



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 12:01 AM EDT

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 Full wwPDB X-ray Structure Validation 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
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) : 2.37.1

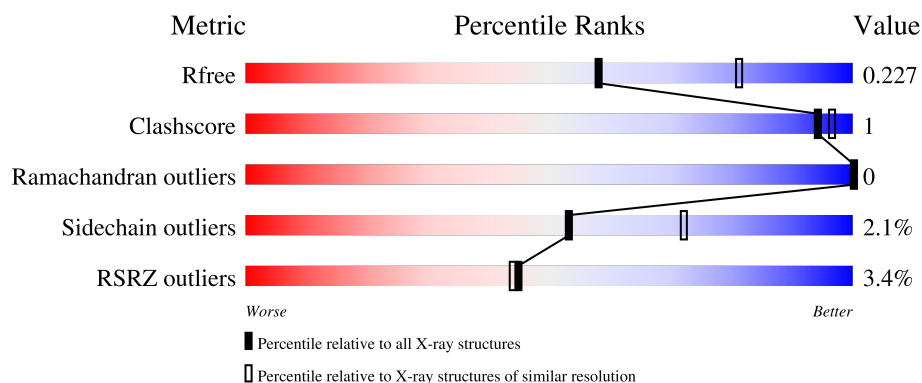
# 1 Overall quality at a glance

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 of 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	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>8%</div> </div> </div>
1	B	345	<div> <div></div> <div>87%</div> <div>8%</div> </div>
1	C	345	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>10%</div> </div> </div>
1	D	345	<div> <div></div> <div>87%</div> <div>9%</div> </div>
1	E	345	<div> <div></div> <div>87%</div> <div>8%</div> </div>

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

## 2 Entry composition

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

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
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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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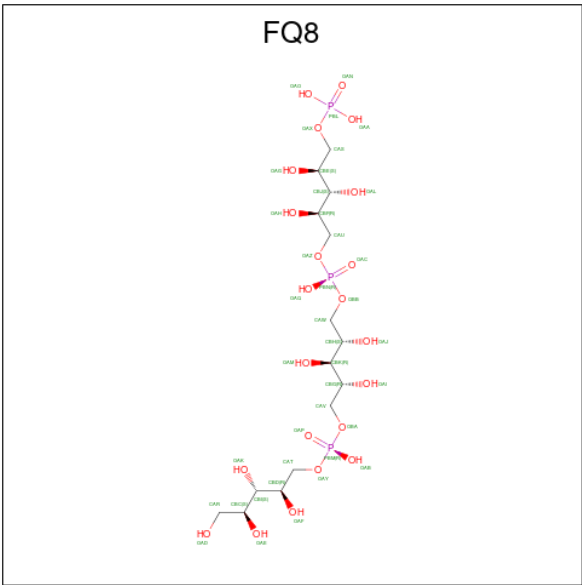
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	SER	-	expression tag	UNP A0A0H3JNB0
D	-5	LEU	-	expression tag	UNP A0A0H3JNB0
D	-4	VAL	-	expression tag	UNP A0A0H3JNB0
D	-3	PRO	-	expression tag	UNP A0A0H3JNB0
D	-2	ARG	-	expression tag	UNP A0A0H3JNB0
D	-1	GLY	-	expression tag	UNP A0A0H3JNB0
D	0	SER	-	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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Chain	Residue	Modelled	Actual	Comment	Reference
I	0	SER	-	expression tag	UNP A0A0H3JNB0

- Molecule 2 is [(2 {R},3 {S},4 {S})-2,3,4,5-tetrakis(oxidanyl)pentyl] [(2 {R},3 {R},4 {S})-2,3,4-tris(oxidanyl)-5-[oxidanyl-[(2 {R},3 {S},4 {S})-2,3,4-tris(oxidanyl)-5-phosphonooxy-pentoxyl]phosphoryl]oxy-pentyl] hydrogen phosphate (three-letter code: FQ8) (formula: C<sub>15</sub>H<sub>35</sub>O<sub>22</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			40	15	22	3		
2	C	1	Total	C	O	P	0	0
			40	15	22	3		
2	F	1	Total	C	O	P	0	0
			40	15	22	3		
2	O	1	Total	C	O	P	0	0
			40	15	22	3		
2	P	1	Total	C	O	P	0	0
			40	15	22	3		
2	E	1	Total	C	O	P	0	0
			40	15	22	3		
2	G	1	Total	C	O	P	0	0
			40	15	22	3		
2	Q	1	Total	C	O	P	0	0
			40	15	22	3		
2	A	1	Total	C	O	P	0	0
			40	15	22	3		

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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	E	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	I	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	B	5	Total	Cl	0	0
			5	5		
4	F	1	Total	Cl	0	0
			1	1		
4	E	2	Total	Cl	0	0
			2	2		
4	G	1	Total	Cl	0	0
			1	1		
4	Q	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	D	2	Total	Cl	0	0
			2	2		
4	H	3	Total	Cl	0	0
			3	3		
4	I	1	Total	Cl	0	0
			1	1		

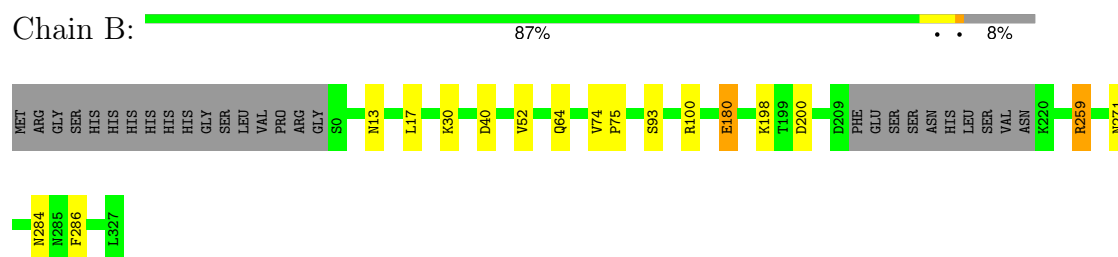
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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

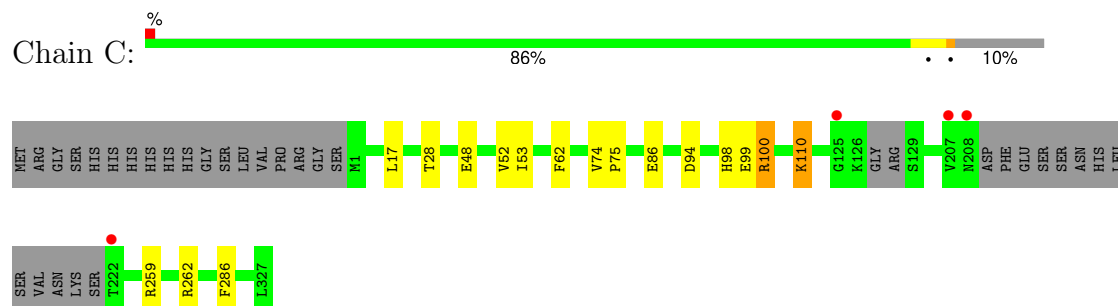
### 3 Residue-property plots [i](#)

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.

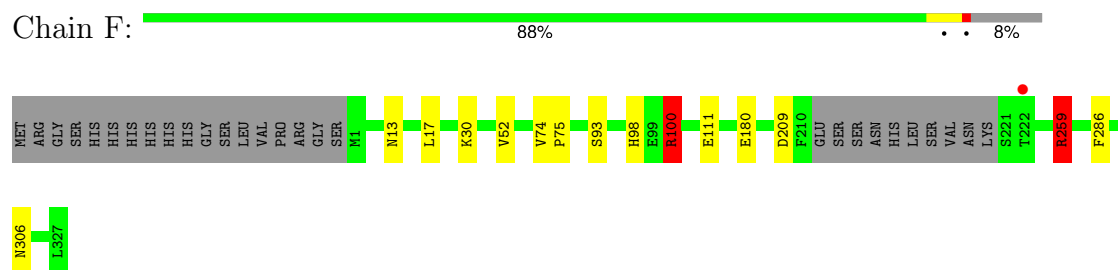
- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase



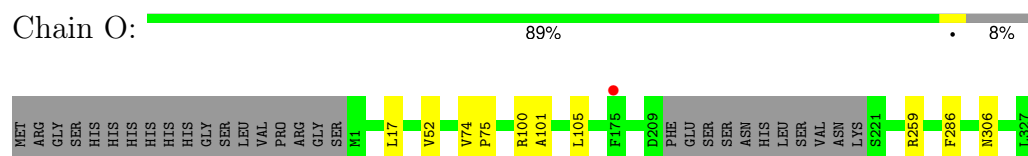
- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase



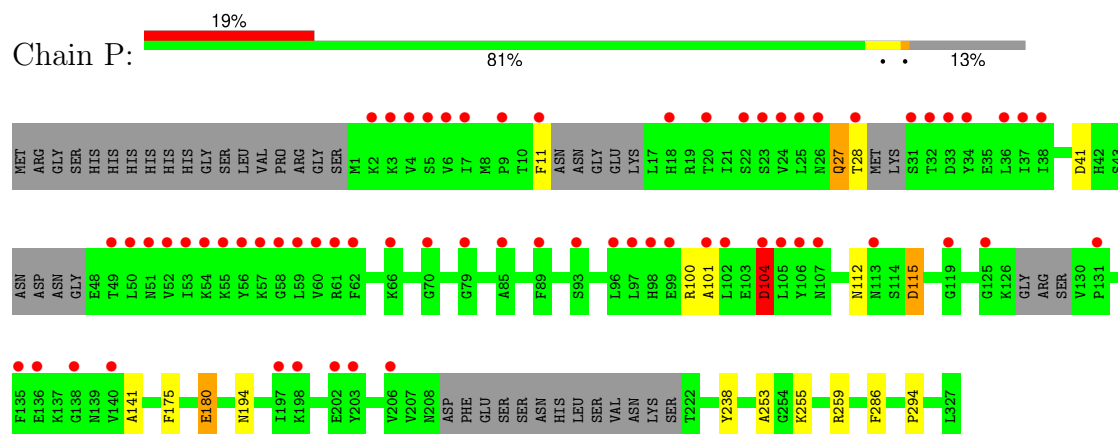
- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase



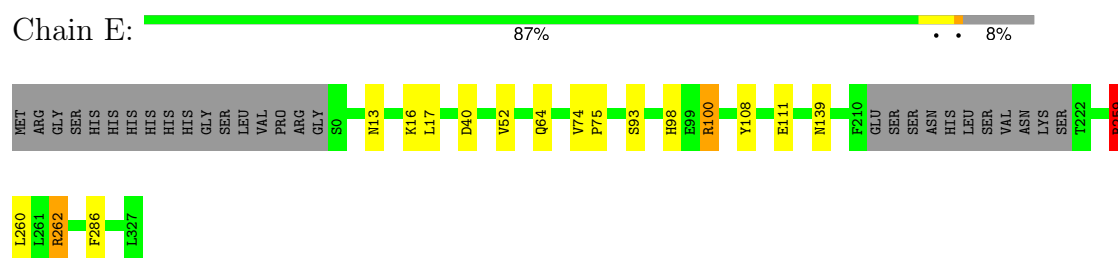
- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase



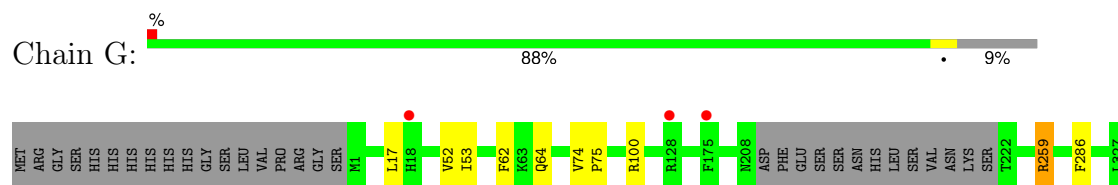
- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase



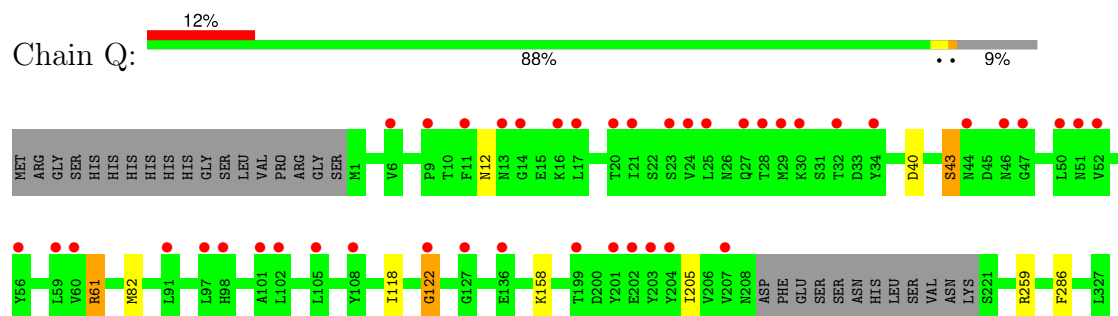
- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase



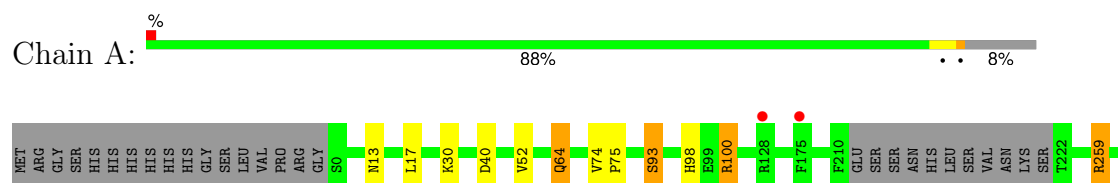
- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase



