



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 03:18 AM UTC

PDB ID : 8JWO / pdb_00008jwo
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

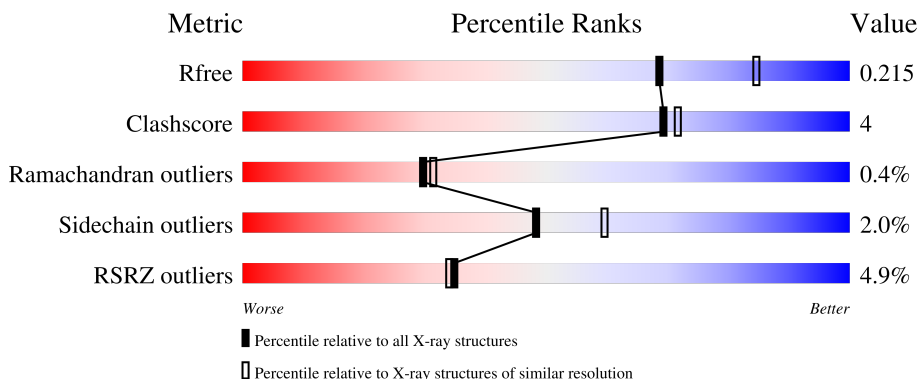
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	351	5% 74% 11% • 15%
1	B	351	5% 79% 9% • 11%
1	C	351	5% 75% 9% • 15%
1	D	351	3% 79% 8% • 12%
1	E	351	5% 74% 10% 17%

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Mol	Chain	Length	Quality of chain
1	F	351	
1	G	351	
1	H	351	
1	I	351	
1	J	351	
1	K	351	
1	L	351	
1	M	351	
1	N	351	
1	O	351	
1	P	351	

2 Entry composition

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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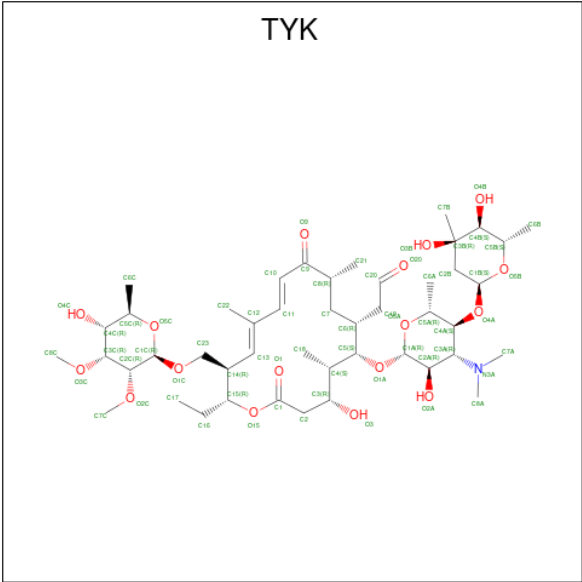
Chain	Residue	Modelled	Actual	Comment	Reference
M	-7	GLY	-	expression tag	UNP A0A3R7J519
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M	-5	VAL	-	expression tag	UNP A0A3R7J519
M	-4	PRO	-	expression tag	UNP A0A3R7J519
M	-3	ARG	-	expression tag	UNP A0A3R7J519
M	-2	GLY	-	expression tag	UNP A0A3R7J519
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 (CCD ID: 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	0	0
			64	46	1	17		
2	P	1	Total	C	N	O	0	0
			64	46	1	17		

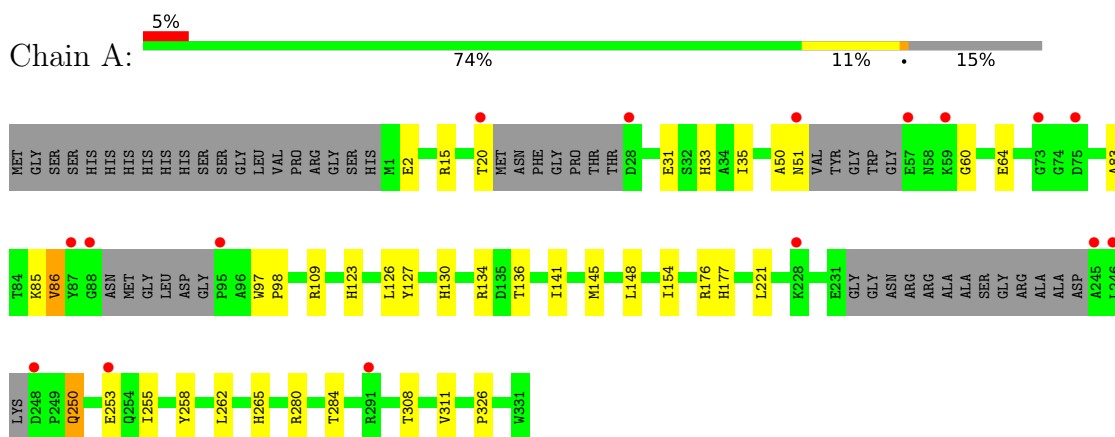
- Molecule 3 is water.

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

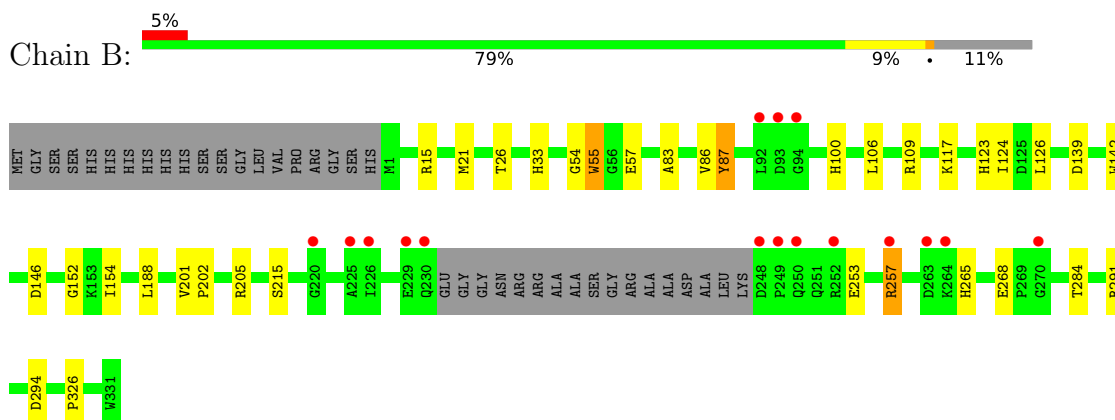
3 Residue-property plots [i](#)

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.

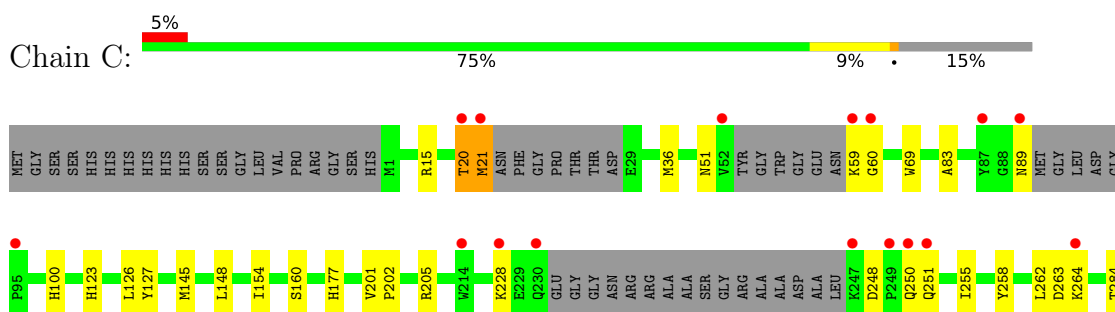
- Molecule 1: Aldo/keto reductase



- Molecule 1: Aldo/keto reductase

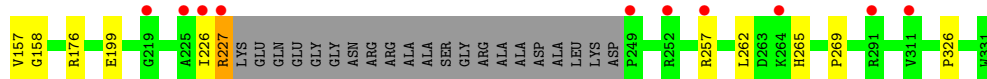
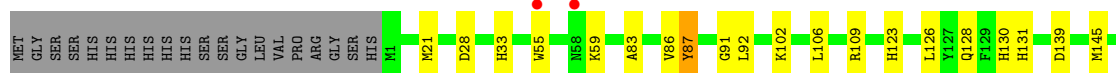
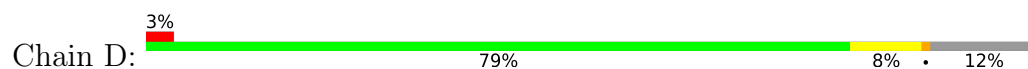


- Molecule 1: Aldo/keto reductase

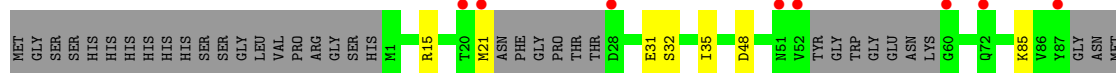




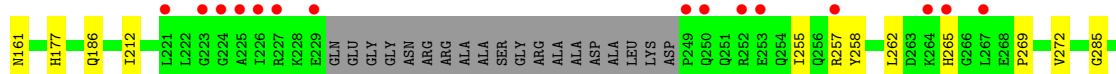
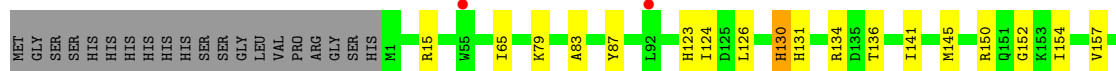
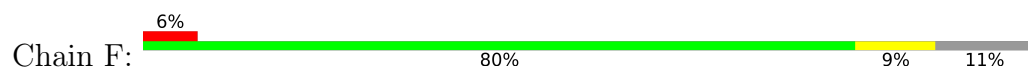
- Molecule 1: Aldo/keto reductase



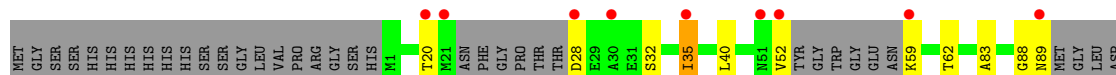
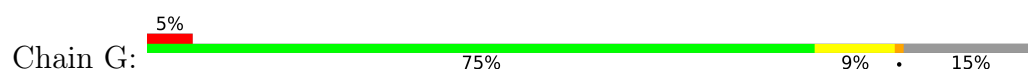
- Molecule 1: Aldo/keto reductase

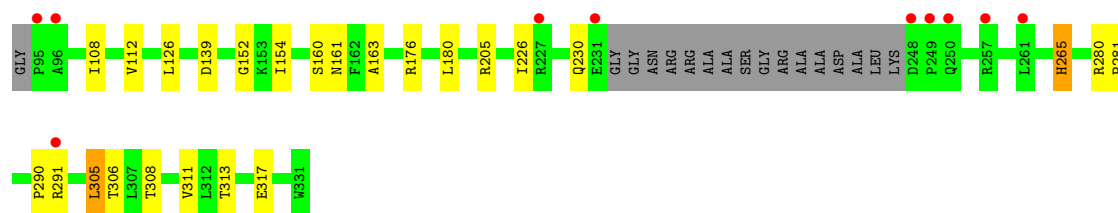


- Molecule 1: Aldo/keto reductase

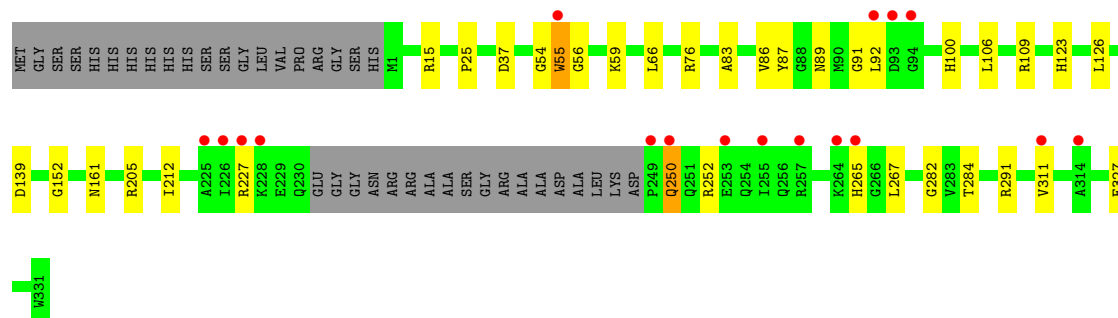
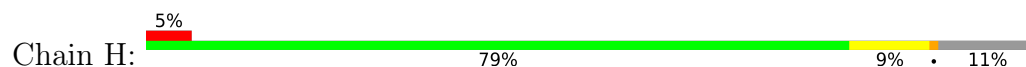


