



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:22 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 Full wwPDB X-ray Structure Validation 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

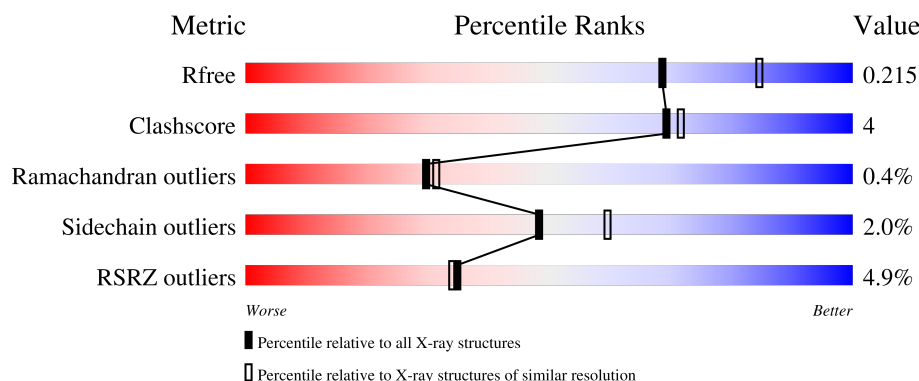
1 Overall quality at a glance

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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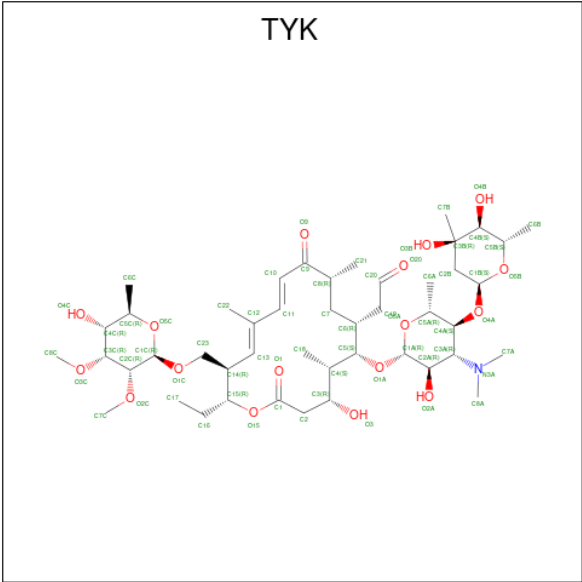
Chain	Residue	Modelled	Actual	Comment	Reference
M	-7	GLY	-	expression tag	UNP A0A3R7J519
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M	-5	VAL	-	expression tag	UNP A0A3R7J519
M	-4	PRO	-	expression tag	UNP A0A3R7J519
M	-3	ARG	-	expression tag	UNP A0A3R7J519
M	-2	GLY	-	expression tag	UNP A0A3R7J519
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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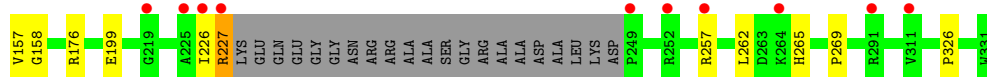
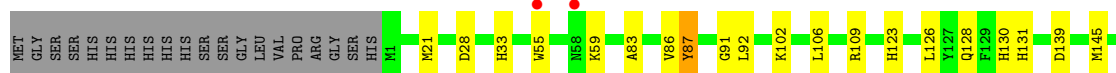
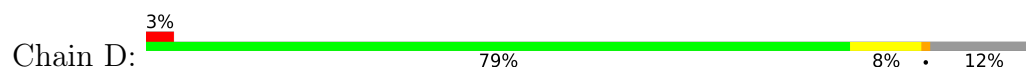
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total	C	N	O	0	0
			64	46	1	17		
2	P	1	Total	C	N	O	0	0
			64	46	1	17		

- Molecule 3 is water.

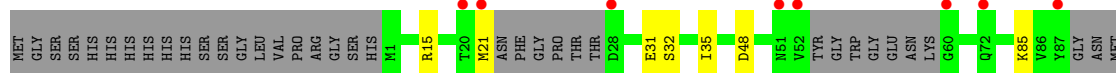
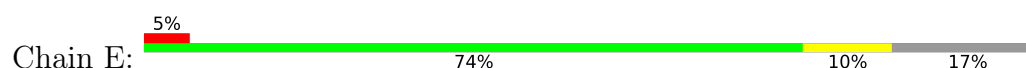
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total	O	0	0
			110	110		
3	B	144	Total	O	0	0
			144	144		
3	C	112	Total	O	0	0
			112	112		
3	D	128	Total	O	0	0
			128	128		
3	E	104	Total	O	0	0
			104	104		
3	F	118	Total	O	0	0
			118	118		
3	G	109	Total	O	0	0
			109	109		
3	H	126	Total	O	0	0
			126	126		
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		



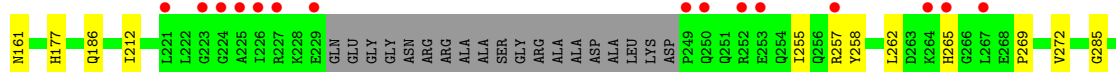
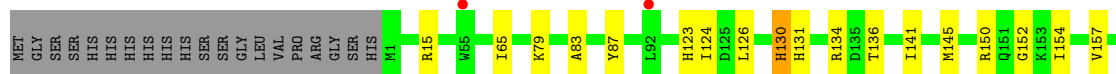
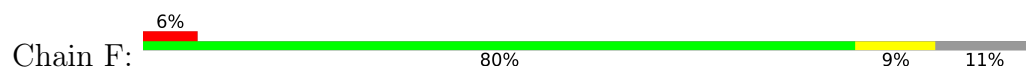
- Molecule 1: Aldo/keto reductase



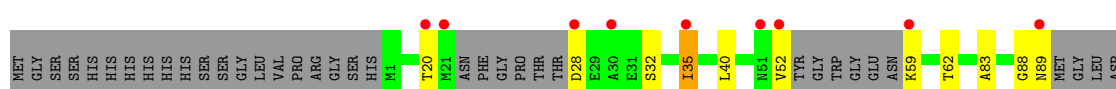
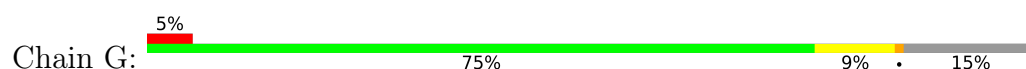
- Molecule 1: Aldo/keto reductase

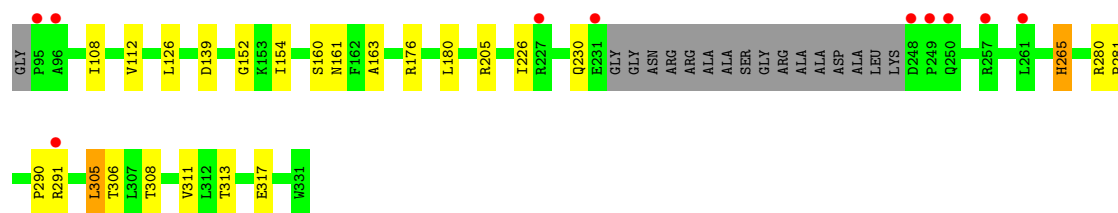


- Molecule 1: Aldo/keto reductase

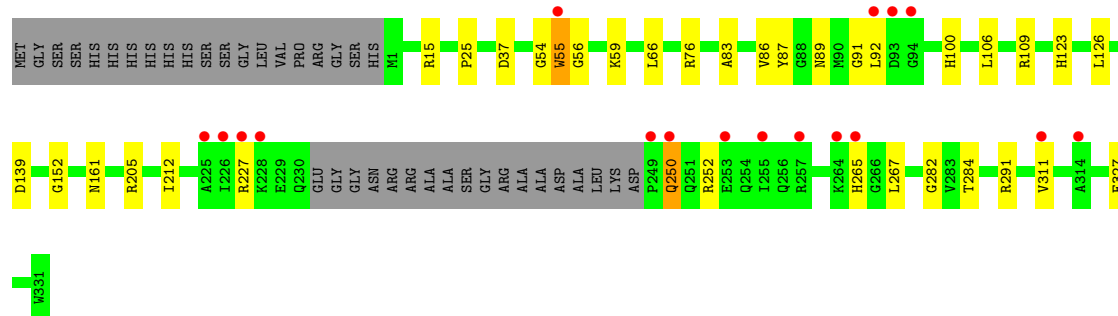
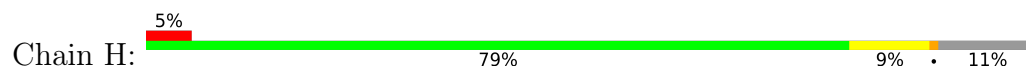


- Molecule 1: Aldo/keto reductase

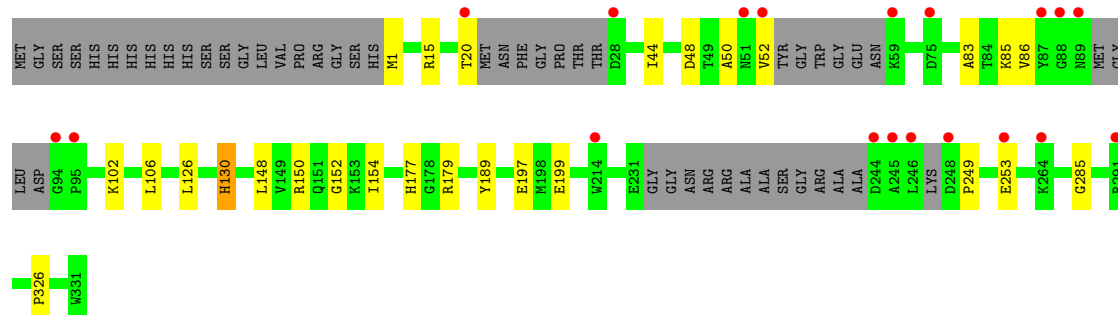
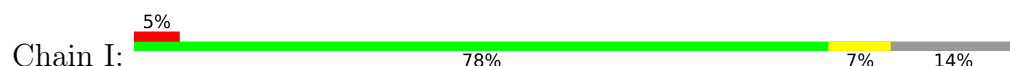




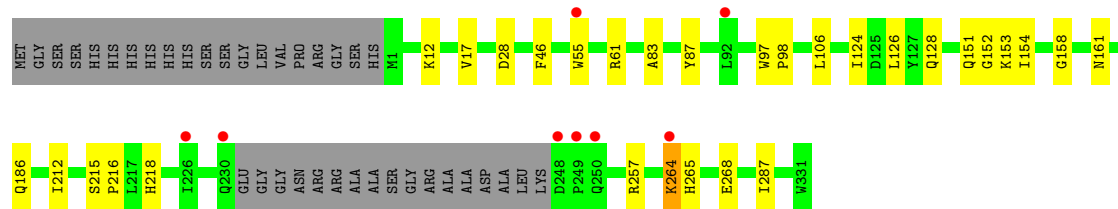
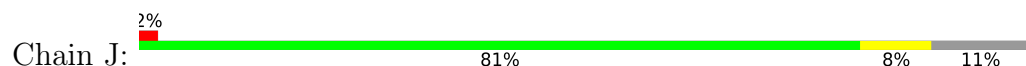
- Molecule 1: Aldo/keto reductase



- Molecule 1: Aldo/keto reductase

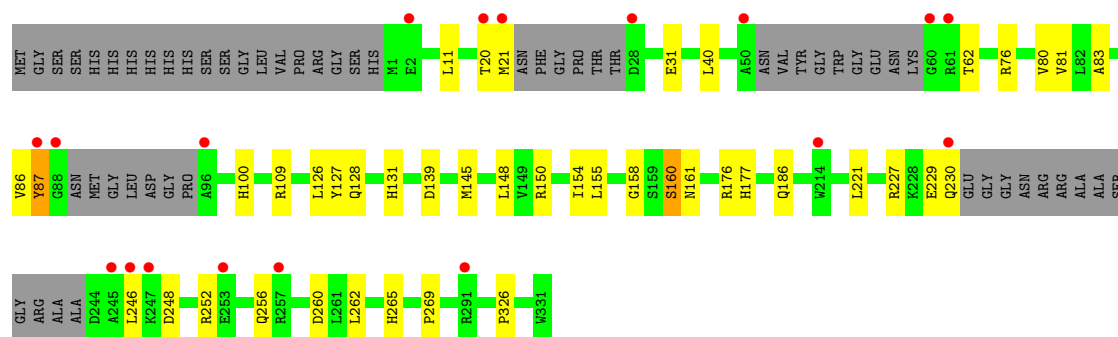


- Molecule 1: Aldo/keto reductase

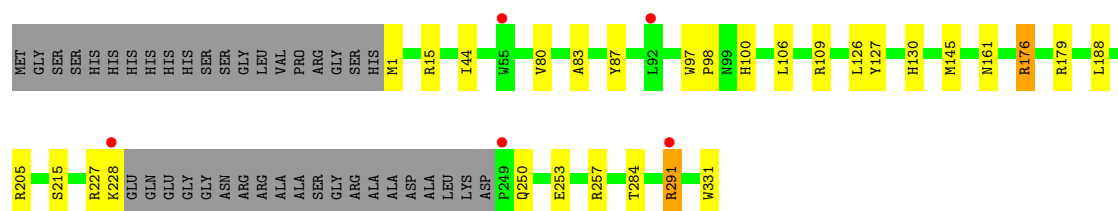
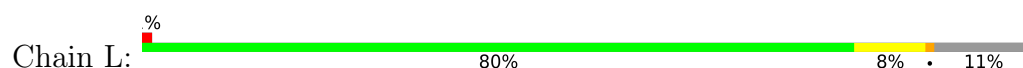


- Molecule 1: Aldo/keto reductase

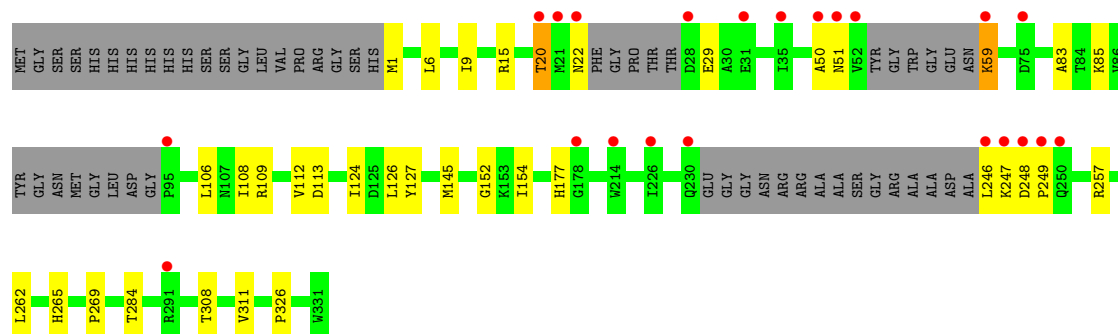
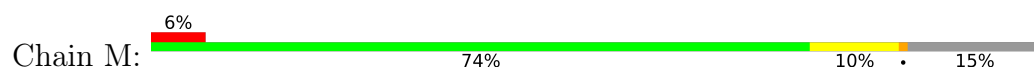




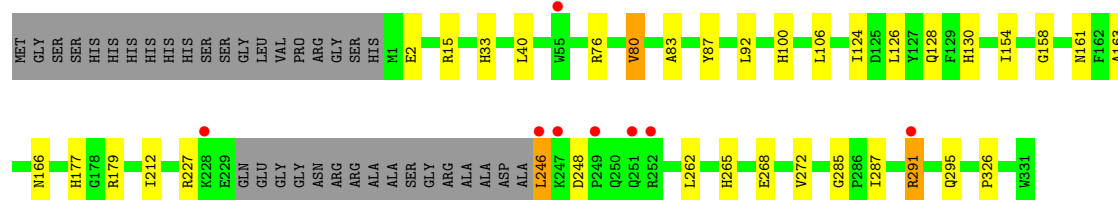
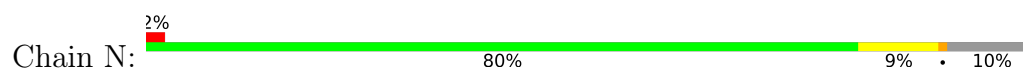
- Molecule 1: Aldo/keto reductase



