



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2024 – 12:40 PM JST

PDB ID : 8JWO
Title : Crystal structure of AKRtyl-tylosin complex
Authors : Lin, S.; Dai, S.; Xiao, Z.
Deposited on : 2023-06-29
Resolution : 2.25 Å(reported)

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

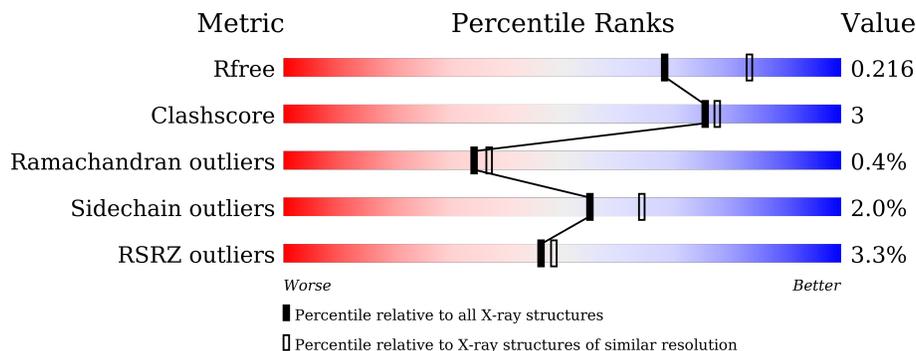
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 3% 75% 10% • 15%
1	B	351	 3% 81% 7% • 11%
1	C	351	 4% 77% 8% • 15%
1	D	351	 5% 83% 5% • 12%
1	E	351	 2% 75% 9% 17%
1	F	351	 5% 81% 8% 11%

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Mol	Chain	Length	Quality of chain
1	G	351	
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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TYK	B	401	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 41183 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Aldo/keto reductase.

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

There are 320 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

- Molecule 2 is TYLOSIN (three-letter code: TYK) (formula: C₄₆H₇₇NO₁₇) (labeled as "Ligand of Interest" by depositor).

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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		

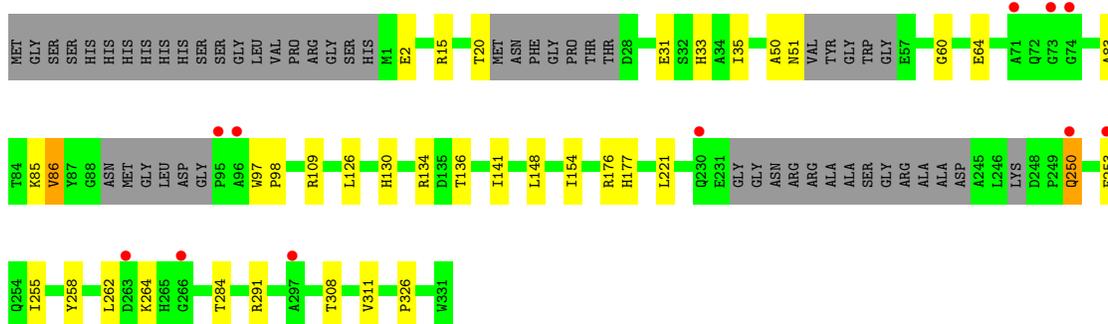
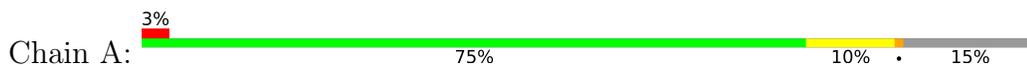
- Molecule 3 is water.

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		

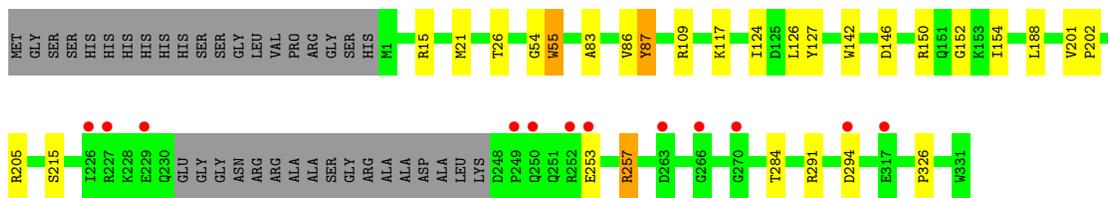
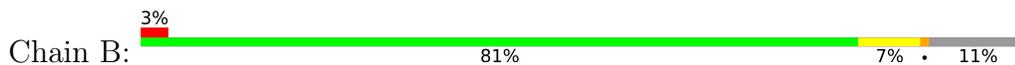
3 Residue-property plots [i](#)

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.

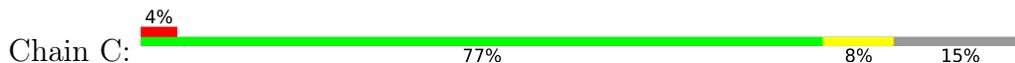
- Molecule 1: Aldo/keto reductase



- Molecule 1: Aldo/keto reductase

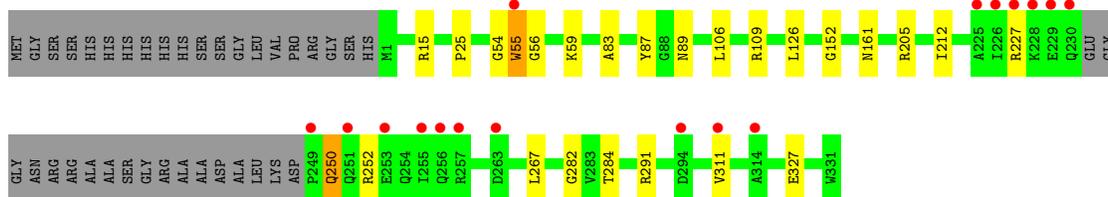


- Molecule 1: Aldo/keto reductase



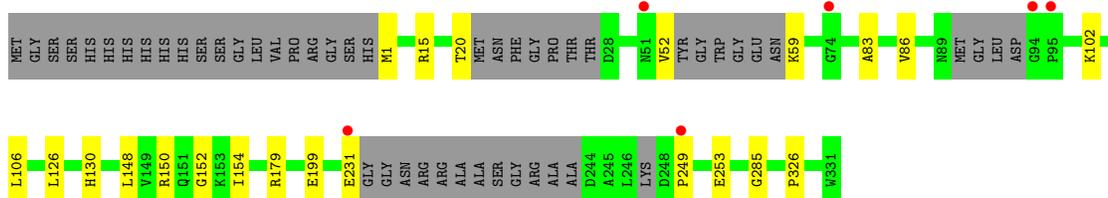
- Molecule 1: Aldo/keto reductase

Chain H: 



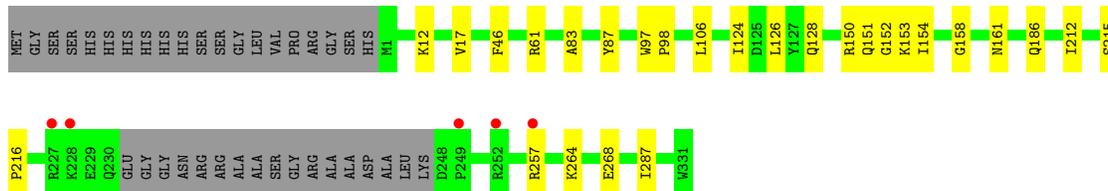
- Molecule 1: Aldo/keto reductase

Chain I: 



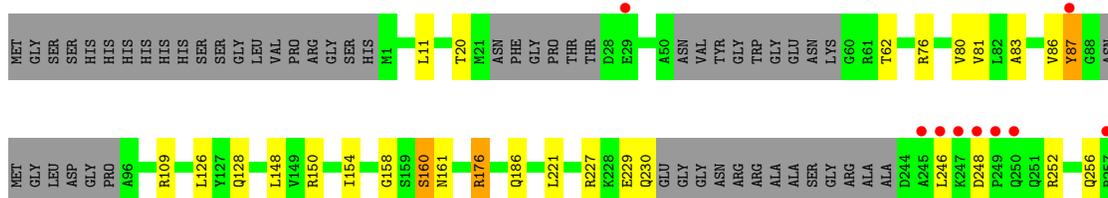
- Molecule 1: Aldo/keto reductase

Chain J: 



- Molecule 1: Aldo/keto reductase

Chain K: 



- Molecule 1: Aldo/keto reductase

Chain L: 



4 Data and refinement statistics i

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:THR:HG21	1:G:62:THR:HG21	1.51	0.90
1:B:26:THR:HG21	1:B:291:ARG:HD3	1.66	0.76
1:D:176:ARG:HD3	1:G:176:ARG:HG2	1.69	0.74
1:K:176:ARG:NH1	3:K:502:HOH:O	2.22	0.71
2:E:401:TYK:H221	2:E:401:TYK:C23	2.20	0.71
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: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:D:226:ILE:O	1:D:227:ARG:HB2	1.95	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: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:C:21:MET:C	1:C:51:ASN:HA	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:G:177:HIS:ND1	3:G:503:HOH:O	2.33	0.53
1:I:1:MET:N	3:I:503:HOH:O	2.42	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:H:15:ARG:HD2	1:H:284:THR:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:C:20:THR:O	1:C:21:MET:C	2.49	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: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:K:83:ALA:HA	1:K:126:LEU:O	2.12	0.49
1:L:161:ASN:O	1:O:326:PRO:HG3	2.13	0.49
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
1:J:83:ALA:HA	1:J:126:LEU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:K:227:ARG:HH21	1:K:227:ARG:HG3	1.79	0.46
1:H:250:GLN:H	1:H:250:GLN:CD	2.18	0.46
1:J:212:ILE:HG22	1:J:287:ILE:HG13	1.97	0.46
1:C:36:MET:HE3	1:C:69:TRP:CD1	2.50	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:I:199:GLU:CD	1:P:163:ALA:HB1	2.36	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: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: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
1:B:54:GLY:O	1:B:55:TRP:HB2	2.16	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:J:264:LYS:NZ	3:J:511:HOH:O	2.50	0.45
1:P:145:MET:HE2	1:P:157:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:106:LEU:C	1:M:106:LEU:HD23	2.37	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:N	2.71	0.44
1:E:229:GLU:HG3	1:E:230:GLN:N	2.33	0.44
1:F:15:ARG:O	1:F:285:GLY:HA3	2.17	0.44
1:C:326:PRO:HG3	1:F:161:ASN:O	2.18	0.43
1:F:79:LYS:NZ	3:F:502:HOH:O	2.30	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: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: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: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:128:GLN:HA	1:K:158:GLY:O	2.18	0.43
1:M:6:LEU:O	1:M:9:ILE:HG12	2.19	0.43
1:D:102:LYS:HD3	3:D:509:HOH:O	2.19	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:A:148:LEU:CD1	1:A:154:ILE:HD12	2.50	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:O:217:LEU:HD22	1:O:273:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:11:LEU:HD21	1:K:81:VAL:HG11	2.01	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
2:F:401:TYK:H14	2:F:401:TYK:H221	1.89	0.41
1:I:106:LEU:C	1:I:106:LEU:HD23	2.40	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
2:A:401:TYK:H14	2:A:401:TYK:H221	1.89	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:L:205:ARG:HH21	1:L:205:ARG:CG	2.32	0.41
1:H:106:LEU:HD23	1:H:106:LEU:C	2.41	0.41
1:J:106:LEU:C	1:J:106:LEU:HD23	2.41	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	287/351 (82%)	281 (98%)	6 (2%)	0	100	100
1	B	310/351 (88%)	299 (96%)	9 (3%)	2 (1%)	25	25
1	C	287/351 (82%)	278 (97%)	8 (3%)	1 (0%)	41	46
1	D	306/351 (87%)	293 (96%)	11 (4%)	2 (1%)	22	21
1	E	282/351 (80%)	275 (98%)	6 (2%)	1 (0%)	34	37
1	F	308/351 (88%)	296 (96%)	11 (4%)	1 (0%)	41	46
1	G	288/351 (82%)	279 (97%)	9 (3%)	0	100	100
1	H	309/351 (88%)	299 (97%)	7 (2%)	3 (1%)	15	13
1	I	289/351 (82%)	281 (97%)	8 (3%)	0	100	100
1	J	310/351 (88%)	300 (97%)	9 (3%)	1 (0%)	41	46
1	K	286/351 (82%)	276 (96%)	9 (3%)	1 (0%)	41	46
1	L	307/351 (88%)	298 (97%)	8 (3%)	1 (0%)	41	46
1	M	287/351 (82%)	279 (97%)	7 (2%)	1 (0%)	41	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	311/351 (89%)	300 (96%)	10 (3%)	1 (0%)	41	46
1	O	293/351 (84%)	288 (98%)	5 (2%)	0	100	100
1	P	312/351 (89%)	299 (96%)	11 (4%)	2 (1%)	25	25
All	All	4772/5616 (85%)	4621 (97%)	134 (3%)	17 (0%)	34	37