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



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





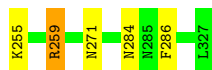
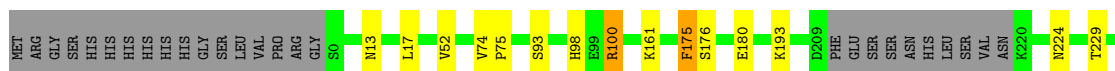
- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

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

### 5.1 Standard geometry

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

All (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
1	F	100	ARG	CG-CD-NE	-7.55	95.95	111.80
1	E	262	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	F	259	ARG	CG-CD-NE	-6.18	98.81	111.80
1	B	259	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	E	262	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	Q	61	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	P	104	ASP	CB-CG-OD2	5.91	123.62	118.30
1	G	259	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	F	259	ARG	CD-NE-CZ	5.44	131.21	123.60
1	E	259	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	H	175	PHE	CA-C-O	-5.27	109.04	120.10
1	H	259	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	259	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	H	161	LYS	CB-CG-CD	5.07	124.77	111.60

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 ⓘ

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

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

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

All (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
1:H:176:SER:HB3	1:H:180:GLU:OE2	2.04	0.58
1:E:13:ASN:O	1:E:16:LYS:HG2	2.04	0.58
1:P:11:PHE:HE1	1:P:41:ASP:O	1.88	0.57
1:P:115:ASP:OD1	1:P:194:ASN:O	2.23	0.56
1:O:101:ALA:O	1:O:105:LEU:HG	2.06	0.55
1:H:175:PHE:HE1	1:H:229:THR:OG1	1.90	0.52
1:E:259:ARG:HG3	1:E:260:LEU:N	2.25	0.51
1:E:108:TYR:O	1:E:111:GLU:HG2	2.10	0.51
1:P:180:GLU:HA	1:P:180:GLU:OE1	2.12	0.50
1:C:53:ILE:HG21	1:C:62:PHE:CD2	2.47	0.50
1:E:13:ASN:ND2	1:E:93:SER:HB2	2.27	0.50
1:B:17:LEU:HB3	1:B:52:VAL:HG11	1.94	0.48
1:A:13:ASN:ND2	1:A:93:SER:HB2	2.28	0.48
1:G:17:LEU:HB3	1:G:52:VAL:HG11	1.95	0.47
1:O:17:LEU:HB3	1:O:52:VAL:HG11	1.96	0.47
1:H:255:LYS:NZ	2:H:401:FQ8:OAA	2.43	0.47
1:F:17:LEU:HB3	1:F:52:VAL:HG11	1.96	0.47
1:P:27:GLN:HE21	1:P:27:GLN:HB2	1.51	0.47
2:E:401:FQ8:OAJ	2:E:401:FQ8:OAI	2.32	0.47
1:H:17:LEU:HB3	1:H:52:VAL:HG11	1.95	0.47
1:H:74:VAL:HB	1:H:75:PRO:HD3	1.96	0.47
1:B:74:VAL:HB	1:B:75:PRO:HD3	1.97	0.47
1:D:74:VAL:HB	1:D:75:PRO:HD3	1.97	0.46
1:B:180:GLU:OE1	1:B:180:GLU:HA	2.15	0.46
1:C:17:LEU:HB3	1:C:52:VAL:HG11	1.98	0.46
1:C:86:GLU:OE2	1:C:110:LYS:HE3	2.16	0.46
1:F:13:ASN:ND2	1:F:93:SER:HB2	2.30	0.46
1:G:74:VAL:HB	1:G:75:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:LEU:HB3	1:D:52:VAL:HG11	1.97	0.45
1:G:53:ILE:HG21	1:G:62:PHE:CD2	2.50	0.45
1:Q:12:ASN:H	1:Q:43:SER:HB3	1.82	0.45
1:C:98:HIS:CE1	1:C:100:ARG:HG3	2.51	0.45
1:P:11:PHE:CE1	1:P:41:ASP:O	2.69	0.45
1:E:17:LEU:HB3	1:E:52:VAL:HG11	1.98	0.45
1:F:180:GLU:HB2	4:F:402:CL:CL	2.54	0.45
1:Q:118:ILE:HG12	1:Q:158:LYS:HD3	1.98	0.45
1:A:17:LEU:HB3	1:A:52:VAL:HG11	1.98	0.45
1:P:238:TYR:HE1	1:P:253:ALA:HB2	1.81	0.45
1:B:271:ASN:OD1	1:F:306:ASN:ND2	2.41	0.44
1:C:28:THR:HG23	1:C:99:GLU:HG2	1.99	0.44
1:F:74:VAL:HB	1:F:75:PRO:HD3	1.99	0.44
1:H:13:ASN:ND2	1:H:93:SER:HB2	2.32	0.44
1:B:198:LYS:CE	1:B:200:ASP:OD2	2.63	0.44
1:Q:122:GLY:O	1:Q:205:ILE:HA	2.17	0.44
1:C:74:VAL:HB	1:C:75:PRO:HD3	1.98	0.44
1:B:13:ASN:ND2	1:B:93:SER:HB2	2.32	0.43
1:C:110:LYS:HA	1:C:110:LYS:HD2	1.69	0.43
1:D:13:ASN:ND2	1:D:93:SER:HB2	2.34	0.43
1:I:74:VAL:HB	1:I:75:PRO:HD3	1.99	0.43
1:P:238:TYR:CE2	1:P:294:PRO:HG2	2.53	0.43
1:Q:61:ARG:NH1	1:Q:82:MET:O	2.31	0.43
1:O:306:ASN:ND2	1:H:271:ASN:OD1	2.44	0.43
1:E:13:ASN:O	1:E:16:LYS:CG	2.67	0.43
1:E:139:ASN:OD1	1:H:224:ASN:ND2	2.52	0.43
1:O:74:VAL:HB	1:O:75:PRO:HD3	2.01	0.42
1:E:40:ASP:OD2	1:E:64:GLN:NE2	2.51	0.42
1:P:27:GLN:OE1	1:P:101:ALA:N	2.53	0.42
1:A:40:ASP:OD2	1:A:64:GLN:NE2	2.51	0.42
1:D:46:ASN:OD1	1:H:193:LYS:CD	2.68	0.42
1:F:259:ARG:NH1	2:F:401:FQ8:OAP	2.49	0.42
1:A:98:HIS:CE1	1:A:100:ARG:HG3	2.55	0.41
1:E:98:HIS:CE1	1:E:100:ARG:HG3	2.56	0.41
1:B:40:ASP:OD2	1:B:64:GLN:NE2	2.52	0.41
1:C:262:ARG:NH2	2:C:401:FQ8:OAA	2.52	0.41
1:E:74:VAL:HB	1:E:75:PRO:HD3	2.02	0.40
1:F:98:HIS:CE1	1:F:100:ARG:HG3	2.56	0.40
1:A:74:VAL:HB	1:A:75:PRO:HD3	2.02	0.40
1:H:98:HIS:CE1	1:H:100:ARG:HG3	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	30	LYS
1	B	100	ARG
1	B	259	ARG
1	B	284	ASN
1	B	286	PHE
1	C	48	GLU
1	C	94	ASP
1	C	100	ARG
1	C	110	LYS
1	C	259	ARG
1	C	286	PHE
1	F	30	LYS
1	F	111	GLU
1	F	209	ASP
1	F	259	ARG
1	F	286	PHE
1	O	100	ARG
1	O	259	ARG
1	O	286	PHE
1	P	27	GLN
1	P	28	THR
1	P	104	ASP
1	P	115	ASP

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Mol	Chain	Res	Type
1	P	175	PHE
1	P	255	LYS
1	P	259	ARG
1	P	286	PHE
1	E	100	ARG
1	E	259	ARG
1	E	286	PHE
1	G	64	GLN
1	G	100	ARG
1	G	259	ARG
1	G	286	PHE
1	Q	40	ASP
1	Q	43	SER
1	Q	259	ARG
1	Q	286	PHE
1	A	30	LYS
1	A	64	GLN
1	A	93	SER
1	A	100	ARG
1	A	259	ARG
1	A	286	PHE
1	D	100	ARG
1	D	146	ILE
1	D	198	LYS
1	D	255	LYS
1	D	259	ARG
1	D	286	PHE
1	H	100	ARG
1	H	259	ARG
1	H	284	ASN
1	H	286	PHE
1	I	46	ASN
1	I	64	GLN
1	I	100	ARG
1	I	259	ARG
1	I	267	LYS
1	I	286	PHE

Sometimes 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

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	G	401	-	39,39,39	1.26	2 (5%)	53,56,56	0.98	3 (5%)
2	FQ8	A	401	-	39,39,39	1.26	4 (10%)	53,56,56	1.17	5 (9%)
2	FQ8	B	401	-	39,39,39	1.61	4 (10%)	53,56,56	1.09	4 (7%)
2	FQ8	F	401	-	39,39,39	1.21	3 (7%)	53,56,56	1.21	5 (9%)
2	FQ8	P	401	-	39,39,39	1.20	2 (5%)	53,56,56	1.01	4 (7%)
2	FQ8	D	401	-	39,39,39	1.23	3 (7%)	53,56,56	0.97	3 (5%)
2	FQ8	Q	401	-	39,39,39	1.16	3 (7%)	53,56,56	0.92	1 (1%)
2	FQ8	H	401	-	39,39,39	1.45	3 (7%)	53,56,56	0.73	1 (1%)
2	FQ8	I	401	-	39,39,39	1.25	3 (7%)	53,56,56	1.03	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FQ8	O	401	-	39,39,39	1.25	2 (5%)	53,56,56	1.14	5 (9%)
2	FQ8	C	401	-	39,39,39	1.20	3 (7%)	53,56,56	1.12	5 (9%)
2	FQ8	E	401	-	39,39,39	1.28	3 (7%)	53,56,56	0.98	3 (5%)

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	G	401	-	-	41/56/56/56	-
2	FQ8	A	401	-	-	37/56/56/56	-
2	FQ8	B	401	-	-	29/56/56/56	-
2	FQ8	F	401	-	-	32/56/56/56	-
2	FQ8	P	401	-	-	32/56/56/56	-
2	FQ8	D	401	-	-	35/56/56/56	-
2	FQ8	Q	401	-	-	37/56/56/56	-
2	FQ8	H	401	-	-	24/56/56/56	-
2	FQ8	I	401	-	-	30/56/56/56	-
2	FQ8	O	401	-	-	34/56/56/56	-
2	FQ8	C	401	-	-	34/56/56/56	-
2	FQ8	E	401	-	-	30/56/56/56	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	FQ8	PBL-OAN	6.79	1.71	1.50
2	H	401	FQ8	PBL-OAN	5.61	1.67	1.50
2	O	401	FQ8	PBL-OAN	5.11	1.66	1.50
2	G	401	FQ8	PBL-OAN	4.94	1.65	1.50
2	F	401	FQ8	PBL-OAN	4.86	1.65	1.50
2	P	401	FQ8	PBL-OAN	4.56	1.64	1.50
2	Q	401	FQ8	PBL-OAN	4.41	1.64	1.50
2	H	401	FQ8	PBM-OAP	4.36	1.65	1.50
2	D	401	FQ8	PBL-OAN	4.32	1.63	1.50
2	E	401	FQ8	PBL-OAN	4.30	1.63	1.50
2	E	401	FQ8	PBM-OAP	4.16	1.65	1.50
2	I	401	FQ8	PBL-OAN	4.05	1.63	1.50
2	A	401	FQ8	PBM-OAP	3.84	1.64	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FQ8	PBL-OAN	3.77	1.62	1.50
2	B	401	FQ8	PBM-OAP	3.72	1.63	1.50
2	A	401	FQ8	PBL-OAN	3.66	1.61	1.50
2	D	401	FQ8	PBM-OAP	3.64	1.63	1.50
2	O	401	FQ8	PBM-OAP	3.58	1.63	1.50
2	I	401	FQ8	PBM-OAP	3.53	1.63	1.50
2	G	401	FQ8	PBM-OAP	3.25	1.62	1.50
2	P	401	FQ8	PBM-OAP	3.18	1.61	1.50
2	F	401	FQ8	PBM-OAP	3.18	1.61	1.50
2	C	401	FQ8	PBM-OAP	3.08	1.61	1.50
2	I	401	FQ8	PBL-OAO	2.77	1.65	1.54
2	B	401	FQ8	CAW-CBH	2.77	1.55	1.51
2	D	401	FQ8	PBL-OAO	2.73	1.65	1.54
2	Q	401	FQ8	PBM-OAP	2.60	1.59	1.50
2	A	401	FQ8	PBL-OAO	2.45	1.63	1.54
2	C	401	FQ8	PBL-OAO	2.39	1.63	1.54
2	A	401	FQ8	CBH-CBK	2.32	1.57	1.53
2	E	401	FQ8	PBL-OAO	2.23	1.63	1.54
2	B	401	FQ8	PBL-OAO	2.21	1.63	1.54
2	Q	401	FQ8	PBL-OAO	2.19	1.62	1.54
2	H	401	FQ8	PBL-OAO	2.04	1.62	1.54
2	F	401	FQ8	PBN-OAZ	2.02	1.67	1.59

