



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 08:54 pm BST

PDB ID : 6HNQ  
Title : TarP-6RboP-(CH<sub>2</sub>)<sub>6</sub>NH<sub>2</sub>  
Authors : Guo, Y.; Stehle, T.  
Deposited on : 2018-09-17  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.11  
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) : 2.11

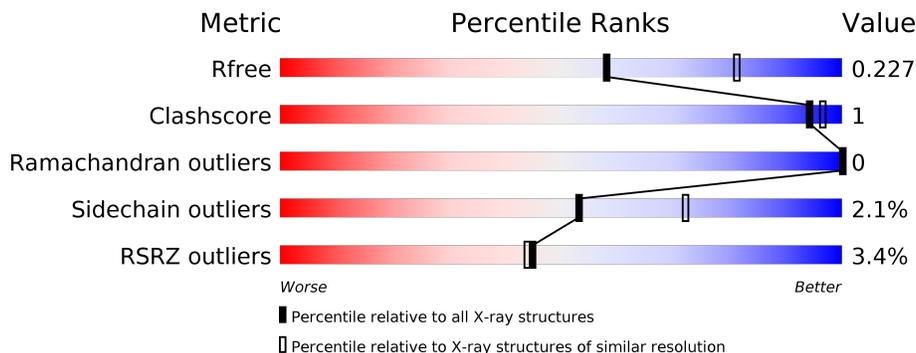
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	345	
1	B	345	
1	C	345	
1	D	345	
1	E	345	
1	F	345	

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Mol	Chain	Length	Quality of chain
1	G	345	<p>88% 9%</p>
1	H	345	<p>86% 5% 8%</p>
1	I	345	<p>2% 89% 9%</p>
1	O	345	<p>89% 8%</p>
1	P	345	<p>19% 81% 13%</p>
1	Q	345	<p>12% 88% 9%</p>

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 31221 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 Probable ss-1,3-N-acetylglucosaminyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	318	Total 2535	C 1632	N 423	O 472	S 8	0	0	0
1	C	312	Total 2451	C 1580	N 403	O 460	S 8	0	0	0
1	F	317	Total 2493	C 1602	N 413	O 470	S 8	0	0	0
1	O	316	Total 2496	C 1606	N 412	O 470	S 8	0	0	0
1	P	300	Total 2074	C 1330	N 357	O 382	S 5	0	0	0
1	E	317	Total 2512	C 1615	N 419	O 470	S 8	0	1	0
1	G	314	Total 2481	C 1589	N 415	O 469	S 8	0	0	0
1	Q	315	Total 2272	C 1450	N 385	O 429	S 8	0	0	0
1	A	317	Total 2507	C 1611	N 416	O 472	S 8	0	0	0
1	D	314	Total 2479	C 1593	N 411	O 467	S 8	0	0	0
1	H	318	Total 2536	C 1631	N 424	O 473	S 8	0	0	0
1	I	314	Total 2448	C 1572	N 408	O 460	S 8	0	0	0

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	initiating methionine	UNP A0A0H3JNB0
B	-16	ARG	-	expression tag	UNP A0A0H3JNB0
B	-15	GLY	-	expression tag	UNP A0A0H3JNB0
B	-14	SER	-	expression tag	UNP A0A0H3JNB0
B	-13	HIS	-	expression tag	UNP A0A0H3JNB0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP A0A0H3JNB0
B	-11	HIS	-	expression tag	UNP A0A0H3JNB0
B	-10	HIS	-	expression tag	UNP A0A0H3JNB0
B	-9	HIS	-	expression tag	UNP A0A0H3JNB0
B	-8	HIS	-	expression tag	UNP A0A0H3JNB0
B	-7	GLY	-	expression tag	UNP A0A0H3JNB0
B	-6	SER	-	expression tag	UNP A0A0H3JNB0
B	-5	LEU	-	expression tag	UNP A0A0H3JNB0
B	-4	VAL	-	expression tag	UNP A0A0H3JNB0
B	-3	PRO	-	expression tag	UNP A0A0H3JNB0
B	-2	ARG	-	expression tag	UNP A0A0H3JNB0
B	-1	GLY	-	expression tag	UNP A0A0H3JNB0
B	0	SER	-	expression tag	UNP A0A0H3JNB0
C	-17	MET	-	initiating methionine	UNP A0A0H3JNB0
C	-16	ARG	-	expression tag	UNP A0A0H3JNB0
C	-15	GLY	-	expression tag	UNP A0A0H3JNB0
C	-14	SER	-	expression tag	UNP A0A0H3JNB0
C	-13	HIS	-	expression tag	UNP A0A0H3JNB0
C	-12	HIS	-	expression tag	UNP A0A0H3JNB0
C	-11	HIS	-	expression tag	UNP A0A0H3JNB0
C	-10	HIS	-	expression tag	UNP A0A0H3JNB0
C	-9	HIS	-	expression tag	UNP A0A0H3JNB0
C	-8	HIS	-	expression tag	UNP A0A0H3JNB0
C	-7	GLY	-	expression tag	UNP A0A0H3JNB0
C	-6	SER	-	expression tag	UNP A0A0H3JNB0
C	-5	LEU	-	expression tag	UNP A0A0H3JNB0
C	-4	VAL	-	expression tag	UNP A0A0H3JNB0
C	-3	PRO	-	expression tag	UNP A0A0H3JNB0
C	-2	ARG	-	expression tag	UNP A0A0H3JNB0
C	-1	GLY	-	expression tag	UNP A0A0H3JNB0
C	0	SER	-	expression tag	UNP A0A0H3JNB0
F	-17	MET	-	initiating methionine	UNP A0A0H3JNB0
F	-16	ARG	-	expression tag	UNP A0A0H3JNB0
F	-15	GLY	-	expression tag	UNP A0A0H3JNB0
F	-14	SER	-	expression tag	UNP A0A0H3JNB0
F	-13	HIS	-	expression tag	UNP A0A0H3JNB0
F	-12	HIS	-	expression tag	UNP A0A0H3JNB0
F	-11	HIS	-	expression tag	UNP A0A0H3JNB0
F	-10	HIS	-	expression tag	UNP A0A0H3JNB0
F	-9	HIS	-	expression tag	UNP A0A0H3JNB0
F	-8	HIS	-	expression tag	UNP A0A0H3JNB0
F	-7	GLY	-	expression tag	UNP A0A0H3JNB0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-6	SER	-	expression tag	UNP A0A0H3JNB0
F	-5	LEU	-	expression tag	UNP A0A0H3JNB0
F	-4	VAL	-	expression tag	UNP A0A0H3JNB0
F	-3	PRO	-	expression tag	UNP A0A0H3JNB0
F	-2	ARG	-	expression tag	UNP A0A0H3JNB0
F	-1	GLY	-	expression tag	UNP A0A0H3JNB0
F	0	SER	-	expression tag	UNP A0A0H3JNB0
O	-17	MET	-	initiating methionine	UNP A0A0H3JNB0
O	-16	ARG	-	expression tag	UNP A0A0H3JNB0
O	-15	GLY	-	expression tag	UNP A0A0H3JNB0
O	-14	SER	-	expression tag	UNP A0A0H3JNB0
O	-13	HIS	-	expression tag	UNP A0A0H3JNB0
O	-12	HIS	-	expression tag	UNP A0A0H3JNB0
O	-11	HIS	-	expression tag	UNP A0A0H3JNB0
O	-10	HIS	-	expression tag	UNP A0A0H3JNB0
O	-9	HIS	-	expression tag	UNP A0A0H3JNB0
O	-8	HIS	-	expression tag	UNP A0A0H3JNB0
O	-7	GLY	-	expression tag	UNP A0A0H3JNB0
O	-6	SER	-	expression tag	UNP A0A0H3JNB0
O	-5	LEU	-	expression tag	UNP A0A0H3JNB0
O	-4	VAL	-	expression tag	UNP A0A0H3JNB0
O	-3	PRO	-	expression tag	UNP A0A0H3JNB0
O	-2	ARG	-	expression tag	UNP A0A0H3JNB0
O	-1	GLY	-	expression tag	UNP A0A0H3JNB0
O	0	SER	-	expression tag	UNP A0A0H3JNB0
P	-17	MET	-	initiating methionine	UNP A0A0H3JNB0
P	-16	ARG	-	expression tag	UNP A0A0H3JNB0
P	-15	GLY	-	expression tag	UNP A0A0H3JNB0
P	-14	SER	-	expression tag	UNP A0A0H3JNB0
P	-13	HIS	-	expression tag	UNP A0A0H3JNB0
P	-12	HIS	-	expression tag	UNP A0A0H3JNB0
P	-11	HIS	-	expression tag	UNP A0A0H3JNB0
P	-10	HIS	-	expression tag	UNP A0A0H3JNB0
P	-9	HIS	-	expression tag	UNP A0A0H3JNB0
P	-8	HIS	-	expression tag	UNP A0A0H3JNB0
P	-7	GLY	-	expression tag	UNP A0A0H3JNB0
P	-6	SER	-	expression tag	UNP A0A0H3JNB0
P	-5	LEU	-	expression tag	UNP A0A0H3JNB0
P	-4	VAL	-	expression tag	UNP A0A0H3JNB0
P	-3	PRO	-	expression tag	UNP A0A0H3JNB0
P	-2	ARG	-	expression tag	UNP A0A0H3JNB0
P	-1	GLY	-	expression tag	UNP A0A0H3JNB0

