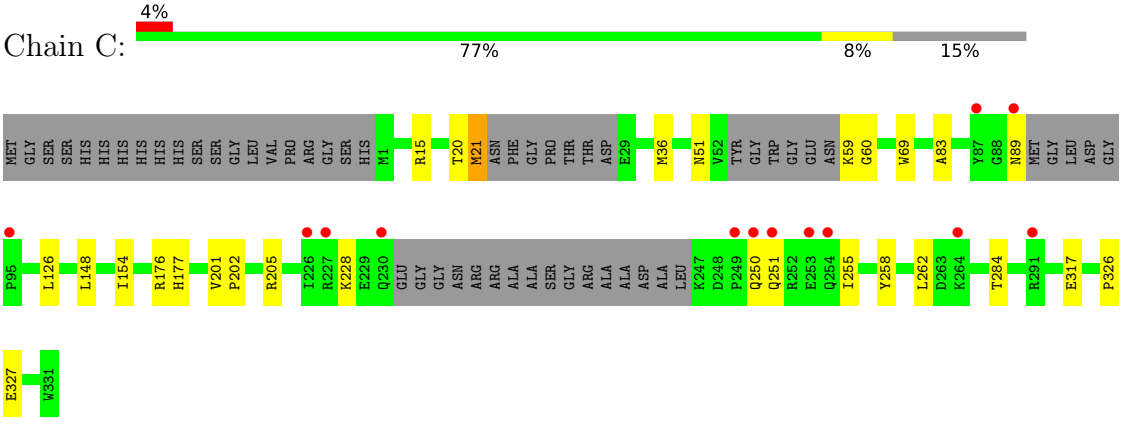
• Molecule 1: Aldo/keto reductase

Chain B:



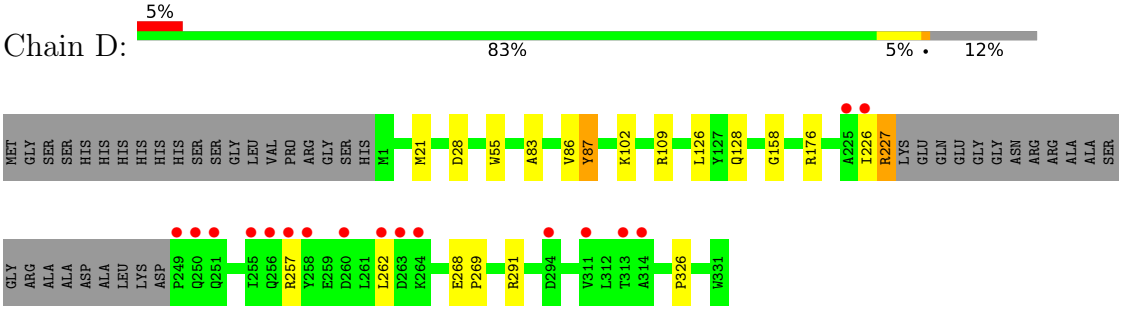
• Molecule 1: Aldo/keto reductase

Chain C:



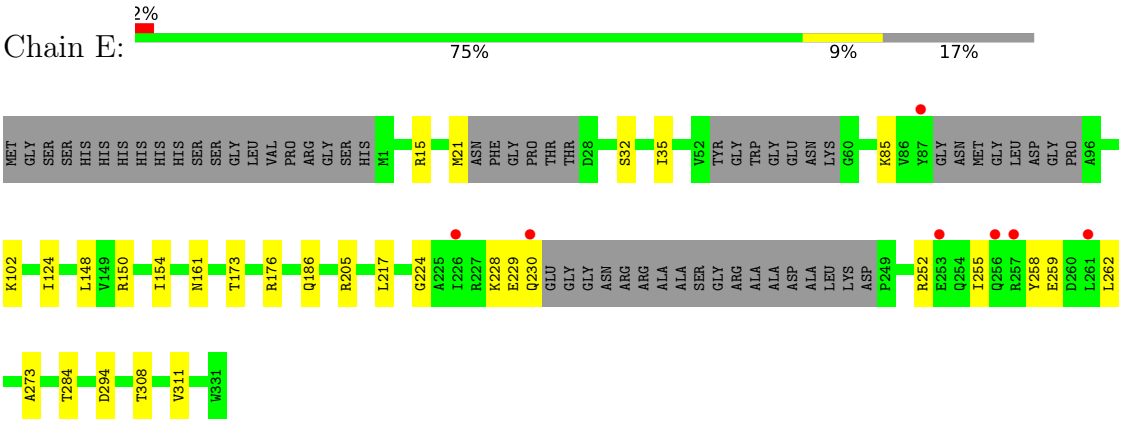
• Molecule 1: Aldo/keto reductase

Chain D:



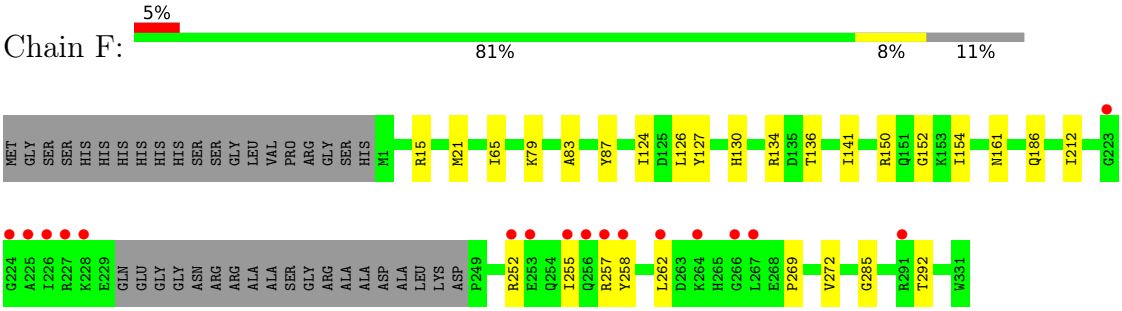
• Molecule 1: Aldo/keto reductase

Chain E:



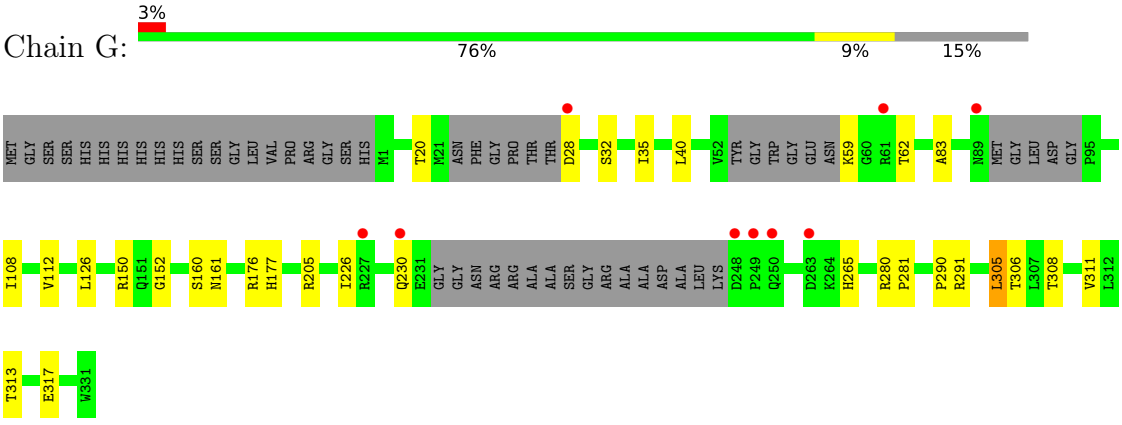
• Molecule 1: Aldo/keto reductase

Chain F:



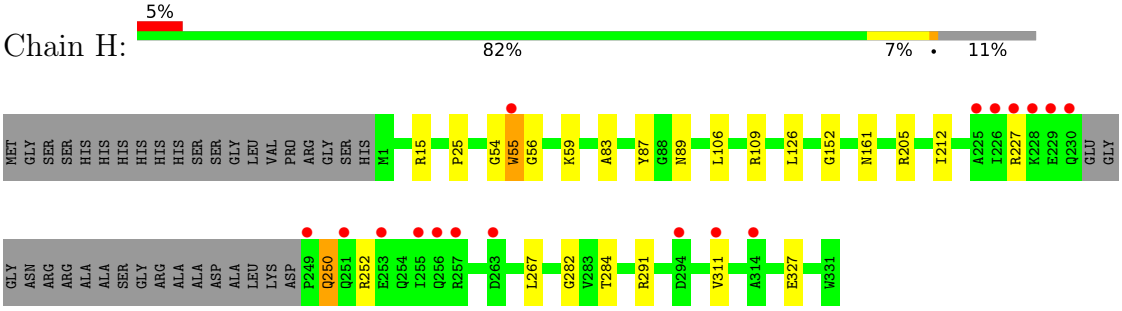
• Molecule 1: Aldo/keto reductase

Chain G:



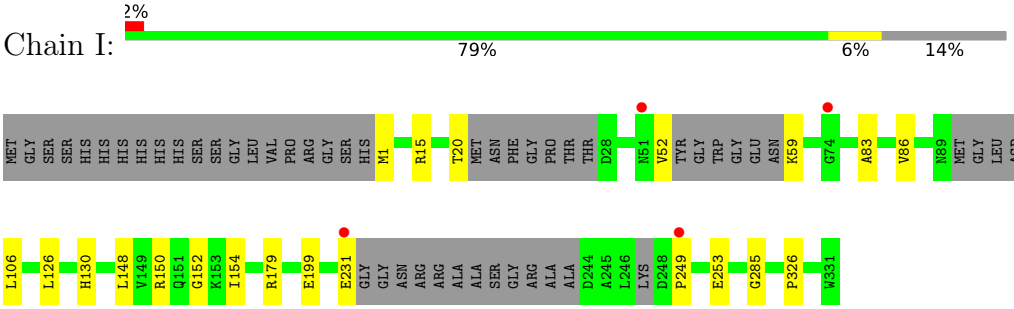
• Molecule 1: Aldo/keto reductase

Chain H:



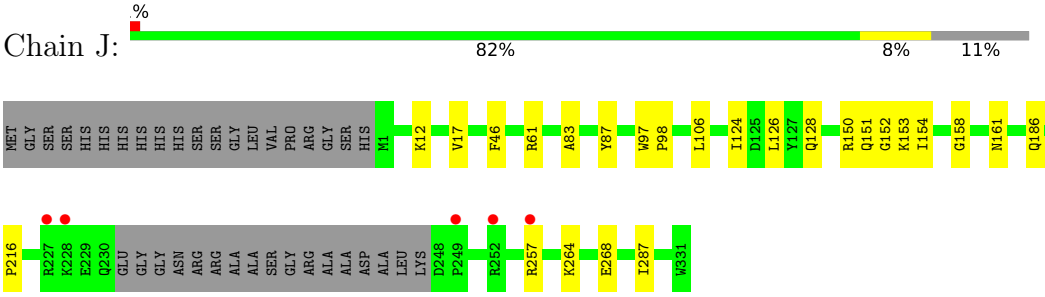
• Molecule 1: Aldo/keto reductase

Chain I:



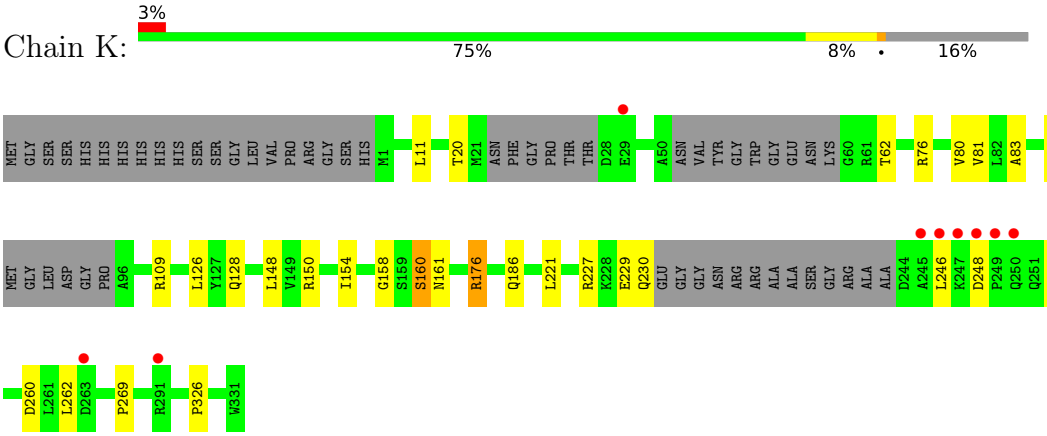
• Molecule 1: Aldo/keto reductase

Chain J:



