



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 03:12 AM UTC

PDB ID : 6HNQ / pdb_00006hnq
Title : TarP-6RboP-(CH₂)₆NH₂
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

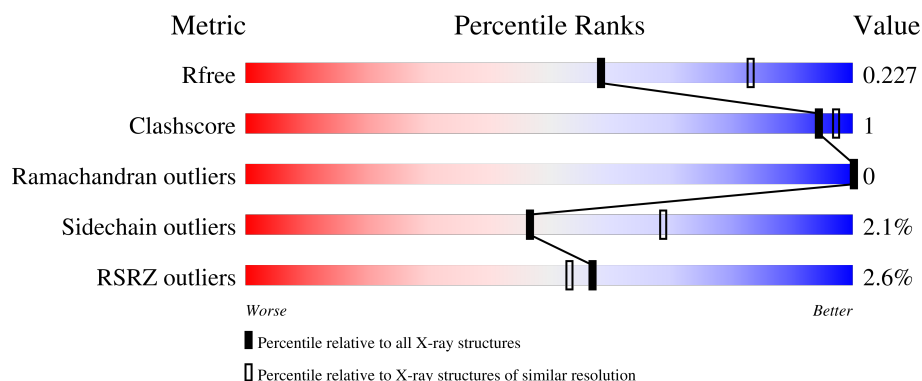
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



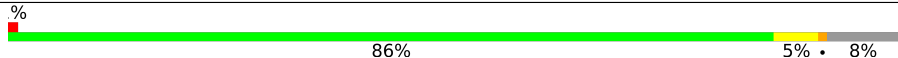
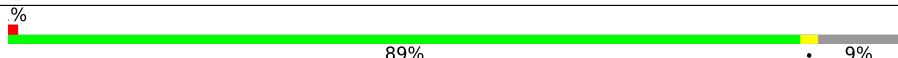
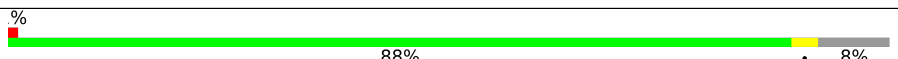
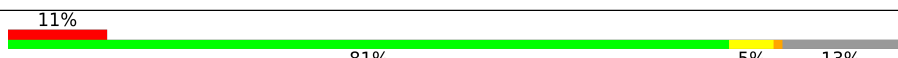
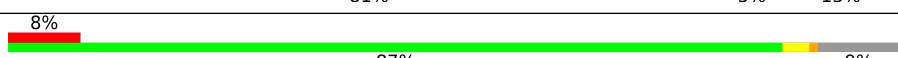
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 ≥ 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	2% 88% 8%
1	B	345	86% 5% 8%
1	C	345	% 86% 10%
1	D	345	% 87% 9%
1	E	345	% 86% 8%

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Mol	Chain	Length	Quality of chain
1	F	345	 88% • • 8%
1	G	345	 88% • 9%
1	H	345	 86% 5% • 8%
1	I	345	 89% • 9%
1	O	345	 88% • 8%
1	P	345	 81% 5% • 13%
1	Q	345	 87% • • 9%

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
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
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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
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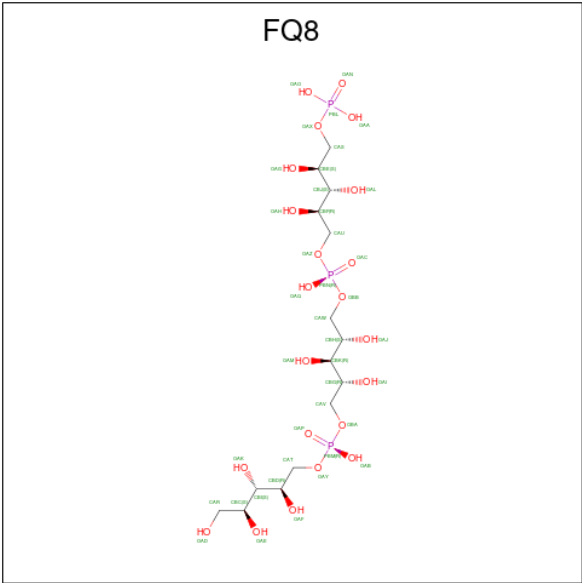
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	SER	-	expression tag	UNP A0A0H3JNB0
D	-5	LEU	-	expression tag	UNP A0A0H3JNB0
D	-4	VAL	-	expression tag	UNP A0A0H3JNB0
D	-3	PRO	-	expression tag	UNP A0A0H3JNB0
D	-2	ARG	-	expression tag	UNP A0A0H3JNB0
D	-1	GLY	-	expression tag	UNP A0A0H3JNB0
D	0	SER	-	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-pentoxy]phosphoryl]oxy-pentyl] hydrogen phosphate (CCD ID: FQ8) (formula: C₁₅H₃₅O₂₂P₃) (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 (CCD ID: 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 (CCD ID: 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.

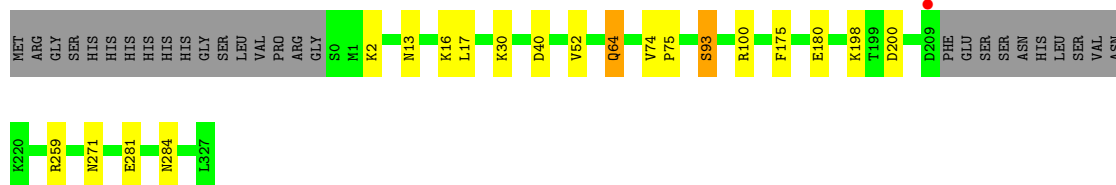
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	165	Total 165	O 165	0	0
5	C	114	Total 114	O 114	0	0
5	F	132	Total 132	O 132	0	0
5	O	138	Total 138	O 138	0	0
5	P	47	Total 47	O 47	0	0
5	E	124	Total 124	O 124	0	0
5	G	133	Total 133	O 133	0	0
5	Q	64	Total 64	O 64	0	0
5	A	124	Total 124	O 124	0	0
5	D	113	Total 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.

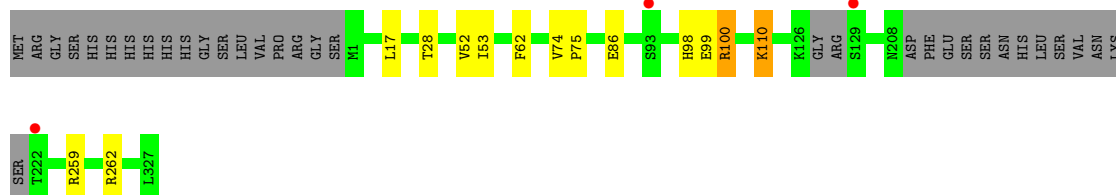
- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

Chain B: 



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

Chain C: 



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

Chain F: 

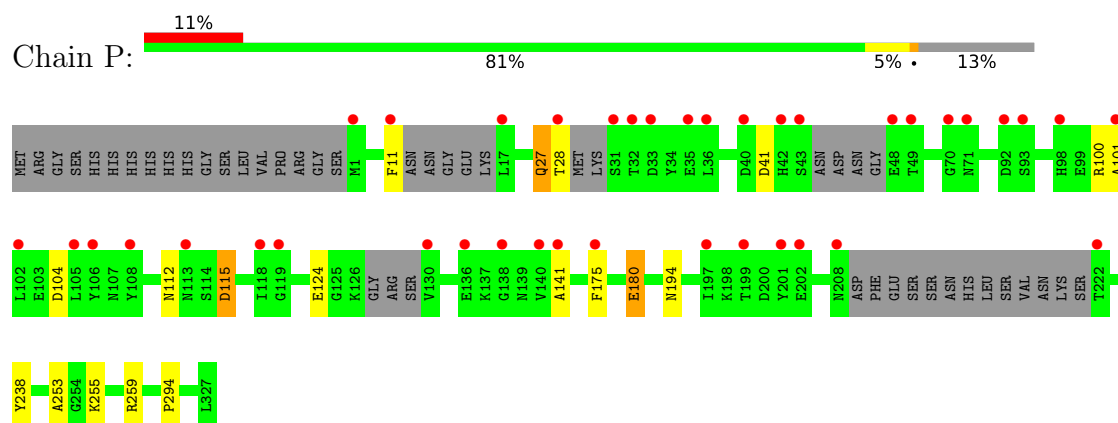


- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

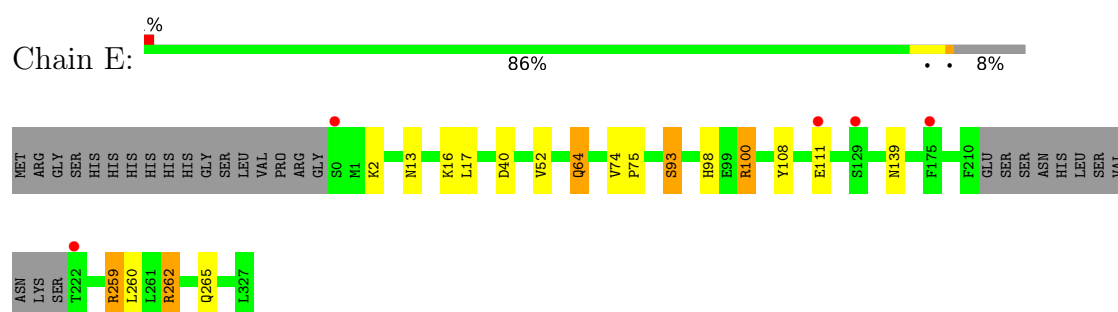
Chain O: 