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Chain	Residue	Modelled	Actual	Comment	Reference
P	0	SER	-	expression tag	UNP A0A0H3JNB0
E	-17	MET	-	initiating methionine	UNP A0A0H3JNB0
E	-16	ARG	-	expression tag	UNP A0A0H3JNB0
E	-15	GLY	-	expression tag	UNP A0A0H3JNB0
E	-14	SER	-	expression tag	UNP A0A0H3JNB0
E	-13	HIS	-	expression tag	UNP A0A0H3JNB0
E	-12	HIS	-	expression tag	UNP A0A0H3JNB0
E	-11	HIS	-	expression tag	UNP A0A0H3JNB0
E	-10	HIS	-	expression tag	UNP A0A0H3JNB0
E	-9	HIS	-	expression tag	UNP A0A0H3JNB0
E	-8	HIS	-	expression tag	UNP A0A0H3JNB0
E	-7	GLY	-	expression tag	UNP A0A0H3JNB0
E	-6	SER	-	expression tag	UNP A0A0H3JNB0
E	-5	LEU	-	expression tag	UNP A0A0H3JNB0
E	-4	VAL	-	expression tag	UNP A0A0H3JNB0
E	-3	PRO	-	expression tag	UNP A0A0H3JNB0
E	-2	ARG	-	expression tag	UNP A0A0H3JNB0
E	-1	GLY	-	expression tag	UNP A0A0H3JNB0
E	0	SER	-	expression tag	UNP A0A0H3JNB0
G	-17	MET	-	initiating methionine	UNP A0A0H3JNB0
G	-16	ARG	-	expression tag	UNP A0A0H3JNB0
G	-15	GLY	-	expression tag	UNP A0A0H3JNB0
G	-14	SER	-	expression tag	UNP A0A0H3JNB0
G	-13	HIS	-	expression tag	UNP A0A0H3JNB0
G	-12	HIS	-	expression tag	UNP A0A0H3JNB0
G	-11	HIS	-	expression tag	UNP A0A0H3JNB0
G	-10	HIS	-	expression tag	UNP A0A0H3JNB0
G	-9	HIS	-	expression tag	UNP A0A0H3JNB0
G	-8	HIS	-	expression tag	UNP A0A0H3JNB0
G	-7	GLY	-	expression tag	UNP A0A0H3JNB0
G	-6	SER	-	expression tag	UNP A0A0H3JNB0
G	-5	LEU	-	expression tag	UNP A0A0H3JNB0
G	-4	VAL	-	expression tag	UNP A0A0H3JNB0
G	-3	PRO	-	expression tag	UNP A0A0H3JNB0
G	-2	ARG	-	expression tag	UNP A0A0H3JNB0
G	-1	GLY	-	expression tag	UNP A0A0H3JNB0
G	0	SER	-	expression tag	UNP A0A0H3JNB0
Q	-17	MET	-	initiating methionine	UNP A0A0H3JNB0
Q	-16	ARG	-	expression tag	UNP A0A0H3JNB0
Q	-15	GLY	-	expression tag	UNP A0A0H3JNB0
Q	-14	SER	-	expression tag	UNP A0A0H3JNB0
Q	-13	HIS	-	expression tag	UNP A0A0H3JNB0

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-12	HIS	-	expression tag	UNP A0A0H3JNB0
Q	-11	HIS	-	expression tag	UNP A0A0H3JNB0
Q	-10	HIS	-	expression tag	UNP A0A0H3JNB0
Q	-9	HIS	-	expression tag	UNP A0A0H3JNB0
Q	-8	HIS	-	expression tag	UNP A0A0H3JNB0
Q	-7	GLY	-	expression tag	UNP A0A0H3JNB0
Q	-6	SER	-	expression tag	UNP A0A0H3JNB0
Q	-5	LEU	-	expression tag	UNP A0A0H3JNB0
Q	-4	VAL	-	expression tag	UNP A0A0H3JNB0
Q	-3	PRO	-	expression tag	UNP A0A0H3JNB0
Q	-2	ARG	-	expression tag	UNP A0A0H3JNB0
Q	-1	GLY	-	expression tag	UNP A0A0H3JNB0
Q	0	SER	-	expression tag	UNP A0A0H3JNB0
A	-17	MET	-	initiating methionine	UNP A0A0H3JNB0
A	-16	ARG	-	expression tag	UNP A0A0H3JNB0
A	-15	GLY	-	expression tag	UNP A0A0H3JNB0
A	-14	SER	-	expression tag	UNP A0A0H3JNB0
A	-13	HIS	-	expression tag	UNP A0A0H3JNB0
A	-12	HIS	-	expression tag	UNP A0A0H3JNB0
A	-11	HIS	-	expression tag	UNP A0A0H3JNB0
A	-10	HIS	-	expression tag	UNP A0A0H3JNB0
A	-9	HIS	-	expression tag	UNP A0A0H3JNB0
A	-8	HIS	-	expression tag	UNP A0A0H3JNB0
A	-7	GLY	-	expression tag	UNP A0A0H3JNB0
A	-6	SER	-	expression tag	UNP A0A0H3JNB0
A	-5	LEU	-	expression tag	UNP A0A0H3JNB0
A	-4	VAL	-	expression tag	UNP A0A0H3JNB0
A	-3	PRO	-	expression tag	UNP A0A0H3JNB0
A	-2	ARG	-	expression tag	UNP A0A0H3JNB0
A	-1	GLY	-	expression tag	UNP A0A0H3JNB0
A	0	SER	-	expression tag	UNP A0A0H3JNB0
D	-17	MET	-	initiating methionine	UNP A0A0H3JNB0
D	-16	ARG	-	expression tag	UNP A0A0H3JNB0
D	-15	GLY	-	expression tag	UNP A0A0H3JNB0
D	-14	SER	-	expression tag	UNP A0A0H3JNB0
D	-13	HIS	-	expression tag	UNP A0A0H3JNB0
D	-12	HIS	-	expression tag	UNP A0A0H3JNB0
D	-11	HIS	-	expression tag	UNP A0A0H3JNB0
D	-10	HIS	-	expression tag	UNP A0A0H3JNB0
D	-9	HIS	-	expression tag	UNP A0A0H3JNB0
D	-8	HIS	-	expression tag	UNP A0A0H3JNB0
D	-7	GLY	-	expression tag	UNP A0A0H3JNB0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	SER	-	expression tag	UNP A0A0H3JNB0
D	-5	LEU	-	expression tag	UNP A0A0H3JNB0
D	-4	VAL	-	expression tag	UNP A0A0H3JNB0
D	-3	PRO	-	expression tag	UNP A0A0H3JNB0
D	-2	ARG	-	expression tag	UNP A0A0H3JNB0
D	-1	GLY	-	expression tag	UNP A0A0H3JNB0
D	0	SER	-	expression tag	UNP A0A0H3JNB0
H	-17	MET	-	initiating methionine	UNP A0A0H3JNB0
H	-16	ARG	-	expression tag	UNP A0A0H3JNB0
H	-15	GLY	-	expression tag	UNP A0A0H3JNB0
H	-14	SER	-	expression tag	UNP A0A0H3JNB0
H	-13	HIS	-	expression tag	UNP A0A0H3JNB0
H	-12	HIS	-	expression tag	UNP A0A0H3JNB0
H	-11	HIS	-	expression tag	UNP A0A0H3JNB0
H	-10	HIS	-	expression tag	UNP A0A0H3JNB0
H	-9	HIS	-	expression tag	UNP A0A0H3JNB0
H	-8	HIS	-	expression tag	UNP A0A0H3JNB0
H	-7	GLY	-	expression tag	UNP A0A0H3JNB0
H	-6	SER	-	expression tag	UNP A0A0H3JNB0
H	-5	LEU	-	expression tag	UNP A0A0H3JNB0
H	-4	VAL	-	expression tag	UNP A0A0H3JNB0
H	-3	PRO	-	expression tag	UNP A0A0H3JNB0
H	-2	ARG	-	expression tag	UNP A0A0H3JNB0
H	-1	GLY	-	expression tag	UNP A0A0H3JNB0
H	0	SER	-	expression tag	UNP A0A0H3JNB0
I	-17	MET	-	initiating methionine	UNP A0A0H3JNB0
I	-16	ARG	-	expression tag	UNP A0A0H3JNB0
I	-15	GLY	-	expression tag	UNP A0A0H3JNB0
I	-14	SER	-	expression tag	UNP A0A0H3JNB0
I	-13	HIS	-	expression tag	UNP A0A0H3JNB0
I	-12	HIS	-	expression tag	UNP A0A0H3JNB0
I	-11	HIS	-	expression tag	UNP A0A0H3JNB0
I	-10	HIS	-	expression tag	UNP A0A0H3JNB0
I	-9	HIS	-	expression tag	UNP A0A0H3JNB0
I	-8	HIS	-	expression tag	UNP A0A0H3JNB0
I	-7	GLY	-	expression tag	UNP A0A0H3JNB0
I	-6	SER	-	expression tag	UNP A0A0H3JNB0
I	-5	LEU	-	expression tag	UNP A0A0H3JNB0
I	-4	VAL	-	expression tag	UNP A0A0H3JNB0
I	-3	PRO	-	expression tag	UNP A0A0H3JNB0
I	-2	ARG	-	expression tag	UNP A0A0H3JNB0
I	-1	GLY	-	expression tag	UNP A0A0H3JNB0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	O	P	0	0
			40	15	22	3		
2	H	1	Total	C	O	P	0	0
			40	15	22	3		
2	I	1	Total	C	O	P	0	0
			40	15	22	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Cl	0	0
			1	1		
4	Q	1	Total	Cl	0	0
			1	1		
4	D	2	Total	Cl	0	0
			2	2		
4	E	2	Total	Cl	0	0
			2	2		
4	H	3	Total	Cl	0	0
			3	3		
4	B	5	Total	Cl	0	0
			5	5		
4	I	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	B	165	Total 165	O 165	0	0
5	C	114	Total 114	O 114	0	0
5	F	132	Total 132	O 132	0	0
5	O	138	Total 138	O 138	0	0
5	P	47	Total 47	O 47	0	0
5	E	124	Total 124	O 124	0	0
5	G	133	Total 133	O 133	0	0
5	Q	64	Total 64	O 64	0	0
5	A	124	Total 124	O 124	0	0
5	D	113	Total 113	O 113	0	0
5	H	168	Total 168	O 168	0	0
5	I	114	Total 114	O 114	0	0







- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

Chain D: 87% 9%



- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

Chain H: 86% 5% 8%



- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

Chain I: 2% 89% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.41Å 211.25Å 122.68Å 90.00° 91.61° 90.00°	Depositor
Resolution (Å)	48.51 – 2.40 48.51 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.51-2.40) 100.0 (48.51-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, $R_{free}$	0.184 , 0.228 0.187 , 0.227	Depositor DCC
$R_{free}$ test set	9436 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	31221	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FQ8, CL

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	0.66	0/2550	0.71	1/3437 (0.0%)
1	B	0.64	1/2578 (0.0%)	0.73	1/3466 (0.0%)
1	C	0.63	0/2492	0.68	0/3361
1	D	0.65	1/2521 (0.0%)	0.70	0/3400
1	E	0.67	0/2558	0.76	4/3448 (0.1%)
1	F	0.65	0/2535	0.78	5/3417 (0.1%)
1	G	0.64	0/2523	0.70	1/3402 (0.0%)
1	H	0.64	0/2579	0.75	3/3470 (0.1%)
1	I	0.62	0/2489	0.70	0/3358
1	O	0.63	0/2539	0.70	0/3424
1	P	0.73	1/2100 (0.0%)	0.78	2/2847 (0.1%)
1	Q	0.68	1/2307 (0.0%)	0.75	2/3128 (0.1%)
All	All	0.65	4/29771 (0.0%)	0.73	19/40158 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	180	GLU	CD-OE2	-10.47	1.14	1.25
1	B	180	GLU	CD-OE2	-6.11	1.19	1.25
1	D	180	GLU	CD-OE1	-5.85	1.19	1.25
1	Q	122	GLY	C-O	-5.76	1.14	1.23

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	259	ARG	NE-CZ-NH1	-13.26	113.67	120.30
1	P	104	ASP	CB-CG-OD1	-8.91	110.28	118.30
1	Q	61	ARG	NE-CZ-NH2	8.77	124.69	120.30
1	F	259	ARG	NE-CZ-NH2	8.54	124.57	120.30
1	E	262	ARG	CG-CD-NE	-7.78	95.47	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	100	ARG	Sidechain
1	F	259	ARG	Sidechain

## 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	2507	0	2453	5	0
1	B	2535	0	2520	8	0
1	C	2451	0	2382	8	0
1	D	2479	0	2424	4	0
1	E	2512	0	2464	11	0
1	F	2493	0	2423	7	0
1	G	2481	0	2419	3	0
1	H	2536	0	2511	11	0
1	I	2448	0	2365	1	0
1	O	2496	0	2426	4	0
1	P	2074	0	1703	10	0
1	Q	2272	0	1982	4	0
2	A	40	0	0	0	0
2	B	40	0	0	0	0
2	C	40	0	0	1	0
2	D	40	0	0	0	0
2	E	40	0	0	2	0
2	F	40	0	0	1	0
2	G	40	0	0	0	0
2	H	40	0	0	1	0
2	I	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	40	0	0	0	0
2	P	40	0	0	0	0
2	Q	40	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	I	1	0	0	0	0
4	A	1	0	0	0	0
4	B	5	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	1	0
4	G	1	0	0	0	0
4	H	3	0	0	0	0
4	I	1	0	0	0	0
4	Q	1	0	0	0	0
5	A	124	0	0	0	0
5	B	165	0	0	0	0
5	C	114	0	0	0	0
5	D	113	0	0	0	0
5	E	124	0	0	0	0
5	F	132	0	0	0	0
5	G	133	0	0	0	0
5	H	168	0	0	0	0
5	I	114	0	0	0	0
5	O	138	0	0	0	0
5	P	47	0	0	0	0
5	Q	64	0	0	0	0
All	All	31221	0	28072	73	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 1.

The worst 5 of 73 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:H:175:PHE:HE1	1:H:229:THR:HG1	1.33	0.77
1:P:100:ARG:O	1:P:104:ASP:HB2	1.86	0.74
1:B:198:LYS:HE2	1:B:200:ASP:OD2	1.92	0.68
1:P:112:ASN:OD1	1:P:141:ALA:HB1	1.95	0.66
1:E:262:ARG:NH2	2:E:401:FQ8:OAO	2.33	0.61

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	313/345 (91%)	304 (97%)	9 (3%)	0	100	100
1	B	314/345 (91%)	306 (98%)	8 (2%)	0	100	100
1	C	306/345 (89%)	300 (98%)	6 (2%)	0	100	100
1	D	310/345 (90%)	303 (98%)	7 (2%)	0	100	100
1	E	314/345 (91%)	305 (97%)	9 (3%)	0	100	100
1	F	313/345 (91%)	306 (98%)	7 (2%)	0	100	100
1	G	310/345 (90%)	303 (98%)	7 (2%)	0	100	100
1	H	314/345 (91%)	306 (98%)	8 (2%)	0	100	100
1	I	310/345 (90%)	303 (98%)	7 (2%)	0	100	100
1	O	312/345 (90%)	305 (98%)	7 (2%)	0	100	100
1	P	288/345 (84%)	282 (98%)	6 (2%)	0	100	100
1	Q	311/345 (90%)	300 (96%)	11 (4%)	0	100	100
All	All	3715/4140 (90%)	3623 (98%)	92 (2%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	260/313 (83%)	254 (98%)	6 (2%)	50	70
1	B	265/313 (85%)	260 (98%)	5 (2%)	57	75
1	C	250/313 (80%)	244 (98%)	6 (2%)	49	68
1	D	256/313 (82%)	250 (98%)	6 (2%)	50	70
1	E	260/313 (83%)	257 (99%)	3 (1%)	71	85
1	F	254/313 (81%)	249 (98%)	5 (2%)	55	74
1	G	258/313 (82%)	254 (98%)	4 (2%)	62	79
1	H	264/313 (84%)	260 (98%)	4 (2%)	65	80
1	I	246/313 (79%)	240 (98%)	6 (2%)	49	68
1	O	255/313 (82%)	252 (99%)	3 (1%)	71	85
1	P	143/313 (46%)	135 (94%)	8 (6%)	21	34
1	Q	184/313 (59%)	180 (98%)	4 (2%)	52	71
All	All	2895/3756 (77%)	2835 (98%)	60 (2%)	53	72

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

Mol	Chain	Res	Type
1	E	100	ARG
1	G	286	PHE
1	I	64	GLN
1	G	64	GLN
1	Q	43	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	231	ASN
1	I	46	ASN
1	I	51	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 21 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FQ8	B	401	-	39,39,39	1.55	4 (10%)	54,56,56	1.05	3 (5%)
2	FQ8	Q	401	-	39,39,39	1.12	3 (7%)	54,56,56	0.88	1 (1%)
2	FQ8	D	401	-	39,39,39	1.19	3 (7%)	54,56,56	0.93	1 (1%)
2	FQ8	E	401	-	39,39,39	1.23	3 (7%)	54,56,56	0.95	3 (5%)
2	FQ8	H	401	-	39,39,39	1.40	2 (5%)	54,56,56	0.73	1 (1%)
2	FQ8	G	401	-	39,39,39	1.22	2 (5%)	54,56,56	0.94	2 (3%)
2	FQ8	A	401	-	39,39,39	1.22	4 (10%)	54,56,56	1.10	3 (5%)
2	FQ8	C	401	-	39,39,39	1.16	3 (7%)	54,56,56	1.05	4 (7%)
2	FQ8	P	401	-	39,39,39	1.16	2 (5%)	54,56,56	0.96	2 (3%)
2	FQ8	O	401	-	39,39,39	1.21	2 (5%)	54,56,56	1.07	4 (7%)
2	FQ8	I	401	-	39,39,39	1.21	3 (7%)	54,56,56	1.02	2 (3%)
2	FQ8	F	401	-	39,39,39	1.17	2 (5%)	54,56,56	1.17	5 (9%)

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	FQ8	B	401	-	-	28/56/56/56	-
2	FQ8	Q	401	-	-	36/56/56/56	-
2	FQ8	D	401	-	-	35/56/56/56	-
2	FQ8	E	401	-	-	30/56/56/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FQ8	H	401	-	-	24/56/56/56	-
2	FQ8	G	401	-	-	42/56/56/56	-
2	FQ8	A	401	-	-	36/56/56/56	-
2	FQ8	C	401	-	-	35/56/56/56	-
2	FQ8	P	401	-	-	31/56/56/56	-
2	FQ8	O	401	-	-	35/56/56/56	-
2	FQ8	I	401	-	-	29/56/56/56	-
2	FQ8	F	401	-	-	32/56/56/56	-

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	FQ8	PBL-OAN	6.53	1.71	1.50
2	H	401	FQ8	PBL-OAN	5.39	1.67	1.50
2	O	401	FQ8	PBL-OAN	4.90	1.66	1.50
2	G	401	FQ8	PBL-OAN	4.74	1.65	1.50
2	F	401	FQ8	PBL-OAN	4.66	1.65	1.50

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	FQ8	OAA-PBL-OAX	3.65	116.46	106.73
2	I	401	FQ8	OAA-PBL-OAX	3.34	115.63	106.73
2	A	401	FQ8	OAD-CAR-CBC	-3.23	104.03	111.07
2	C	401	FQ8	OAA-PBL-OAX	3.14	115.10	106.73
2	A	401	FQ8	OAA-PBL-OAX	3.07	114.89	106.73

There are no chirality outliers.