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	FQ8	OAA-PBL-OAX	3.75	116.46	106.67
2	I	401	FQ8	OAA-PBL-OAX	3.44	115.63	106.67
2	A	401	FQ8	OAD-CAR-CBC	-3.39	104.03	111.16
2	C	401	FQ8	OAA-PBL-OAX	3.23	115.10	106.67
2	A	401	FQ8	OAA-PBL-OAX	3.15	114.89	106.67
2	D	401	FQ8	OAD-CAR-CBC	-3.13	104.59	111.16
2	C	401	FQ8	CBC-CBI-CBD	-3.08	108.45	113.57
2	P	401	FQ8	CAU-CBF-CBJ	-3.01	106.54	112.22
2	B	401	FQ8	OAD-CAR-CBC	-3.00	104.86	111.16
2	F	401	FQ8	CAU-CBF-CBJ	-2.98	106.60	112.22
2	B	401	FQ8	OAA-PBL-OAX	2.97	114.41	106.67
2	P	401	FQ8	OAA-PBL-OAX	2.82	114.01	106.67
2	E	401	FQ8	OAD-CAR-CBC	-2.77	105.34	111.16
2	E	401	FQ8	OAA-PBL-OAX	2.65	113.59	106.67
2	O	401	FQ8	CBG-CBK-CBH	-2.63	109.20	113.57
2	A	401	FQ8	CBF-CBJ-CBE	-2.43	109.53	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	401	FQ8	CBC-CBI-CBD	-2.39	109.60	113.57
2	O	401	FQ8	CAU-CBF-CBJ	-2.37	107.75	112.22
2	H	401	FQ8	OAD-CAR-CBC	-2.35	106.23	111.16
2	F	401	FQ8	OAD-CAR-CBC	-2.34	106.23	111.16
2	G	401	FQ8	OAA-PBL-OAX	2.33	112.75	106.67
2	A	401	FQ8	CBC-CBI-CBD	-2.30	109.74	113.57
2	F	401	FQ8	OAB-PBM-OAY	2.29	117.96	107.57
2	O	401	FQ8	OAZ-CAU-CBF	-2.28	103.27	109.36
2	E	401	FQ8	CAV-CBG-CBK	-2.25	107.97	112.22
2	O	401	FQ8	OAA-PBL-OAX	2.25	112.53	106.67
2	Q	401	FQ8	OBA-PBM-OAP	-2.18	100.30	108.94
2	D	401	FQ8	CBG-CBK-CBH	-2.15	109.99	113.57
2	F	401	FQ8	OAX-PBL-OAN	-2.12	100.71	106.44
2	C	401	FQ8	CAU-CBF-CBJ	-2.12	108.23	112.22
2	C	401	FQ8	CAV-CBG-CBK	-2.10	108.26	112.22
2	A	401	FQ8	CAV-CBG-CBK	-2.10	108.26	112.22
2	P	401	FQ8	OAD-CAR-CBC	-2.09	106.76	111.16
2	C	401	FQ8	OAE-CBC-CAR	2.09	113.78	109.03
2	G	401	FQ8	OAD-CAR-CBC	-2.08	106.79	111.16
2	P	401	FQ8	CBG-CBK-CBH	-2.07	110.13	113.57
2	G	401	FQ8	CAV-CBG-CBK	-2.06	108.32	112.22
2	B	401	FQ8	OAQ-PBL-OAX	-2.03	101.38	106.67
2	B	401	FQ8	CBF-CBJ-CBE	-2.03	110.20	113.57
2	I	401	FQ8	OAD-CAR-CBC	-2.02	106.90	111.16
2	D	401	FQ8	CBF-CBJ-CBE	-2.00	110.24	113.57

There are no chirality outliers.

All (395) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	FQ8	CAS-OAX-PBL-OAO
2	B	401	FQ8	CAS-OAX-PBL-OAA
2	B	401	FQ8	OAX-CAS-CBE-OAG
2	B	401	FQ8	CAU-OAZ-PBN-OAQ
2	B	401	FQ8	CAU-OAZ-PBN-OAC
2	B	401	FQ8	CAU-OAZ-PBN-OBQ
2	B	401	FQ8	OBQ-CAW-CBH-OAJ
2	B	401	FQ8	OBQ-CAW-CBH-CBK
2	B	401	FQ8	OAI-CBG-CBK-CBH
2	B	401	FQ8	CAV-CBG-CBK-CBH
2	B	401	FQ8	OAI-CBG-CBK-OAM
2	B	401	FQ8	CAV-CBG-CBK-OAM

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Mol	Chain	Res	Type	Atoms
2	B	401	FQ8	OBA-CAV-CBG-CBK
2	B	401	FQ8	OBA-CAV-CBG-OAI
2	B	401	FQ8	CAT-OAY-PBM-OAP
2	B	401	FQ8	OAY-CAT-CBD-OAF
2	C	401	FQ8	CAS-OAX-PBL-OAN
2	C	401	FQ8	CAS-OAX-PBL-OAO
2	C	401	FQ8	CAS-OAX-PBL-OAA
2	C	401	FQ8	CAU-OAZ-PBN-OAC
2	C	401	FQ8	CAU-OAZ-PBN-OB
2	C	401	FQ8	CAW-OB
2	C	401	FQ8	OB
2	C	401	FQ8	OAI-CBG-CBK-CBH
2	C	401	FQ8	CAV-CBG-CBK-CBH
2	C	401	FQ8	OAI-CBG-CBK-OAM
2	C	401	FQ8	CAV-CBG-CBK-OAM
2	C	401	FQ8	CAV-OBA-PBM-OAP
2	C	401	FQ8	CAV-OBA-PBM-OAY
2	C	401	FQ8	CAT-OAY-PBM-OBA
2	C	401	FQ8	CAT-OAY-PBM-OAP
2	C	401	FQ8	CAT-OAY-PBM-OAB
2	C	401	FQ8	OAY-CAT-CBD-CBI
2	C	401	FQ8	CAT-CBD-CBI-OAK
2	C	401	FQ8	OAF-CBD-CBI-OAK
2	C	401	FQ8	OAF-CBD-CBI-CBC
2	C	401	FQ8	CAR-CBC-CBI-OAK
2	C	401	FQ8	OAD-CAR-CBC-OAE
2	F	401	FQ8	CAS-OAX-PBL-OAO
2	F	401	FQ8	CAS-OAX-PBL-OAA
2	F	401	FQ8	CAU-OAZ-PBN-OAC
2	F	401	FQ8	CAU-OAZ-PBN-OB
2	F	401	FQ8	OB
2	F	401	FQ8	OB
2	F	401	FQ8	OBA-CAV-CBG-CBK
2	F	401	FQ8	OBA-CAV-CBG-OAI
2	F	401	FQ8	CAV-OBA-PBM-OAP
2	F	401	FQ8	CAV-OBA-PBM-OAB
2	F	401	FQ8	CAV-OBA-PBM-OAY
2	F	401	FQ8	CAT-OAY-PBM-OBA
2	F	401	FQ8	CAT-OAY-PBM-OAP
2	F	401	FQ8	CAT-OAY-PBM-OAB
2	F	401	FQ8	OAY-CAT-CBD-OAF

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Mol	Chain	Res	Type	Atoms
2	F	401	FQ8	OAY-CAT-CBD-CBI
2	F	401	FQ8	CAT-CBD-CBI-OAK
2	F	401	FQ8	OAF-CBD-CBI-OAK
2	F	401	FQ8	OAF-CBD-CBI-CBC
2	O	401	FQ8	CAS-OAX-PBL-OAN
2	O	401	FQ8	CAS-OAX-PBL-OAO
2	O	401	FQ8	CAS-OAX-PBL-OAA
2	O	401	FQ8	CAU-OAZ-PBN-OAQ
2	O	401	FQ8	CAU-OAZ-PBN-OAC
2	O	401	FQ8	CAU-OAZ-PBN-OB
2	O	401	FQ8	OB-CAW-CBH-OAJ
2	O	401	FQ8	OB-CAW-CBH-CBK
2	O	401	FQ8	OBA-CAV-CBG-CBK
2	O	401	FQ8	OBA-CAV-CBG-OAI
2	O	401	FQ8	CAV-OBA-PBM-OAP
2	O	401	FQ8	CAV-OBA-PBM-OAB
2	O	401	FQ8	CAV-OBA-PBM-OAY
2	O	401	FQ8	OAY-CAT-CBD-OAF
2	O	401	FQ8	OAY-CAT-CBD-CBI
2	O	401	FQ8	CAT-CBD-CBI-OAK
2	O	401	FQ8	CAT-CBD-CBI-CBC
2	O	401	FQ8	OAF-CBD-CBI-OAK
2	O	401	FQ8	OAF-CBD-CBI-CBC
2	O	401	FQ8	OAD-CAR-CBC-CBI
2	O	401	FQ8	OAD-CAR-CBC-OAE
2	P	401	FQ8	CAS-OAX-PBL-OAN
2	P	401	FQ8	CAS-OAX-PBL-OAO
2	P	401	FQ8	CAS-OAX-PBL-OAA
2	P	401	FQ8	CAU-OAZ-PBN-OAQ
2	P	401	FQ8	CAU-OAZ-PBN-OAC
2	P	401	FQ8	CAU-OAZ-PBN-OB
2	P	401	FQ8	OB-CAW-CBH-OAJ
2	P	401	FQ8	CAT-OAY-PBM-OBA
2	P	401	FQ8	CAT-OAY-PBM-OAP
2	P	401	FQ8	OAY-CAT-CBD-OAF
2	P	401	FQ8	OAY-CAT-CBD-CBI
2	E	401	FQ8	OAZ-CAU-CBF-CBJ
2	E	401	FQ8	CAU-OAZ-PBN-OAC
2	E	401	FQ8	CAW-OB-PBN-OAZ
2	E	401	FQ8	CAW-OB-PBN-OAQ
2	E	401	FQ8	OAI-CBG-CBK-CBH
2	E	401	FQ8	CAV-CBG-CBK-CBH

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Mol	Chain	Res	Type	Atoms
2	E	401	FQ8	OAI-CBG-CBK-OAM
2	E	401	FQ8	CAV-CBG-CBK-OAM
2	E	401	FQ8	OBA-CAV-CBG-OAI
2	E	401	FQ8	CAV-OBA-PBM-OAP
2	E	401	FQ8	CAV-OBA-PBM-OAB
2	E	401	FQ8	CAV-OBA-PBM-OAY
2	E	401	FQ8	CAT-OAY-PBM-OAP
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
2	G	401	FQ8	CAU-OAZ-PBN-OAQ
2	G	401	FQ8	CAW-OBB-PBN-OAZ
2	G	401	FQ8	CAW-OBB-PBN-OAQ
2	G	401	FQ8	CAW-OBB-PBN-OAC
2	G	401	FQ8	OBB-CAW-CBH-OAJ
2	G	401	FQ8	CAV-OBA-PBM-OAY
2	G	401	FQ8	OAY-CAT-CBD-OAF
2	Q	401	FQ8	CAS-OAX-PBL-OAO
2	Q	401	FQ8	CAS-OAX-PBL-OAA
2	Q	401	FQ8	OAX-CAS-CBE-OAG
2	Q	401	FQ8	OAZ-CAU-CBF-CBJ
2	Q	401	FQ8	OAZ-CAU-CBF-OAH
2	Q	401	FQ8	CAW-OBB-PBN-OAZ
2	Q	401	FQ8	CAW-OBB-PBN-OAQ
2	Q	401	FQ8	CAW-OBB-PBN-OAC
2	Q	401	FQ8	OBA-CAV-CBG-OAI
2	Q	401	FQ8	CAV-OBA-PBM-OAP
2	Q	401	FQ8	CAV-OBA-PBM-OAB
2	Q	401	FQ8	CAV-OBA-PBM-OAY
2	Q	401	FQ8	CAT-OAY-PBM-OAP
2	A	401	FQ8	CAS-OAX-PBL-OAO
2	A	401	FQ8	CAS-OAX-PBL-OAA
2	A	401	FQ8	OAX-CAS-CBE-OAG
2	A	401	FQ8	OAX-CAS-CBE-CBJ
2	A	401	FQ8	OAJ-CBH-CBK-OAM
2	A	401	FQ8	OAJ-CBH-CBK-CBG
2	A	401	FQ8	OBA-CAV-CBG-OAI
2	A	401	FQ8	CAV-OBA-PBM-OAY
2	A	401	FQ8	CAT-OAY-PBM-OBA
2	A	401	FQ8	CAT-OAY-PBM-OAB

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Mol	Chain	Res	Type	Atoms
2	D	401	FQ8	CAS-OAX-PBL-OAO
2	D	401	FQ8	CAS-OAX-PBL-OAA
2	D	401	FQ8	OAX-CAS-CBE-OAG
2	D	401	FQ8	CAU-OAZ-PBN-OAQ
2	D	401	FQ8	CAU-OAZ-PBN-OAC
2	D	401	FQ8	CAU-OAZ-PBN-OB
2	D	401	FQ8	OB-CAW-CBH-OAJ
2	D	401	FQ8	OB-CAW-CBH-CBK
2	D	401	FQ8	CAV-CBG-CBK-CBH
2	D	401	FQ8	OAI-CBG-CBK-OAM
2	D	401	FQ8	CAV-CBG-CBK-OAM
2	D	401	FQ8	CAT-OAY-PBM-OBA
2	D	401	FQ8	OAY-CAT-CBD-CBI
2	H	401	FQ8	CAS-CBE-CBJ-OAL
2	H	401	FQ8	CAS-CBE-CBJ-CBF
2	H	401	FQ8	OAG-CBE-CBJ-OAL
2	H	401	FQ8	OAG-CBE-CBJ-CBF
2	H	401	FQ8	CAU-OAZ-PBN-OAC
2	H	401	FQ8	CAU-OAZ-PBN-OB
2	H	401	FQ8	OB-CAW-CBH-OAJ
2	H	401	FQ8	OB-CAW-CBH-CBK
2	H	401	FQ8	OBA-CAV-CBG-CBK
2	H	401	FQ8	OBA-CAV-CBG-OAI
2	H	401	FQ8	CAV-OBA-PBM-OAB
2	H	401	FQ8	CAV-OBA-PBM-OAY
2	H	401	FQ8	OAY-CAT-CBD-OAF
2	I	401	FQ8	CAS-OAX-PBL-OAO
2	I	401	FQ8	CAS-OAX-PBL-OAA
2	I	401	FQ8	CAS-CBE-CBJ-OAL
2	I	401	FQ8	CAS-CBE-CBJ-CBF
2	I	401	FQ8	OAG-CBE-CBJ-OAL
2	I	401	FQ8	OAG-CBE-CBJ-CBF
2	I	401	FQ8	OAZ-CAU-CBF-CBJ
2	I	401	FQ8	OAZ-CAU-CBF-OAH
2	I	401	FQ8	CAW-OB-PBN-OAZ
2	I	401	FQ8	CAW-OB-PBN-OAQ
2	I	401	FQ8	CAW-OB-PBN-OAC
2	I	401	FQ8	OB-CAW-CBH-OAJ
2	I	401	FQ8	CAT-OAY-PBM-OAP
2	I	401	FQ8	OAY-CAT-CBD-OAF
2	I	401	FQ8	OAY-CAT-CBD-CBI
2	I	401	FQ8	OAD-CAR-CBC-CBI