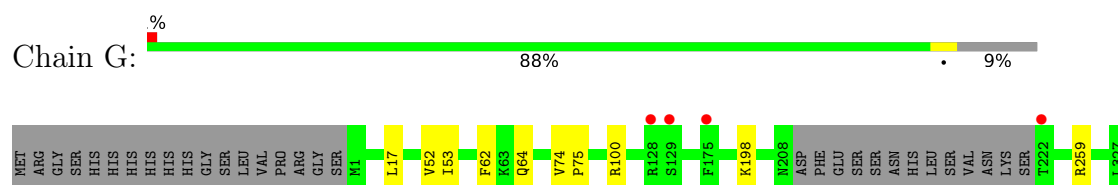
- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase



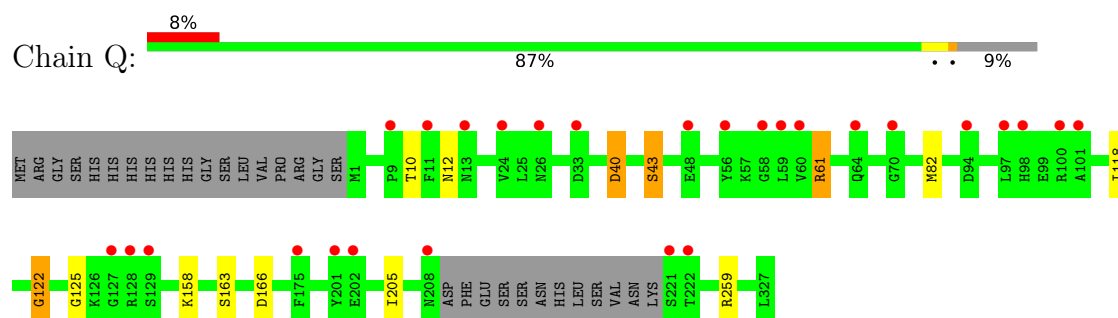
- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase



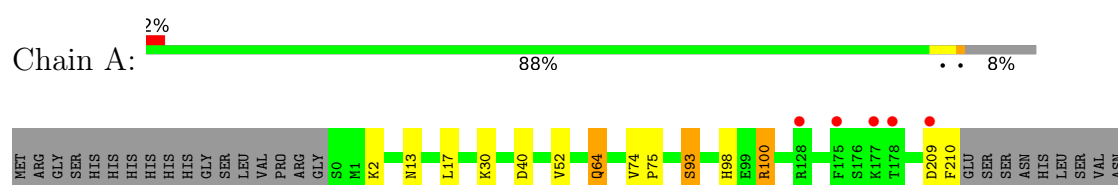
- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

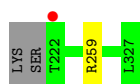


- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

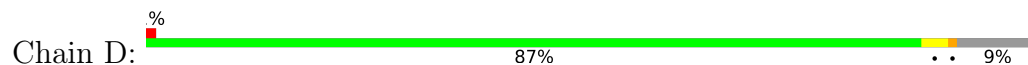


- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase

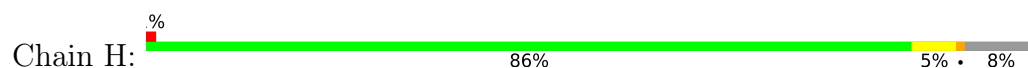




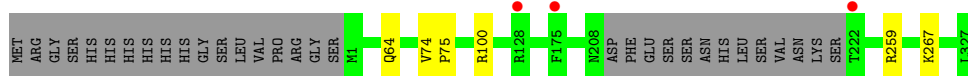
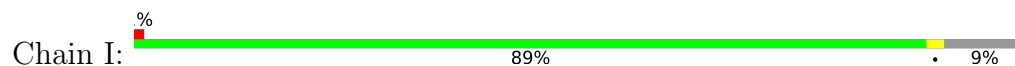
- Molecule 1: Probable ss-1,3-N-acetylglucosaminyltransferase



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 99.9 (48.51-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	40.9	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FQ8, MG, 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	0.95	0/2550	1.26	0/3437
1	B	0.94	0/2578	1.28	2/3466 (0.1%)
1	C	0.92	0/2492	1.24	0/3361
1	D	0.93	0/2521	1.25	0/3400
1	E	0.96	0/2558	1.27	1/3448 (0.0%)
1	F	0.95	0/2535	1.27	4/3417 (0.1%)
1	G	0.93	0/2523	1.25	0/3402
1	H	0.94	0/2579	1.29	3/3470 (0.1%)
1	I	0.92	0/2489	1.25	0/3358
1	O	0.93	0/2539	1.25	0/3424
1	P	1.03	1/2100 (0.0%)	1.33	1/2847 (0.0%)
1	Q	1.00	1/2307 (0.0%)	1.32	3/3128 (0.1%)
All	All	0.95	2/29771 (0.0%)	1.27	14/40158 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	122	GLY	C-O	-7.24	1.14	1.23
1	P	180	GLU	CD-OE2	-5.91	1.14	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	175	PHE	CA-C-O	-7.87	109.04	119.11
1	F	259	ARG	NE-CZ-NH1	-7.83	113.67	121.50
1	E	262	ARG	CG-CD-NE	-7.51	95.47	112.00
1	F	100	ARG	CG-CD-NE	-7.30	95.95	112.00
1	B	175	PHE	CA-C-O	-6.83	110.37	119.11
1	Q	61	ARG	NE-CZ-NH2	6.10	124.69	119.20
1	F	259	ARG	CG-CD-NE	-5.99	98.81	112.00
1	F	259	ARG	NE-CZ-NH2	5.97	124.57	119.20
1	H	161	LYS	CB-CG-CD	5.86	124.77	111.30
1	B	281	GLU	CB-CG-CD	5.80	122.45	112.60
1	P	124	GLU	CA-C-O	-5.71	113.11	119.67
1	Q	122	GLY	CA-C-O	-5.53	115.55	120.75
1	H	176	SER	CA-C-O	-5.20	115.71	121.33
1	Q	125	GLY	CA-C-O	-5.11	116.40	120.79

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	6	0
1	B	2535	0	2520	8	0
1	C	2451	0	2382	8	0
1	D	2479	0	2424	5	0
1	E	2512	0	2464	11	0
1	F	2493	0	2423	7	0
1	G	2481	0	2419	3	0
1	H	2536	0	2511	11	0
1	I	2448	0	2365	1	0
1	O	2496	0	2426	4	0
1	P	2074	0	1703	10	0
1	Q	2272	0	1982	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	31221	0	28072	77	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 (77) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:10:THR:OG1	1:Q:40:ASP:CG	2.61	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:D:146:ILE:HD12	1:D:251:GLN:CD	2.45	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:Q:163:SER:HA	1:Q:166:ASP:CG	2.46	0.40
1:A:74:VAL:HB	1:A:75:PRO:HD3	2.02	0.40
1:A:209:ASP:O	1:A:210:PHE:C	2.64	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%)	44	66
1	B	265/313 (85%)	257 (97%)	8 (3%)	36	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	250/313 (80%)	247 (99%)	3 (1%)	63	81
1	D	256/313 (82%)	249 (97%)	7 (3%)	39	62
1	E	260/313 (83%)	254 (98%)	6 (2%)	44	66
1	F	254/313 (81%)	249 (98%)	5 (2%)	48	70
1	G	258/313 (82%)	254 (98%)	4 (2%)	55	76
1	H	264/313 (84%)	258 (98%)	6 (2%)	44	66
1	I	246/313 (79%)	242 (98%)	4 (2%)	55	76
1	O	255/313 (82%)	251 (98%)	4 (2%)	55	76
1	P	143/313 (46%)	137 (96%)	6 (4%)	26	45
1	Q	184/313 (59%)	181 (98%)	3 (2%)	55	76
All	All	2895/3756 (77%)	2833 (98%)	62 (2%)	47	69