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
1	P	55	TRP
1	K	87	TYR
1	H	56	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/275 (86%)	232 (98%)	6 (2%)	47	56
1	B	249/275 (90%)	243 (98%)	6 (2%)	49	58
1	C	237/275 (86%)	233 (98%)	4 (2%)	60	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	245/275 (89%)	240 (98%)	5 (2%)	55	64
1	E	233/275 (85%)	231 (99%)	2 (1%)	78	86
1	F	247/275 (90%)	241 (98%)	6 (2%)	49	58
1	G	238/275 (86%)	231 (97%)	7 (3%)	42	51
1	H	248/275 (90%)	241 (97%)	7 (3%)	43	52
1	I	239/275 (87%)	235 (98%)	4 (2%)	60	71
1	J	249/275 (90%)	247 (99%)	2 (1%)	81	88
1	K	235/275 (86%)	231 (98%)	4 (2%)	60	71
1	L	246/275 (90%)	244 (99%)	2 (1%)	81	88
1	M	238/275 (86%)	229 (96%)	9 (4%)	33	39
1	N	250/275 (91%)	244 (98%)	6 (2%)	49	58
1	O	242/275 (88%)	239 (99%)	3 (1%)	71	80
1	P	250/275 (91%)	246 (98%)	4 (2%)	62	73
All	All	3884/4400 (88%)	3807 (98%)	77 (2%)	55	64

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

Mol	Chain	Res	Type
1	A	20	THR
1	A	86	VAL
1	A	250	GLN
1	A	253	GLU
1	A	264	LYS
1	A	291	ARG
1	B	21	MET
1	B	117	LYS
1	B	127	TYR
1	B	150	ARG
1	B	257	ARG
1	B	294	ASP
1	C	21	MET
1	C	59	LYS
1	C	89	ASN
1	C	176	ARG
1	D	21	MET
1	D	28	ASP
1	D	227	ARG

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Mol	Chain	Res	Type
1	D	268	GLU
1	D	291	ARG
1	E	21	MET
1	E	150	ARG
1	F	21	MET
1	F	65	ILE
1	F	127	TYR
1	F	150	ARG
1	F	252	ARG
1	F	292	THR
1	G	40	LEU
1	G	59	LYS
1	G	150	ARG
1	G	160	SER
1	G	265	HIS
1	G	291	ARG
1	G	305	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
1	I	59	LYS
1	I	231	GLU
1	J	150	ARG
1	J	257	ARG
1	K	160	SER
1	K	176	ARG
1	K	248	ASP
1	K	252	ARG
1	L	228	LYS
1	L	252	ARG
1	M	20	THR
1	M	22	ASN
1	M	28	ASP
1	M	46	PHE
1	M	59	LYS
1	M	113	ASP

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Mol	Chain	Res	Type
1	M	150	ARG
1	M	246	LEU
1	M	257	ARG
1	N	40	LEU
1	N	92	LEU
1	N	127	TYR
1	N	227	ARG
1	N	246	LEU
1	N	291	ARG
1	O	21	MET
1	O	179	ARG
1	O	229	GLU
1	P	21	MET
1	P	27	THR
1	P	244	ASP
1	P	253	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	186	GLN
1	D	130	HIS
1	E	251	GLN
1	F	130	HIS
1	H	256	GLN
1	I	51	ASN
1	I	89	ASN
1	J	130	HIS
1	J	256	GLN
1	L	128	GLN
1	L	130	HIS
1	L	186	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TYK	P	401	-	67,67,67	0.75	2 (2%)	83,97,97	0.92	5 (6%)
2	TYK	E	401	-	67,67,67	0.73	3 (4%)	83,97,97	0.82	2 (2%)
2	TYK	C	401	-	67,67,67	0.66	1 (1%)	83,97,97	1.24	4 (4%)
2	TYK	K	401	-	67,67,67	0.65	2 (2%)	83,97,97	0.68	0
2	TYK	M	401	-	67,67,67	0.67	0	83,97,97	1.01	4 (4%)
2	TYK	I	401	-	67,67,67	0.69	1 (1%)	83,97,97	0.83	2 (2%)
2	TYK	D	401	-	67,67,67	0.73	2 (2%)	83,97,97	1.20	7 (8%)
2	TYK	N	401	-	67,67,67	0.79	2 (2%)	83,97,97	0.84	4 (4%)
2	TYK	H	401	-	67,67,67	0.64	1 (1%)	83,97,97	0.75	3 (3%)
2	TYK	O	401	-	67,67,67	0.71	1 (1%)	83,97,97	0.74	1 (1%)
2	TYK	L	401	-	67,67,67	0.71	1 (1%)	83,97,97	0.90	4 (4%)
2	TYK	J	401	-	67,67,67	0.74	2 (2%)	83,97,97	0.74	3 (3%)
2	TYK	G	401	-	67,67,67	0.75	2 (2%)	83,97,97	0.83	1 (1%)
2	TYK	A	401	-	67,67,67	0.74	2 (2%)	83,97,97	1.20	5 (6%)
2	TYK	B	401	-	67,67,67	0.69	1 (1%)	83,97,97	1.02	4 (4%)
2	TYK	F	401	-	67,67,67	0.73	2 (2%)	83,97,97	1.09	3 (3%)

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

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

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	401	TYK	C6-C5	3.24	1.59	1.52
2	F	401	TYK	C11-C10	3.17	1.42	1.33
2	D	401	TYK	C6-C5	3.06	1.58	1.52
2	F	401	TYK	C6-C5	3.02	1.58	1.52
2	J	401	TYK	O1C-C23	3.01	1.49	1.43
2	D	401	TYK	C11-C10	3.01	1.42	1.33
2	A	401	TYK	C11-C10	2.88	1.41	1.33
2	G	401	TYK	C11-C10	2.66	1.41	1.33
2	A	401	TYK	C6-C5	2.65	1.57	1.52
2	C	401	TYK	C11-C10	2.61	1.41	1.33
2	E	401	TYK	C11-C10	2.58	1.40	1.33
2	G	401	TYK	C6-C5	2.56	1.57	1.52
2	L	401	TYK	C6-C5	2.55	1.57	1.52
2	K	401	TYK	C11-C10	2.38	1.40	1.33
2	P	401	TYK	C6-C5	2.38	1.57	1.52
2	E	401	TYK	C6-C5	2.32	1.57	1.52
2	K	401	TYK	C6-C5	2.30	1.57	1.52
2	H	401	TYK	C6-C5	2.30	1.57	1.52
2	B	401	TYK	C6-C5	2.22	1.57	1.52
2	J	401	TYK	C11-C10	2.22	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	401	TYK	C11-C10	2.20	1.39	1.33
2	N	401	TYK	C11-C10	2.18	1.39	1.33
2	I	401	TYK	C11-C12	-2.10	1.41	1.45
2	E	401	TYK	C22-C12	-2.08	1.46	1.50
2	O	401	TYK	C6-C5	2.07	1.56	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	TYK	C10-C11-C12	7.42	137.45	126.23
2	A	401	TYK	C10-C11-C12	7.35	137.34	126.23
2	F	401	TYK	C10-C11-C12	7.26	137.21	126.23
2	D	401	TYK	C10-C11-C12	6.95	136.74	126.23
2	B	401	TYK	O1A-C5-C4	4.33	113.44	108.22
2	E	401	TYK	C10-C11-C12	4.13	132.47	126.23
2	M	401	TYK	C10-C11-C12	4.09	132.42	126.23
2	P	401	TYK	O1A-C5-C4	3.75	112.74	108.22
2	C	401	TYK	O1A-C5-C4	3.74	112.73	108.22
2	G	401	TYK	O1A-C5-C4	3.74	112.73	108.22
2	I	401	TYK	O1A-C5-C4	3.65	112.61	108.22
2	N	401	TYK	O1A-C5-C4	3.63	112.60	108.22
2	M	401	TYK	O5C-C1C-C2C	3.37	116.19	109.51
2	A	401	TYK	O1A-C5-C4	3.29	112.19	108.22
2	H	401	TYK	C10-C11-C12	3.20	131.07	126.23
2	L	401	TYK	C10-C11-C12	3.03	130.82	126.23
2	N	401	TYK	C1B-O4A-C4A	2.89	120.51	114.66
2	M	401	TYK	C1C-C2C-C3C	2.87	116.47	110.75
2	C	401	TYK	C22-C12-C11	-2.84	113.60	118.08
2	L	401	TYK	O1A-C5-C4	2.84	111.64	108.22
2	J	401	TYK	O1A-C5-C4	2.82	111.62	108.22
2	B	401	TYK	C10-C11-C12	2.81	130.48	126.23
2	E	401	TYK	O1A-C5-C4	2.79	111.58	108.22
2	A	401	TYK	C11-C12-C13	2.76	128.50	119.42
2	D	401	TYK	O1A-C5-C6	2.75	116.36	109.23
2	A	401	TYK	C22-C12-C11	-2.73	113.77	118.08
2	P	401	TYK	C10-C11-C12	2.72	130.34	126.23
2	B	401	TYK	O15-C15-C14	2.70	113.35	107.42
2	I	401	TYK	C1B-O4A-C4A	2.69	120.11	114.66
2	J	401	TYK	C1B-O4A-C4A	2.64	120.00	114.66
2	C	401	TYK	C11-C12-C13	2.63	128.06	119.42
2	H	401	TYK	O1A-C5-C4	2.59	111.34	108.22
2	N	401	TYK	C10-C11-C12	2.58	130.13	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	401	TYK	O1A-C5-C4	2.55	111.30	108.22
2	D	401	TYK	O1A-C5-C4	2.53	111.27	108.22
2	B	401	TYK	C15-O15-C1	2.43	122.56	117.83
2	L	401	TYK	O15-C15-C14	2.28	112.42	107.42
2	O	401	TYK	C1B-O4A-C4A	2.26	119.24	114.66
2	D	401	TYK	O15-C15-C14	-2.23	102.52	107.42
2	J	401	TYK	C10-C11-C12	2.22	129.59	126.23
2	D	401	TYK	C22-C12-C11	-2.18	114.64	118.08
2	N	401	TYK	O5C-C1C-C2C	2.18	113.83	109.51
2	P	401	TYK	O4B-C4B-C5B	-2.17	105.58	109.39
2	D	401	TYK	C11-C10-C9	2.17	133.42	121.46
2	H	401	TYK	O5C-C1C-C2C	2.13	113.73	109.51
2	F	401	TYK	C1B-O4A-C4A	2.09	118.88	114.66
2	P	401	TYK	C1B-O4A-C4A	2.07	118.85	114.66
2	D	401	TYK	C11-C12-C13	2.06	126.19	119.42
2	F	401	TYK	C11-C12-C13	2.06	126.17	119.42
2	P	401	TYK	C1A-C2A-C3A	2.03	112.58	109.24
2	L	401	TYK	O5C-C1C-C2C	2.03	113.53	109.51
2	A	401	TYK	C1B-O4A-C4A	2.02	118.75	114.66

There are no chirality outliers.