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Mol	Chain	Res	Type	Atoms
2	I	401	FQ8	OAD-CAR-CBC-OAE
2	Q	401	FQ8	OAD-CAR-CBC-OAE
2	G	401	FQ8	OAG-CBE-CBJ-OAL
2	C	401	FQ8	OAG-CBE-CBJ-CBF
2	G	401	FQ8	OAG-CBE-CBJ-CBF
2	G	401	FQ8	OAE-CBC-CBI-CBD
2	D	401	FQ8	OAI-CBG-CBK-CBH
2	C	401	FQ8	CAS-CBE-CBJ-OAL
2	F	401	FQ8	CAW-CBH-CBK-OAM
2	G	401	FQ8	CAV-CBG-CBK-OAM
2	Q	401	FQ8	CAV-CBG-CBK-OAM
2	A	401	FQ8	CAW-CBH-CBK-OAM
2	C	401	FQ8	CAS-CBE-CBJ-CBF
2	C	401	FQ8	CAT-CBD-CBI-CBC
2	F	401	FQ8	CAT-CBD-CBI-CBC
2	G	401	FQ8	CAS-CBE-CBJ-CBF
2	G	401	FQ8	CAV-CBG-CBK-CBH
2	G	401	FQ8	CAR-CBC-CBI-CBD
2	Q	401	FQ8	CAV-CBG-CBK-CBH
2	A	401	FQ8	CAW-CBH-CBK-CBG
2	C	401	FQ8	OAD-CAR-CBC-CBI
2	Q	401	FQ8	OAD-CAR-CBC-CBI
2	G	401	FQ8	OAE-CBC-CBI-OAK
2	B	401	FQ8	OAH-CBF-CBJ-CBE
2	E	401	FQ8	OAJ-CBH-CBK-CBG
2	G	401	FQ8	OAI-CBG-CBK-CBH
2	Q	401	FQ8	OAI-CBG-CBK-CBH
2	H	401	FQ8	OAJ-CBH-CBK-CBG
2	F	401	FQ8	CAU-CBF-CBJ-OAL
2	P	401	FQ8	CAS-CBE-CBJ-OAL
2	P	401	FQ8	CAR-CBC-CBI-OAK
2	E	401	FQ8	CAW-CBH-CBK-OAM
2	G	401	FQ8	CAR-CBC-CBI-OAK
2	Q	401	FQ8	CAS-CBE-CBJ-OAL
2	H	401	FQ8	CAW-CBH-CBK-OAM
2	H	401	FQ8	CAR-CBC-CBI-OAK
2	B	401	FQ8	CAU-CBF-CBJ-CBE
2	C	401	FQ8	CAR-CBC-CBI-CBD
2	F	401	FQ8	CAU-CBF-CBJ-CBE
2	F	401	FQ8	CAW-CBH-CBK-CBG
2	O	401	FQ8	CAW-CBH-CBK-CBG
2	P	401	FQ8	CAT-CBD-CBI-CBC

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Mol	Chain	Res	Type	Atoms
2	P	401	FQ8	CAR-CBC-CBI-CBD
2	E	401	FQ8	CAW-CBH-CBK-CBG
2	Q	401	FQ8	CAS-CBE-CBJ-CBF
2	D	401	FQ8	CAW-CBH-CBK-CBG
2	D	401	FQ8	CAR-CBC-CBI-CBD
2	H	401	FQ8	CAW-CBH-CBK-CBG
2	H	401	FQ8	CAR-CBC-CBI-CBD
2	C	401	FQ8	OAG-CBE-CBJ-OAL
2	P	401	FQ8	OAG-CBE-CBJ-OAL
2	E	401	FQ8	OAJ-CBH-CBK-OAM
2	H	401	FQ8	OAJ-CBH-CBK-OAM
2	F	401	FQ8	OAJ-CBH-CBK-CBG
2	P	401	FQ8	OAG-CBE-CBJ-CBF
2	P	401	FQ8	OAE-CBC-CBI-CBD
2	Q	401	FQ8	OAG-CBE-CBJ-CBF
2	D	401	FQ8	OAE-CBC-CBI-CBD
2	H	401	FQ8	OAE-CBC-CBI-CBD
2	B	401	FQ8	CAS-CBE-CBJ-OAL
2	D	401	FQ8	CAS-CBE-CBJ-OAL
2	D	401	FQ8	CAU-CBF-CBJ-CBE
2	C	401	FQ8	OAE-CBC-CBI-OAK
2	F	401	FQ8	OAJ-CBH-CBK-OAM
2	P	401	FQ8	OAF-CBD-CBI-OAK
2	G	401	FQ8	OAI-CBG-CBK-OAM
2	Q	401	FQ8	OAI-CBG-CBK-OAM
2	F	401	FQ8	OAH-CBF-CBJ-CBE
2	D	401	FQ8	OAG-CBE-CBJ-CBF
2	D	401	FQ8	OAY-CAT-CBD-OAF
2	B	401	FQ8	CAU-CBF-CBJ-OAL
2	P	401	FQ8	CAT-CBD-CBI-OAK
2	D	401	FQ8	CAW-CBH-CBK-OAM
2	B	401	FQ8	OAG-CBE-CBJ-OAL
2	Q	401	FQ8	OAG-CBE-CBJ-OAL
2	D	401	FQ8	OAG-CBE-CBJ-OAL
2	H	401	FQ8	OAE-CBC-CBI-OAK
2	P	401	FQ8	CAS-CBE-CBJ-CBF
2	D	401	FQ8	CAS-CBE-CBJ-CBF
2	B	401	FQ8	OAG-CBE-CBJ-CBF
2	P	401	FQ8	OAF-CBD-CBI-CBC
2	E	401	FQ8	OAG-CBE-CBJ-CBF
2	G	401	FQ8	OAJ-CBH-CBK-CBG
2	P	401	FQ8	OAE-CBC-CBI-OAK

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Mol	Chain	Res	Type	Atoms
2	E	401	FQ8	OAG-CBE-CBJ-OAL
2	O	401	FQ8	CAW-CBH-CBK-OAM
2	E	401	FQ8	CAS-CBE-CBJ-OAL
2	B	401	FQ8	OAX-CAS-CBE-CBJ
2	O	401	FQ8	OAZ-CAU-CBF-CBJ
2	P	401	FQ8	OBB-CAW-CBH-CBK
2	Q	401	FQ8	OAX-CAS-CBE-CBJ
2	Q	401	FQ8	OBA-CAV-CBG-CBK
2	A	401	FQ8	OBB-CAW-CBH-CBK
2	A	401	FQ8	OBA-CAV-CBG-CBK
2	A	401	FQ8	CBF-CAU-OAZ-PBN
2	B	401	FQ8	OAHCBF-CBJ-OAL
2	D	401	FQ8	OAJ-CBH-CBK-OAM
2	D	401	FQ8	OAJ-CBH-CBK-CBG
2	G	401	FQ8	CAW-CBH-CBK-OAM
2	Q	401	FQ8	CAW-CBH-CBK-OAM
2	D	401	FQ8	CAR-CBC-CBI-OAK
2	B	401	FQ8	CAS-CBE-CBJ-CBF
2	E	401	FQ8	CAS-CBE-CBJ-CBF
2	B	401	FQ8	CAS-OAX-PBL-OAN
2	F	401	FQ8	CAS-OAX-PBL-OAN
2	G	401	FQ8	CAS-OAX-PBL-OAN
2	I	401	FQ8	CAS-OAX-PBL-OAN
2	D	401	FQ8	OAHCBF-CBJ-CBE
2	I	401	FQ8	OAF-CBD-CBI-CBC
2	P	401	FQ8	CAW-CBH-CBK-OAM
2	P	401	FQ8	CAW-CBH-CBK-CBG
2	I	401	FQ8	CAT-CBD-CBI-CBC
2	F	401	FQ8	OAHCBF-CBJ-OAL
2	G	401	FQ8	OAJ-CBH-CBK-OAM
2	C	401	FQ8	OAY-CAT-CBD-OAF
2	O	401	FQ8	OAZ-CAU-CBF-OAH
2	E	401	FQ8	OAZ-CAU-CBF-OAH
2	D	401	FQ8	CAU-CBF-CBJ-OAL
2	G	401	FQ8	OAD-CAR-CBC-OAE
2	O	401	FQ8	OAJ-CBH-CBK-CBG
2	O	401	FQ8	CAS-CBE-CBJ-CBF
2	E	401	FQ8	OAE-CBC-CBI-CBD
2	Q	401	FQ8	OAJ-CBH-CBK-CBG
2	Q	401	FQ8	OAE-CBC-CBI-CBD
2	G	401	FQ8	OAD-CAR-CBC-CBI
2	C	401	FQ8	OAE-CBC-CBI-CBD

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Mol	Chain	Res	Type	Atoms
2	P	401	FQ8	OAJ-CBH-CBK-CBG
2	A	401	FQ8	OAE-CBC-CBI-CBD
2	I	401	FQ8	OAH-CBF-CBJ-CBE
2	G	401	FQ8	OAH-CBF-CBJ-CBE
2	A	401	FQ8	OAF-CBD-CBI-CBC
2	A	401	FQ8	CAV-CBG-CBK-OAM
2	Q	401	FQ8	OAY-CAT-CBD-OAF
2	A	401	FQ8	OBB-CAW-CBH-OAJ
2	O	401	FQ8	OAJ-CBH-CBK-OAM
2	P	401	FQ8	OAJ-CBH-CBK-OAM
2	Q	401	FQ8	OAJ-CBH-CBK-OAM
2	A	401	FQ8	OAE-CBC-CBI-OAK
2	D	401	FQ8	OAH-CBF-CBJ-OAL
2	D	401	FQ8	OAE-CBC-CBI-OAK
2	I	401	FQ8	OAF-CBD-CBI-OAK
2	P	401	FQ8	CBE-CAS-OAX-PBL
2	I	401	FQ8	OAH-CBF-CBJ-OAL
2	B	401	FQ8	CAT-OAY-PBM-OBA
2	P	401	FQ8	CAV-OBA-PBM-OAP
2	E	401	FQ8	CAT-OAY-PBM-OBA
2	G	401	FQ8	CAU-OAZ-PBN-OAC
2	G	401	FQ8	CAU-OAZ-PBN-OB
2	G	401	FQ8	CAV-OBA-PBM-OAP
2	G	401	FQ8	CAT-OAY-PBM-OAP
2	Q	401	FQ8	CAT-OAY-PBM-OBA
2	Q	401	FQ8	CAT-OAY-PBM-OAB
2	A	401	FQ8	CAV-OBA-PBM-OAP
2	A	401	FQ8	CAT-OAY-PBM-OAP
2	D	401	FQ8	CAT-OAY-PBM-OAP
2	G	401	FQ8	OAF-CBD-CBI-CBC
2	C	401	FQ8	CBD-CAT-OAY-PBM
2	F	401	FQ8	CBD-CAT-OAY-PBM
2	O	401	FQ8	CBD-CAT-OAY-PBM
2	A	401	FQ8	CAS-OAX-PBL-OAN
2	D	401	FQ8	CAS-OAX-PBL-OAN
2	A	401	FQ8	CAV-CBG-CBK-CBH
2	A	401	FQ8	CBD-CAT-OAY-PBM
2	O	401	FQ8	OAI-CBG-CBK-OAM
2	A	401	FQ8	CAR-CBC-CBI-OAK
2	G	401	FQ8	CAW-CBH-CBK-CBG
2	E	401	FQ8	CBE-CAS-OAX-PBL
2	A	401	FQ8	CAR-CBC-CBI-CBD

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Mol	Chain	Res	Type	Atoms
2	A	401	FQ8	OAG-CBE-CBJ-OAL
2	H	401	FQ8	OAH-CBF-CBJ-OAL
2	A	401	FQ8	OAY-CAT-CBD-CBI
2	E	401	FQ8	CAR-CBC-CBI-OAK
2	A	401	FQ8	CAS-CBE-CBJ-OAL
2	H	401	FQ8	CAU-CBF-CBJ-OAL
2	G	401	FQ8	CAT-CBD-CBI-CBC
2	Q	401	FQ8	CAW-CBH-CBK-CBG
2	A	401	FQ8	CAU-CBF-CBJ-CBE
2	Q	401	FQ8	CBD-CAT-OAY-PBM
2	D	401	FQ8	CBD-CAT-OAY-PBM
2	I	401	FQ8	OAI-CBG-CBK-OAM
2	Q	401	FQ8	CAR-CBC-CBI-OAK
2	I	401	FQ8	CAU-CBF-CBJ-OAL
2	Q	401	FQ8	CAR-CBC-CBI-CBD
2	A	401	FQ8	OAG-CBE-CBJ-CBF
2	H	401	FQ8	OAH-CBF-CBJ-CBE
2	E	401	FQ8	OAE-CBC-CBI-OAK
2	F	401	FQ8	CBF-CAU-OAZ-PBN
2	O	401	FQ8	CAU-CBF-CBJ-OAL
2	O	401	FQ8	CAV-CBG-CBK-OAM
2	I	401	FQ8	CAT-CBD-CBI-OAK
2	E	401	FQ8	CAR-CBC-CBI-CBD
2	G	401	FQ8	OAH-CBF-CBJ-OAL
2	A	401	FQ8	OAY-CAT-CBD-OAF
2	O	401	FQ8	OAG-CBE-CBJ-OAL
2	P	401	FQ8	OAI-CBG-CBK-OAM
2	A	401	FQ8	OAI-CBG-CBK-OAM
2	B	401	FQ8	OAY-CAT-CBD-CBI
2	E	401	FQ8	OBA-CAV-CBG-CBK
2	G	401	FQ8	OAY-CAT-CBD-CBI
2	D	401	FQ8	OAX-CAS-CBE-CBJ
2	I	401	FQ8	OBB-CAW-CBH-CBK
2	A	401	FQ8	CAT-CBD-CBI-OAK
2	E	401	FQ8	CAT-CBD-CBI-CBC
2	G	401	FQ8	OAF-CBD-CBI-OAK
2	Q	401	FQ8	OAE-CBC-CBI-OAK
2	A	401	FQ8	OAF-CBD-CBI-OAK
2	I	401	FQ8	OAI-CBG-CBK-CBH
2	I	401	FQ8	OAE-CBC-CBI-CBD
2	G	401	FQ8	CBD-CAT-OAY-PBM
2	F	401	FQ8	OAI-CBG-CBK-OAM