5 of 393 torsion outliers are listed below:

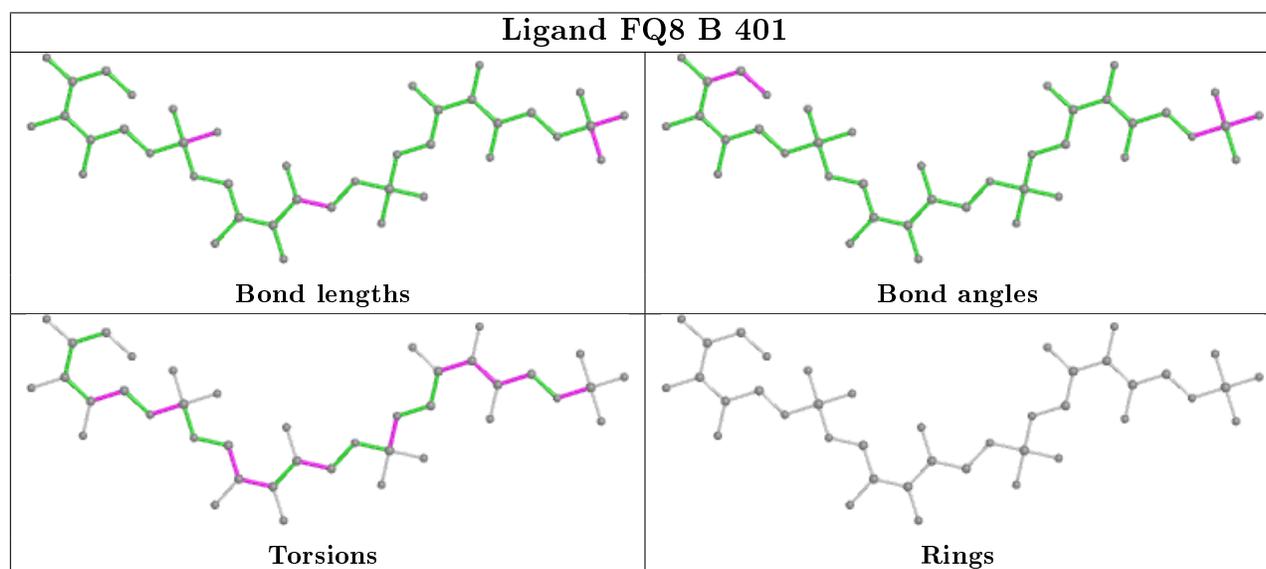
Mol	Chain	Res	Type	Atoms
2	G	401	FQ8	CAS-OAX-PBL-OAO
2	G	401	FQ8	CAS-OAX-PBL-OAA
2	G	401	FQ8	CAS-CBE-CBJ-OAL
2	G	401	FQ8	OAZ-CAU-CBF-CBJ
2	G	401	FQ8	OAZ-CAU-CBF-OAH

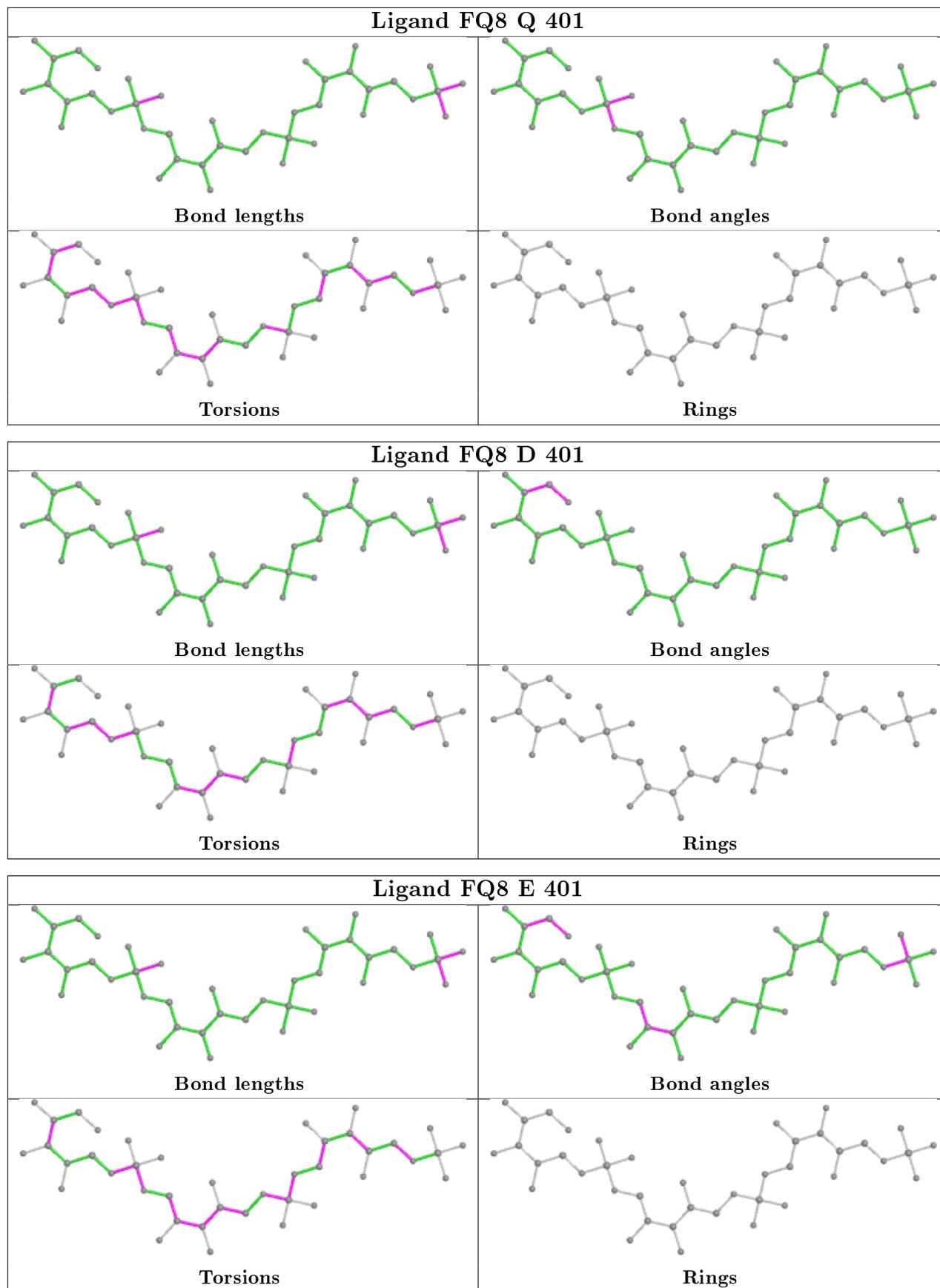
There are no ring outliers.

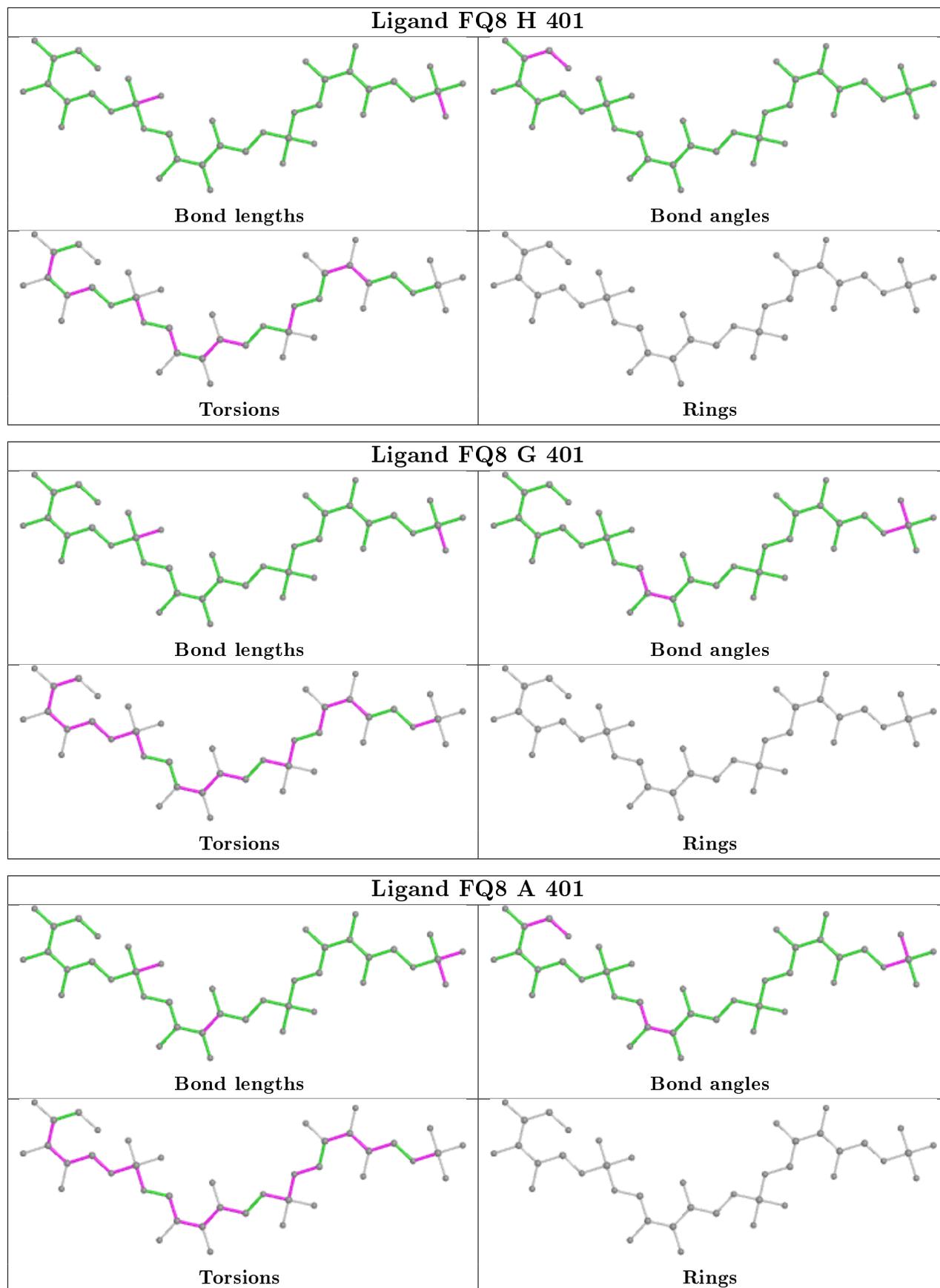
4 monomers are involved in 5 short contacts:

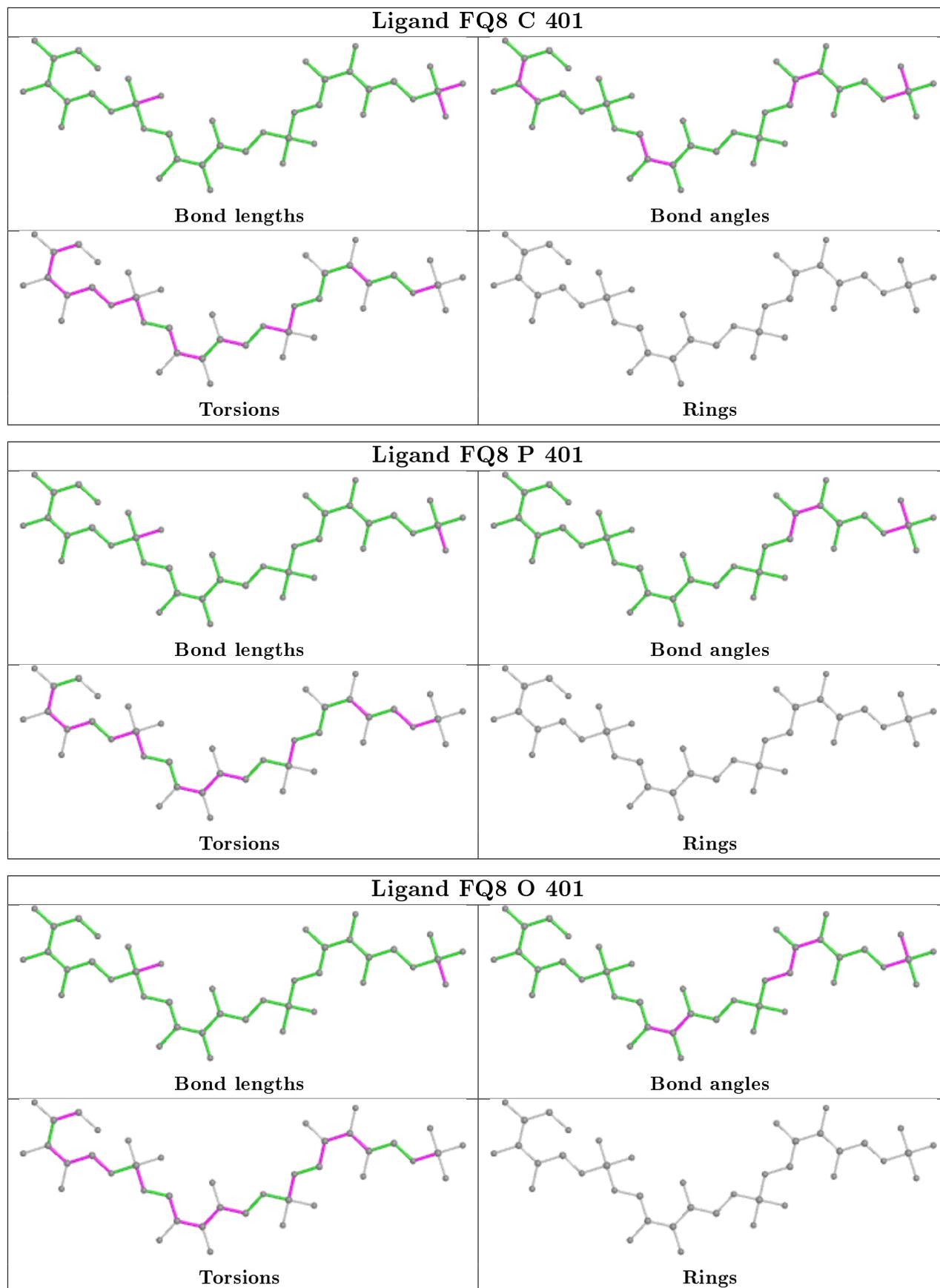
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	FQ8	2	0
2	H	401	FQ8	1	0
2	C	401	FQ8	1	0
2	F	401	FQ8	1	0

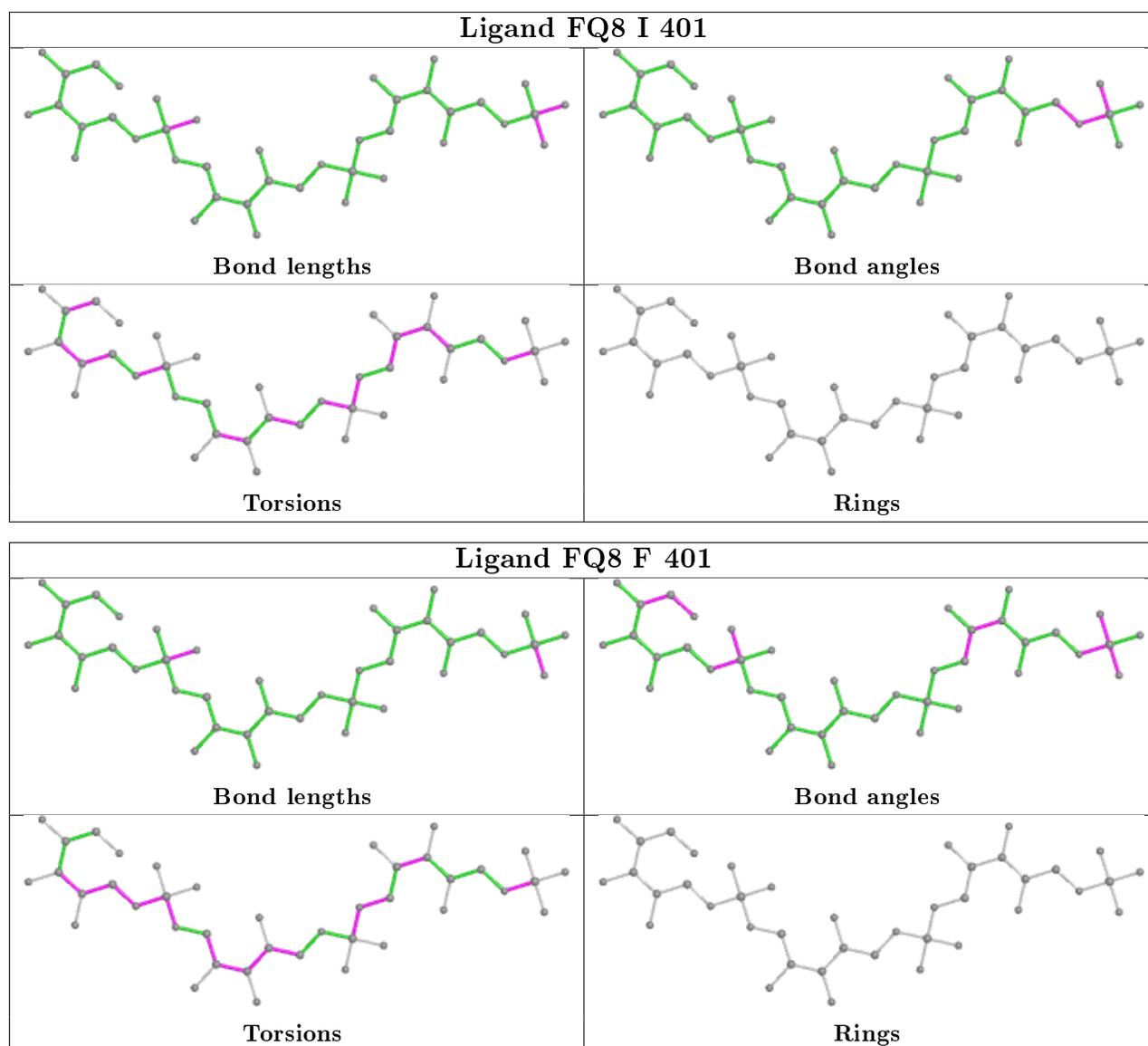
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	317/345 (91%)	-0.34	2 (0%) 89 88	30, 44, 75, 121	0
1	B	318/345 (92%)	-0.40	0 100 100	27, 40, 65, 94	0
1	C	312/345 (90%)	-0.19	4 (1%) 77 75	29, 49, 84, 100	0
1	D	314/345 (91%)	-0.45	1 (0%) 94 93	33, 49, 72, 120	0
1	E	317/345 (91%)	-0.33	0 100 100	29, 44, 76, 112	0
1	F	317/345 (91%)	-0.23	1 (0%) 94 93	32, 45, 70, 106	0
1	G	314/345 (91%)	-0.37	3 (0%) 82 80	34, 48, 74, 118	0
1	H	318/345 (92%)	-0.42	0 100 100	27, 39, 64, 91	0
1	I	314/345 (91%)	-0.09	8 (2%) 57 55	31, 52, 92, 115	0
1	O	316/345 (91%)	-0.27	1 (0%) 94 93	29, 43, 69, 98	0
1	P	300/345 (86%)	0.83	66 (22%) 0 0	45, 83, 138, 164	0
1	Q	315/345 (91%)	0.40	43 (13%) 3 2	38, 70, 129, 153	0
All	All	3772/4140 (91%)	-0.16	129 (3%) 45 44	27, 48, 101, 164	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	26	ASN	7.8
1	Q	24	VAL	7.4
1	P	197	ILE	5.8
1	I	128	ARG	5.6
1	Q	59	LEU	5.6