All (248) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	B	401	TYK	C23-C14-C15-O15
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	C10-C11-C12-C13
2	C	401	TYK	C10-C11-C12-C22
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	C10-C11-C12-C13
2	D	401	TYK	C10-C11-C12-C22
2	D	401	TYK	O15-C15-C16-C17
2	E	401	TYK	C20-C19-C6-C7
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	C10-C11-C12-C13
2	F	401	TYK	C10-C11-C12-C22
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	C2C-C1C-O1C-C23
2	F	401	TYK	O5C-C1C-O1C-C23
2	G	401	TYK	C12-C13-C14-C23

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Mol	Chain	Res	Type	Atoms
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
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	I	401	TYK	C2C-C1C-O1C-C23
2	I	401	TYK	O5C-C1C-O1C-C23
2	J	401	TYK	C20-C19-C6-C7
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

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Mol	Chain	Res	Type	Atoms
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	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	B	401	TYK	C19-C6-C7-C8
2	P	401	TYK	C19-C6-C7-C8
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	O	401	TYK	C2C-C1C-O1C-C23
2	B	401	TYK	C18-C4-C5-C6
2	H	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	D	401	TYK	C2C-C1C-O1C-C23
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	G	401	TYK	C15-C14-C23-O1C
2	J	401	TYK	C15-C14-C23-O1C
2	A	401	TYK	C20-C19-C6-C5
2	O	401	TYK	C20-C19-C6-C5
2	L	401	TYK	C18-C4-C5-C6
2	A	401	TYK	C20-C19-C6-C7
2	D	401	TYK	C20-C19-C6-C7
2	F	401	TYK	C20-C19-C6-C7

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Mol	Chain	Res	Type	Atoms
2	G	401	TYK	C20-C19-C6-C7
2	H	401	TYK	C20-C19-C6-C7
2	K	401	TYK	C20-C19-C6-C7
2	L	401	TYK	C20-C19-C6-C7
2	P	401	TYK	C20-C19-C6-C7
2	J	401	TYK	C12-C13-C14-C15
2	M	401	TYK	C12-C13-C14-C15
2	O	401	TYK	C12-C13-C14-C15
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	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	D	401	TYK	C13-C14-C23-O1C
2	G	401	TYK	C13-C14-C23-O1C
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	N	401	TYK	C13-C14-C23-O1C
2	O	401	TYK	C13-C14-C23-O1C
2	P	401	TYK	C13-C14-C15-C16
2	A	401	TYK	C14-C23-O1C-C1C
2	B	401	TYK	C14-C23-O1C-C1C
2	D	401	TYK	C12-C13-C14-C23

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Mol	Chain	Res	Type	Atoms
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	K	401	TYK	C14-C23-O1C-C1C
2	O	401	TYK	C14-C23-O1C-C1C
2	O	401	TYK	C18-C4-C5-C6
2	I	401	TYK	C6-C7-C8-C9
2	J	401	TYK	C13-C14-C15-O15
2	M	401	TYK	C6-C7-C8-C9
2	B	401	TYK	C5-C6-C7-C8
2	P	401	TYK	C5-C6-C7-C8
2	H	401	TYK	C18-C4-C5-O1A
2	J	401	TYK	C18-C4-C5-O1A
2	C	401	TYK	C18-C4-C5-C6
2	L	401	TYK	C1-C2-C3-C4
2	B	401	TYK	C18-C4-C5-O1A
2	B	401	TYK	C12-C13-C14-C15
2	G	401	TYK	C12-C13-C14-C15
2	I	401	TYK	C12-C13-C14-C15
2	I	401	TYK	C6-C19-C20-O20
2	I	401	TYK	C4-C5-C6-C19
2	J	401	TYK	C6-C19-C20-O20
2	J	401	TYK	C4-C5-C6-C19
2	K	401	TYK	C6-C19-C20-O20
2	A	401	TYK	C18-C4-C5-C6
2	F	401	TYK	C18-C4-C5-C6
2	A	401	TYK	C6-C7-C8-C21
2	E	401	TYK	O1A-C5-C6-C19
2	H	401	TYK	O1A-C5-C6-C19
2	L	401	TYK	O1A-C5-C6-C19
2	P	401	TYK	O1A-C5-C6-C19
2	H	401	TYK	C2C-C3C-O3C-C8C
2	D	401	TYK	C18-C4-C5-O1A
2	D	401	TYK	C5-C6-C7-C8
2	F	401	TYK	C5-C6-C7-C8
2	E	401	TYK	C20-C19-C6-C5
2	J	401	TYK	C20-C19-C6-C5
2	L	401	TYK	C20-C19-C6-C5
2	A	401	TYK	O15-C15-C16-C17
2	C	401	TYK	C4A-C3A-N3A-C7A
2	K	401	TYK	C4A-C3A-N3A-C7A
2	B	401	TYK	C20-C19-C6-C7

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Mol	Chain	Res	Type	Atoms
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	P	401	TYK	C12-C13-C14-C15
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	G	401	TYK	C18-C4-C5-O1A
2	G	401	TYK	C22-C12-C13-C14
2	J	401	TYK	C2C-C1C-O1C-C23
2	K	401	TYK	C2C-C1C-O1C-C23
2	E	401	TYK	C19-C6-C7-C8
2	I	401	TYK	C21-C8-C9-O9
2	K	401	TYK	C21-C8-C9-O9
2	A	401	TYK	C13-C14-C23-O1C
2	E	401	TYK	C9-C10-C11-C12
2	H	401	TYK	C13-C14-C23-O1C
2	L	401	TYK	C4A-C3A-N3A-C7A
2	C	401	TYK	C14-C23-O1C-C1C
2	E	401	TYK	C14-C23-O1C-C1C

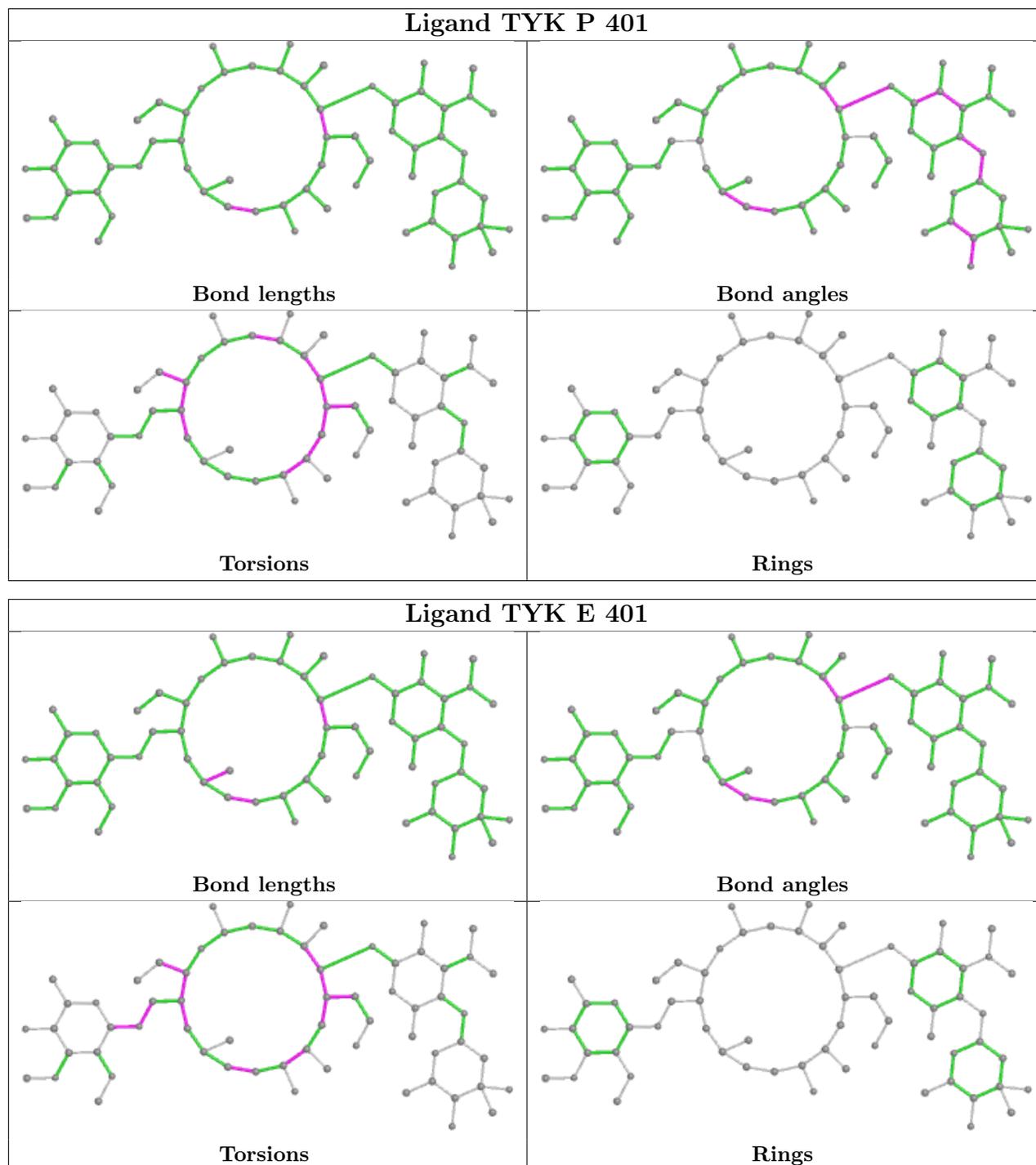
There are no ring outliers.

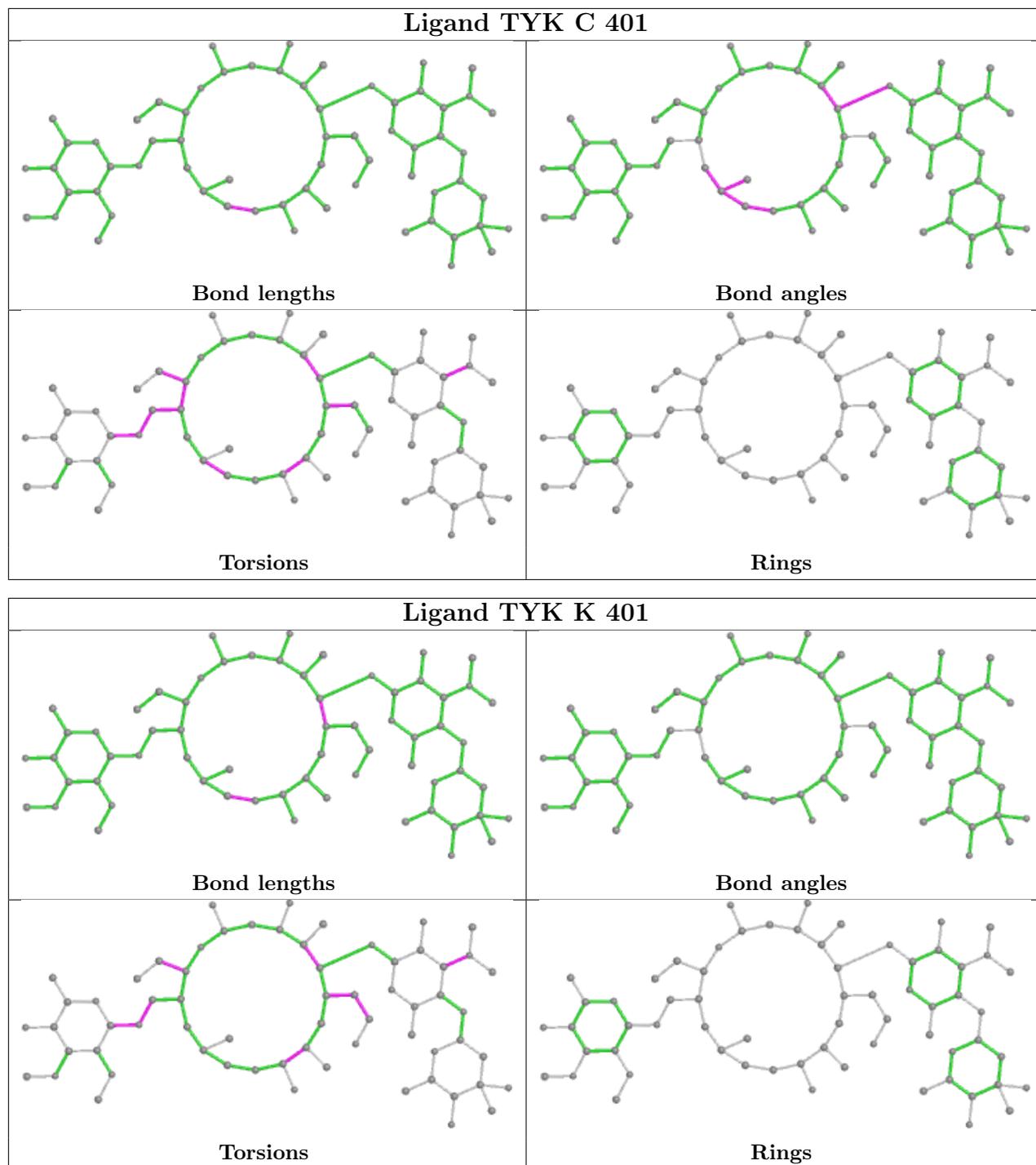
7 monomers are involved in 18 short contacts:

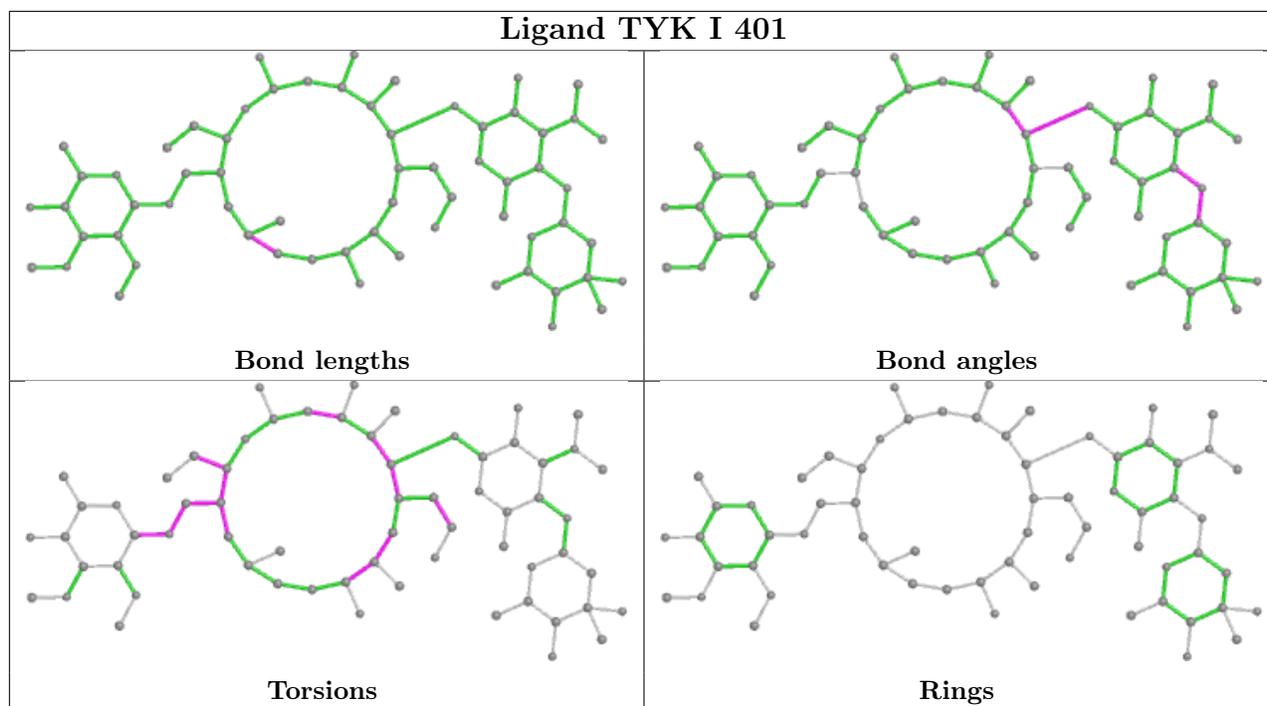
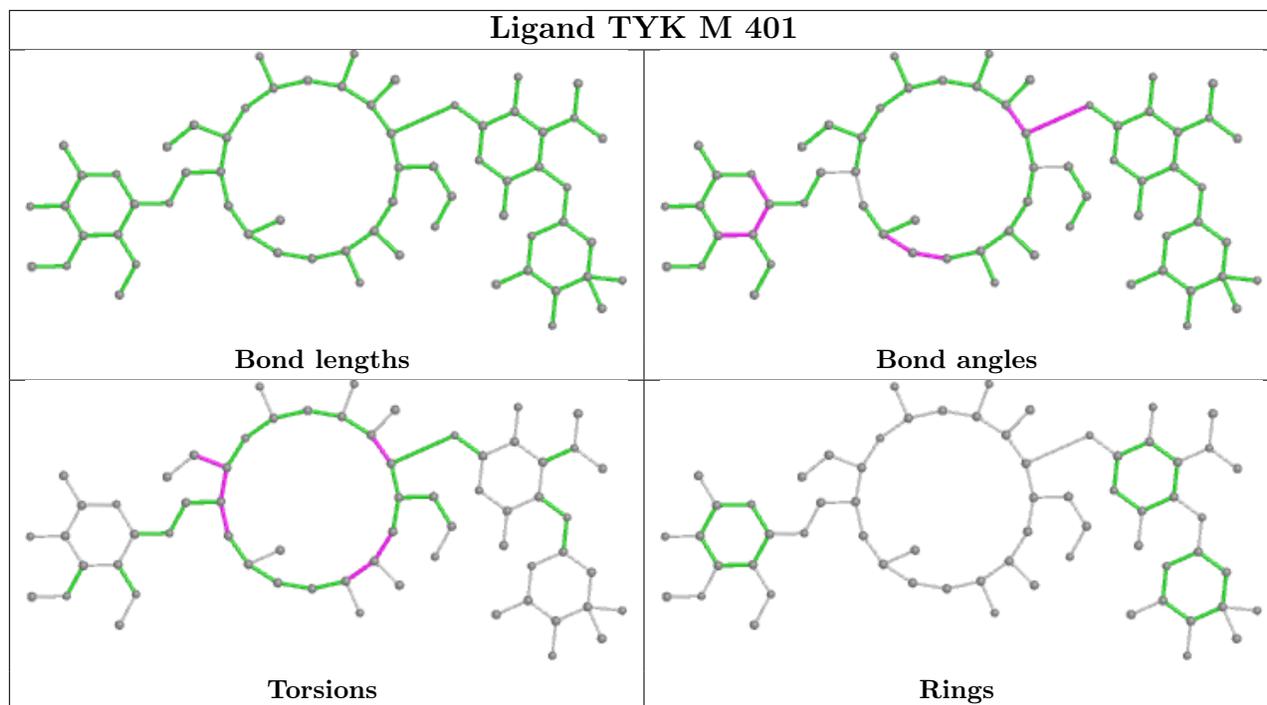
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	TYK	4	0
2	C	401	TYK	5	0
2	K	401	TYK	1	0
2	D	401	TYK	1	0
2	O	401	TYK	2	0
2	A	401	TYK	2	0
2	F	401	TYK	3	0

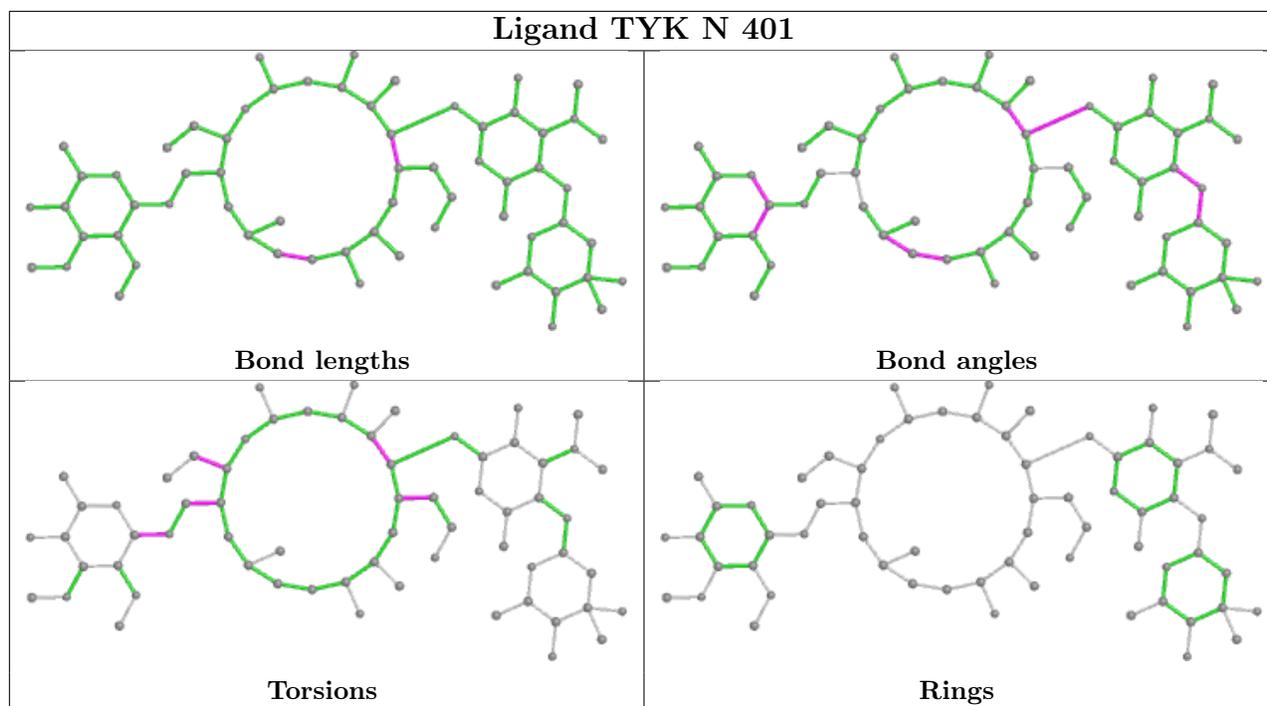
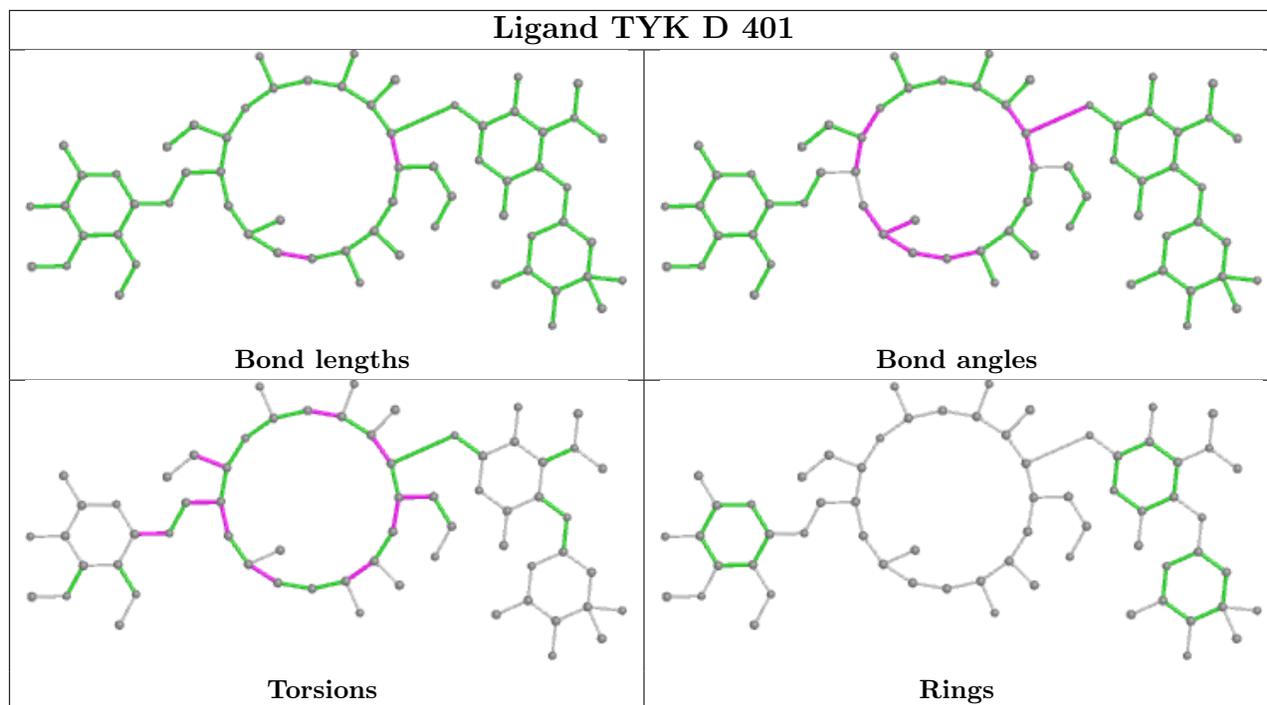
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