- Molecule 1: Aldo/keto reductase

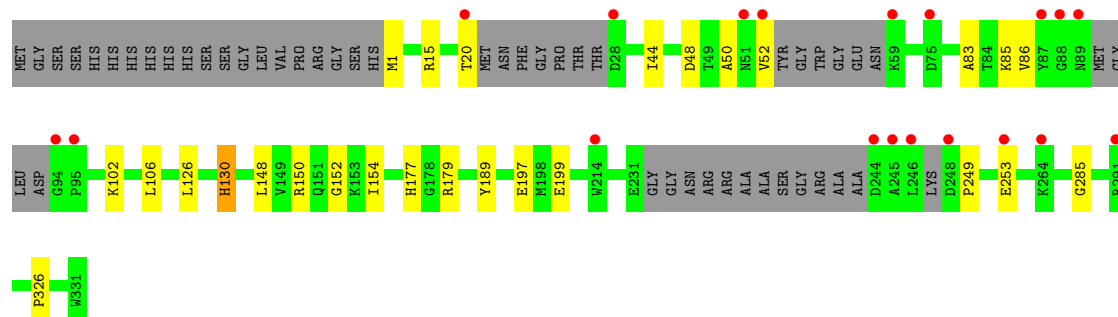
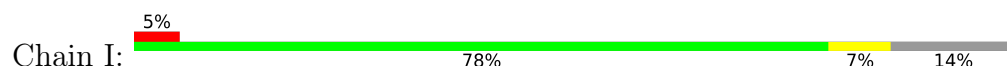




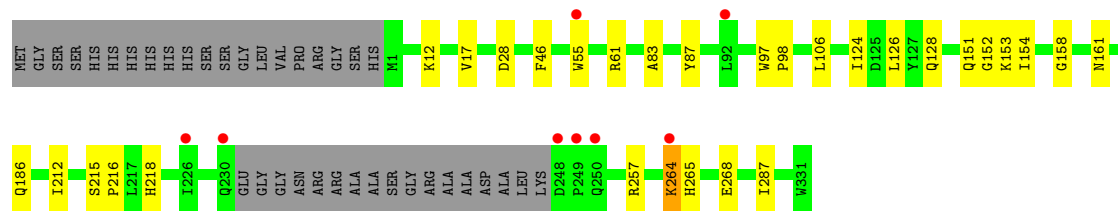
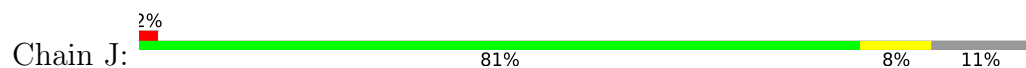
- Molecule 1: Aldo/keto reductase



- Molecule 1: Aldo/keto reductase

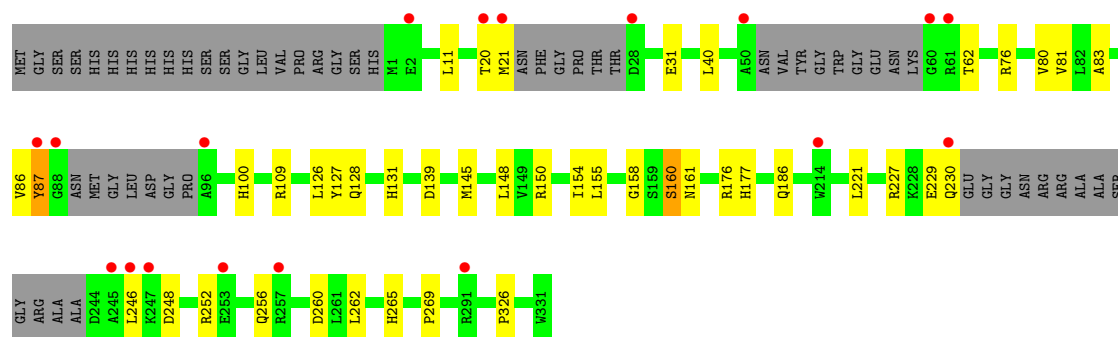


- Molecule 1: Aldo/keto reductase

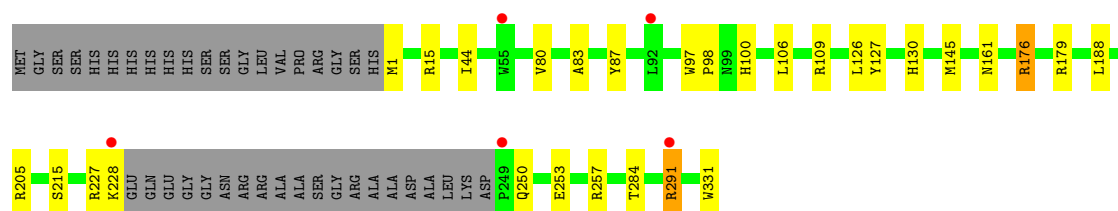
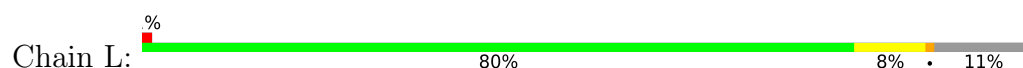


- Molecule 1: Aldo/keto reductase

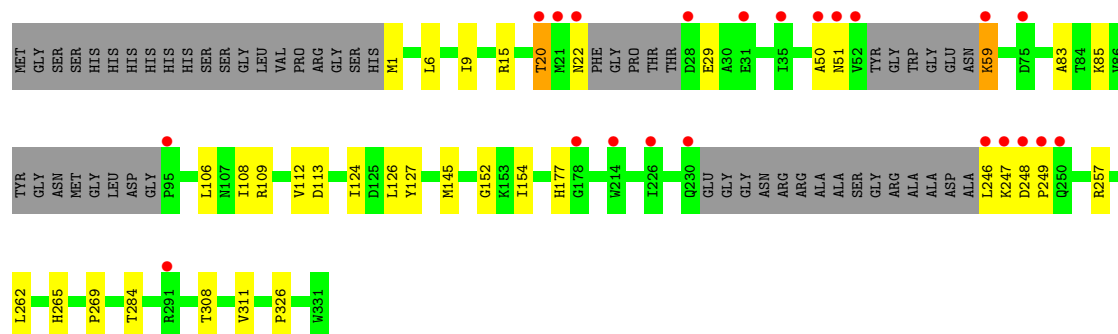
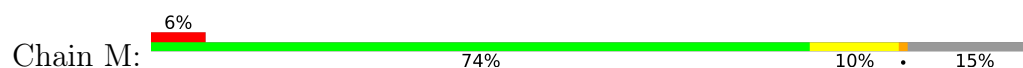




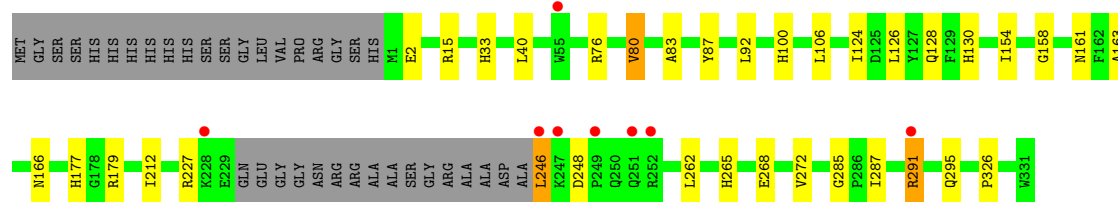
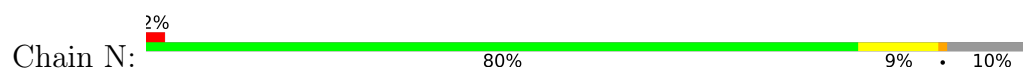
- Molecule 1: Aldo/keto reductase



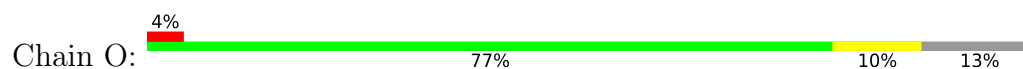
- Molecule 1: Aldo/keto reductase

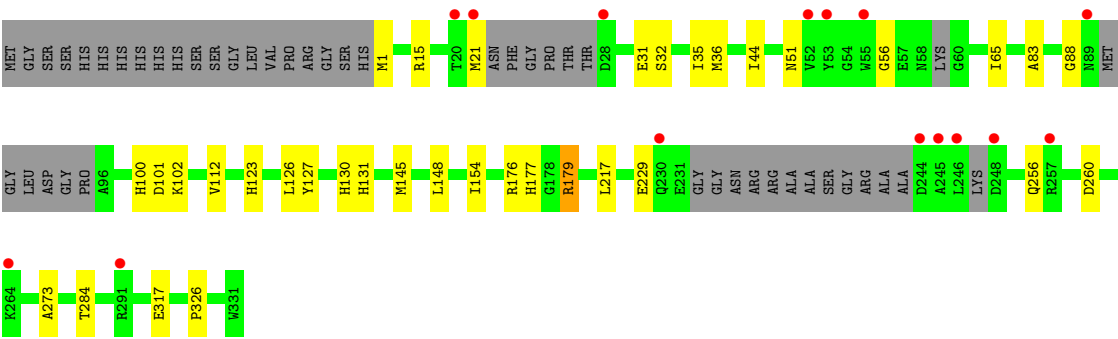


- Molecule 1: Aldo/keto reductase

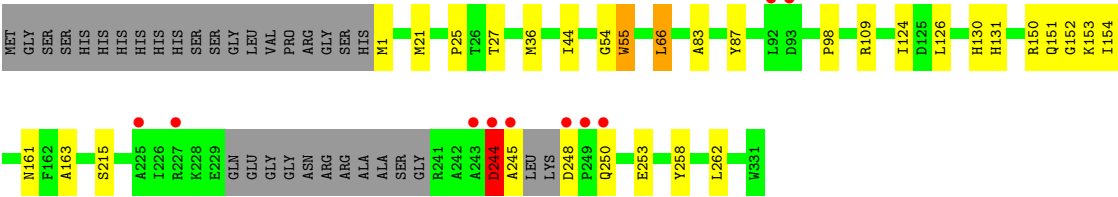
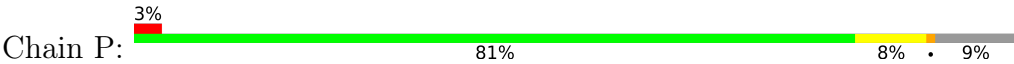