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

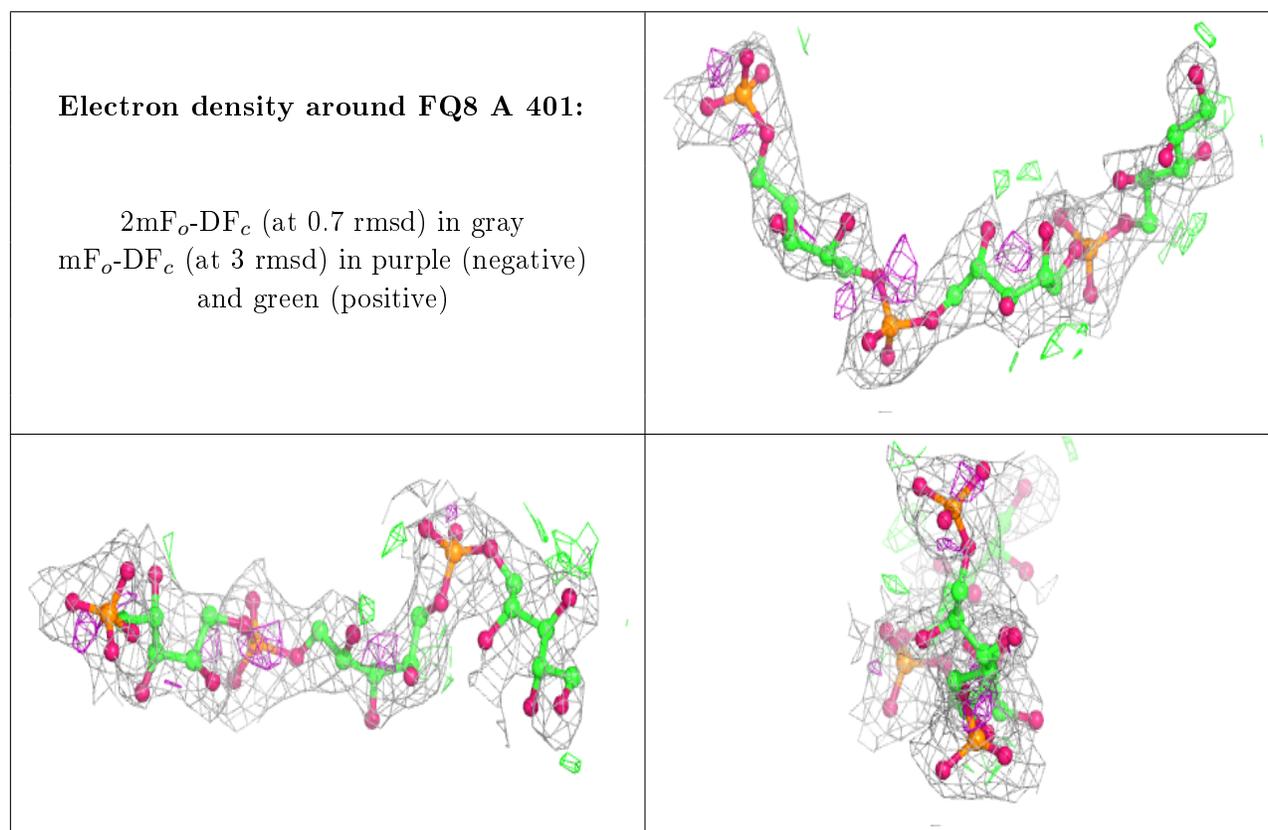
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	D	402	1/1	0.80	0.27	71,71,71,71	0
3	MG	E	402	1/1	0.84	0.37	60,60,60,60	0
4	CL	F	402	1/1	0.87	0.08	77,77,77,77	0
2	FQ8	A	401	40/40	0.88	0.18	50,79,126,130	0
2	FQ8	E	401	40/40	0.88	0.19	61,85,121,137	0
3	MG	B	402	1/1	0.89	0.50	63,63,63,63	0
4	CL	D	404	1/1	0.89	0.14	72,72,72,72	0
4	CL	B	407	1/1	0.91	0.09	71,71,71,71	0
2	FQ8	D	401	40/40	0.92	0.19	44,77,125,130	0
3	MG	I	402	1/1	0.92	0.53	66,66,66,66	0
2	FQ8	P	401	40/40	0.93	0.18	51,100,151,161	0
2	FQ8	Q	401	40/40	0.94	0.17	51,81,129,143	0
2	FQ8	B	401	40/40	0.94	0.18	34,72,101,113	0
2	FQ8	I	401	40/40	0.94	0.17	48,74,95,118	0
2	FQ8	H	401	40/40	0.95	0.17	36,69,91,100	0
4	CL	I	403	1/1	0.95	0.09	57,57,57,57	0
4	CL	Q	402	1/1	0.95	0.10	71,71,71,71	0
2	FQ8	O	401	40/40	0.95	0.18	36,58,99,124	0
2	FQ8	C	401	40/40	0.95	0.17	49,72,104,121	0
2	FQ8	G	401	40/40	0.95	0.15	50,73,124,142	0
4	CL	D	403	1/1	0.95	0.13	73,73,73,73	0
4	CL	E	404	1/1	0.96	0.08	61,61,61,61	0
2	FQ8	F	401	40/40	0.96	0.19	43,64,94,108	0
4	CL	E	403	1/1	0.96	0.10	40,40,40,40	0
4	CL	B	405	1/1	0.96	0.08	57,57,57,57	0
4	CL	B	403	1/1	0.96	0.12	44,44,44,44	0
4	CL	H	403	1/1	0.97	0.09	40,40,40,40	0
4	CL	G	402	1/1	0.98	0.12	64,64,64,64	0
4	CL	A	402	1/1	0.98	0.12	38,38,38,38	0
4	CL	H	404	1/1	0.98	0.10	48,48,48,48	0
4	CL	H	402	1/1	0.98	0.12	56,56,56,56	0
4	CL	B	404	1/1	0.99	0.07	51,51,51,51	0

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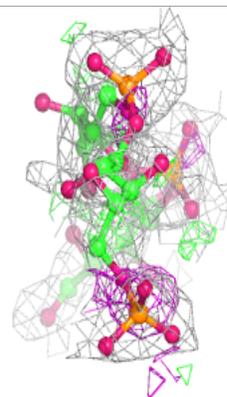
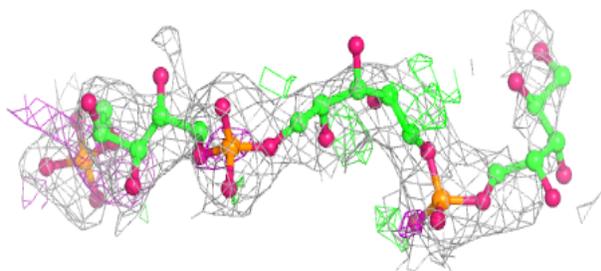
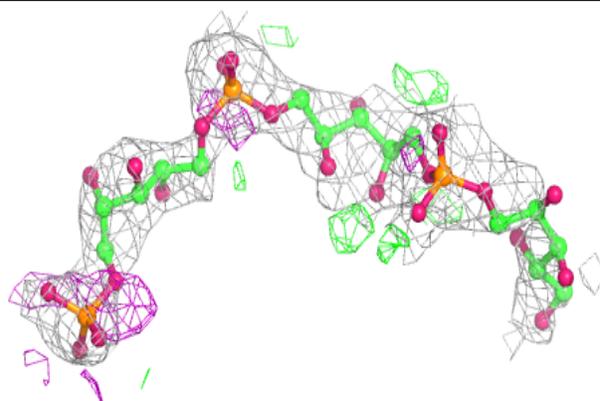
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	B	406	1/1	0.99	0.09	44,44,44,44	0

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.