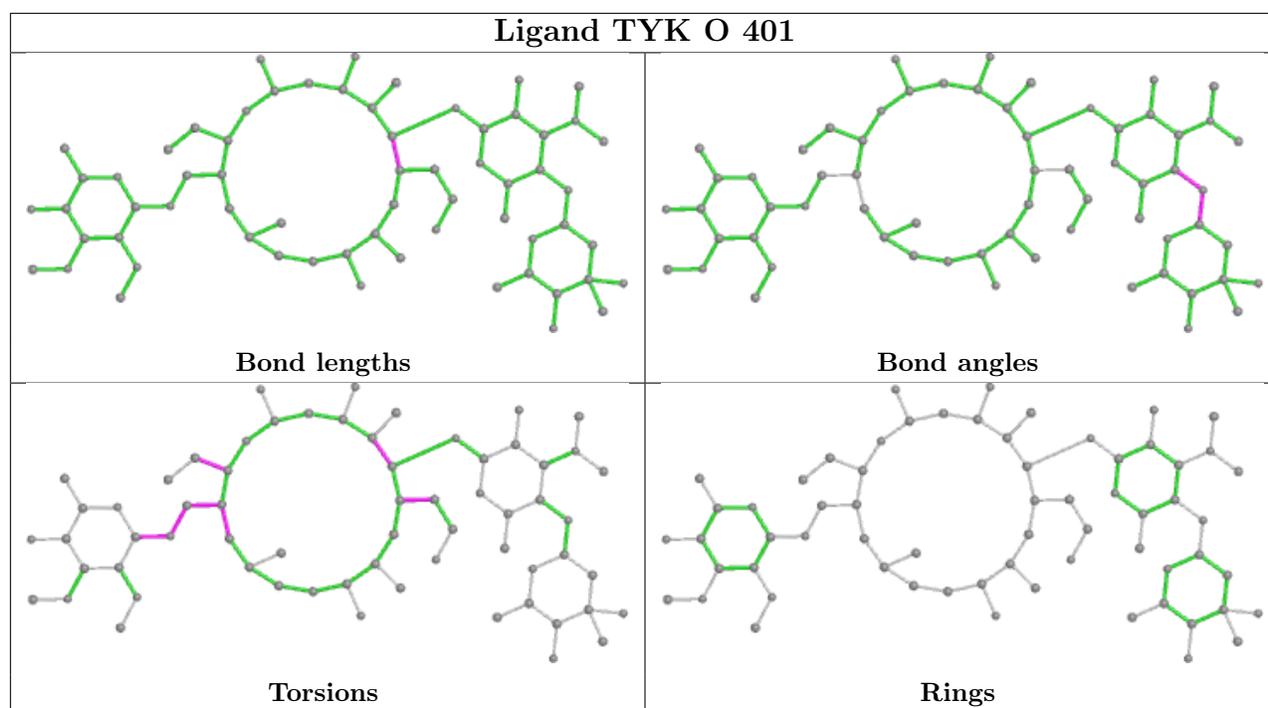
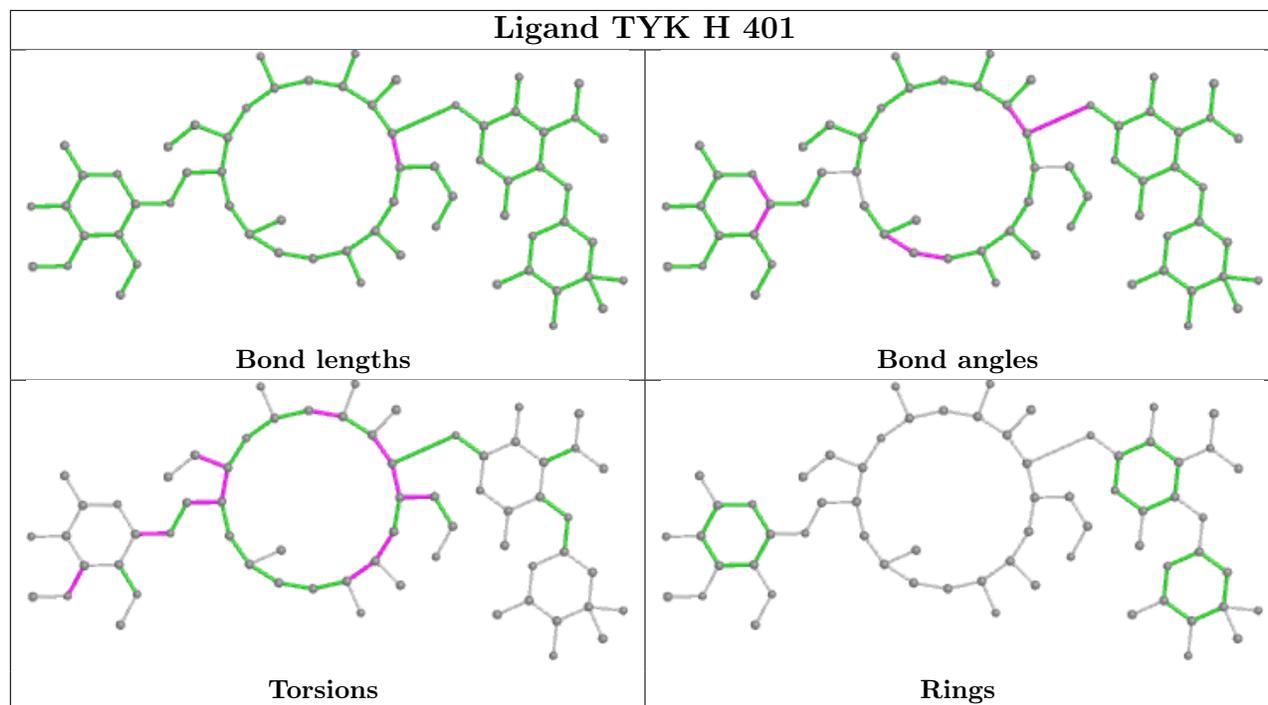
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

