



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 07:21 am BST

PDB ID : 3FOF  
Title : Structural insight into the quinolone-DNA cleavage complex of type IIA topoisomerases  
Authors : Laponogov, I.; Sohi, M.K.; Veselkov, D.A.; Pan, X.-S.; Sawhney, R.; Thompson, A.W.; McAuley, K.E.; Fisher, L.M.; Sanderson, M.R.  
Deposited on : 2008-12-30  
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

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

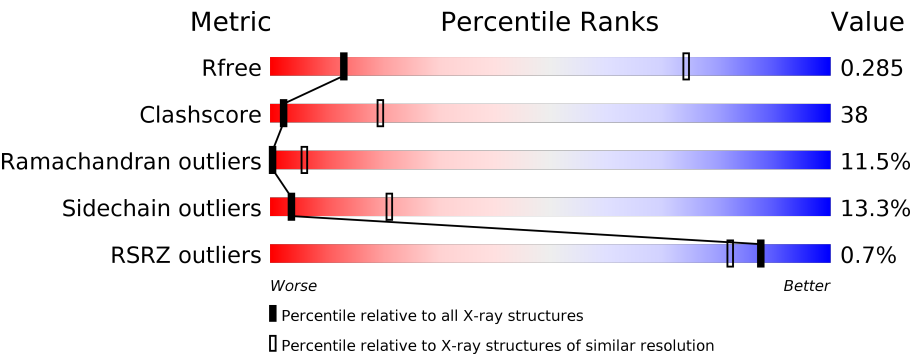
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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.




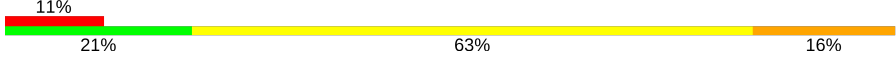
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	496	<div><div></div><div>52%28%7%12%</div></div>
1	B	496	<div><div></div><div>54%26%7%13%</div></div>
2	C	268	<div><div></div><div>41%27%•27%</div></div>
2	D	268	<div><div></div><div>44%25%5%26%</div></div>
3	E	15	<div><div>7%</div><div>33%60%7%</div></div>
4	F	19	<div><div>11%</div><div>21%68%11%</div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
5	G	15	
6	H	19	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MFx	F	0	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8498 atoms, of which 46 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 DNA topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			2482	1520	483	477	2			
1	B	432	Total	C	N	O	S	0	0	0
			2439	1494	476	467	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	489	LEU	-	EXPRESSION TAG	UNP P72525
A	490	GLU	-	EXPRESSION TAG	UNP P72525
A	491	HIS	-	EXPRESSION TAG	UNP P72525
A	492	HIS	-	EXPRESSION TAG	UNP P72525
A	493	HIS	-	EXPRESSION TAG	UNP P72525
A	494	HIS	-	EXPRESSION TAG	UNP P72525
A	495	HIS	-	EXPRESSION TAG	UNP P72525
A	496	HIS	-	EXPRESSION TAG	UNP P72525
B	489	LEU	-	EXPRESSION TAG	UNP P72525
B	490	GLU	-	EXPRESSION TAG	UNP P72525
B	491	HIS	-	EXPRESSION TAG	UNP P72525
B	492	HIS	-	EXPRESSION TAG	UNP P72525
B	493	HIS	-	EXPRESSION TAG	UNP P72525
B	494	HIS	-	EXPRESSION TAG	UNP P72525
B	495	HIS	-	EXPRESSION TAG	UNP P72525
B	496	HIS	-	EXPRESSION TAG	UNP P72525