- Molecule 1: Aldo/keto reductase





● Molecule 1: Aldo/keto reductase



4 Data and refinement statistics

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) 99.1 (49.74-2.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.181 , 0.216 0.181 , 0.215	Depositor DCC
R_{free} test set	15542 reflections (4.89%)	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)	0.36 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.69	2/2373 (0.1%)	1.02	1/3216 (0.0%)
1	B	0.67	4/2493 (0.2%)	1.03	1/3387 (0.0%)
1	C	0.67	2/2359 (0.1%)	1.05	2/3197 (0.1%)
1	D	0.68	5/2458 (0.2%)	1.02	1/3340 (0.0%)
1	E	0.65	3/2321 (0.1%)	1.02	1/3147 (0.0%)
1	F	0.66	5/2476 (0.2%)	1.00	0/3363
1	G	0.65	1/2367 (0.0%)	1.02	3/3209 (0.1%)
1	H	0.67	3/2485 (0.1%)	1.03	1/3375 (0.0%)
1	I	0.68	2/2383 (0.1%)	1.03	1/3231 (0.0%)
1	J	0.67	2/2493 (0.1%)	0.99	1/3387 (0.0%)
1	K	0.68	4/2348 (0.2%)	1.04	1/3183 (0.0%)
1	L	0.70	2/2467 (0.1%)	1.02	5/3351 (0.1%)
1	M	0.67	2/2358 (0.1%)	1.04	0/3196
1	N	0.70	5/2501 (0.2%)	1.04	1/3397 (0.0%)
1	O	0.71	5/2424 (0.2%)	1.03	1/3287 (0.0%)
1	P	0.67	2/2517 (0.1%)	1.06	2/3418 (0.1%)
All	All	0.68	49/38823 (0.1%)	1.03	22/52684 (0.0%)

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	100	HIS	CE1-NE2	7.54	1.40	1.32
1	D	123	HIS	CE1-NE2	6.54	1.39	1.32
1	F	131	HIS	CE1-NE2	6.43	1.39	1.32
1	O	131	HIS	CE1-NE2	6.37	1.39	1.32
1	M	177	HIS	CE1-NE2	6.34	1.38	1.32

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	291	ARG	N-CA-C	-7.45	104.03	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	139	ASP	CA-CB-CG	7.37	119.97	112.60
1	L	227	ARG	N-CA-C	-6.25	105.41	113.16
1	B	139	ASP	CA-CB-CG	6.25	118.84	112.60
1	L	250	GLN	N-CA-C	-6.06	104.59	112.23

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	26	0
1	B	2438	0	2375	16	0
1	C	2312	0	2276	20	0
1	D	2403	0	2345	15	0
1	E	2275	0	2234	20	0
1	F	2421	0	2364	16	0
1	G	2320	0	2273	18	0
1	H	2430	0	2372	15	0
1	I	2337	0	2285	16	0
1	J	2438	0	2375	17	0
1	K	2302	0	2258	22	0
1	L	2412	0	2358	15	0
1	M	2312	0	2279	21	0
1	N	2446	0	2391	15	0
1	O	2376	0	2308	19	0
1	P	2463	0	2398	18	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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
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	273	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 4.

The worst 5 of 273 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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	287/351 (82%)	281 (98%)	6 (2%)	0	100	100
1	B	310/351 (88%)	299 (96%)	9 (3%)	2 (1%)	21	21
1	C	287/351 (82%)	278 (97%)	8 (3%)	1 (0%)	36	40
1	D	306/351 (87%)	293 (96%)	11 (4%)	2 (1%)	18	17
1	E	282/351 (80%)	275 (98%)	6 (2%)	1 (0%)	30	31
1	F	308/351 (88%)	296 (96%)	11 (4%)	1 (0%)	36	40
1	G	288/351 (82%)	279 (97%)	9 (3%)	0	100	100
1	H	309/351 (88%)	299 (97%)	7 (2%)	3 (1%)	12	10
1	I	289/351 (82%)	281 (97%)	8 (3%)	0	100	100
1	J	310/351 (88%)	300 (97%)	9 (3%)	1 (0%)	36	40
1	K	286/351 (82%)	276 (96%)	9 (3%)	1 (0%)	36	40
1	L	307/351 (88%)	298 (97%)	8 (3%)	1 (0%)	36	40
1	M	287/351 (82%)	279 (97%)	7 (2%)	1 (0%)	36	40
1	N	311/351 (89%)	300 (96%)	10 (3%)	1 (0%)	36	40
1	O	293/351 (84%)	288 (98%)	5 (2%)	0	100	100
1	P	312/351 (89%)	299 (96%)	11 (4%)	2 (1%)	21	21
All	All	4772/5616 (85%)	4621 (97%)	134 (3%)	17 (0%)	30	31

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 ⓘ

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%)	234 (98%)	4 (2%)	53	65
1	B	249/275 (90%)	243 (98%)	6 (2%)	43	54
1	C	237/275 (86%)	233 (98%)	4 (2%)	53	65
1	D	245/275 (89%)	241 (98%)	4 (2%)	55	66
1	E	233/275 (85%)	232 (100%)	1 (0%)	84	89
1	F	247/275 (90%)	244 (99%)	3 (1%)	63	74
1	G	238/275 (86%)	229 (96%)	9 (4%)	29	36
1	H	248/275 (90%)	238 (96%)	10 (4%)	28	34
1	I	239/275 (87%)	237 (99%)	2 (1%)	73	80
1	J	249/275 (90%)	247 (99%)	2 (1%)	73	80
1	K	235/275 (86%)	229 (97%)	6 (3%)	40	50
1	L	246/275 (90%)	243 (99%)	3 (1%)	63	74
1	M	238/275 (86%)	232 (98%)	6 (2%)	42	52
1	N	250/275 (91%)	242 (97%)	8 (3%)	34	43
1	O	242/275 (88%)	238 (98%)	4 (2%)	53	65
1	P	250/275 (91%)	245 (98%)	5 (2%)	48	59
All	All	3884/4400 (88%)	3807 (98%)	77 (2%)	48	59

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

Mol	Chain	Res	Type
1	M	113	ASP
1	O	229	GLU
1	M	257	ARG
1	N	227	ARG
1	P	244	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	256	GLN
1	O	177	HIS
1	I	89	ASN
1	P	143	GLN
1	L	254	GLN

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 oligosaccharides 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	B	401	-	67,67,67	0.69	1 (1%)	87,97,97	1.05	4 (4%)
2	TYK	M	401	-	67,67,67	0.67	0	87,97,97	1.04	4 (4%)
2	TYK	P	401	-	67,67,67	0.76	2 (2%)	87,97,97	0.93	5 (5%)
2	TYK	G	401	-	67,67,67	0.77	3 (4%)	87,97,97	0.87	2 (2%)
2	TYK	L	401	-	67,67,67	0.72	1 (1%)	87,97,97	0.91	5 (5%)
2	TYK	D	401	-	67,67,67	0.74	2 (2%)	87,97,97	1.21	7 (8%)
2	TYK	E	401	-	67,67,67	0.74	3 (4%)	87,97,97	0.83	2 (2%)
2	TYK	F	401	-	67,67,67	0.74	2 (2%)	87,97,97	1.12	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TYK	C	401	-	67,67,67	0.67	1 (1%)	87,97,97	1.26	5 (5%)
2	TYK	H	401	-	67,67,67	0.64	1 (1%)	87,97,97	0.76	3 (3%)
2	TYK	K	401	-	67,67,67	0.66	2 (2%)	87,97,97	0.68	0
2	TYK	A	401	-	67,67,67	0.76	3 (4%)	87,97,97	1.23	5 (5%)
2	TYK	O	401	-	67,67,67	0.72	1 (1%)	87,97,97	0.74	1 (1%)
2	TYK	J	401	-	67,67,67	0.76	2 (2%)	87,97,97	0.74	3 (3%)
2	TYK	I	401	-	67,67,67	0.69	1 (1%)	87,97,97	0.82	2 (2%)
2	TYK	N	401	-	67,67,67	0.80	2 (2%)	87,97,97	0.84	4 (4%)

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	B	401	-	-	22/67/126/126	0/3/4/4
2	TYK	M	401	-	-	11/67/126/126	0/3/4/4
2	TYK	P	401	-	-	14/67/126/126	0/3/4/4
2	TYK	G	401	-	-	17/67/126/126	0/3/4/4
2	TYK	L	401	-	-	17/67/126/126	0/3/4/4
2	TYK	D	401	-	-	15/67/126/126	0/3/4/4
2	TYK	E	401	-	-	17/67/126/126	0/3/4/4
2	TYK	F	401	-	-	16/67/126/126	0/3/4/4
2	TYK	C	401	-	-	18/67/126/126	0/3/4/4
2	TYK	H	401	-	-	17/67/126/126	0/3/4/4
2	TYK	K	401	-	-	8/67/126/126	0/3/4/4
2	TYK	A	401	-	-	16/67/126/126	0/3/4/4
2	TYK	O	401	-	-	10/67/126/126	0/3/4/4
2	TYK	J	401	-	-	16/67/126/126	0/3/4/4
2	TYK	I	401	-	-	16/67/126/126	0/3/4/4
2	TYK	N	401	-	-	8/67/126/126	0/3/4/4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	401	TYK	C6-C5	3.30	1.59	1.52
2	F	401	TYK	C11-C10	3.21	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	401	TYK	O1C-C23	3.14	1.49	1.43
2	D	401	TYK	C6-C5	3.11	1.58	1.52
2	F	401	TYK	C6-C5	3.07	1.58	1.52

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	TYK	C10-C11-C12	7.58	137.45	126.23
2	A	401	TYK	C10-C11-C12	7.51	137.34	126.23
2	F	401	TYK	C10-C11-C12	7.42	137.21	126.23
2	D	401	TYK	C10-C11-C12	7.10	136.74	126.23
2	B	401	TYK	O1A-C5-C4	4.42	113.44	108.23

There are no chirality outliers.

5 of 238 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	C13-C14-C15-C16
2	A	401	TYK	C13-C14-C15-O15
2	A	401	TYK	C23-C14-C15-C16

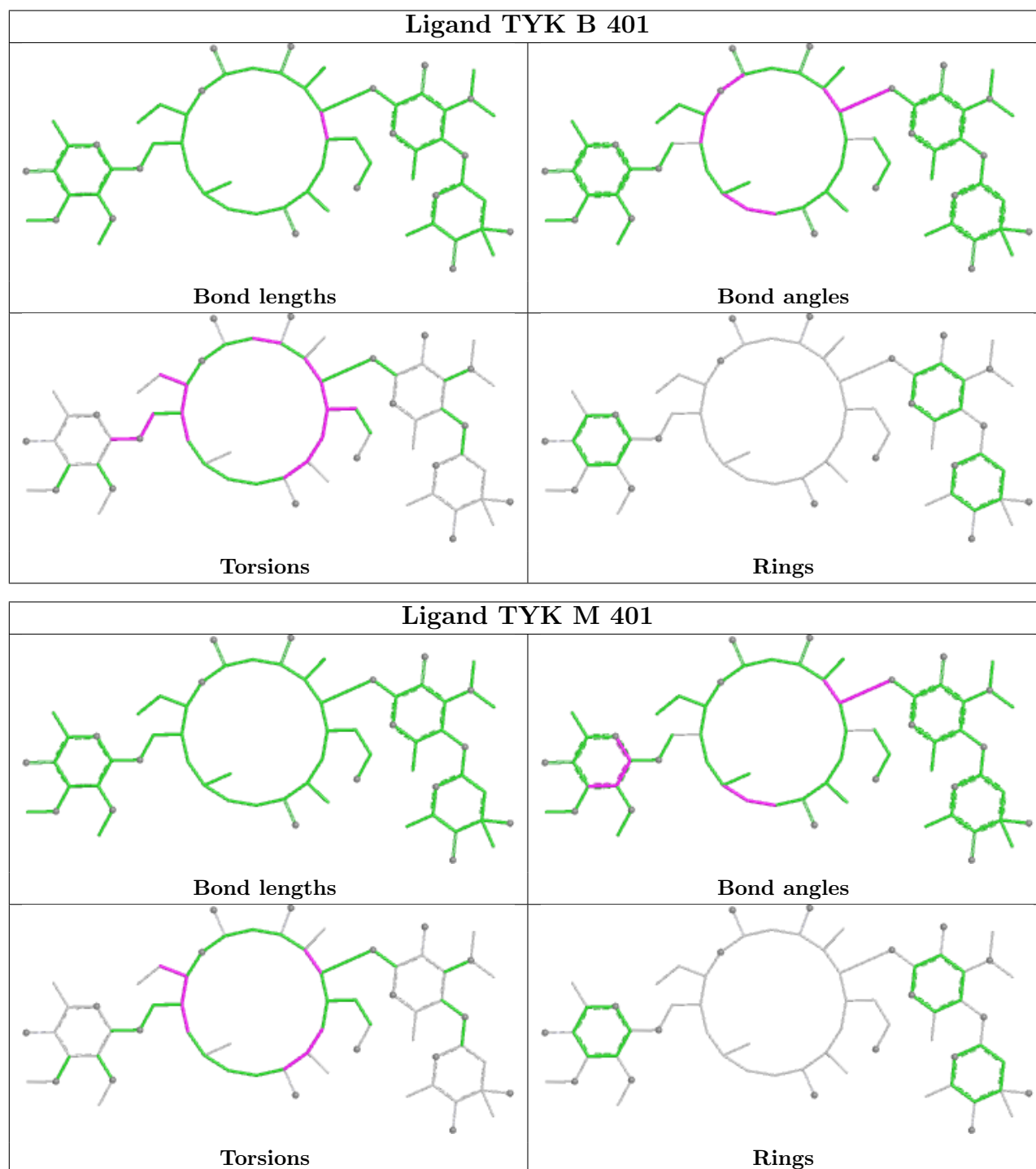
There are no ring outliers.