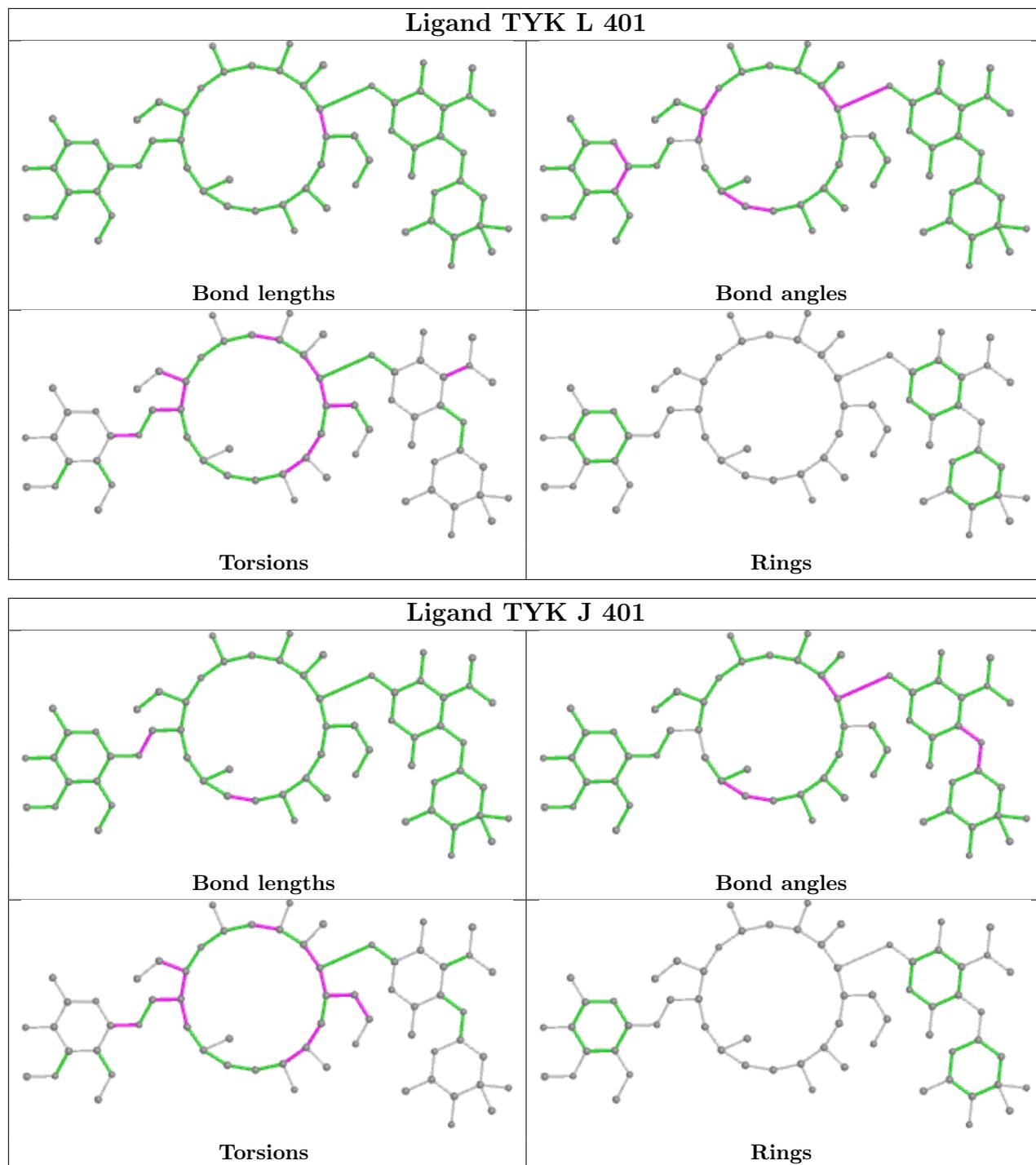


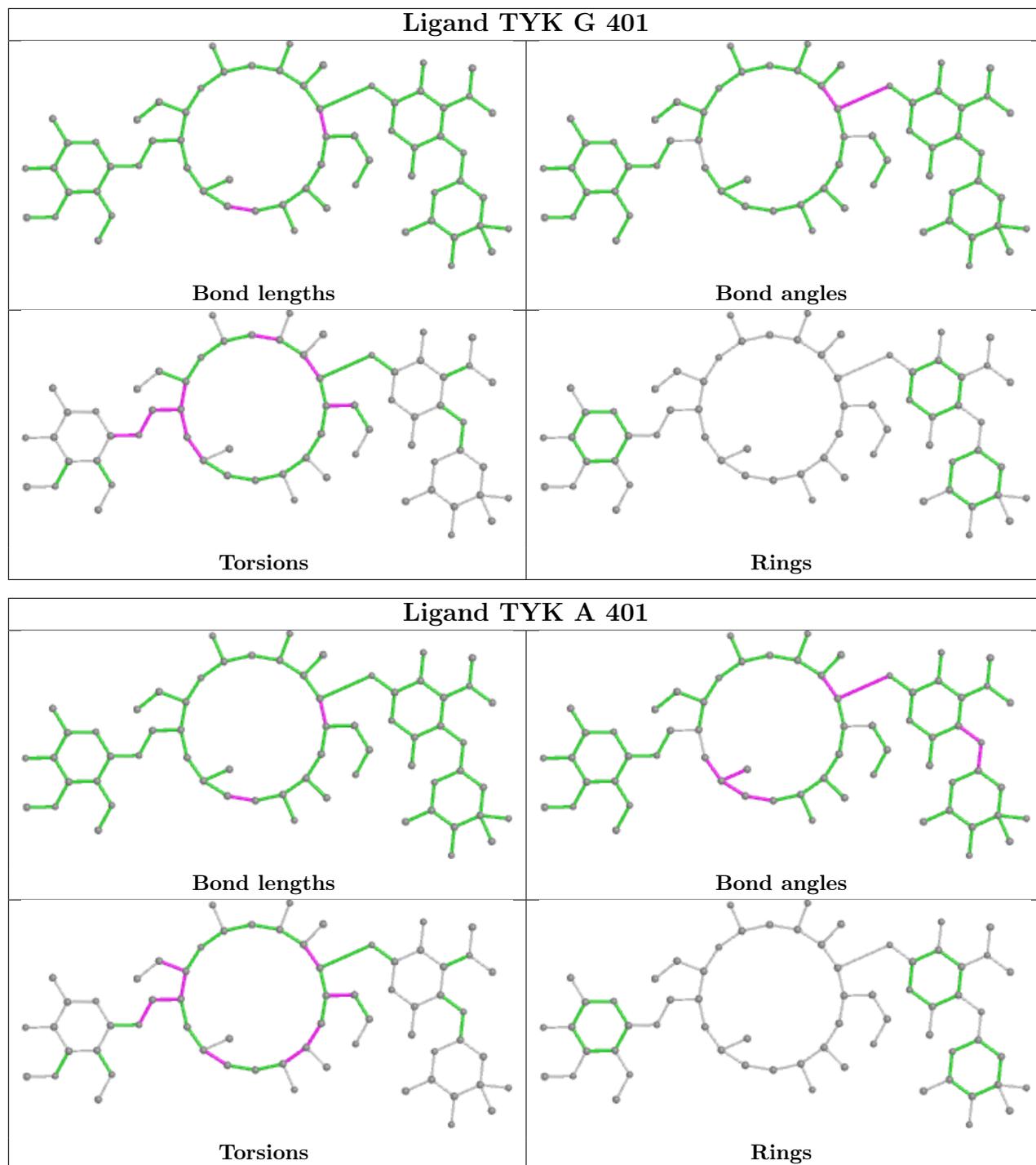


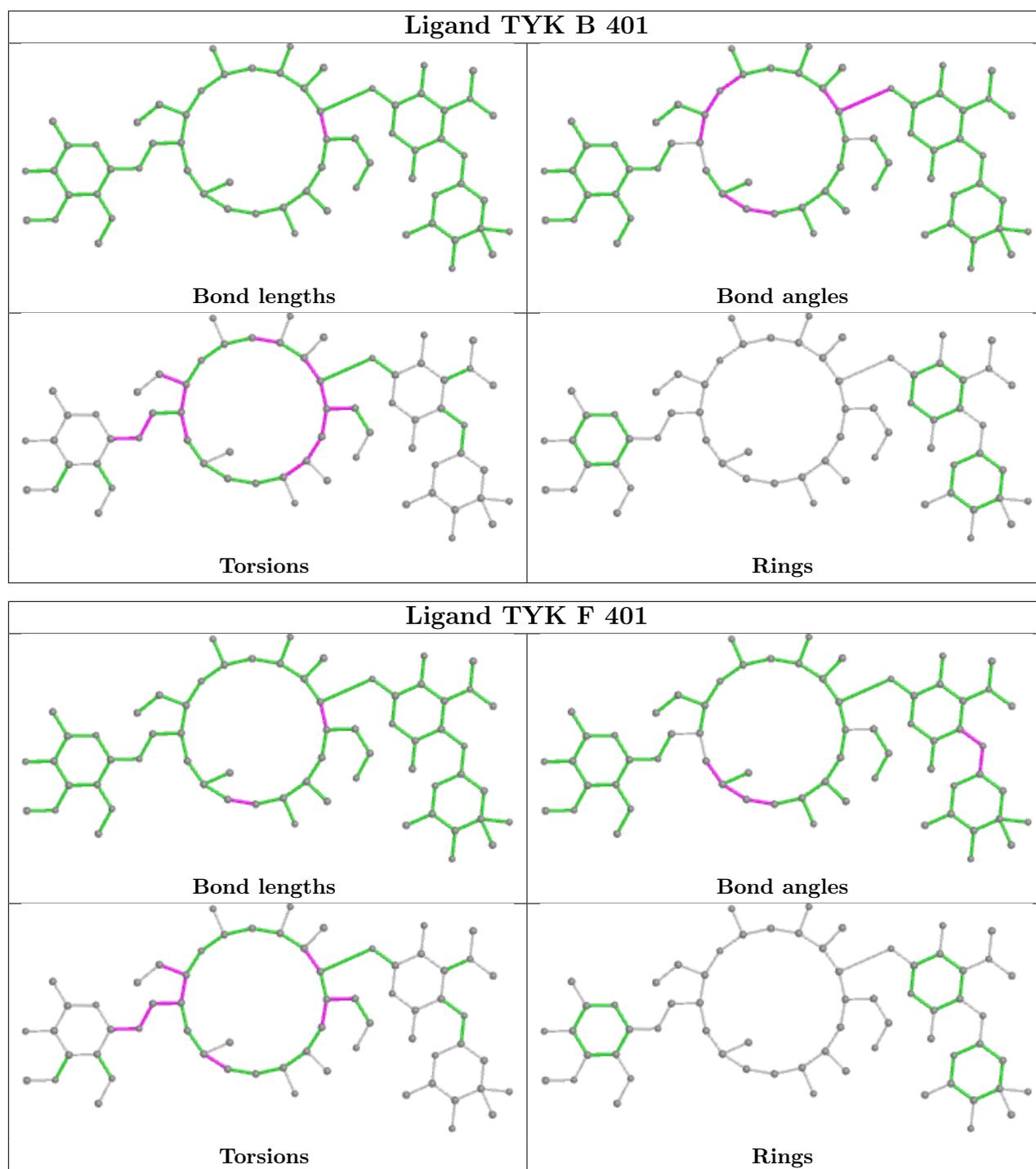












5.7 Other polymers [i](#)

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

All (162) RSRZ outliers are listed below:

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

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Mol	Chain	Res	Type	RSRZ
1	K	291	ARG	4.4
1	M	95	PRO	4.3
1	K	247	LYS	4.1
1	C	87	TYR	4.0
1	P	242	ALA	3.9
1	B	227	ARG	3.9
1	K	248	ASP	3.8
1	H	55	TRP	3.8
1	H	253	GLU	3.8
1	O	248	ASP	3.8
1	E	253	GLU	3.7
1	D	255	ILE	3.7
1	O	246	LEU	3.6
1	I	94	GLY	3.6
1	K	246	LEU	3.6
1	B	226	ILE	3.5
1	M	247	LYS	3.5
1	H	226	ILE	3.5
1	D	250	GLN	3.5
1	G	230	GLN	3.4
1	M	226	ILE	3.4
1	K	245	ALA	3.4
1	I	95	PRO	3.4
1	G	248	ASP	3.4
1	P	243	ALA	3.3
1	A	230	GLN	3.2
1	D	263	ASP	3.2
1	C	264	LYS	3.1
1	D	225	ALA	3.1
1	F	266	GLY	3.1
1	I	231	GLU	3.1
1	C	95	PRO	3.0
1	H	227	ARG	3.0
1	F	227	ARG	3.0
1	C	251	GLN	3.0
1	K	250	GLN	3.0
1	H	225	ALA	3.0
1	I	249	PRO	3.0
1	C	89	ASN	3.0
1	J	227	ARG	3.0
1	F	264	LYS	3.0
1	G	249	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	248	ASP	2.9
1	B	266	GLY	2.9
1	H	314	ALA	2.9
1	C	249	PRO	2.9
1	J	252	ARG	2.9
1	M	51	ASN	2.9
1	K	249	PRO	2.9
1	N	249	PRO	2.9
1	C	253	GLU	2.9
1	M	225	ALA	2.9
1	H	251	GLN	2.8
1	E	257	ARG	2.8
1	B	263	ASP	2.8
1	F	291	ARG	2.8
1	L	227	ARG	2.8
1	K	257	ARG	2.8
1	B	252	ARG	2.8
1	D	260	ASP	2.8
1	O	55	TRP	2.8
1	K	263	ASP	2.8
1	J	249	PRO	2.7
1	D	249	PRO	2.7
1	B	270	GLY	2.7
1	C	230	GLN	2.7
1	B	229	GLU	2.7
1	D	262	LEU	2.7
1	B	250	GLN	2.7
1	A	95	PRO	2.7
1	E	230	GLN	2.7
1	M	21	MET	2.7
1	G	227	ARG	2.6
1	A	297	ALA	2.6
1	D	258	TYR	2.6
1	F	224	GLY	2.6
1	A	266	GLY	2.6
1	G	263	ASP	2.6
1	C	250	GLN	2.6
1	F	258	TYR	2.6
1	I	74	GLY	2.6
1	A	263	ASP	2.6
1	D	311	VAL	2.6
1	P	253	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	226	ILE	2.6
1	F	257	ARG	2.5
1	A	253	GLU	2.5
1	P	244	ASP	2.5
1	P	227	ARG	2.5
1	H	256	GLN	2.5
1	L	250	GLN	2.5
1	N	251	GLN	2.5
1	D	256	GLN	2.5
1	O	53	TYR	2.5
1	F	226	ILE	2.5
1	F	262	LEU	2.5
1	D	251	GLN	2.4
1	N	252	ARG	2.4
1	G	61	ARG	2.4
1	H	257	ARG	2.4
1	B	253	GLU	2.4
1	H	249	PRO	2.4
1	C	291	ARG	2.4
1	H	263	ASP	2.4
1	E	261	LEU	2.4
1	F	225	ALA	2.4
1	H	230	GLN	2.4
1	E	226	ILE	2.4
1	F	253	GLU	2.4
1	M	257	ARG	2.3
1	H	228	LYS	2.3
1	N	253	GLU	2.3
1	A	74	GLY	2.3
1	J	228	LYS	2.3
1	O	245	ALA	2.3
1	M	75	ASP	2.3
1	M	22	ASN	2.3
1	A	96	ALA	2.3
1	L	253	GLU	2.3
1	G	28	ASP	2.3
1	D	313	THR	2.2
1	A	73	GLY	2.2
1	N	248	ASP	2.2
1	F	255	ILE	2.2
1	M	253	GLU	2.2
1	B	294	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	311	VAL	2.2
1	C	227	ARG	2.2
1	L	225	ALA	2.2
1	H	255	ILE	2.2
1	I	51	ASN	2.2
1	F	256	GLN	2.2
1	N	250	GLN	2.2
1	E	256	GLN	2.1
1	D	257	ARG	2.1
1	F	252	ARG	2.1
1	H	229	GLU	2.1
1	F	228	LYS	2.1
1	M	264	LYS	2.1
1	F	267	LEU	2.1
1	B	317	GLU	2.1
1	K	29	GLU	2.1
1	D	314	ALA	2.1
1	E	87	TYR	2.1
1	N	263	ASP	2.1
1	A	71	ALA	2.1
1	P	225	ALA	2.1
1	J	257	ARG	2.1
1	F	223	GLY	2.1
1	D	226	ILE	2.1
1	D	264	LYS	2.1
1	A	250	GLN	2.1
1	C	254	GLN	2.1
1	D	294	ASP	2.1
1	M	31	GLU	2.0
1	H	294	ASP	2.0
1	G	250	GLN	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 monosaccharides in this entry.

6.4 Ligands

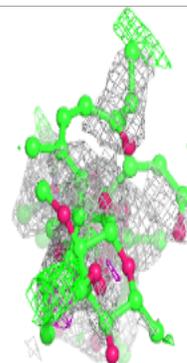
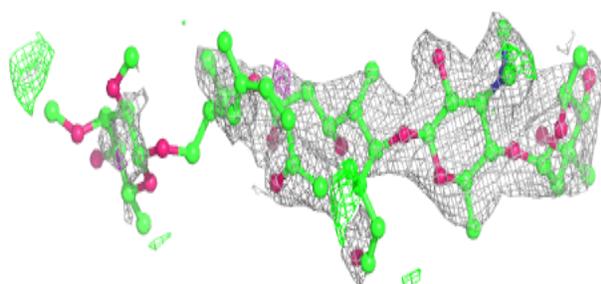
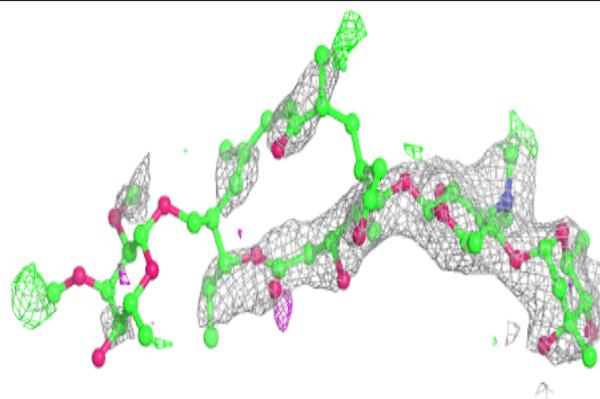
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

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

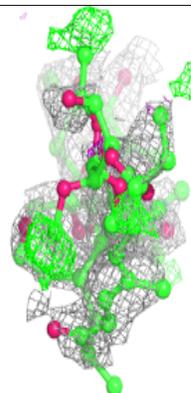
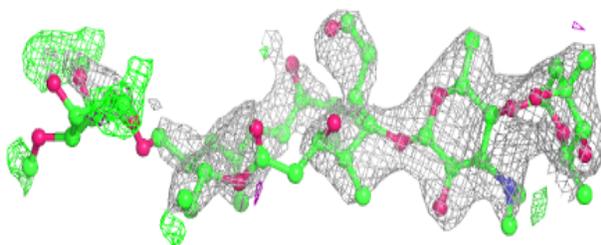
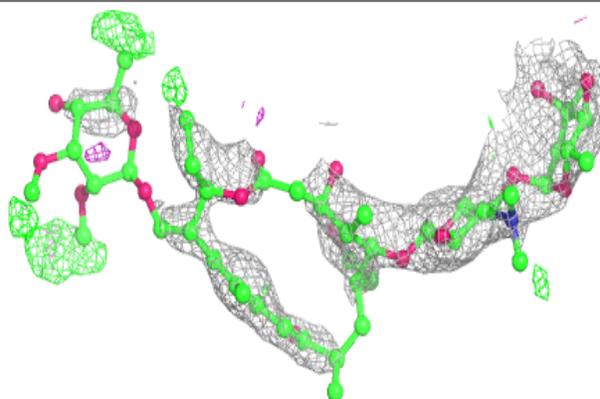
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TYK F 401:

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

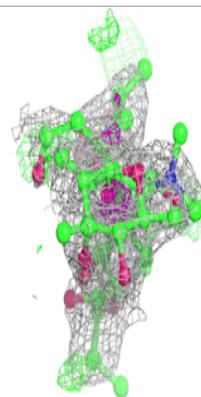
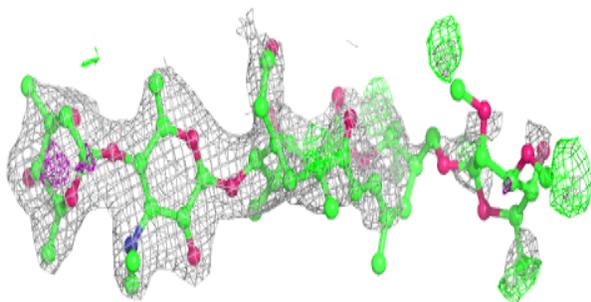
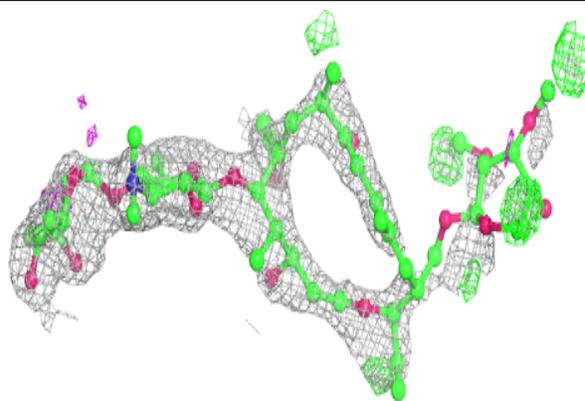
**Electron density around TYK H 401:**

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

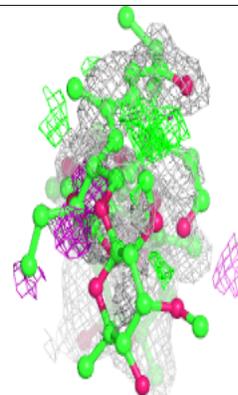
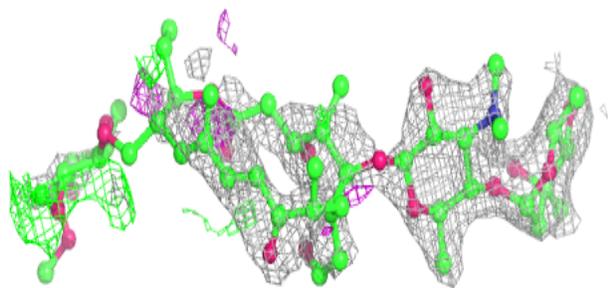
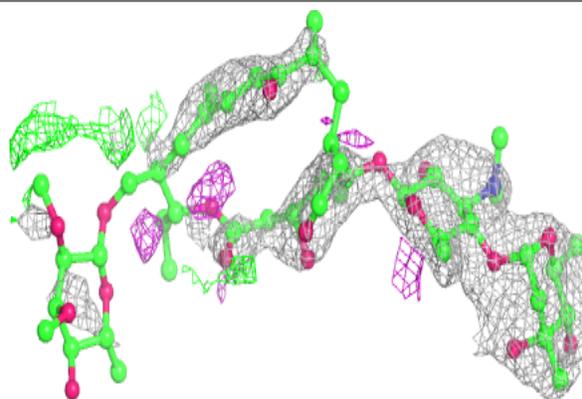


Electron density around TYK G 401:

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

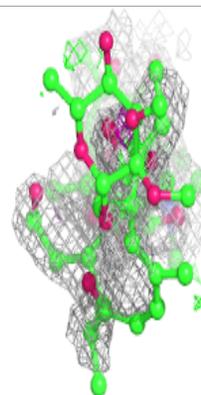
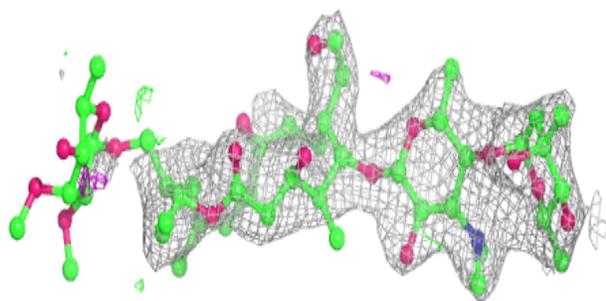
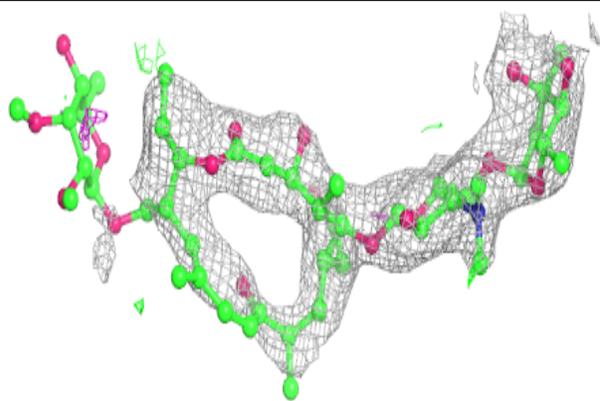
**Electron density around TYK B 401:**

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

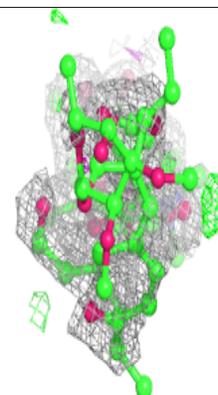
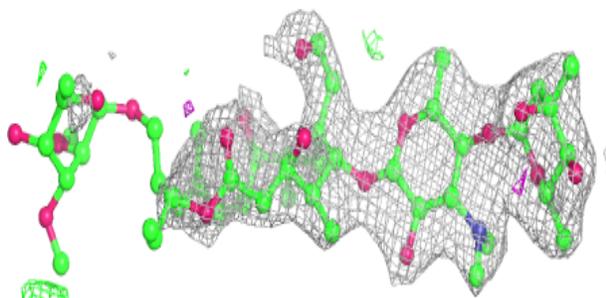
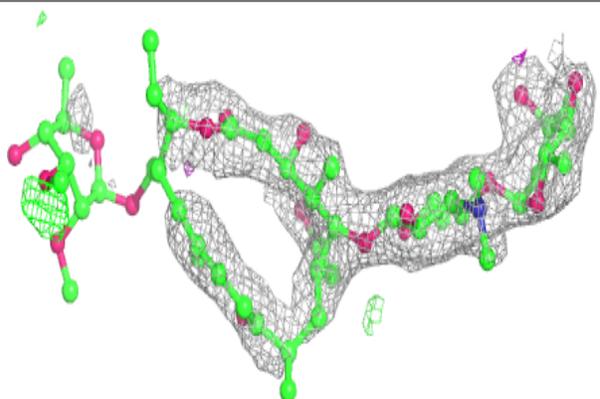


Electron density around TYK C 401:

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

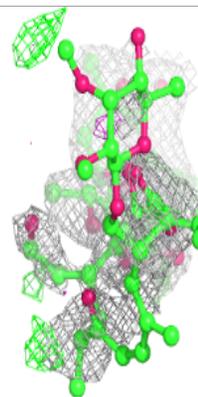
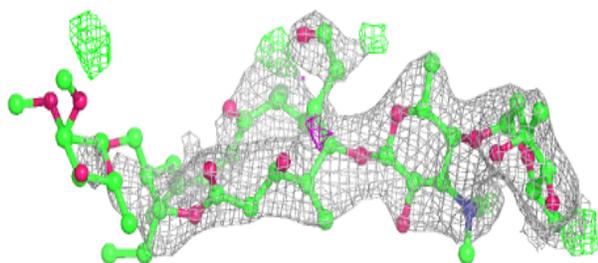
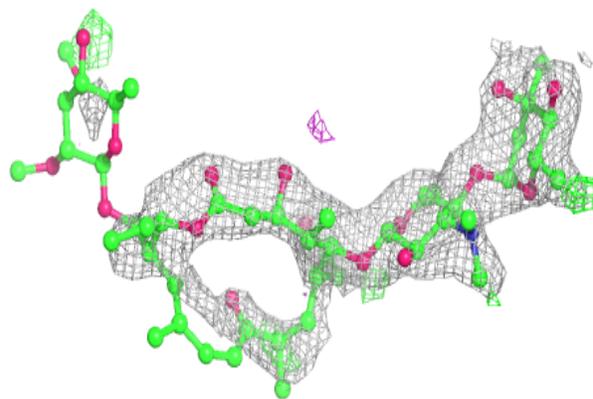
**Electron density around TYK E 401:**

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

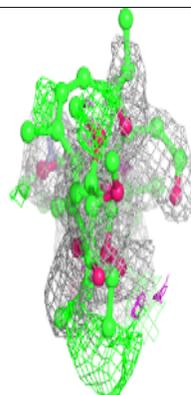
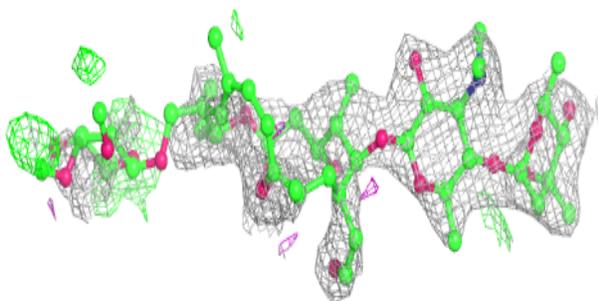
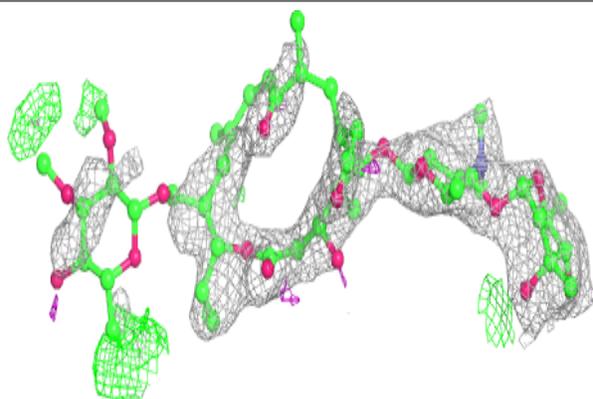


Electron density around TYK A 401:

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

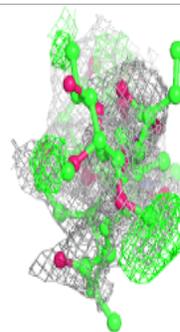
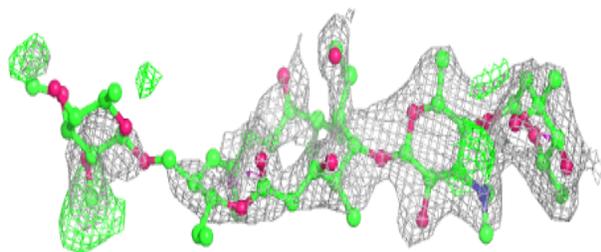
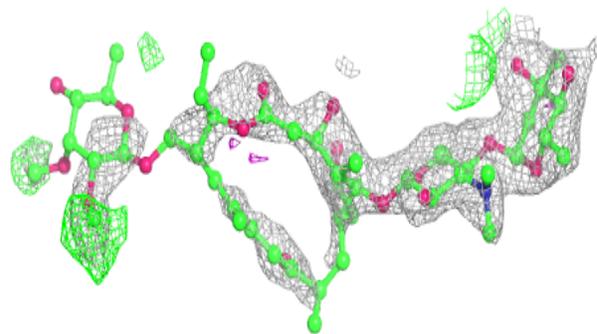
**Electron density around TYK D 401:**