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	LYS
1	B	16	LYS
1	B	30	LYS
1	B	64	GLN
1	B	93	SER
1	B	100	ARG
1	B	259	ARG
1	B	284	ASN
1	C	100	ARG
1	C	110	LYS
1	C	259	ARG
1	F	30	LYS
1	F	64	GLN
1	F	93	SER
1	F	111	GLU
1	F	162	LYS
1	O	2	LYS
1	O	64	GLN
1	O	100	ARG
1	O	259	ARG
1	P	27	GLN
1	P	28	THR
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	E	2	LYS
1	E	64	GLN
1	E	93	SER
1	E	100	ARG
1	E	259	ARG
1	E	265	GLN
1	G	64	GLN
1	G	100	ARG
1	G	198	LYS
1	G	259	ARG
1	Q	40	ASP
1	Q	43	SER
1	Q	259	ARG
1	A	2	LYS
1	A	30	LYS
1	A	64	GLN
1	A	93	SER
1	A	100	ARG
1	A	259	ARG
1	D	2	LYS
1	D	93	SER
1	D	100	ARG
1	D	146	ILE
1	D	198	LYS
1	D	255	LYS
1	D	259	ARG
1	H	2	LYS
1	H	50	LEU
1	H	93	SER
1	H	100	ARG
1	H	259	ARG
1	H	284	ASN
1	I	64	GLN
1	I	100	ARG
1	I	259	ARG
1	I	267	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	68	ASN
1	B	224	ASN
1	B	245	ASN
1	B	285	ASN
1	C	191	ASN
1	C	245	ASN
1	F	26	ASN
1	F	112	ASN
1	F	245	ASN
1	F	303	GLN
1	O	112	ASN
1	O	168	ASN
1	O	191	ASN
1	O	245	ASN
1	O	303	GLN
1	P	231	ASN
1	P	245	ASN
1	E	68	ASN
1	E	306	ASN
1	G	68	ASN
1	G	245	ASN
1	Q	68	ASN
1	Q	245	ASN
1	A	68	ASN
1	A	112	ASN
1	A	194	ASN
1	A	265	GLN
1	A	306	ASN
1	D	68	ASN
1	D	231	ASN
1	D	245	ASN
1	D	271	ASN
1	H	68	ASN
1	H	224	ASN
1	H	245	ASN
1	H	285	ASN
1	H	303	GLN
1	I	51	ASN
1	I	245	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FQ8	Q	401	-	39,39,39	1.16	3 (7%)	53,56,56	0.92	1 (1%)
2	FQ8	F	401	-	39,39,39	1.21	3 (7%)	53,56,56	1.21	5 (9%)
2	FQ8	G	401	-	39,39,39	1.26	2 (5%)	53,56,56	0.98	3 (5%)
2	FQ8	O	401	-	39,39,39	1.25	2 (5%)	53,56,56	1.14	5 (9%)
2	FQ8	B	401	-	39,39,39	1.61	4 (10%)	53,56,56	1.09	4 (7%)
2	FQ8	D	401	-	39,39,39	1.23	3 (7%)	53,56,56	0.97	3 (5%)
2	FQ8	I	401	-	39,39,39	1.25	3 (7%)	53,56,56	1.03	2 (3%)
2	FQ8	E	401	-	39,39,39	1.28	3 (7%)	53,56,56	0.98	3 (5%)
2	FQ8	H	401	-	39,39,39	1.45	3 (7%)	53,56,56	0.73	1 (1%)
2	FQ8	C	401	-	39,39,39	1.20	3 (7%)	53,56,56	1.12	5 (9%)
2	FQ8	P	401	-	39,39,39	1.20	2 (5%)	53,56,56	1.01	4 (7%)
2	FQ8	A	401	-	39,39,39	1.26	4 (10%)	53,56,56	1.17	5 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FQ8	Q	401	-	-	37/56/56/56	-
2	FQ8	F	401	-	-	32/56/56/56	-
2	FQ8	G	401	-	-	41/56/56/56	-
2	FQ8	O	401	-	-	34/56/56/56	-
2	FQ8	B	401	-	-	29/56/56/56	-
2	FQ8	D	401	-	-	35/56/56/56	-
2	FQ8	I	401	-	-	30/56/56/56	-
2	FQ8	E	401	-	-	30/56/56/56	-
2	FQ8	H	401	-	-	24/56/56/56	-
2	FQ8	C	401	-	-	34/56/56/56	-
2	FQ8	P	401	-	-	32/56/56/56	-
2	FQ8	A	401	-	-	37/56/56/56	-

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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	OAO-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-OB
2	B	401	FQ8	OB-CAW-CBH-OAJ
2	B	401	FQ8	OB-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
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-PBN-OAC
2	C	401	FQ8	OB-CAW-CBH-OAJ
2	C	401	FQ8	OB-CAW-CBH-CBK

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Mol	Chain	Res	Type	Atoms
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-CAW-CBH-OAJ
2	F	401	FQ8	OB-CAW-CBH-CBK
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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-OBB
2	D	401	FQ8	OBB-CAW-CBH-OAJ
2	D	401	FQ8	OBB-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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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	OAH-CBF-CBJ-OAL

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Mol	Chain	Res	Type	Atoms
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	OAH-CBF-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	OAH-CBF-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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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:

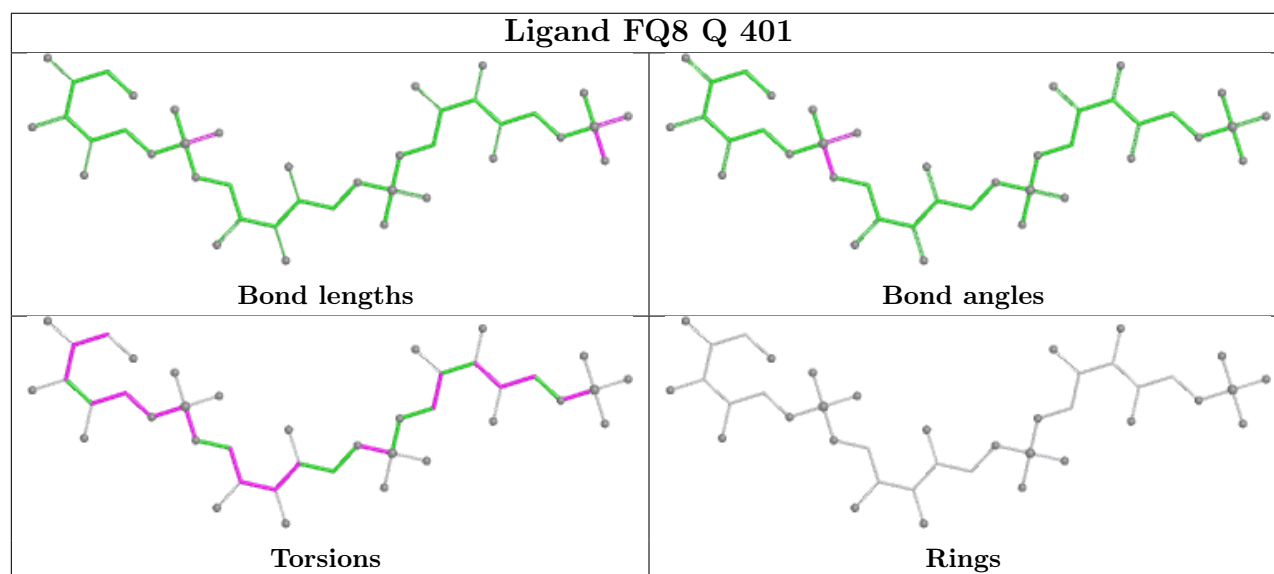
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	FQ8	1	0
2	E	401	FQ8	2	0

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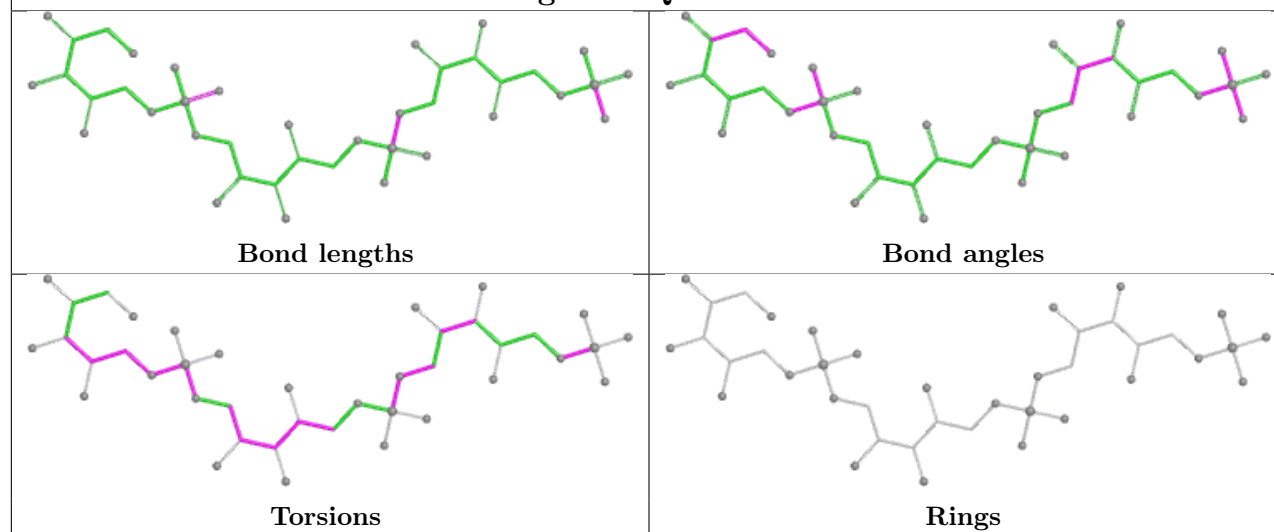
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	401	FQ8	1	0
2	C	401	FQ8	1	0