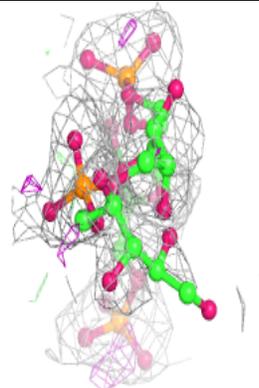
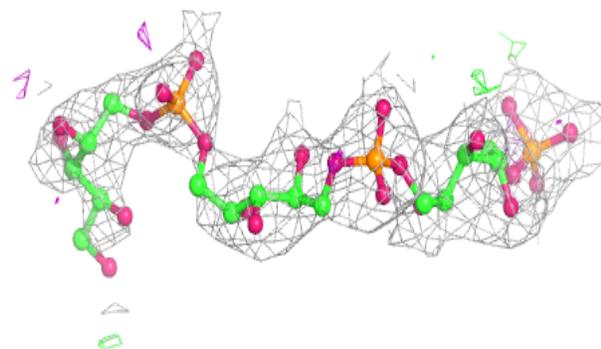
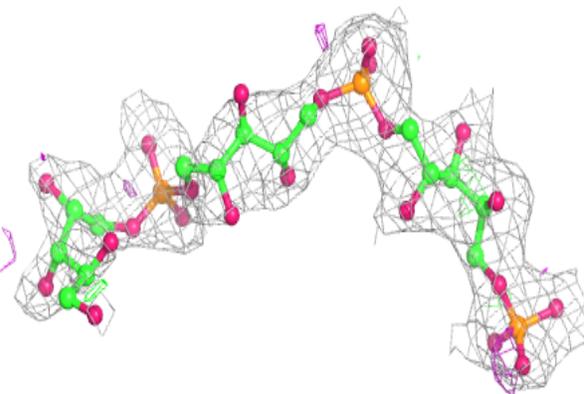


**Electron density around FQ8 E 401:**

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

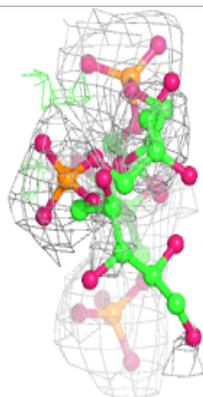
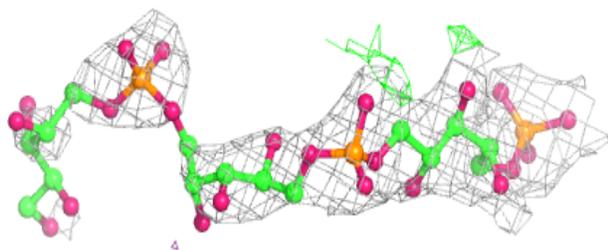
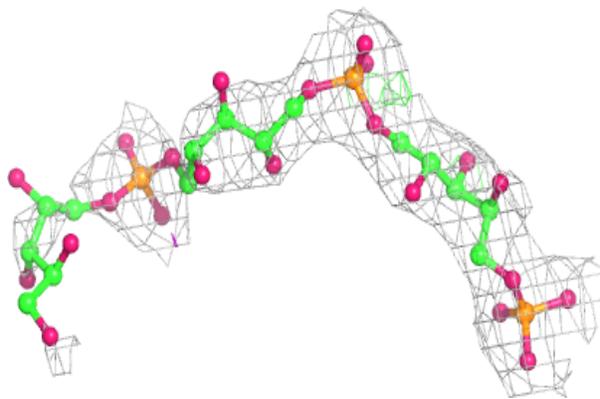
**Electron density around FQ8 D 401:**

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

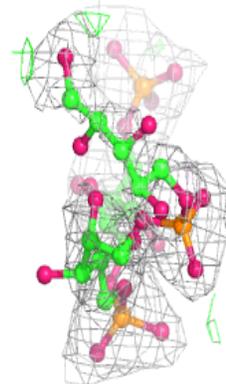
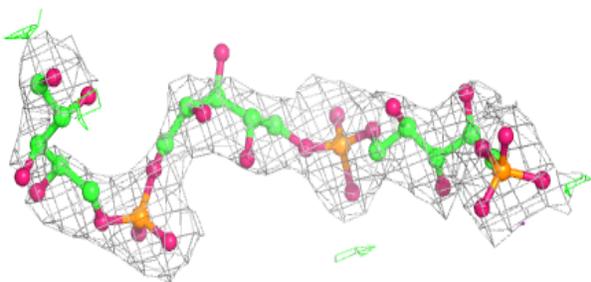
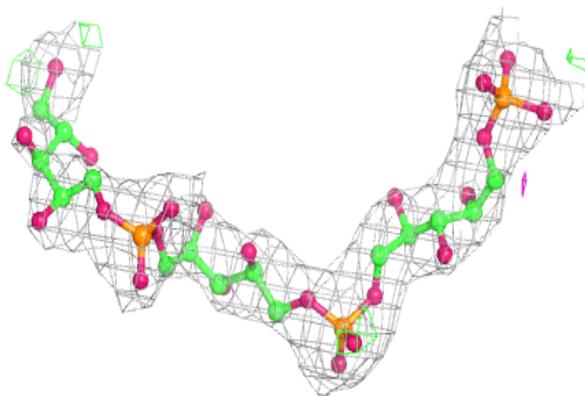


**Electron density around FQ8 P 401:**

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

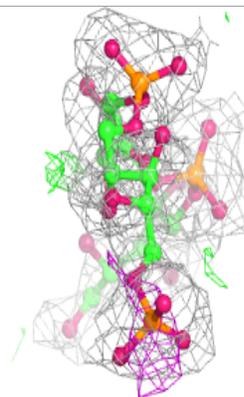
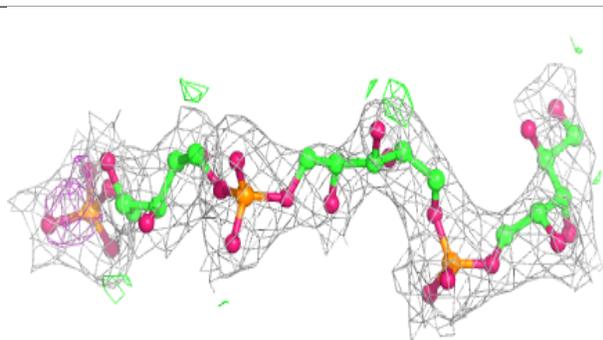
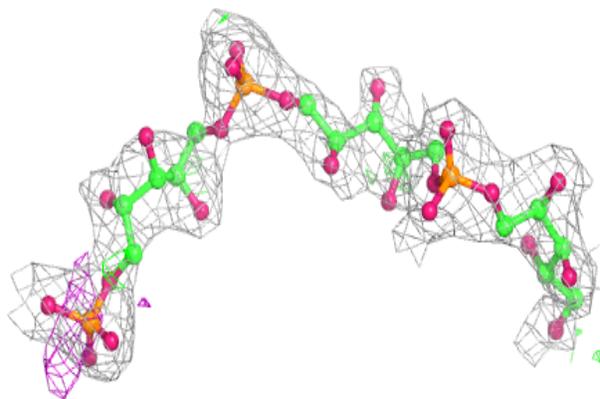
**Electron density around FQ8 Q 401:**

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

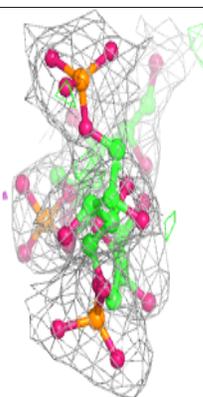
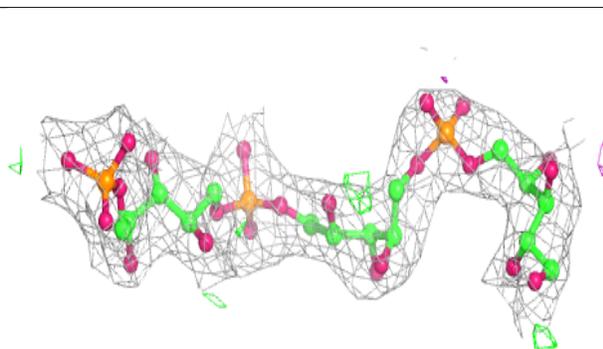
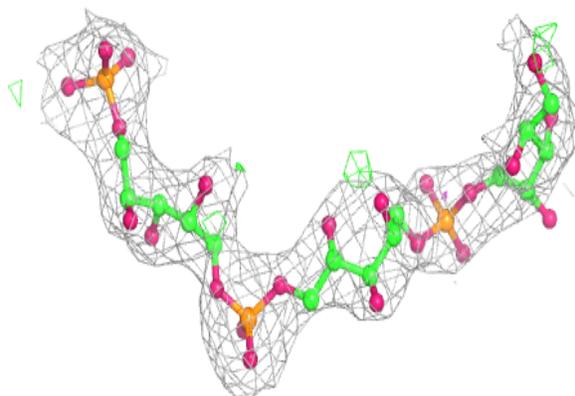


**Electron density around FQ8 B 401:**

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

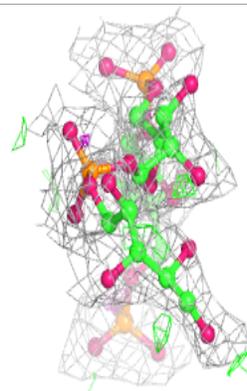
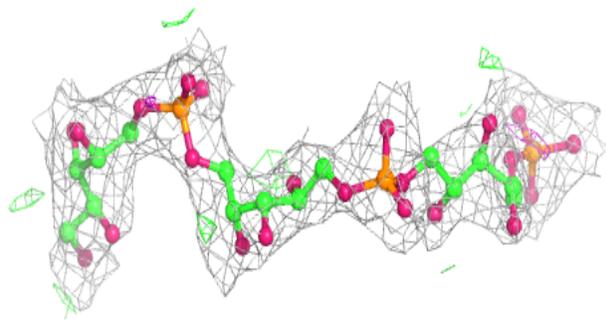
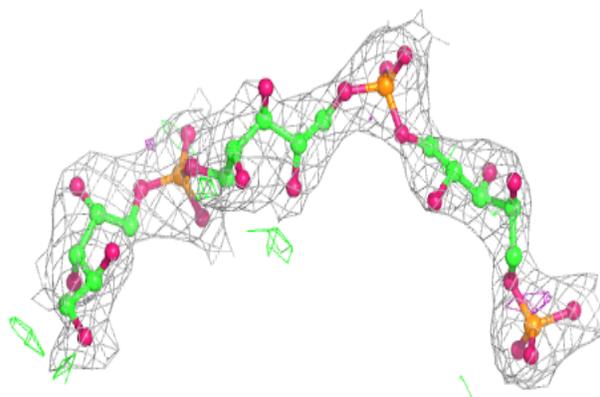
**Electron density around FQ8 I 401:**