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

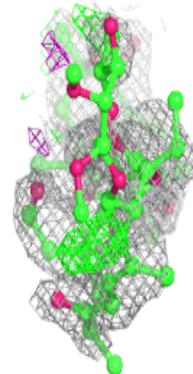
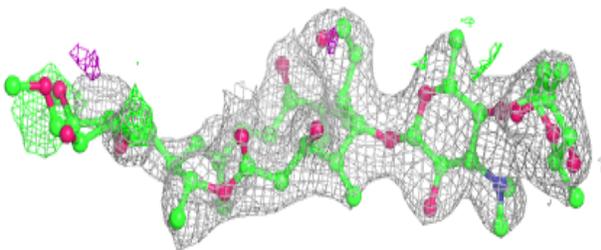
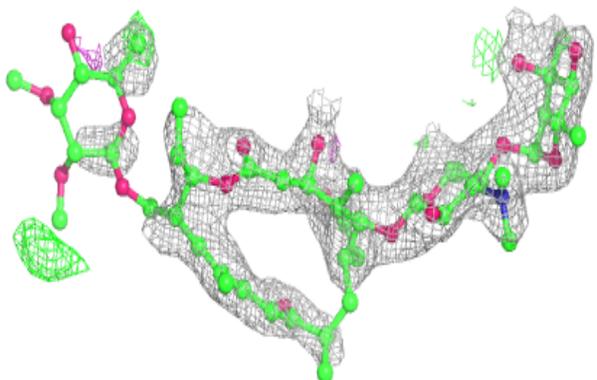


Electron density around TYK J 401:

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

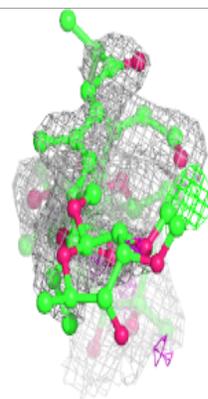
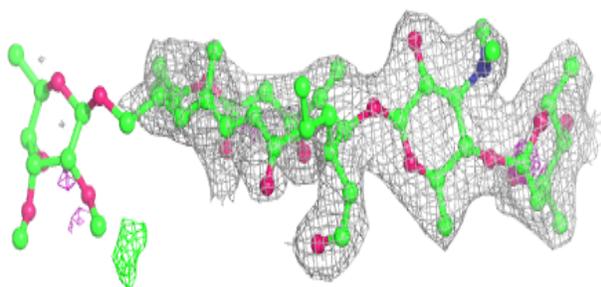
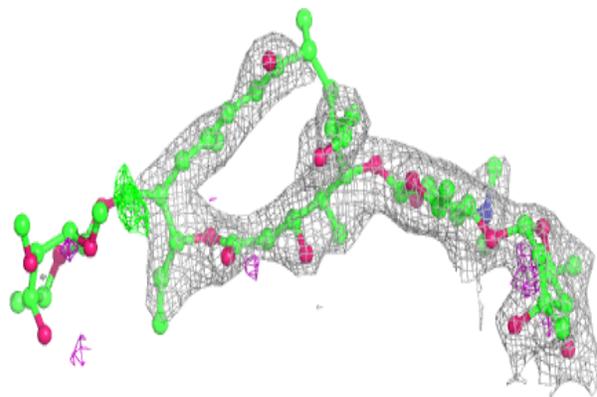
**Electron density around TYK M 401:**

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

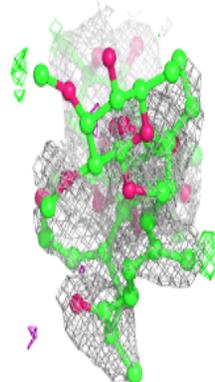
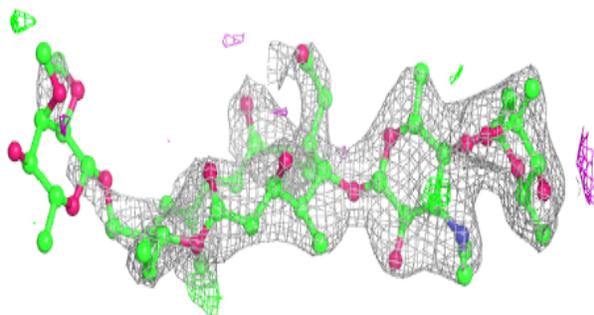
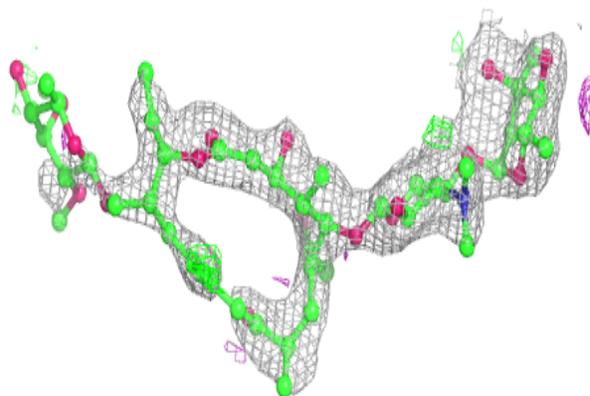


Electron density around TYK O 401:

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

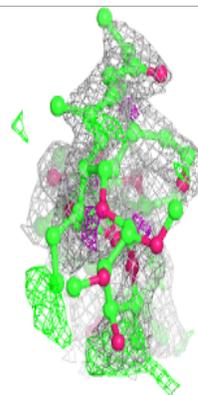
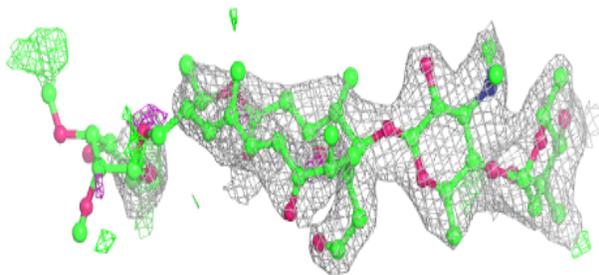
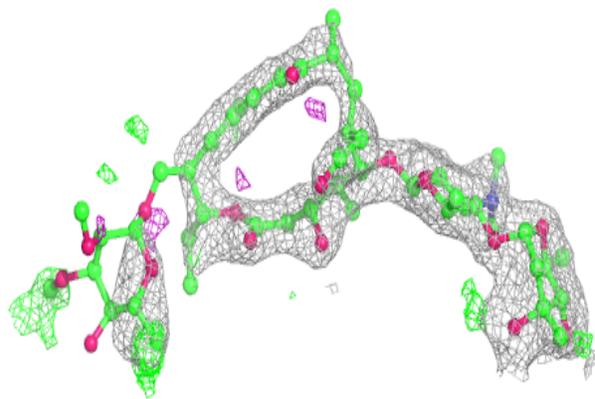
**Electron density around TYK K 401:**

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

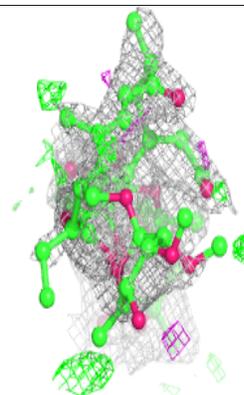
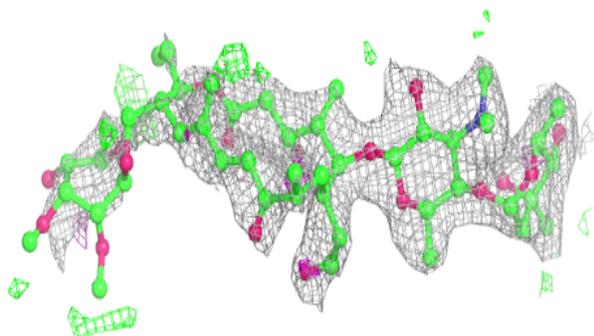
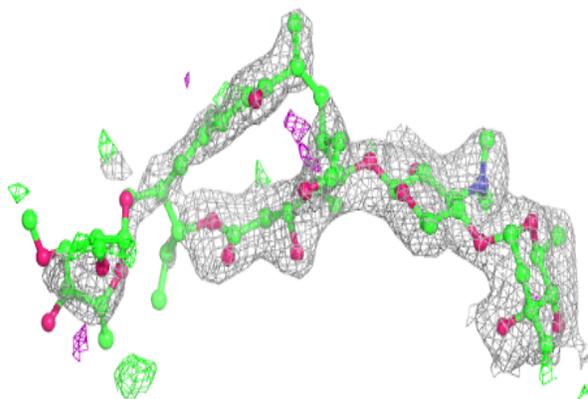


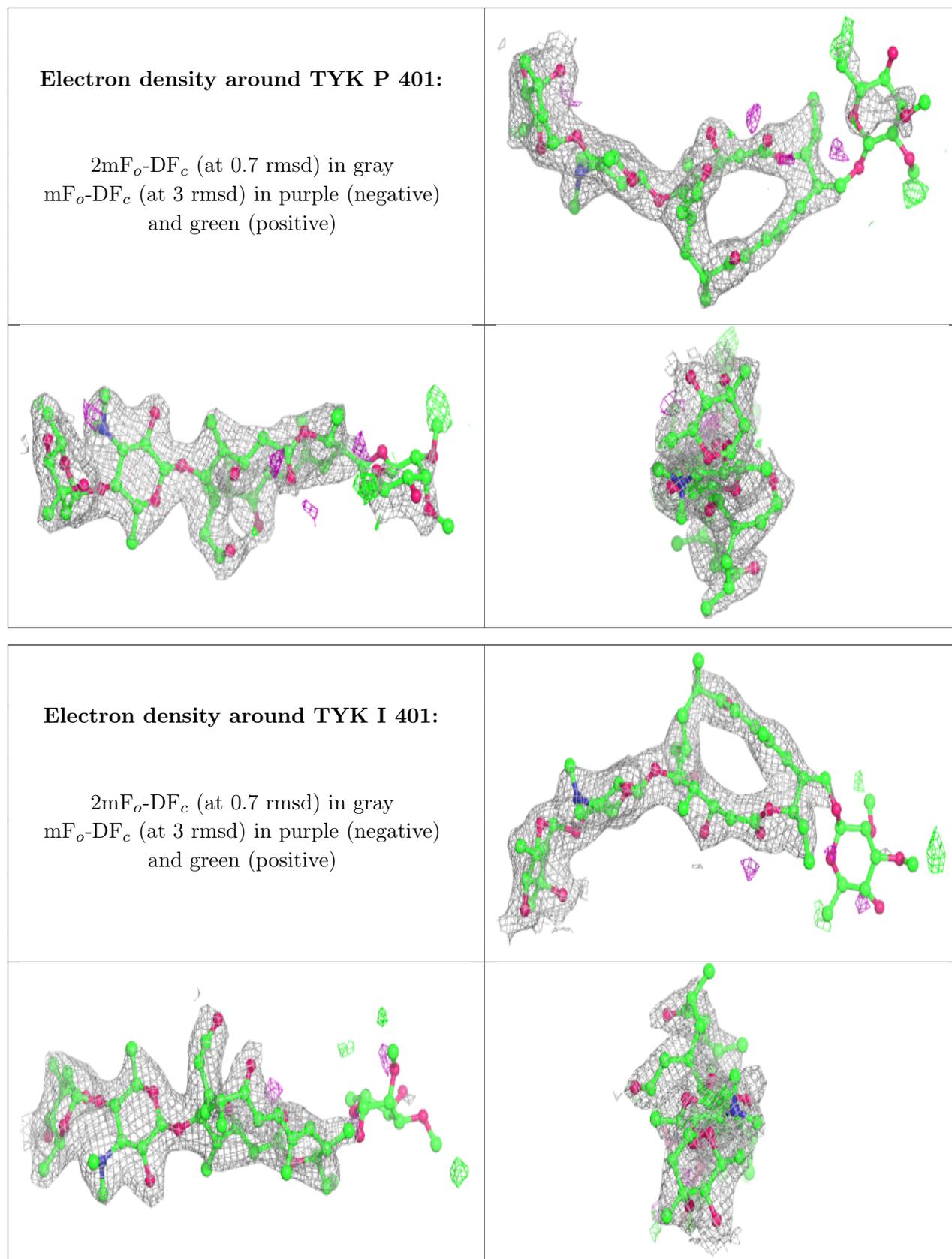
Electron density around TYK L 401:

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

**Electron density around TYK N 401:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.