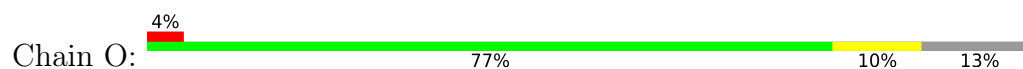
- Molecule 1: Aldo/keto reductase

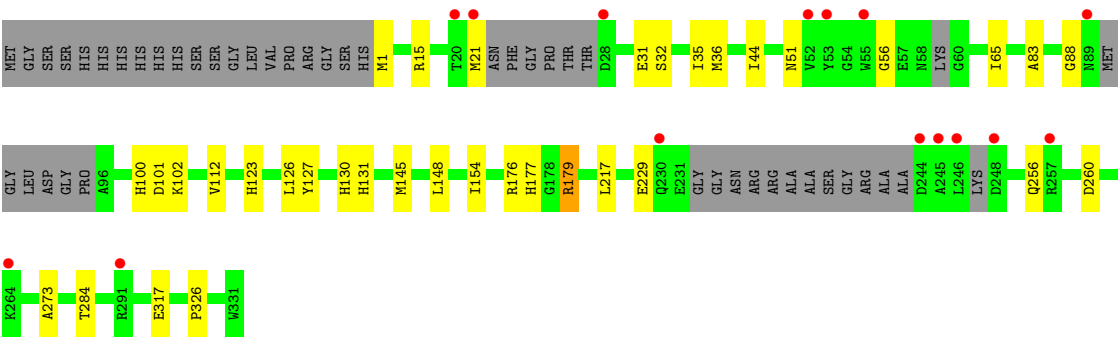


- Molecule 1: Aldo/keto reductase

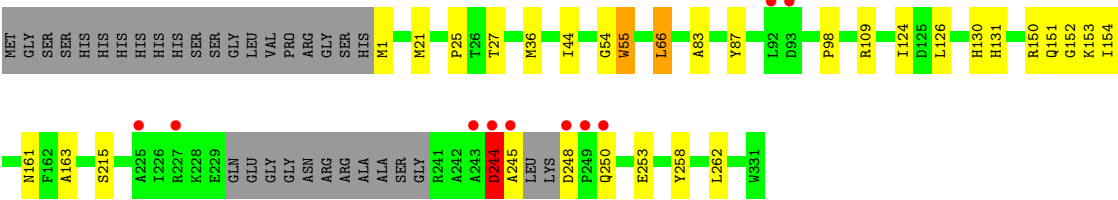
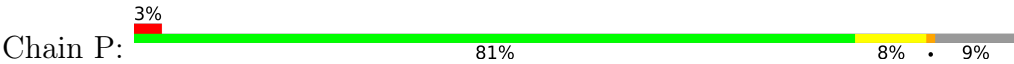


- Molecule 1: Aldo/keto reductase





● 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%)

All (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
1	B	265	HIS	CE1-NE2	6.30	1.38	1.32
1	B	100	HIS	CE1-NE2	6.29	1.38	1.32
1	L	130	HIS	CE1-NE2	6.29	1.38	1.32
1	D	131	HIS	CE1-NE2	6.12	1.38	1.32
1	A	123	HIS	CE1-NE2	6.08	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	100	HIS	CE1-NE2	6.00	1.38	1.32
1	K	131	HIS	CE1-NE2	5.96	1.38	1.32
1	A	265	HIS	CE1-NE2	5.95	1.38	1.32
1	F	130	HIS	CE1-NE2	5.82	1.38	1.32
1	K	177	HIS	CE1-NE2	5.82	1.38	1.32
1	F	177	HIS	CE1-NE2	5.72	1.38	1.32
1	C	100	HIS	CE1-NE2	5.69	1.38	1.32
1	H	123	HIS	CE1-NE2	5.65	1.38	1.32
1	C	123	HIS	CE1-NE2	5.63	1.38	1.32
1	D	33	HIS	CE1-NE2	5.59	1.38	1.32
1	F	265	HIS	CE1-NE2	5.58	1.38	1.32
1	P	130	HIS	CE1-NE2	5.57	1.38	1.32
1	D	130	HIS	CE1-NE2	5.57	1.38	1.32
1	E	131	HIS	CE1-NE2	5.57	1.38	1.32
1	J	265	HIS	CE1-NE2	5.56	1.38	1.32
1	B	33	HIS	CE1-NE2	5.52	1.38	1.32
1	E	265	HIS	CE1-NE2	5.50	1.38	1.32
1	N	177	HIS	CE1-NE2	5.42	1.38	1.32
1	J	218	HIS	CE1-NE2	5.39	1.38	1.32
1	O	100	HIS	CE1-NE2	5.35	1.37	1.32
1	O	177	HIS	CE1-NE2	5.34	1.37	1.32
1	L	100	HIS	CE1-NE2	5.30	1.37	1.32
1	I	130	HIS	CE1-NE2	5.29	1.37	1.32
1	H	265	HIS	CE1-NE2	5.29	1.37	1.32
1	F	123	HIS	CE1-NE2	5.28	1.37	1.32
1	O	123	HIS	CE1-NE2	5.26	1.37	1.32
1	I	177	HIS	CE1-NE2	5.25	1.37	1.32
1	K	100	HIS	CE1-NE2	5.24	1.37	1.32
1	P	131	HIS	CE1-NE2	5.18	1.37	1.32
1	N	265	HIS	CE1-NE2	5.15	1.37	1.32
1	O	130	HIS	CE1-NE2	5.11	1.37	1.32
1	N	130	HIS	CE1-NE2	5.07	1.37	1.32
1	B	123	HIS	CE1-NE2	5.07	1.37	1.32
1	K	265	HIS	CE1-NE2	5.07	1.37	1.32
1	G	265	HIS	CE1-NE2	5.04	1.37	1.32
1	D	265	HIS	CE1-NE2	5.04	1.37	1.32
1	N	33	HIS	CE1-NE2	5.03	1.37	1.32
1	M	265	HIS	CE1-NE2	5.01	1.37	1.32
1	E	177	HIS	CE1-NE2	5.01	1.37	1.32

All (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
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
1	J	28	ASP	CA-CB-CG	6.06	118.66	112.60
1	O	179	ARG	N-CA-C	6.05	119.23	110.28
1	G	139	ASP	CA-CB-CG	5.97	118.57	112.60
1	D	139	ASP	CA-CB-CG	5.78	118.38	112.60
1	C	20	THR	CB-CA-C	5.73	121.82	110.42
1	L	331	TRP	CA-C-O	-5.51	111.43	120.80
1	N	248	ASP	CA-CB-CG	5.47	118.07	112.60
1	P	215	SER	CB-CA-C	5.37	115.01	111.20
1	H	139	ASP	CA-CB-CG	5.27	117.87	112.60
1	L	176	ARG	CB-CA-C	-5.23	101.79	110.68
1	A	280	ARG	N-CA-C	5.22	116.23	109.65
1	I	48	ASP	CA-CB-CG	5.22	117.82	112.60
1	E	48	ASP	CA-CB-CG	5.20	117.80	112.60
1	P	244	ASP	CA-CB-CG	5.16	117.76	112.60
1	G	180	LEU	CA-C-N	-5.11	116.93	122.55
1	G	180	LEU	C-N-CA	-5.11	116.93	122.55
1	C	248	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

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

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

All (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
2:O:401:TYK:H8C3	2:O:401:TYK:H7C2	1.73	0.70
1:A:177:HIS:ND1	3:A:501:HOH:O	2.24	0.70
1:O:148:LEU:HD13	1:O:154:ILE:HD12	1.74	0.69
1:P:248:ASP:N	3:P:502:HOH:O	2.25	0.68
1:F:262:LEU:HD11	1:F:272:VAL:HG11	1.75	0.68
1:C:21:MET:C	1:C:51:ASN:HA	2.19	0.68
1:G:28:ASP:N	3:G:501:HOH:O	2.26	0.67
2:E:401:TYK:H221	2:E:401:TYK:H231	1.75	0.67
1:I:249:PRO:O	1:I:253:GLU:HG2	1.95	0.67
1:K:221:LEU:HD11	1:K:246:LEU:HD13	1.77	0.66
1:K:160:SER:HB3	1:K:186:GLN:HB3	1.77	0.66
1:M:20:THR:HG22	1:M:51:ASN:HA	1.78	0.65
2:C:401:TYK:HC2C	2:C:401:TYK:H162	1.79	0.65
1:D:226:ILE:O	1:D:227:ARG:HB2	1.95	0.64
1:L:205:ARG:HG2	1:L:205:ARG:HH21	1.62	0.64
1:A:86:VAL:HG22	1:A:130:HIS:ND1	2.14	0.63
1:M:145:MET:HE3	1:M:154:ILE:CD1	2.29	0.63
1:J:12:LYS:HD2	1:P:98:PRO:HB3	1.80	0.63
1:M:50:ALA:HB2	1:M:85:LYS:HE3	1.81	0.62
1:O:15:ARG:HD2	1:O:284:THR:O	2.00	0.61
2:E:401:TYK:C22	2:E:401:TYK:O9	2.49	0.61
1:I:86:VAL:CG2	1:I:130:HIS:ND1	2.64	0.61
1:M:15:ARG:HD2	1:M:284:THR:O	2.00	0.61
1:L:15:ARG:HD2	1:L:284:THR:O	2.02	0.60
2:E:401:TYK:O9	2:E:401:TYK:H223	2.02	0.60
1:H:54:GLY:O	1:H:55:TRP:HB2	2.02	0.60
1:A:86:VAL:CG2	1:A:130:HIS:ND1	2.66	0.59
1:N:291:ARG:NH1	1:N:295:GLN:HE22	2.01	0.58
1:O:127:TYR:HD2	1:O:145:MET:HE1	1.68	0.58
1:P:36:MET:SD	1:P:66:LEU:HD22	2.43	0.58
1:G:313:THR:O	1:G:317:GLU:HG3	2.04	0.58
1:M:112:VAL:HG22	1:M:127:TYR:CE2	2.39	0.58
1:B:152:GLY:O	1:H:109:ARG:NH1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:LYS:HE3	1:H:89:ASN:O	2.04	0.57
1:M:108:ILE:O	1:M:112:VAL:HG23	2.05	0.57
1:G:20:THR:HG21	1:G:62:THR:CG2	2.31	0.57
1:D:257:ARG:NH1	2:D:401:TYK:O1	2.38	0.57
1:A:109:ARG:NH1	1:G:152:GLY:O	2.37	0.56
1:A:221:LEU:HD13	1:A:255:ILE:HD11	1.86	0.56
1:P:83:ALA:HA	1:P:126:LEU:O	2.05	0.56
1:K:229:GLU:O	1:K:230:GLN:HG2	2.06	0.56
1:A:127:TYR:HD2	1:A:145:MET:HE1	1.70	0.56
1:N:262:LEU:HD13	1:N:272:VAL:HG21	1.88	0.56
1:A:50:ALA:O	1:A:51:ASN:HB2	2.04	0.55
1:C:228:LYS:HE2	3:C:534:HOH:O	2.05	0.55
1:A:50:ALA:HB2	1:A:85:LYS:HE3	1.87	0.55
1:A:15:ARG:HD2	1:A:284:THR:O	2.07	0.55
1:C:20:THR:O	1:C:21:MET:C	2.49	0.55
1:C:205:ARG:HG2	1:C:205:ARG:HH21	1.71	0.55
1:P:54:GLY:O	1:P:55:TRP:HB2	2.07	0.55
1:A:148:LEU:HD13	1:A:154:ILE:HD12	1.89	0.54
1:E:252:ARG:NH1	1:E:252:ARG:HB3	2.22	0.54
1:E:15:ARG:HD2	1:E:284:THR:O	2.07	0.54
1:M:112:VAL:HG22	1:M:127:TYR:CZ	2.43	0.54
1:B:15:ARG:HD2	1:B:284:THR:O	2.06	0.54
1:C:228:LYS:CE	3:C:534:HOH:O	2.56	0.54
1:I:152:GLY:O	1:M:109:ARG:NH1	2.38	0.54
1:G:308:THR:OG1	1:G:311:VAL:HG23	2.08	0.53
1:A:31:GLU:O	1:A:35:ILE:HG12	2.09	0.53
1:C:148:LEU:HD13	1:C:154:ILE:HD12	1.90	0.53
1:K:86:VAL:O	1:K:87:TYR:HB2	2.07	0.53
1:K:148:LEU:HD13	1:K:154:ILE:HD12	1.89	0.53
1:C:251:GLN:O	1:C:255:ILE:HG12	2.09	0.53
1:L:1:MET:HE3	1:L:44:ILE:HG13	1.91	0.53
1:E:258:TYR:CE1	1:E:262:LEU:HD11	2.43	0.53
1:E:308:THR:OG1	1:E:311:VAL:HG23	2.09	0.52
1:O:36:MET:HE1	1:O:65:ILE:HG22	1.90	0.52
1:H:15:ARG:HD2	1:H:284:THR:O	2.09	0.52
1:I:326:PRO:HG3	1:P:161:ASN:O	2.09	0.52
1:A:176:ARG:HG3	1:A:177:HIS:CD2	2.43	0.52
1:C:83:ALA:HA	1:C:126:LEU:O	2.10	0.52
1:C:127:TYR:HD2	1:C:145:MET:HE1	1.75	0.52
1:E:294:ASP:OD2	1:J:61:ARG:NH2	2.40	0.52
1:E:32:SER:O	1:E:35:ILE:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:THR:HA	1:E:176:ARG:HD3	1.91	0.51
1:K:161:ASN:O	1:N:326:PRO:HG3	2.10	0.51
1:G:35:ILE:HD13	1:G:290:PRO:O	2.11	0.51
1:F:269:PRO:O	1:F:272:VAL:HG12	2.10	0.51
1:H:250:GLN:H	1:H:250:GLN:CD	2.18	0.51
1:P:25:PRO:HB3	1:P:55:TRP:CE2	2.46	0.51
1:F:262:LEU:CD1	1:F:272:VAL:HG11	2.41	0.51
1:M:1:MET:N	3:M:506:HOH:O	2.44	0.51
1:P:124:ILE:O	1:P:154:ILE:HA	2.10	0.51
1:I:199:GLU:CD	1:P:163:ALA:HB1	2.36	0.50
1:K:109:ARG:NH1	1:M:152:GLY:O	2.39	0.50
1:N:246:LEU:HD23	1:N:246:LEU:N	2.27	0.50
1:D:109:ARG:NH1	1:H:152:GLY:O	2.45	0.50
1:O:256:GLN:NE2	1:O:260:ASP:OD1	2.45	0.50
1:D:326:PRO:HG3	1:G:161:ASN:O	2.12	0.50
1:O:148:LEU:HD13	1:O:154:ILE:CD1	2.39	0.50
1:P:1:MET:HE3	1:P:44:ILE:HG13	1.93	0.50
1:A:326:PRO:HG3	1:H:161:ASN:O	2.12	0.49
1:J:268:GLU:HB3	3:J:601:HOH:O	2.13	0.49
1:E:217:LEU:CD2	1:E:273:ALA:HB3	2.43	0.49
1:H:83:ALA:HA	1:H:126:LEU:O	2.12	0.49
1:A:60:GLY:O	1:A:64:GLU:HG2	2.12	0.49
1:I:148:LEU:HD13	1:I:154:ILE:HD12	1.94	0.49
2:K:401:TYK:O20	3:K:501:HOH:O	2.20	0.49
3:B:540:HOH:O	1:E:176:ARG:HD2	2.13	0.49
1:I:1:MET:HE3	1:I:44:ILE:HG13	1.93	0.49
1:K:83:ALA:HA	1:K:126:LEU:O	2.12	0.49
1:A:2:GLU:CD	1:A:2:GLU:N	2.71	0.49
1:M:106:LEU:C	1:M:106:LEU:HD23	2.37	0.49
1:L:161:ASN:O	1:O:326:PRO:HG3	2.13	0.49
1:C:36:MET:HE3	1:C:69:TRP:CD1	2.48	0.48
1:D:262:LEU:CD2	1:D:269:PRO:HA	2.43	0.48
1:H:25:PRO:HB3	1:H:55:TRP:CE2	2.47	0.48
1:B:83:ALA:HA	1:B:126:LEU:O	2.14	0.48
1:J:124:ILE:O	1:J:154:ILE:HA	2.13	0.48
1:B:201:VAL:O	1:B:205:ARG:HG3	2.13	0.48
1:O:101:ASP:O	1:O:102:LYS:HB2	2.13	0.48
1:E:85:LYS:HE2	1:E:186:GLN:HE22	1.78	0.48
1:J:152:GLY:O	1:P:109:ARG:NH1	2.46	0.48
1:K:262:LEU:HD12	1:K:269:PRO:HA	1.96	0.48
1:N:124:ILE:O	1:N:154:ILE:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:83:ALA:HA	1:J:126:LEU:O	2.14	0.48
1:O:1:MET:HE3	1:O:44:ILE:HG13	1.94	0.48
1:D:128:GLN:HA	1:D:158:GLY:O	2.14	0.48
1:O:217:LEU:CD2	1:O:273:ALA:HB3	2.44	0.47
1:A:97:TRP:CD2	1:A:98:PRO:HD2	2.49	0.47
2:A:401:TYK:O9	2:A:401:TYK:H13	2.14	0.47
1:O:112:VAL:HG21	1:O:154:ILE:HD11	1.95	0.47
1:E:229:GLU:OE2	1:E:252:ARG:NH2	2.47	0.47
1:I:150:ARG:HH12	1:K:150:ARG:HG2	1.79	0.47
1:J:186:GLN:HA	1:J:212:ILE:O	2.14	0.47
1:L:97:TRP:CD2	1:L:98:PRO:HD2	2.49	0.47
1:F:145:MET:HE2	1:F:157:VAL:HG13	1.95	0.47
1:L:83:ALA:HA	1:L:126:LEU:O	2.15	0.47
1:F:124:ILE:O	1:F:154:ILE:HA	2.15	0.47
1:M:124:ILE:O	1:M:154:ILE:HA	2.15	0.47
1:A:83:ALA:HA	1:A:126:LEU:O	2.15	0.47
1:B:253:GLU:O	1:B:257:ARG:HG2	2.15	0.46
1:D:83:ALA:HA	1:D:126:LEU:O	2.15	0.46
1:A:148:LEU:HD13	1:A:154:ILE:CD1	2.45	0.46
1:F:79:LYS:NZ	3:F:502:HOH:O	2.30	0.46
1:K:227:ARG:HH21	1:K:227:ARG:HG3	1.79	0.46
1:I:106:LEU:C	1:I:106:LEU:HD23	2.40	0.46
1:J:212:ILE:HG22	1:J:287:ILE:HG13	1.97	0.46
1:I:1:MET:N	3:I:503:HOH:O	2.42	0.46
1:N:83:ALA:HA	1:N:126:LEU:O	2.15	0.46
1:L:109:ARG:NH1	1:P:152:GLY:O	2.48	0.46
1:H:106:LEU:C	1:H:106:LEU:HD23	2.41	0.46
1:J:106:LEU:C	1:J:106:LEU:HD23	2.41	0.46
1:M:59:LYS:HE2	1:M:59:LYS:HA	1.97	0.46
1:E:148:LEU:HD13	1:E:154:ILE:HD12	1.98	0.46
1:I:189:TYR:OH	1:I:197:GLU:OE2	2.27	0.46
1:M:83:ALA:HA	1:M:126:LEU:O	2.15	0.46
1:M:308:THR:OG1	1:M:311:VAL:HG23	2.16	0.46
1:A:308:THR:OG1	1:A:311:VAL:HG23	2.16	0.45
2:F:401:TYK:H13	2:F:401:TYK:O9	2.15	0.45
1:C:15:ARG:HD2	1:C:284:THR:O	2.15	0.45
1:C:327:GLU:OE1	1:F:134:ARG:NH1	2.49	0.45
1:I:50:ALA:HB2	1:I:85:LYS:HZ3	1.80	0.45
1:L:253:GLU:O	1:L:257:ARG:HG3	2.16	0.45
1:P:248:ASP:OD1	1:P:250:GLN:HG2	2.16	0.45
1:O:83:ALA:HA	1:O:126:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLY:O	1:B:55:TRP:HB2	2.16	0.45
1:D:59:LYS:NZ	1:D:91:GLY:O	2.43	0.45
1:E:224:GLY:O	1:E:228:LYS:HG2	2.16	0.45
1:E:205:ARG:HH21	1:E:205:ARG:HG2	1.82	0.45
1:K:256:GLN:NE2	1:K:260:ASP:OD1	2.45	0.45
1:N:212:ILE:HG22	1:N:287:ILE:HG13	1.99	0.45
1:K:76:ARG:O	1:K:80:VAL:HG13	2.17	0.44
1:O:32:SER:O	1:O:35:ILE:HG22	2.17	0.44
1:I:102:LYS:HD3	3:I:507:HOH:O	2.17	0.44
1:H:205:ARG:HD2	1:H:282:GLY:HA3	2.00	0.44
1:J:97:TRP:CD2	1:J:98:PRO:HD2	2.52	0.44
1:M:29:GLU:N	3:M:512:HOH:O	2.51	0.44
2:C:401:TYK:O9	2:C:401:TYK:H13	2.17	0.44
1:G:83:ALA:HA	1:G:126:LEU:O	2.17	0.44
1:A:258:TYR:CE1	1:A:262:LEU:HD11	2.52	0.44
1:A:2:GLU:CD	1:A:2:GLU:H	2.26	0.44
1:E:229:GLU:HG3	1:E:230:GLN:N	2.33	0.44
1:L:127:TYR:CD2	1:L:145:MET:HE1	2.53	0.44
1:F:15:ARG:O	1:F:285:GLY:HA3	2.17	0.44
1:H:37:ASP:CG	1:H:76:ARG:HH11	2.24	0.44
1:C:326:PRO:HG3	1:F:161:ASN:O	2.18	0.43
1:D:86:VAL:O	1:D:87:TYR:HB2	2.17	0.43
1:C:20:THR:O	1:C:21:MET:O	2.35	0.43
1:G:205:ARG:HG2	1:G:205:ARG:HH21	1.83	0.43
1:H:25:PRO:HB3	1:H:55:TRP:CD2	2.53	0.43
1:H:59:LYS:NZ	1:H:91:GLY:O	2.43	0.43
1:K:262:LEU:CD1	1:K:269:PRO:HA	2.47	0.43
1:C:177:HIS:ND1	3:C:502:HOH:O	2.36	0.43
1:C:201:VAL:HB	1:C:202:PRO:HD3	2.00	0.43
1:D:86:VAL:O	1:D:87:TYR:CB	2.66	0.43
1:N:106:LEU:C	1:N:106:LEU:HD23	2.43	0.43
1:N:268:GLU:O	1:N:272:VAL:HG23	2.19	0.43
1:N:76:ARG:O	1:N:80:VAL:HG13	2.19	0.43
1:F:136:THR:HG22	1:F:141:ILE:HG13	2.01	0.43
1:A:250:GLN:H	1:A:250:GLN:HG2	1.53	0.43
1:F:255:ILE:O	1:F:258:TYR:HB3	2.19	0.43
1:L:106:LEU:HD23	1:L:106:LEU:C	2.44	0.43
1:F:257:ARG:NE	2:F:401:TYK:O1	2.52	0.43
1:J:151:GLN:OE1	1:J:153:LYS:HE2	2.19	0.43
1:K:127:TYR:HD2	1:K:145:MET:HE1	1.83	0.43
1:K:128:GLN:HA	1:K:158:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:6:LEU:O	1:M:9:ILE:HG12	2.19	0.43
1:M:127:TYR:HD2	1:M:145:MET:HE1	1.84	0.43
1:D:102:LYS:HD3	3:D:509:HOH:O	2.19	0.42
1:K:229:GLU:C	1:K:230:GLN:HG2	2.44	0.42
1:K:326:PRO:HG3	1:N:161:ASN:O	2.20	0.42
1:L:176:ARG:HG2	1:O:176:ARG:HD3	2.00	0.42
1:C:250:GLN:O	2:C:401:TYK:H20	2.19	0.42
1:C:317:GLU:O	2:C:401:TYK:H22	2.19	0.42
1:M:247:LYS:O	1:M:248:ASP:CG	2.63	0.42
1:A:148:LEU:CD1	1:A:154:ILE:HD12	2.50	0.42
1:G:88:GLY:O	1:G:89:ASN:C	2.61	0.42
1:M:262:LEU:CD1	1:M:269:PRO:HA	2.49	0.42
1:O:317:GLU:O	2:O:401:TYK:H22	2.20	0.42
1:D:199:GLU:CD	1:G:163:ALA:HB1	2.45	0.42
1:O:217:LEU:HD22	1:O:273:ALA:HB3	2.01	0.42
1:K:11:LEU:HD21	1:K:81:VAL:HG11	2.01	0.42
1:K:20:THR:O	1:K:21:MET:C	2.61	0.42
1:E:35:ILE:HD12	1:E:35:ILE:HA	1.91	0.42
1:F:130:HIS:HD2	3:F:576:HOH:O	2.01	0.42
1:G:108:ILE:O	1:G:112:VAL:HG23	2.19	0.42
1:L:188:LEU:HD13	1:L:215:SER:HB3	2.02	0.42
1:B:326:PRO:HG3	1:E:161:ASN:O	2.19	0.42
1:G:32:SER:O	1:G:35:ILE:HG13	2.20	0.42
1:B:188:LEU:HD13	1:B:215:SER:HB3	2.00	0.42
1:I:179:ARG:NH1	3:I:514:HOH:O	2.51	0.42
1:E:31:GLU:CD	1:J:55:TRP:HB3	2.46	0.41
2:F:401:TYK:H14	2:F:401:TYK:H221	1.89	0.41
1:A:136:THR:HG22	1:A:141:ILE:HG13	2.02	0.41
1:N:15:ARG:O	1:N:285:GLY:HA3	2.20	0.41
1:G:226:ILE:O	1:G:230:GLN:HG2	2.20	0.41
1:P:151:GLN:OE1	1:P:153:LYS:HE2	2.20	0.41
1:B:142:TRP:O	1:B:146:ASP:HB2	2.20	0.41
1:J:264:LYS:NZ	3:J:511:HOH:O	2.50	0.41
2:A:401:TYK:H14	2:A:401:TYK:H221	1.89	0.41
1:B:106:LEU:HD23	1:B:106:LEU:C	2.45	0.41
1:B:124:ILE:O	1:B:154:ILE:HA	2.20	0.41
1:L:179:ARG:NH1	1:P:150:ARG:HH12	2.18	0.41
1:P:244:ASP:O	1:P:245:ALA:C	2.63	0.41
1:L:205:ARG:HH21	1:L:205:ARG:CG	2.32	0.41
1:N:212:ILE:CG2	1:N:287:ILE:HG13	2.51	0.41
1:P:258:TYR:CE1	1:P:262:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:VAL:HB	1:B:202:PRO:HD3	2.02	0.41
1:F:83:ALA:HA	1:F:126:LEU:O	2.20	0.41
1:J:128:GLN:HA	1:J:158:GLY:O	2.20	0.41
1:O:51:ASN:O	1:O:56:GLY:HA2	2.21	0.41
1:C:263:ASP:O	1:C:264:LYS:C	2.62	0.41
1:E:255:ILE:O	1:E:259:GLU:HG3	2.20	0.41
1:F:186:GLN:HA	1:F:212:ILE:O	2.21	0.41
1:G:305:LEU:HD23	1:G:306:THR:N	2.36	0.41
1:I:15:ARG:O	1:I:285:GLY:HA3	2.21	0.41
1:J:17:VAL:HG22	1:J:46:PHE:CD2	2.56	0.41
1:N:163:ALA:HB3	1:N:166:ASN:OD1	2.21	0.41
1:O:32:SER:HB3	1:O:36:MET:HE3	2.03	0.41
1:A:134:ARG:NH1	1:H:327:GLU:OE2	2.54	0.41
1:B:86:VAL:O	1:B:87:TYR:CB	2.68	0.41
1:B:86:VAL:O	1:B:87:TYR:HB2	2.21	0.41
2:C:401:TYK:H221	2:C:401:TYK:H14	1.85	0.41
1:N:128:GLN:HA	1:N:158:GLY:O	2.21	0.41
1:E:124:ILE:O	1:E:154:ILE:HA	2.21	0.40
1:C:258:TYR:CE1	1:C:262:LEU:HD11	2.57	0.40
1:D:106:LEU:C	1:D:106:LEU:HD23	2.46	0.40
1:D:145:MET:HE3	1:D:157:VAL:HG22	2.03	0.40
1:I:83:ALA:HA	1:I:126:LEU:O	2.21	0.40
1:J:161:ASN:O	1:M:326:PRO:HG3	2.21	0.40
1:O:88:GLY:HA2	1:O:101:ASP:OD1	2.22	0.40
1:B:109:ARG:NH1	1:F:152:GLY:O	2.53	0.40
1:G:280:ARG:HA	1:G:281:PRO:HD3	1.96	0.40
1:J:215:SER:N	1:J:216:PRO:CD	2.84	0.40
1:A:33:HIS:HB3	3:A:581:HOH:O	2.21	0.40
1:K:20:THR:OG1	1:K:62:THR:HG21	2.22	0.40
1:L:179:ARG:HH11	1:P:150:ARG:NH1	2.20	0.40

