wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 10:25 pm BST

PDB ID	:	6H4M
Title	:	TarP-UDP-GlcNAc-3RboP
Authors	:	Guo, Y.; Stehle, T.
Deposited on	:	2018-07-22
Resolution	:	2.73 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

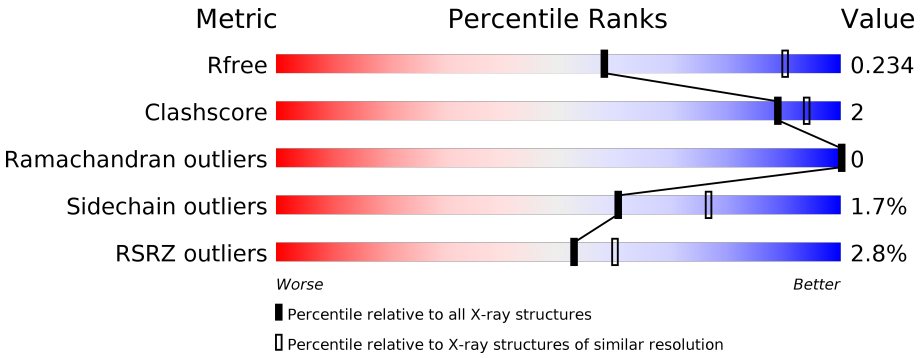
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 >=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 <=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	88% 8%
1	B	345	88% 8%
1	C	345	2% 87% 9%
1	D	345	87% 10%
1	E	345	88% 8%
1	F	345	87% 8%

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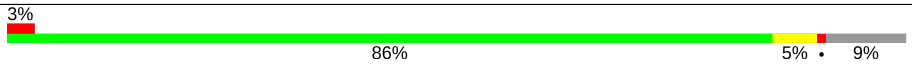
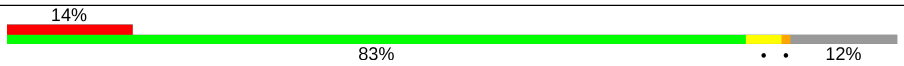
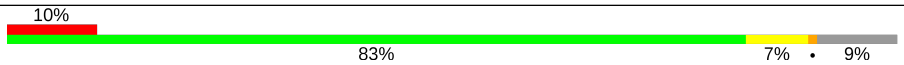
Mol	Chain	Length	Quality of chain
1	G	345	
1	H	345	
1	I	345	
1	O	345	
1	P	345	
1	Q	345	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 30905 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	317	Total	C	N	O	S	0	0	0
			2496	1606	412	470	8			
1	C	314	Total	C	N	O	S	0	0	0
			2431	1564	400	459	8			
1	F	316	Total	C	N	O	S	0	0	0
			2440	1574	395	463	8			
1	O	316	Total	C	N	O	S	0	0	0
			2464	1582	406	468	8			
1	P	305	Total	C	N	O	S	0	0	0
			2121	1355	359	401	6			
1	E	317	Total	C	N	O	S	0	0	0
			2476	1600	406	462	8			
1	G	314	Total	C	N	O	S	0	0	0
			2423	1562	398	455	8			
1	Q	314	Total	C	N	O	S	0	0	0
			2217	1413	377	421	6			
1	A	317	Total	C	N	O	S	0	0	0
			2488	1604	410	466	8			
1	D	312	Total	C	N	O	S	0	0	0
			2401	1549	398	446	8			
1	H	318	Total	C	N	O	S	0	0	0
			2522	1621	415	478	8			
1	I	315	Total	C	N	O	S	0	0	0
			2427	1558	400	461	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
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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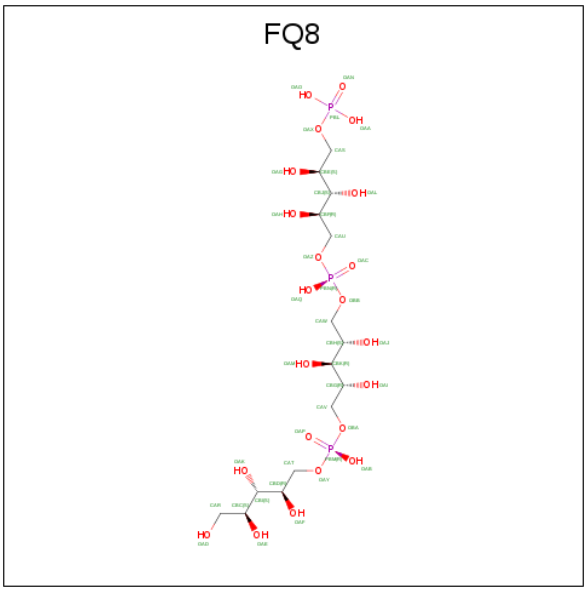
Chain	Residue	Modelled	Actual	Comment	Reference
I	0	SER	-	expression tag	UNP A0A0H3JNB0

- 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-phosphonoo xy-pentoxy]phosphoryl]oxy-pentyl] hydrogen phosphate (three-letter code: FQ8) (formula: $C_{15}H_{35}O_{22}P_3$).



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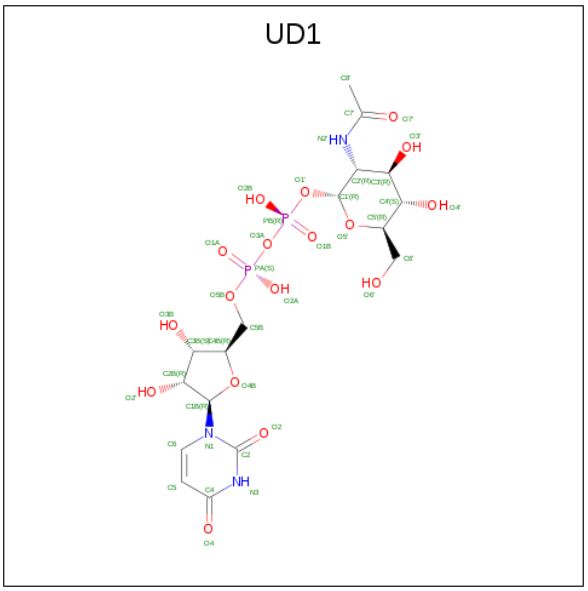
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	O	P	0	0
			40	15	22	3		
2	H	1	Total	C	O	P	0	0
			40	15	22	3		
2	I	1	Total	C	O	P	0	0
			40	15	22	3		

- Molecule 3 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	F	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	O	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	E	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	G	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	Q	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C N O P 39 17 3 17 2	0	0
3	H	1	Total C N O P 39 17 3 17 2	0	0
3	I	1	Total C N O P 39 17 3 17 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	Q	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	H	2	Total Mg 2 2	0	0
4	B	2	Total Mg 2 2	0	0
4	I	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	A	2	Total Mg 2 2	0	0
4	O	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0

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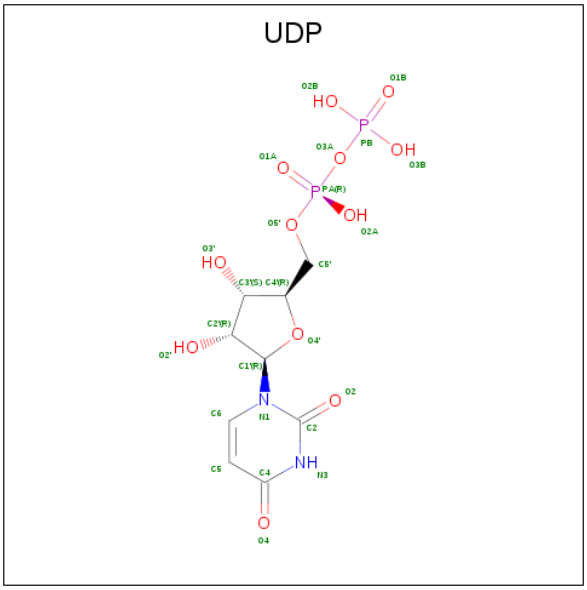
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total Cl 1 1	0	0
5	H	2	Total Cl 2 2	0	0
5	B	2	Total Cl 2 2	0	0
5	I	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	A	1	Total Cl 1 1	0	0
5	O	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0

- Molecule 6 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	P	1	Total C N O P 25 9 2 12 2	0	0

- Molecule 7 is water.

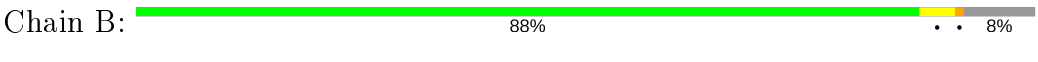
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	125	Total O 125 125	0	0
7	C	86	Total O 86 86	0	0
7	F	80	Total O 80 80	0	0
7	O	93	Total O 93 93	0	0
7	P	53	Total O 53 53	0	0
7	E	103	Total O 103 103	0	0
7	G	79	Total O 79 79	0	0
7	Q	48	Total O 48 48	0	0
7	A	108	Total O 108 108	0	0
7	D	89	Total O 89 89	0	0
7	H	105	Total O 105 105	0	0
7	I	69	Total O 69 69	0	0

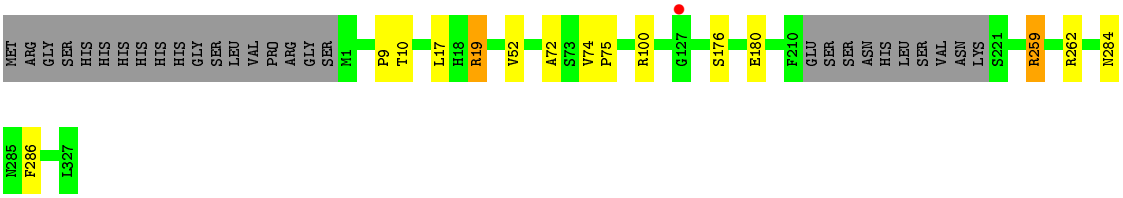
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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

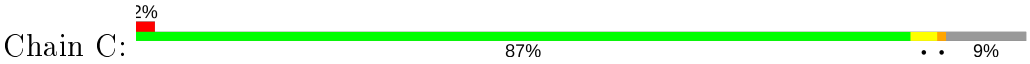
Chain B:

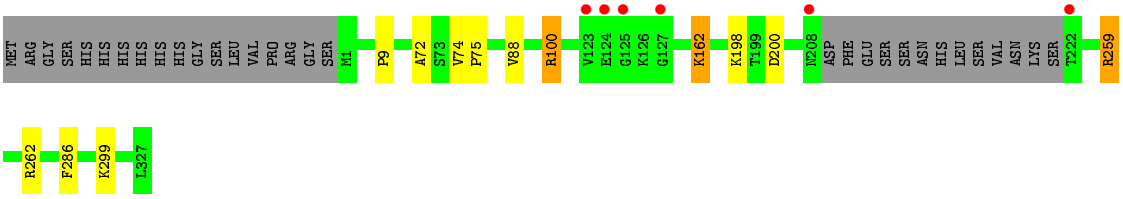




- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

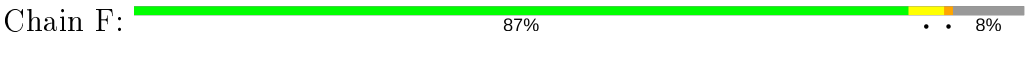
Chain C:

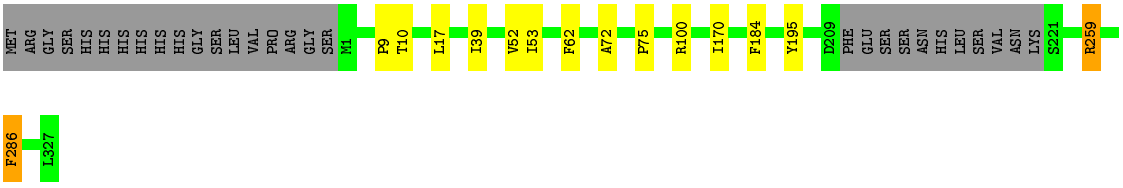




- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

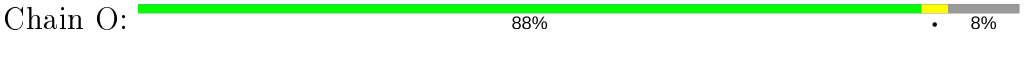
Chain F:

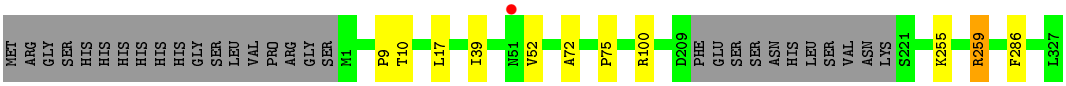




- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

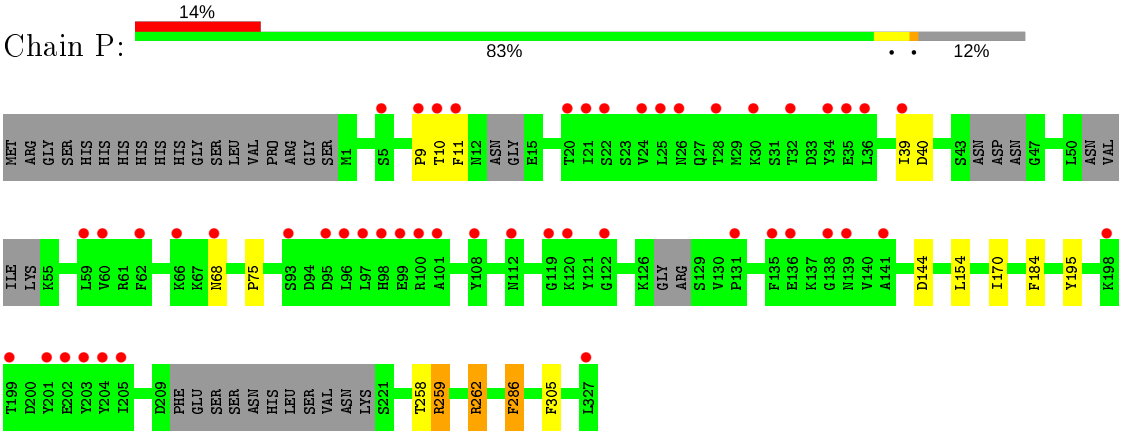
Chain O:





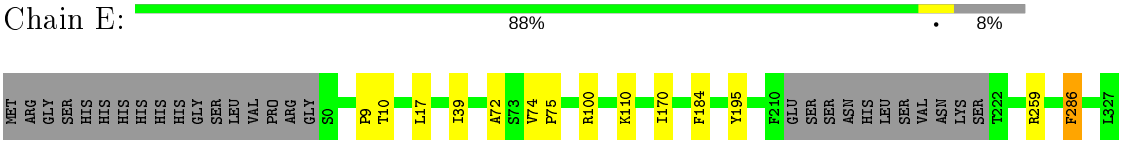
• Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

Chain P:



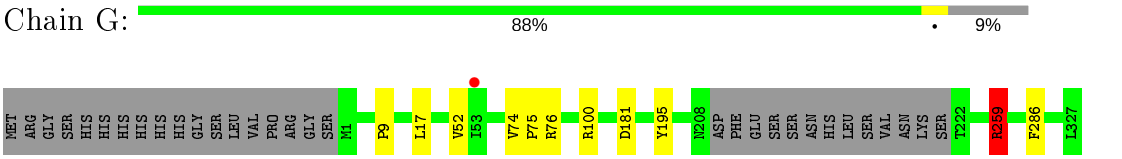
• Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

Chain E:



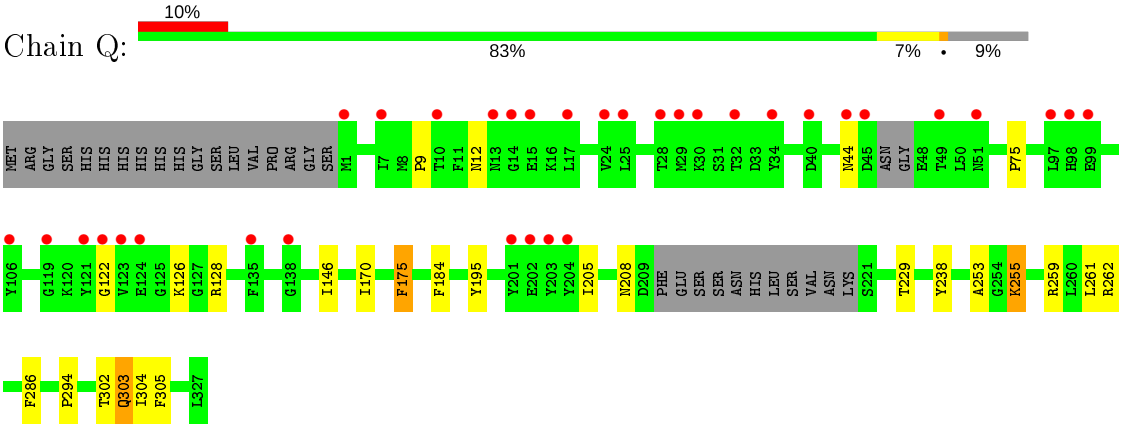
• Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

Chain G:



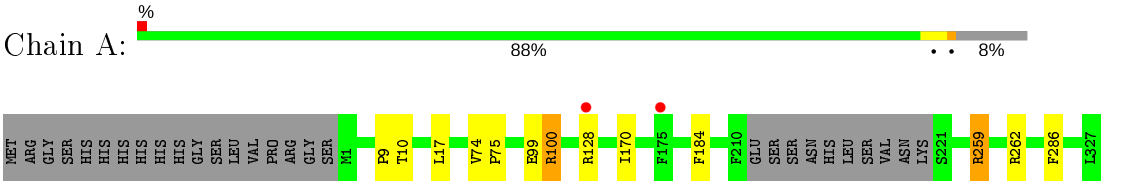
• Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

Chain Q:



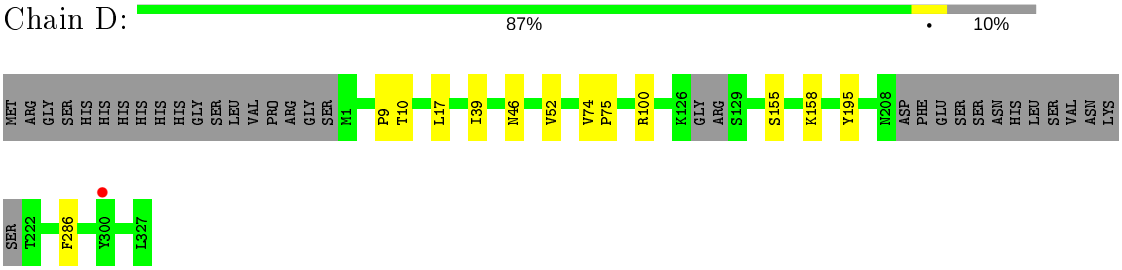
• Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

Chain A:



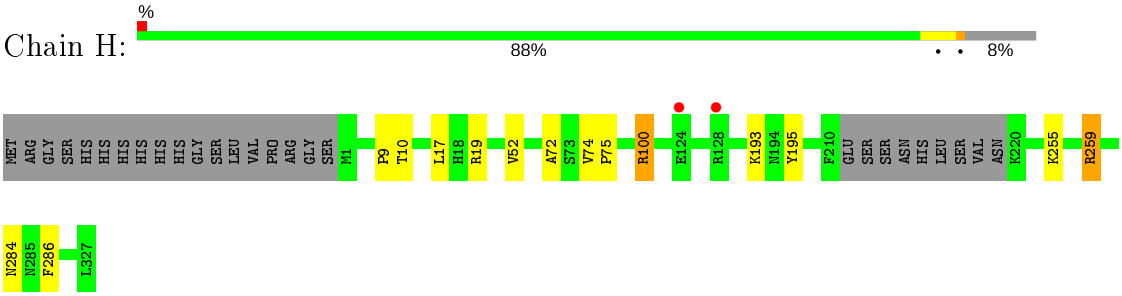
• Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

Chain D:



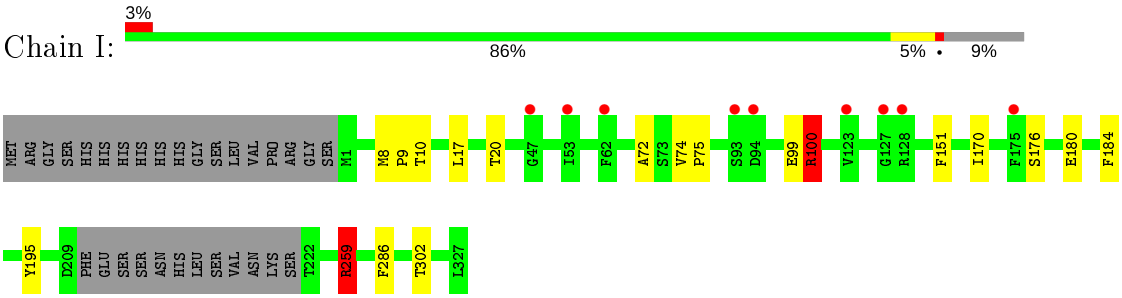
• Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

Chain H:



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

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.17Å 210.75Å 123.20Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	48.44 – 2.73 48.44 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.44-2.73) 99.9 (48.44-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.189 , 0.233 0.191 , 0.234	Depositor DCC
R_{free} test set	6412 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	45.3	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	30905	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FQ8, MG, UD1, UDP, 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	0.41	0/2532	0.55	0/3417
1	B	0.40	0/2538	0.56	0/3423
1	C	0.38	0/2472	0.53	0/3341
1	D	0.40	0/2442	0.55	0/3303
1	E	0.41	0/2519	0.55	0/3399
1	F	0.39	0/2481	0.54	0/3354
1	G	0.39	0/2464	0.55	0/3332
1	H	0.41	0/2565	0.59	0/3456
1	I	0.38	0/2468	0.54	0/3338
1	O	0.39	0/2506	0.54	0/3384
1	P	0.39	0/2152	0.55	1/2922 (0.0%)
1	Q	0.42	0/2250	0.56	0/3060
All	All	0.40	0/29389	0.55	1/39729 (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	A	0	1
1	B	0	3
1	C	0	2
1	D	0	1
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	O	0	2
1	P	0	1
1	Q	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	19

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	144	ASP	CB-CG-OD1	5.42	123.18	118.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	100	ARG	Sidechain
1	B	19	ARG	Sidechain
1	B	259	ARG	Sidechain
1	C	100	ARG	Sidechain
1	C	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	2488	0	2398	7	0
1	B	2496	0	2423	8	0
1	C	2431	0	2308	7	0
1	D	2401	0	2274	7	0
1	E	2476	0	2387	7	0
1	F	2440	0	2303	8	0
1	G	2423	0	2299	5	0
1	H	2522	0	2459	8	0
1	I	2427	0	2288	13	0
1	O	2464	0	2360	6	0
1	P	2121	0	1726	13	0
1	Q	2217	0	1853	17	0
2	A	40	0	0	1	0
2	B	40	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	40	0	0	2	0
2	D	40	0	0	0	0
2	E	40	0	0	0	0
2	F	40	0	0	1	0
2	G	40	0	0	1	0
2	H	40	0	0	0	0
2	I	40	0	0	3	0
2	O	40	0	0	1	0
2	P	40	0	0	3	0
2	Q	40	0	0	1	0
3	A	39	0	25	1	0
3	B	39	0	25	1	0
3	C	39	0	25	1	0
3	D	39	0	25	0	0
3	E	39	0	25	1	0
3	F	39	0	25	1	0
3	G	39	0	25	0	0
3	H	39	0	25	1	0
3	I	39	0	25	1	0
3	O	39	0	25	1	0
3	Q	39	0	25	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
4	I	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	H	2	0	0	0	0
5	I	1	0	0	0	0
5	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	1	0	0	0	0
6	P	25	0	11	1	0
7	A	108	0	0	0	0
7	B	125	0	0	0	0
7	C	86	0	0	0	0
7	D	89	0	0	0	0
7	E	103	0	0	0	0
7	F	80	0	0	0	0
7	G	79	0	0	0	0
7	H	105	0	0	0	0
7	I	69	0	0	0	0
7	O	93	0	0	0	0
7	P	53	0	0	0	0
7	Q	48	0	0	0	0
All	All	30905	0	27364	108	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 2.

The worst 5 of 108 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:P:9:PRO:O	6:P:402:UDP:O2'	2.02	0.78
1:B:262:ARG:NH1	2:B:401:FQ8:OAO	2.23	0.70
2:C:401:FQ8:OAP	2:C:401:FQ8:OAF	2.09	0.69
1:Q:302:THR:HG22	1:Q:304:ILE:HG22	1.76	0.68
1:P:259:ARG:NH2	2:P:401:FQ8:OAP	2.27	0.67

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	313/345 (91%)	306 (98%)	7 (2%)	0	100	100
1	C	310/345 (90%)	302 (97%)	8 (3%)	0	100	100
1	D	306/345 (89%)	298 (97%)	8 (3%)	0	100	100
1	E	313/345 (91%)	304 (97%)	9 (3%)	0	100	100
1	F	312/345 (90%)	305 (98%)	7 (2%)	0	100	100
1	G	310/345 (90%)	302 (97%)	8 (3%)	0	100	100
1	H	314/345 (91%)	306 (98%)	8 (2%)	0	100	100
1	I	311/345 (90%)	303 (97%)	8 (3%)	0	100	100
1	O	312/345 (90%)	304 (97%)	8 (3%)	0	100	100
1	P	293/345 (85%)	283 (97%)	10 (3%)	0	100	100
1	Q	308/345 (89%)	300 (97%)	8 (3%)	0	100	100
All	All	3715/4140 (90%)	3617 (97%)	98 (3%)	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	250/313 (80%)	247 (99%)	3 (1%)	71	83
1	B	253/313 (81%)	249 (98%)	4 (2%)	62	78
1	C	238/313 (76%)	233 (98%)	5 (2%)	53	72
1	D	233/313 (74%)	231 (99%)	2 (1%)	78	87
1	E	246/313 (79%)	241 (98%)	5 (2%)	55	72
1	F	235/313 (75%)	232 (99%)	3 (1%)	69	82
1	G	235/313 (75%)	232 (99%)	3 (1%)	69	82
1	H	260/313 (83%)	254 (98%)	6 (2%)	50	70
1	I	236/313 (75%)	232 (98%)	4 (2%)	60	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	248/313 (79%)	246 (99%)	2 (1%)	81 89
1	P	154/313 (49%)	151 (98%)	3 (2%)	57 74
1	Q	169/313 (54%)	163 (96%)	6 (4%)	35 55
All	All	2757/3756 (73%)	2711 (98%)	46 (2%)	60 76

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	259	ARG
1	Q	175	PHE
1	I	100	ARG
1	E	286	PHE
1	G	259	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	303	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 51 ligands modelled in this entry, 27 are monoatomic - leaving 24 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	1.03	2 (5%)	54,56,56	0.86	1 (1%)
3	UD1	Q	402	-	34,41,41	0.74	1 (2%)	45,62,62	1.11	4 (8%)
2	FQ8	G	401	-	39,39,39	1.17	4 (10%)	54,56,56	1.02	3 (5%)
2	FQ8	E	401	-	39,39,39	1.21	3 (7%)	54,56,56	0.95	1 (1%)
2	FQ8	C	401	-	39,39,39	1.00	2 (5%)	54,56,56	0.82	1 (1%)
2	FQ8	D	401	-	39,39,39	1.01	2 (5%)	54,56,56	0.83	1 (1%)
3	UD1	B	402	4	34,41,41	0.66	1 (2%)	45,62,62	1.01	2 (4%)
2	FQ8	Q	401	-	39,39,39	1.04	2 (5%)	54,56,56	0.85	3 (5%)
2	FQ8	I	401	-	39,39,39	1.08	2 (5%)	54,56,56	1.02	3 (5%)
3	UD1	G	402	4	34,41,41	0.70	1 (2%)	45,62,62	1.03	3 (6%)
2	FQ8	P	401	-	39,39,39	1.11	4 (10%)	54,56,56	0.97	2 (3%)
2	FQ8	A	401	-	39,39,39	1.03	2 (5%)	54,56,56	0.85	1 (1%)
3	UD1	D	402	4	34,41,41	0.66	0	45,62,62	1.07	3 (6%)
3	UD1	I	402	4	34,41,41	0.61	1 (2%)	45,62,62	1.06	2 (4%)
3	UD1	F	402	4	34,41,41	0.64	0	45,62,62	1.42	5 (11%)
2	FQ8	F	401	-	39,39,39	1.34	5 (12%)	54,56,56	1.02	3 (5%)
3	UD1	O	402	4	34,41,41	0.64	1 (2%)	45,62,62	1.10	2 (4%)
3	UD1	E	402	4	34,41,41	0.65	1 (2%)	45,62,62	1.12	5 (11%)
3	UD1	H	402	4	34,41,41	0.63	0	45,62,62	1.28	5 (11%)
3	UD1	C	402	4	34,41,41	0.60	0	45,62,62	0.97	1 (2%)
3	UD1	A	402	4	34,41,41	0.63	1 (2%)	45,62,62	0.98	1 (2%)
2	FQ8	H	401	-	39,39,39	1.04	2 (5%)	54,56,56	0.84	2 (3%)
6	UDP	P	402	-	20,26,26	0.90	1 (5%)	25,40,40	1.29	2 (8%)
2	FQ8	O	401	-	39,39,39	1.11	2 (5%)	54,56,56	1.30	9 (16%)

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	-	-	31/56/56/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UD1	Q	402	-	-	7/24/63/63	0/3/3/3
2	FQ8	G	401	-	-	31/56/56/56	-
2	FQ8	E	401	-	-	34/56/56/56	-
2	FQ8	C	401	-	-	34/56/56/56	-
2	FQ8	D	401	-	-	30/56/56/56	-
3	UD1	B	402	4	-	10/24/63/63	0/3/3/3
2	FQ8	Q	401	-	-	34/56/56/56	-
2	FQ8	I	401	-	-	34/56/56/56	-
3	UD1	G	402	4	-	10/24/63/63	0/3/3/3
2	FQ8	P	401	-	-	34/56/56/56	-
2	FQ8	A	401	-	-	35/56/56/56	-
3	UD1	D	402	4	-	10/24/63/63	0/3/3/3
3	UD1	I	402	4	-	9/24/63/63	0/3/3/3
3	UD1	F	402	4	-	10/24/63/63	0/3/3/3
2	FQ8	F	401	-	-	28/56/56/56	-
3	UD1	O	402	4	-	9/24/63/63	0/3/3/3
3	UD1	E	402	4	-	6/24/63/63	0/3/3/3
3	UD1	H	402	4	-	7/24/63/63	0/3/3/3
3	UD1	C	402	4	-	10/24/63/63	0/3/3/3
3	UD1	A	402	4	-	8/24/63/63	0/3/3/3
2	FQ8	H	401	-	-	36/56/56/56	-
6	UDP	P	402	-	-	7/14/32/32	0/2/2/2
2	FQ8	O	401	-	-	21/56/56/56	-

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	FQ8	PBL-OAN	4.43	1.64	1.50
2	E	401	FQ8	PBL-OAN	4.27	1.64	1.50
2	G	401	FQ8	PBL-OAN	3.71	1.62	1.50
2	F	401	FQ8	PBM-OAP	3.67	1.63	1.50
2	A	401	FQ8	PBL-OAN	3.53	1.61	1.50

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	402	UD1	C8'-C7'-N2'	-4.28	108.84	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	402	UD1	C8'-C7'-N2'	-3.81	109.65	116.10
3	C	402	UD1	PB-O3A-PA	-3.79	119.83	132.83
6	P	402	UDP	PA-O3A-PB	-3.78	119.87	132.83
3	I	402	UD1	PB-O3A-PA	-3.54	120.69	132.83

There are no chirality outliers.

5 of 485 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	FQ8	CAU-OAZ-PBN-OAQ
2	B	401	FQ8	CAU-OAZ-PBN-OBB
2	B	401	FQ8	OBB-CAW-CBH-OAJ
2	B	401	FQ8	OBB-CAW-CBH-CBK
2	B	401	FQ8	OBA-CAV-CBG-CBK

There are no ring outliers.

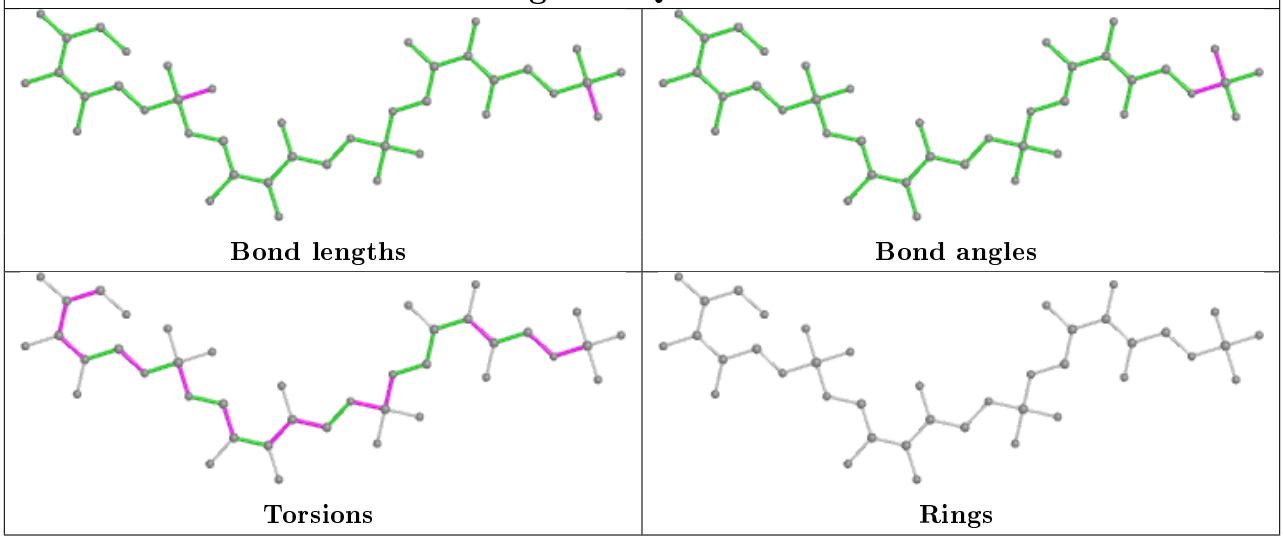
18 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	FQ8	1	0
2	G	401	FQ8	1	0
2	C	401	FQ8	2	0
3	B	402	UD1	1	0
2	Q	401	FQ8	1	0
2	I	401	FQ8	3	0
2	P	401	FQ8	3	0
2	A	401	FQ8	1	0
3	I	402	UD1	1	0
3	F	402	UD1	1	0
2	F	401	FQ8	1	0
3	O	402	UD1	1	0
3	E	402	UD1	1	0
3	H	402	UD1	1	0
3	C	402	UD1	1	0
3	A	402	UD1	1	0
6	P	402	UDP	1	0
2	O	401	FQ8	1	0

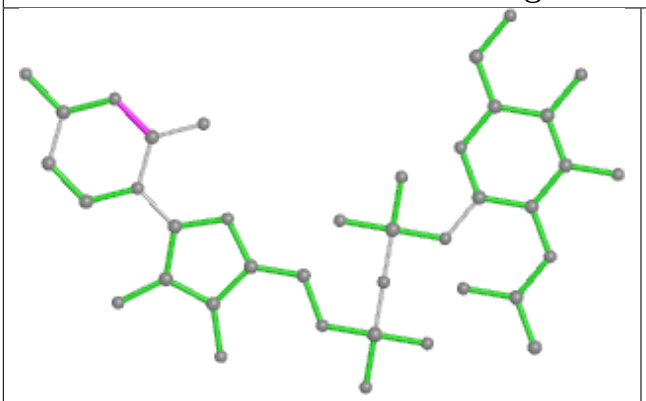
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

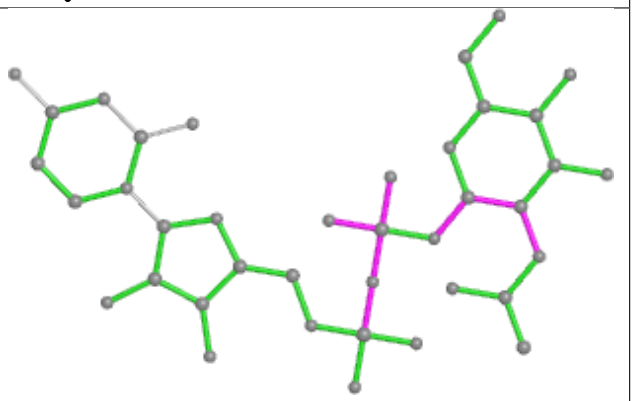
Ligand FQ8 B 401



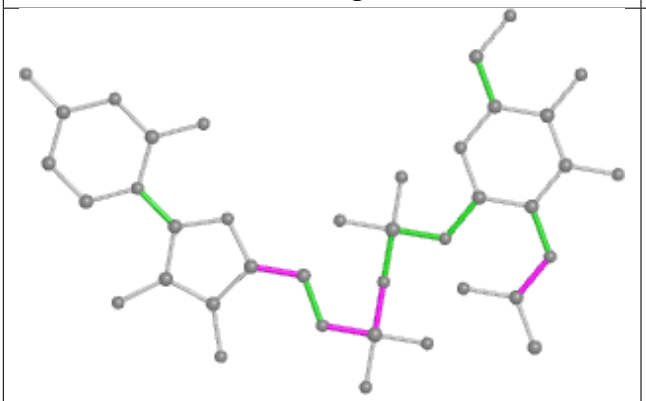
Ligand UD1 Q 402



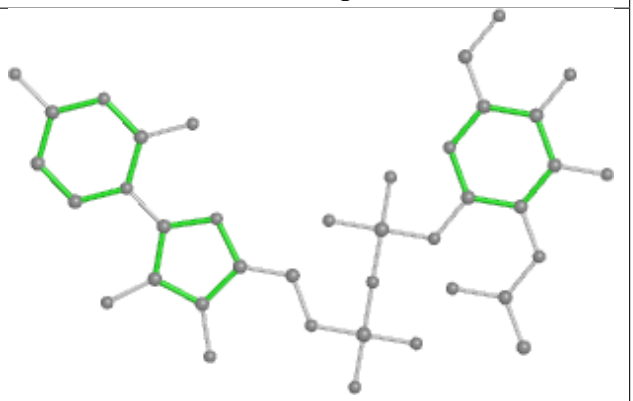
Bond lengths



Bond angles

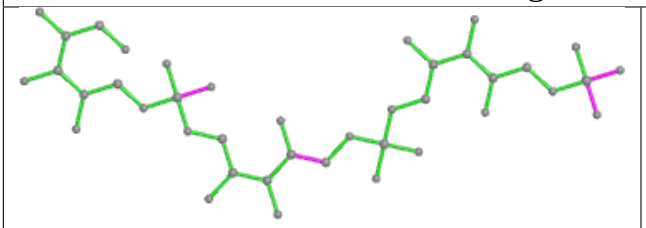


Torsions



Rings

Ligand FQ8 G 401



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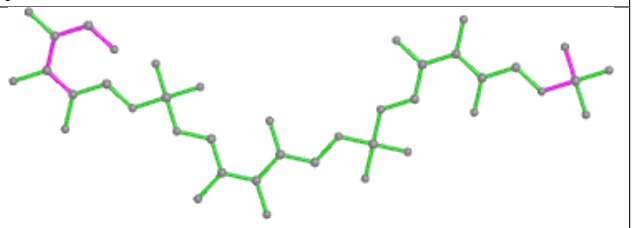

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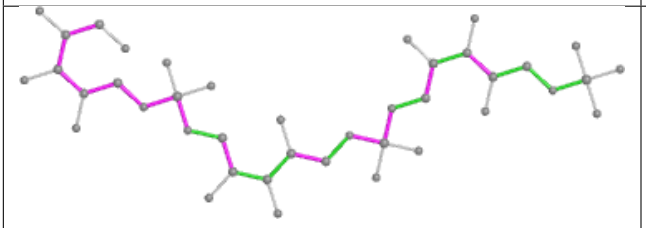