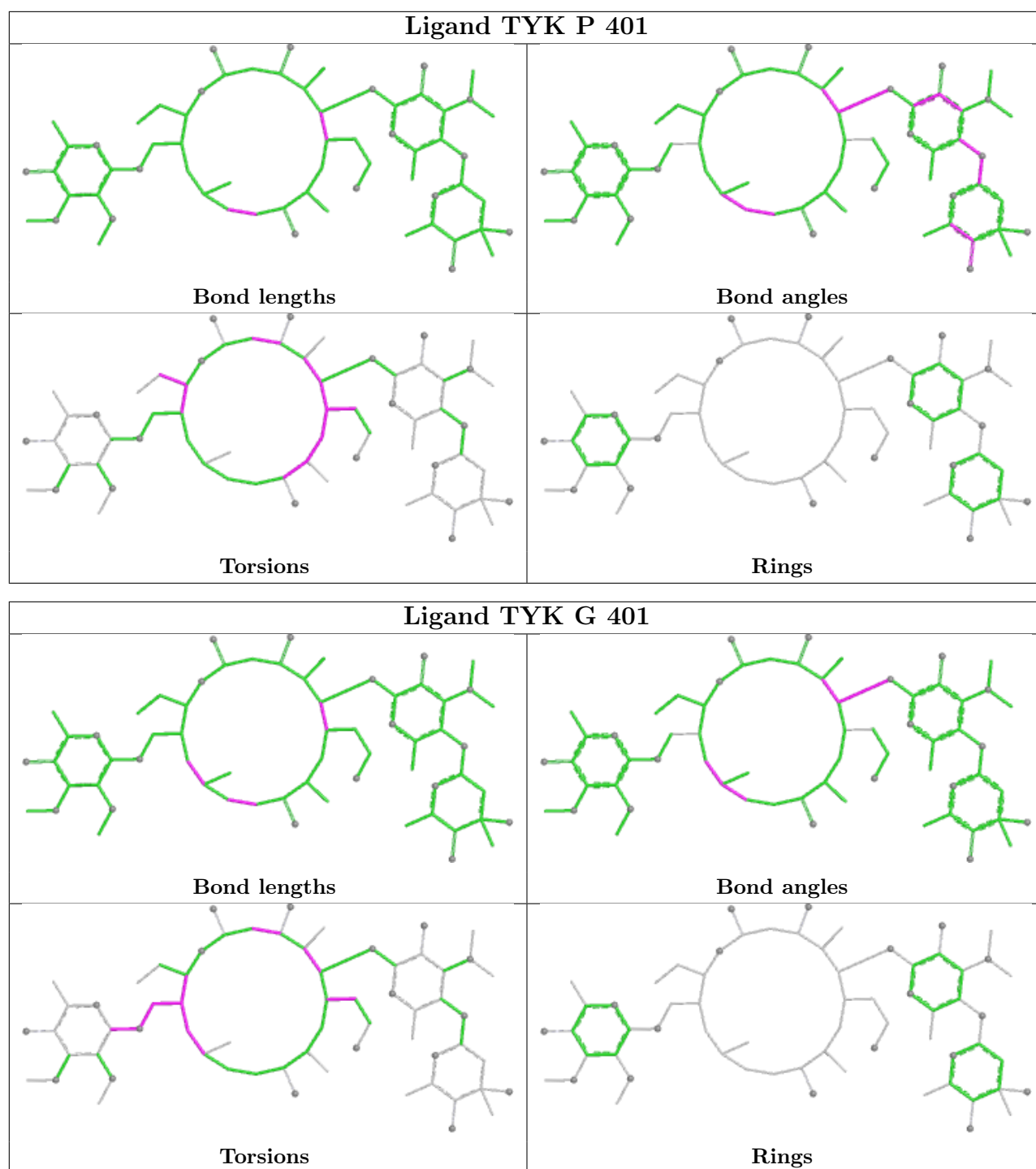
7 monomers are involved in 18 short contacts:

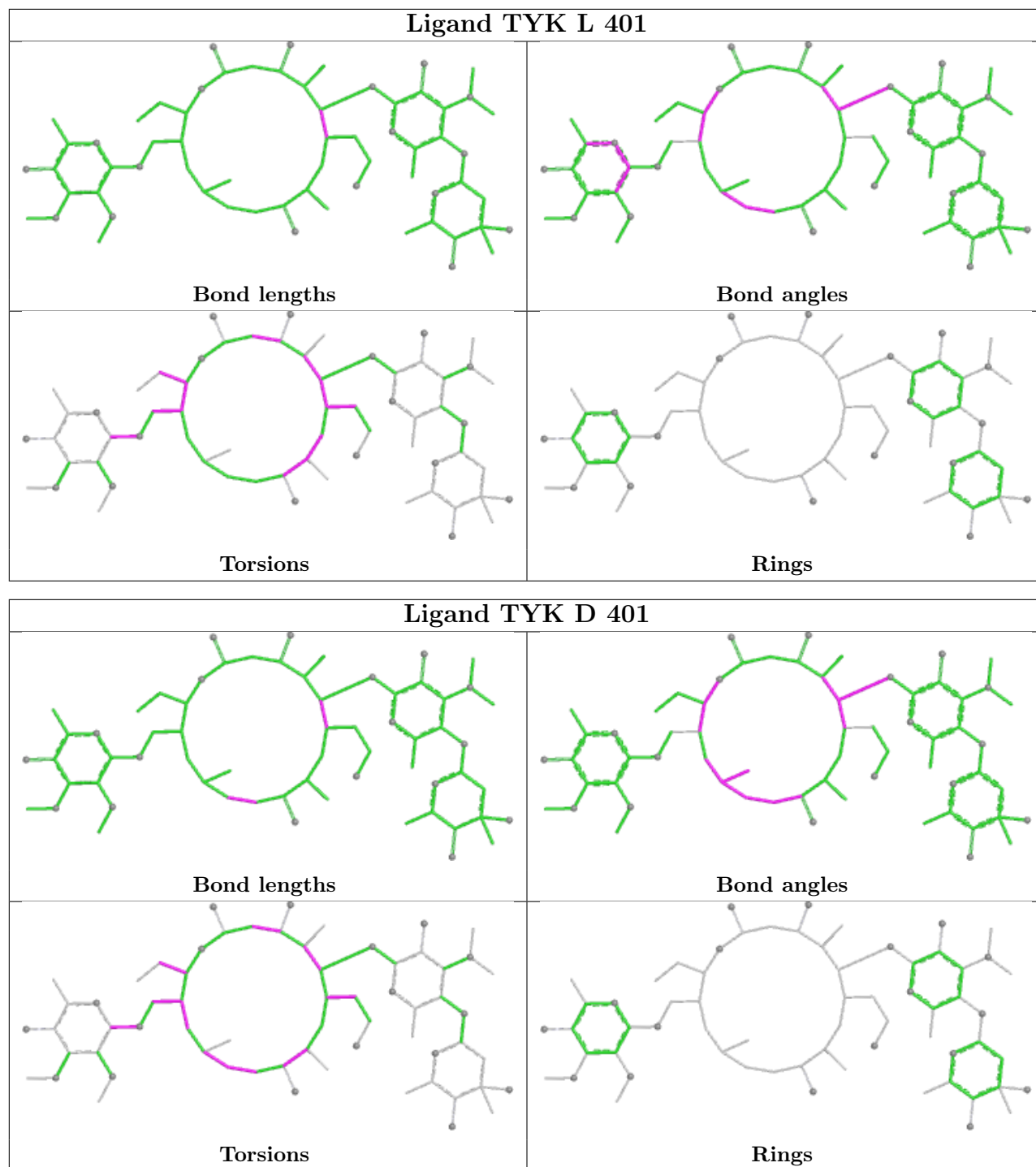
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	TYK	1	0
2	E	401	TYK	4	0
2	F	401	TYK	3	0
2	C	401	TYK	5	0
2	K	401	TYK	1	0
2	A	401	TYK	2	0
2	O	401	TYK	2	0

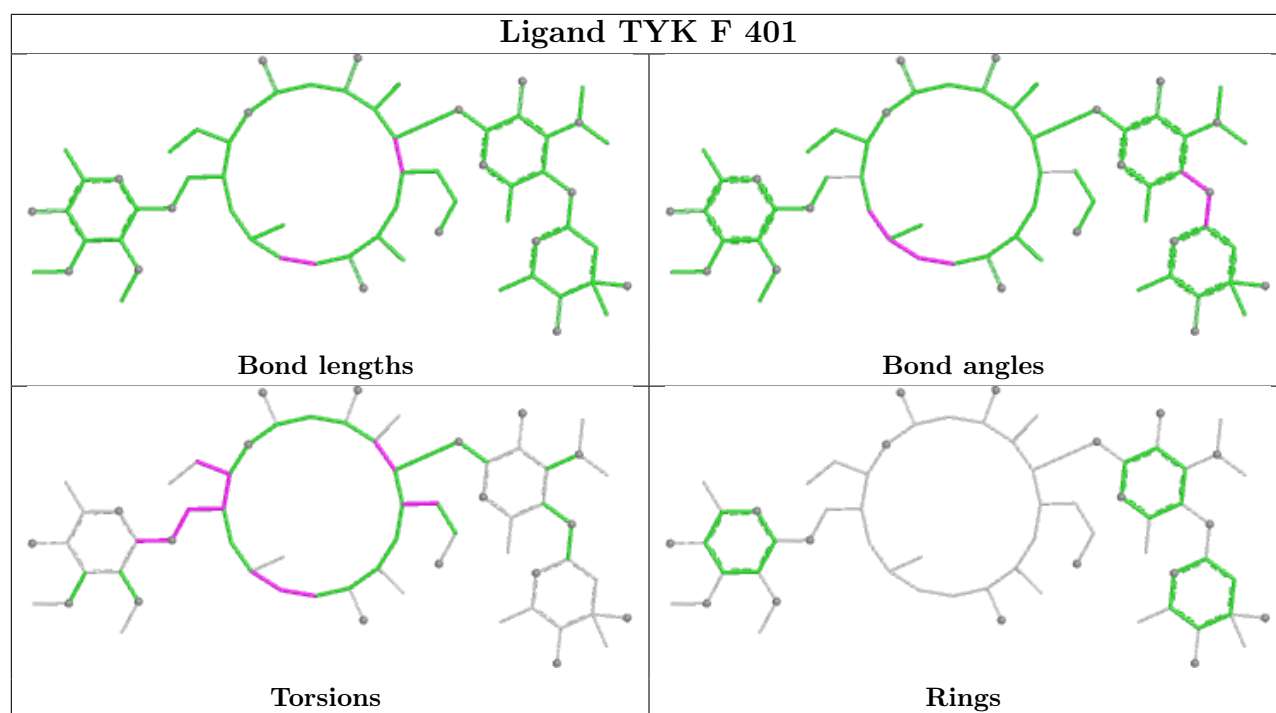
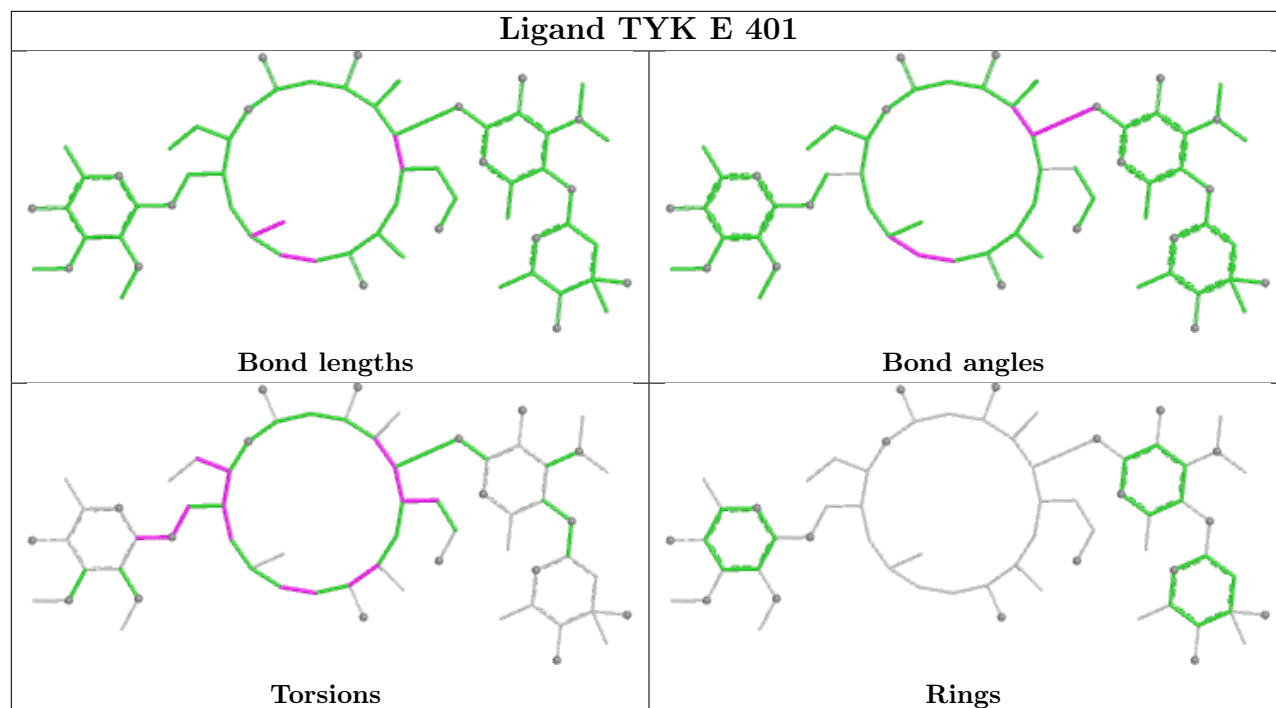
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