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

All (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
1	L	87	TYR
1	M	249	PRO
1	N	87	TYR
1	P	87	TYR
1	C	60	GLY
1	E	102	LYS
1	H	55	TRP
1	B	55	TRP
1	D	55	TRP

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Mol	Chain	Res	Type
1	P	55	TRP
1	K	87	TYR
1	H	56	GLY

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

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR

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Mol	Chain	Res	Type
1	A	86	VAL
1	A	250	GLN
1	A	253	GLU
1	B	21	MET
1	B	57	GLU
1	B	117	LYS
1	B	257	ARG
1	B	268	GLU
1	B	294	ASP
1	C	21	MET
1	C	59	LYS
1	C	89	ASN
1	C	160	SER
1	D	21	MET
1	D	28	ASP
1	D	92	LEU
1	D	227	ARG
1	E	21	MET
1	F	65	ILE
1	F	150	ARG
1	F	292	THR
1	G	35	ILE
1	G	40	LEU
1	G	52	VAL
1	G	59	LYS
1	G	154	ILE
1	G	160	SER
1	G	265	HIS
1	G	291	ARG
1	G	305	LEU
1	H	66	LEU
1	H	86	VAL
1	H	92	LEU
1	H	212	ILE
1	H	227	ARG
1	H	250	GLN
1	H	252	ARG
1	H	267	LEU
1	H	291	ARG
1	H	311	VAL
1	I	20	THR
1	I	52	VAL

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Mol	Chain	Res	Type
1	J	257	ARG
1	J	264	LYS
1	K	31	GLU
1	K	40	LEU
1	K	155	LEU
1	K	160	SER
1	K	248	ASP
1	K	252	ARG
1	L	80	VAL
1	L	228	LYS
1	L	291	ARG
1	M	20	THR
1	M	22	ASN
1	M	59	LYS
1	M	113	ASP
1	M	246	LEU
1	M	257	ARG
1	N	2	GLU
1	N	40	LEU
1	N	80	VAL
1	N	92	LEU
1	N	179	ARG
1	N	227	ARG
1	N	246	LEU
1	N	291	ARG
1	O	21	MET
1	O	31	GLU
1	O	179	ARG
1	O	229	GLU
1	P	21	MET
1	P	27	THR
1	P	66	LEU
1	P	244	ASP
1	P	253	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	C	5	GLN
1	C	143	GLN
1	C	151	GLN

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Mol	Chain	Res	Type
1	D	72	GLN
1	D	143	GLN
1	E	169	GLN
1	E	177	HIS
1	E	251	GLN
1	F	130	HIS
1	F	256	GLN
1	G	33	HIS
1	G	230	GLN
1	H	169	GLN
1	H	256	GLN
1	I	51	ASN
1	I	72	GLN
1	I	89	ASN
1	J	256	GLN
1	K	177	HIS
1	L	128	GLN
1	L	130	HIS
1	L	169	GLN
1	L	186	GLN
1	L	254	GLN
1	N	186	GLN
1	O	72	GLN
1	O	177	HIS
1	O	256	GLN
1	P	143	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
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
2	D	401	TYK	C11-C10	3.04	1.42	1.33
2	A	401	TYK	C11-C10	2.91	1.41	1.33
2	G	401	TYK	C11-C10	2.69	1.41	1.33
2	A	401	TYK	C6-C5	2.69	1.57	1.52
2	C	401	TYK	C11-C10	2.64	1.41	1.33
2	E	401	TYK	C11-C10	2.61	1.40	1.33
2	G	401	TYK	C6-C5	2.60	1.57	1.52
2	L	401	TYK	C6-C5	2.59	1.57	1.52
2	P	401	TYK	C6-C5	2.41	1.57	1.52
2	K	401	TYK	C11-C10	2.40	1.40	1.33
2	E	401	TYK	C6-C5	2.35	1.57	1.52
2	K	401	TYK	C6-C5	2.33	1.57	1.52
2	H	401	TYK	C6-C5	2.33	1.57	1.52
2	B	401	TYK	C6-C5	2.26	1.57	1.52
2	J	401	TYK	C11-C10	2.24	1.39	1.33
2	P	401	TYK	C11-C10	2.22	1.39	1.33
2	N	401	TYK	C11-C10	2.20	1.39	1.33
2	I	401	TYK	C11-C12	-2.12	1.41	1.46
2	E	401	TYK	C22-C12	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	401	TYK	C6-C5	2.10	1.56	1.52
2	G	401	TYK	C13-C12	2.09	1.40	1.34
2	A	401	TYK	C13-C12	2.04	1.39	1.34

All (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
2	E	401	TYK	C10-C11-C12	4.22	132.47	126.23
2	M	401	TYK	C10-C11-C12	4.18	132.42	126.23
2	P	401	TYK	O1A-C5-C4	3.83	112.74	108.23
2	C	401	TYK	O1A-C5-C4	3.82	112.73	108.23
2	G	401	TYK	O1A-C5-C4	3.81	112.73	108.23
2	I	401	TYK	O1A-C5-C4	3.72	112.61	108.23
2	N	401	TYK	O1A-C5-C4	3.70	112.60	108.23
2	A	401	TYK	C11-C12-C13	3.61	128.50	118.82
2	C	401	TYK	C11-C12-C13	3.45	128.06	118.82
2	M	401	TYK	O5C-C1C-C2C	3.45	116.19	109.49
2	A	401	TYK	O1A-C5-C4	3.36	112.19	108.23
2	H	401	TYK	C10-C11-C12	3.27	131.07	126.23
2	L	401	TYK	C10-C11-C12	3.10	130.82	126.23
2	M	401	TYK	C1C-C2C-C3C	2.95	116.47	110.74
2	C	401	TYK	C22-C12-C11	-2.94	113.60	118.09
2	N	401	TYK	C1B-O4A-C4A	2.91	120.51	114.72
2	L	401	TYK	O1A-C5-C4	2.89	111.64	108.23
2	J	401	TYK	O1A-C5-C4	2.87	111.62	108.23
2	B	401	TYK	C10-C11-C12	2.87	130.48	126.23
2	E	401	TYK	O1A-C5-C4	2.84	111.58	108.23
2	A	401	TYK	C22-C12-C11	-2.82	113.77	118.09
2	P	401	TYK	C10-C11-C12	2.78	130.34	126.23
2	D	401	TYK	C11-C12-C13	2.75	126.19	118.82
2	D	401	TYK	O1A-C5-C6	2.75	116.36	109.23
2	F	401	TYK	C11-C12-C13	2.74	126.17	118.82
2	I	401	TYK	C1B-O4A-C4A	2.71	120.11	114.72
2	J	401	TYK	C1B-O4A-C4A	2.65	120.00	114.72
2	B	401	TYK	O15-C15-C14	2.65	113.35	107.60
2	H	401	TYK	O1A-C5-C4	2.64	111.34	108.23
2	N	401	TYK	C10-C11-C12	2.64	130.13	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	401	TYK	O1A-C5-C4	2.60	111.30	108.23
2	D	401	TYK	O1A-C5-C4	2.58	111.27	108.23
2	B	401	TYK	C15-O15-C1	2.50	122.56	117.81
2	G	401	TYK	C11-C12-C13	2.45	125.39	118.82
2	D	401	TYK	O15-C15-C14	-2.34	102.52	107.60
2	O	401	TYK	C1B-O4A-C4A	2.27	119.24	114.72
2	J	401	TYK	C10-C11-C12	2.27	129.59	126.23
2	D	401	TYK	C22-C12-C11	-2.25	114.64	118.09
2	P	401	TYK	O4B-C4B-C5B	-2.25	105.58	109.46
2	D	401	TYK	C11-C10-C9	2.23	133.42	121.58
2	N	401	TYK	O5C-C1C-C2C	2.23	113.83	109.49
2	L	401	TYK	O15-C15-C14	2.23	112.42	107.60
2	H	401	TYK	O5C-C1C-C2C	2.18	113.73	109.49
2	P	401	TYK	C1A-C2A-C3A	2.10	112.58	109.20
2	F	401	TYK	C1B-O4A-C4A	2.09	118.88	114.72
2	L	401	TYK	O5C-C1C-C2C	2.08	113.53	109.49
2	P	401	TYK	C1B-O4A-C4A	2.07	118.85	114.72
2	C	401	TYK	O5C-C1C-C2C	2.04	113.45	109.49
2	L	401	TYK	C1C-O5C-C5C	2.03	117.10	113.63
2	A	401	TYK	C1B-O4A-C4A	2.02	118.75	114.72

There are no chirality outliers.