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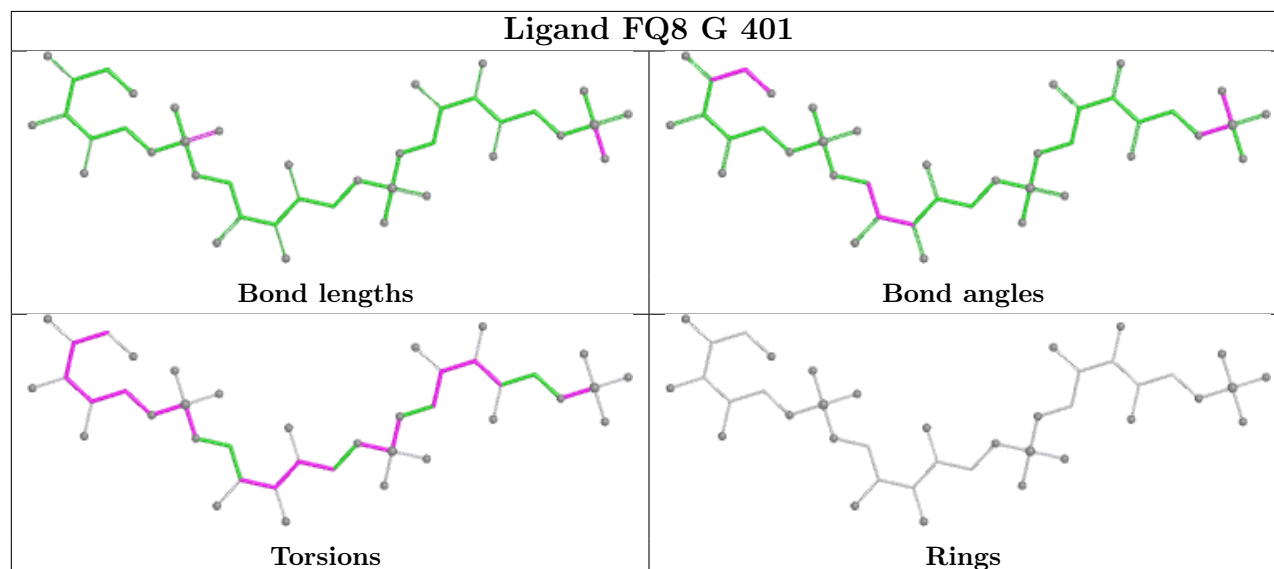
Mol	Chain	Res	Type	Atoms
2	O	401	FQ8	CAV-CBG-CBK-CBH
2	I	401	FQ8	CAU-CBF-CBJ-CBE
2	P	401	FQ8	OAD-CAR-CBC-OAE
2	B	401	FQ8	OAE-CBC-CBI-CBD
2	A	401	FQ8	CAS-CBE-CBJ-CBF

There are no ring outliers.

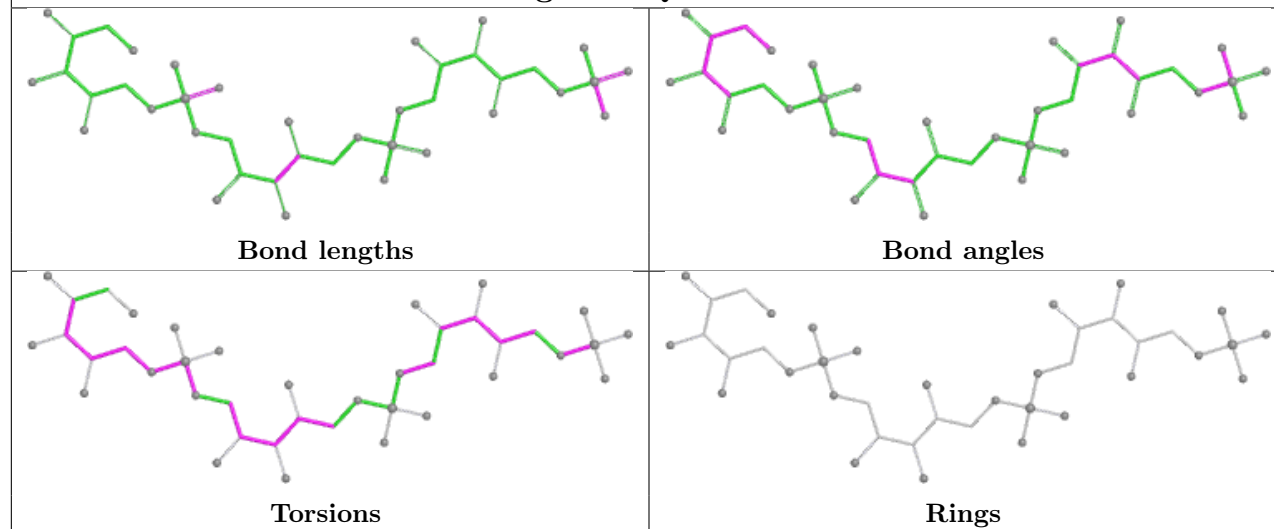
4 monomers are involved in 5 short contacts:

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

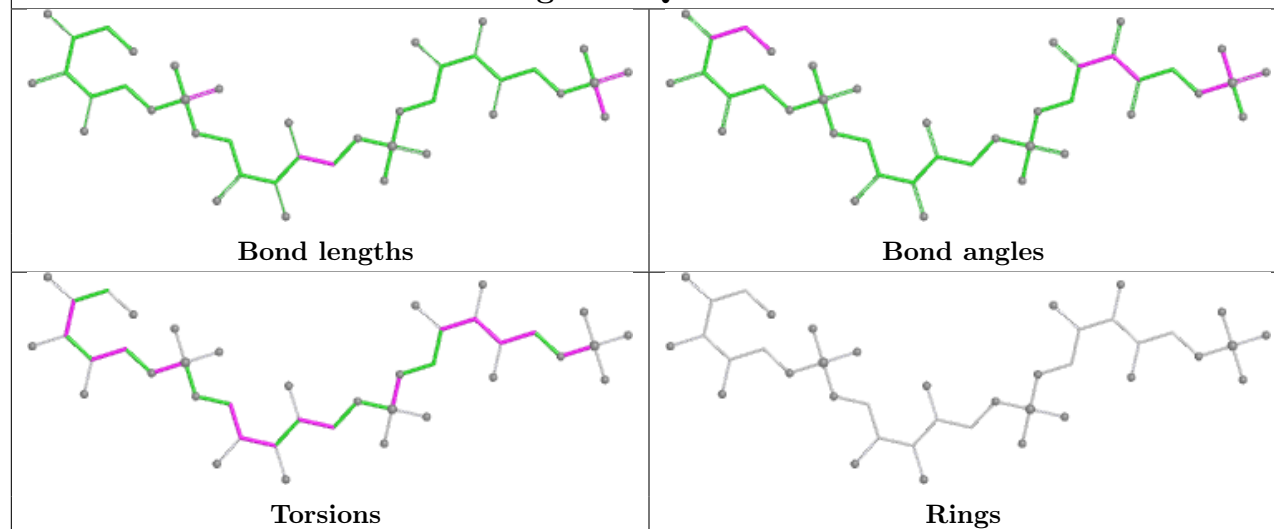
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