- Molecule 2 is a protein called DNA topoisomerase 4 subunit B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	196	Total	C	N	O	0	0	0
			1040	630	202	208			
2	D	199	Total	C	N	O	0	0	0
			1059	639	208	212			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	380	MET	-	INITIATING METHIONINE	UNP Q59961
C	381	GLY	-	EXPRESSION TAG	UNP Q59961
C	382	HIS	-	EXPRESSION TAG	UNP Q59961
C	383	HIS	-	EXPRESSION TAG	UNP Q59961
C	384	HIS	-	EXPRESSION TAG	UNP Q59961
C	385	HIS	-	EXPRESSION TAG	UNP Q59961
C	386	HIS	-	EXPRESSION TAG	UNP Q59961
C	387	HIS	-	EXPRESSION TAG	UNP Q59961
C	388	HIS	-	EXPRESSION TAG	UNP Q59961
C	389	HIS	-	EXPRESSION TAG	UNP Q59961
C	390	HIS	-	EXPRESSION TAG	UNP Q59961
C	391	HIS	-	EXPRESSION TAG	UNP Q59961
C	392	SER	-	EXPRESSION TAG	UNP Q59961
C	393	SER	-	EXPRESSION TAG	UNP Q59961
C	394	GLY	-	EXPRESSION TAG	UNP Q59961
C	395	HIS	-	EXPRESSION TAG	UNP Q59961
C	396	ILE	-	EXPRESSION TAG	UNP Q59961
C	397	ASP	-	EXPRESSION TAG	UNP Q59961
C	398	ASP	-	EXPRESSION TAG	UNP Q59961
C	399	ASP	-	EXPRESSION TAG	UNP Q59961
C	400	ASP	-	EXPRESSION TAG	UNP Q59961
C	401	LYS	-	EXPRESSION TAG	UNP Q59961
C	402	HIS	-	EXPRESSION TAG	UNP Q59961
C	403	MET	-	EXPRESSION TAG	UNP Q59961
D	380	MET	-	INITIATING METHIONINE	UNP Q59961
D	381	GLY	-	EXPRESSION TAG	UNP Q59961
D	382	HIS	-	EXPRESSION TAG	UNP Q59961
D	383	HIS	-	EXPRESSION TAG	UNP Q59961
D	384	HIS	-	EXPRESSION TAG	UNP Q59961
D	385	HIS	-	EXPRESSION TAG	UNP Q59961
D	386	HIS	-	EXPRESSION TAG	UNP Q59961
D	387	HIS	-	EXPRESSION TAG	UNP Q59961
D	388	HIS	-	EXPRESSION TAG	UNP Q59961
D	389	HIS	-	EXPRESSION TAG	UNP Q59961
D	390	HIS	-	EXPRESSION TAG	UNP Q59961
D	391	HIS	-	EXPRESSION TAG	UNP Q59961
D	392	SER	-	EXPRESSION TAG	UNP Q59961
D	393	SER	-	EXPRESSION TAG	UNP Q59961
D	394	GLY	-	EXPRESSION TAG	UNP Q59961
D	395	HIS	-	EXPRESSION TAG	UNP Q59961
D	396	ILE	-	EXPRESSION TAG	UNP Q59961
D	397	ASP	-	EXPRESSION TAG	UNP Q59961

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	398	ASP	-	EXPRESSION TAG	UNP Q59961
D	399	ASP	-	EXPRESSION TAG	UNP Q59961
D	400	ASP	-	EXPRESSION TAG	UNP Q59961
D	401	LYS	-	EXPRESSION TAG	UNP Q59961
D	402	HIS	-	EXPRESSION TAG	UNP Q59961
D	403	MET	-	EXPRESSION TAG	UNP Q59961

- Molecule 3 is a DNA chain called DNA (5'-D(P\*AP\*CP\*CP\*AP\*AP\*GP\*GP\*TP\*CP\*AP\*TP\*GP\*AP\*AP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	15	Total	C	N	O	P	0	0	0
			306	144	60	87	15			

- Molecule 4 is a DNA chain called DNA (5'-D(P\*AP\*GP\*TP\*CP\*AP\*TP\*TP\*CP\*AP\*TP\*GP\*AP\*CP\*CP\*TP\*TP\*GP\*GP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	19	Total	C	N	O	P	0	0	0
			381	179	66	117	19			

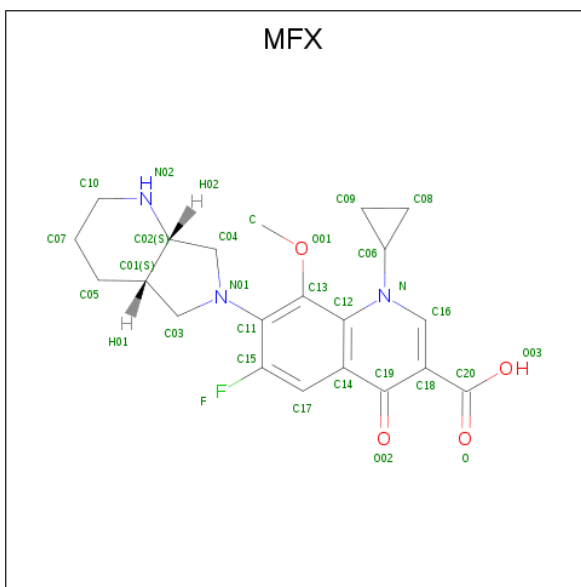
- Molecule 5 is a DNA chain called DNA (5'-D(P\*CP\*TP\*GP\*TP\*TP\*TP\*TP\*AP\*CP\*GP\*TP\*GP\*CP\*AP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	15	Total	C	N	O	P	0	0	0
			298	140	48	95	15			

- Molecule 6 is a DNA chain called DNA (5'-D(P\*GP\*AP\*CP\*TP\*AP\*TP\*GP\*CP\*AP\*CP\*GP\*TP\*AP\*AP\*AP\*AP\*CP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	19	Total	C	N	O	P	0	0	0
			389	183	78	109	19			

- Molecule 7 is 1-cyclopropyl-6-fluoro-8-methoxy-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (three-letter code: MFX) (formula: C<sub>21</sub>H<sub>24</sub>FN<sub>3</sub>O<sub>4</sub>).