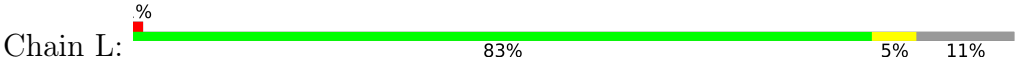
• Molecule 1: Aldo/keto reductase

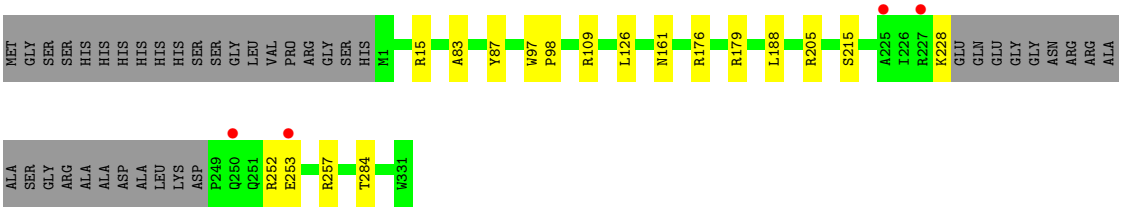
Chain K:



• Molecule 1: Aldo/keto reductase

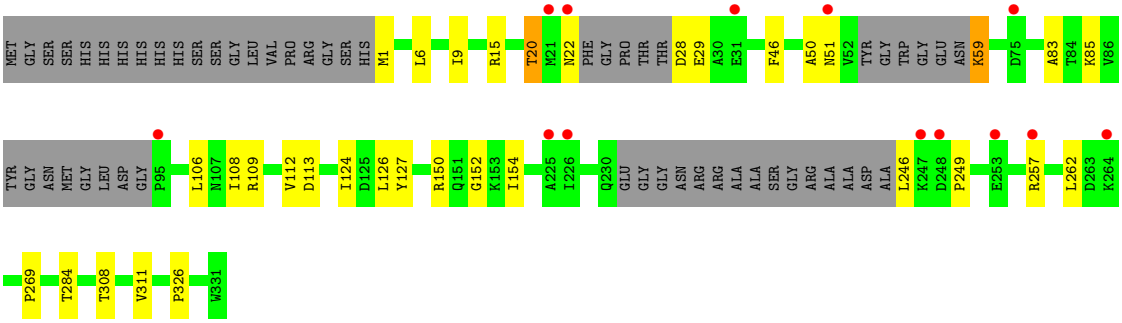
Chain L:





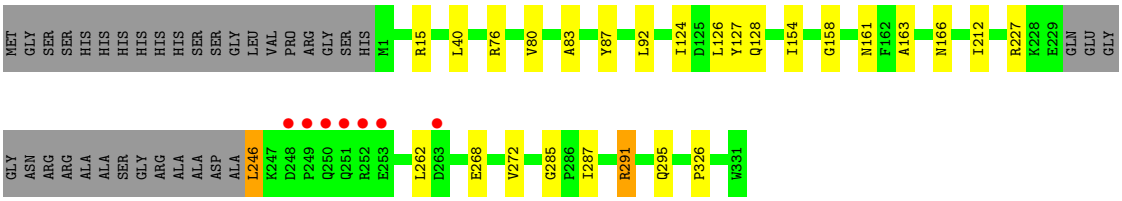
• Molecule 1: Aldo/keto reductase

Chain M:



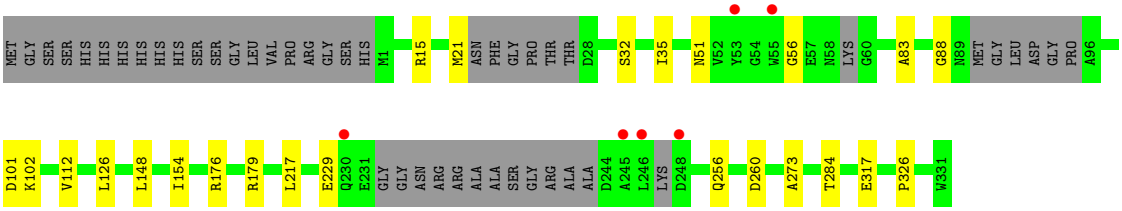
• Molecule 1: Aldo/keto reductase

Chain N:



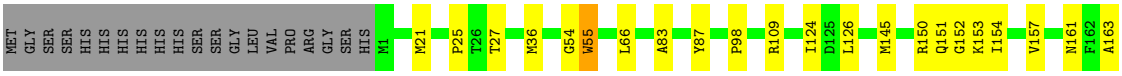
• Molecule 1: Aldo/keto reductase

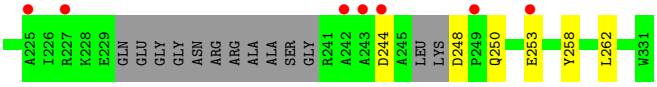
Chain O:



• Molecule 1: Aldo/keto reductase

Chain P:




A225
I226
R227
K228
E229
GLN
GLU
GLY
GLY
ASN
ARG
ARG
ALA
ALA
SER
GLY
R241
A242
A243
D244
A245
LEU
LYS
D248
P249
Q250
E253
Y258
L262
W331

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	111.02Å 111.02Å 560.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 2.25 49.74 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.74-2.25) 99.2 (49.74-2.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.181 , 0.216 0.181 , 0.216	Depositor DCC
R_{free} test set	15542 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.041 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	41183	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3485e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: TYK

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	A	0.45	0/2373	0.69	0/3216
1	B	0.44	0/2493	0.73	0/3387
1	C	0.44	0/2359	0.71	0/3197
1	D	0.45	0/2458	0.71	0/3340
1	E	0.42	0/2321	0.70	0/3147
1	F	0.43	0/2476	0.72	0/3363
1	G	0.43	0/2367	0.70	0/3209
1	H	0.44	0/2485	0.73	0/3375
1	I	0.45	0/2383	0.73	0/3231
1	J	0.45	0/2493	0.71	0/3387
1	K	0.45	0/2348	0.71	0/3183
1	L	0.47	0/2467	0.72	0/3351
1	M	0.43	0/2358	0.73	0/3196
1	N	0.48	0/2501	0.73	0/3397
1	O	0.47	0/2424	0.71	0/3287
1	P	0.46	0/2517	0.74	0/3418
All	All	0.45	0/38823	0.72	0/52684

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2327	0	2276	24	0
1	B	2438	0	2375	15	0
1	C	2312	0	2276	18	0
1	D	2403	0	2345	11	0
1	E	2275	0	2234	19	0
1	F	2421	0	2364	15	0
1	G	2320	0	2273	17	0
1	H	2430	0	2372	13	0
1	I	2337	0	2285	13	0
1	J	2438	0	2375	16	0
1	K	2302	0	2258	19	0
1	L	2412	0	2358	12	0
1	M	2312	0	2279	18	0
1	N	2446	0	2391	14	0
1	O	2376	0	2308	15	0
1	P	2463	0	2398	17	0
2	A	64	0	77	2	0
2	B	64	0	77	0	0
2	C	64	0	77	5	0
2	D	64	0	77	1	0
2	E	64	0	77	4	0
2	F	64	0	77	3	0
2	G	64	0	77	0	0
2	H	64	0	77	0	0
2	I	64	0	77	0	0
2	J	64	0	77	0	0
2	K	64	0	77	1	0
2	L	64	0	77	0	0
2	M	64	0	77	0	0
2	N	64	0	77	0	0
2	O	64	0	77	2	0
2	P	64	0	77	0	0
3	A	110	0	0	2	0
3	B	144	0	0	1	0
3	C	112	0	0	3	0
3	D	128	0	0	1	0
3	E	104	0	0	0	0
3	F	118	0	0	2	0
3	G	109	0	0	2	0
3	H	126	0	0	0	0
3	I	137	0	0	3	0
3	J	163	0	0	2	0
3	K	121	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	183	0	0	0	0
3	M	117	0	0	2	0
3	N	169	0	0	0	0
3	O	132	0	0	0	0
3	P	174	0	0	1	0
All	All	41183	0	38399	242	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 3.

The worst 5 of 242 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:G:20:THR:HG21	1:G:62:THR:HG21	1.51	0.90
1:B:26:THR:HG21	1:B:291:ARG:HD3	1.66	0.76
1:D:176:ARG:HD3	1:G:176:ARG:HG2	1.69	0.74
1:K:176:ARG:NH1	3:K:502:HOH:O	2.22	0.71
2:E:401:TYK:H221	2:E:401:TYK:C23	2.20	0.71

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	A	287/351 (82%)	281 (98%)	6 (2%)	0	100	100
1	B	310/351 (88%)	299 (96%)	9 (3%)	2 (1%)	25	25
1	C	287/351 (82%)	278 (97%)	8 (3%)	1 (0%)	41	46
1	D	306/351 (87%)	293 (96%)	11 (4%)	2 (1%)	22	21
1	E	282/351 (80%)	275 (98%)	6 (2%)	1 (0%)	34	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	308/351 (88%)	296 (96%)	11 (4%)	1 (0%)	41	46
1	G	288/351 (82%)	279 (97%)	9 (3%)	0	100	100
1	H	309/351 (88%)	299 (97%)	7 (2%)	3 (1%)	15	13
1	I	289/351 (82%)	281 (97%)	8 (3%)	0	100	100
1	J	310/351 (88%)	300 (97%)	9 (3%)	1 (0%)	41	46
1	K	286/351 (82%)	276 (96%)	9 (3%)	1 (0%)	41	46
1	L	307/351 (88%)	298 (97%)	8 (3%)	1 (0%)	41	46
1	M	287/351 (82%)	279 (97%)	7 (2%)	1 (0%)	41	46
1	N	311/351 (89%)	300 (96%)	10 (3%)	1 (0%)	41	46
1	O	293/351 (84%)	288 (98%)	5 (2%)	0	100	100
1	P	312/351 (89%)	299 (96%)	11 (4%)	2 (1%)	25	25
All	All	4772/5616 (85%)	4621 (97%)	134 (3%)	17 (0%)	34	37

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	87	TYR
1	D	87	TYR
1	F	87	TYR
1	H	87	TYR
1	J	87	TYR

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	A	238/275 (86%)	232 (98%)	6 (2%)	47	56
1	B	249/275 (90%)	243 (98%)	6 (2%)	49	58
1	C	237/275 (86%)	233 (98%)	4 (2%)	60	71
1	D	245/275 (89%)	240 (98%)	5 (2%)	55	64
1	E	233/275 (85%)	231 (99%)	2 (1%)	78	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	247/275 (90%)	241 (98%)	6 (2%)	49	58
1	G	238/275 (86%)	231 (97%)	7 (3%)	42	51
1	H	248/275 (90%)	241 (97%)	7 (3%)	43	52
1	I	239/275 (87%)	235 (98%)	4 (2%)	60	71
1	J	249/275 (90%)	247 (99%)	2 (1%)	81	88
1	K	235/275 (86%)	231 (98%)	4 (2%)	60	71
1	L	246/275 (90%)	244 (99%)	2 (1%)	81	88
1	M	238/275 (86%)	229 (96%)	9 (4%)	33	39
1	N	250/275 (91%)	244 (98%)	6 (2%)	49	58
1	O	242/275 (88%)	239 (99%)	3 (1%)	71	80
1	P	250/275 (91%)	246 (98%)	4 (2%)	62	73
All	All	3884/4400 (88%)	3807 (98%)	77 (2%)	55	64

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	28	ASP
1	O	179	ARG
1	M	59	LYS
1	N	92	LEU
1	P	244	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	130	HIS
1	J	256	GLN
1	L	186	GLN
1	L	128	GLN
1	F	130	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)

16 ligands 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	$\#\|Z\| > 2$
2	TYK	P	401	-	67,67,67	0.75	2 (2%)	83,97,97	0.92	5 (6%)
2	TYK	E	401	-	67,67,67	0.73	3 (4%)	83,97,97	0.82	2 (2%)
2	TYK	C	401	-	67,67,67	0.66	1 (1%)	83,97,97	1.24	4 (4%)
2	TYK	K	401	-	67,67,67	0.65	2 (2%)	83,97,97	0.68	0
2	TYK	M	401	-	67,67,67	0.67	0	83,97,97	1.01	4 (4%)
2	TYK	I	401	-	67,67,67	0.69	1 (1%)	83,97,97	0.83	2 (2%)
2	TYK	D	401	-	67,67,67	0.73	2 (2%)	83,97,97	1.20	7 (8%)
2	TYK	N	401	-	67,67,67	0.79	2 (2%)	83,97,97	0.84	4 (4%)
2	TYK	H	401	-	67,67,67	0.64	1 (1%)	83,97,97	0.75	3 (3%)
2	TYK	O	401	-	67,67,67	0.71	1 (1%)	83,97,97	0.74	1 (1%)
2	TYK	L	401	-	67,67,67	0.71	1 (1%)	83,97,97	0.90	4 (4%)
2	TYK	J	401	-	67,67,67	0.74	2 (2%)	83,97,97	0.74	3 (3%)
2	TYK	G	401	-	67,67,67	0.75	2 (2%)	83,97,97	0.83	1 (1%)
2	TYK	A	401	-	67,67,67	0.74	2 (2%)	83,97,97	1.20	5 (6%)
2	TYK	B	401	-	67,67,67	0.69	1 (1%)	83,97,97	1.02	4 (4%)
2	TYK	F	401	-	67,67,67	0.73	2 (2%)	83,97,97	1.09	3 (3%)