All (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
2	A	401	TYK	C23-C14-C15-O15
2	A	401	TYK	C14-C15-C16-C17
2	B	401	TYK	C4-C5-C6-C19
2	B	401	TYK	O1A-C5-C6-C19
2	B	401	TYK	C6-C7-C8-C9
2	B	401	TYK	C6-C7-C8-C21
2	B	401	TYK	C21-C8-C9-C10
2	B	401	TYK	C21-C8-C9-O9
2	B	401	TYK	C13-C14-C15-C16
2	B	401	TYK	C13-C14-C15-O15
2	B	401	TYK	C23-C14-C15-C16
2	B	401	TYK	C23-C14-C15-O15

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Mol	Chain	Res	Type	Atoms
2	B	401	TYK	C2C-C1C-O1C-C23
2	C	401	TYK	C21-C8-C9-C10
2	C	401	TYK	C21-C8-C9-O9
2	C	401	TYK	C13-C14-C15-C16
2	C	401	TYK	C13-C14-C15-O15
2	C	401	TYK	C23-C14-C15-C16
2	C	401	TYK	C23-C14-C15-O15
2	C	401	TYK	C13-C14-C23-O1C
2	C	401	TYK	C15-C14-C23-O1C
2	C	401	TYK	O15-C15-C16-C17
2	C	401	TYK	C2C-C1C-O1C-C23
2	C	401	TYK	O5C-C1C-O1C-C23
2	D	401	TYK	O15-C15-C16-C17
2	E	401	TYK	C4-C5-C6-C19
2	E	401	TYK	C21-C8-C9-O9
2	E	401	TYK	C12-C13-C14-C23
2	E	401	TYK	C13-C14-C15-C16
2	E	401	TYK	C13-C14-C15-O15
2	E	401	TYK	C23-C14-C15-C16
2	E	401	TYK	C23-C14-C15-O15
2	E	401	TYK	C14-C15-C16-C17
2	E	401	TYK	O15-C15-C16-C17
2	E	401	TYK	C2C-C1C-O1C-C23
2	E	401	TYK	O5C-C1C-O1C-C23
2	F	401	TYK	C13-C14-C15-C16
2	F	401	TYK	C13-C14-C15-O15
2	F	401	TYK	C23-C14-C15-C16
2	F	401	TYK	C23-C14-C15-O15
2	F	401	TYK	C13-C14-C23-O1C
2	F	401	TYK	C15-C14-C23-O1C
2	F	401	TYK	O15-C15-C16-C17
2	F	401	TYK	O5C-C1C-O1C-C23
2	G	401	TYK	C12-C13-C14-C23
2	G	401	TYK	C13-C14-C15-C16
2	G	401	TYK	C13-C14-C15-O15
2	G	401	TYK	C23-C14-C15-C16
2	G	401	TYK	C23-C14-C15-O15
2	H	401	TYK	C21-C8-C9-O9
2	H	401	TYK	C13-C14-C15-O15
2	H	401	TYK	C15-C14-C23-O1C
2	H	401	TYK	C14-C15-C16-C17
2	H	401	TYK	O15-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
2	H	401	TYK	C2C-C1C-O1C-C23
2	H	401	TYK	O5C-C1C-O1C-C23
2	I	401	TYK	C13-C14-C15-O15
2	I	401	TYK	C13-C14-C23-O1C
2	I	401	TYK	C15-C14-C23-O1C
2	I	401	TYK	C14-C15-C16-C17
2	I	401	TYK	O15-C15-C16-C17
2	J	401	TYK	C13-C14-C23-O1C
2	J	401	TYK	O15-C15-C16-C17
2	J	401	TYK	O5C-C1C-O1C-C23
2	K	401	TYK	C14-C15-C16-C17
2	K	401	TYK	O15-C15-C16-C17
2	K	401	TYK	O5C-C1C-O1C-C23
2	L	401	TYK	C4-C5-C6-C19
2	L	401	TYK	C21-C8-C9-O9
2	L	401	TYK	C13-C14-C15-O15
2	L	401	TYK	C13-C14-C23-O1C
2	L	401	TYK	C15-C14-C23-O1C
2	L	401	TYK	O15-C15-C16-C17
2	L	401	TYK	C2C-C1C-O1C-C23
2	M	401	TYK	C21-C8-C9-C10
2	M	401	TYK	C21-C8-C9-O9
2	M	401	TYK	C13-C14-C15-C16
2	M	401	TYK	C13-C14-C15-O15
2	M	401	TYK	C23-C14-C15-C16
2	M	401	TYK	C23-C14-C15-O15
2	M	401	TYK	C14-C15-C16-C17
2	M	401	TYK	O15-C15-C16-C17
2	N	401	TYK	C15-C14-C23-O1C
2	N	401	TYK	C14-C15-C16-C17
2	N	401	TYK	O15-C15-C16-C17
2	N	401	TYK	O5C-C1C-O1C-C23
2	O	401	TYK	C14-C15-C16-C17
2	O	401	TYK	O15-C15-C16-C17
2	O	401	TYK	O5C-C1C-O1C-C23
2	P	401	TYK	C4-C5-C6-C19
2	P	401	TYK	C6-C7-C8-C9
2	P	401	TYK	C21-C8-C9-C10
2	P	401	TYK	C21-C8-C9-O9
2	P	401	TYK	O15-C15-C16-C17
2	I	401	TYK	O5C-C1C-O1C-C23
2	F	401	TYK	C2C-C1C-O1C-C23

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Mol	Chain	Res	Type	Atoms
2	I	401	TYK	C2C-C1C-O1C-C23
2	A	401	TYK	C10-C11-C12-C22
2	C	401	TYK	C10-C11-C12-C22
2	D	401	TYK	C10-C11-C12-C22
2	F	401	TYK	C10-C11-C12-C22
2	A	401	TYK	C10-C11-C12-C13
2	C	401	TYK	C10-C11-C12-C13
2	D	401	TYK	C10-C11-C12-C13
2	F	401	TYK	C10-C11-C12-C13
2	B	401	TYK	O5C-C1C-O1C-C23
2	L	401	TYK	O5C-C1C-O1C-C23
2	G	401	TYK	C2C-C1C-O1C-C23
2	N	401	TYK	C2C-C1C-O1C-C23
2	G	401	TYK	O5C-C1C-O1C-C23
2	P	401	TYK	C6-C7-C8-C21
2	J	401	TYK	C18-C4-C5-C6
2	H	401	TYK	C6-C7-C8-C9
2	J	401	TYK	C6-C7-C8-C9
2	L	401	TYK	C6-C7-C8-C9
2	A	401	TYK	C20-C19-C6-C7
2	D	401	TYK	C20-C19-C6-C7
2	E	401	TYK	C20-C19-C6-C7
2	F	401	TYK	C20-C19-C6-C7
2	H	401	TYK	C20-C19-C6-C7
2	J	401	TYK	C20-C19-C6-C7
2	K	401	TYK	C20-C19-C6-C7
2	L	401	TYK	C20-C19-C6-C7
2	B	401	TYK	C18-C4-C5-C6
2	D	401	TYK	C2C-C1C-O1C-C23
2	H	401	TYK	C18-C4-C5-C6
2	B	401	TYK	C1-C2-C3-C4
2	D	401	TYK	C1-C2-C3-C4
2	G	401	TYK	C1-C2-C3-C4
2	H	401	TYK	C1-C2-C3-C4
2	I	401	TYK	C1-C2-C3-C4
2	J	401	TYK	C1-C2-C3-C4
2	P	401	TYK	C1-C2-C3-C4
2	H	401	TYK	C4-C5-C6-C19
2	O	401	TYK	C2C-C1C-O1C-C23
2	A	401	TYK	C20-C19-C6-C5
2	G	401	TYK	C15-C14-C23-O1C
2	J	401	TYK	C15-C14-C23-O1C

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Mol	Chain	Res	Type	Atoms
2	M	401	TYK	C12-C13-C14-C15
2	G	401	TYK	C13-C14-C23-O1C
2	N	401	TYK	C13-C14-C23-O1C
2	L	401	TYK	C18-C4-C5-C6
2	I	401	TYK	C6-C7-C8-C9
2	M	401	TYK	C6-C7-C8-C9
2	D	401	TYK	C18-C4-C5-C6
2	E	401	TYK	C18-C4-C5-C6
2	G	401	TYK	C18-C4-C5-C6
2	I	401	TYK	C18-C4-C5-C6
2	K	401	TYK	C18-C4-C5-C6
2	M	401	TYK	C18-C4-C5-C6
2	N	401	TYK	C18-C4-C5-C6
2	P	401	TYK	C18-C4-C5-C6
2	D	401	TYK	C1-C2-C3-O3
2	G	401	TYK	C20-C19-C6-C7
2	P	401	TYK	C20-C19-C6-C7
2	H	401	TYK	C13-C14-C15-C16
2	I	401	TYK	C13-C14-C15-C16
2	J	401	TYK	C13-C14-C15-C16
2	L	401	TYK	C13-C14-C15-C16
2	P	401	TYK	C13-C14-C15-C16
2	B	401	TYK	C14-C15-C16-C17
2	C	401	TYK	C14-C15-C16-C17
2	D	401	TYK	C21-C8-C9-C10
2	D	401	TYK	C21-C8-C9-O9
2	D	401	TYK	C14-C15-C16-C17
2	E	401	TYK	C21-C8-C9-C10
2	F	401	TYK	C14-C15-C16-C17
2	H	401	TYK	C21-C8-C9-C10
2	J	401	TYK	C21-C8-C9-O9
2	J	401	TYK	C14-C15-C16-C17
2	L	401	TYK	C21-C8-C9-C10
2	L	401	TYK	C14-C15-C16-C17
2	P	401	TYK	C14-C15-C16-C17
2	O	401	TYK	C18-C4-C5-C6
2	A	401	TYK	C14-C23-O1C-C1C
2	B	401	TYK	C14-C23-O1C-C1C
2	F	401	TYK	C14-C23-O1C-C1C
2	G	401	TYK	C14-C23-O1C-C1C
2	I	401	TYK	C14-C23-O1C-C1C
2	J	401	TYK	C13-C14-C15-O15

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Mol	Chain	Res	Type	Atoms
2	K	401	TYK	C14-C23-O1C-C1C
2	O	401	TYK	C14-C23-O1C-C1C
2	D	401	TYK	C12-C13-C14-C23
2	H	401	TYK	C18-C4-C5-O1A
2	J	401	TYK	C18-C4-C5-O1A
2	B	401	TYK	C12-C13-C14-C15
2	G	401	TYK	C12-C13-C14-C15
2	J	401	TYK	C12-C13-C14-C15
2	O	401	TYK	C12-C13-C14-C15
2	C	401	TYK	C18-C4-C5-C6
2	J	401	TYK	C6-C19-C20-O20
2	K	401	TYK	C6-C19-C20-O20
2	L	401	TYK	C1-C2-C3-C4
2	I	401	TYK	C4-C5-C6-C19
2	J	401	TYK	C4-C5-C6-C19
2	B	401	TYK	C18-C4-C5-O1A
2	B	401	TYK	C20-C19-C6-C7
2	C	401	TYK	C20-C19-C6-C7
2	N	401	TYK	C20-C19-C6-C7
2	O	401	TYK	C20-C19-C6-C7
2	G	401	TYK	C22-C12-C13-C14
2	A	401	TYK	C18-C4-C5-C6
2	F	401	TYK	C18-C4-C5-C6
2	L	401	TYK	C20-C19-C6-C5
2	L	401	TYK	O1A-C5-C6-C19
2	A	401	TYK	C6-C7-C8-C21
2	H	401	TYK	C2C-C3C-O3C-C8C
2	D	401	TYK	C18-C4-C5-O1A
2	D	401	TYK	C13-C14-C23-O1C
2	O	401	TYK	C13-C14-C23-O1C
2	A	401	TYK	O15-C15-C16-C17
2	I	401	TYK	C6-C19-C20-O20
2	E	401	TYK	C9-C10-C11-C12
2	B	401	TYK	C1-C2-C3-O3
2	G	401	TYK	C1-C2-C3-O3
2	I	401	TYK	C1-C2-C3-O3
2	B	401	TYK	C5-C6-C7-C8
2	P	401	TYK	C5-C6-C7-C8
2	B	401	TYK	C19-C6-C7-C8
2	E	401	TYK	O1A-C5-C6-C19
2	H	401	TYK	O1A-C5-C6-C19
2	I	401	TYK	C21-C8-C9-O9

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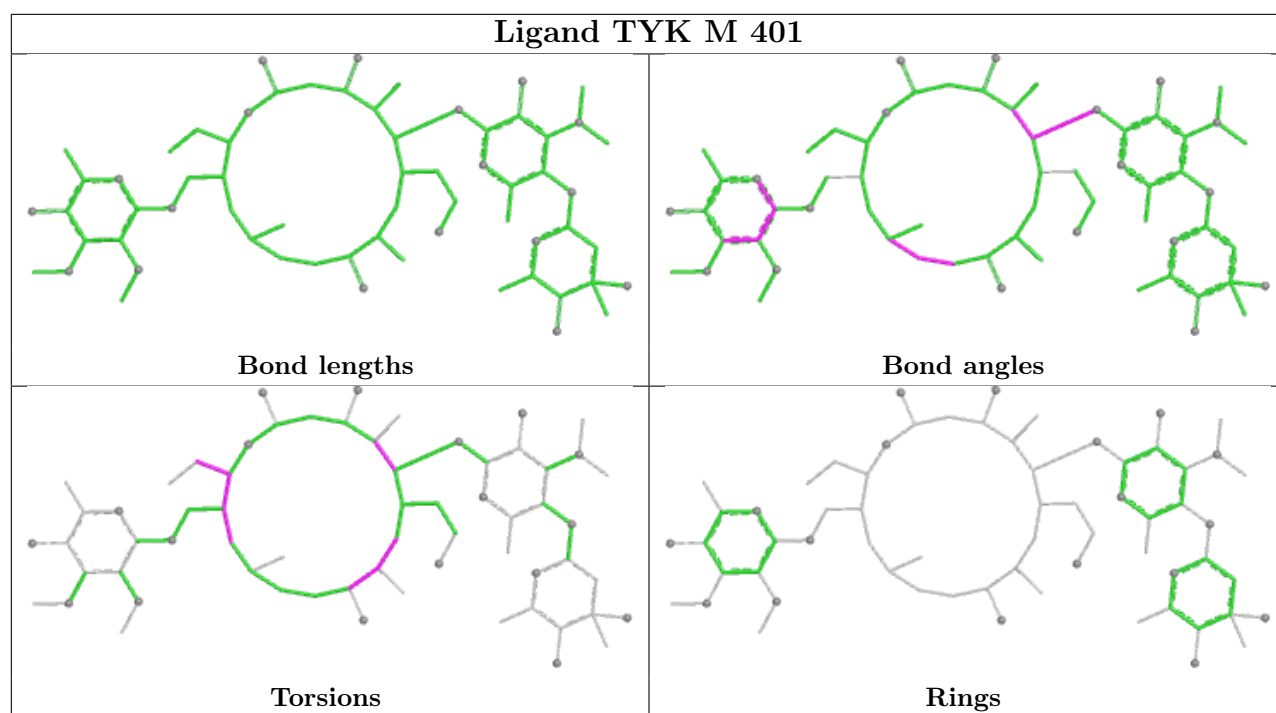
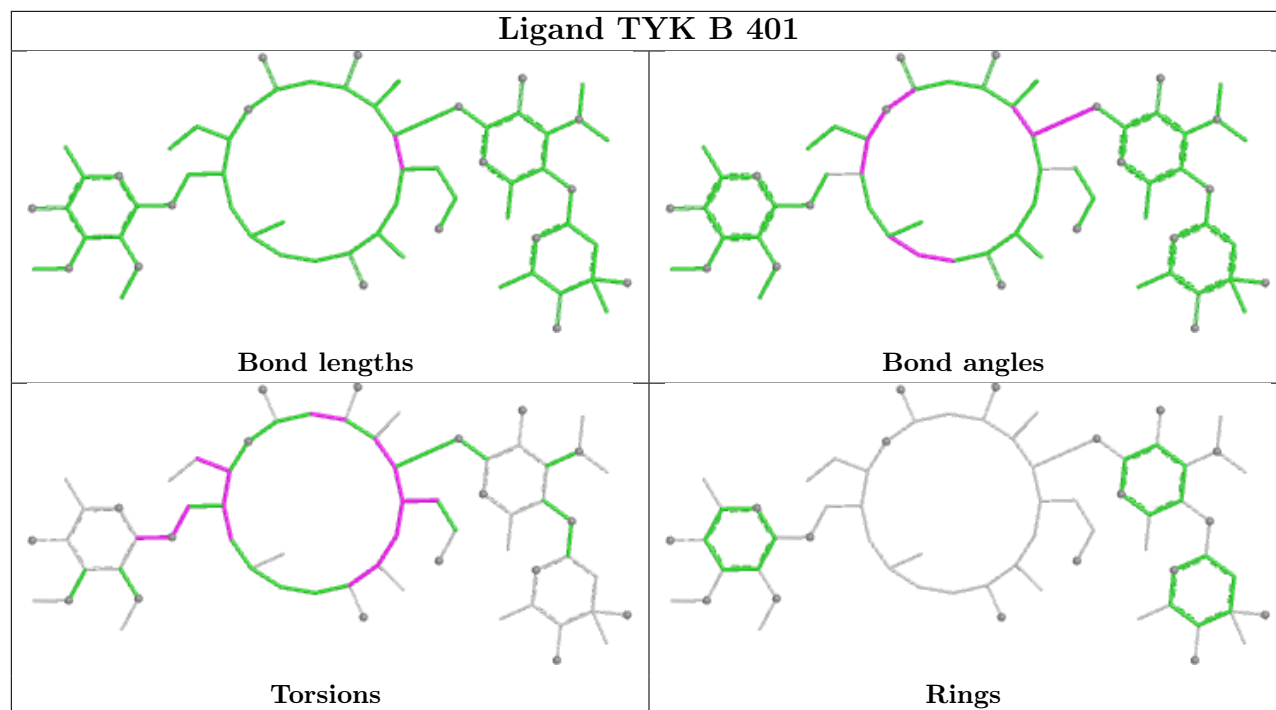
Mol	Chain	Res	Type	Atoms
2	K	401	TYK	C21-C8-C9-O9
2	P	401	TYK	O1A-C5-C6-C19
2	P	401	TYK	C19-C6-C7-C8
2	G	401	TYK	C18-C4-C5-O1A
2	A	401	TYK	C9-C10-C11-C12
2	C	401	TYK	C9-C10-C11-C12
2	D	401	TYK	C9-C10-C11-C12
2	F	401	TYK	C9-C10-C11-C12
2	O	401	TYK	C2C-C3C-O3C-C8C
2	C	401	TYK	C14-C23-O1C-C1C
2	E	401	TYK	C14-C23-O1C-C1C