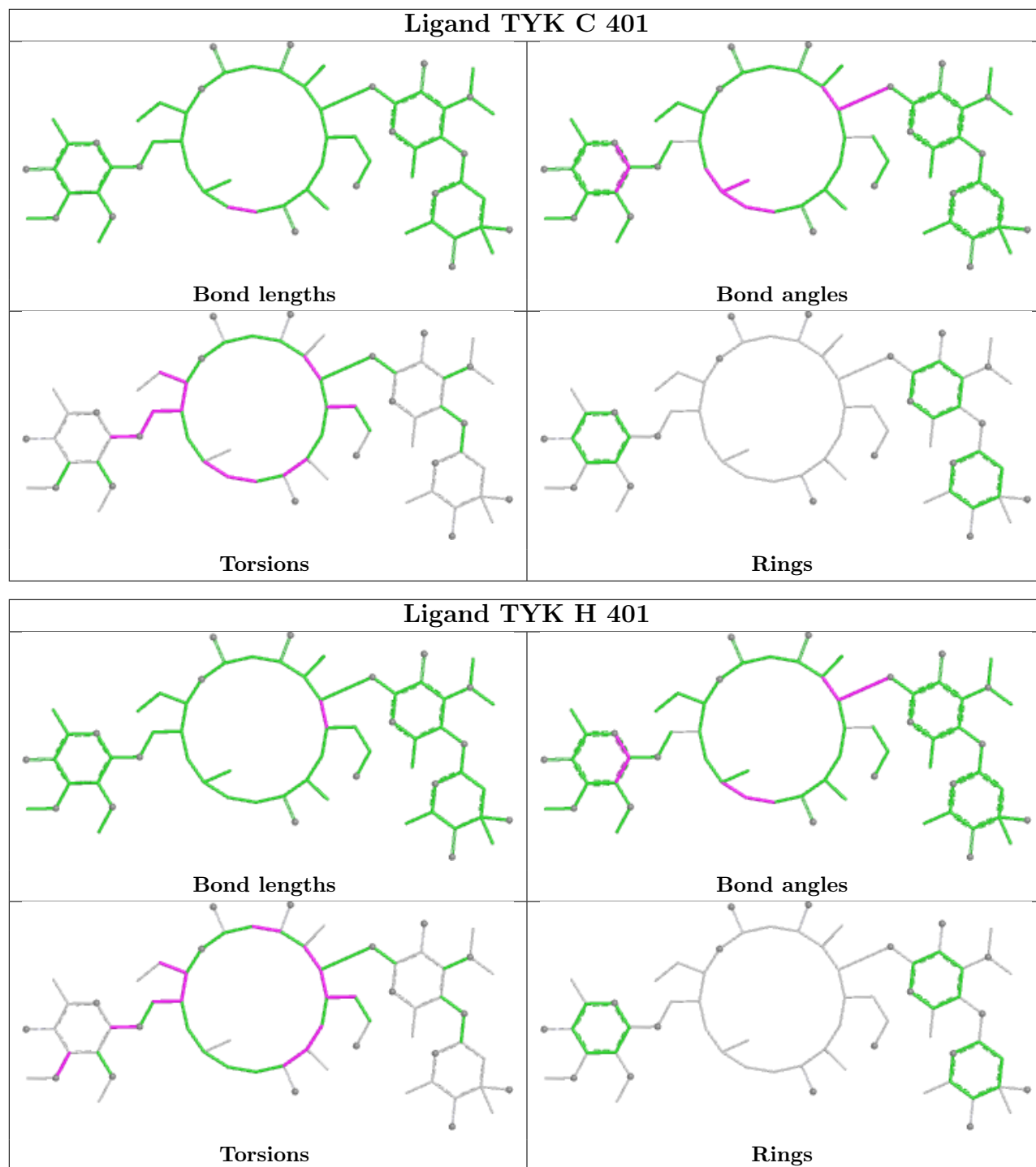
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

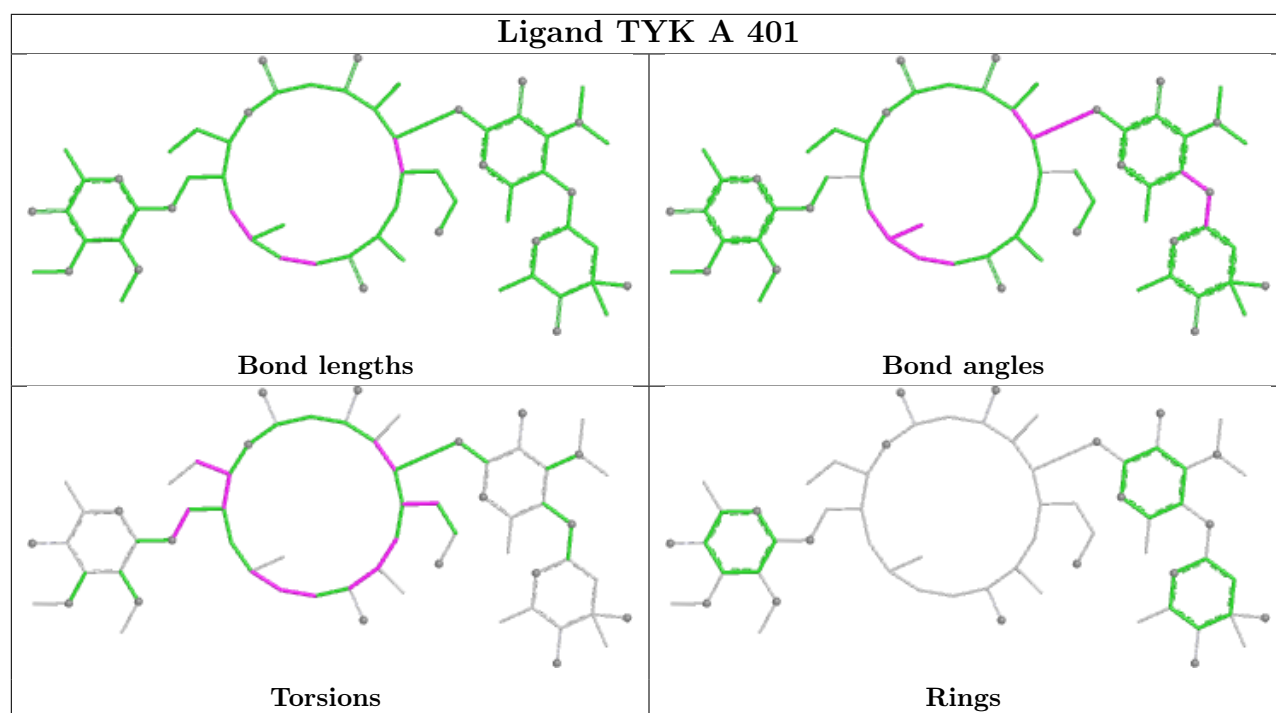
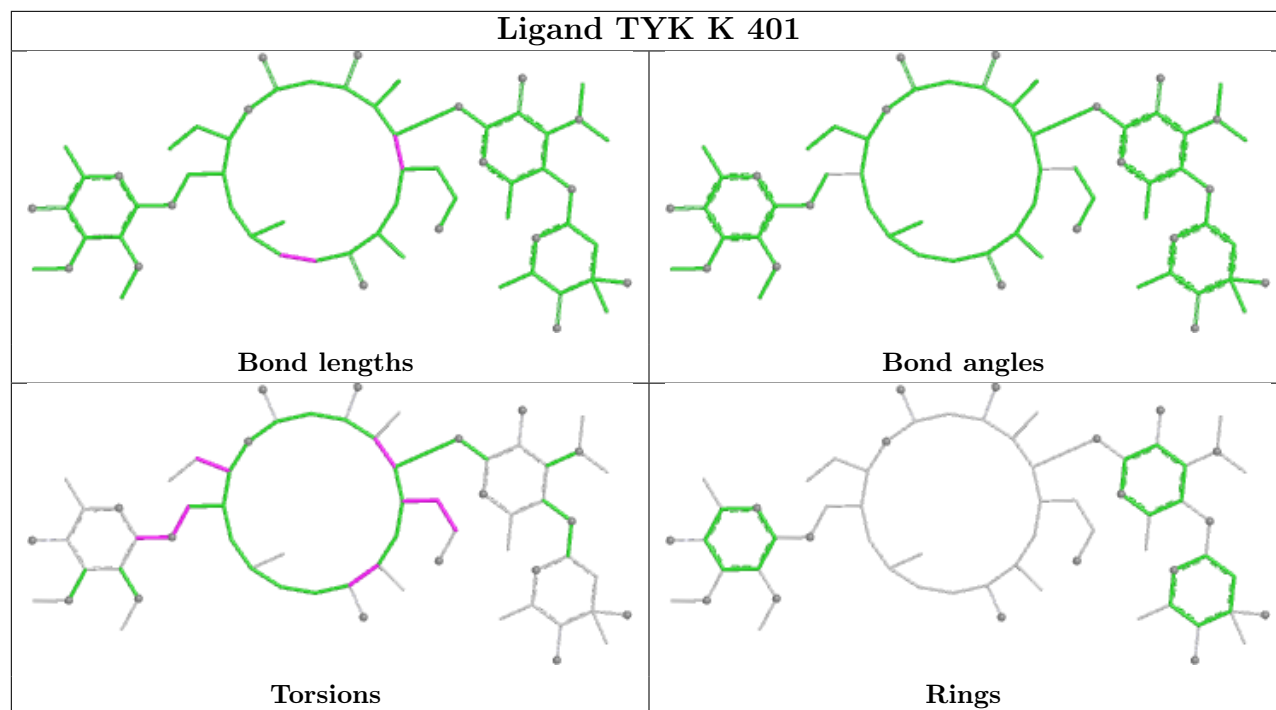