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	TYK	P	401	-	-	15/67/126/126	0/3/4/4
2	TYK	E	401	-	-	19/67/126/126	0/3/4/4
2	TYK	C	401	-	-	18/67/126/126	0/3/4/4
2	TYK	K	401	-	-	10/67/126/126	0/3/4/4
2	TYK	M	401	-	-	11/67/126/126	0/3/4/4
2	TYK	I	401	-	-	17/67/126/126	0/3/4/4
2	TYK	D	401	-	-	15/67/126/126	0/3/4/4
2	TYK	N	401	-	-	8/67/126/126	0/3/4/4
2	TYK	H	401	-	-	18/67/126/126	0/3/4/4
2	TYK	O	401	-	-	10/67/126/126	0/3/4/4
2	TYK	L	401	-	-	18/67/126/126	0/3/4/4
2	TYK	J	401	-	-	18/67/126/126	0/3/4/4
2	TYK	G	401	-	-	17/67/126/126	0/3/4/4
2	TYK	A	401	-	-	16/67/126/126	0/3/4/4
2	TYK	B	401	-	-	22/67/126/126	0/3/4/4
2	TYK	F	401	-	-	16/67/126/126	0/3/4/4

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	401	TYK	C6-C5	3.24	1.59	1.52
2	F	401	TYK	C11-C10	3.17	1.42	1.33
2	D	401	TYK	C6-C5	3.06	1.58	1.52
2	F	401	TYK	C6-C5	3.02	1.58	1.52
2	J	401	TYK	O1C-C23	3.01	1.49	1.43

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	TYK	C10-C11-C12	7.42	137.45	126.23
2	A	401	TYK	C10-C11-C12	7.35	137.34	126.23
2	F	401	TYK	C10-C11-C12	7.26	137.21	126.23
2	D	401	TYK	C10-C11-C12	6.95	136.74	126.23
2	B	401	TYK	O1A-C5-C4	4.33	113.44	108.22

There are no chirality outliers.

5 of 248 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	TYK	C21-C8-C9-C10
2	A	401	TYK	C21-C8-C9-O9
2	A	401	TYK	C10-C11-C12-C13
2	A	401	TYK	C10-C11-C12-C22
2	A	401	TYK	C13-C14-C15-C16

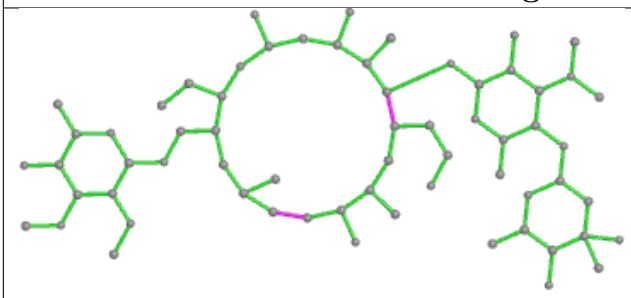
There are no ring outliers.

7 monomers are involved in 18 short contacts:

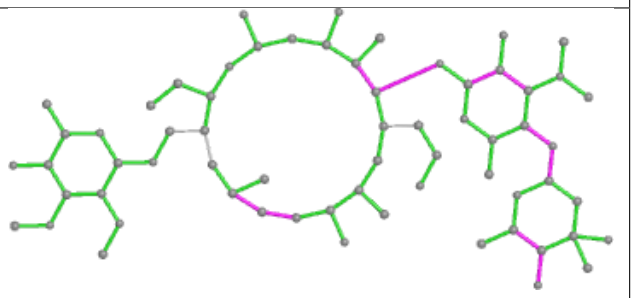
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	TYK	4	0
2	C	401	TYK	5	0
2	K	401	TYK	1	0
2	D	401	TYK	1	0
2	O	401	TYK	2	0
2	A	401	TYK	2	0
2	F	401	TYK	3	0

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.

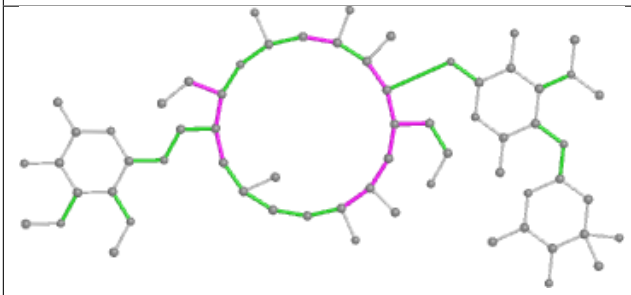
Ligand TYK P 401



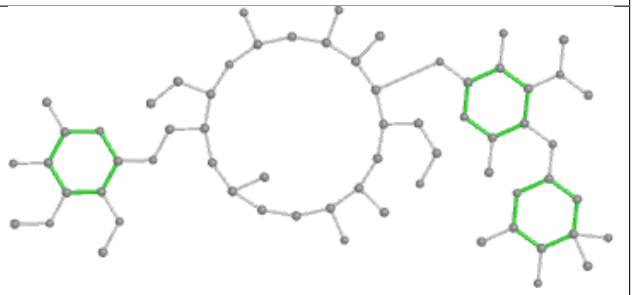
Bond lengths



Bond angles

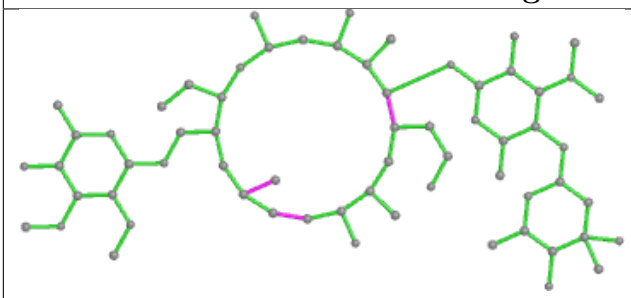


Torsions



Rings

Ligand TYK E 401



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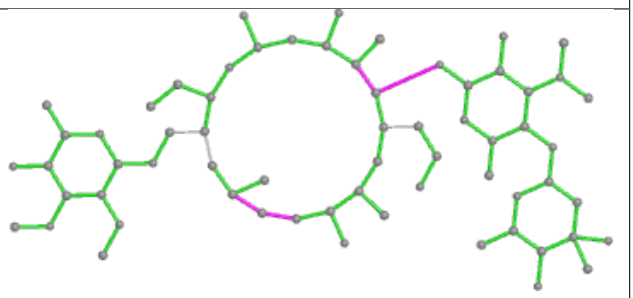

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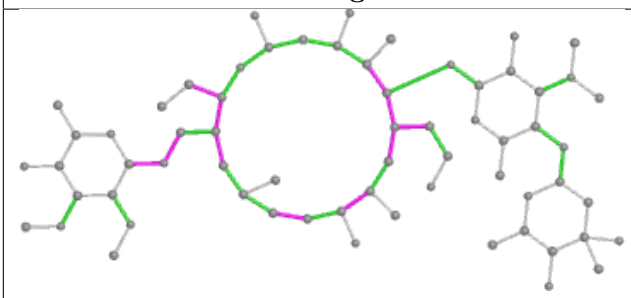

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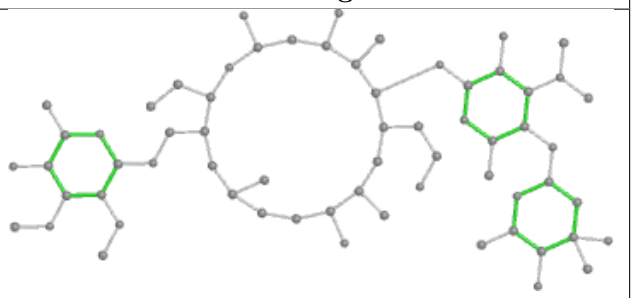

Rings

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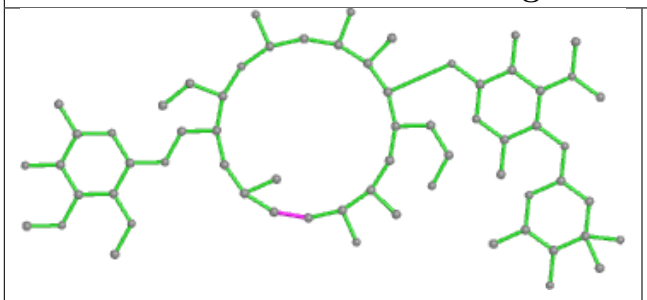

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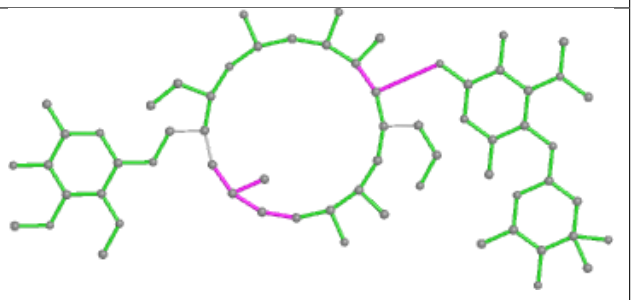

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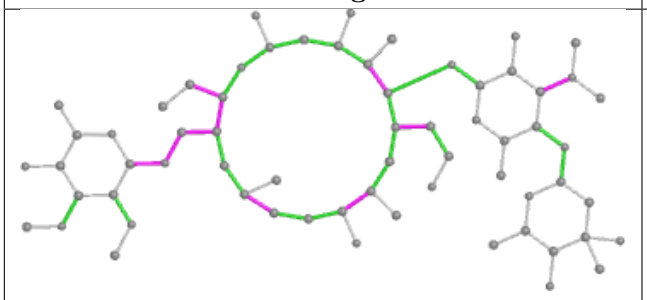

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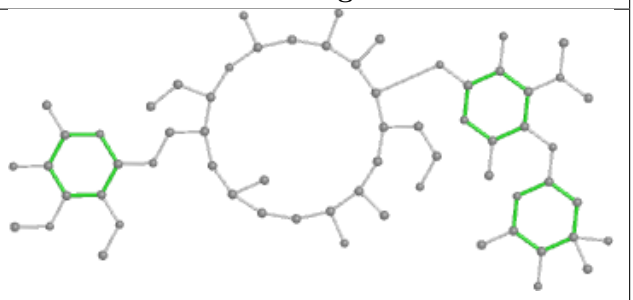

Rings

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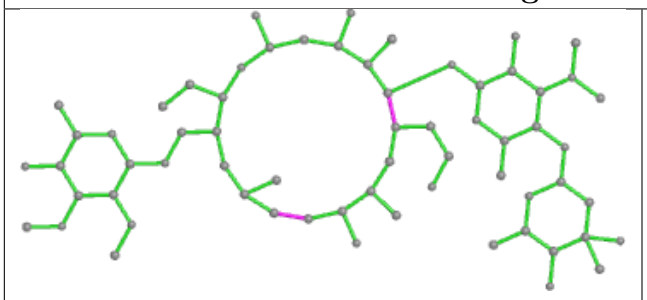

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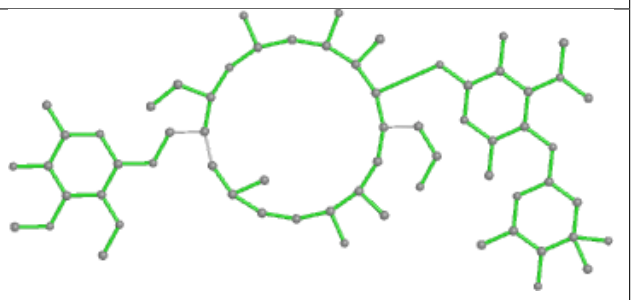

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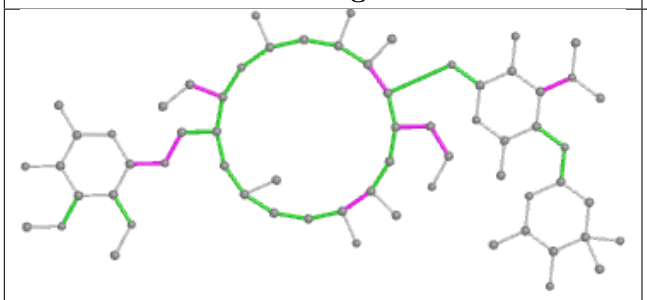