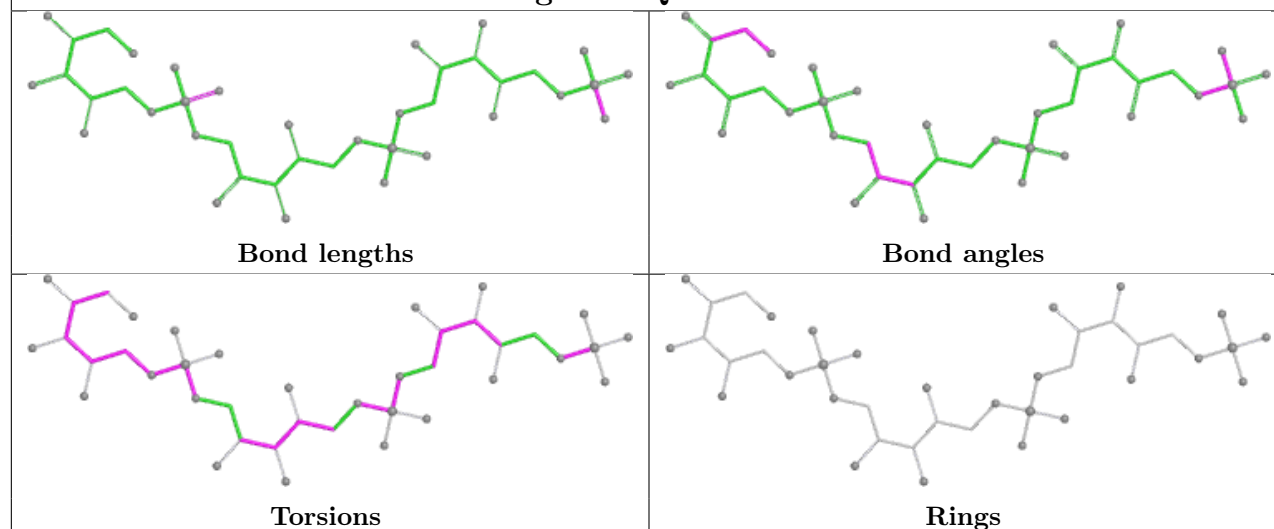
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