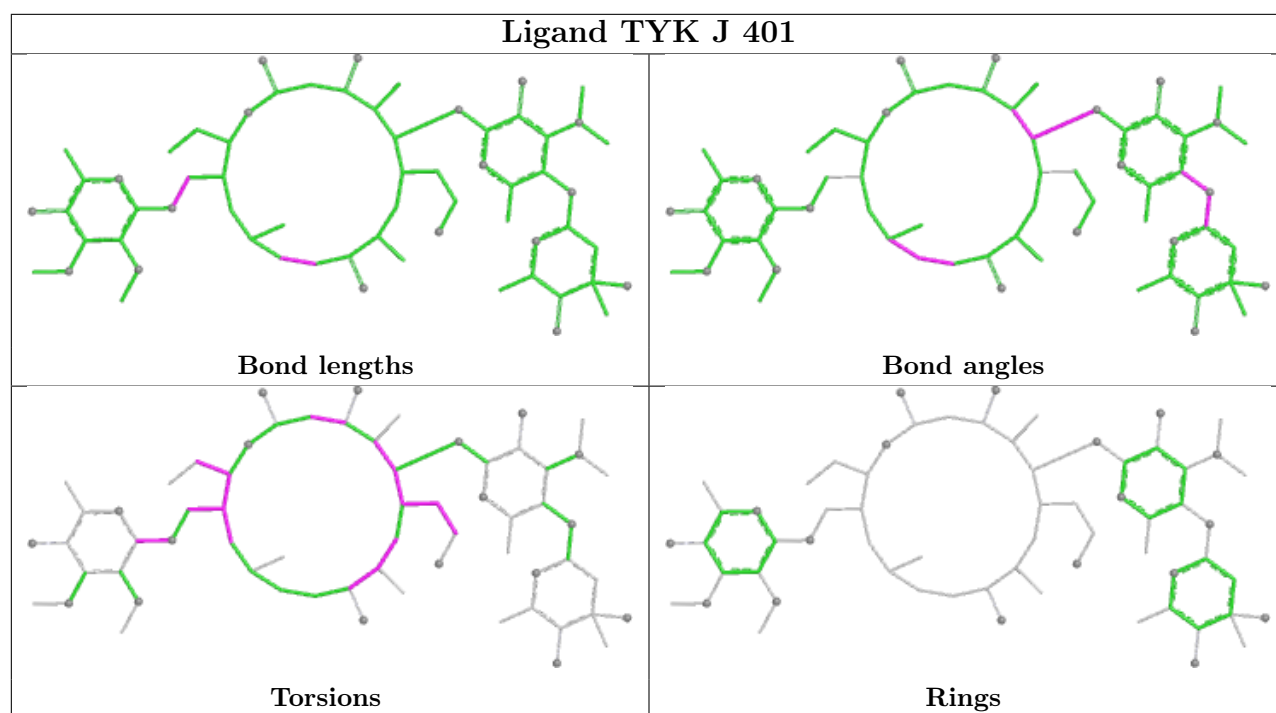
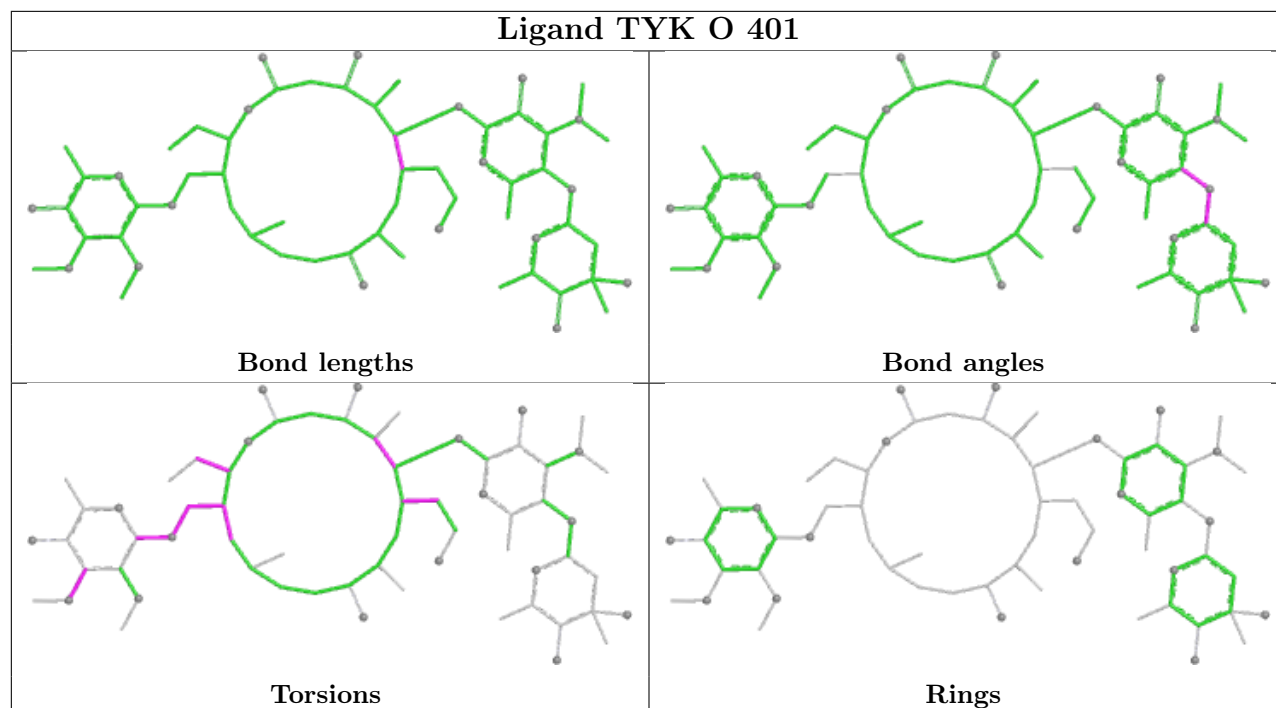


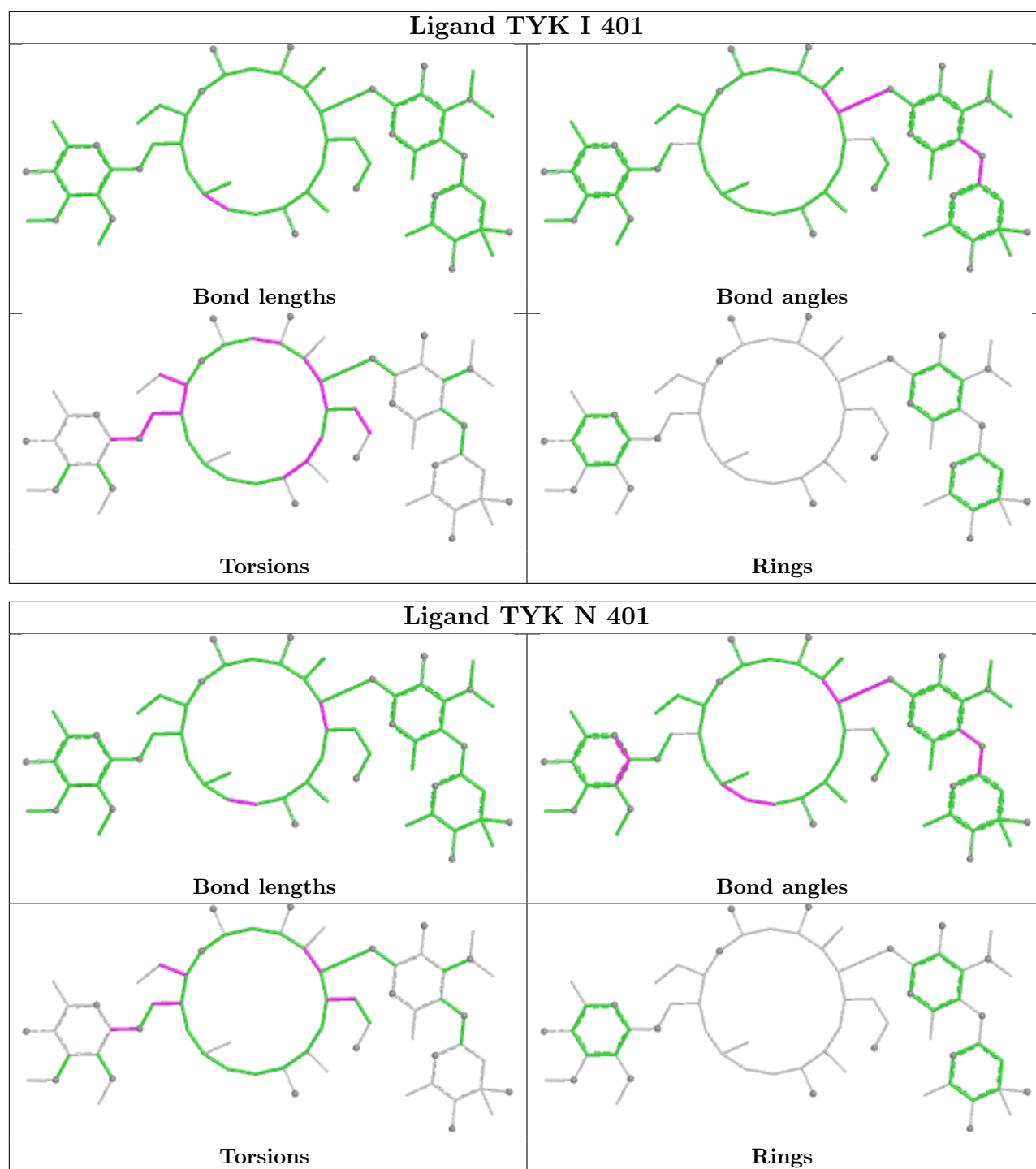












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	299/351 (85%)	0.15	16 (5%) 31 29	18, 34, 69, 85	0
1	B	314/351 (89%)	-0.01	16 (5%) 33 32	16, 29, 69, 106	0
1	C	297/351 (84%)	0.24	16 (5%) 31 29	18, 35, 72, 103	0
1	D	310/351 (88%)	0.09	12 (3%) 43 43	19, 33, 69, 89	0
1	E	292/351 (83%)	0.16	17 (5%) 29 27	18, 35, 69, 100	0
1	F	312/351 (88%)	0.14	20 (6%) 25 24	17, 33, 75, 105	0
1	G	298/351 (84%)	0.26	19 (6%) 25 24	18, 36, 72, 98	0
1	H	313/351 (89%)	0.10	17 (5%) 31 29	17, 31, 74, 104	0
1	I	301/351 (85%)	-0.00	19 (6%) 26 24	16, 29, 68, 87	0
1	J	314/351 (89%)	-0.20	8 (2%) 58 59	15, 27, 63, 94	0
1	K	296/351 (84%)	0.14	18 (6%) 27 25	16, 33, 75, 112	0
1	L	311/351 (88%)	-0.28	5 (1%) 70 71	14, 25, 57, 100	0
1	M	297/351 (84%)	0.13	22 (7%) 20 19	17, 32, 74, 116	0
1	N	315/351 (89%)	-0.22	8 (2%) 58 59	16, 27, 56, 101	0
1	O	305/351 (86%)	0.01	15 (4%) 35 34	15, 31, 67, 94	0
1	P	318/351 (90%)	-0.28	10 (3%) 51 51	15, 25, 62, 102	0
All	All	4892/5616 (87%)	0.02	238 (4%) 35 34	14, 31, 70, 116	0

The worst 5 of 238 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	249	PRO	9.6
1	N	246	LEU	8.4
1	A	245	ALA	7.9
1	F	249	PRO	7.1
1	M	246	LEU	7.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