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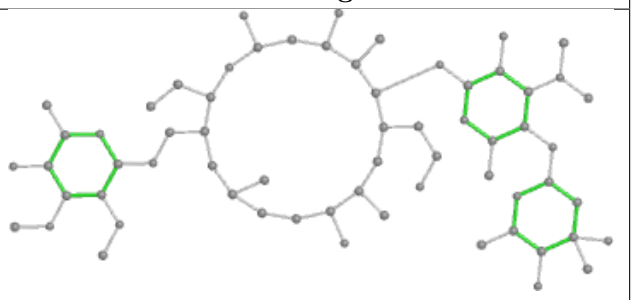
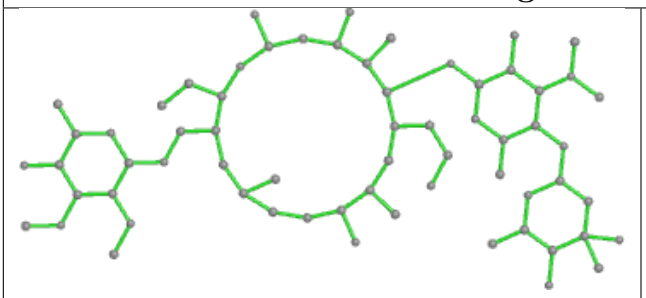


Rings

Ligand TYK M 401



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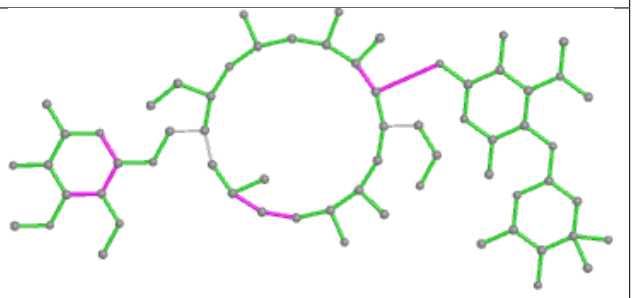

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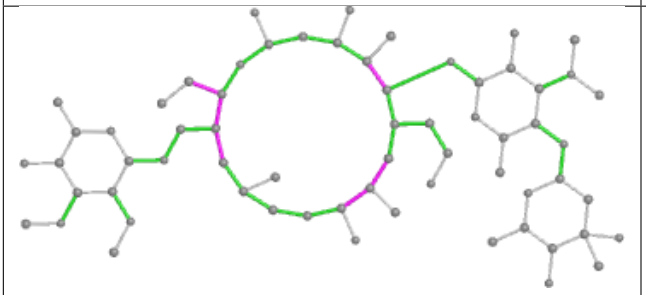

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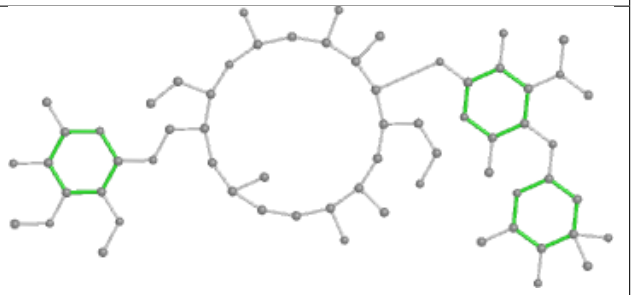
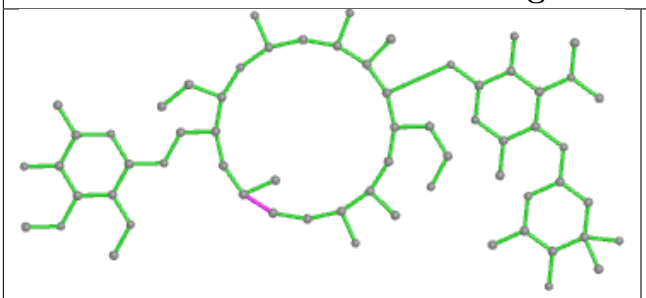


Rings

Ligand TYK I 401



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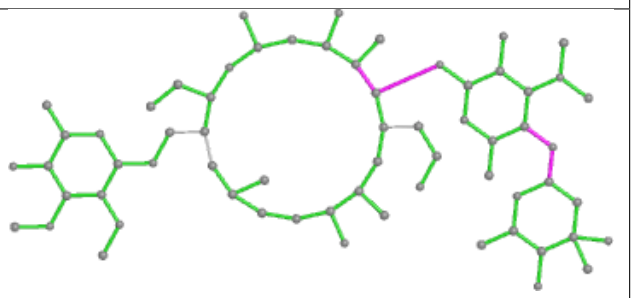

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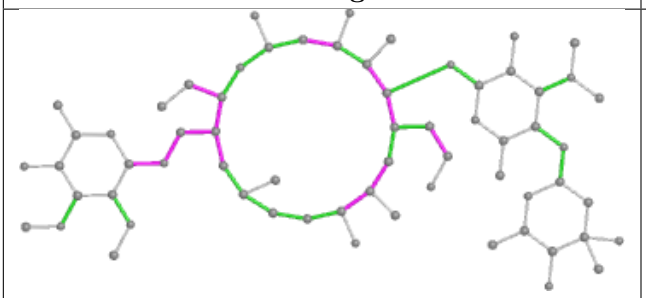
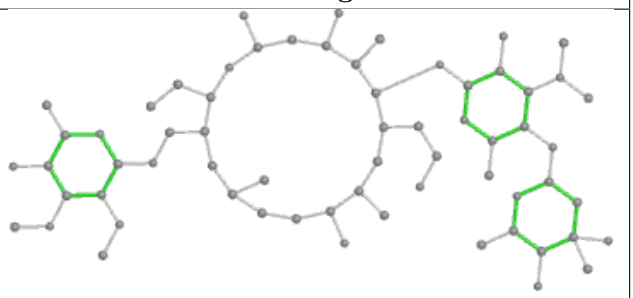
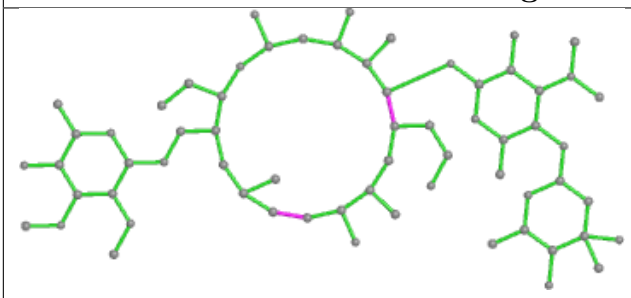


Torsions

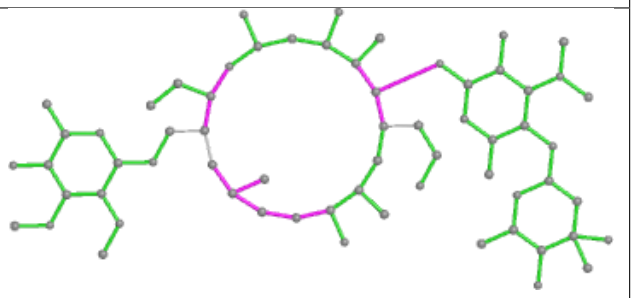


Rings

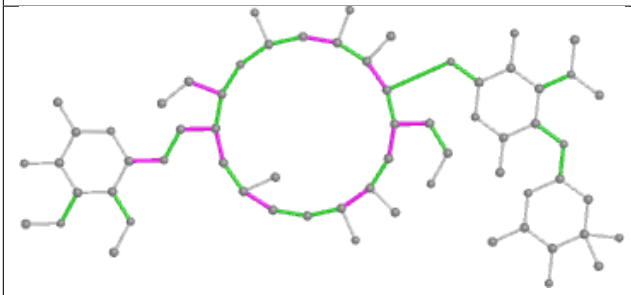
Ligand TYK D 401



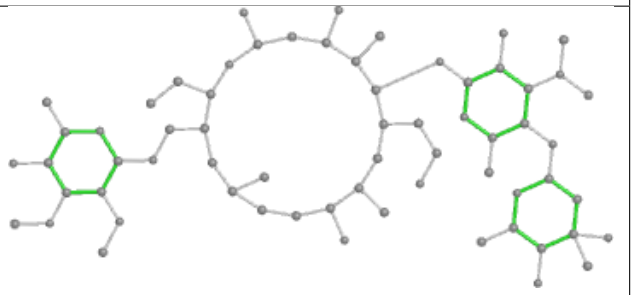
Bond lengths



Bond angles

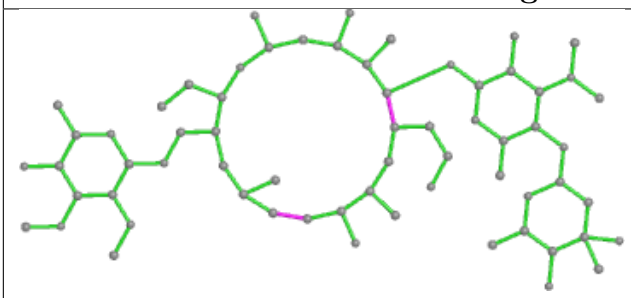


Torsions



Rings

Ligand TYK N 401



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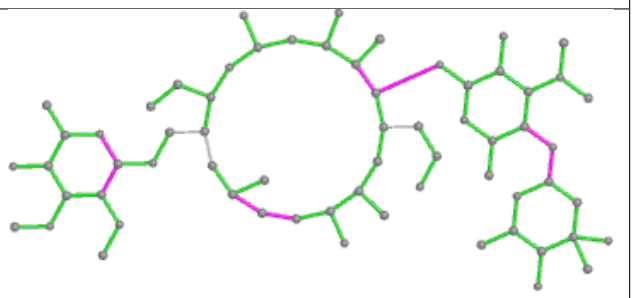
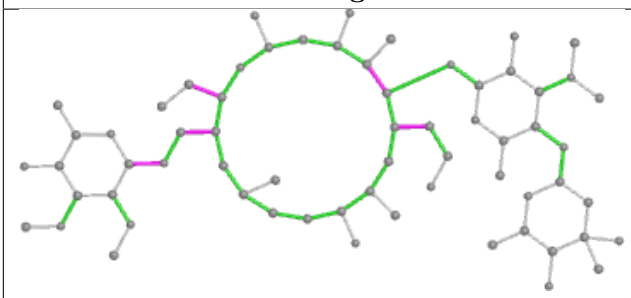


Bond angles



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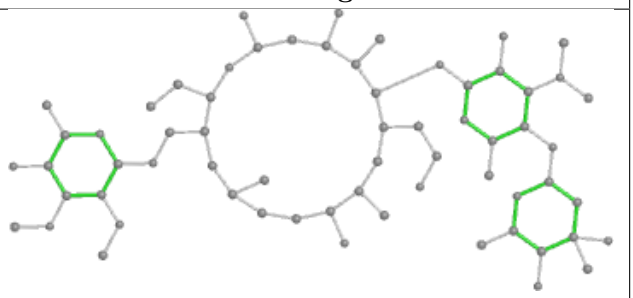
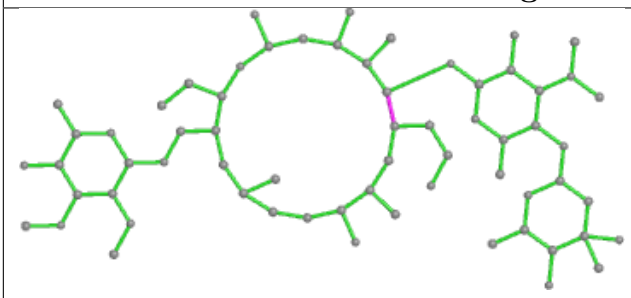


Rings

Ligand TYK H 401



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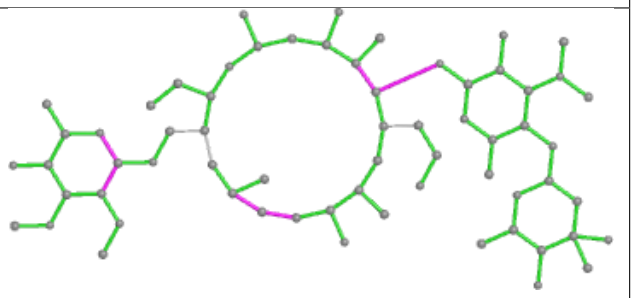