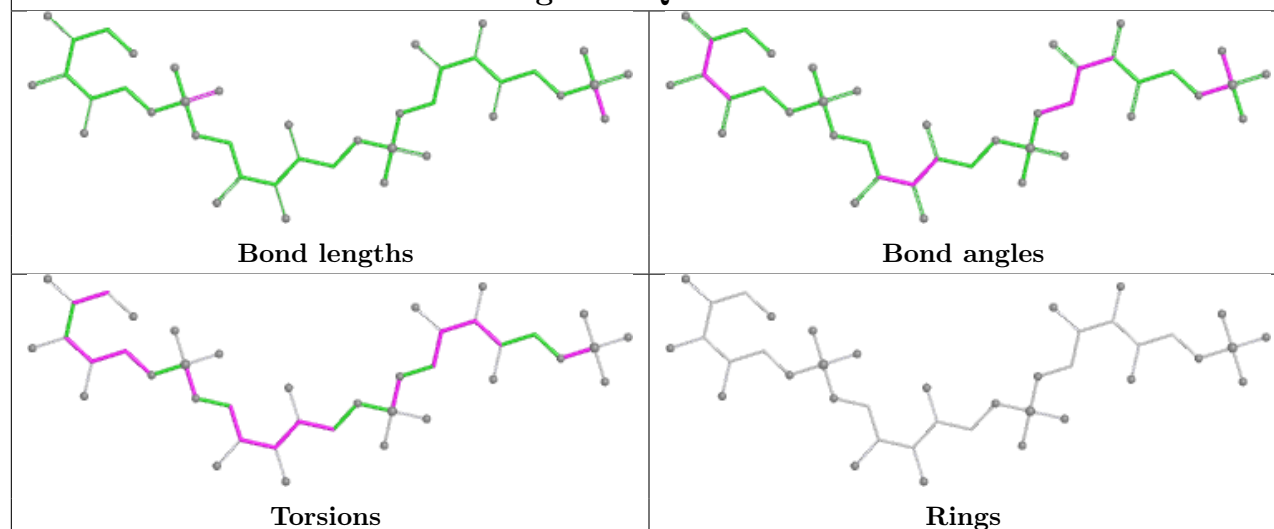
Ligand FQ8 F 401



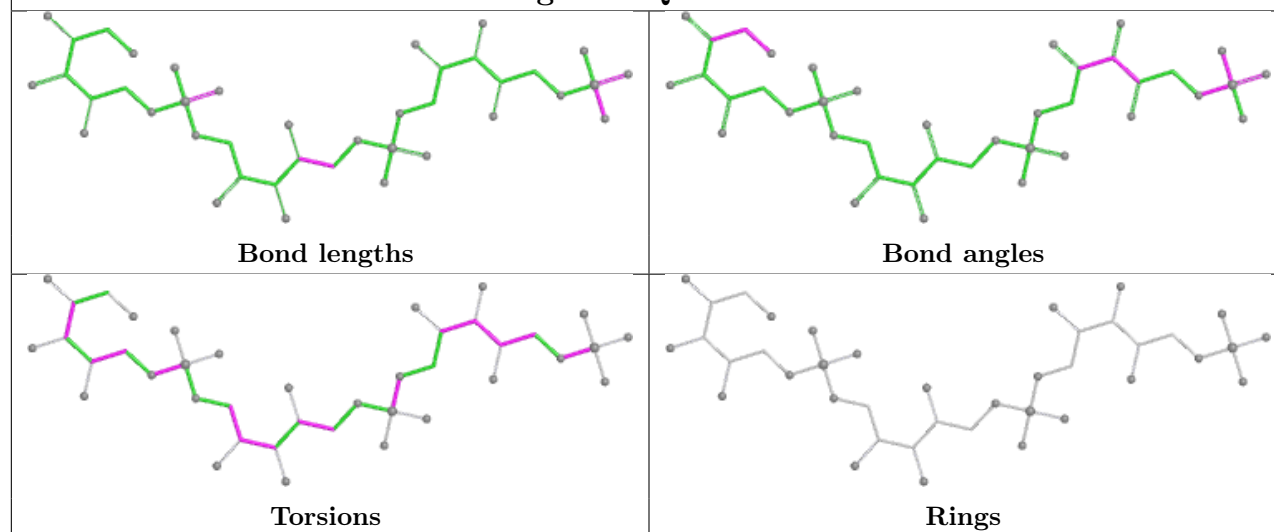
Ligand FQ8 G 401



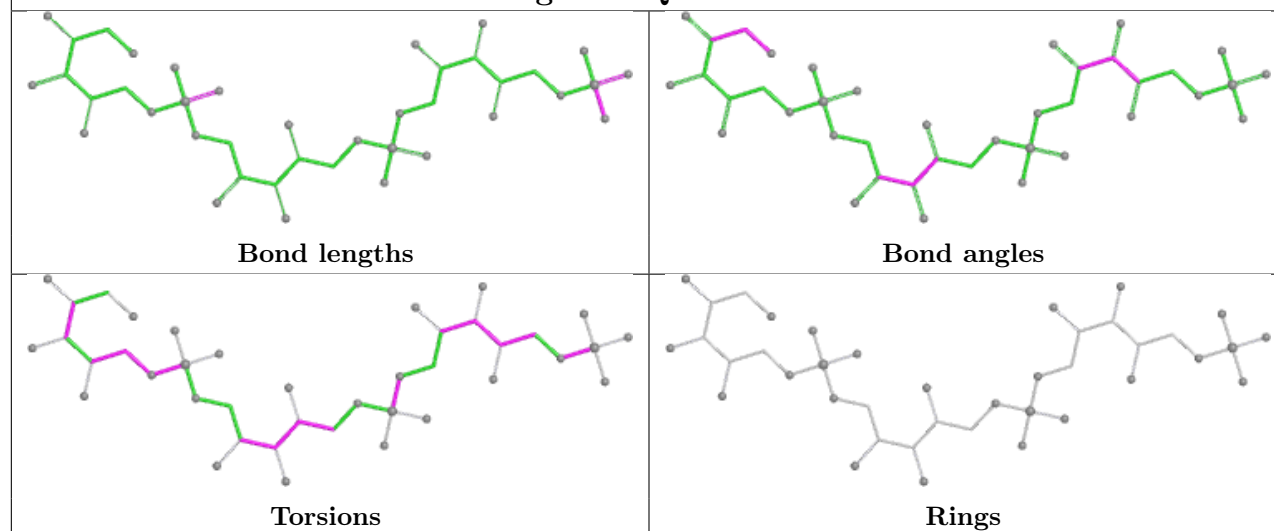
Ligand FQ8 O 401



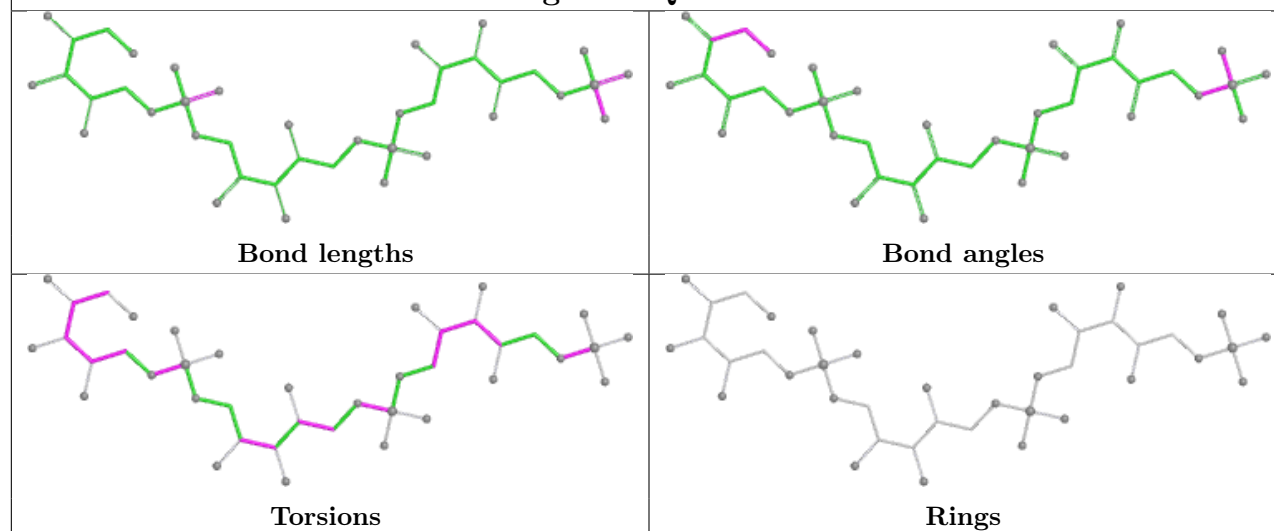
Ligand FQ8 B 401



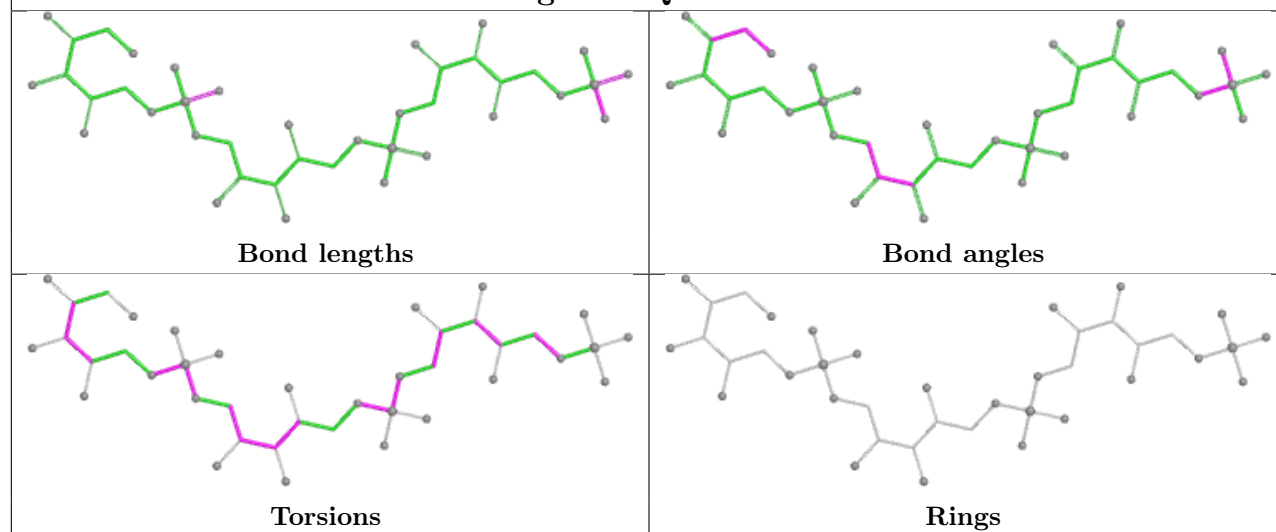
Ligand FQ8 D 401



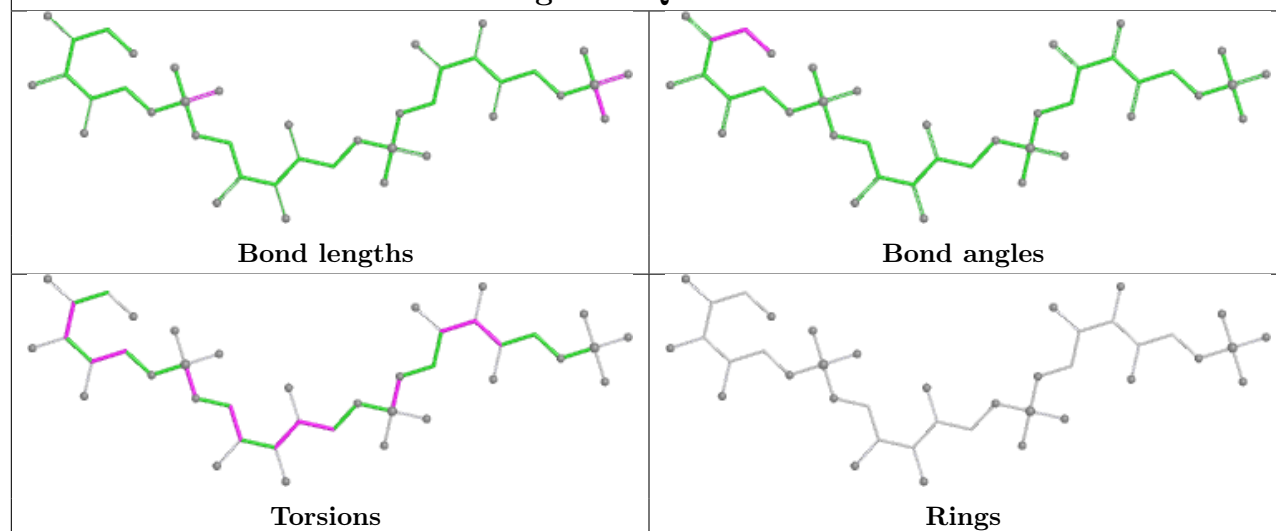
Ligand FQ8 I 401



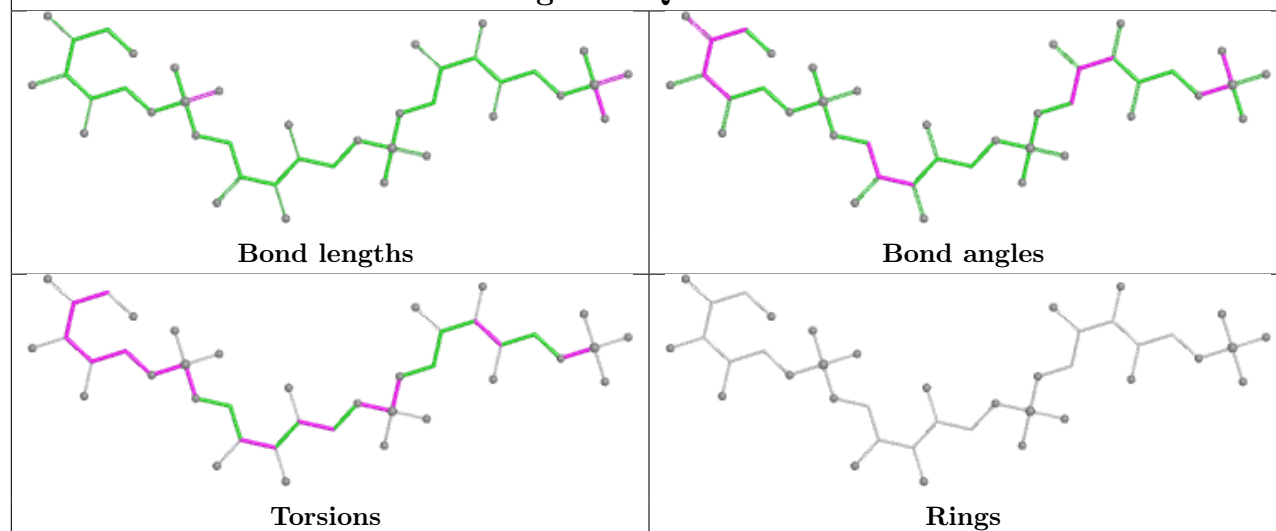
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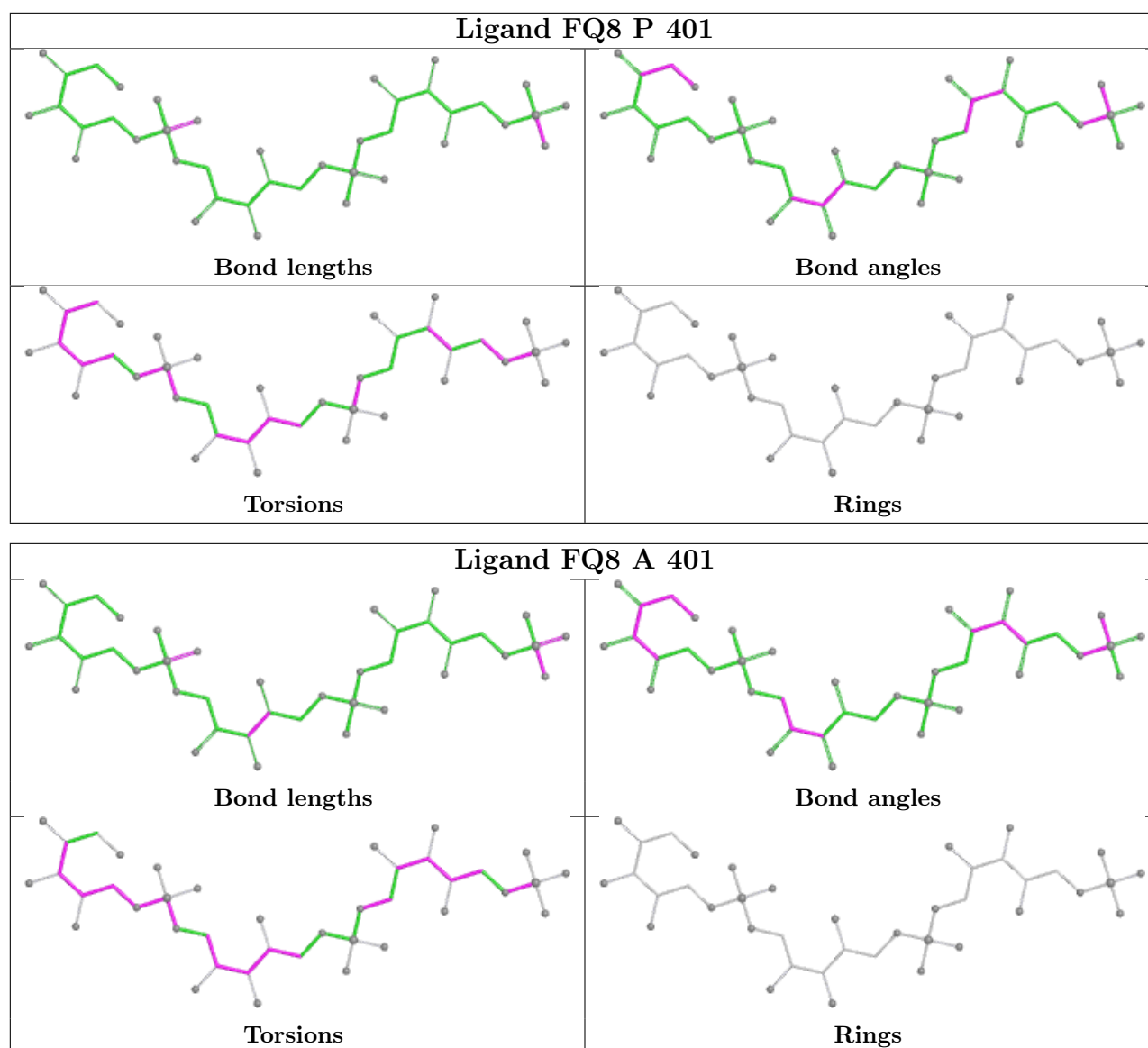