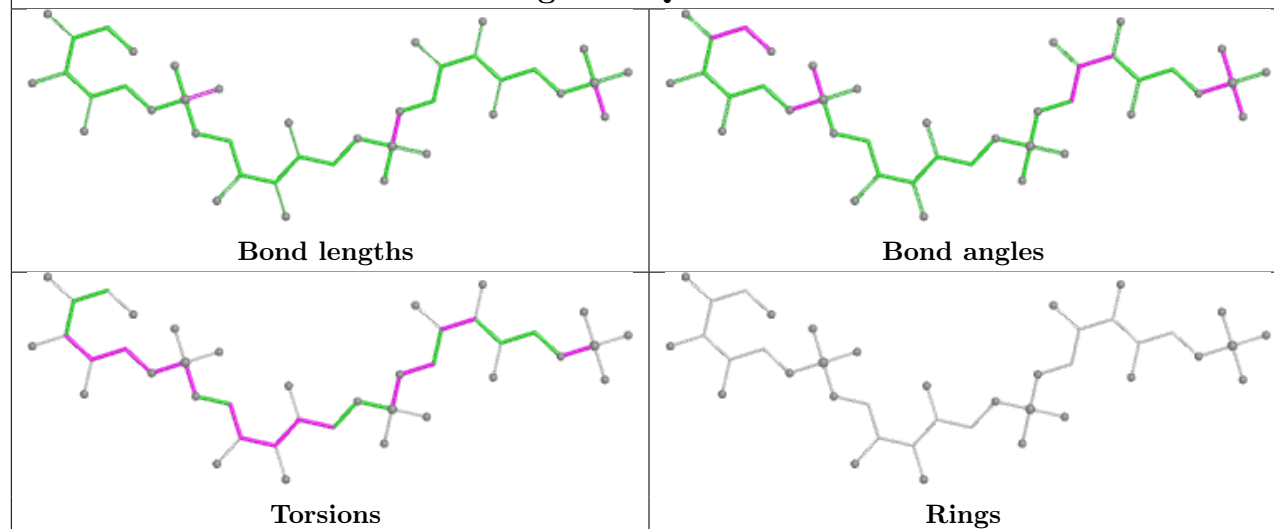
## Ligand FQ8 A 401

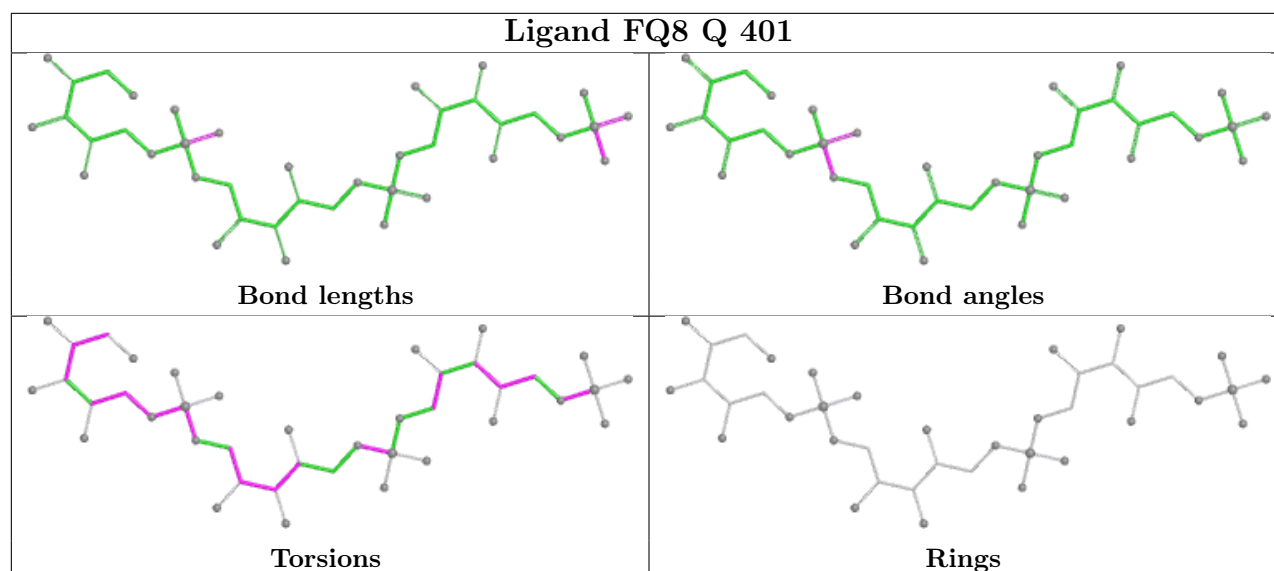
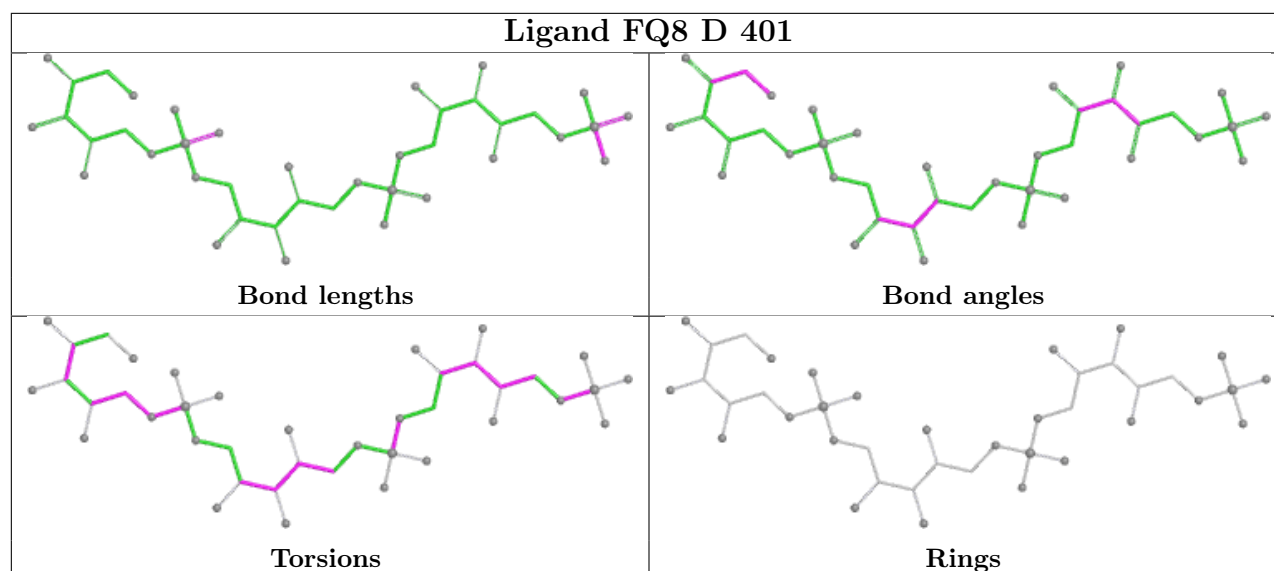
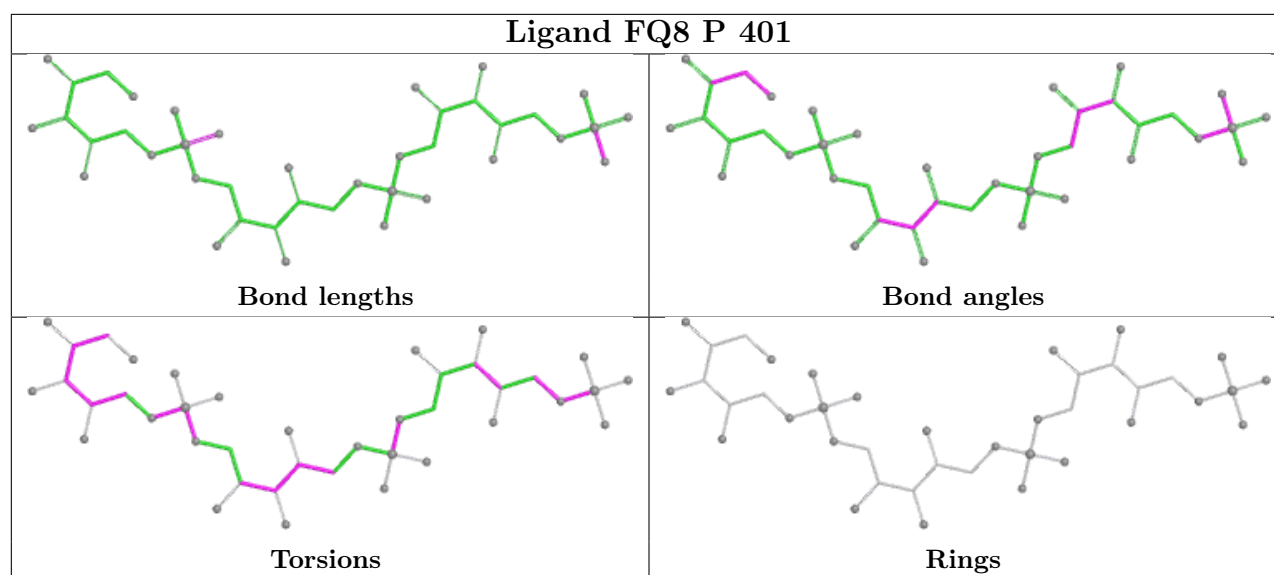


## Ligand FQ8 B 401

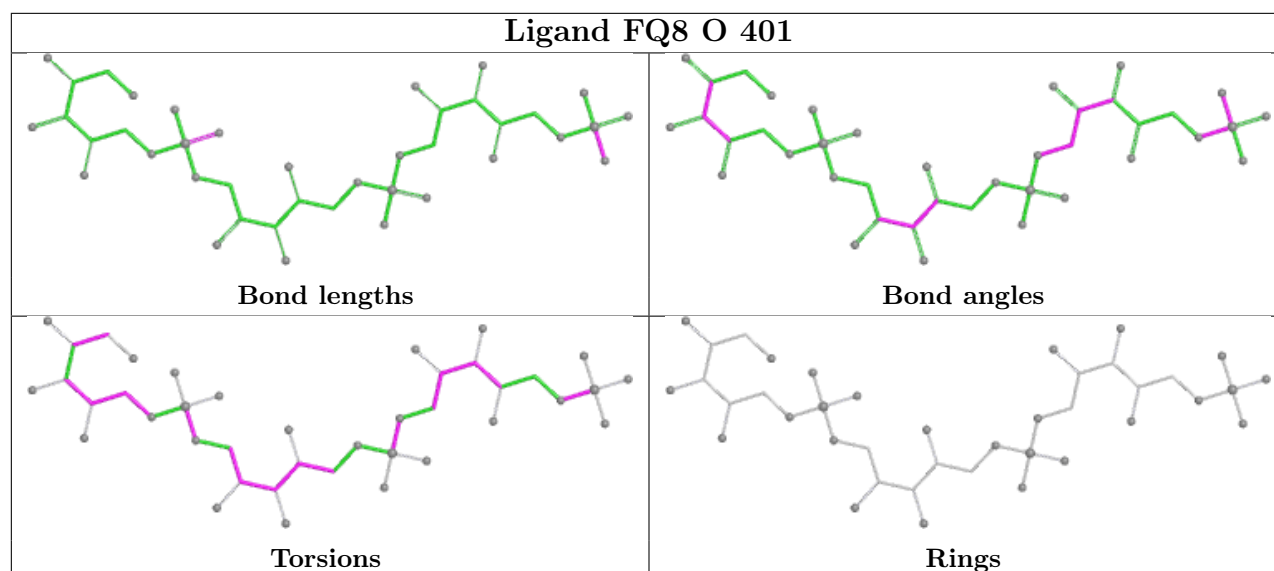
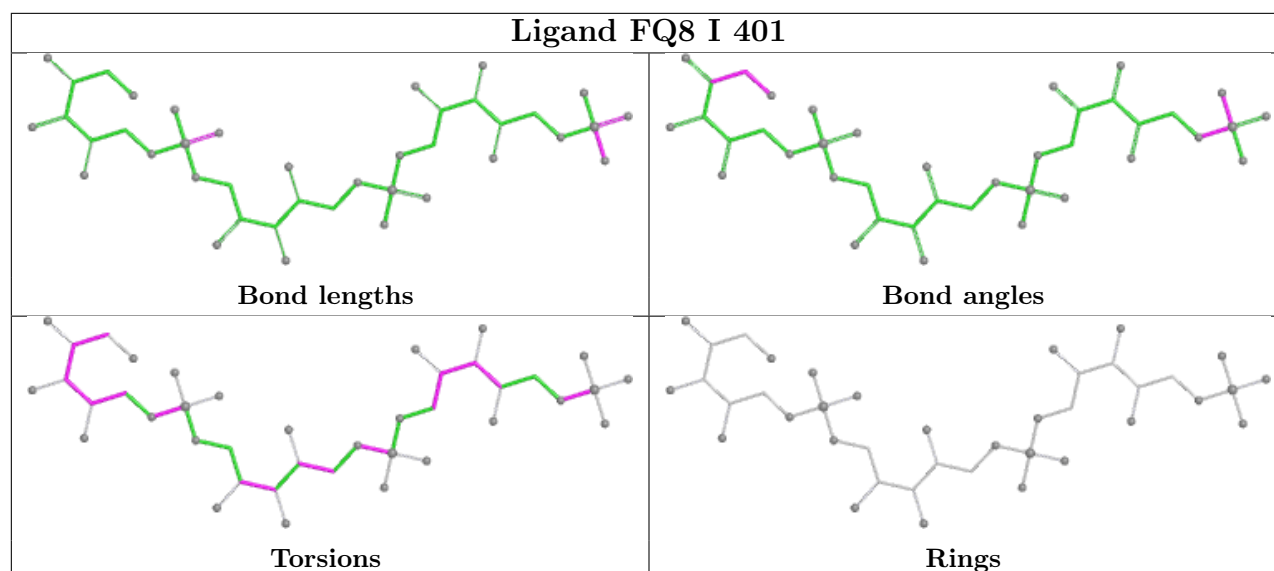
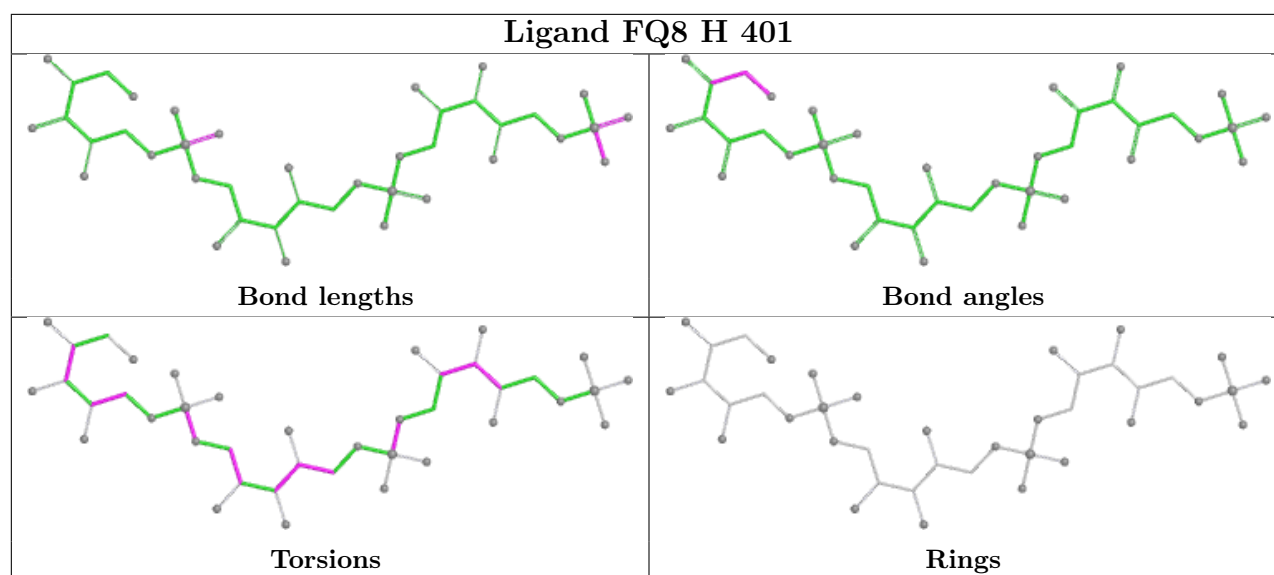


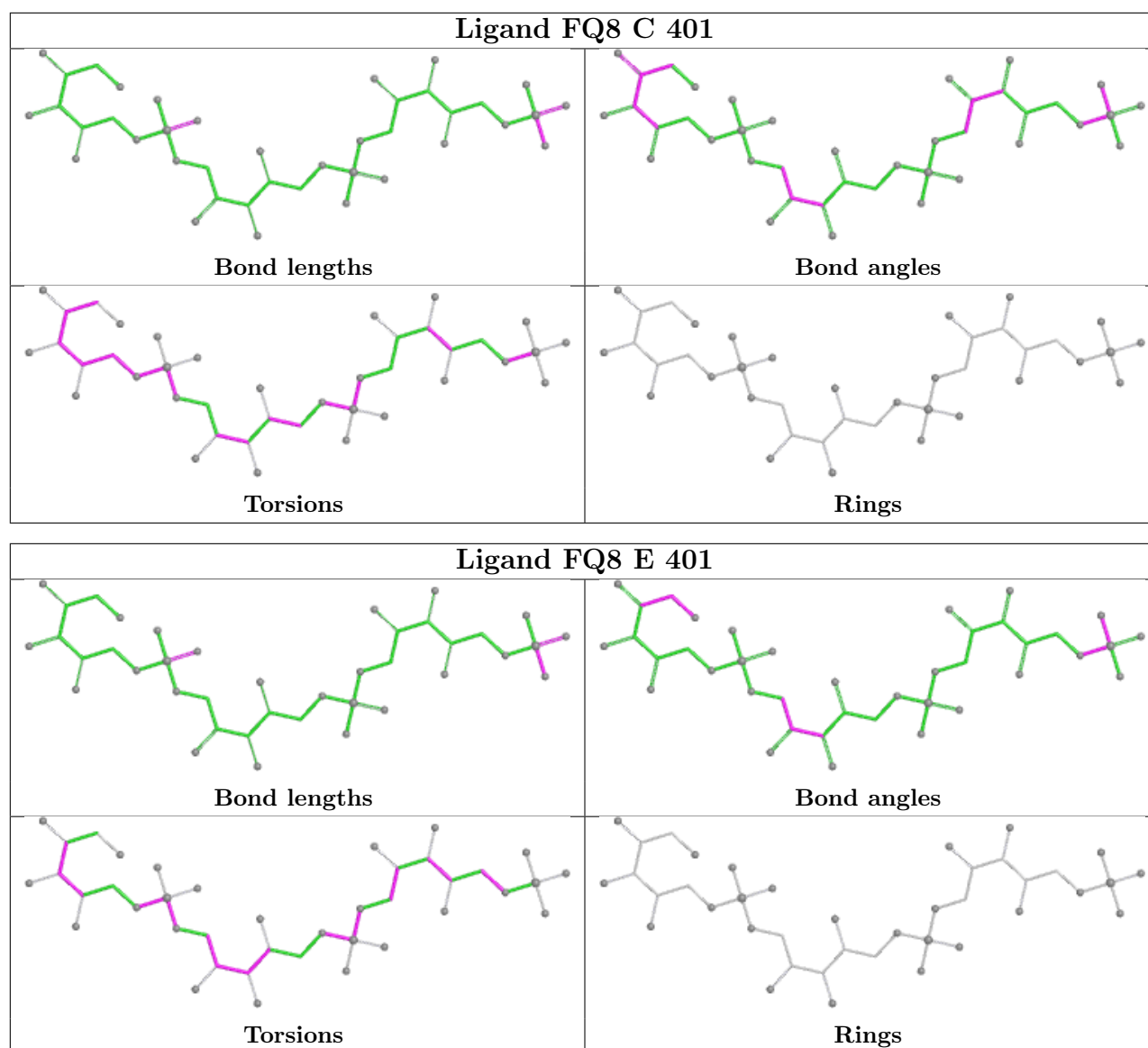
## Ligand FQ8 F 401











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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, 38, 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