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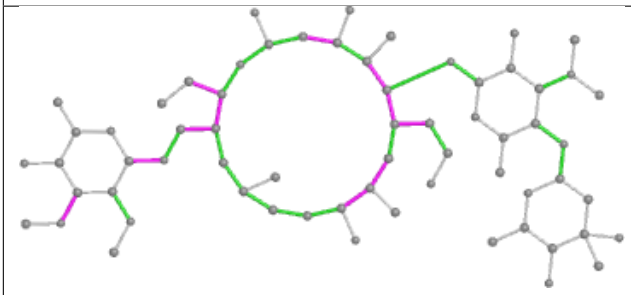
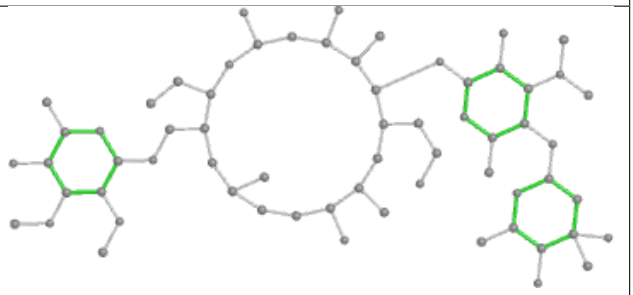
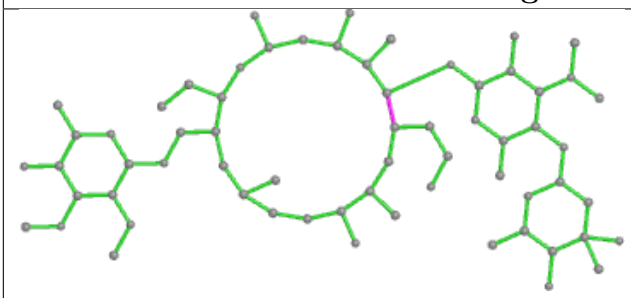


Torsions



Rings

Ligand TYK O 401



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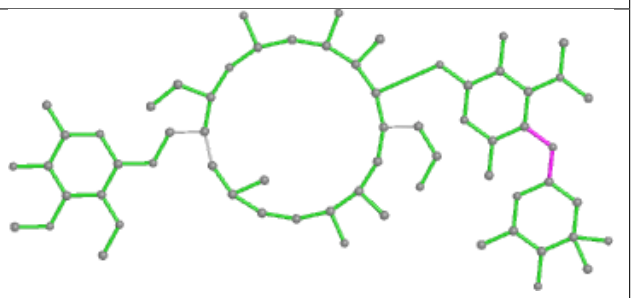
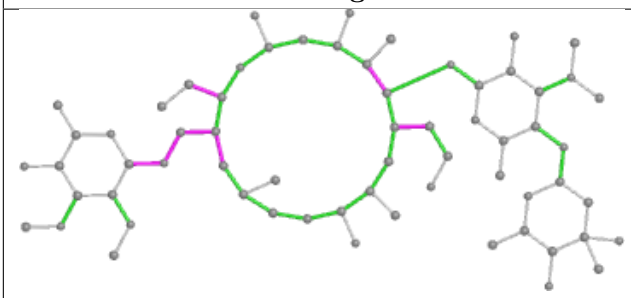


Bond angles



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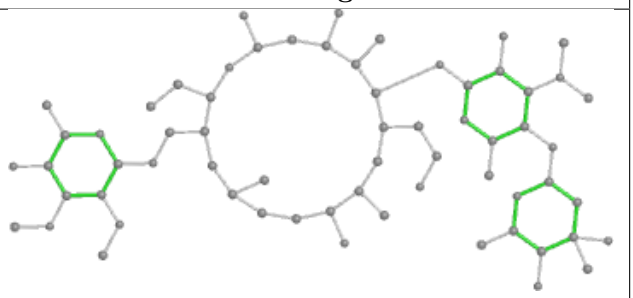
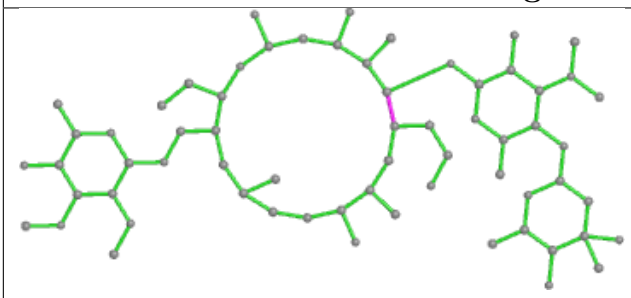


Rings

Ligand TYK L 401



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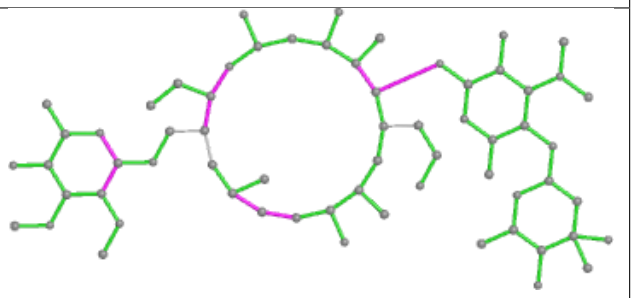
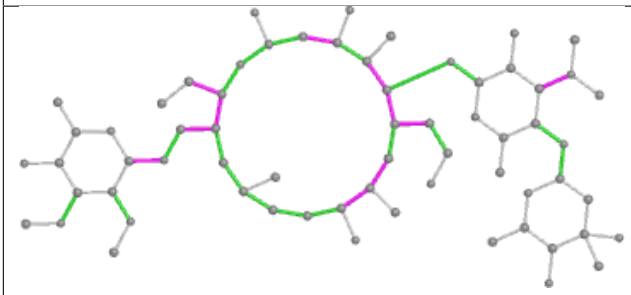


Bond angles



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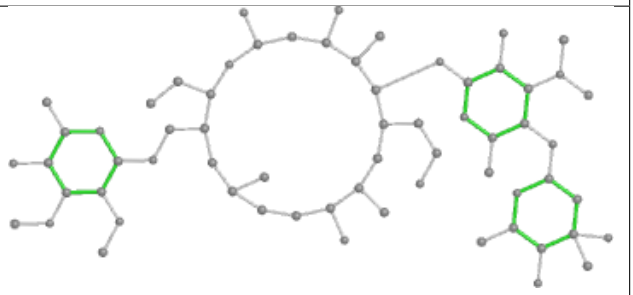
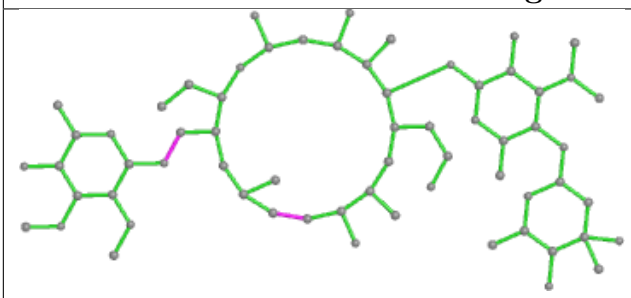


Rings

Ligand TYK J 401



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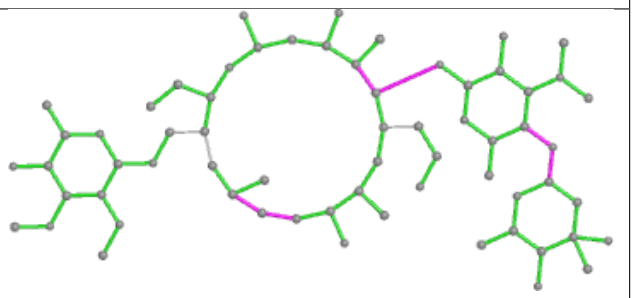
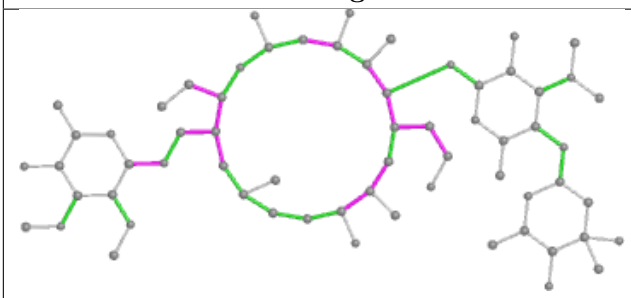


Bond angles



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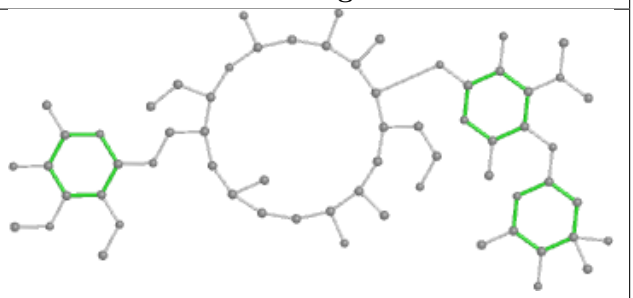
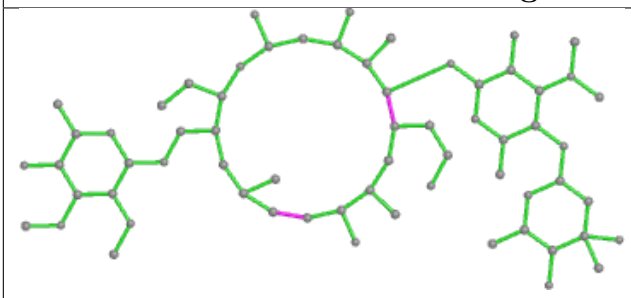
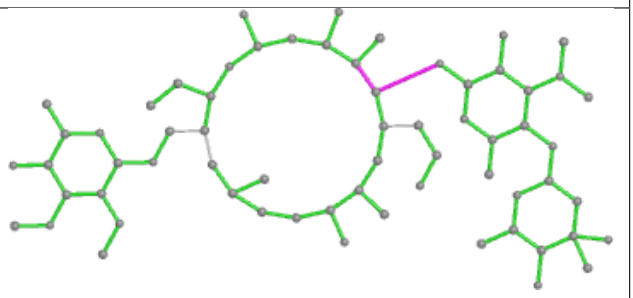


Rings

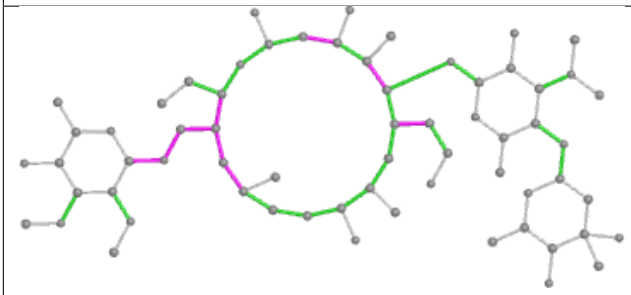
Ligand TYK G 401



Bond lengths



Bond angles



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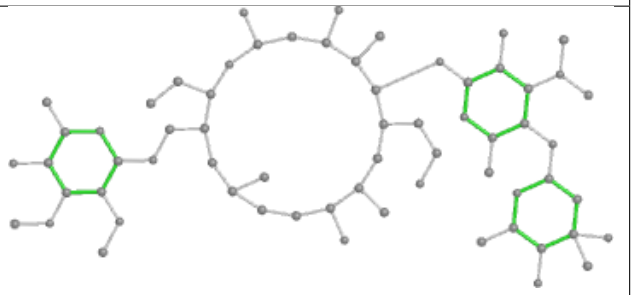
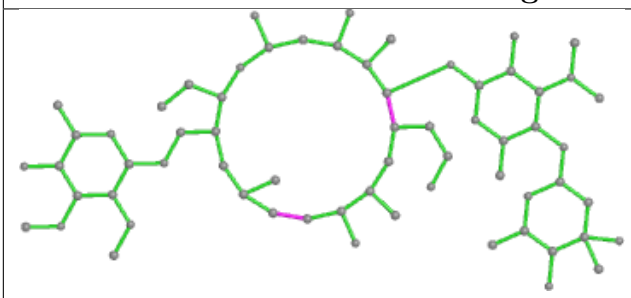
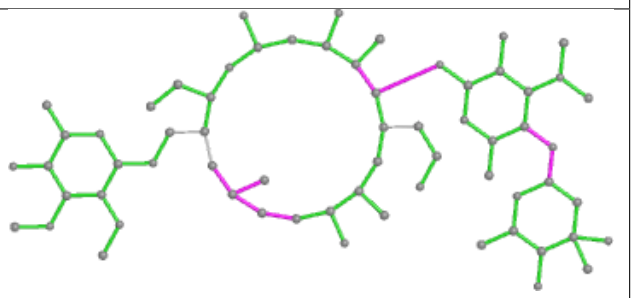