Ligand FQ8 H 401



Ligand FQ8 C 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	317/345 (91%)	-0.23	6 (1%) 66 62	30, 44, 75, 121	0
1	B	318/345 (92%)	-0.41	1 (0%) 90 88	27, 40, 65, 94	0
1	C	312/345 (90%)	-0.19	3 (0%) 79 76	29, 49, 84, 100	0
1	D	314/345 (91%)	-0.24	3 (0%) 79 76	33, 49, 72, 120	0
1	E	317/345 (91%)	-0.25	5 (1%) 70 66	22, 44, 76, 112	1 (0%)
1	F	317/345 (91%)	-0.27	3 (0%) 81 78	32, 45, 70, 106	0
1	G	314/345 (91%)	-0.22	4 (1%) 75 71	34, 48, 74, 118	0
1	H	318/345 (92%)	-0.44	2 (0%) 85 83	27, 39, 64, 91	0
1	I	314/345 (91%)	-0.11	3 (0%) 79 76	31, 52, 92, 115	0
1	O	316/345 (91%)	-0.32	2 (0%) 85 83	29, 43, 69, 98	0
1	P	300/345 (86%)	0.80	39 (13%) 7 5	45, 83, 138, 164	0
1	Q	315/345 (91%)	0.47	27 (8%) 16 13	38, 70, 129, 153	0
All	All	3772/4140 (91%)	-0.12	98 (2%) 57 53	22, 48, 101, 164	1 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	PHE	4.2
1	O	221	SER	3.9
1	P	222	THR	3.8
1	P	208	ASN	3.7
1	E	175	PHE	3.6
1	P	43	SER	3.6
1	A	222	THR	3.5
1	F	210	PHE	3.5
1	P	49	THR	3.5
1	P	40	ASP	3.5
1	P	197	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	222	THR	3.4
1	Q	13	ASN	3.4
1	P	31	SER	3.4
1	P	17	LEU	3.4
1	Q	208	ASN	3.2
1	P	119	GLY	3.2
1	D	222	THR	3.2
1	P	136	GLU	3.1
1	E	222	THR	3.0
1	P	28	THR	3.0
1	Q	48	GLU	3.0
1	Q	59	LEU	2.9
1	G	175	PHE	2.9
1	E	129	SER	2.9
1	C	129	SER	2.8
1	B	209	ASP	2.8
1	Q	128	ARG	2.8
1	P	98	HIS	2.8
1	Q	97	LEU	2.7
1	E	0	SER	2.7
1	P	35	GLU	2.7
1	P	11	PHE	2.6
1	O	209	ASP	2.6
1	P	140	VAL	2.6
1	Q	222	THR	2.6
1	I	128	ARG	2.6
1	P	175	PHE	2.6
1	Q	202	GLU	2.6
1	A	209	ASP	2.6
1	I	175	PHE	2.6
1	P	93	SER	2.6
1	P	101	ALA	2.6
1	I	222	THR	2.6
1	P	92	ASP	2.5
1	Q	129	SER	2.5
1	Q	94	ASP	2.5
1	P	48	GLU	2.5
1	P	113	ASN	2.5
1	Q	201	TYR	2.5
1	P	138	GLY	2.5
1	H	175	PHE	2.5
1	P	106	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	P	105	LEU	2.5
1	P	42	HIS	2.5
1	Q	98	HIS	2.5
1	Q	101	ALA	2.5
1	P	71	ASN	2.4
1	C	222	THR	2.4
1	G	129	SER	2.4
1	P	108	TYR	2.4
1	P	141	ALA	2.4
1	P	118	ILE	2.4
1	Q	26	ASN	2.4
1	G	128	ARG	2.3
1	P	1	MET	2.3
1	P	102	LEU	2.3
1	P	33	ASP	2.3
1	P	202	GLU	2.3
1	F	222	THR	2.3
1	P	199	THR	2.3
1	P	201	TYR	2.3
1	Q	58	GLY	2.2
1	P	36	LEU	2.2
1	F	221	SER	2.2
1	D	93	SER	2.2
1	P	130	VAL	2.1
1	Q	127	GLY	2.1
1	Q	56	TYR	2.1
1	A	177	LYS	2.1
1	Q	175	PHE	2.1
1	Q	64	GLN	2.1
1	Q	221	SER	2.1
1	H	209	ASP	2.1
1	A	178	THR	2.1
1	A	128	ARG	2.1
1	E	111	GLU	2.1
1	Q	11	PHE	2.0
1	Q	24	VAL	2.0
1	Q	60	VAL	2.0
1	D	175	PHE	2.0
1	P	32	THR	2.0
1	Q	9	PRO	2.0
1	Q	100	ARG	2.0
1	P	70	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	Q	70	GLY	2.0
1	Q	33	ASP	2.0
1	C	93	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FQ8	E	401	40/40	0.85	0.13	61,85,121,137	0
3	MG	D	402	1/1	0.85	0.37	71,71,71,71	0
2	FQ8	A	401	40/40	0.86	0.13	50,79,126,130	0
3	MG	E	402	1/1	0.87	0.31	60,60,60,60	0
4	CL	F	402	1/1	0.88	0.12	77,77,77,77	0
2	FQ8	P	401	40/40	0.89	0.10	51,100,151,161	0
2	FQ8	Q	401	40/40	0.90	0.12	51,81,129,143	0
3	MG	I	402	1/1	0.91	0.42	66,66,66,66	0
2	FQ8	D	401	40/40	0.91	0.12	44,77,125,130	0
2	FQ8	I	401	40/40	0.92	0.10	48,74,95,118	0
3	MG	B	402	1/1	0.92	0.42	63,63,63,63	0
4	CL	D	403	1/1	0.92	0.11	73,73,73,73	0
2	FQ8	H	401	40/40	0.93	0.10	36,69,91,100	0
2	FQ8	F	401	40/40	0.93	0.10	43,64,94,108	0
2	FQ8	B	401	40/40	0.93	0.11	34,72,101,113	0
2	FQ8	C	401	40/40	0.93	0.10	49,72,104,121	0
2	FQ8	G	401	40/40	0.94	0.10	50,73,124,142	0
2	FQ8	O	401	40/40	0.94	0.10	36,58,99,124	0
4	CL	D	404	1/1	0.95	0.10	72,72,72,72	0
4	CL	Q	402	1/1	0.96	0.08	71,71,71,71	0

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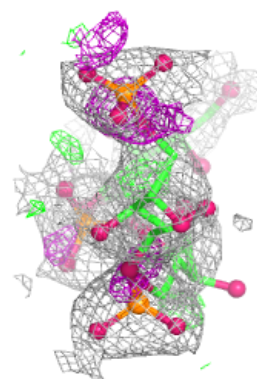
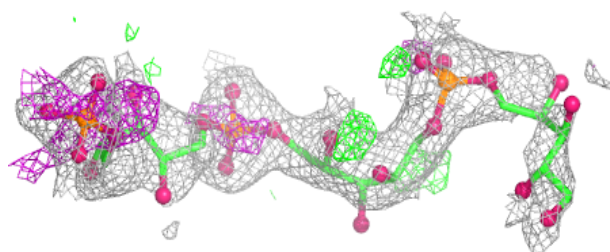
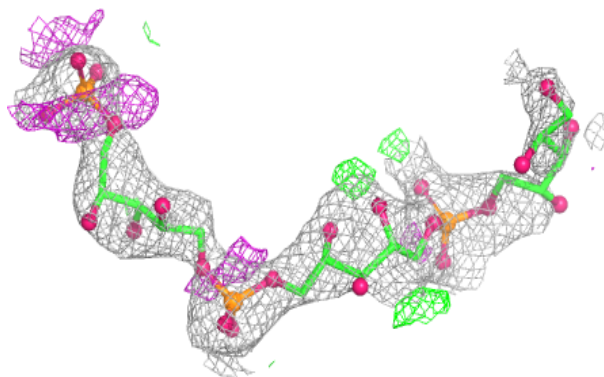
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	B	403	1/1	0.96	0.08	44,44,44,44	0
4	CL	E	403	1/1	0.96	0.06	40,40,40,40	0
4	CL	H	403	1/1	0.96	0.10	40,40,40,40	0
4	CL	H	404	1/1	0.96	0.06	48,48,48,48	0
4	CL	B	407	1/1	0.97	0.13	71,71,71,71	0
4	CL	E	404	1/1	0.97	0.09	61,61,61,61	0
4	CL	H	402	1/1	0.97	0.06	56,56,56,56	0
4	CL	G	402	1/1	0.97	0.09	64,64,64,64	0
4	CL	B	405	1/1	0.97	0.11	57,57,57,57	0
4	CL	I	403	1/1	0.97	0.07	57,57,57,57	0
4	CL	B	404	1/1	0.98	0.06	51,51,51,51	0
4	CL	A	402	1/1	0.98	0.04	38,38,38,38	0
4	CL	B	406	1/1	0.99	0.06	44,44,44,44	0