All (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
1	P	34	TYR	5.6
1	P	36	LEU	5.4
1	P	98	HIS	5.3
1	Q	202	GLU	5.1
1	P	24	VAL	4.9
1	P	20	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	P	50	LEU	4.8
1	P	66	LYS	4.8
1	P	101	ALA	4.7
1	P	52	VAL	4.6
1	P	6	VAL	4.4
1	P	51	ASN	4.4
1	P	25	LEU	4.3
1	O	175	PHE	4.3
1	P	106	TYR	4.1
1	Q	203	TYR	4.1
1	P	203	TYR	4.0
1	P	97	LEU	4.0
1	P	31	SER	4.0
1	P	62	PHE	4.0
1	P	53	ILE	3.9
1	P	93	SER	3.9
1	P	105	LEU	3.7
1	Q	101	ALA	3.7
1	P	140	VAL	3.7
1	P	59	LEU	3.6
1	P	138	GLY	3.6
1	Q	14	GLY	3.6
1	P	49	THR	3.5
1	Q	97	LEU	3.5
1	P	136	GLU	3.5
1	P	119	GLY	3.5
1	P	89	PHE	3.4
1	Q	17	LEU	3.4
1	C	222	THR	3.4
1	P	206	VAL	3.4
1	P	96	LEU	3.4
1	P	22	SER	3.3
1	Q	91	LEU	3.2
1	P	202	GLU	3.2
1	Q	60	VAL	3.2
1	Q	51	ASN	3.1
1	P	5	SER	3.1
1	Q	98	HIS	3.1
1	F	222	THR	3.1
1	P	79	GLY	3.1
1	Q	20	THR	3.1
1	A	175	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	P	99	GLU	3.1
1	P	33	ASP	3.1
1	I	206	VAL	3.0
1	Q	122	GLY	3.0
1	Q	28	THR	3.0
1	P	58	GLY	3.0
1	P	125	GLY	3.0
1	C	207	VAL	3.0
1	P	37	ILE	3.0
1	Q	46	ASN	3.0
1	Q	21	ILE	2.9
1	P	7	ILE	2.9
1	Q	105	LEU	2.8
1	P	60	VAL	2.8
1	Q	6	VAL	2.8
1	Q	32	THR	2.8
1	P	113	ASN	2.8
1	P	23	SER	2.8
1	Q	27	GLN	2.8
1	Q	11	PHE	2.8
1	P	28	THR	2.8
1	C	208	ASN	2.8
1	P	55	LYS	2.8
1	P	11	PHE	2.7
1	P	57	LYS	2.7
1	Q	47	GLY	2.7
1	Q	127	GLY	2.7
1	P	56	TYR	2.7
1	Q	29	MET	2.7
1	Q	44	ASN	2.7
1	P	102	LEU	2.7
1	I	53	ILE	2.7
1	Q	108	TYR	2.7
1	I	127	GLY	2.6
1	Q	102	LEU	2.6
1	G	128	ARG	2.6
1	Q	136	GLU	2.6
1	P	85	ALA	2.5
1	Q	207	VAL	2.5
1	I	94	ASP	2.5
1	P	2	LYS	2.5
1	P	32	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	10	THR	2.4
1	P	107	ASN	2.4
1	Q	52	VAL	2.4
1	P	135	PHE	2.4
1	Q	56	TYR	2.4
1	P	61	ARG	2.3
1	P	104	ASP	2.3
1	Q	30	LYS	2.3
1	G	175	PHE	2.3
1	P	70	GLY	2.3
1	Q	50	LEU	2.3
1	Q	201	TYR	2.3
1	Q	204	TYR	2.3
1	P	3	LYS	2.2
1	P	9	PRO	2.2
1	I	51	ASN	2.2
1	Q	23	SER	2.2
1	G	18	HIS	2.2
1	Q	199	THR	2.2
1	Q	25	LEU	2.2
1	A	128	ARG	2.2
1	Q	34	TYR	2.1
1	P	131	PRO	2.1
1	P	4	VAL	2.1
1	Q	13	ASN	2.1
1	P	198	LYS	2.1
1	Q	9	PRO	2.1
1	I	222	THR	2.1
1	P	54	LYS	2.1
1	P	18	HIS	2.1
1	P	38	ILE	2.0
1	D	327	LEU	2.0
1	C	125	GLY	2.0
1	Q	16	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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, 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	0.15	72,72,72,72	0
4	CL	B	407	1/1	0.91	0.09	71,71,71,71	0
3	MG	I	402	1/1	0.92	0.53	66,66,66,66	0
2	FQ8	D	401	40/40	0.92	0.19	44,77,125,130	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	I	401	40/40	0.94	0.17	48,74,95,118	0
2	FQ8	B	401	40/40	0.94	0.18	34,72,101,113	0
2	FQ8	C	401	40/40	0.95	0.17	49,72,104,121	0
2	FQ8	O	401	40/40	0.95	0.18	36,58,99,124	0
2	FQ8	G	401	40/40	0.95	0.15	50,73,124,142	0
4	CL	Q	402	1/1	0.95	0.10	71,71,71,71	0
4	CL	D	403	1/1	0.95	0.13	73,73,73,73	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	E	404	1/1	0.96	0.08	61,61,61,61	0
4	CL	B	405	1/1	0.96	0.08	57,57,57,57	0
2	FQ8	F	401	40/40	0.96	0.19	43,64,94,108	0
4	CL	B	403	1/1	0.96	0.12	44,44,44,44	0
4	CL	E	403	1/1	0.96	0.10	40,40,40,40	0
4	CL	H	403	1/1	0.97	0.09	40,40,40,40	0
4	CL	H	402	1/1	0.98	0.12	56,56,56,56	0
4	CL	G	402	1/1	0.98	0.12	64,64,64,64	0
4	CL	H	404	1/1	0.98	0.10	48,48,48,48	0
4	CL	A	402	1/1	0.98	0.12	38,38,38,38	0
4	CL	B	406	1/1	0.99	0.09	44,44,44,44	0

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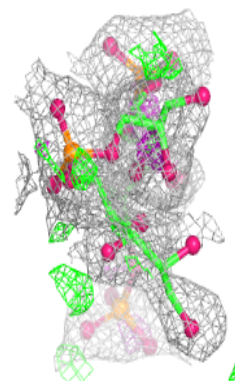
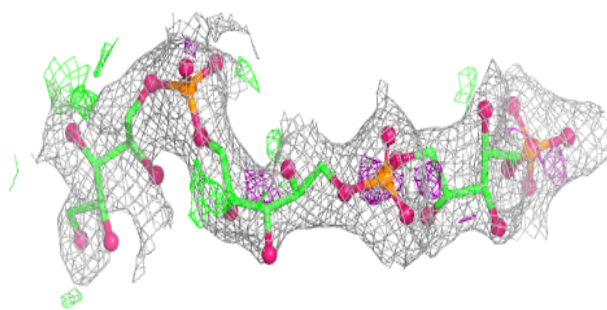
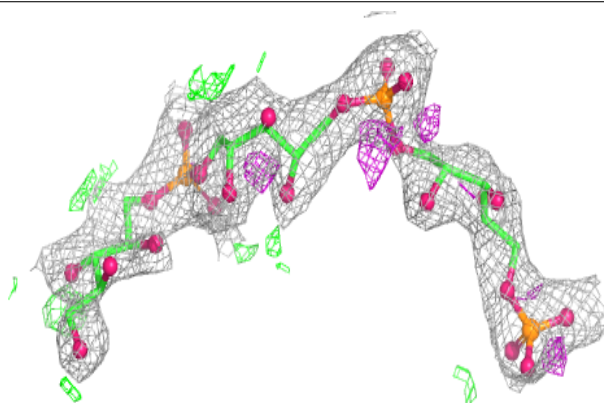
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	B	404	1/1	0.99	0.07	51,51,51,51	0

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 A 401:**

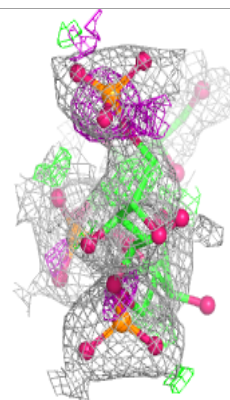
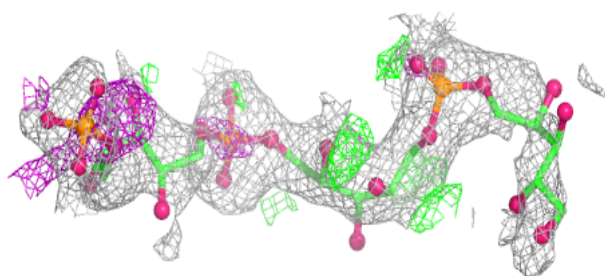
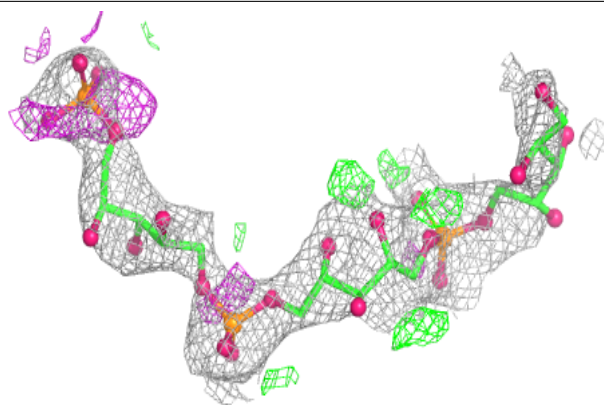
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



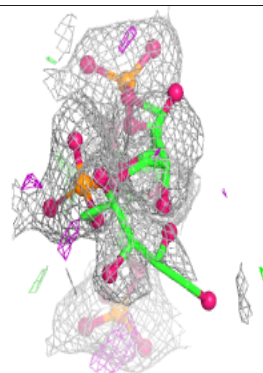
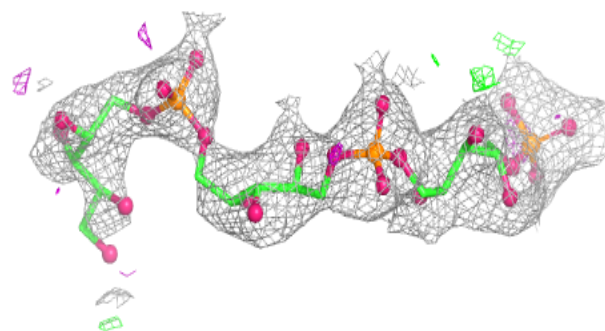
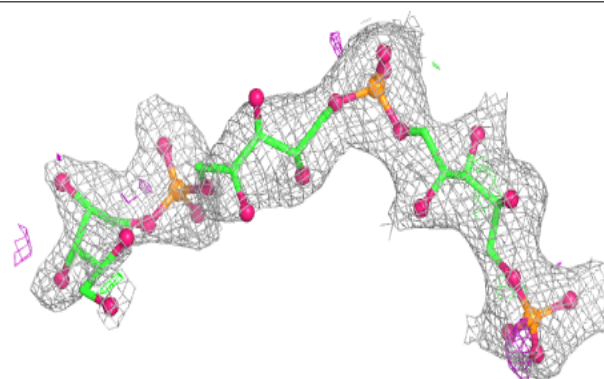


**Electron density around FQ8 E 401:**

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

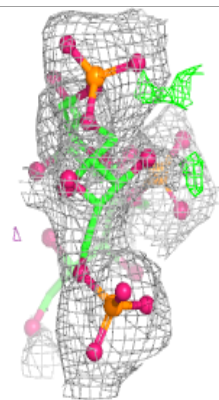
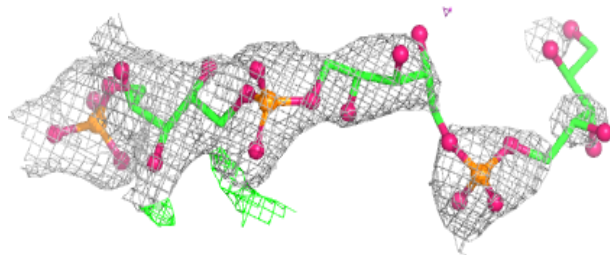
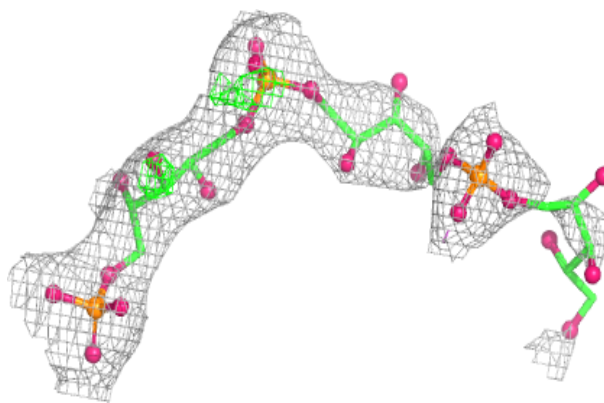
**Electron density around FQ8 D 401:**

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and green (positive)