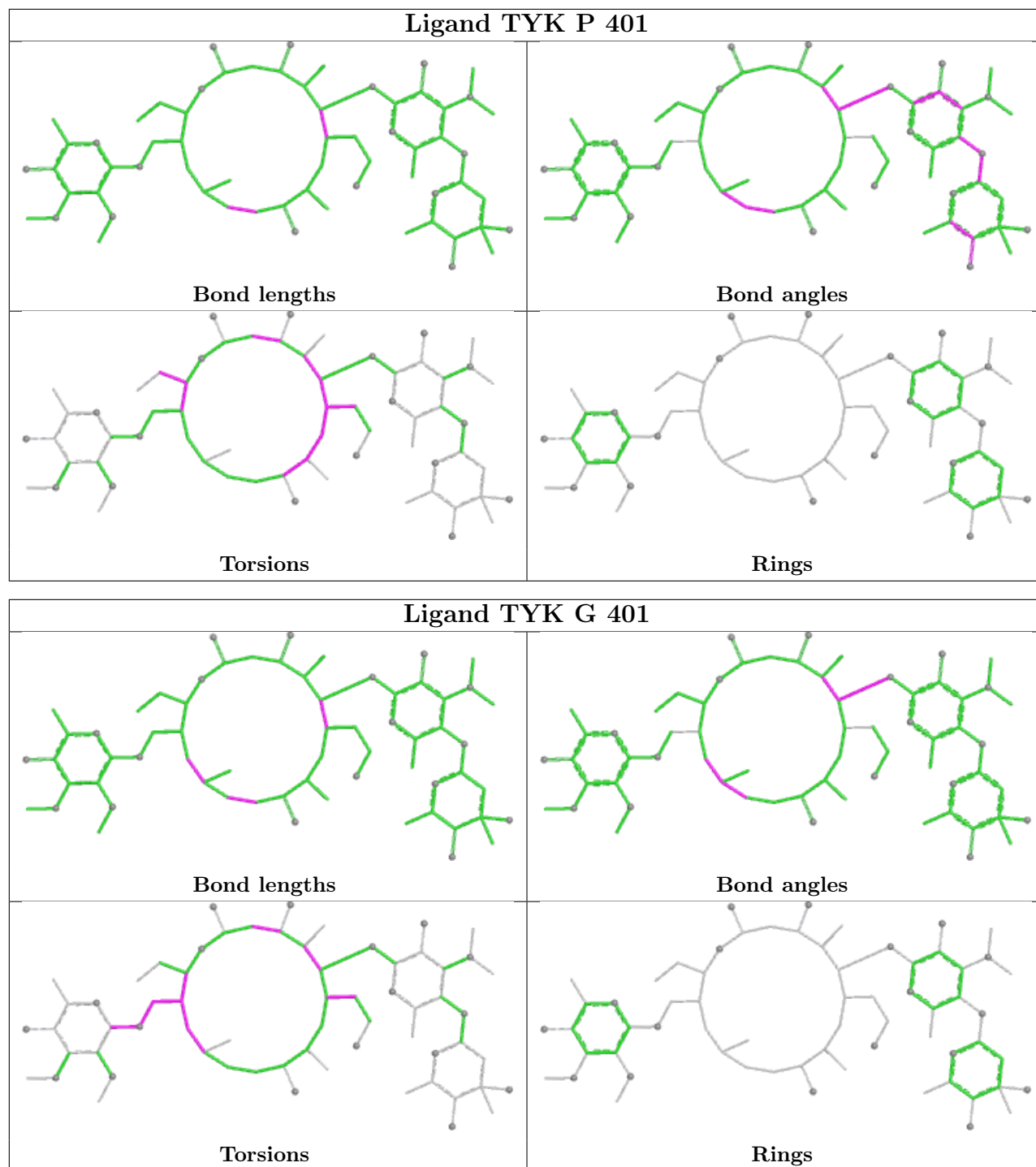
There are no ring outliers.

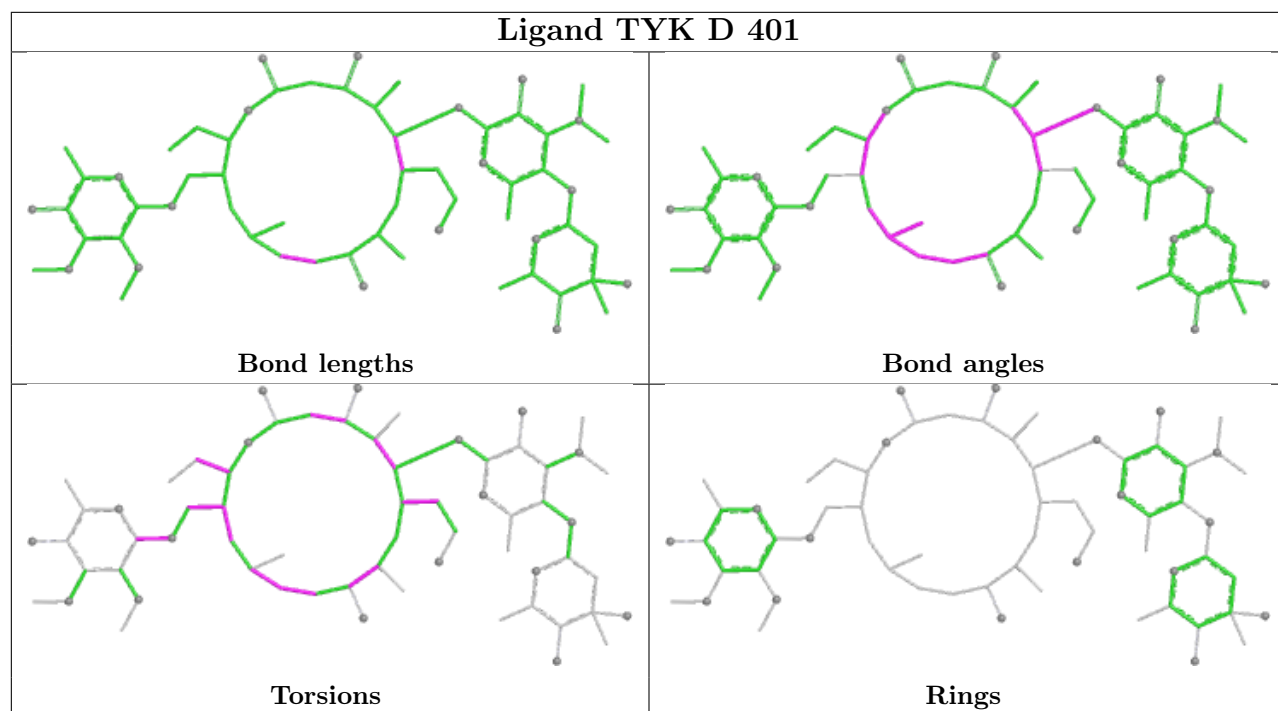
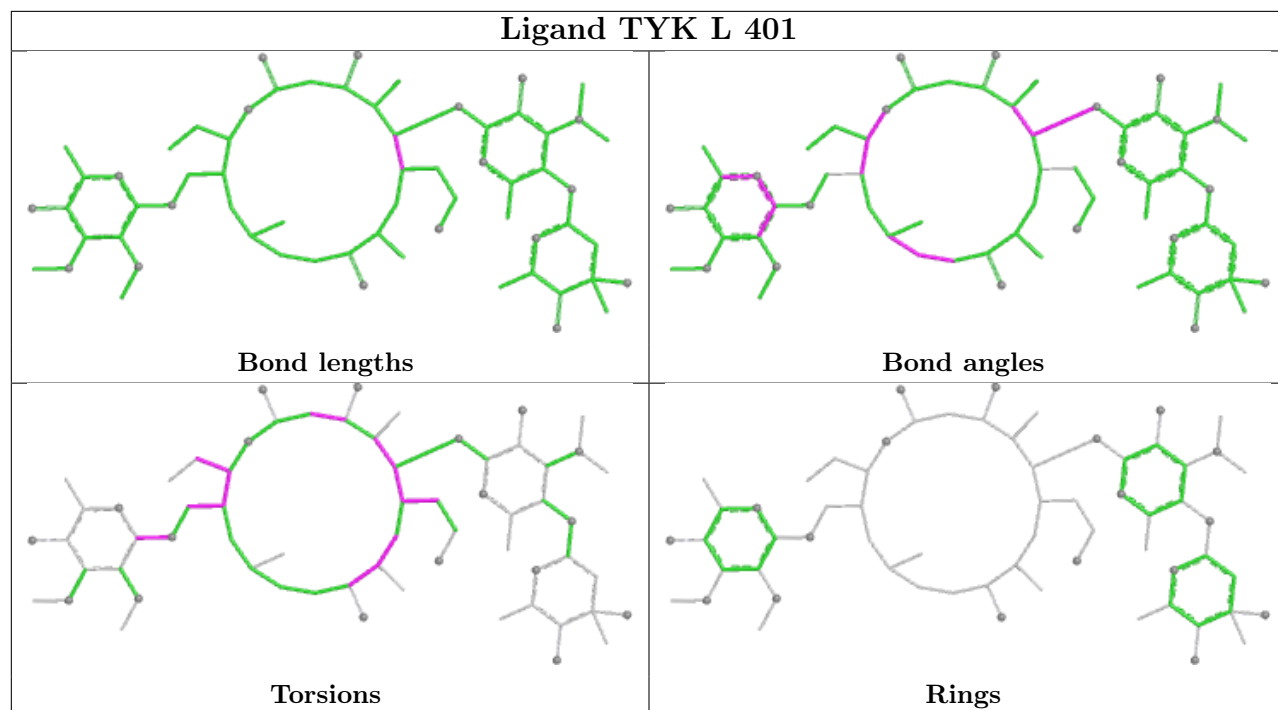
7 monomers are involved in 18 short contacts:

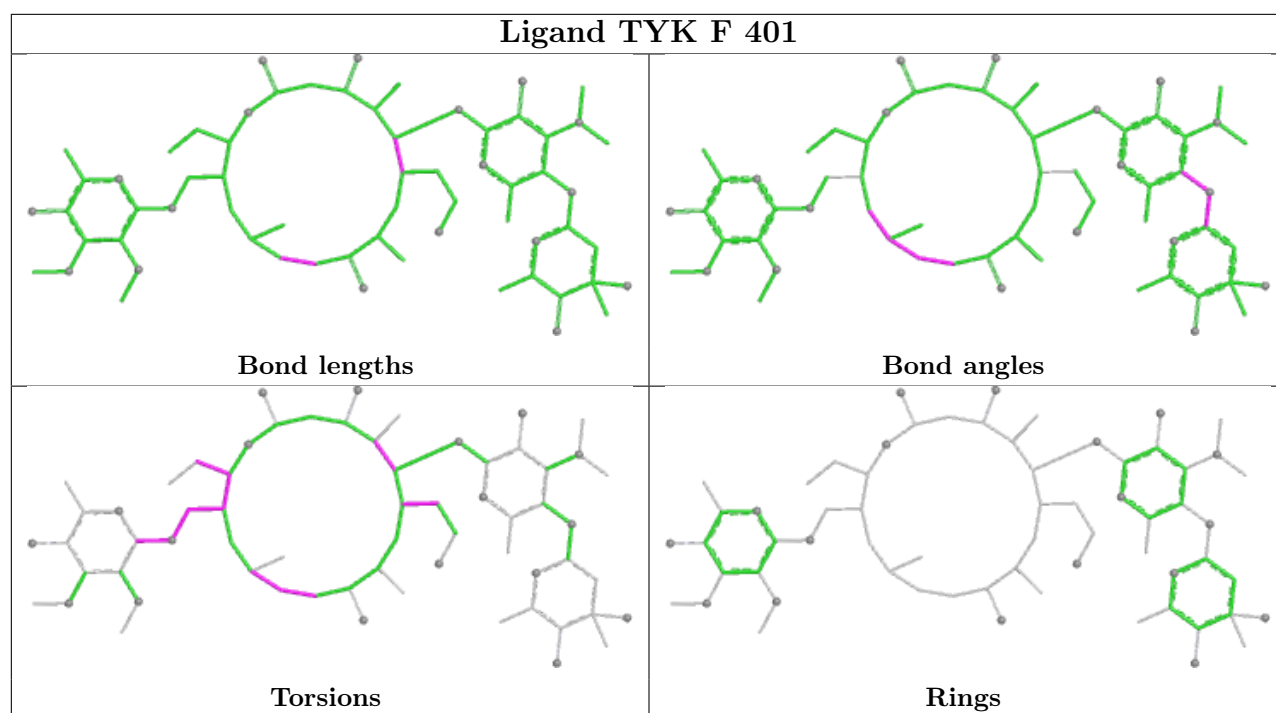
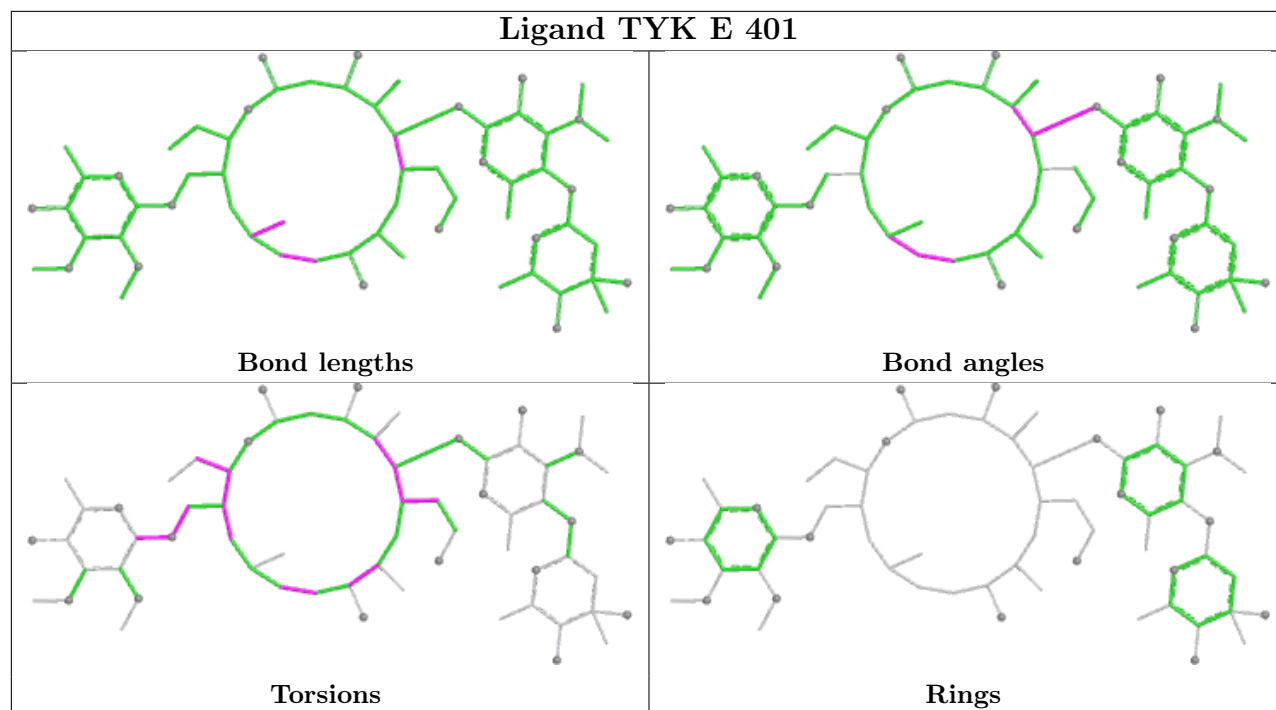
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	TYK	1	0
2	E	401	TYK	4	0
2	F	401	TYK	3	0
2	C	401	TYK	5	0
2	K	401	TYK	1	0
2	A	401	TYK	2	0
2	O	401	TYK	2	0