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

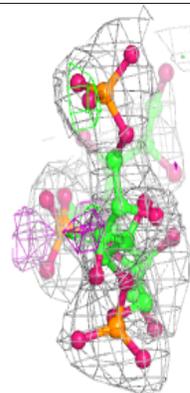
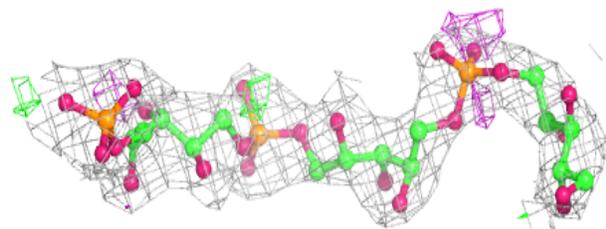
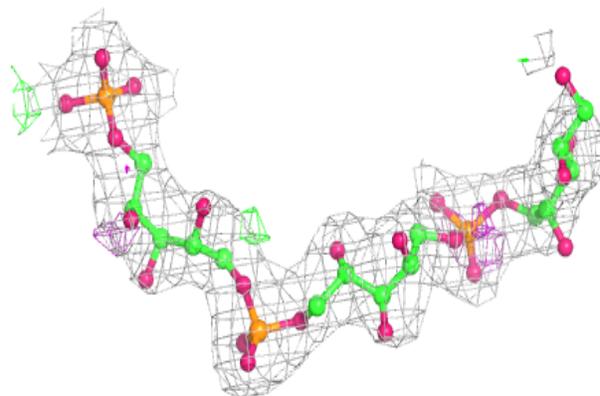


**Electron density around FQ8 H 401:**

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

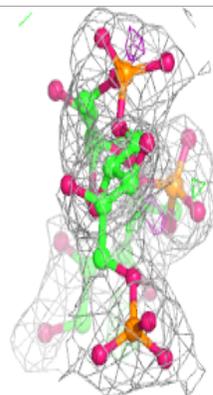
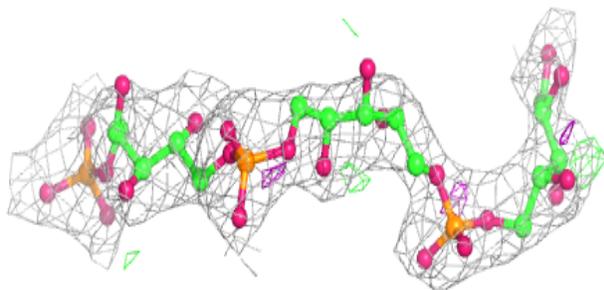
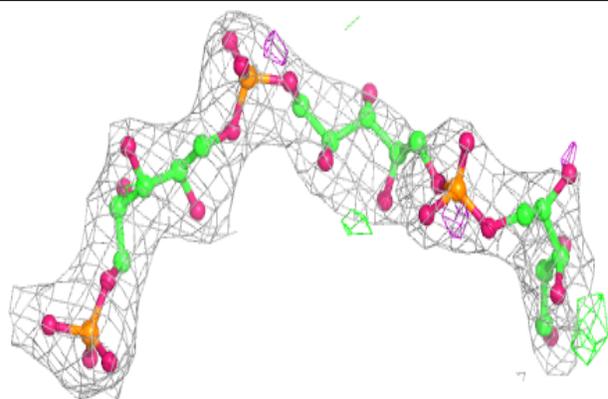
**Electron density around FQ8 O 401:**

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and green (positive)

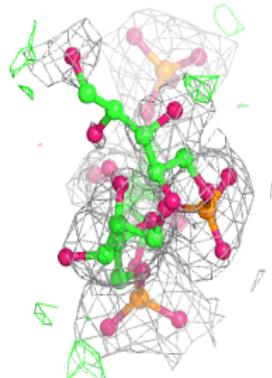
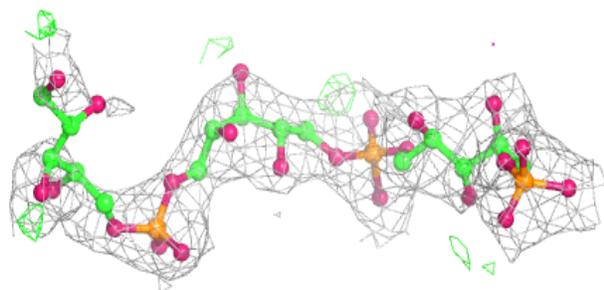
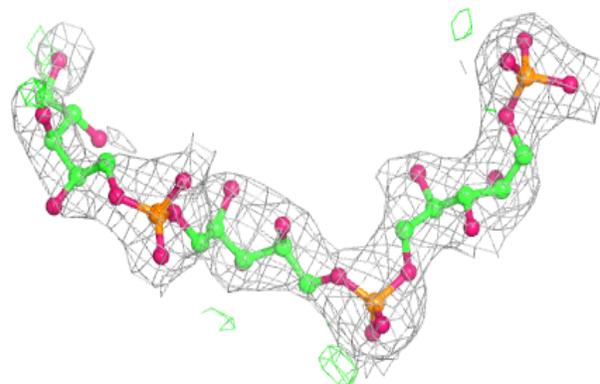


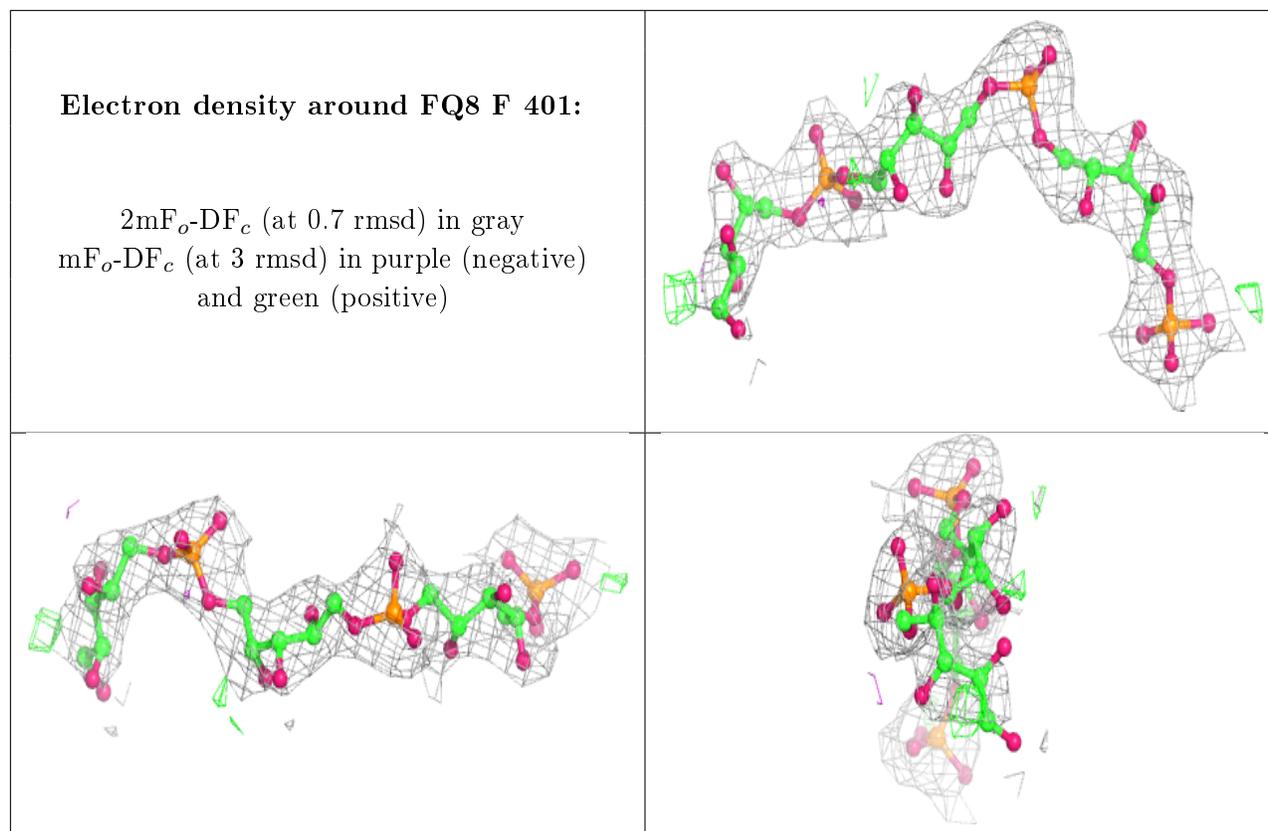
**Electron density around FQ8 C 401:**

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

**Electron density around FQ8 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.