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

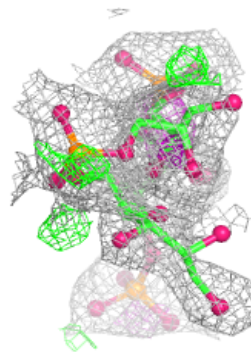
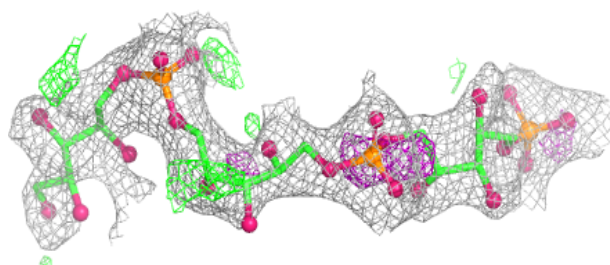
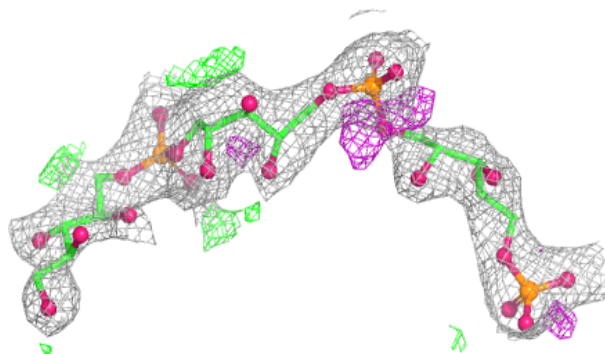
Electron density around FQ8 E 401:

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

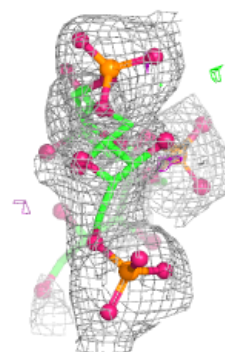
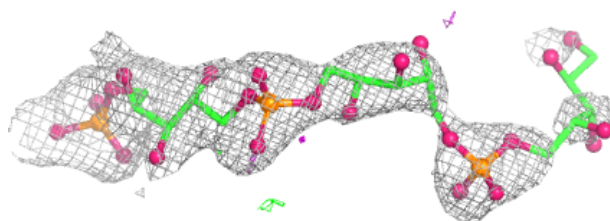
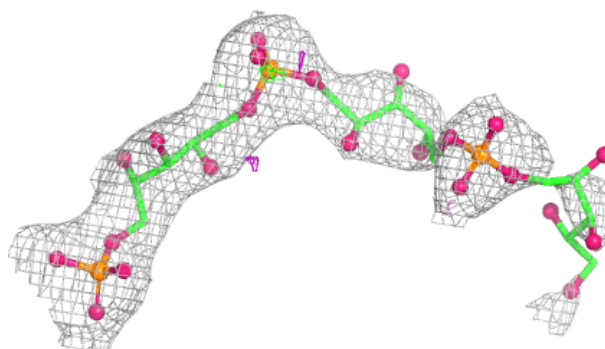


Electron density around FQ8 A 401:

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and green (positive)

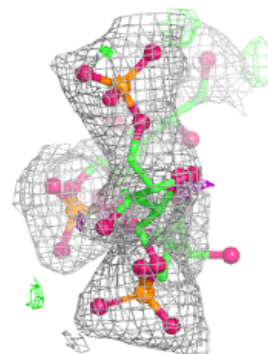
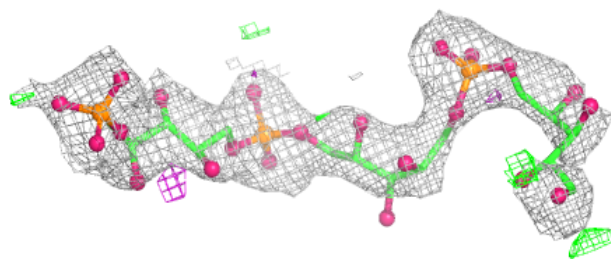
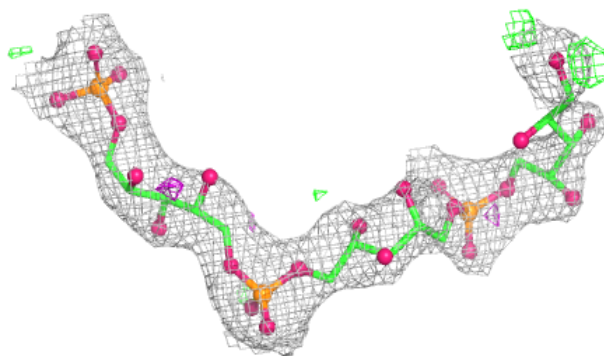
**Electron density around FQ8 P 401:**

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and green (positive)

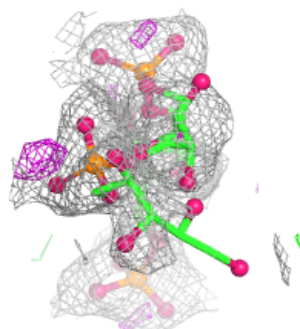
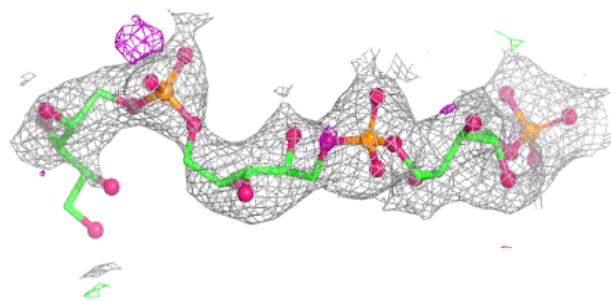
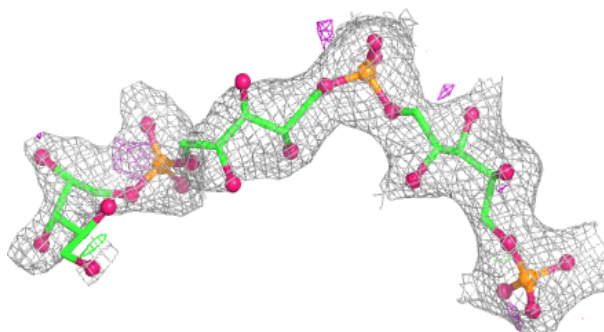


Electron density around FQ8 Q 401:

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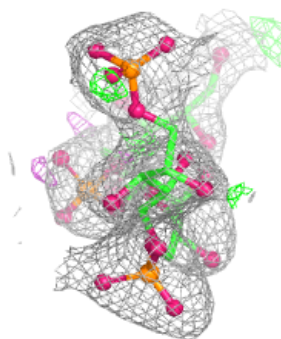
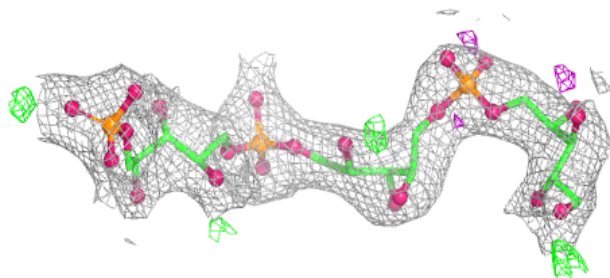
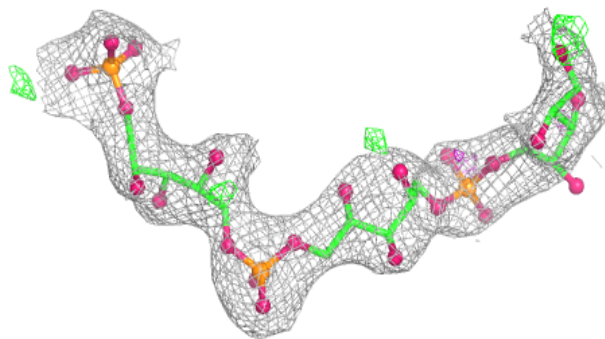
**Electron density around FQ8 D 401:**

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and green (positive)