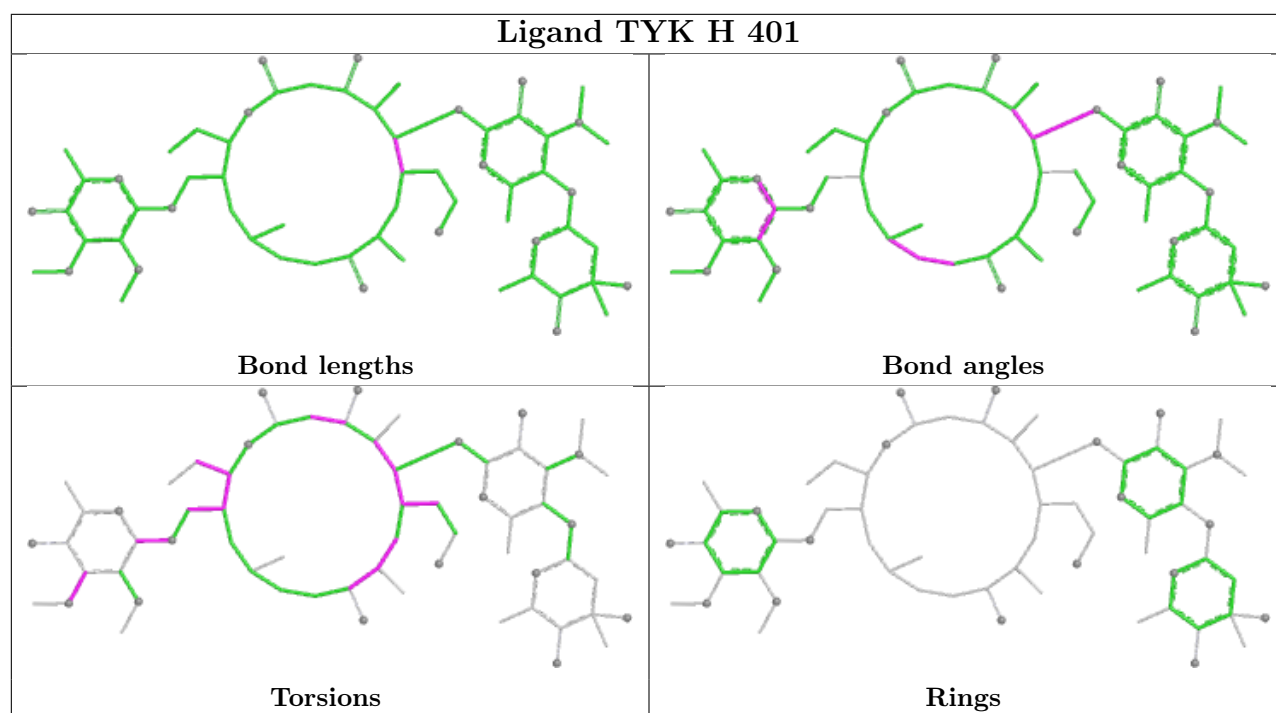
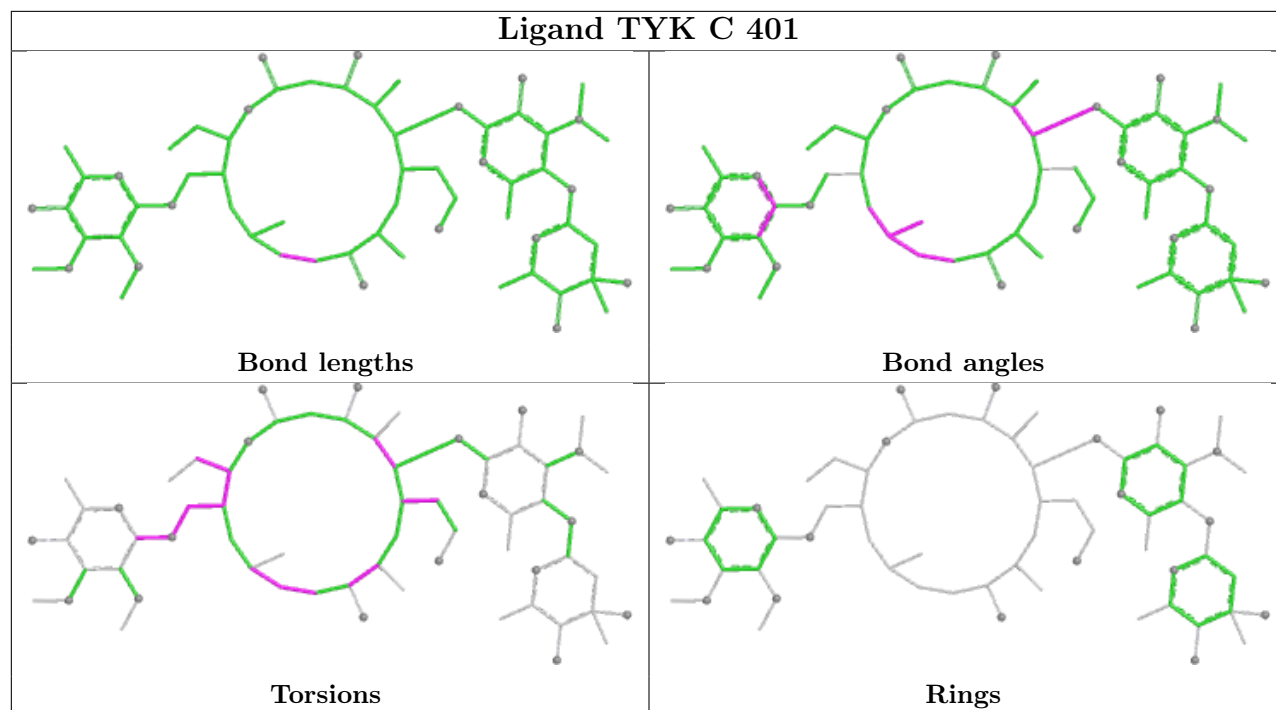
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

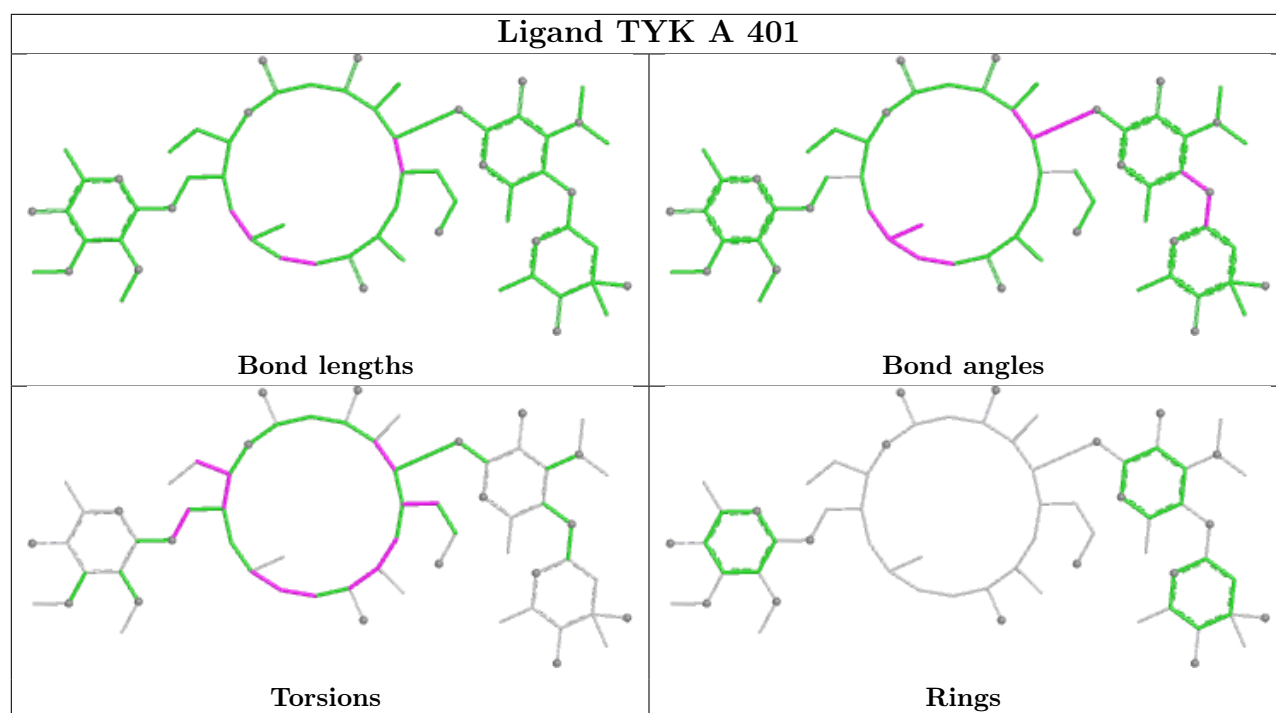
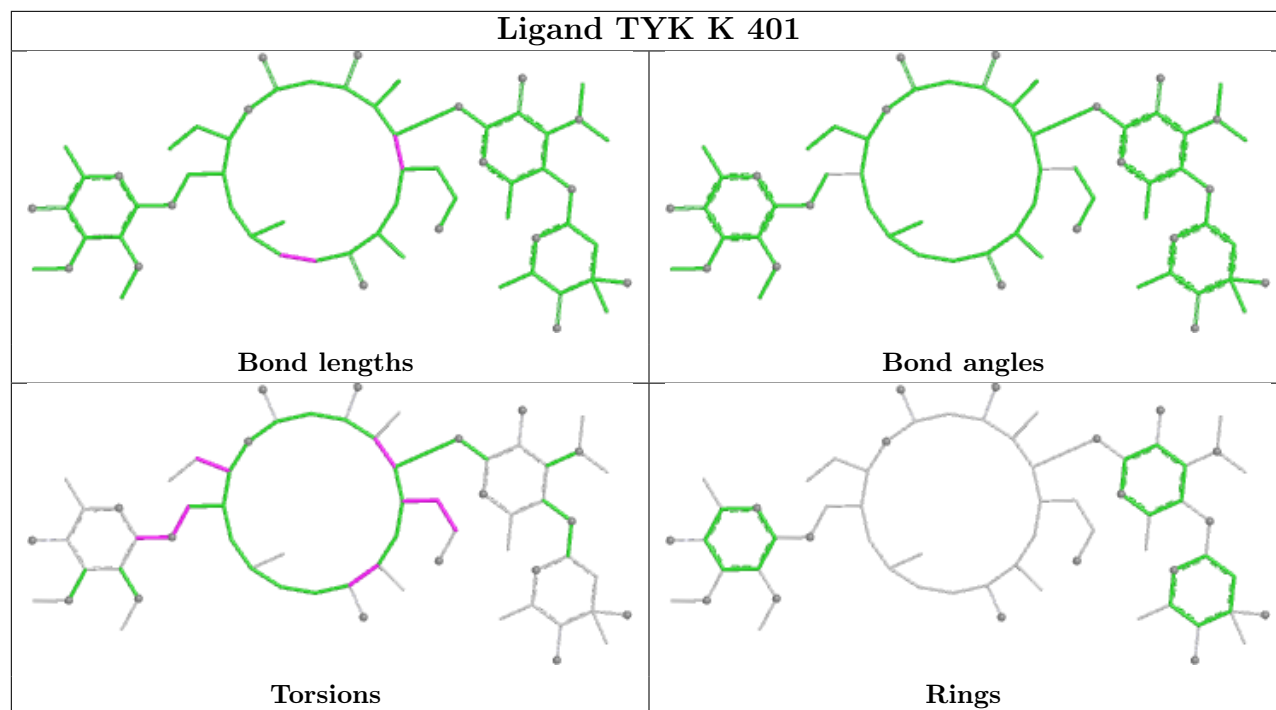


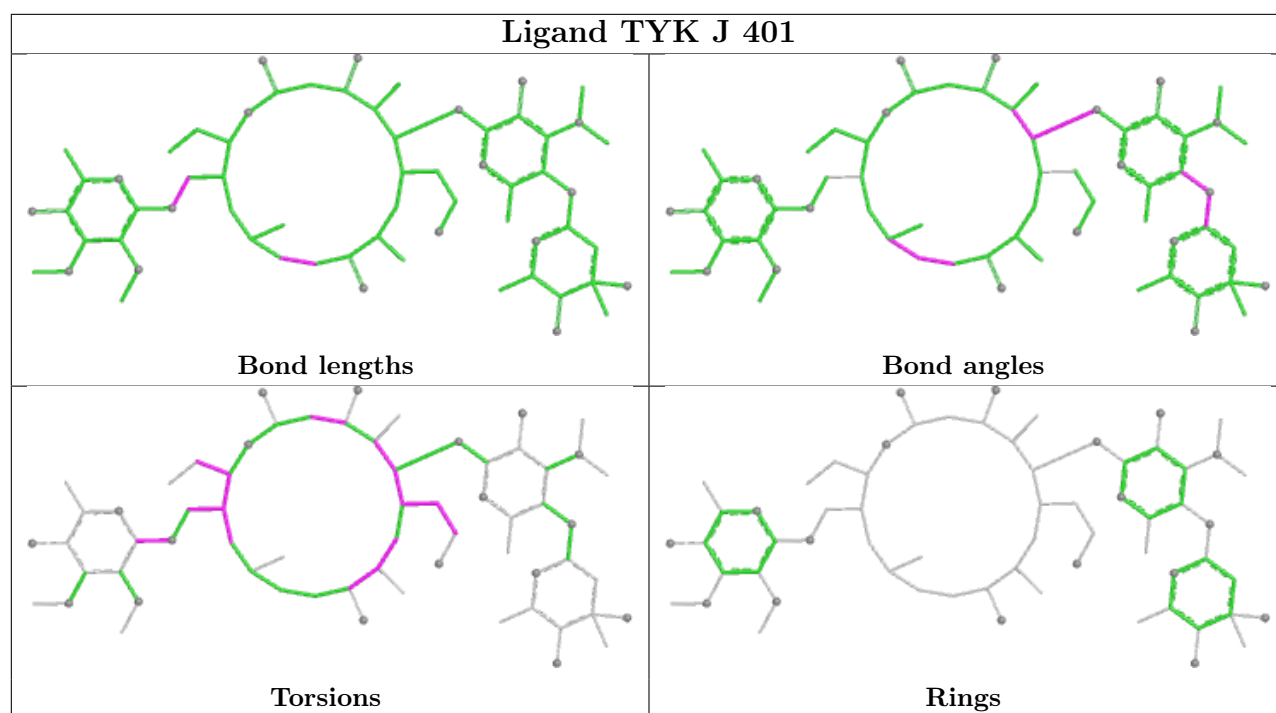
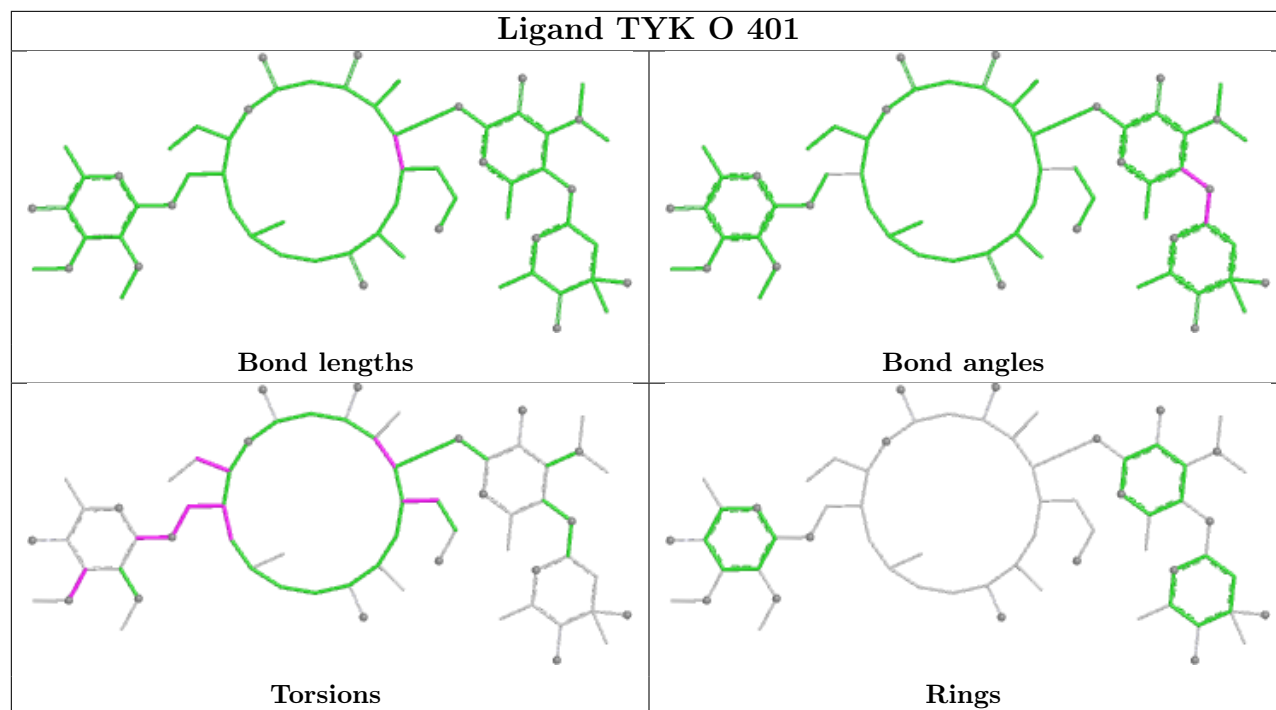