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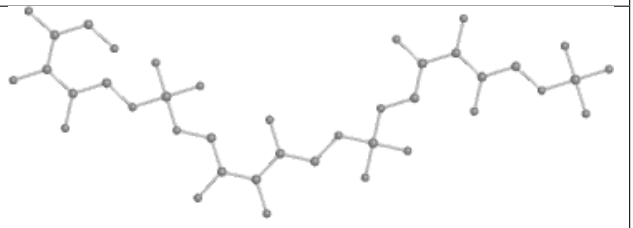
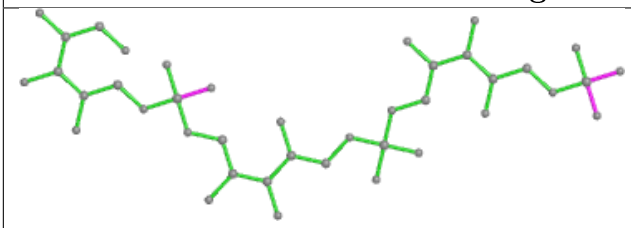
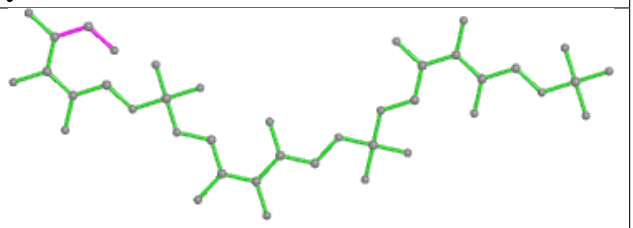


Rings

Ligand FQ8 E 401



Bond lengths



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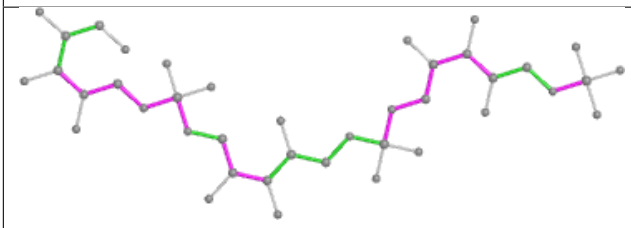

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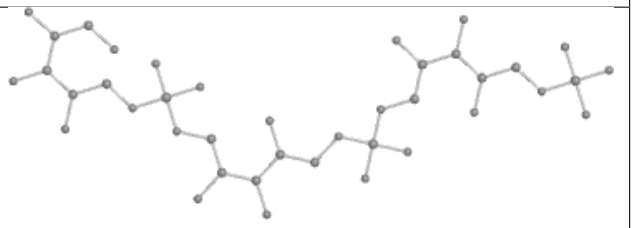
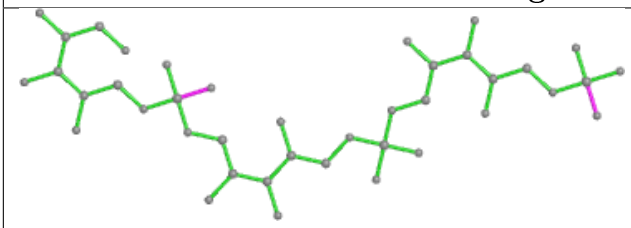
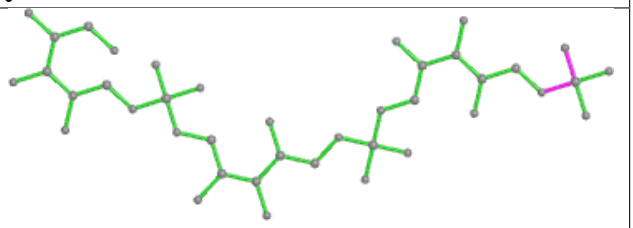


Rings

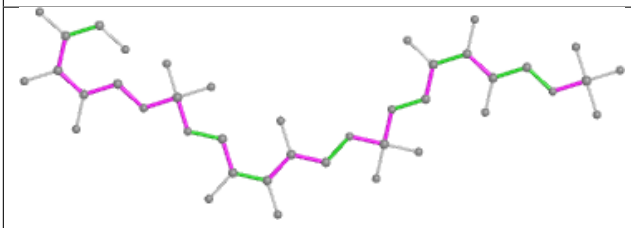
Ligand FQ8 C 401



Bond lengths



Bond angles



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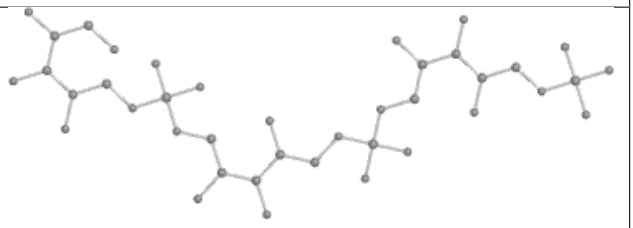
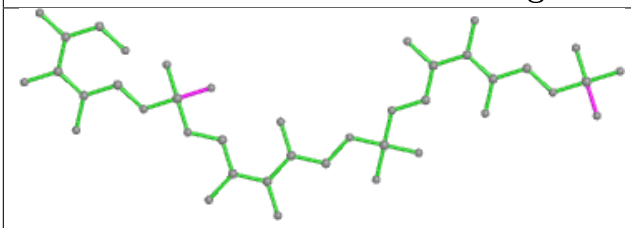


Rings

Ligand FQ8 D 401



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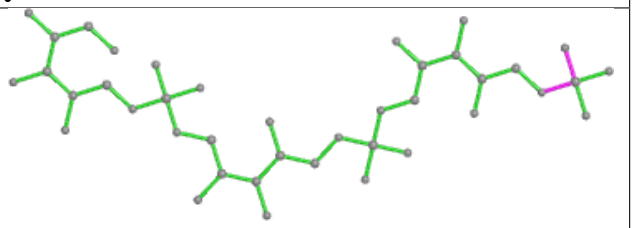
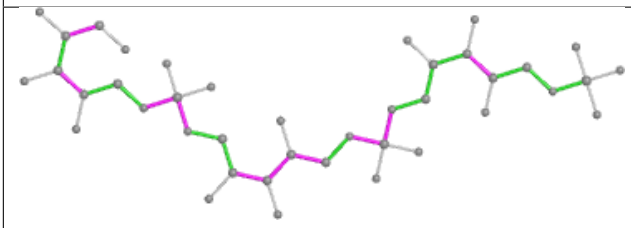


Bond angles



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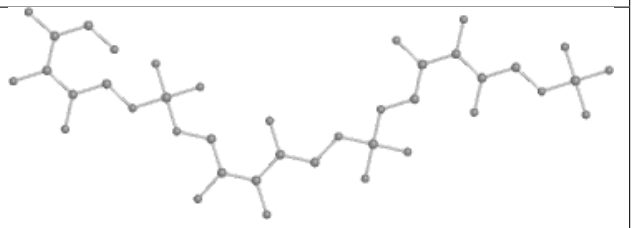
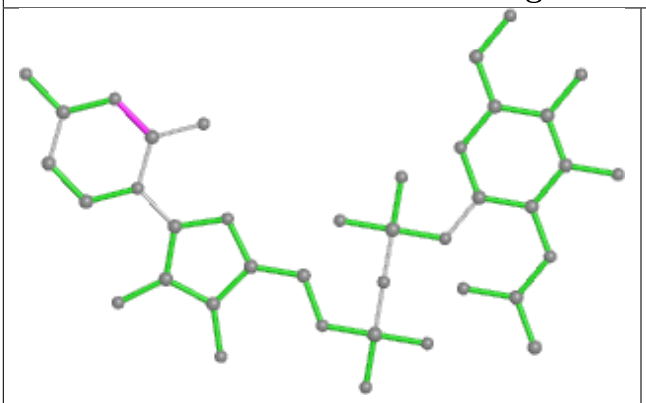


Rings

Ligand UD1 B 402



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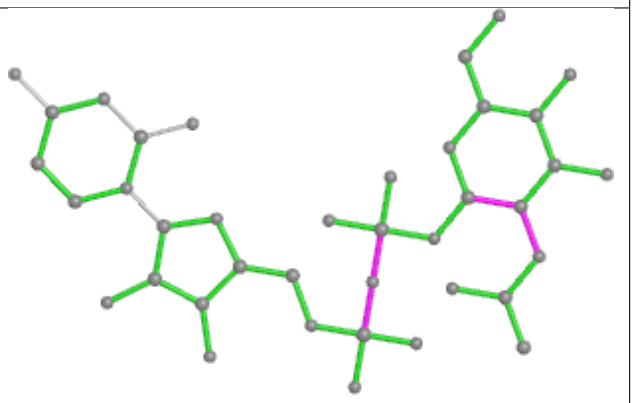
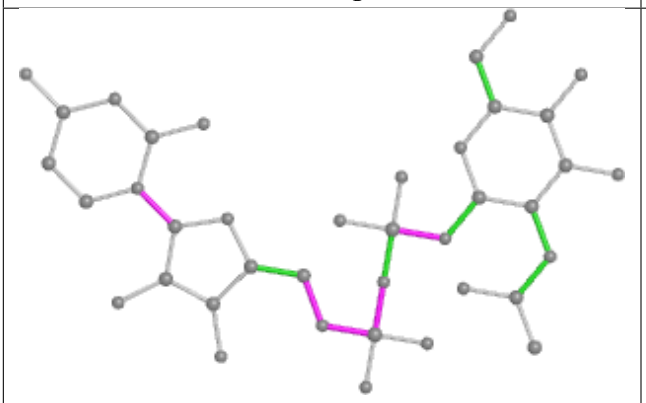


Bond angles



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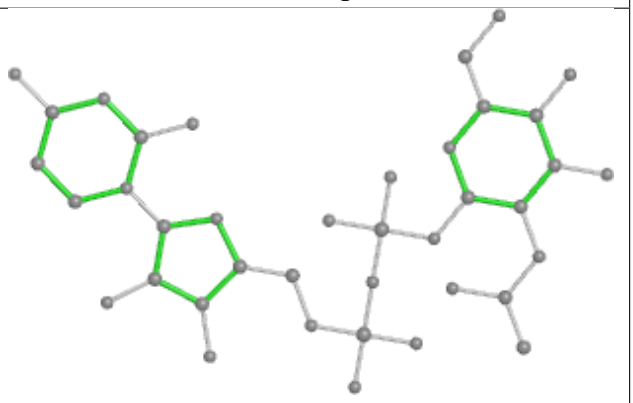
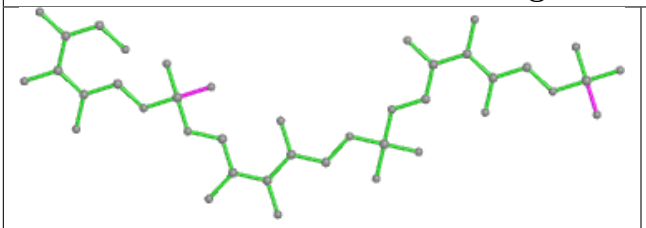


Rings

Ligand FQ8 Q 401



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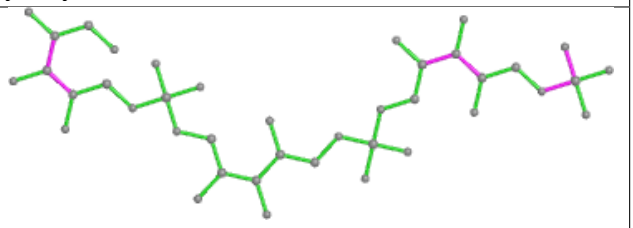
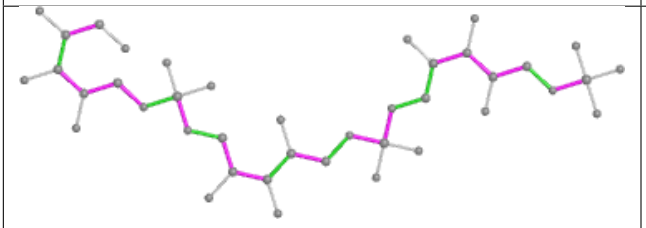


Bond angles



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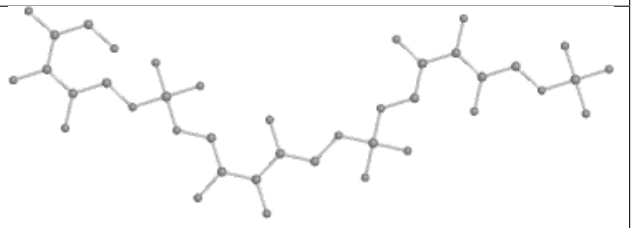
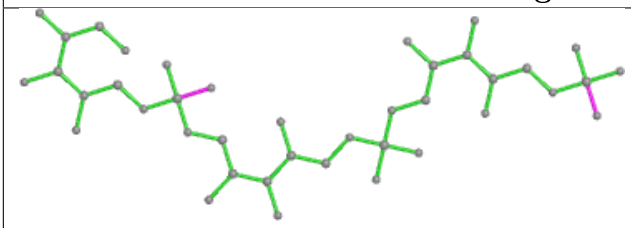


Rings

Ligand FQ8 I 401



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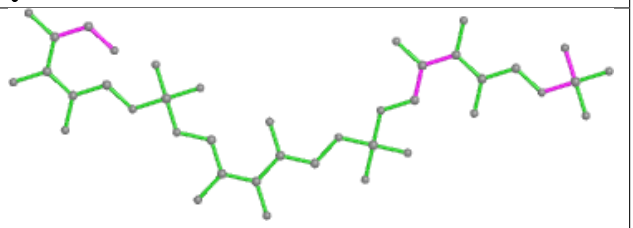
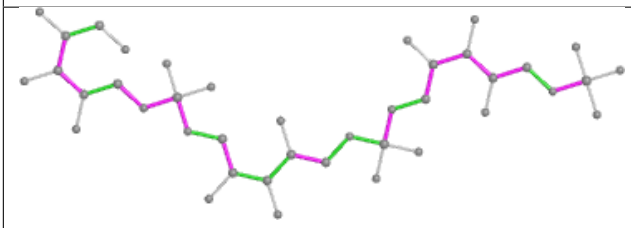
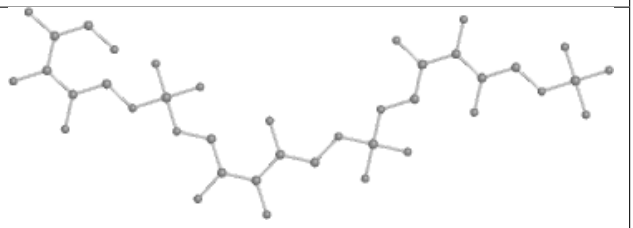


Bond angles

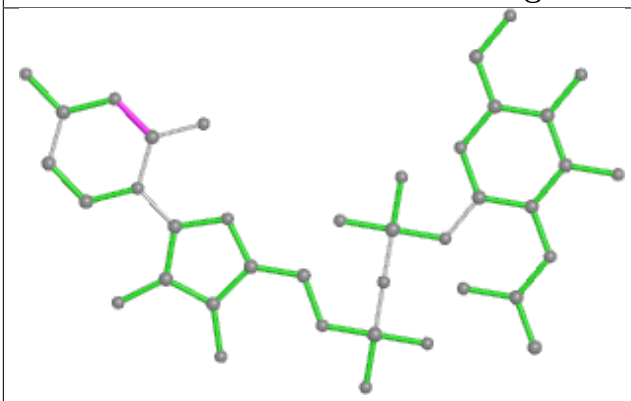


Torsions



Rings

Ligand UD1 G 402



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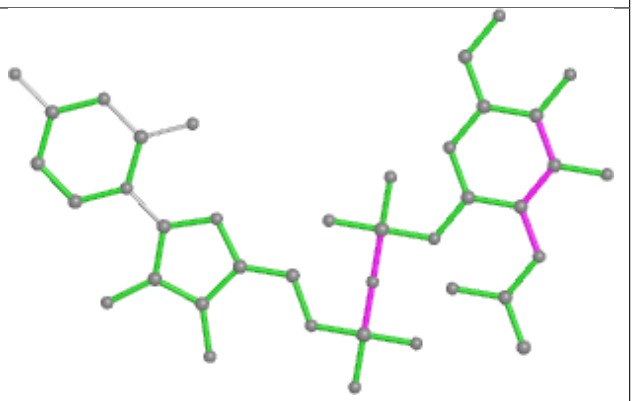
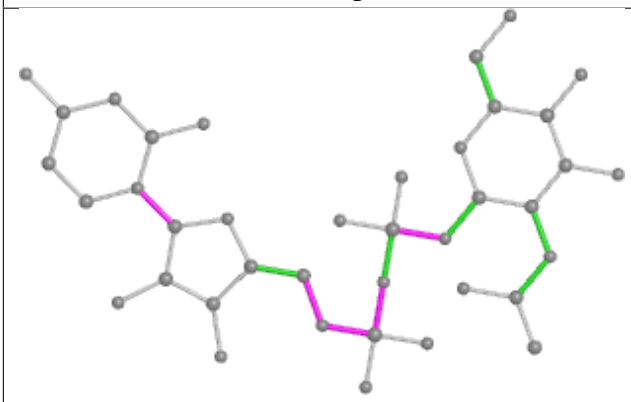


Bond angles



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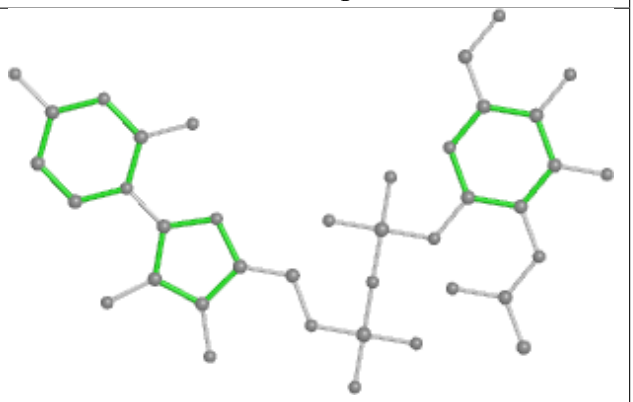
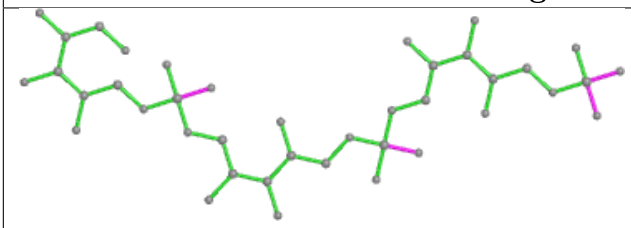


Rings

Ligand FQ8 P 401



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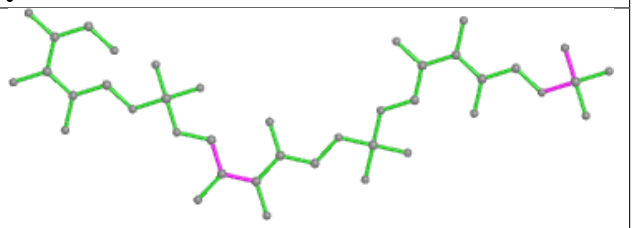

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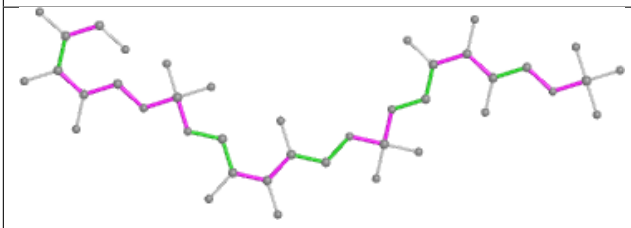