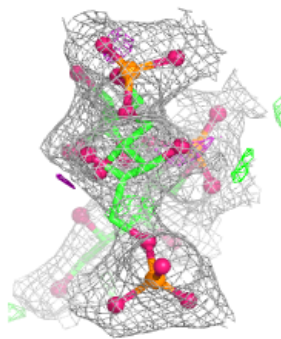
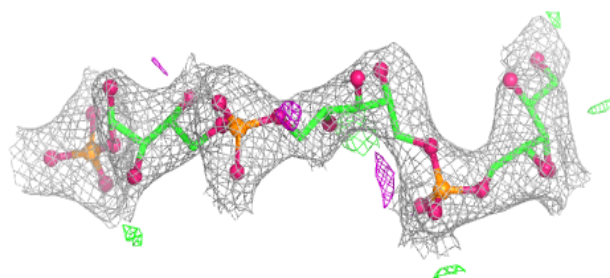
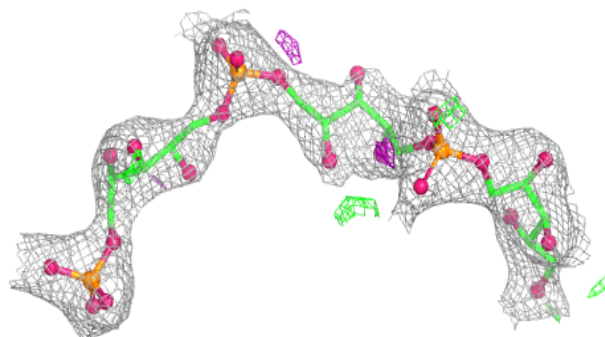


Electron density around FQ8 I 401:

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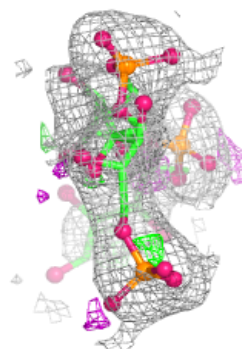
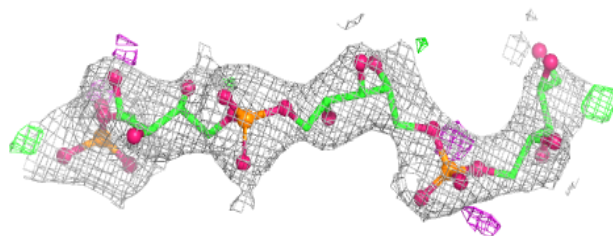
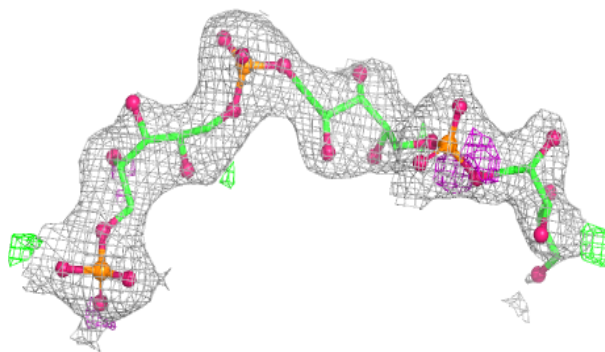
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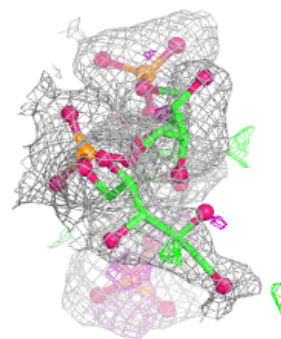
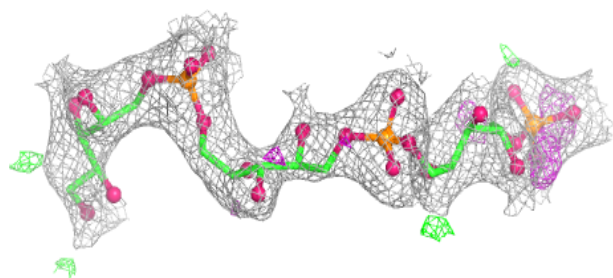
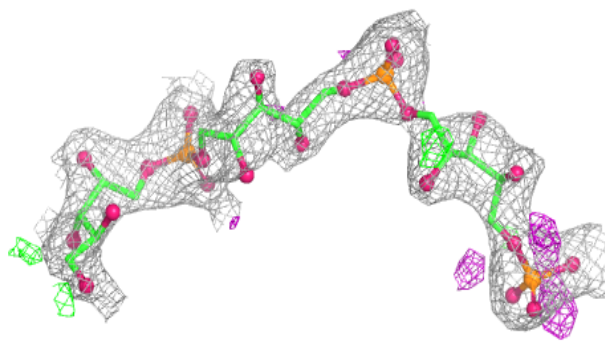


Electron density around FQ8 F 401:

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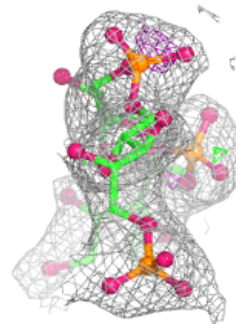
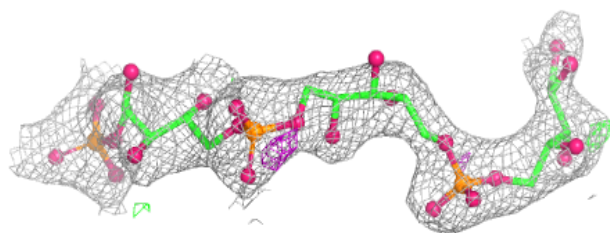
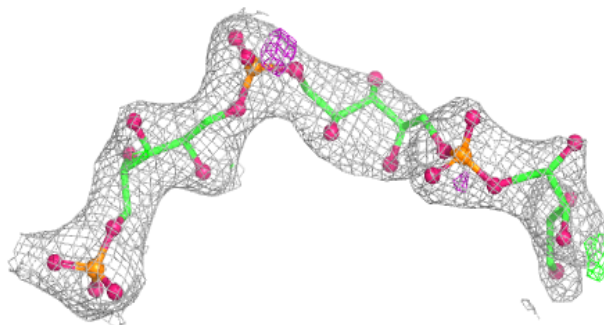
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and green (positive)

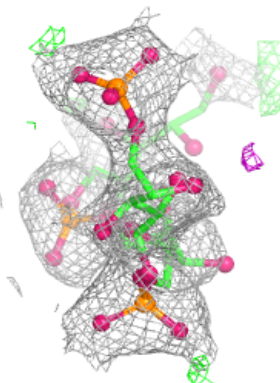
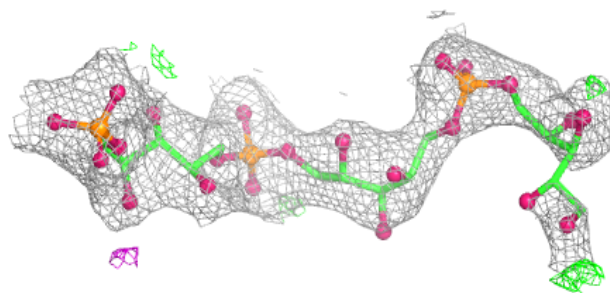
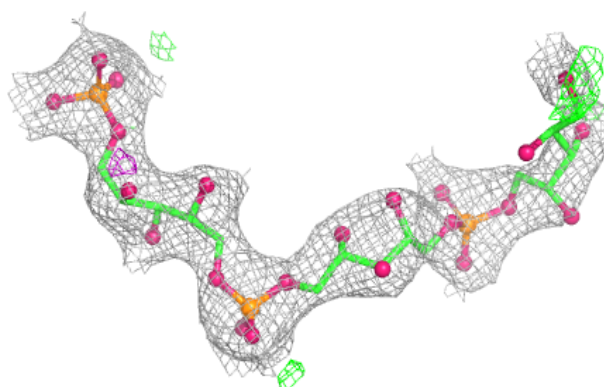


Electron density around FQ8 C 401:

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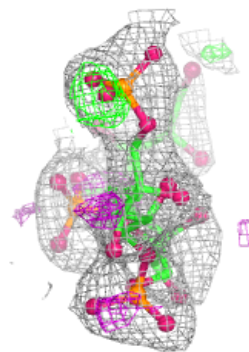
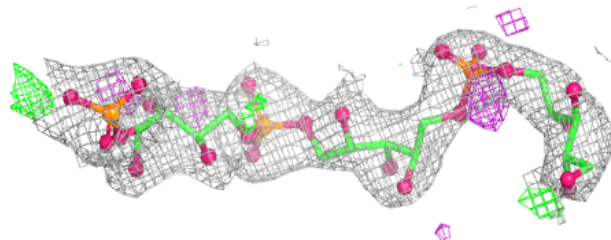
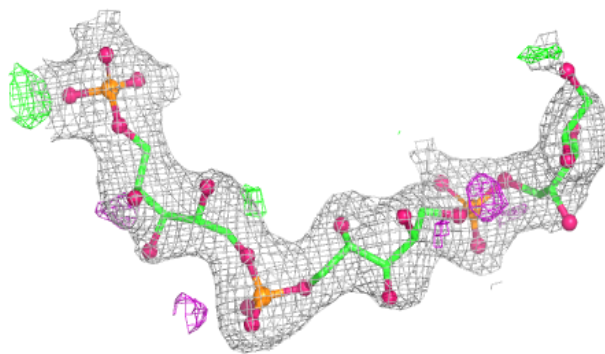
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and green (positive)



Electron density around FQ8 O 401:

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 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.