Rings

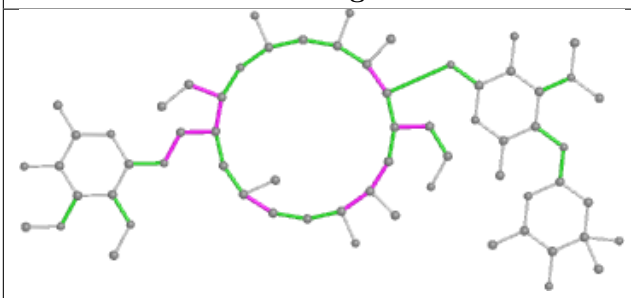
Ligand TYK A 401



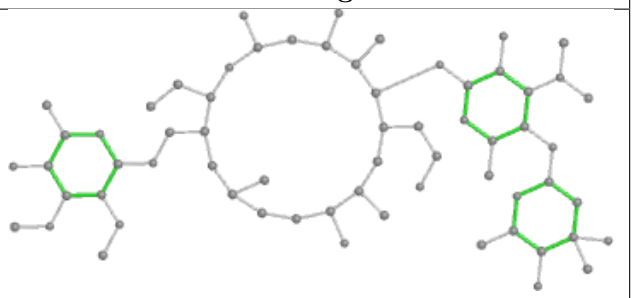
Bond lengths



Bond angles

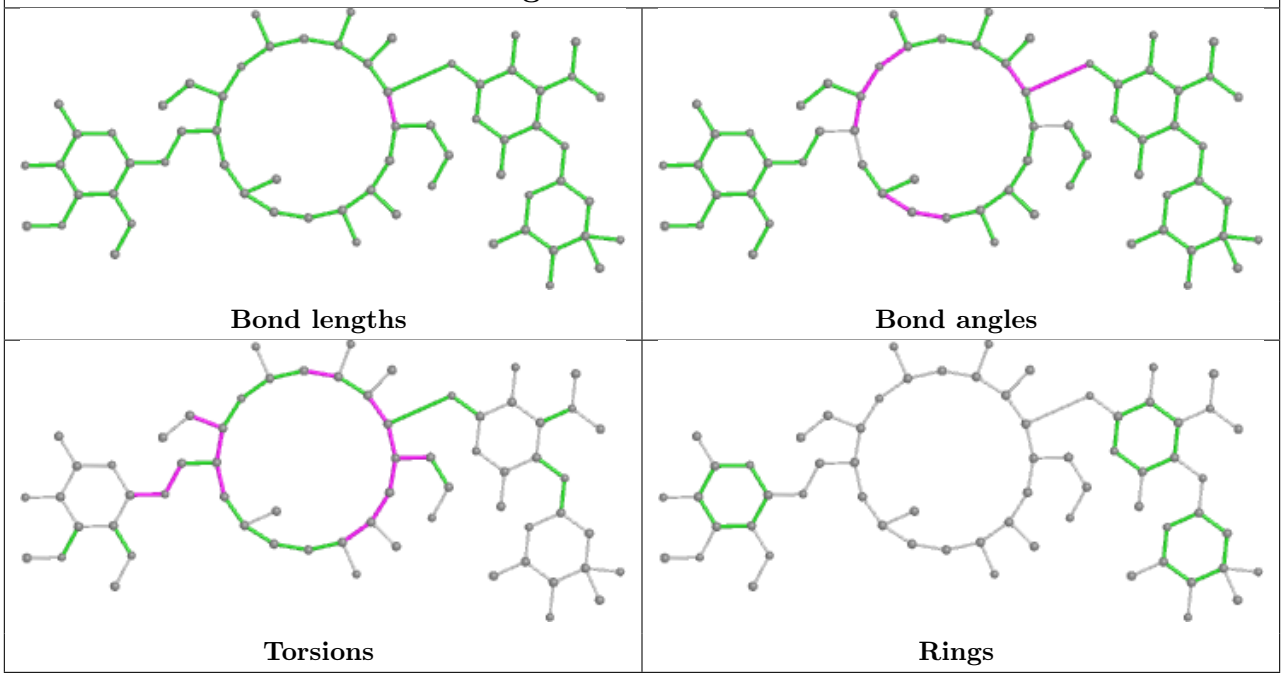


Torsions

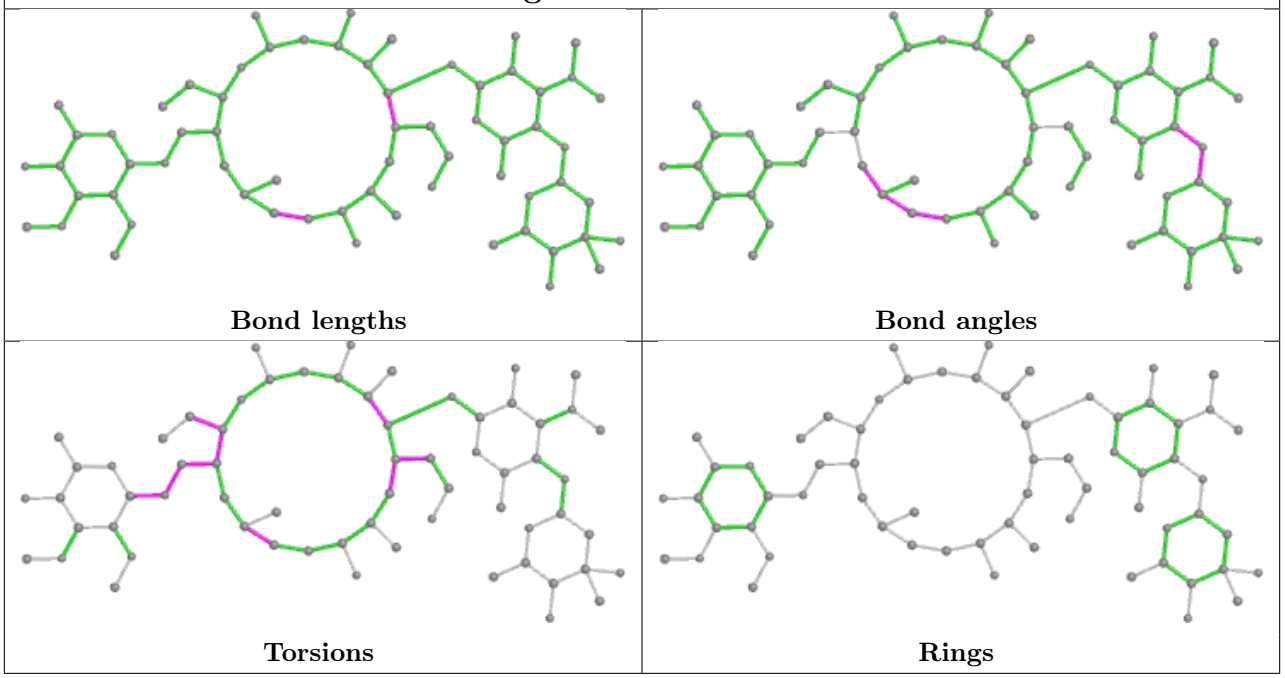


Rings

Ligand TYK B 401



Ligand TYK F 401



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	A	299/351 (85%)	0.09	11 (3%)	41	44	18, 34, 69, 85	0
1	B	314/351 (89%)	-0.10	12 (3%)	40	43	16, 29, 69, 106	0
1	C	297/351 (84%)	0.14	13 (4%)	34	37	18, 35, 72, 103	0
1	D	310/351 (88%)	0.00	17 (5%)	25	27	19, 33, 69, 89	0
1	E	292/351 (83%)	-0.01	7 (2%)	59	62	18, 35, 69, 100	0
1	F	312/351 (88%)	-0.04	17 (5%)	25	28	17, 33, 75, 105	0
1	G	298/351 (84%)	0.15	9 (3%)	50	53	18, 36, 72, 98	0
1	H	313/351 (89%)	-0.05	17 (5%)	25	28	17, 31, 74, 104	0
1	I	301/351 (85%)	-0.02	6 (1%)	65	68	16, 29, 68, 87	0
1	J	314/351 (89%)	-0.22	5 (1%)	72	74	15, 27, 63, 94	0
1	K	296/351 (84%)	0.12	11 (3%)	41	44	16, 33, 75, 112	0
1	L	311/351 (88%)	-0.20	4 (1%)	77	79	14, 25, 57, 100	0
1	M	297/351 (84%)	0.05	13 (4%)	34	37	17, 32, 74, 116	0
1	N	315/351 (89%)	-0.19	7 (2%)	62	65	16, 27, 56, 101	0
1	O	305/351 (86%)	0.01	6 (1%)	65	68	15, 31, 67, 94	0
1	P	318/351 (90%)	-0.23	7 (2%)	62	65	15, 25, 62, 102	0
All	All	4892/5616 (87%)	-0.03	162 (3%)	46	48	14, 31, 70, 116	0

The worst 5 of 162 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	249	PRO	4.9
1	G	89	ASN	4.8
1	O	230	GLN	4.8
1	K	87	TYR	4.6
1	P	249	PRO	4.5

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)

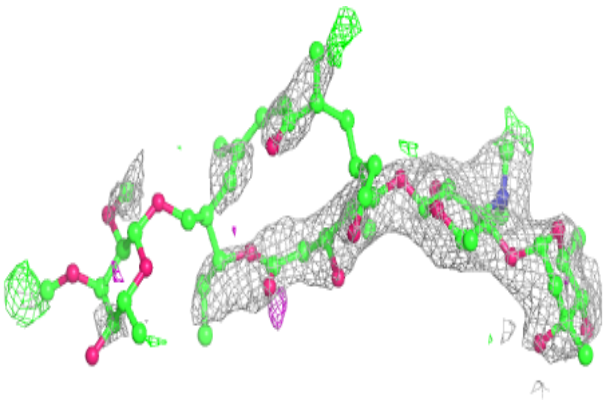
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

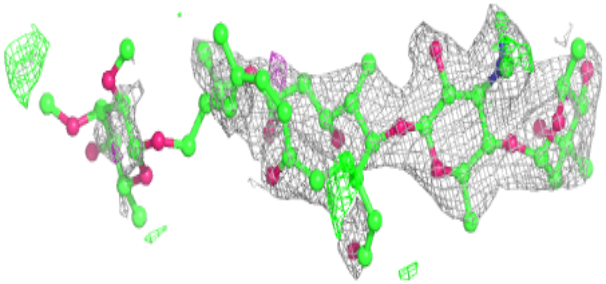
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TYK	F	401	64/64	0.76	0.40	64,86,145,155	0
2	TYK	H	401	64/64	0.76	0.39	57,88,161,170	0
2	TYK	G	401	64/64	0.78	0.39	44,84,151,159	0
2	TYK	B	401	64/64	0.78	0.42	56,91,169,179	0
2	TYK	C	401	64/64	0.79	0.37	53,76,161,172	0
2	TYK	E	401	64/64	0.80	0.36	49,77,167,177	0
2	TYK	A	401	64/64	0.80	0.39	47,77,170,181	0
2	TYK	D	401	64/64	0.82	0.38	43,77,156,167	0
2	TYK	J	401	64/64	0.82	0.34	49,82,151,160	0
2	TYK	M	401	64/64	0.83	0.33	37,64,138,144	0
2	TYK	O	401	64/64	0.83	0.32	37,65,148,159	0
2	TYK	K	401	64/64	0.84	0.37	41,71,161,170	0
2	TYK	L	401	64/64	0.85	0.35	41,64,152,157	0
2	TYK	N	401	64/64	0.86	0.32	45,65,147,152	0
2	TYK	P	401	64/64	0.86	0.32	40,63,143,155	0
2	TYK	I	401	64/64	0.87	0.35	43,63,165,180	0

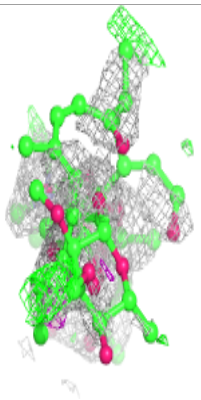
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TYK F 401:

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

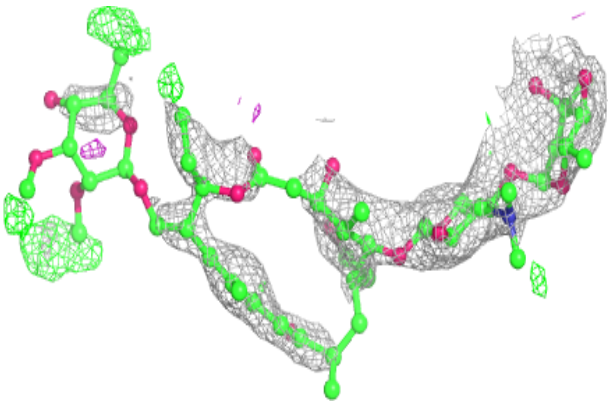


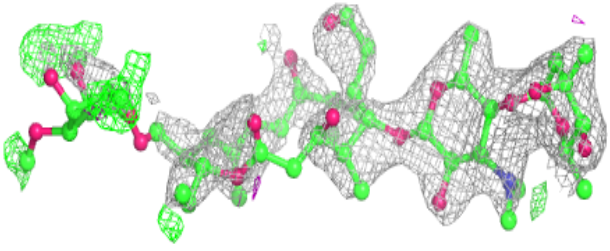


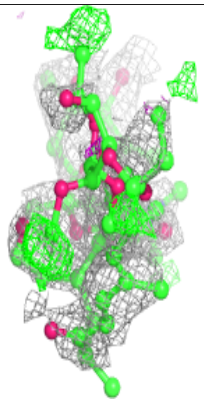


Electron density around TYK H 401:

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

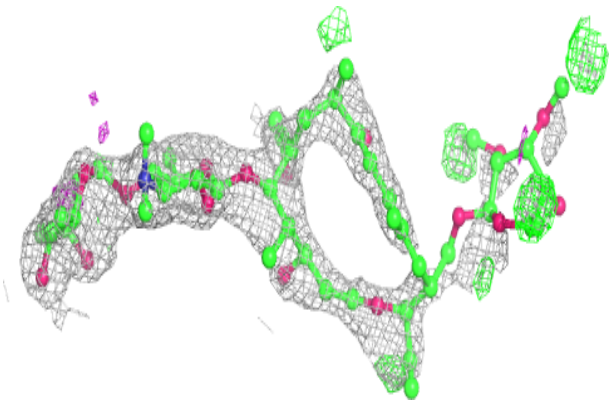


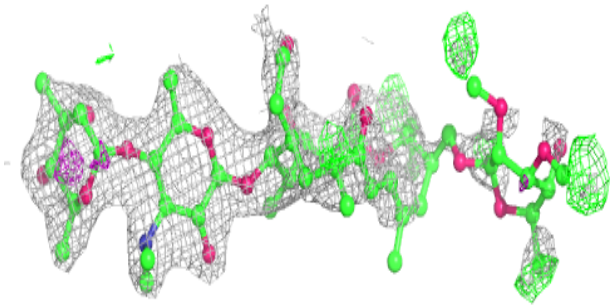


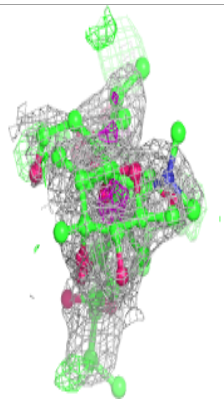


Electron density around TYK G 401:

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

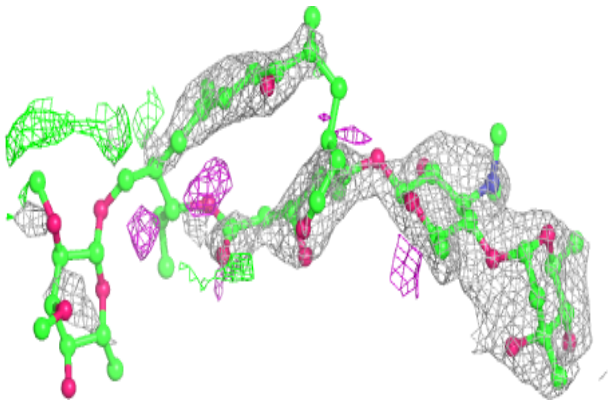


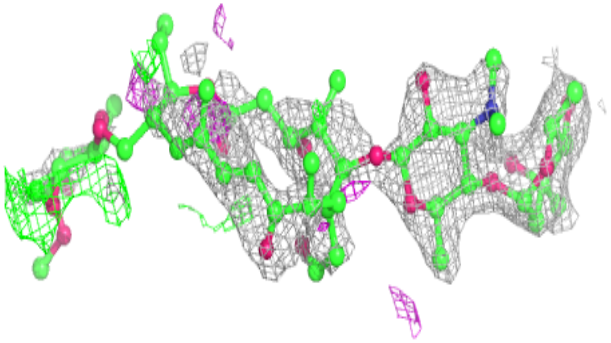


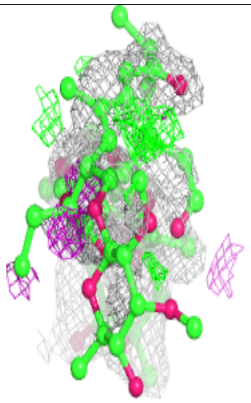


Electron density around TYK B 401:

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

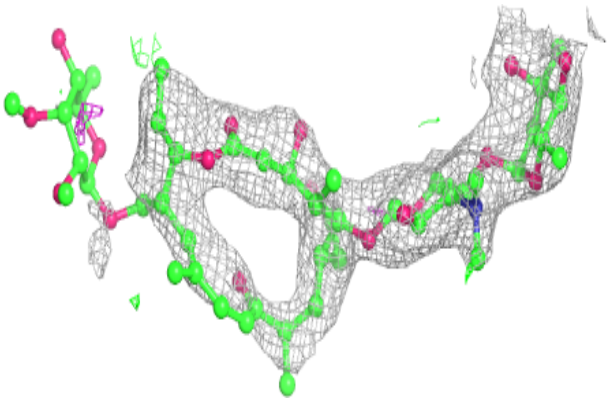


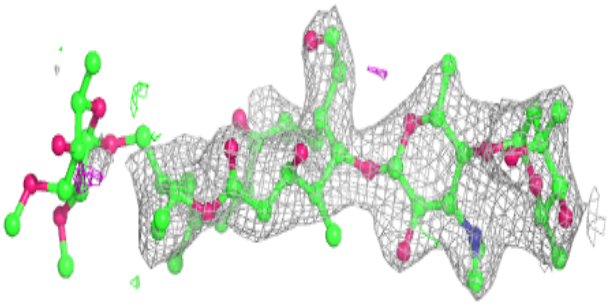


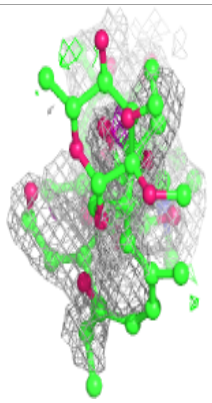


Electron density around TYK C 401:

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

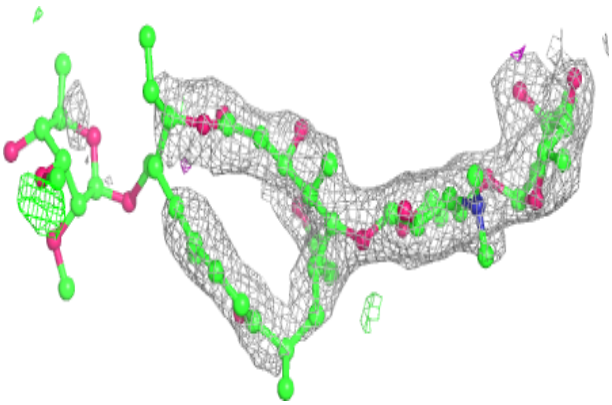


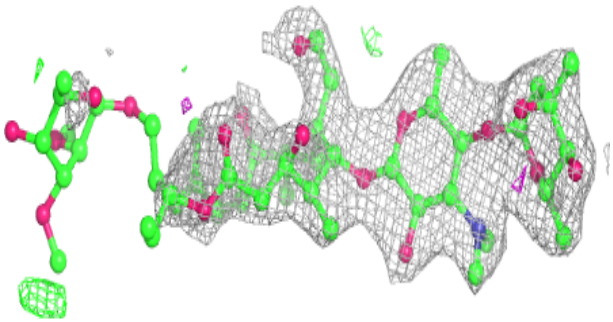


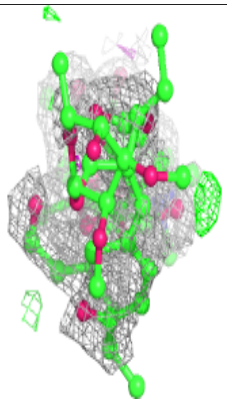


Electron density around TYK E 401:

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

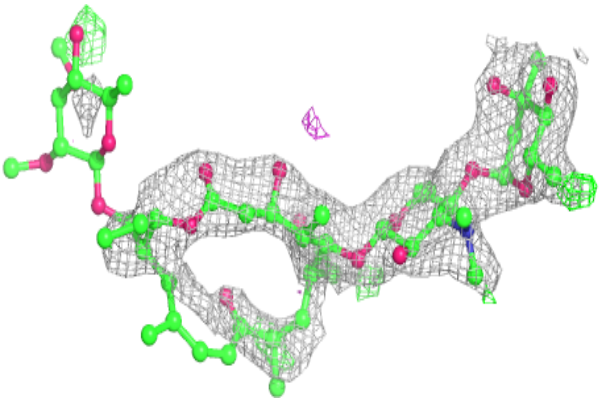


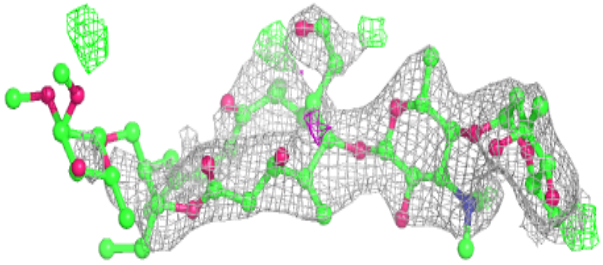


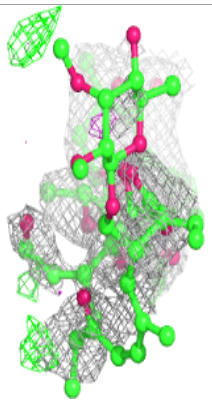


Electron density around TYK A 401:

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

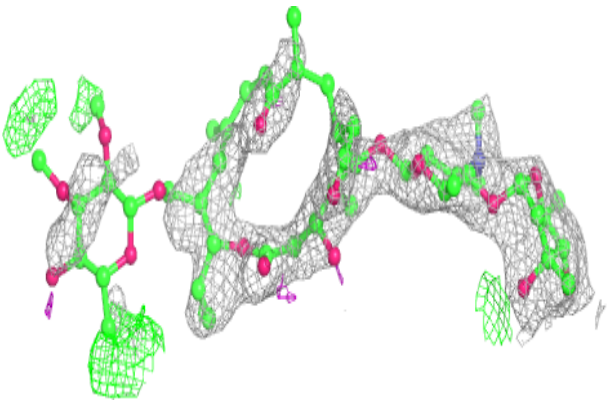


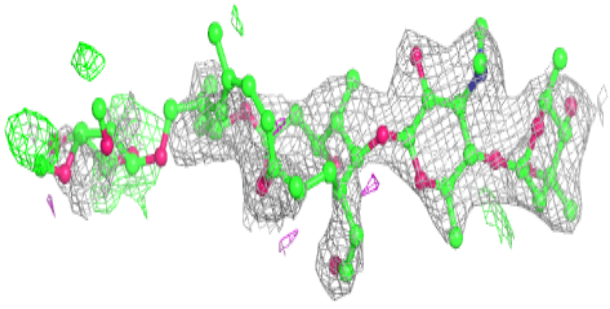


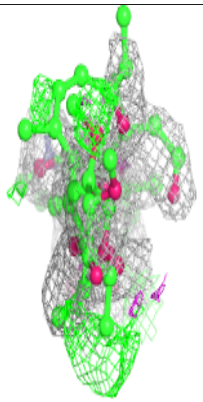


Electron density around TYK D 401:

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

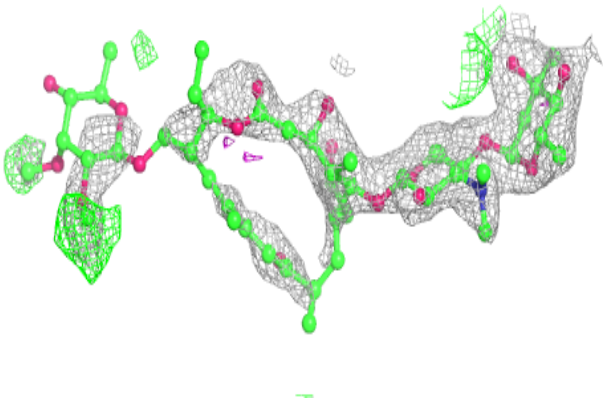


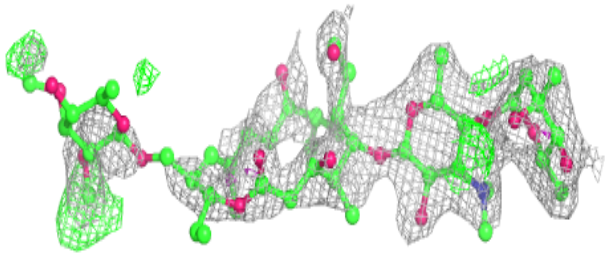


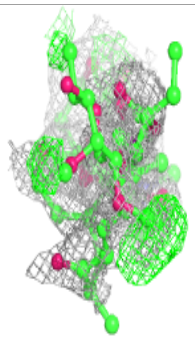


Electron density around TYK J 401:

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

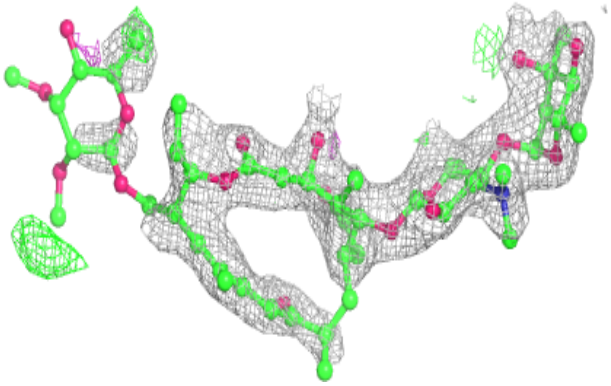


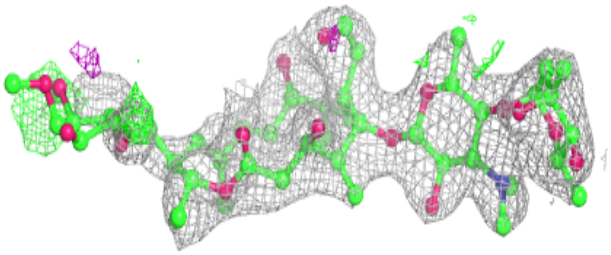


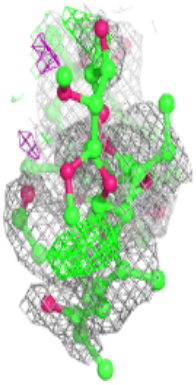


Electron density around TYK M 401:

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

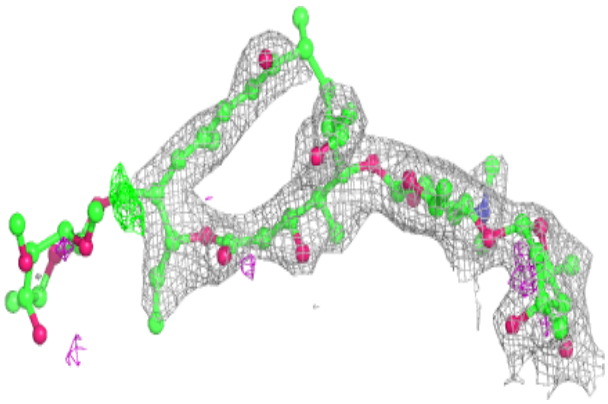


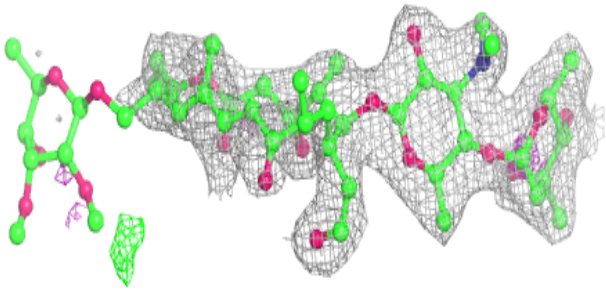


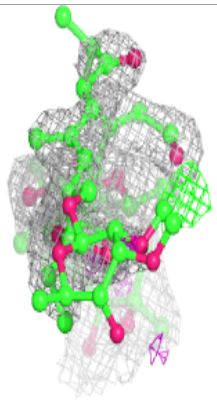


Electron density around TYK O 401:

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

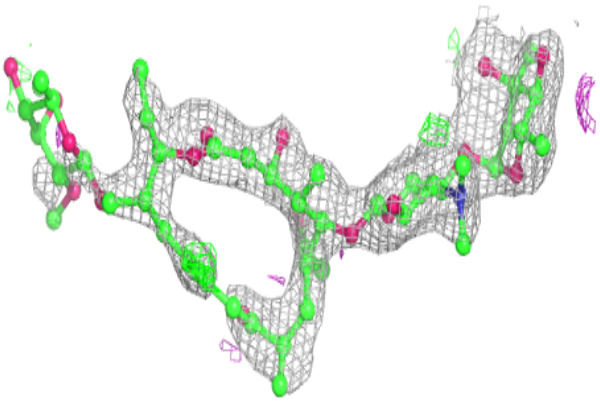


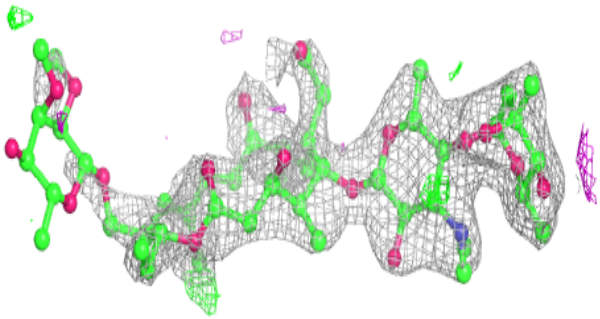


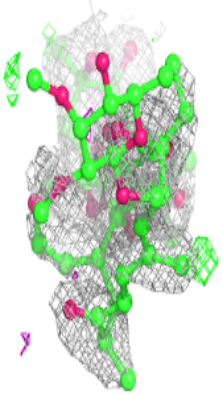


Electron density around TYK K 401:

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

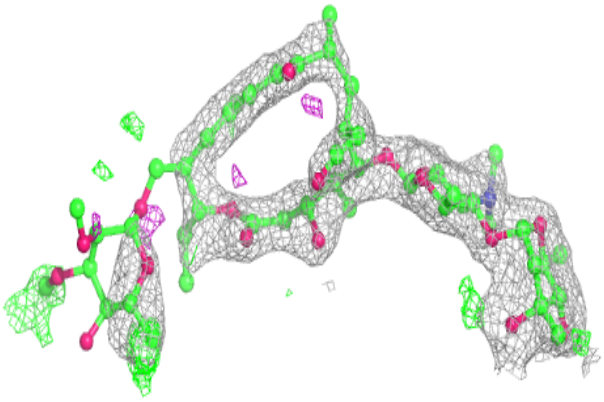


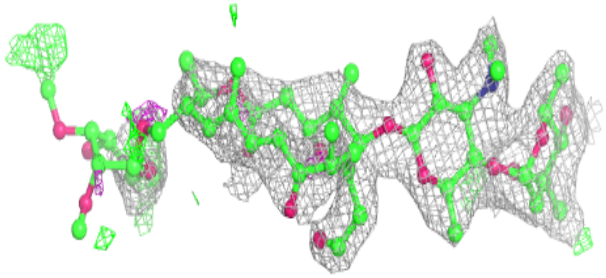


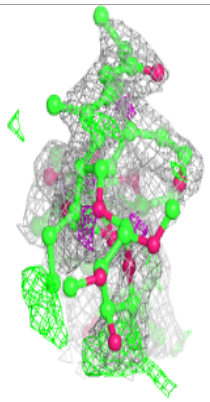


Electron density around TYK L 401:

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

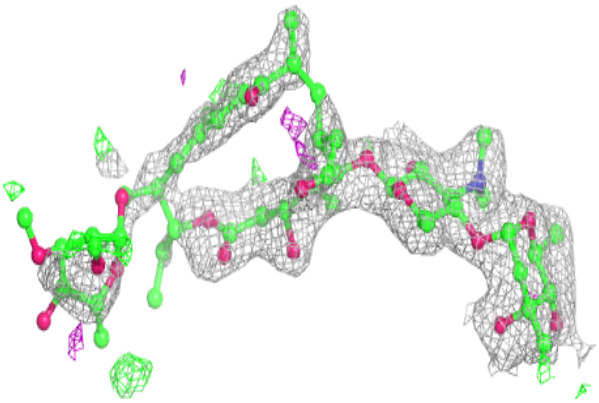


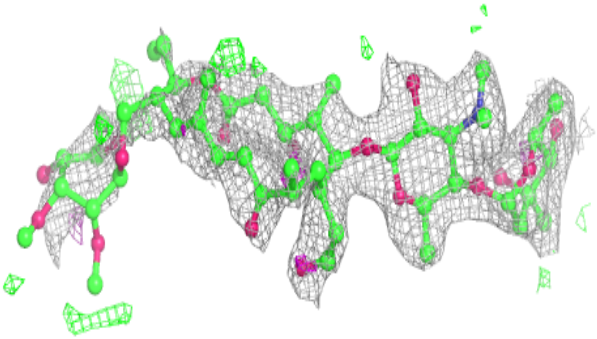


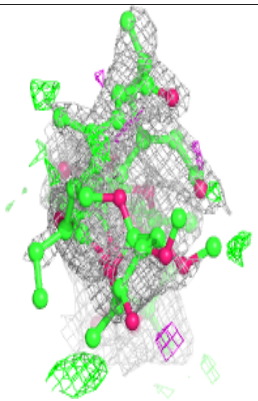


Electron density around TYK N 401:

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

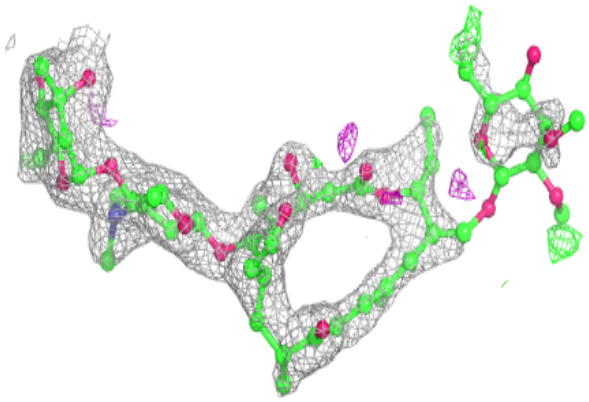


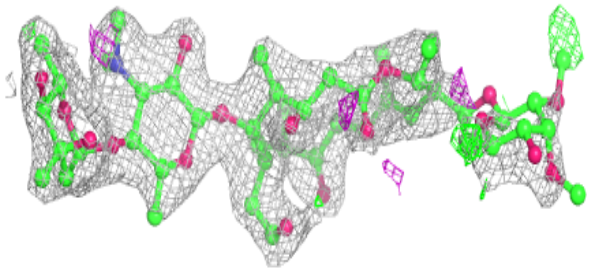


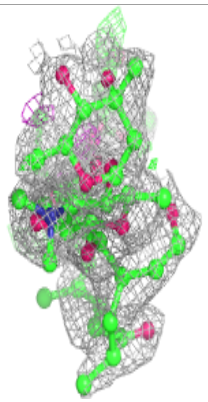


Electron density around TYK P 401:

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

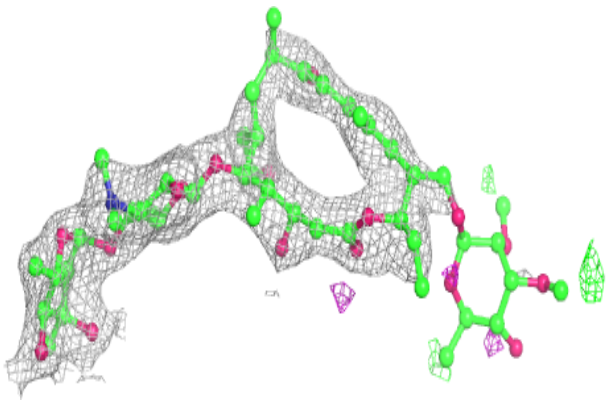


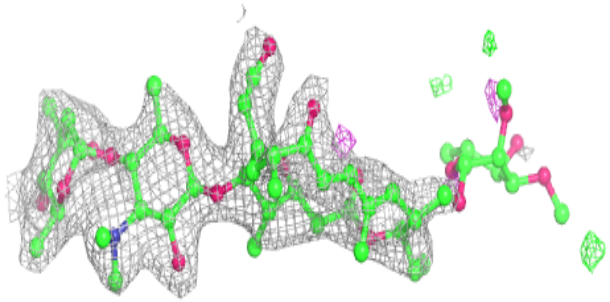


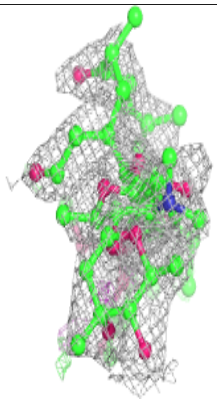


Electron density around TYK I 401:

$2mF_o$-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.