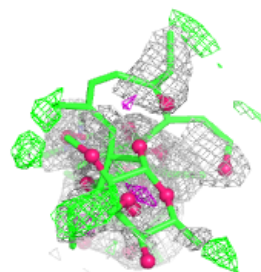
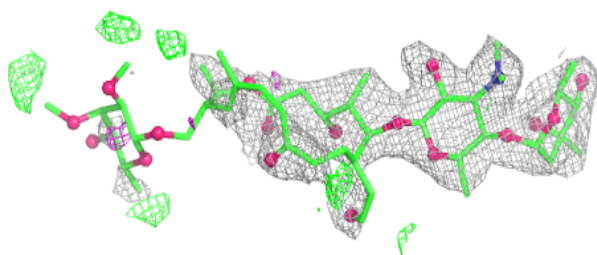
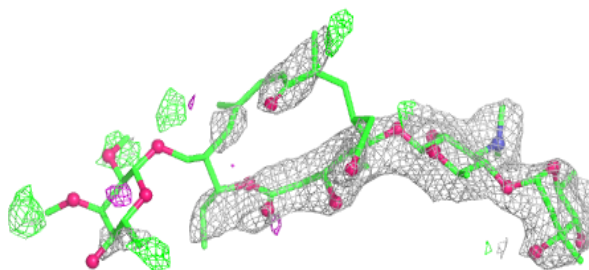
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TYK	F	401	64/64	0.71	0.23	64,86,145,155	0
2	TYK	H	401	64/64	0.73	0.23	57,88,161,170	0
2	TYK	B	401	64/64	0.75	0.25	56,91,169,179	0
2	TYK	G	401	64/64	0.76	0.22	44,84,151,159	0
2	TYK	D	401	64/64	0.76	0.22	43,77,156,167	0
2	TYK	J	401	64/64	0.78	0.20	49,82,151,160	0
2	TYK	A	401	64/64	0.79	0.24	47,77,170,181	0
2	TYK	N	401	64/64	0.80	0.20	45,65,147,152	0
2	TYK	L	401	64/64	0.82	0.19	41,64,152,157	0
2	TYK	C	401	64/64	0.83	0.21	53,76,161,172	0
2	TYK	M	401	64/64	0.83	0.19	37,64,138,144	0
2	TYK	E	401	64/64	0.83	0.20	49,77,167,177	0
2	TYK	P	401	64/64	0.83	0.19	40,63,143,155	0
2	TYK	K	401	64/64	0.84	0.19	41,71,161,170	0
2	TYK	O	401	64/64	0.85	0.18	37,65,148,159	0
2	TYK	I	401	64/64	0.86	0.18	43,63,165,180	0

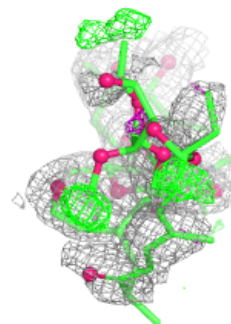
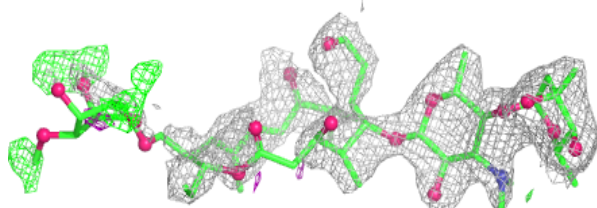
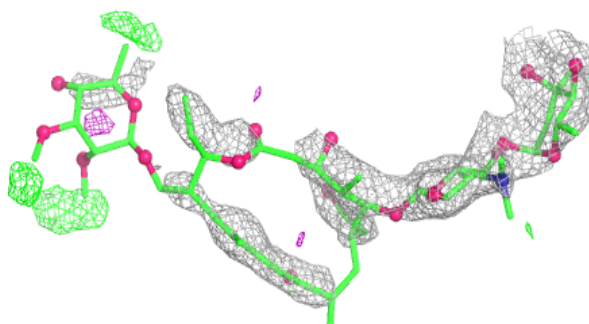
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

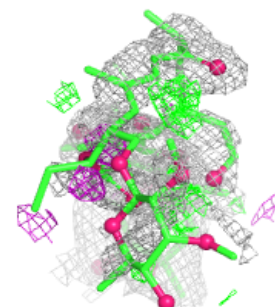
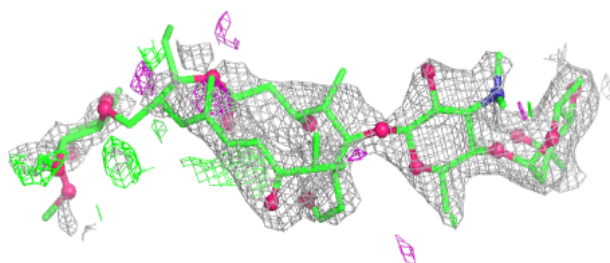
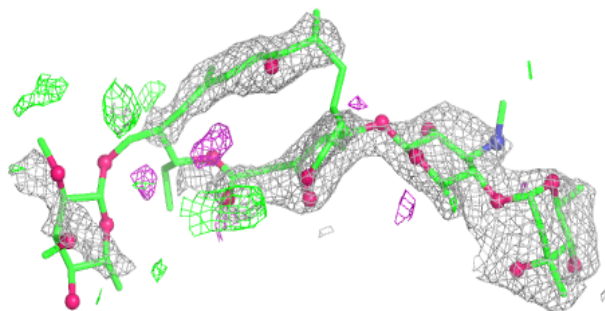
**Electron density around TYK H 401:**

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

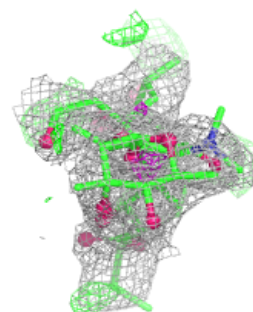
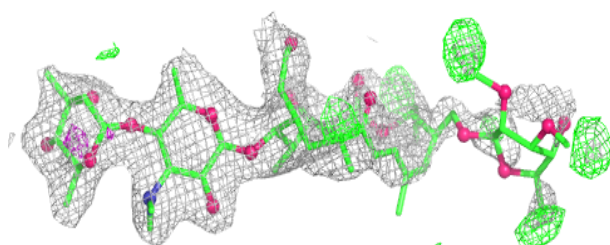
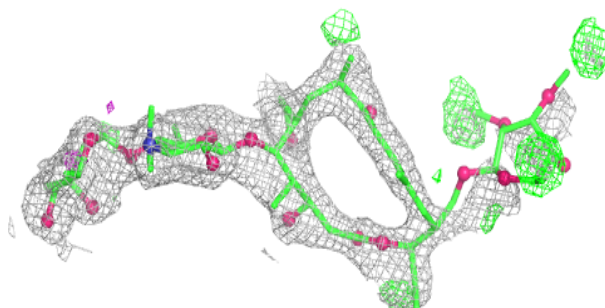


Electron density around TYK B 401:

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

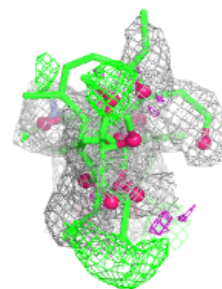
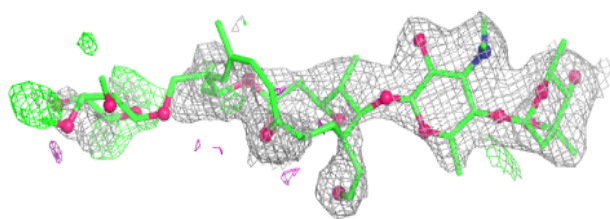
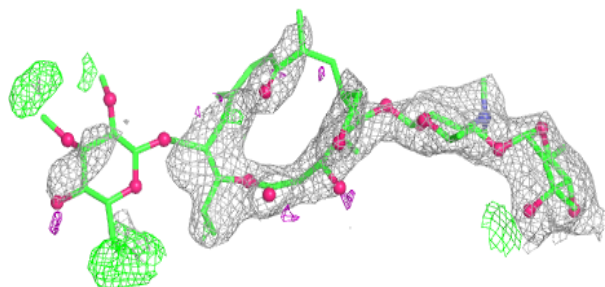
**Electron density around TYK G 401:**

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

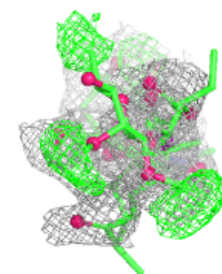
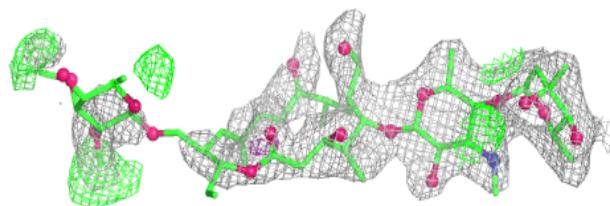
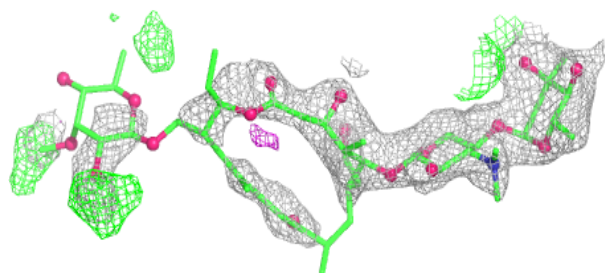


Electron density around TYK D 401:

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

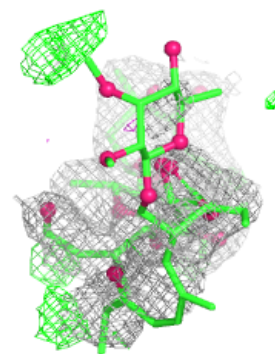
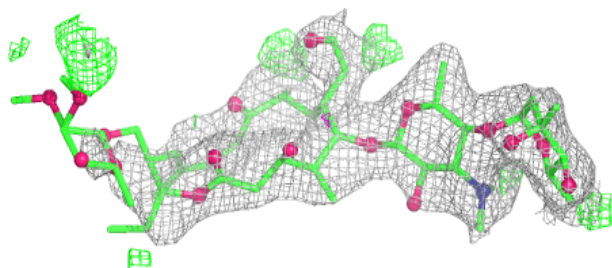
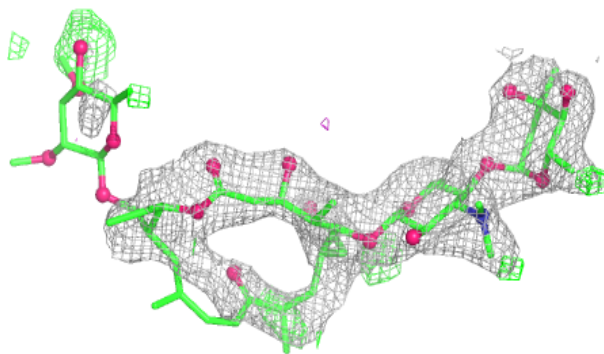
**Electron density around TYK J 401:**

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

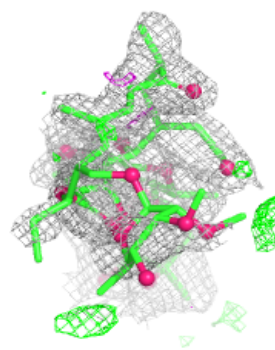
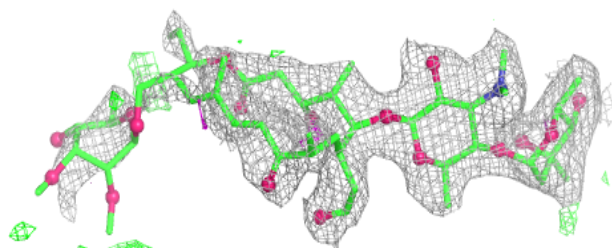
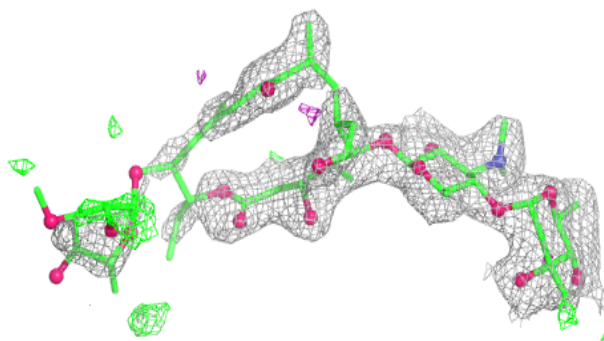