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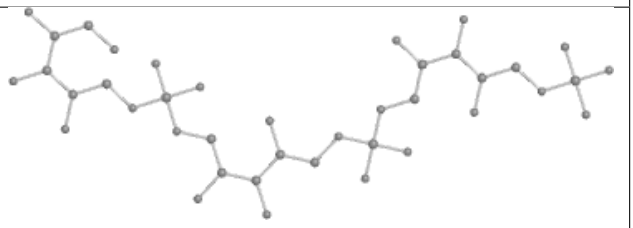
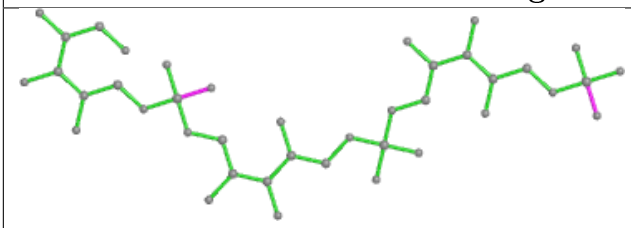


Rings

Ligand FQ8 A 401



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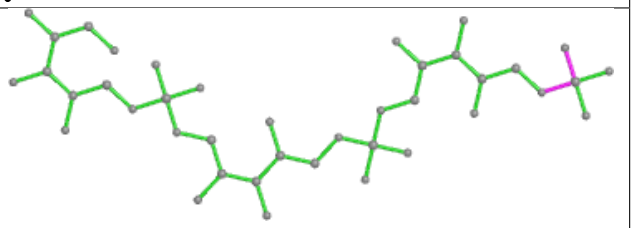
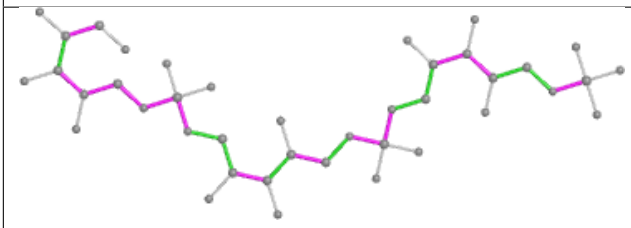


Bond angles



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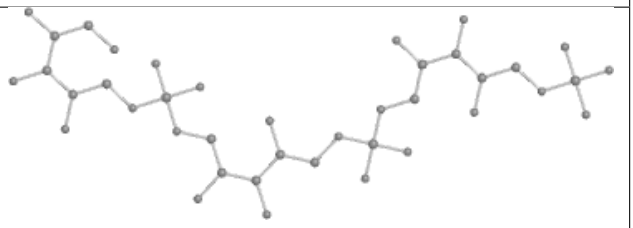
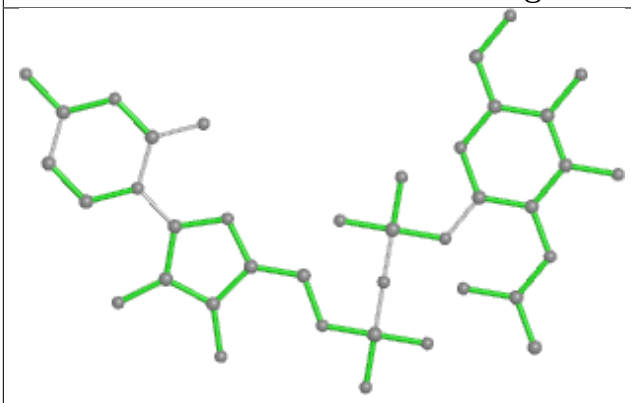


Rings

Ligand UD1 D 402



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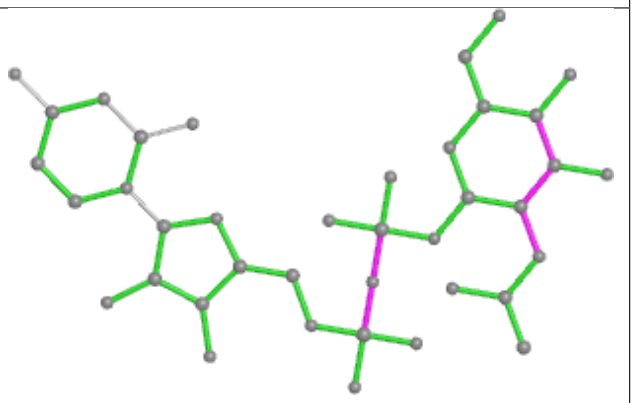

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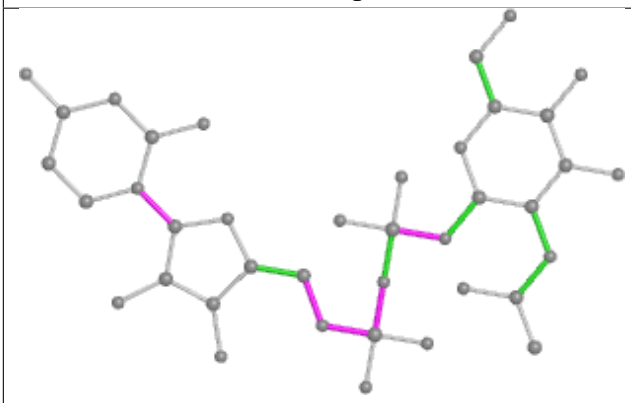

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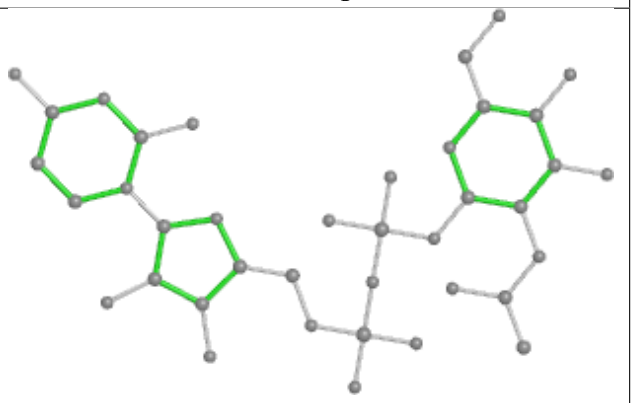
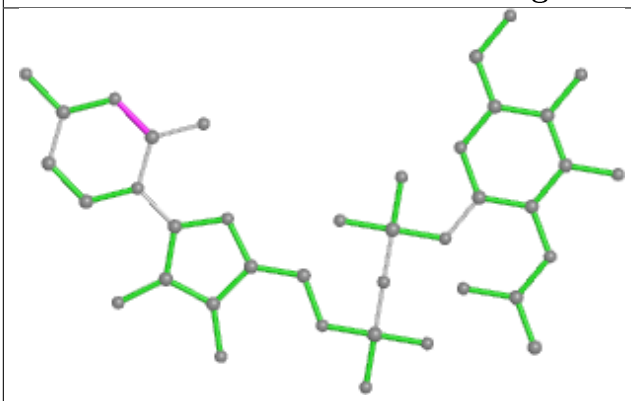


Rings

Ligand UD1 I 402



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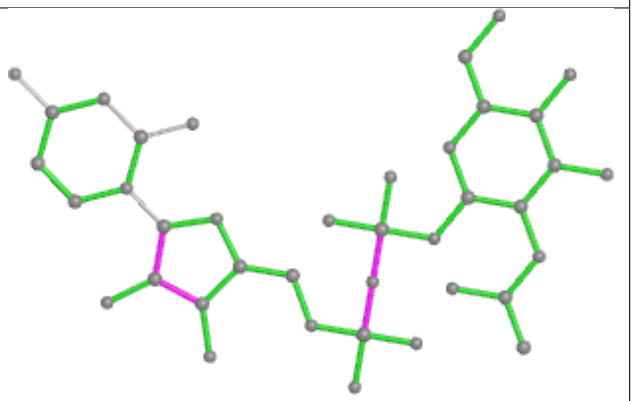

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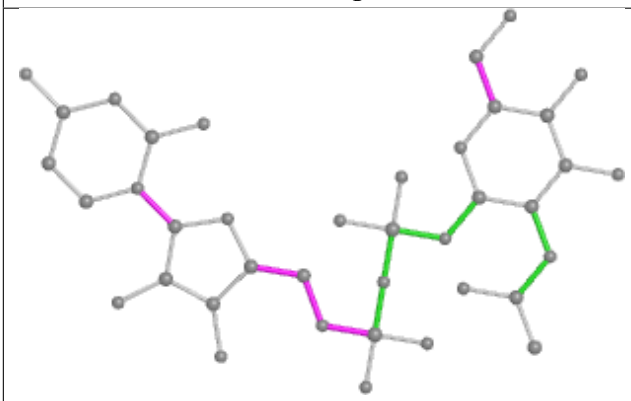

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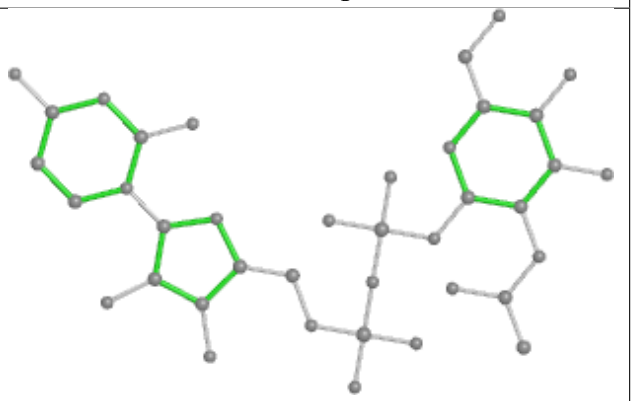
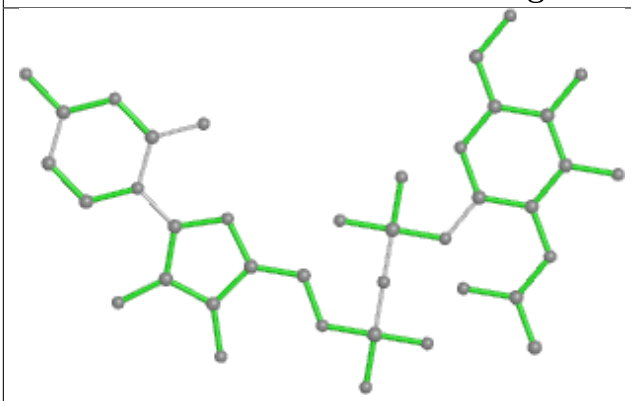


Rings

Ligand UD1 F 402



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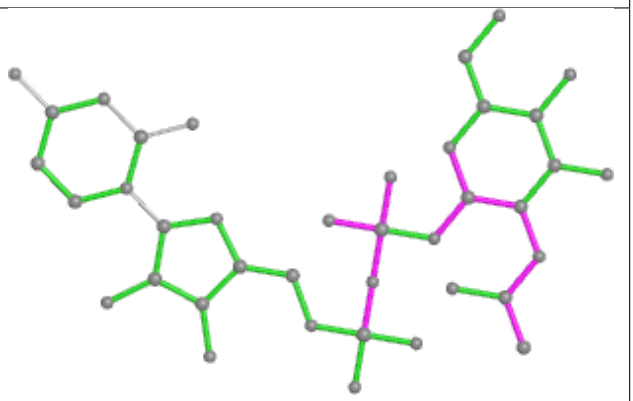

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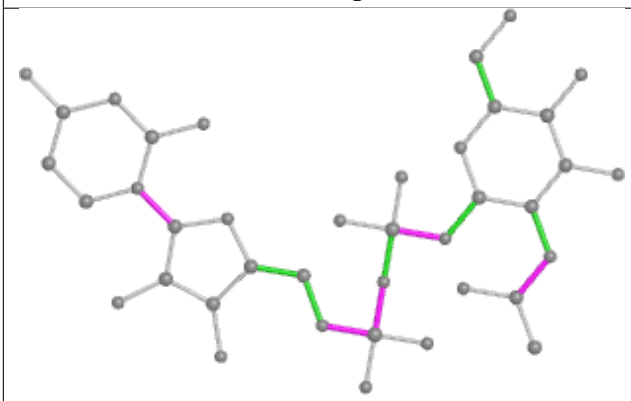

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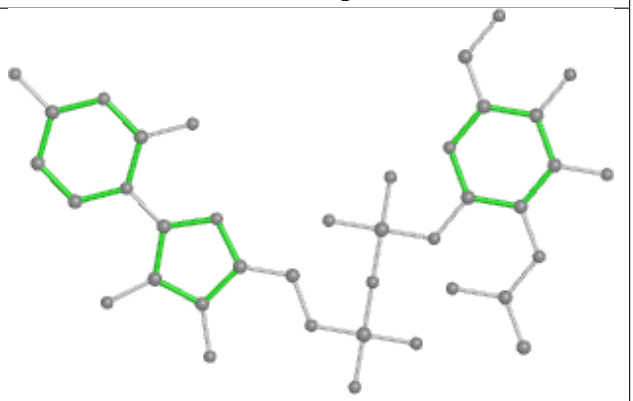
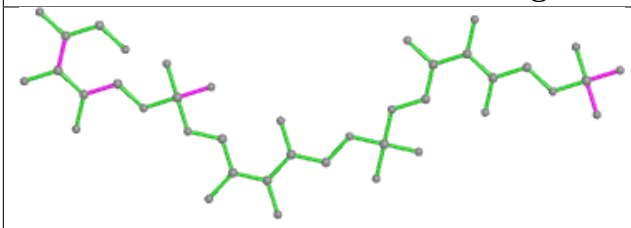


Rings

Ligand FQ8 F 401



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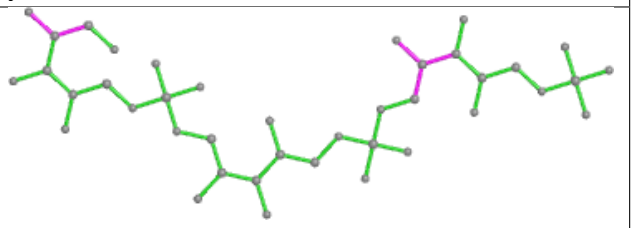

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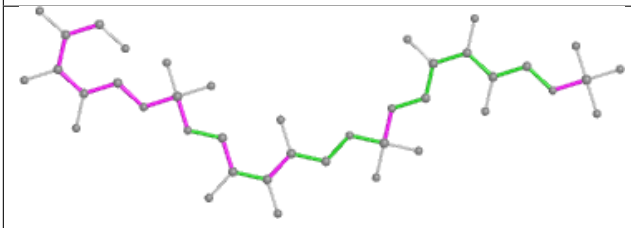

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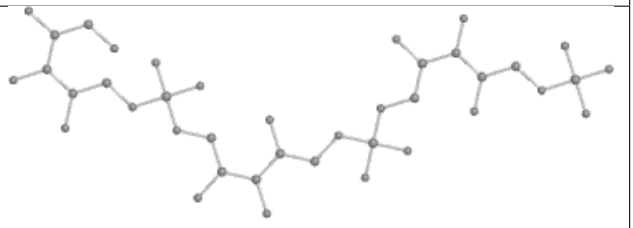
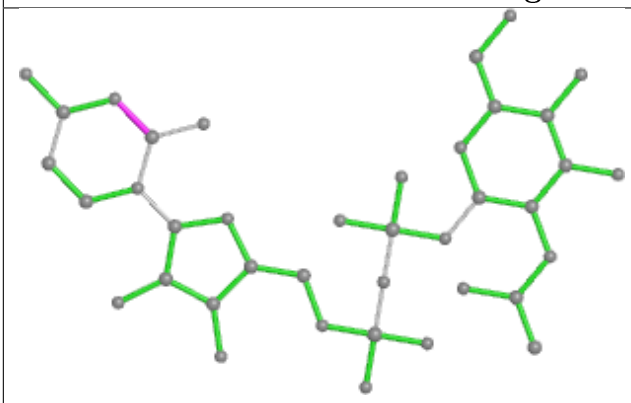


Rings

Ligand UD1 O 402



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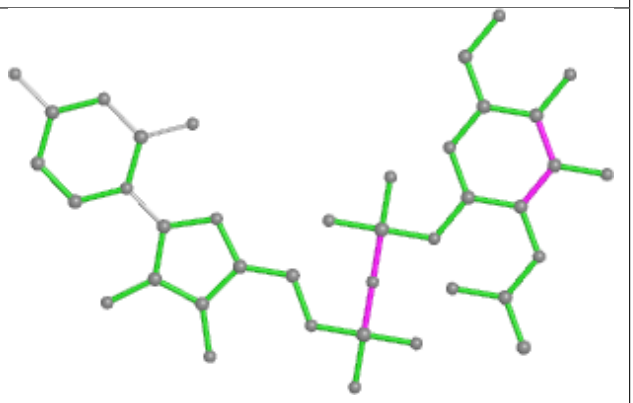
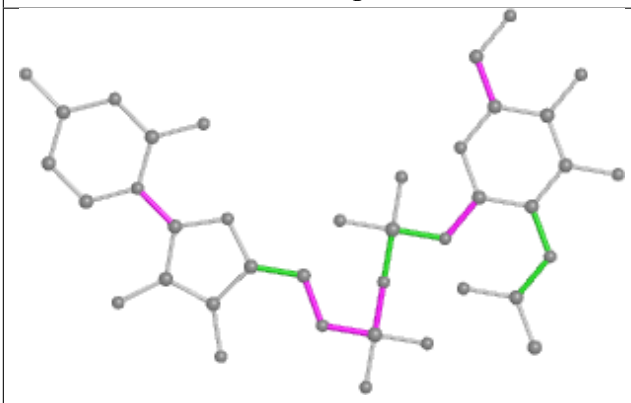


Bond angles



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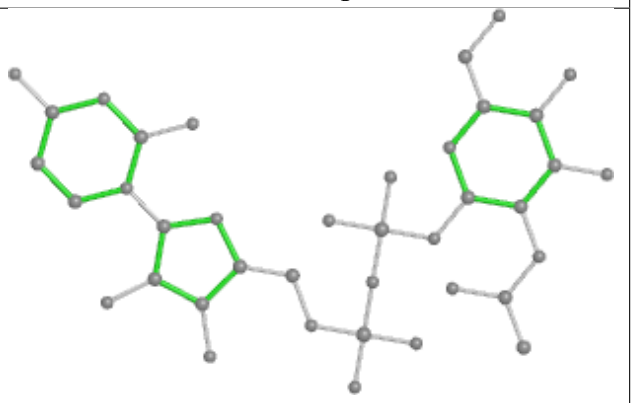
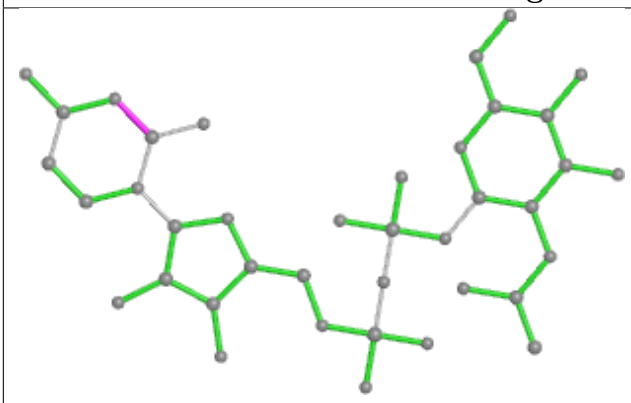


Rings

Ligand UD1 E 402



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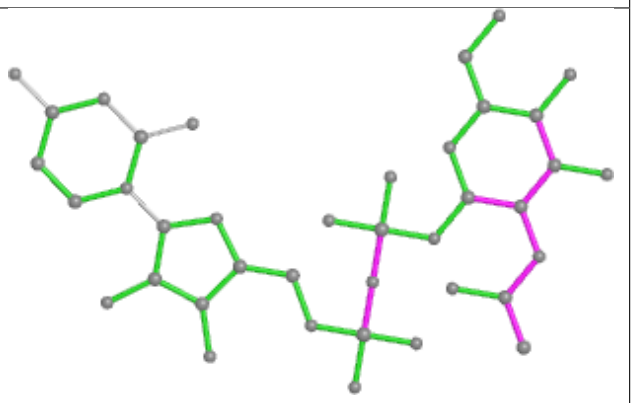
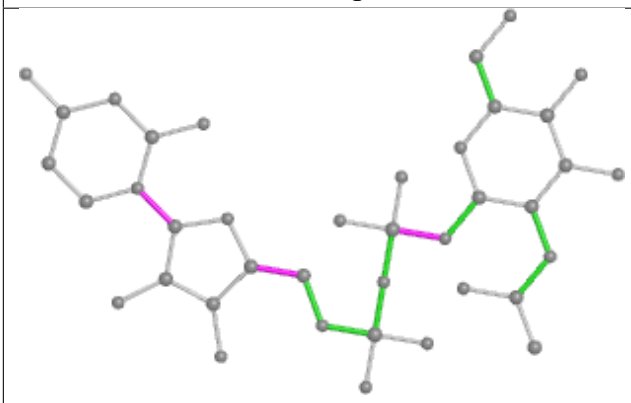