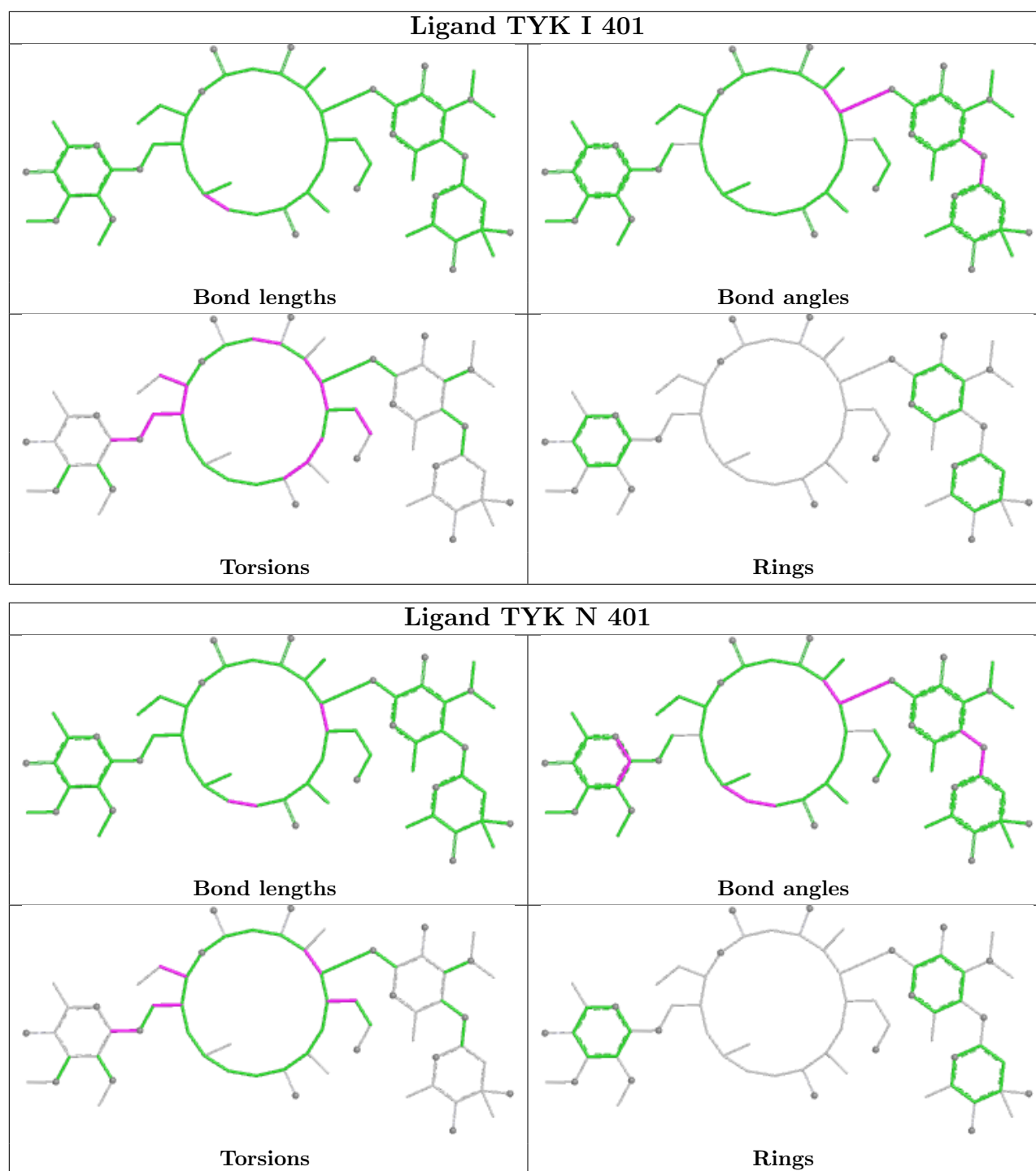












5.7 Other polymers [i](#)

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

All (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

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Mol	Chain	Res	Type	RSRZ
1	K	87	TYR	7.0
1	E	249	PRO	6.7
1	P	92	LEU	6.0
1	I	52	VAL	5.9
1	C	20	THR	5.8
1	C	247	LYS	5.6
1	C	59	LYS	5.6
1	K	21	MET	5.4
1	H	249	PRO	5.3
1	K	88	GLY	5.2
1	G	95	PRO	5.0
1	O	21	MET	5.0
1	L	228	LYS	5.0
1	D	225	ALA	5.0
1	H	55	TRP	5.0
1	M	249	PRO	4.9
1	B	92	LEU	4.8
1	E	28	ASP	4.9
1	D	226	ILE	4.8
1	O	246	LEU	4.8
1	D	249	PRO	4.8
1	H	92	LEU	4.7
1	K	28	ASP	4.6
1	A	88	GLY	4.5
1	C	21	MET	4.5
1	C	95	PRO	4.5
1	F	227	ARG	4.5
1	I	59	LYS	4.5
1	K	20	THR	4.3
1	J	92	LEU	4.2
1	I	88	GLY	4.2
1	O	53	TYR	4.1
1	M	22	ASN	4.1
1	G	28	ASP	4.0
1	L	55	TRP	4.0
1	O	55	TRP	3.9
1	J	249	PRO	3.9
1	D	55	TRP	3.9
1	M	21	MET	3.8
1	E	87	TYR	3.8
1	G	52	VAL	3.8
1	O	248	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	I	94	GLY	3.8
1	A	95	PRO	3.7
1	M	59	LYS	3.7
1	P	245	ALA	3.7
1	F	226	ILE	3.7
1	I	89	ASN	3.7
1	K	257	ARG	3.7
1	E	21	MET	3.6
1	L	92	LEU	3.6
1	F	264	LYS	3.6
1	J	55	TRP	3.6
1	F	224	GLY	3.6
1	A	248	ASP	3.6
1	M	52	VAL	3.6
1	K	60	GLY	3.5
1	C	250	GLN	3.5
1	A	57	GLU	3.5
1	B	226	ILE	3.5
1	G	21	MET	3.4
1	G	248	ASP	3.4
1	H	226	ILE	3.4
1	A	253	GLU	3.4
1	E	291	ARG	3.4
1	C	87	TYR	3.3
1	K	50	ALA	3.3
1	A	59	LYS	3.3
1	K	246	LEU	3.2
1	C	249	PRO	3.2
1	G	20	THR	3.2
1	I	244	ASP	3.2
1	K	245	ALA	3.2
1	M	20	THR	3.2
1	M	31	GLU	3.2
1	P	248	ASP	3.2
1	M	214	TRP	3.1
1	C	264	LYS	3.1
1	A	246	LEU	3.1
1	M	95	PRO	3.1
1	F	291	ARG	3.1
1	C	214	TRP	3.1
1	C	60	GLY	3.0
1	G	250	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	247	LYS	3.0
1	E	60	GLY	3.0
1	F	55	TRP	3.0
1	H	314	ALA	3.0
1	G	89	ASN	3.0
1	F	229	GLU	3.0
1	M	247	LYS	2.9
1	B	257	ARG	2.9
1	A	51	ASN	2.9
1	B	94	GLY	2.9
1	M	28	ASP	2.9
1	M	51	ASN	2.9
1	G	231	GLU	2.9
1	M	248	ASP	2.9
1	D	252	ARG	2.9
1	I	291	ARG	2.9
1	F	92	LEU	2.9
1	C	52	VAL	2.8
1	C	228	LYS	2.8
1	B	93	ASP	2.8
1	B	248	ASP	2.8
1	N	252	ARG	2.8
1	B	225	ALA	2.8
1	E	293	ALA	2.8
1	O	52	VAL	2.8
1	D	58	ASN	2.8
1	I	214	TRP	2.8
1	A	73	GLY	2.8
1	A	87	TYR	2.8
1	F	221	LEU	2.8
1	E	214	TRP	2.7
1	H	94	GLY	2.7
1	I	246	LEU	2.7
1	M	291	ARG	2.7
1	J	230	GLN	2.7
1	I	51	ASN	2.7
1	I	95	PRO	2.7
1	F	253	GLU	2.7
1	G	291	ARG	2.7
1	C	89	ASN	2.7
1	D	227	ARG	2.7
1	F	252	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	227	ARG	2.7
1	P	243	ALA	2.6
1	A	291	ARG	2.6
1	N	249	PRO	2.6
1	K	214	TRP	2.6
1	M	230	GLN	2.6
1	F	225	ALA	2.6
1	G	59	LYS	2.6
1	H	264	LYS	2.6
1	J	226	ILE	2.6
1	M	226	ILE	2.6
1	D	264	LYS	2.6
1	I	245	ALA	2.5
1	C	230	GLN	2.5
1	H	250	GLN	2.5
1	I	87	TYR	2.5
1	G	261	LEU	2.5
1	G	30	ALA	2.5
1	H	228	LYS	2.5
1	N	247	LYS	2.5
1	K	230	GLN	2.5
1	H	225	ALA	2.5
1	G	249	PRO	2.5
1	O	28	ASP	2.5
1	B	229	GLU	2.4
1	H	311	VAL	2.4
1	O	245	ALA	2.4
1	B	250	GLN	2.4
1	P	227	ARG	2.4
1	I	20	THR	2.4
1	G	35	ILE	2.4
1	F	257	ARG	2.4
1	M	75	ASP	2.4
1	O	244	ASP	2.4
1	K	96	ALA	2.4
1	E	228	LYS	2.4
1	G	227	ARG	2.4
1	B	230	GLN	2.4
1	N	55	TRP	2.4
1	O	89	ASN	2.3
1	B	220	GLY	2.3
1	H	253	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	51	ASN	2.3
1	P	244	ASP	2.3
1	A	228	LYS	2.3
1	O	264	LYS	2.3
1	O	230	GLN	2.3
1	I	28	ASP	2.3
1	B	249	PRO	2.3
1	B	270	GLY	2.3
1	P	225	ALA	2.3
1	E	20	THR	2.3
1	K	291	ARG	2.3
1	M	250	GLN	2.3
1	B	252	ARG	2.3
1	D	257	ARG	2.3
1	E	292	THR	2.3
1	F	250	GLN	2.3
1	K	2	GLU	2.3
1	A	28	ASP	2.2
1	H	93	ASP	2.2
1	A	20	THR	2.2
1	E	253	GLU	2.2
1	H	255	ILE	2.2
1	J	248	ASP	2.2
1	O	291	ARG	2.2
1	P	249	PRO	2.2
1	M	178	GLY	2.2
1	F	265	HIS	2.2
1	G	96	ALA	2.2
1	I	264	LYS	2.2
1	P	93	ASP	2.2
1	L	291	ARG	2.2
1	N	291	ARG	2.2
1	F	267	LEU	2.1
1	F	312	LEU	2.1
1	P	250	GLN	2.1
1	B	264	LYS	2.1
1	A	75	ASP	2.1
1	I	75	ASP	2.1
1	E	52	VAL	2.1
1	H	257	ARG	2.1
1	O	257	ARG	2.1
1	I	253	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	265	HIS	2.1
1	J	250	GLN	2.1
1	M	50	ALA	2.1
1	K	253	GLU	2.1
1	E	230	GLN	2.1
1	G	51	ASN	2.1
1	N	251	GLN	2.1
1	D	311	VAL	2.1
1	F	311	VAL	2.1
1	D	219	GLY	2.1
1	F	223	GLY	2.1
1	G	257	ARG	2.1
1	K	61	ARG	2.1
1	O	20	THR	2.0
1	C	251	GLN	2.0
1	E	72	GLN	2.0
1	B	263	ASP	2.0
1	E	267	LEU	2.0
1	I	248	ASP	2.0
1	M	35	ILE	2.0
1	J	264	LYS	2.0
1	D	291	ARG	2.0
1	N	228	LYS	2.0

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.

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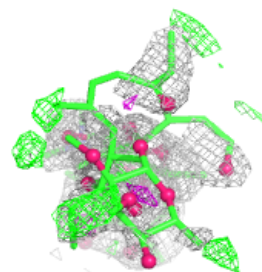
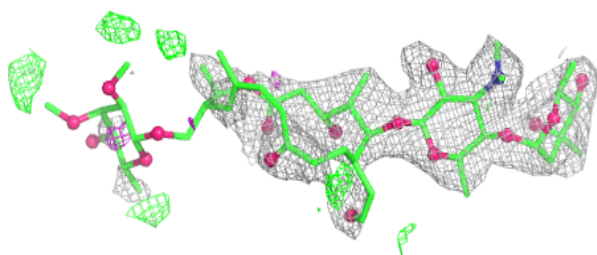
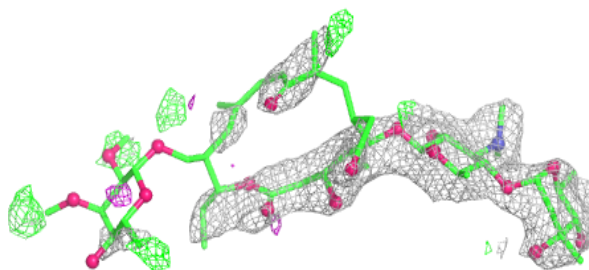
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TYK	F	401	64/64	0.71	0.23	64,86,145,155	0
2	TYK	H	401	64/64	0.73	0.23	57,88,161,170	0
2	TYK	B	401	64/64	0.75	0.25	56,91,169,179	0
2	TYK	G	401	64/64	0.76	0.22	44,84,151,159	0
2	TYK	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

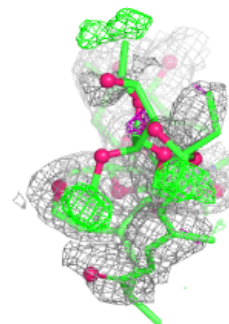
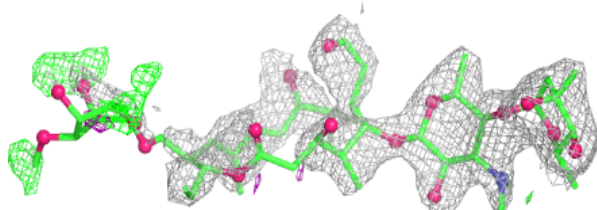
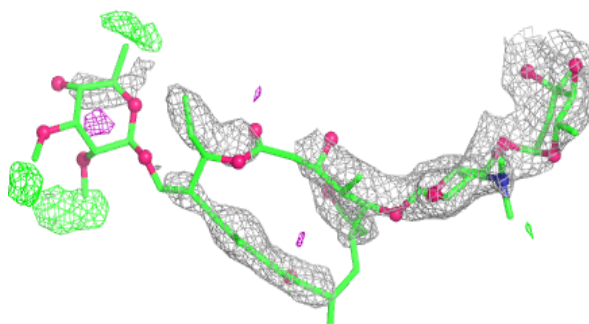
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

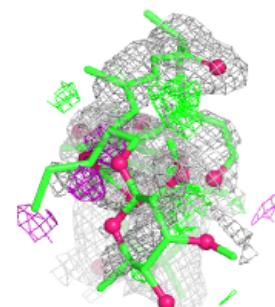
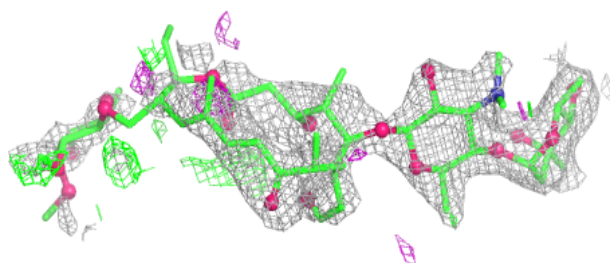
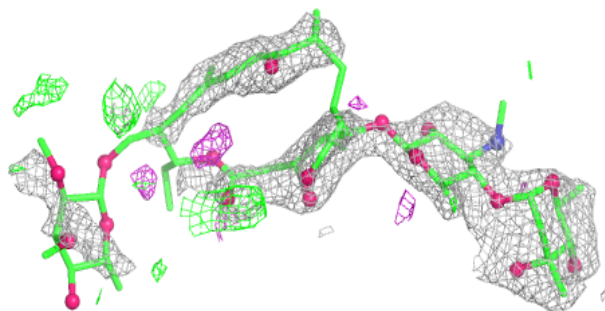
**Electron density around TYK H 401:**