Electron density around TYK A 401:

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

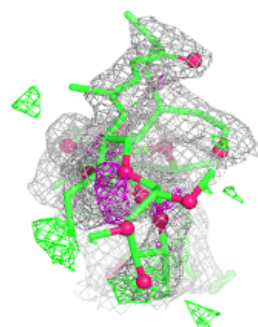
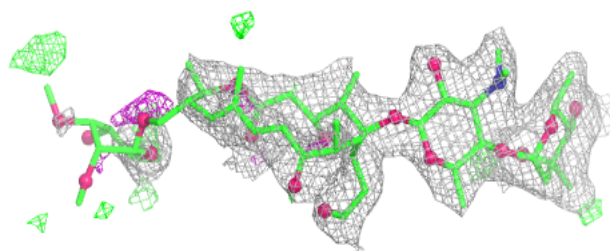
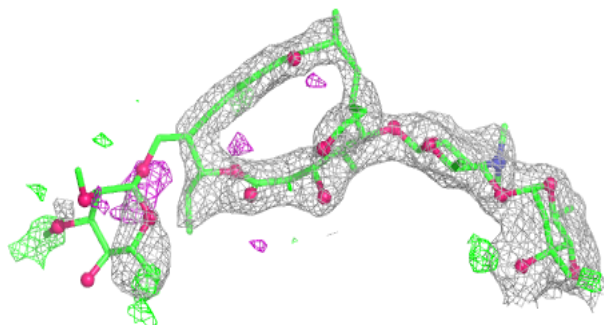
**Electron density around TYK N 401:**

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

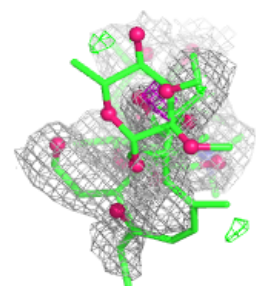
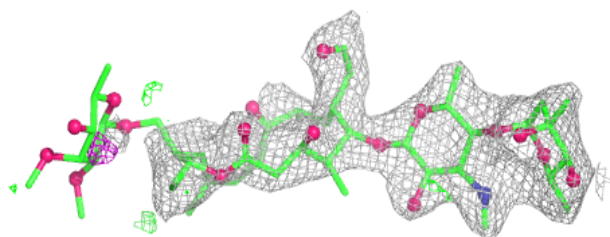
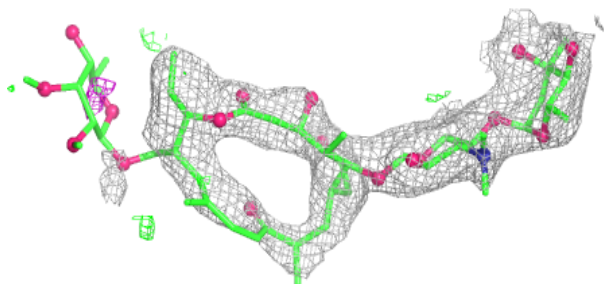


Electron density around TYK L 401:

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

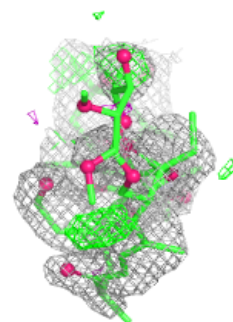
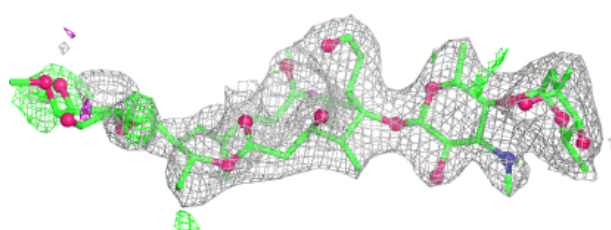
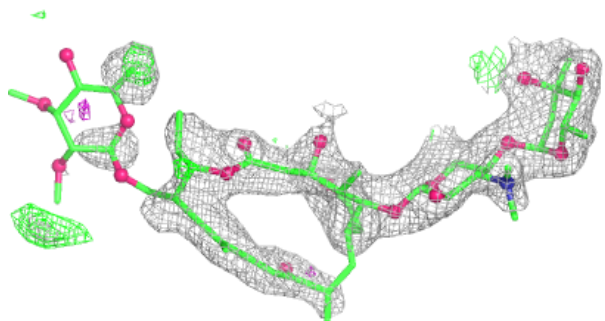
**Electron density around TYK C 401:**

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

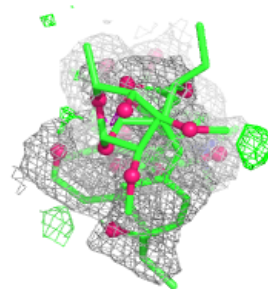
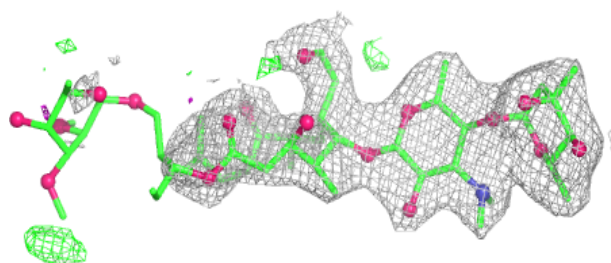
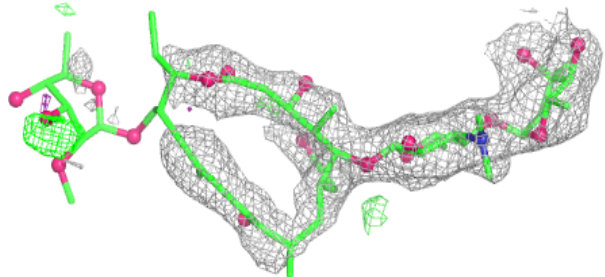


Electron density around TYK M 401:

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

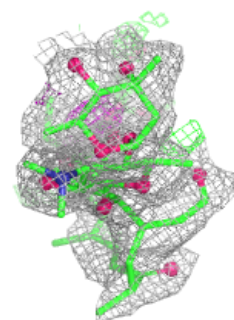
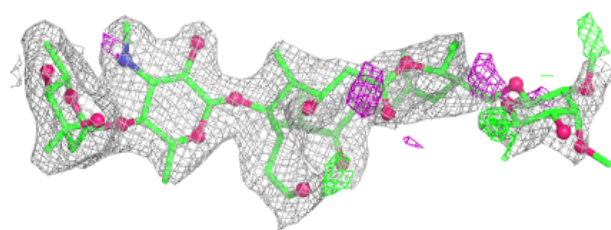
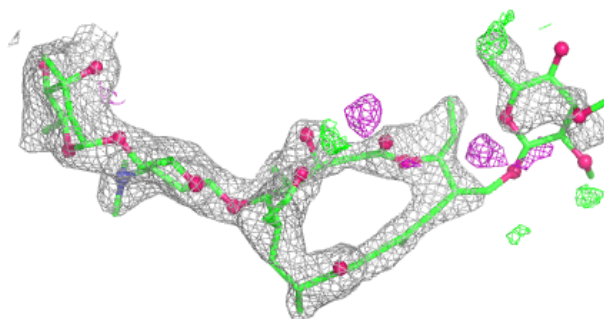
**Electron density around TYK E 401:**

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

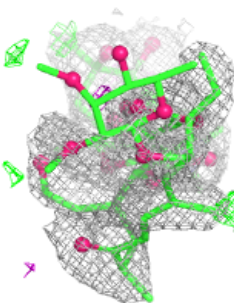
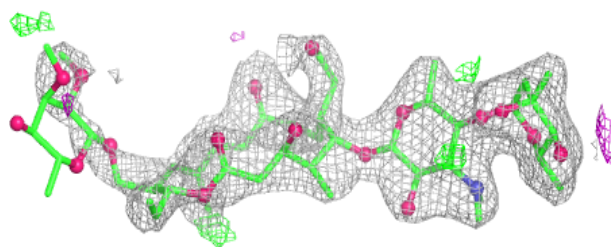
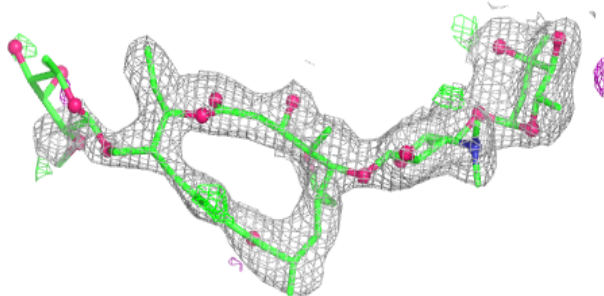


Electron density around TYK P 401:

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

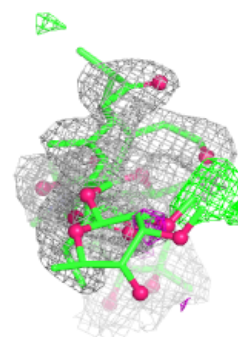
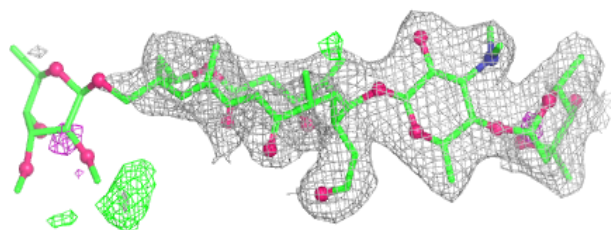
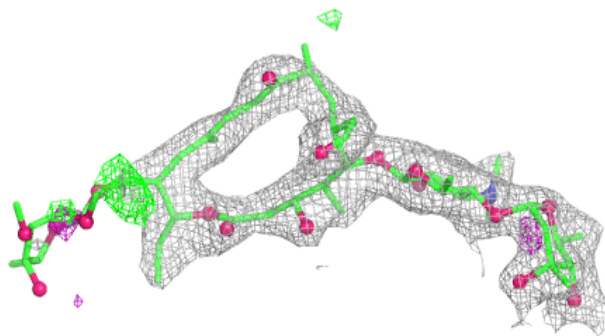
**Electron density around TYK K 401:**

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

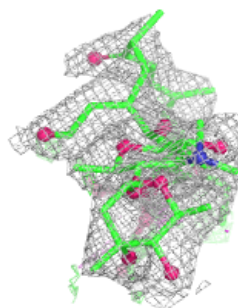
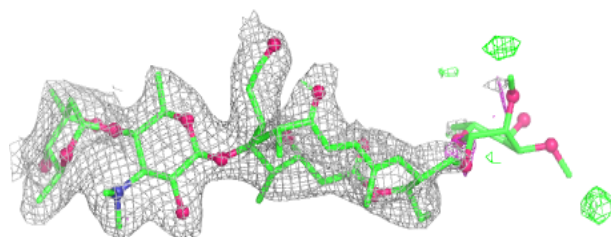
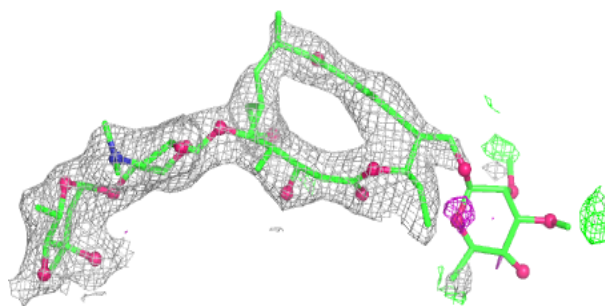


Electron density around TYK O 401:

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

**Electron density around TYK 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.