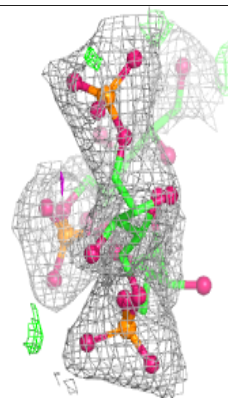
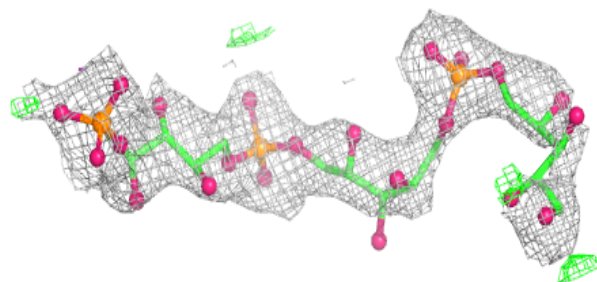
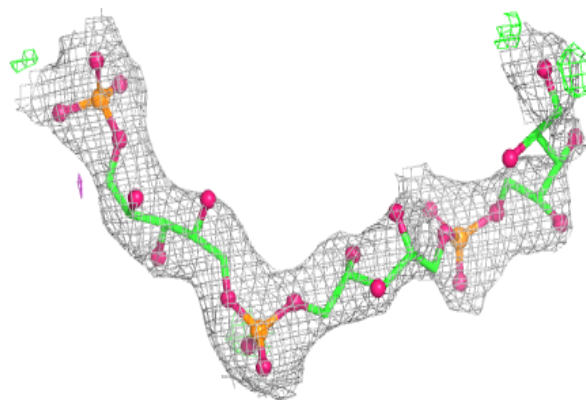


**Electron density around FQ8 P 401:**

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and green (positive)

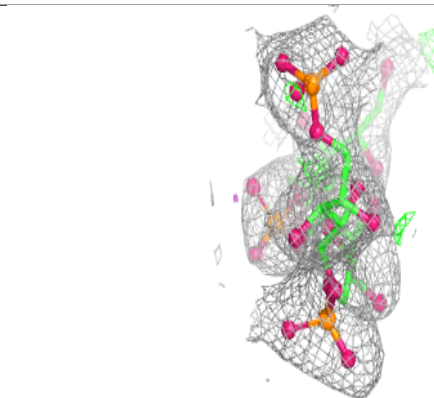
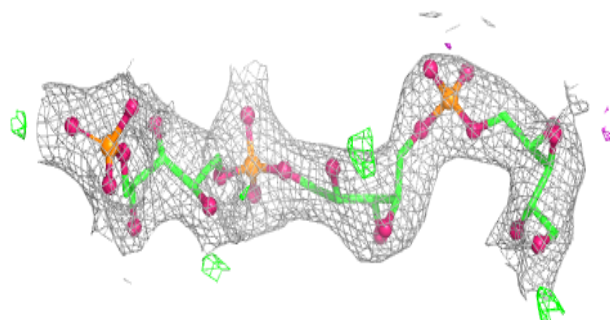
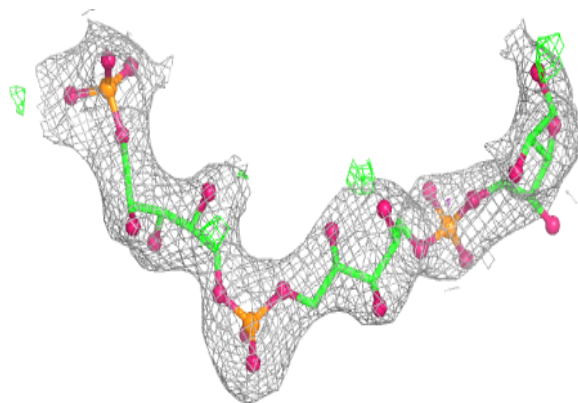
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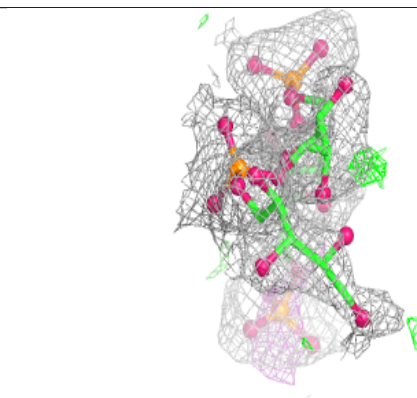
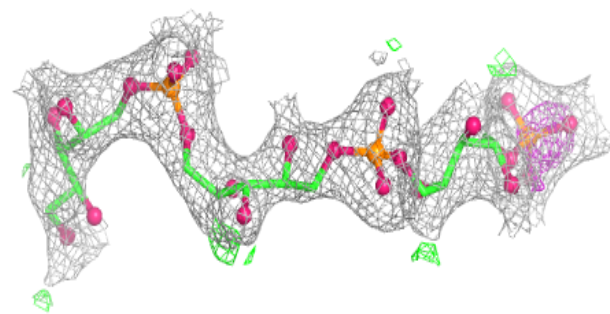
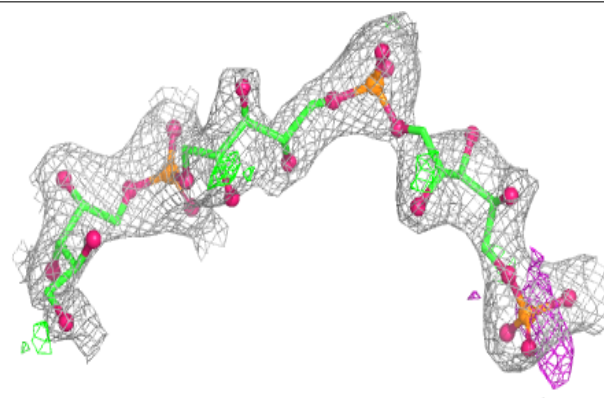


**Electron density around FQ8 I 401:**

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and green (positive)

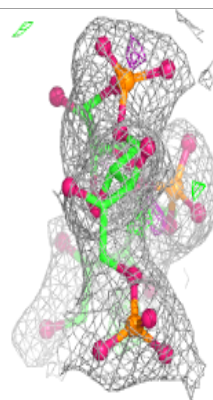
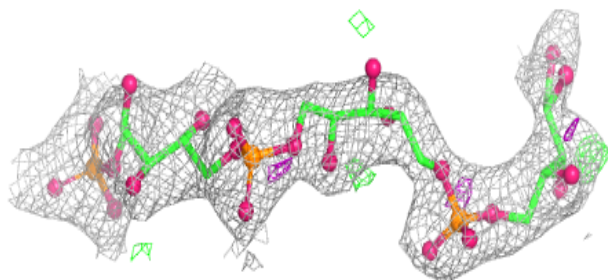
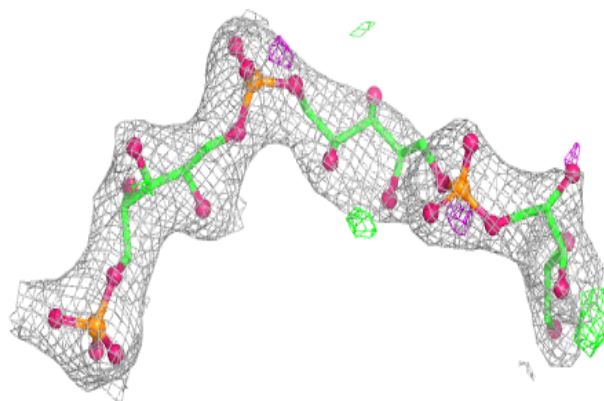
**Electron density around FQ8 B 401:**

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and green (positive)

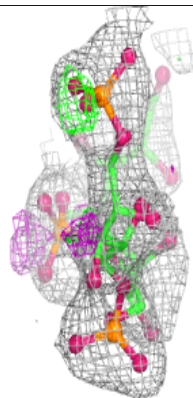
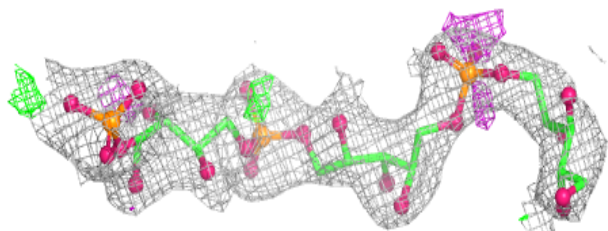
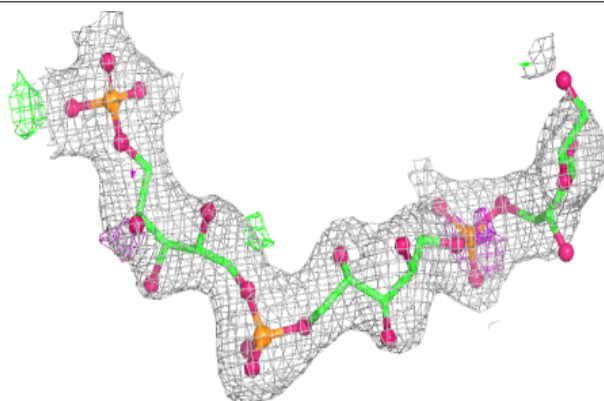


**Electron density around FQ8 C 401:**

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and green (positive)

**Electron density around FQ8 O 401:**

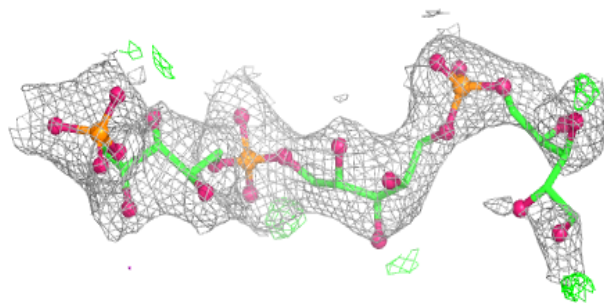
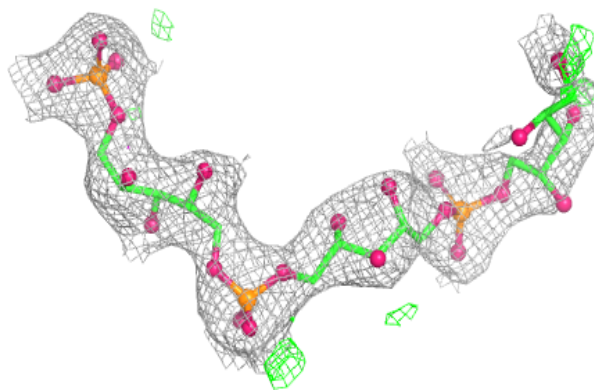
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and green (positive)



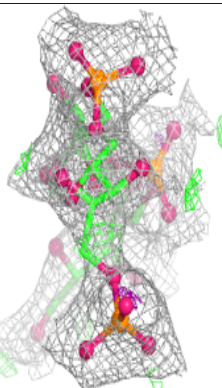
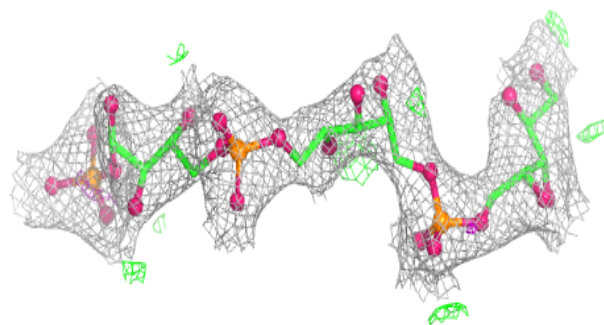
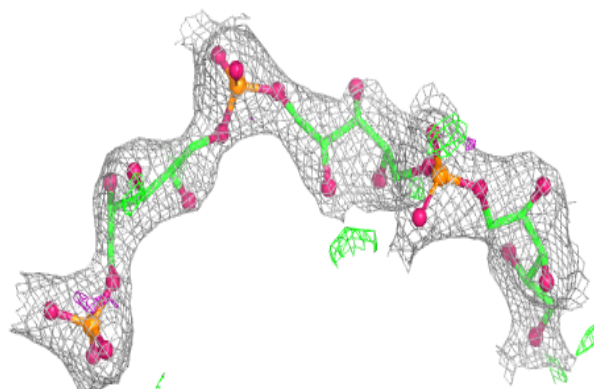


**Electron density around FQ8 G 401:**

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and green (positive)

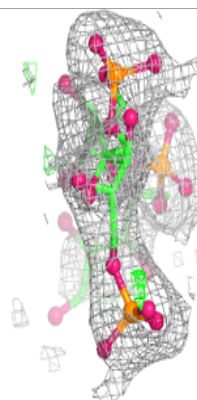
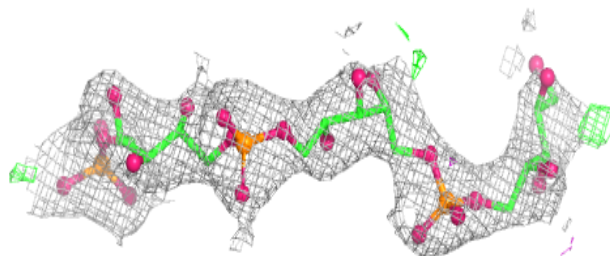
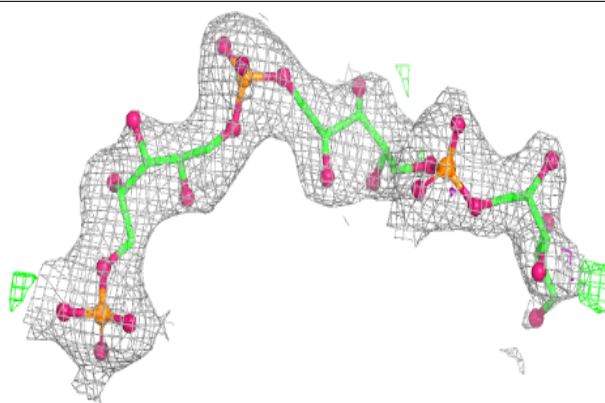
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and green (positive)



**Electron density around FQ8 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.