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

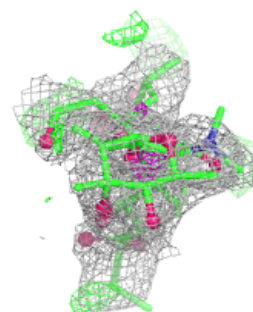
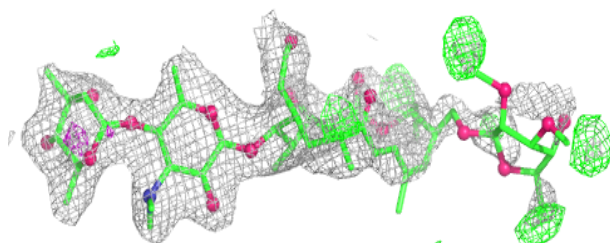
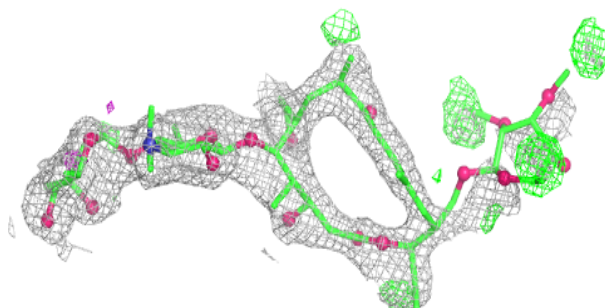


Electron density around TYK B 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

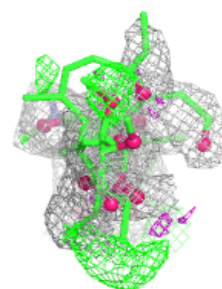
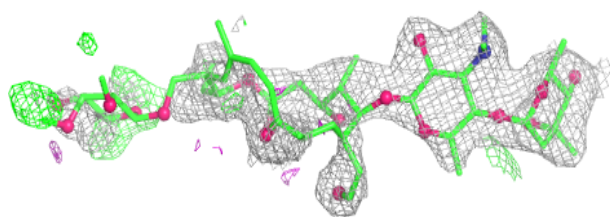
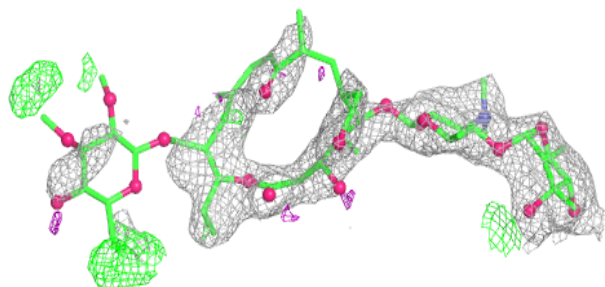
**Electron density around TYK G 401:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

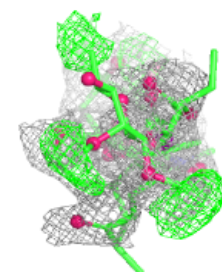
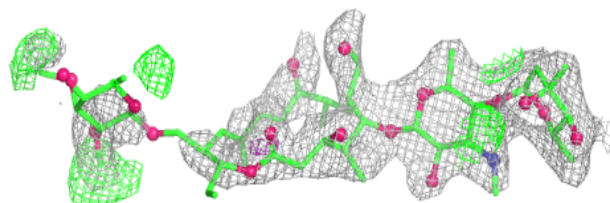
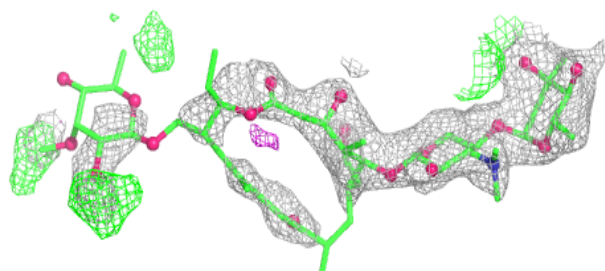


Electron density around TYK D 401:

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

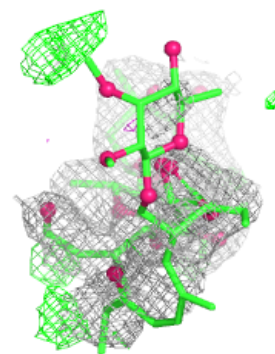
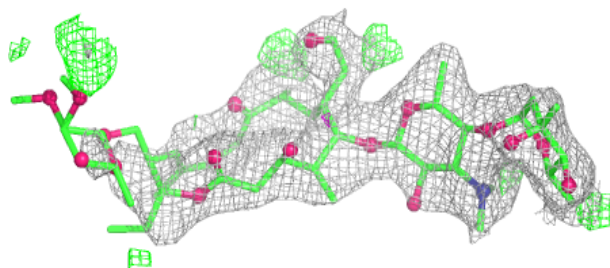
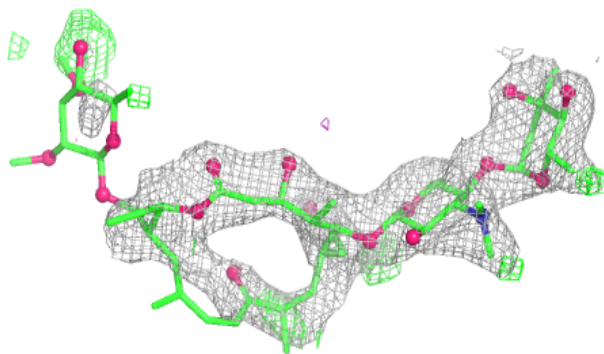
**Electron density around TYK J 401:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

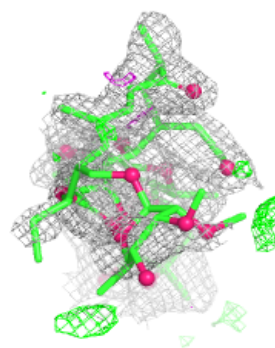
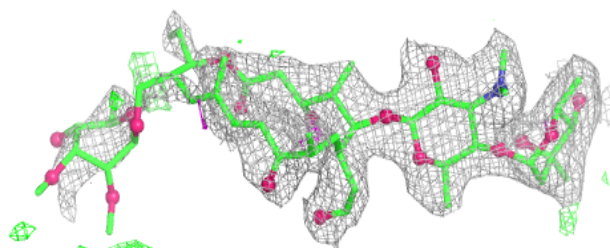
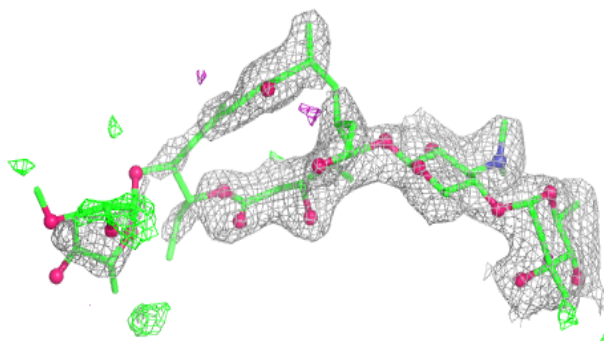


Electron density around TYK A 401:

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

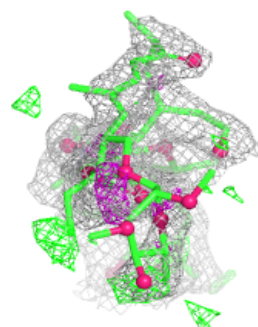
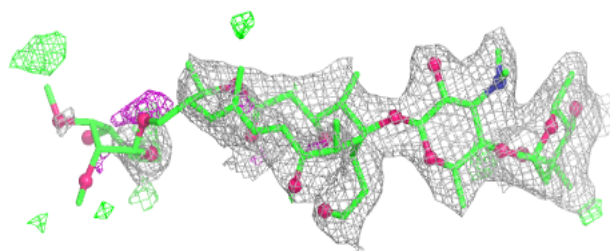
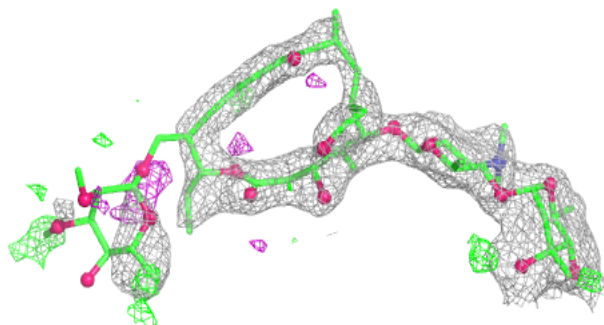
**Electron density around TYK N 401:**

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

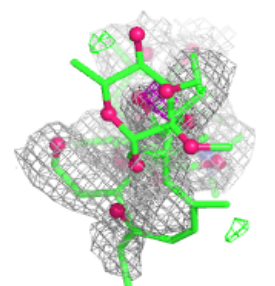
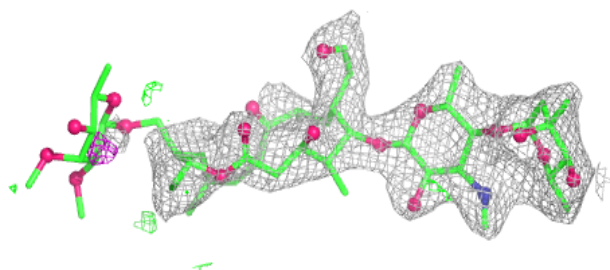
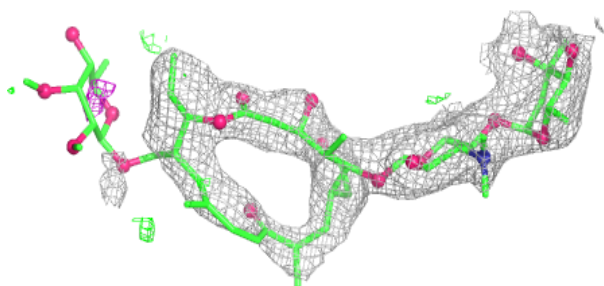


Electron density around TYK L 401:

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

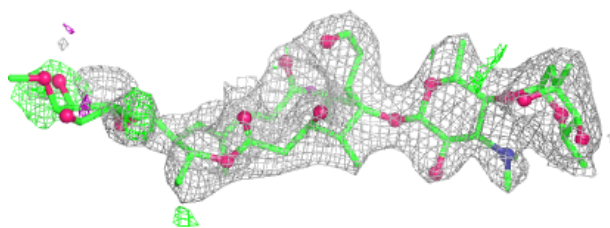
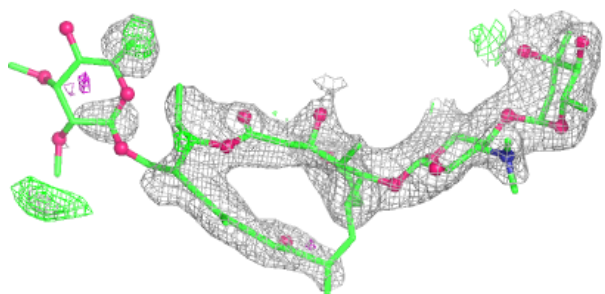
**Electron density around TYK C 401:**

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

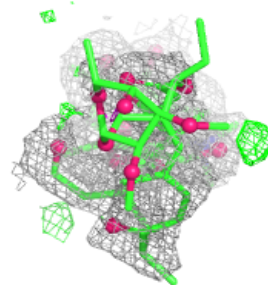
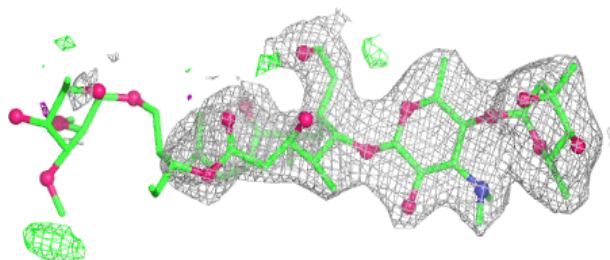
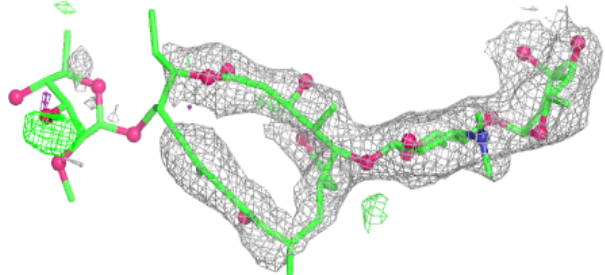


Electron density around TYK M 401:

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

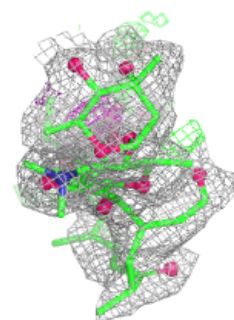
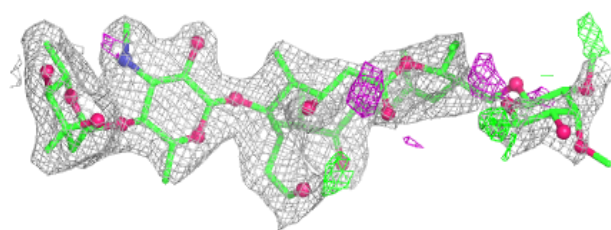
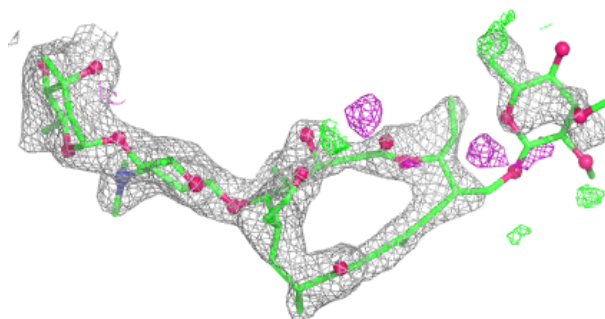
**Electron density around TYK E 401:**

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

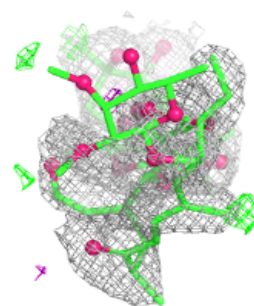
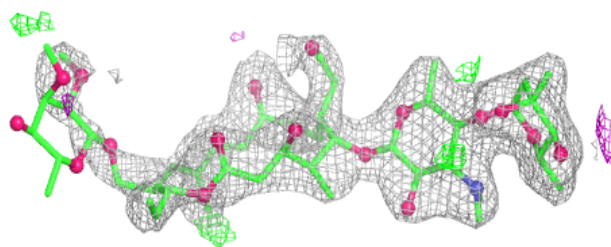
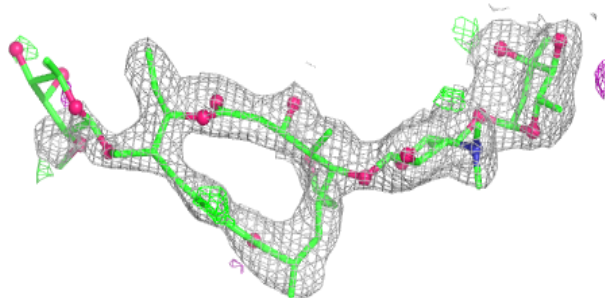


Electron density around TYK P 401:

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

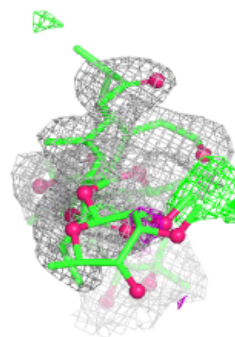
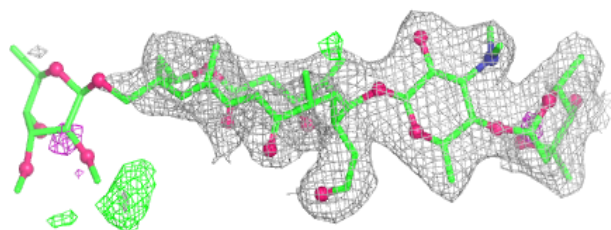
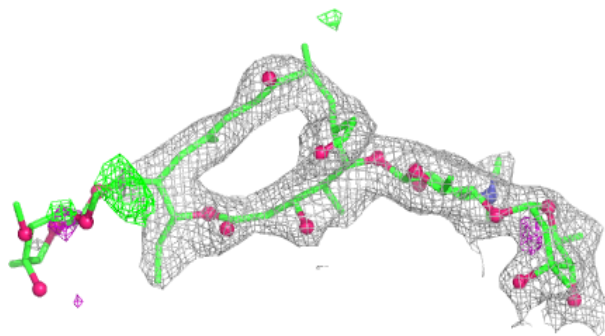
**Electron density around TYK K 401:**

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

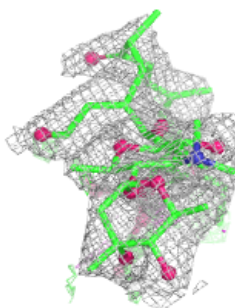
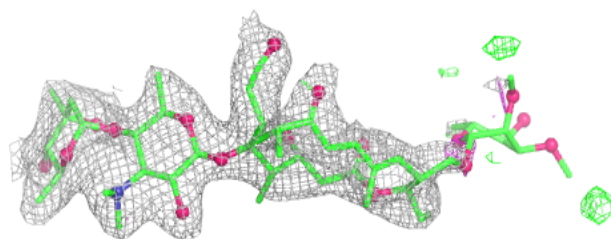
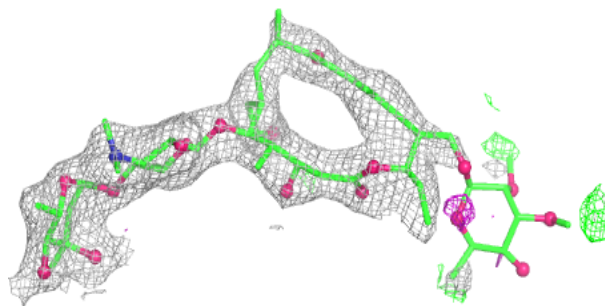


Electron density around TYK O 401:

$2mF_o-DF_c$ (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.