Bond angles



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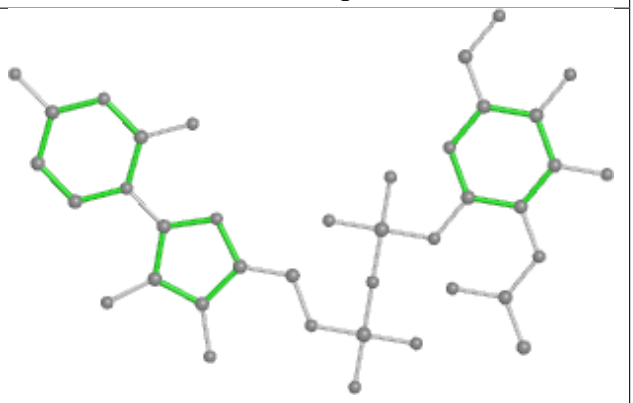
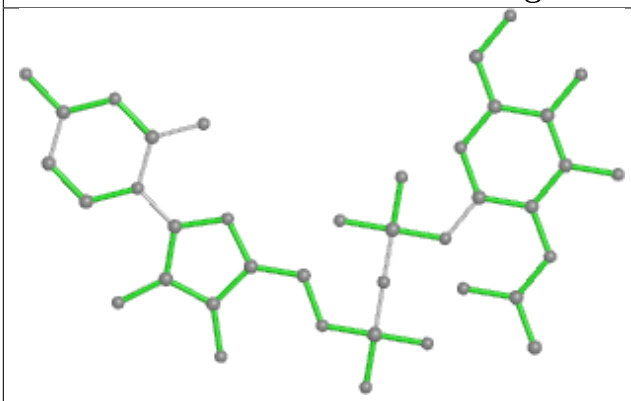


Rings

Ligand UD1 H 402



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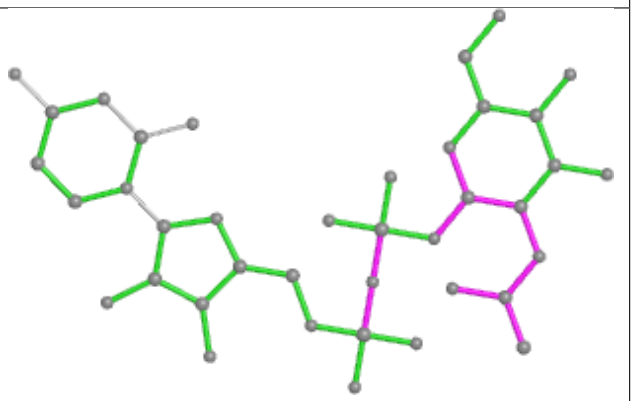
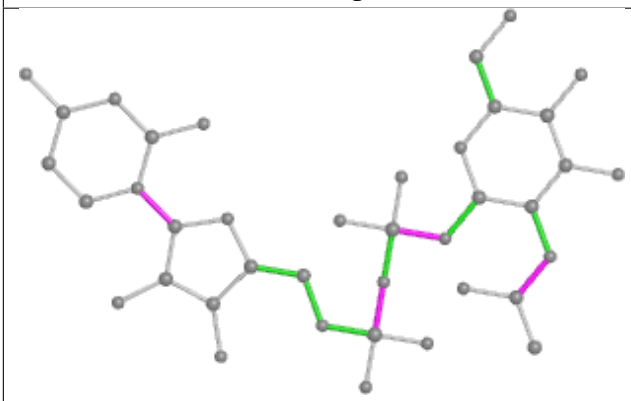
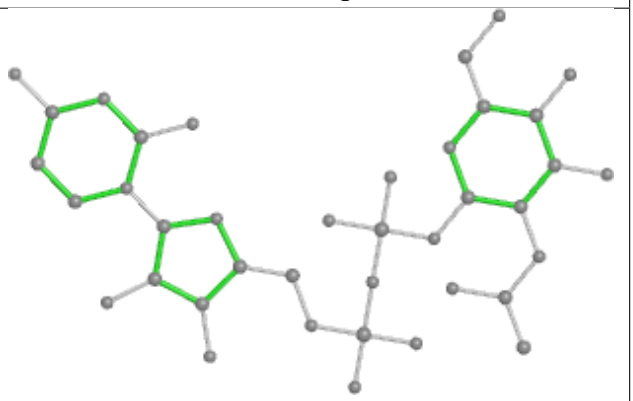


Bond angles

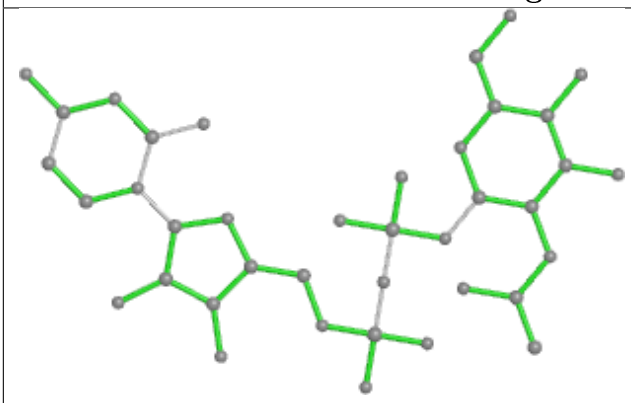


Torsions



Rings

Ligand UD1 C 402



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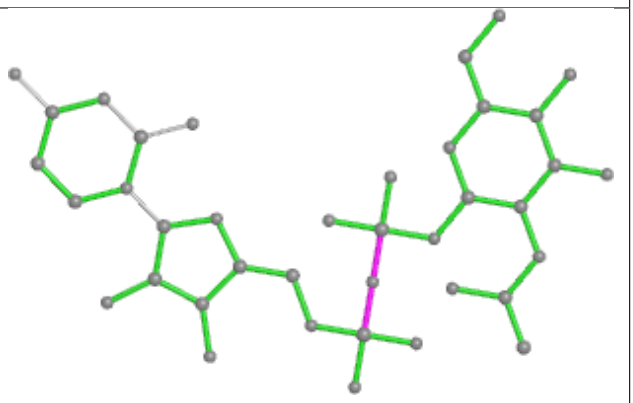

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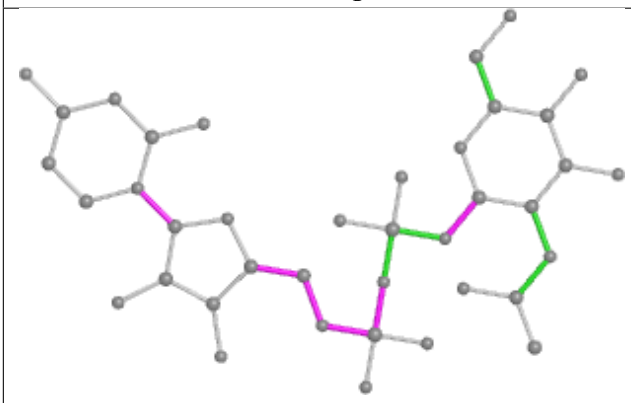

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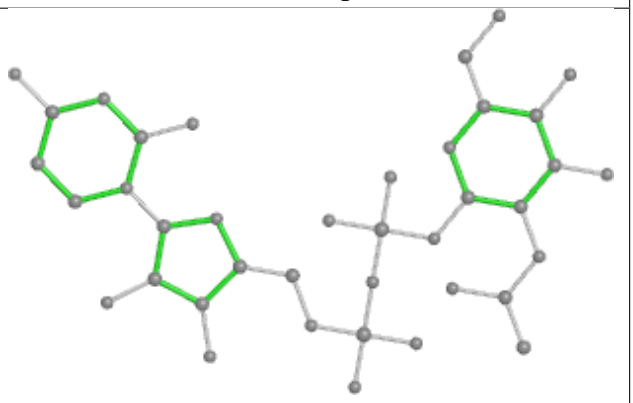
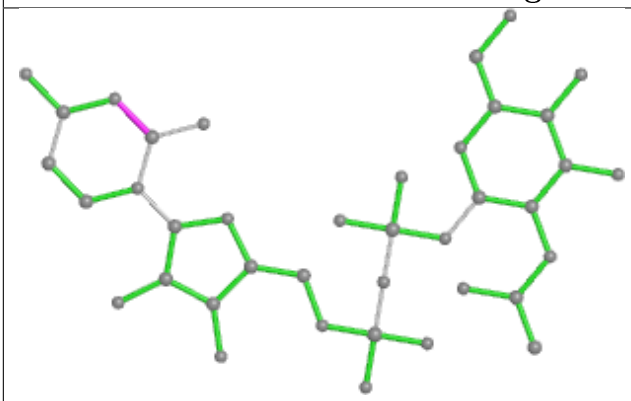


Rings

Ligand UD1 A 402



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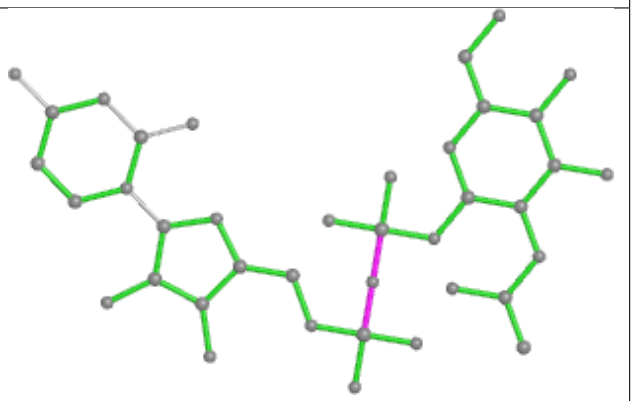
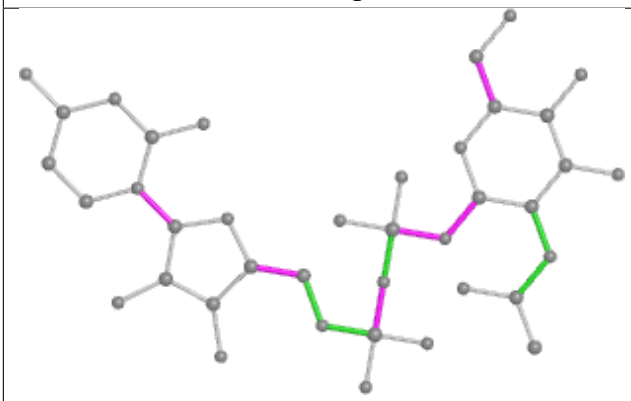
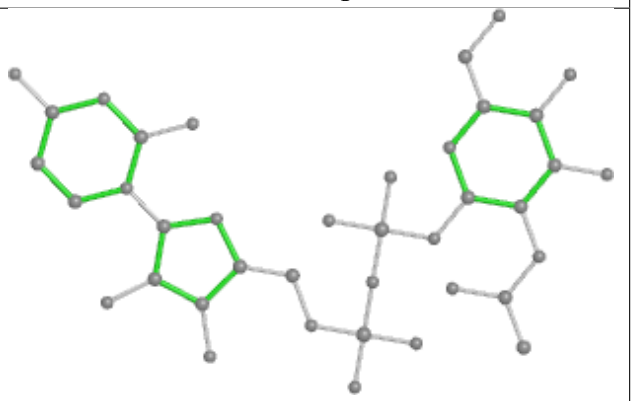


Bond angles

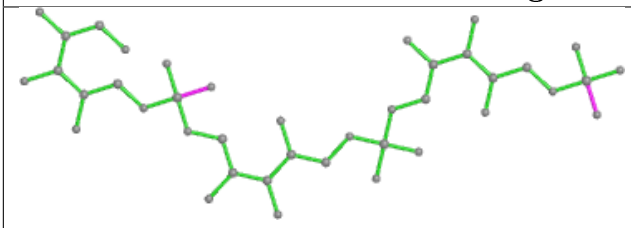


Torsions

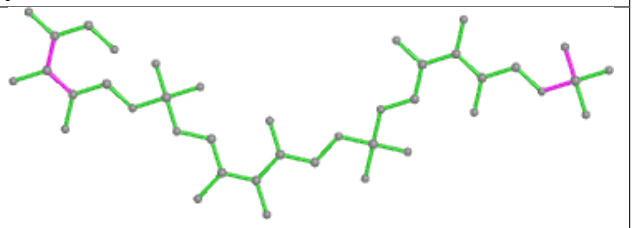


Rings

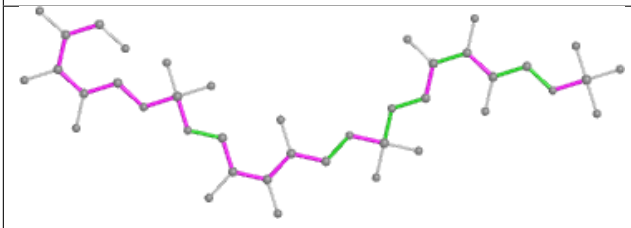
Ligand FQ8 H 401



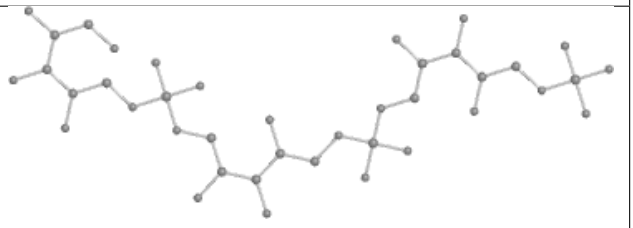
Bond lengths



Bond angles

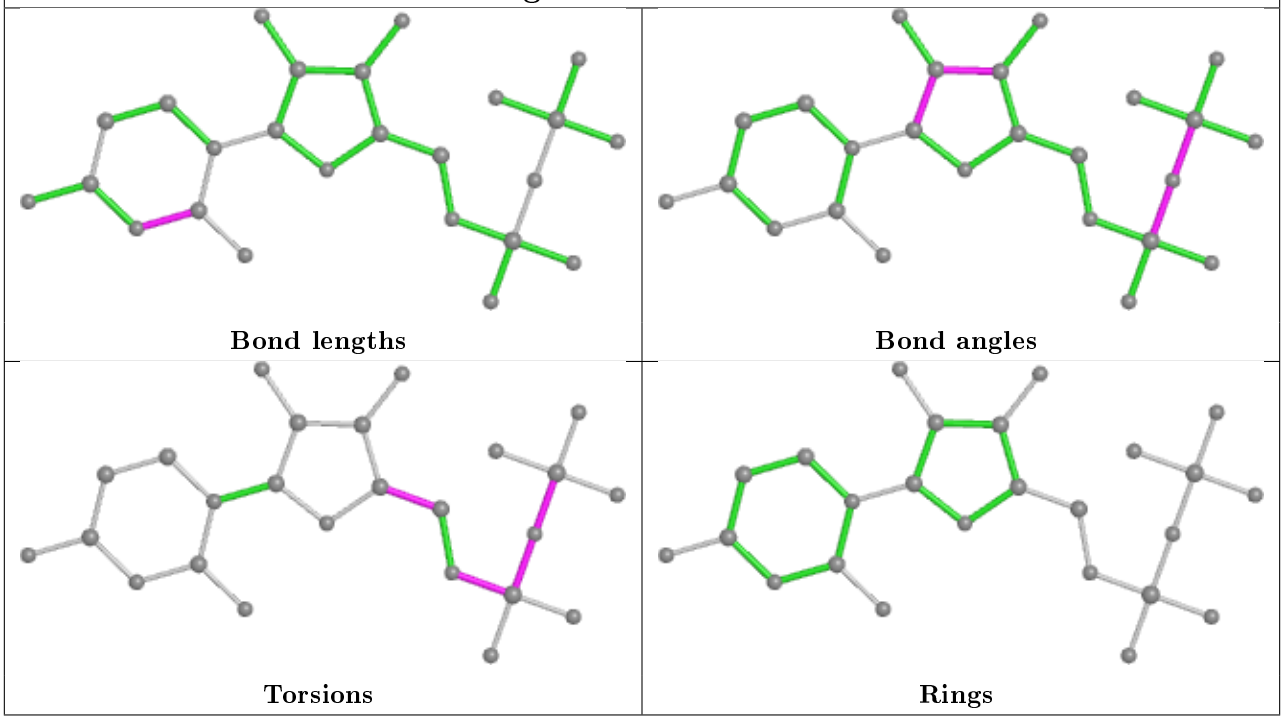


Torsions

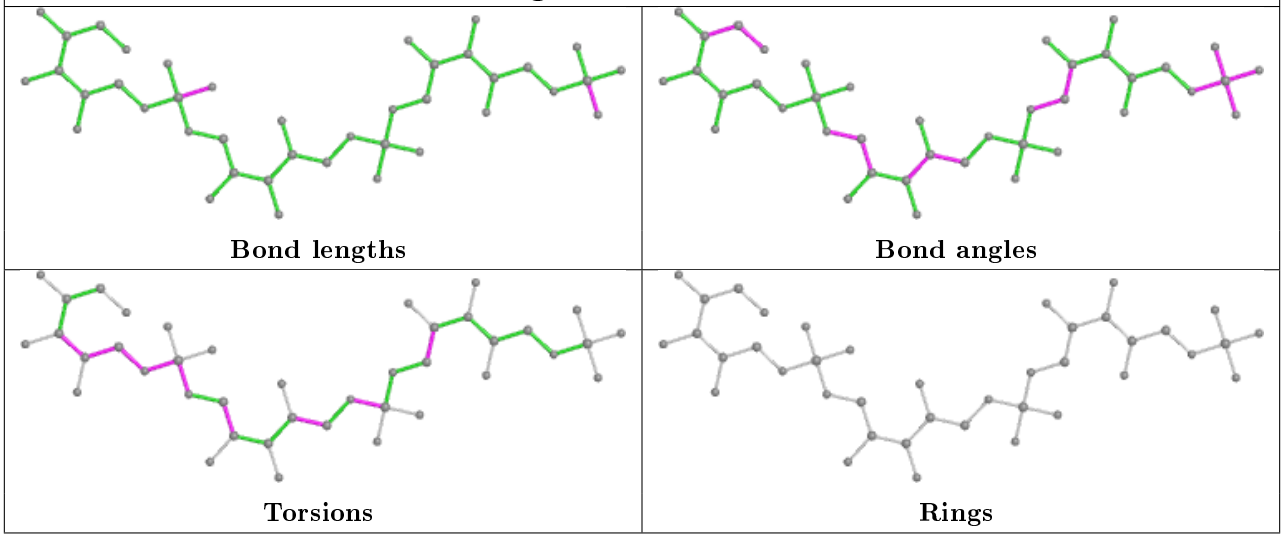


Rings

Ligand UDP P 402



Ligand FQ8 O 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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	317/345 (91%)	-0.17	2 (0%) 89 91	25, 41, 66, 100	0
1	B	317/345 (91%)	-0.16	1 (0%) 94 96	27, 39, 65, 97	0
1	C	314/345 (91%)	-0.08	6 (1%) 66 73	29, 47, 80, 115	0
1	D	312/345 (90%)	-0.09	1 (0%) 94 96	33, 47, 68, 111	0
1	E	317/345 (91%)	-0.19	0 100 100	28, 42, 71, 107	0
1	F	316/345 (91%)	0.01	0 100 100	33, 45, 69, 92	0
1	G	314/345 (91%)	-0.05	1 (0%) 94 96	33, 48, 79, 104	0
1	H	318/345 (92%)	-0.17	2 (0%) 89 91	26, 39, 68, 105	0
1	I	315/345 (91%)	0.02	9 (2%) 51 58	32, 51, 83, 104	0
1	O	316/345 (91%)	0.01	1 (0%) 94 96	31, 44, 69, 98	0
1	P	305/345 (88%)	0.69	49 (16%) 1 1	39, 72, 118, 141	0
1	Q	314/345 (91%)	0.48	34 (10%) 5 5	34, 65, 113, 147	0
All	All	3775/4140 (91%)	0.02	106 (2%) 53 60	25, 47, 91, 147	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	98	HIS	5.1
1	P	136	GLU	5.0
1	P	62	PHE	4.8
1	C	127	GLY	4.8
1	P	34	TYR	4.7

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 (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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FQ8	E	401	40/40	0.82	0.26	60,114,157,186	0
6	UDP	P	402	25/25	0.84	0.21	76,95,121,135	0
2	FQ8	A	401	40/40	0.86	0.25	65,110,158,175	0
4	MG	P	403	1/1	0.86	0.10	56,56,56,56	0
4	MG	O	403	1/1	0.86	0.26	45,45,45,45	0
3	UD1	Q	402	39/39	0.87	0.21	61,94,165,170	0
4	MG	G	403	1/1	0.88	0.22	46,46,46,46	0
2	FQ8	H	401	40/40	0.89	0.30	48,93,137,158	0
4	MG	A	403	1/1	0.90	0.17	52,52,52,52	0
2	FQ8	D	401	40/40	0.90	0.27	48,89,155,199	0
2	FQ8	Q	401	40/40	0.91	0.23	45,99,149,175	0
2	FQ8	B	401	40/40	0.91	0.28	49,92,149,166	0
2	FQ8	P	401	40/40	0.91	0.22	55,92,144,173	0
5	CL	E	404	1/1	0.92	0.10	44,44,44,44	0
4	MG	H	403	1/1	0.92	0.16	45,45,45,45	0
4	MG	D	403	1/1	0.92	0.11	57,57,57,57	0
4	MG	A	404	1/1	0.93	0.20	56,56,56,56	0
3	UD1	G	402	39/39	0.94	0.19	39,77,129,138	0
2	FQ8	G	401	40/40	0.94	0.24	49,78,155,158	0
2	FQ8	C	401	40/40	0.94	0.21	44,75,128,177	0
4	MG	H	404	1/1	0.94	0.36	61,61,61,61	0
2	FQ8	I	401	40/40	0.94	0.24	51,82,128,135	0
3	UD1	C	402	39/39	0.94	0.21	58,73,123,135	0
3	UD1	I	402	39/39	0.94	0.22	55,80,117,133	0
3	UD1	O	402	39/39	0.94	0.26	42,72,120,125	0
5	CL	P	404	1/1	0.94	0.10	76,76,76,76	0
4	MG	B	403	1/1	0.95	0.39	55,55,55,55	0
2	FQ8	F	401	40/40	0.95	0.26	40,74,136,136	0
4	MG	I	403	1/1	0.95	0.11	49,49,49,49	0
5	CL	I	404	1/1	0.95	0.12	53,53,53,53	0
3	UD1	D	402	39/39	0.95	0.16	39,57,89,93	0
3	UD1	A	402	39/39	0.95	0.13	34,61,101,115	0

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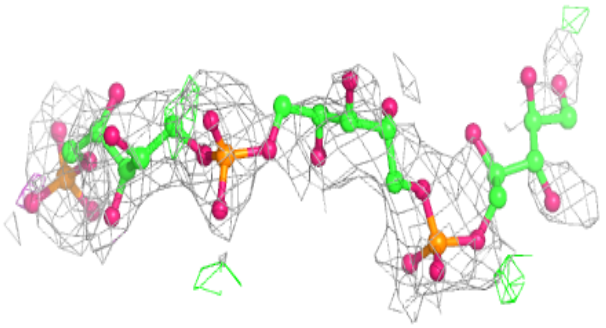
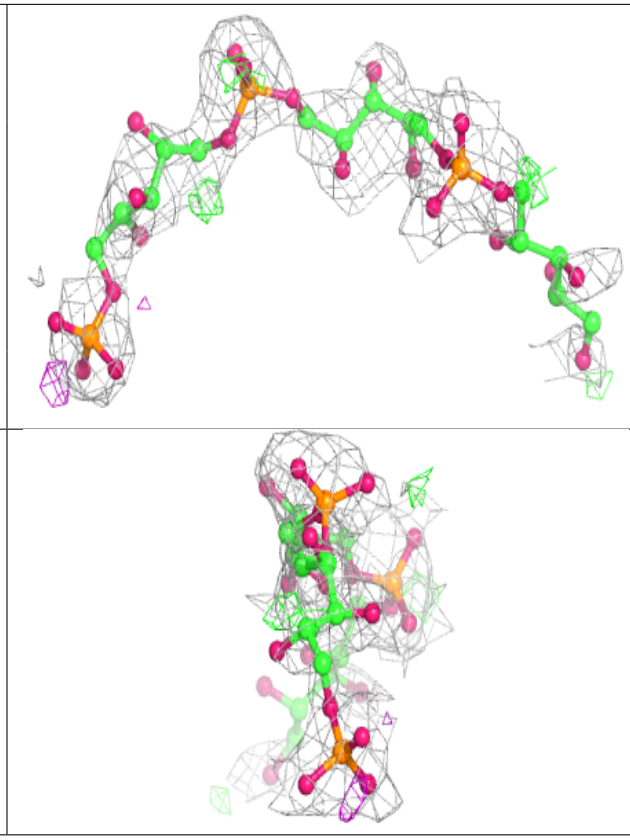
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	UD1	E	402	39/39	0.95	0.14	37,56,109,134	0
4	MG	B	404	1/1	0.95	0.17	40,40,40,40	0
3	UD1	F	402	39/39	0.95	0.21	40,61,104,121	0
3	UD1	H	402	39/39	0.96	0.15	27,47,96,116	0
4	MG	C	403	1/1	0.96	0.16	55,55,55,55	0
5	CL	B	406	1/1	0.96	0.09	49,49,49,49	0
5	CL	D	404	1/1	0.96	0.15	65,65,65,65	0
4	MG	F	403	1/1	0.96	0.20	50,50,50,50	0
3	UD1	B	402	39/39	0.96	0.17	30,54,125,148	0
2	FQ8	O	401	40/40	0.96	0.26	27,59,113,146	0
5	CL	B	405	1/1	0.97	0.08	47,47,47,47	0
4	MG	Q	403	1/1	0.97	0.32	53,53,53,53	0
5	CL	C	404	1/1	0.97	0.12	63,63,63,63	0
4	MG	E	403	1/1	0.97	0.30	44,44,44,44	0
5	CL	H	405	1/1	0.98	0.08	38,38,38,38	0
5	CL	F	404	1/1	0.98	0.15	45,45,45,45	0
5	CL	A	405	1/1	0.98	0.10	48,48,48,48	0
5	CL	H	406	1/1	0.99	0.13	56,56,56,56	0
5	CL	O	404	1/1	0.99	0.11	41,41,41,41	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:

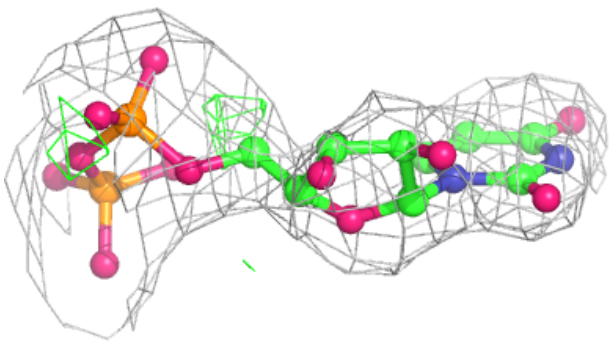
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

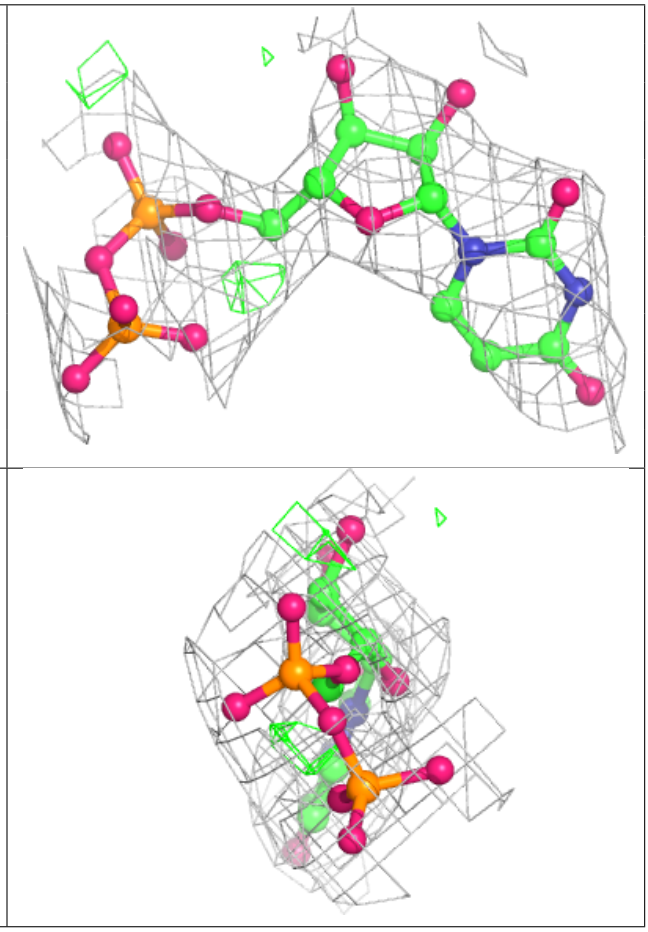




Electron density around UDP P 402:

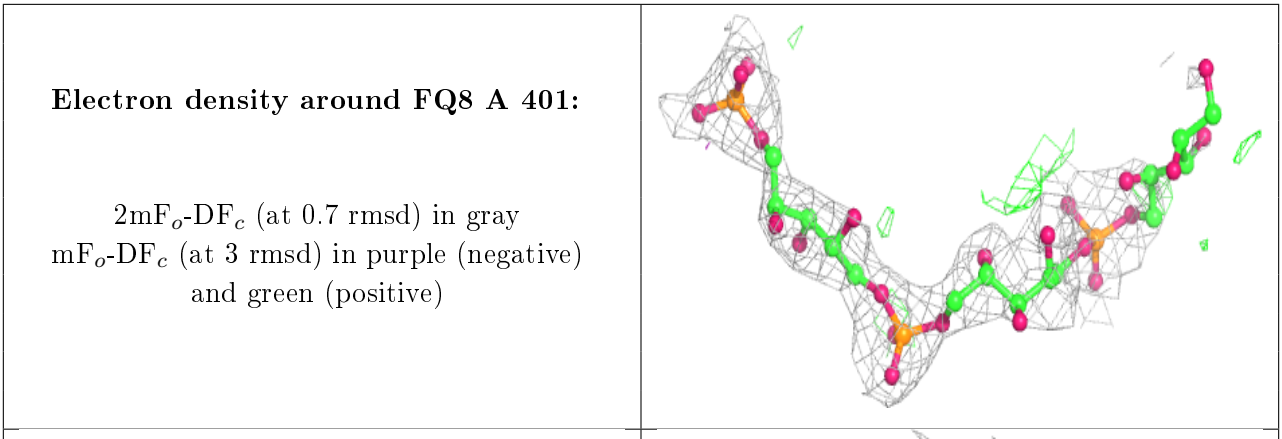
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





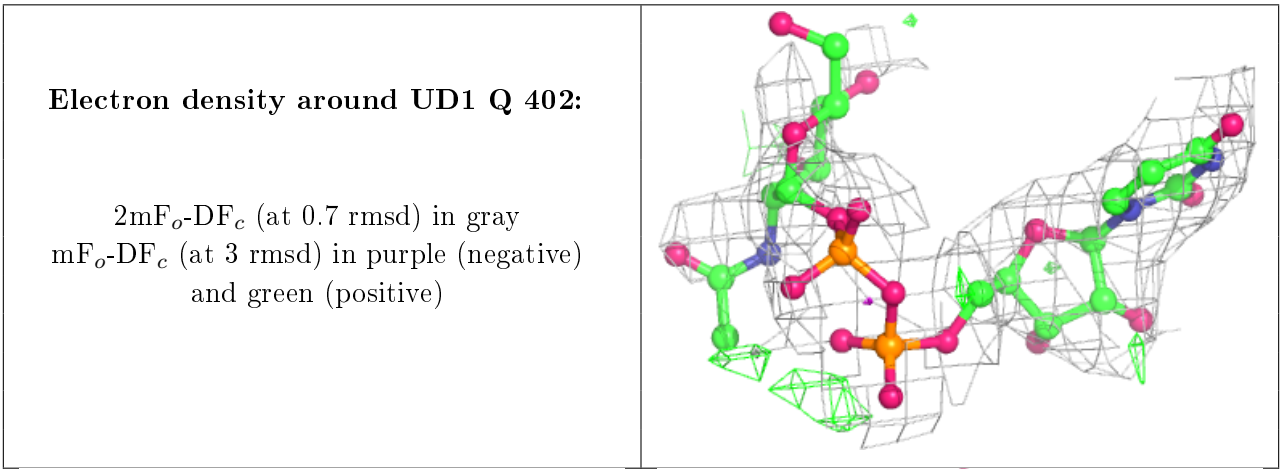
Electron density around FQ8 A 401:

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



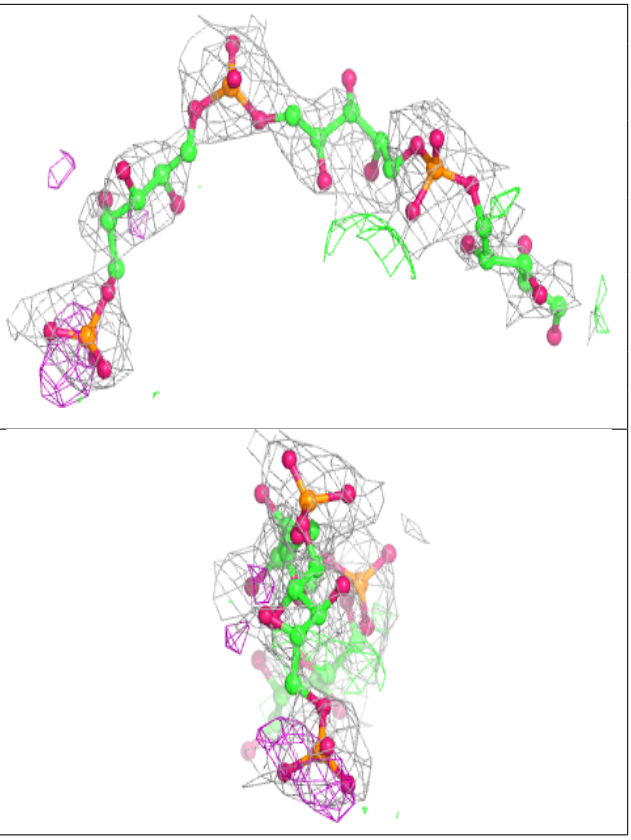
Electron density around UD1 Q 402:

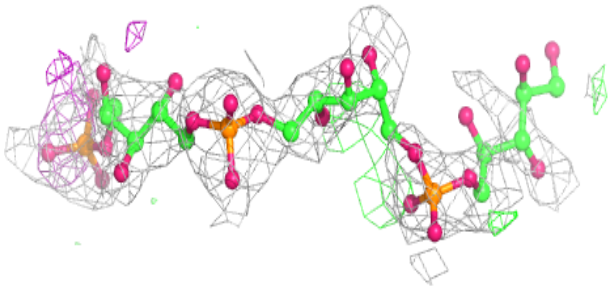
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FQ8 H 401:

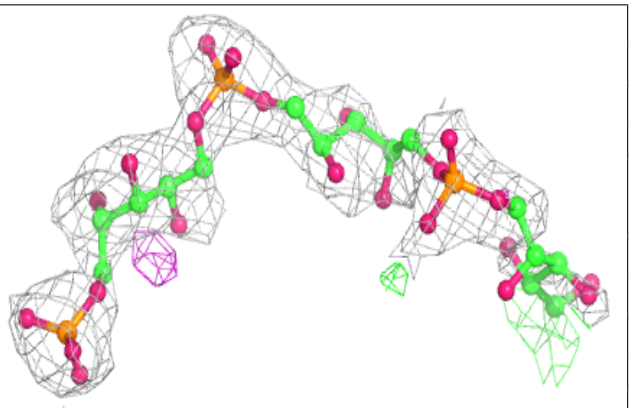
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

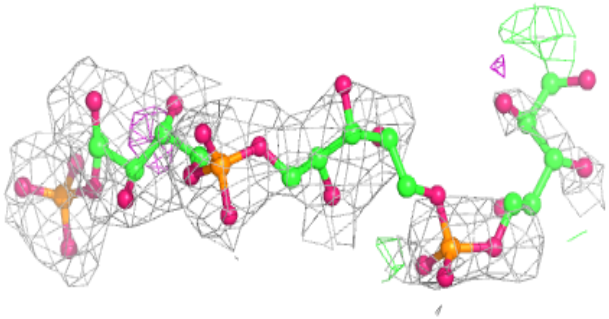


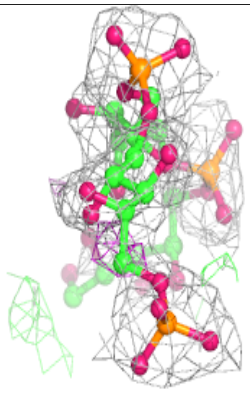


Electron density around FQ8 D 401:

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

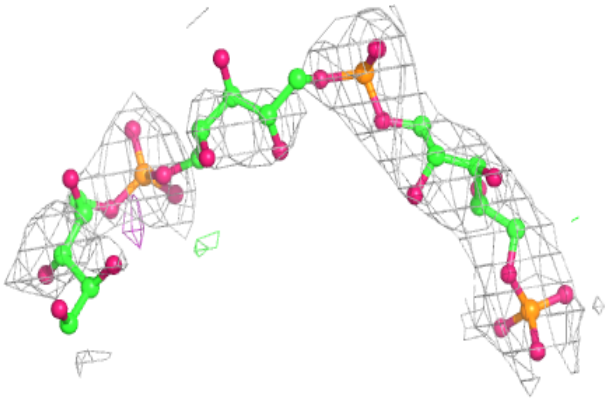


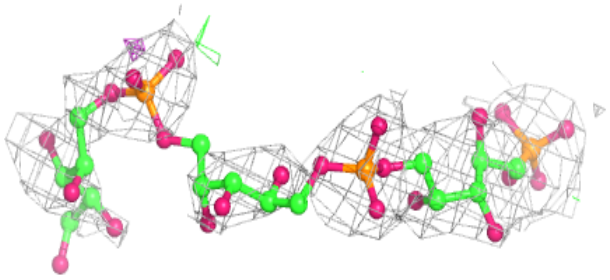


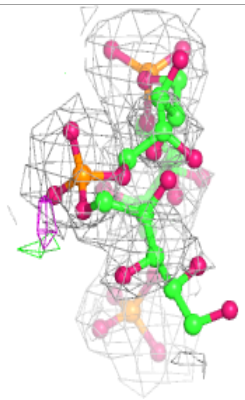


Electron density around FQ8 Q 401:

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

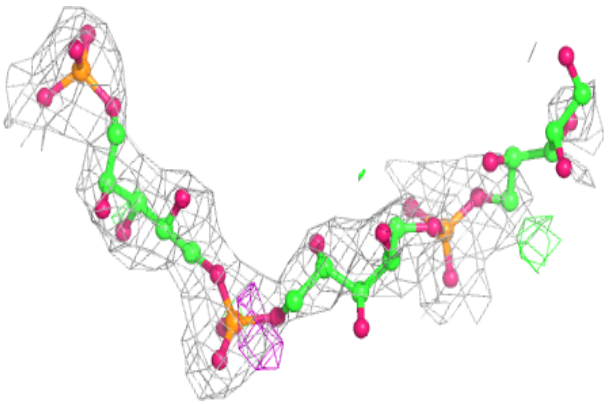


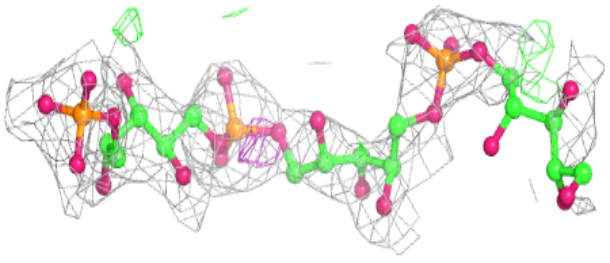




Electron density around FQ8 B 401:

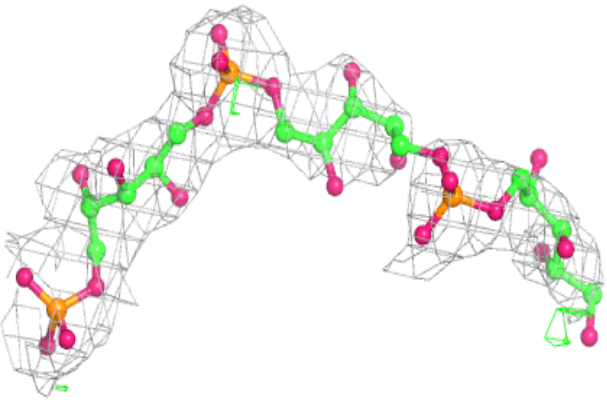
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

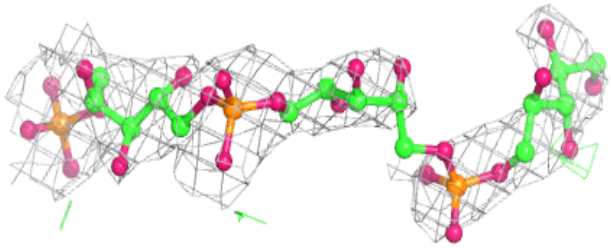


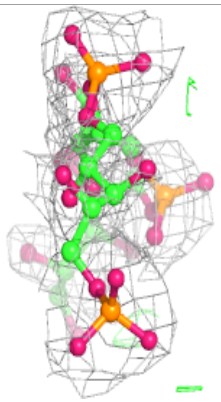


Electron density around FQ8 P 401:

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

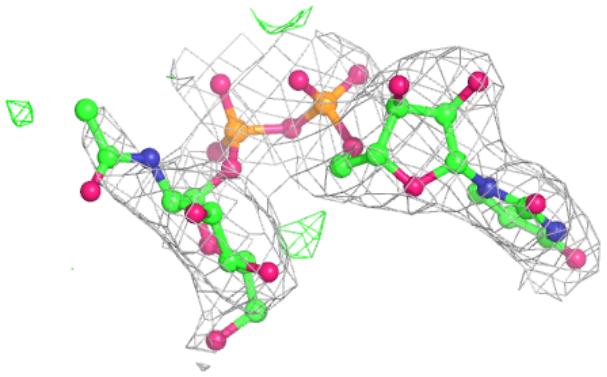


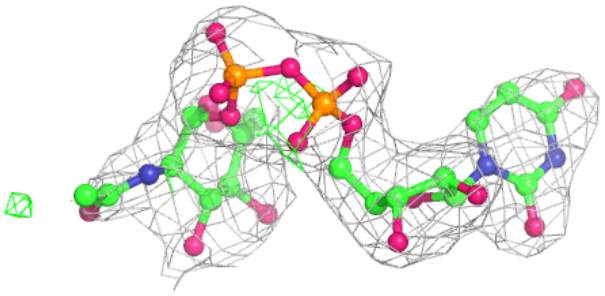


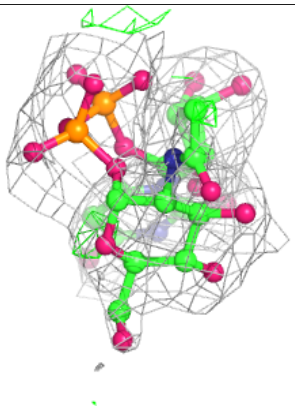


Electron density around UD1 G 402:

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

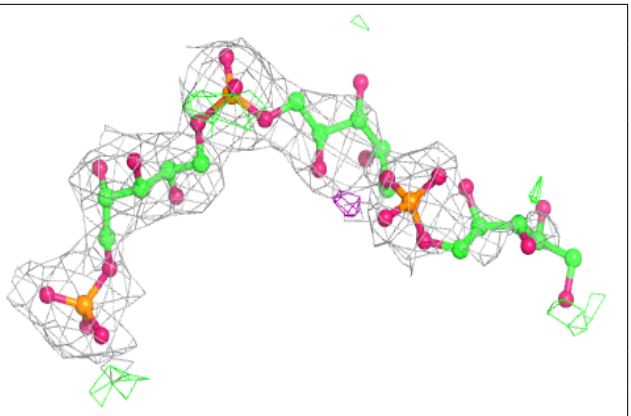


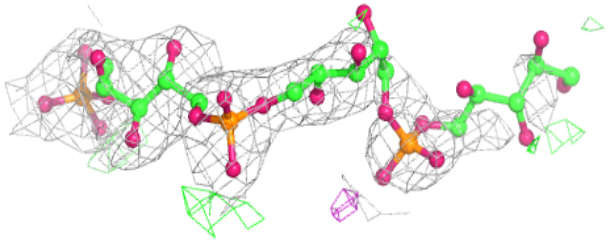


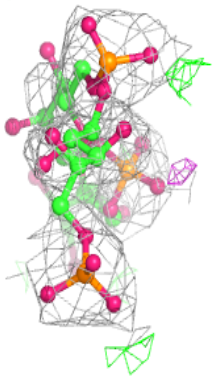


Electron density around FQ8 G 401:

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

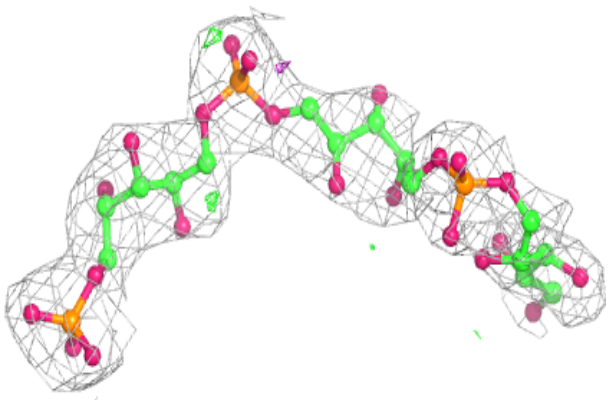


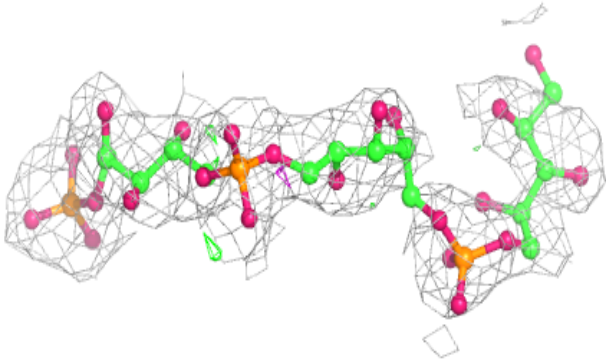


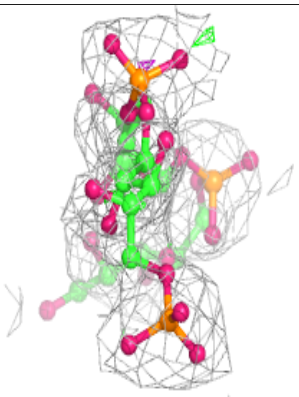


Electron density around FQ8 C 401:

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

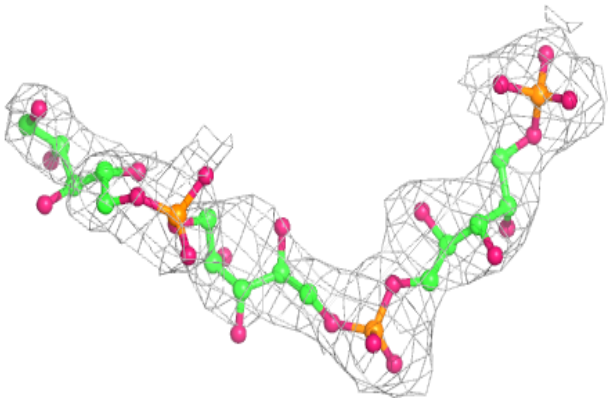


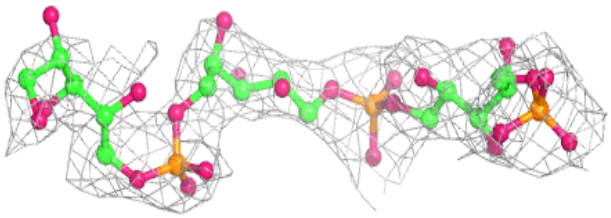


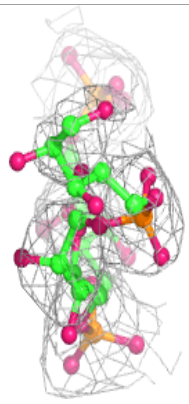


Electron density around FQ8 I 401:

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

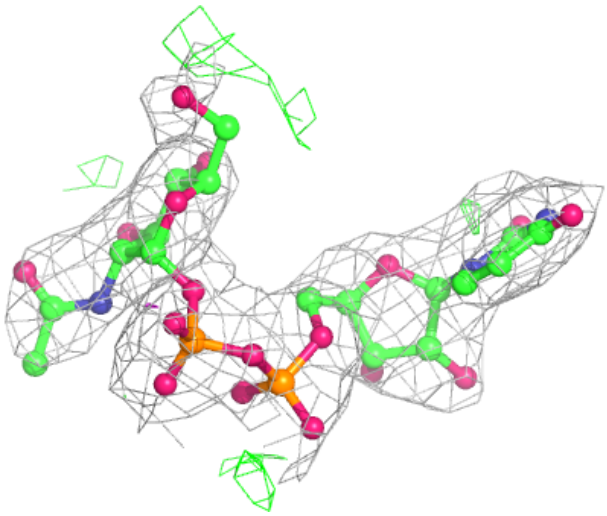


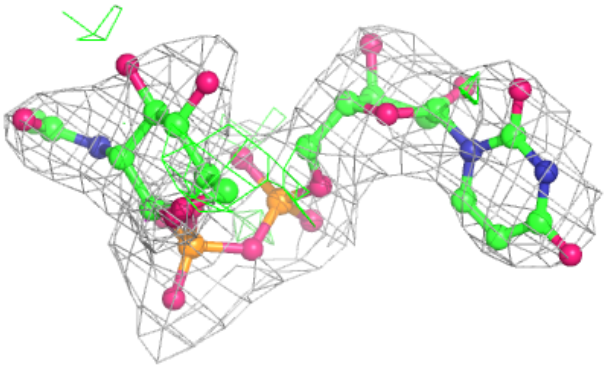


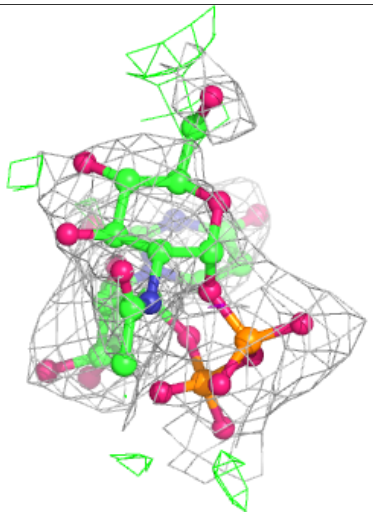


Electron density around UD1 C 402:

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

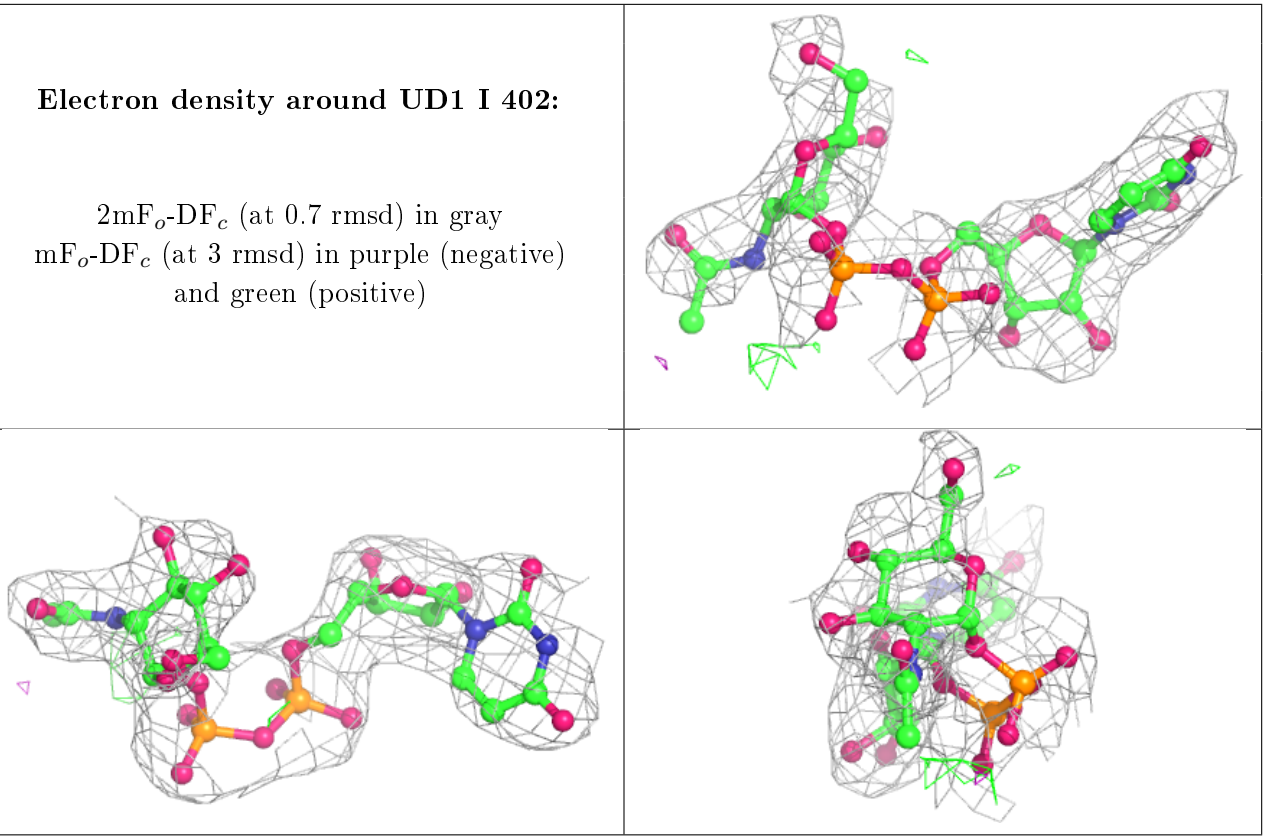






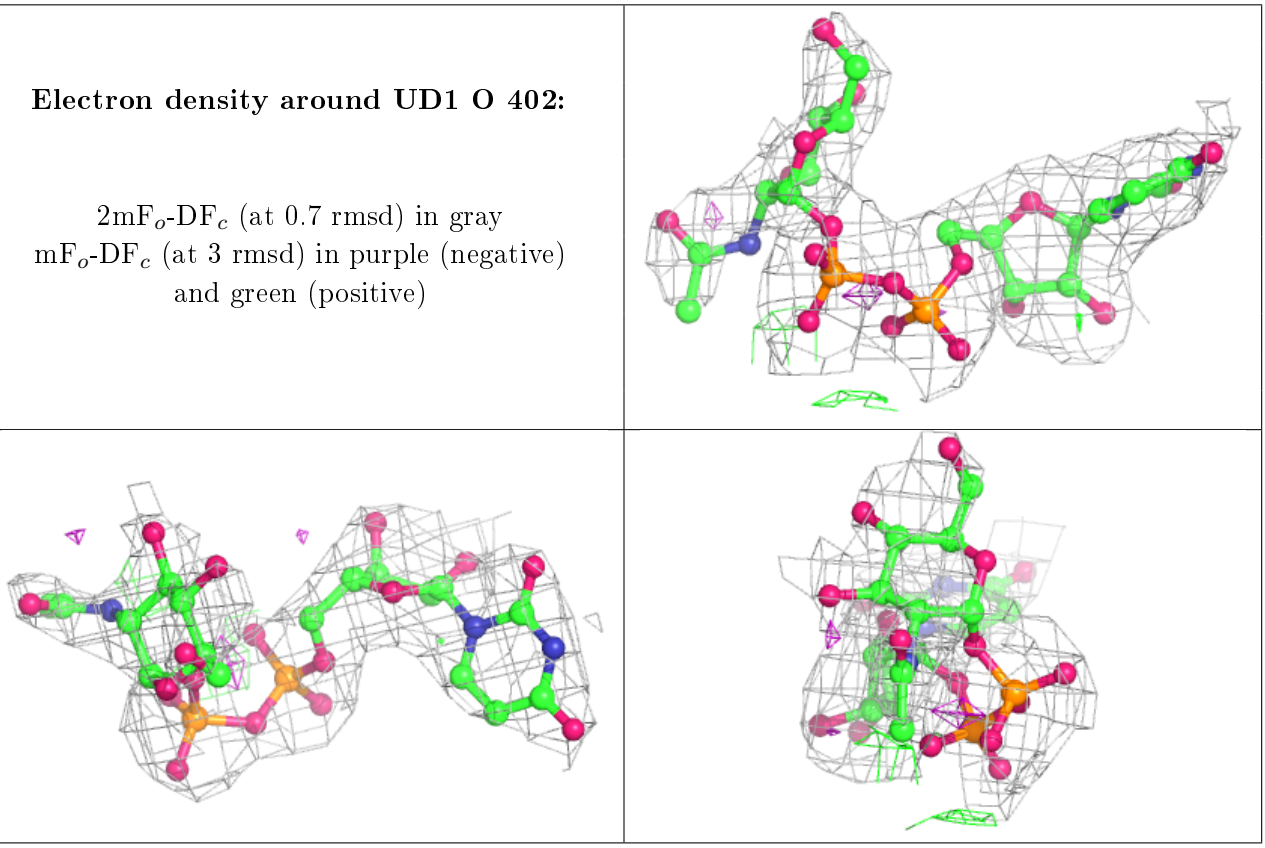
Electron density around UD1 I 402:

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



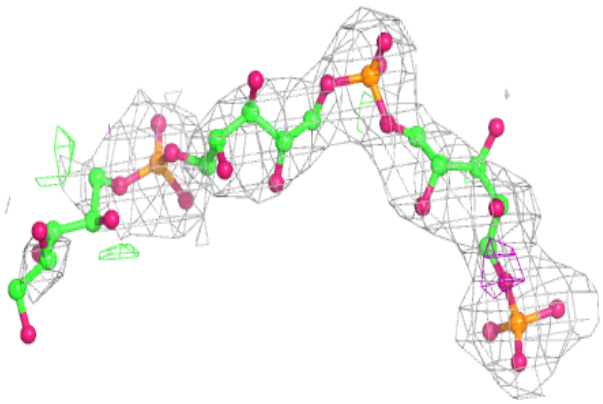
Electron density around UD1 O 402:

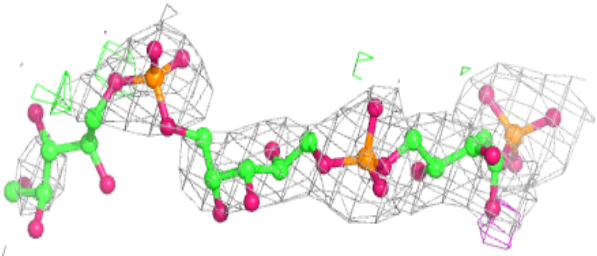
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

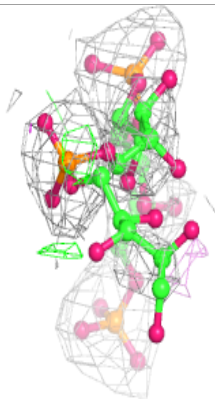


Electron density around FQ8 F 401:

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

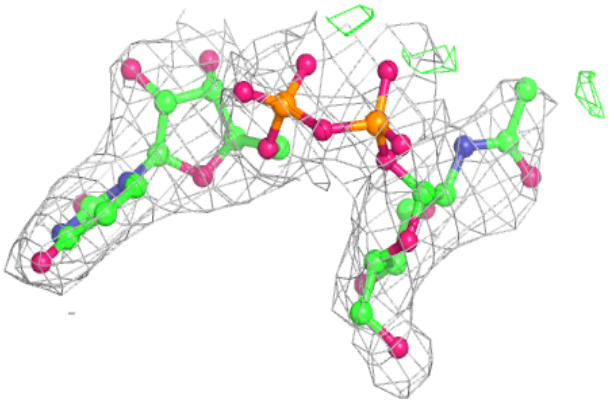


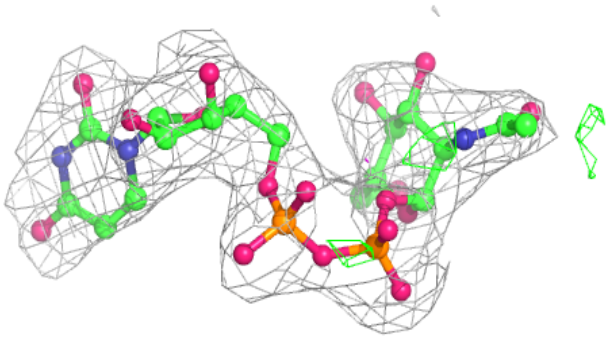


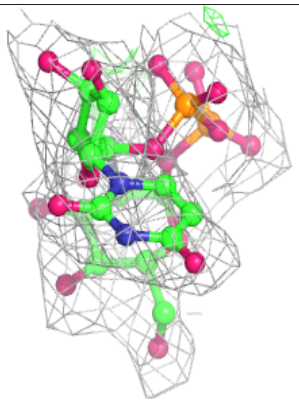


Electron density around UD1 D 402:

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

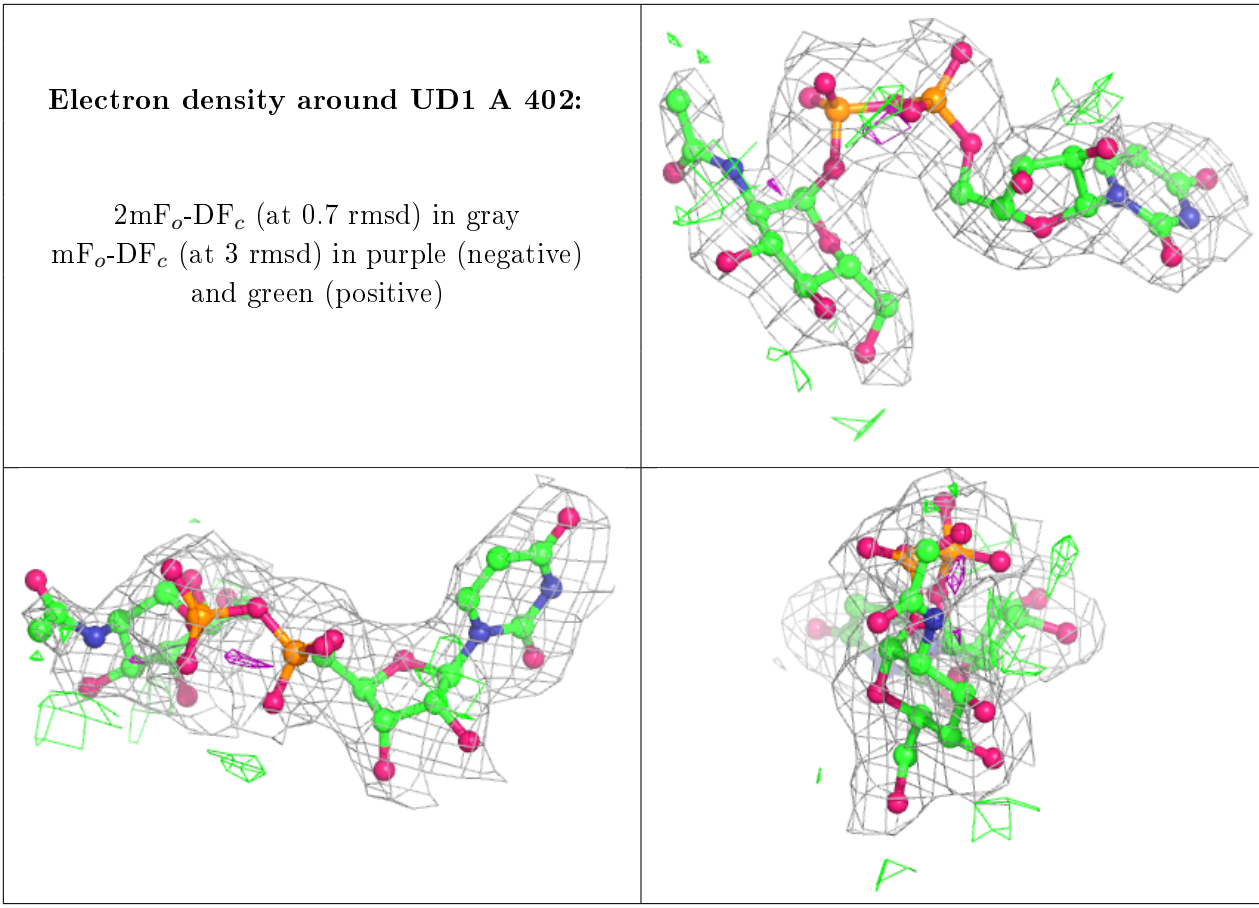






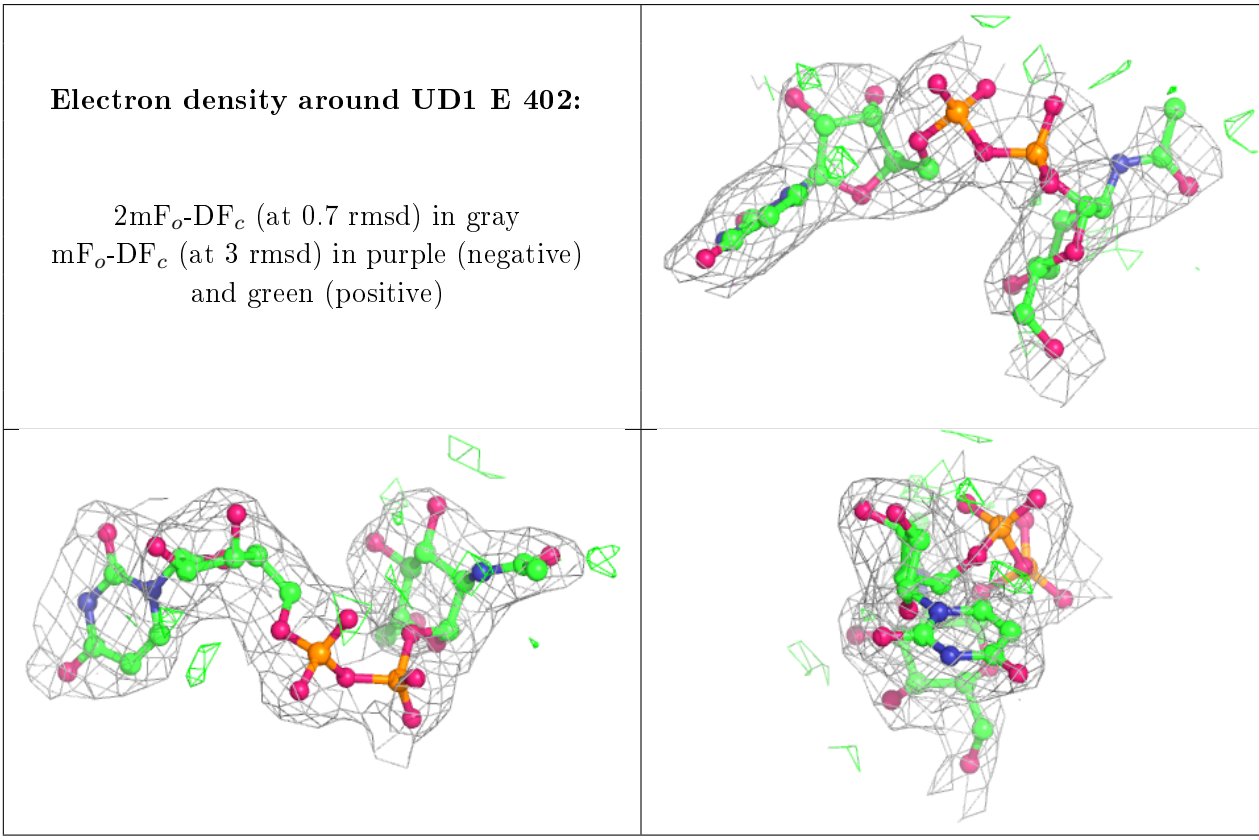
Electron density around UD1 A 402:

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



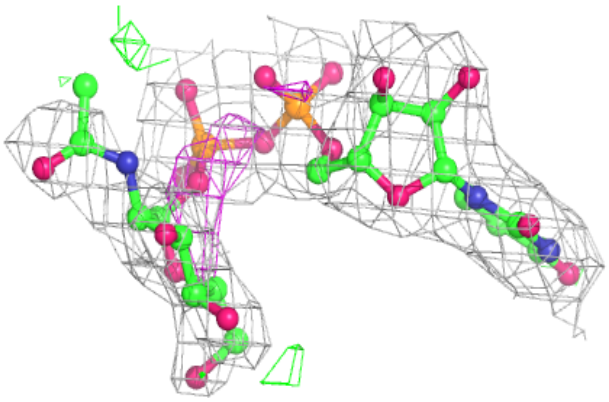
Electron density around UD1 E 402:

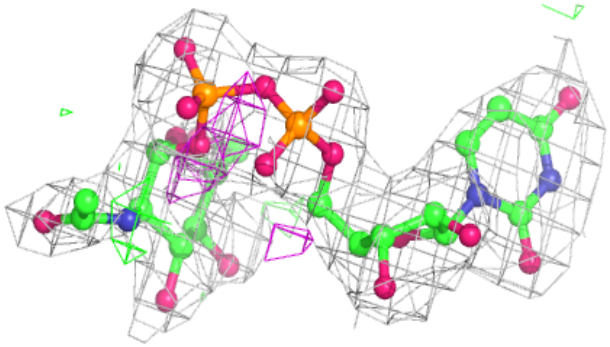
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around UD1 F 402:

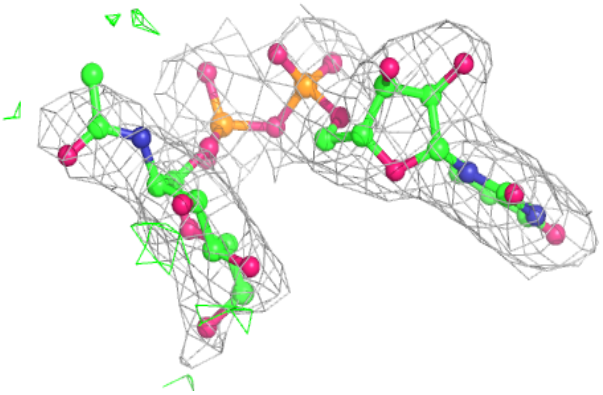
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

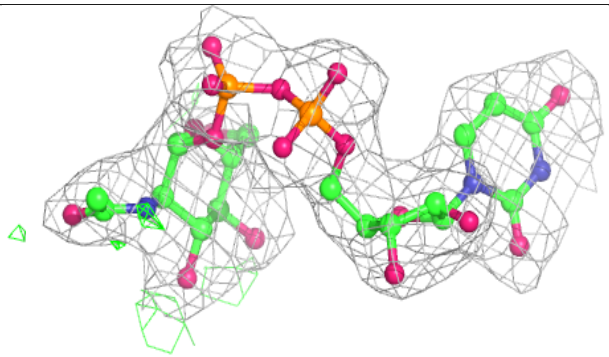


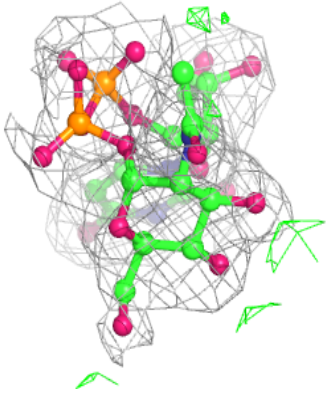


Electron density around UD1 H 402:

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

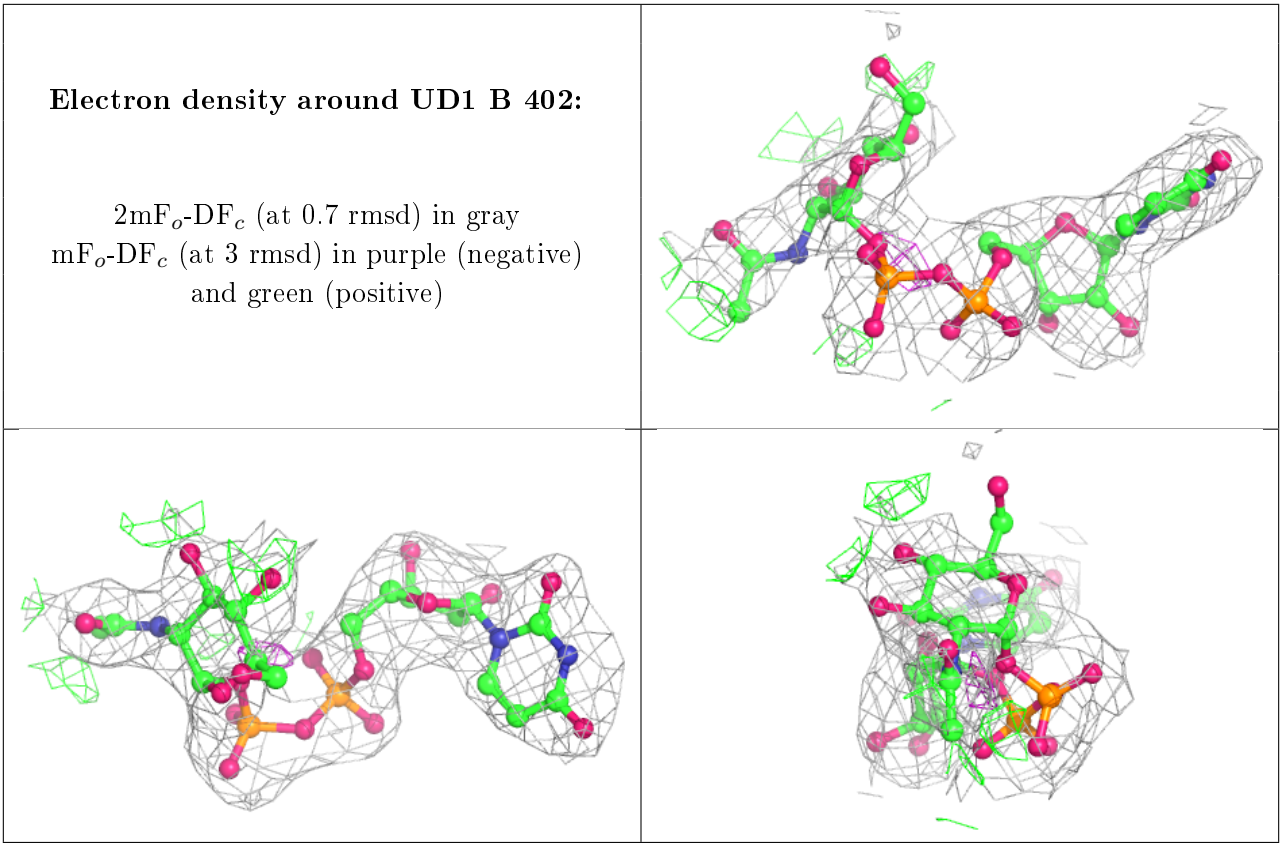






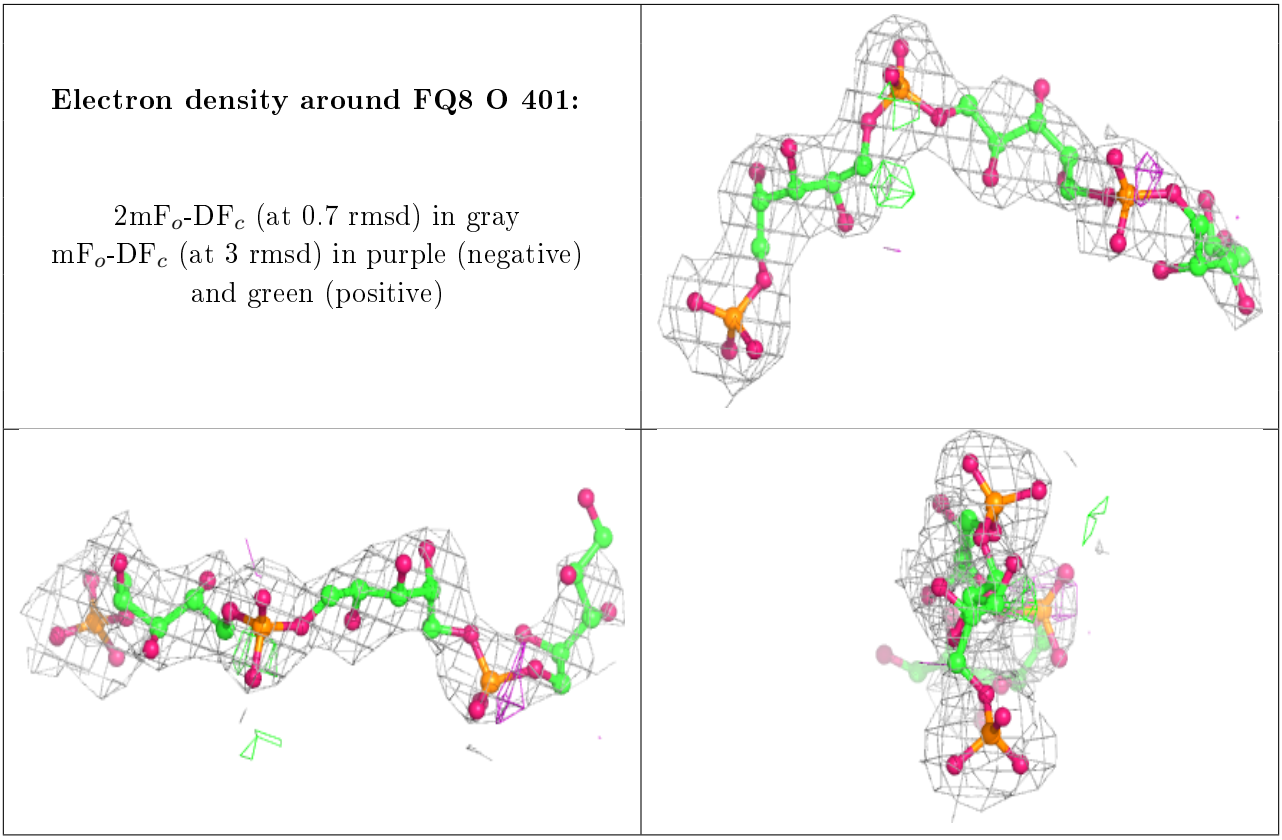
Electron density around UD1 B 402:

$2mF_o$-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 O 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.