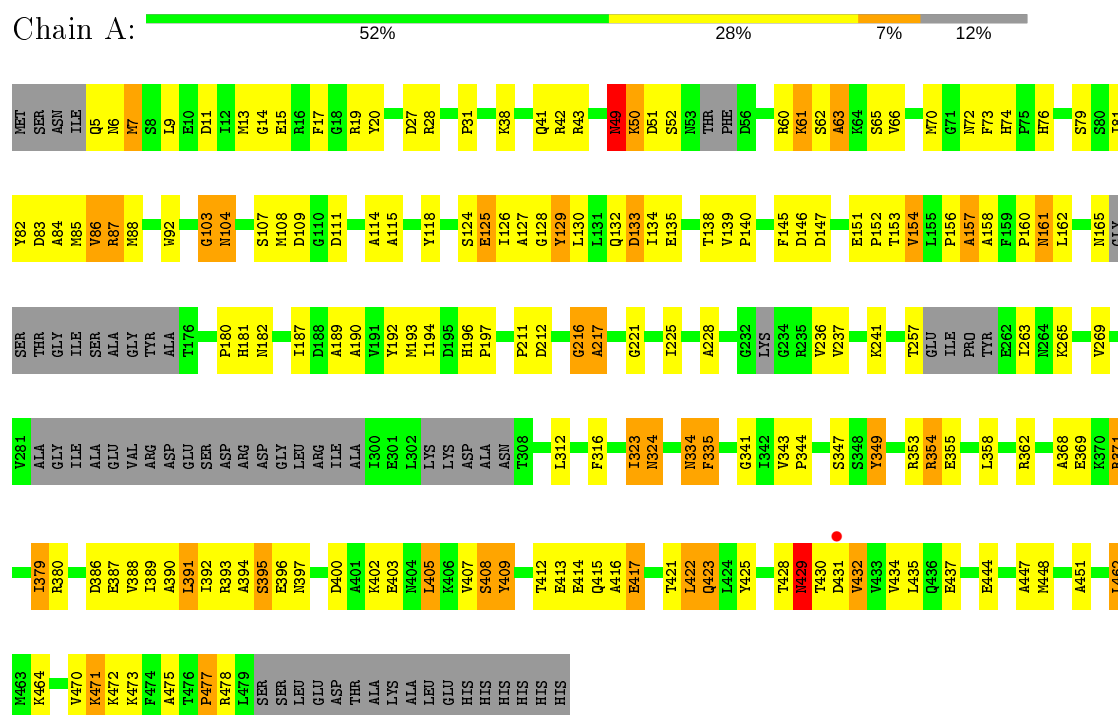


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	F	1	Total	C	F	H	N	O	0	0
			52	21	1	23	3	4		
7	H	1	Total	C	F	H	N	O	0	0
			52	21	1	23	3	4		

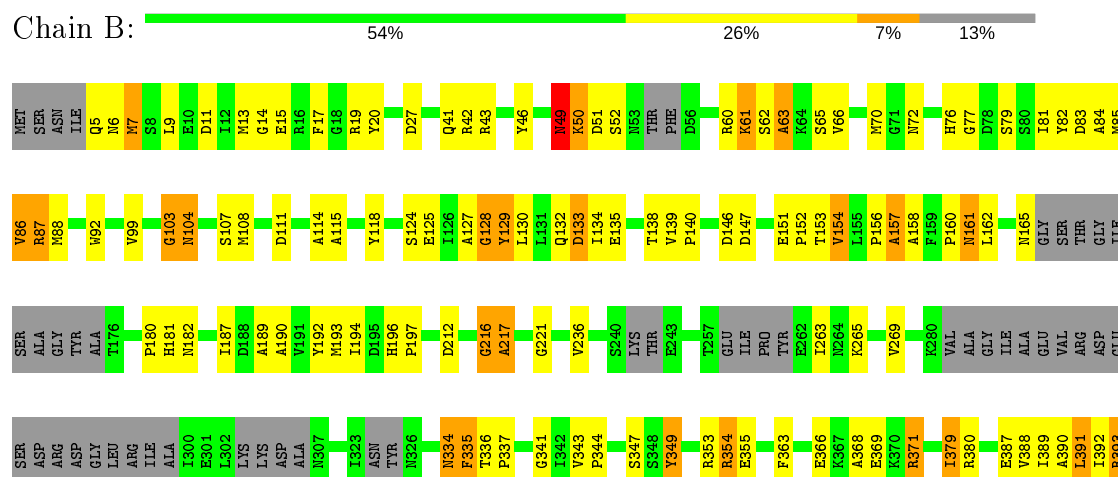
### 3 Residue-property plots [i](#)

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.

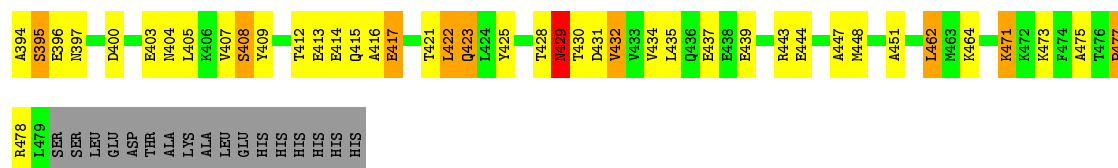
#### • Molecule 1: DNA topoisomerase 4 subunit A



#### • Molecule 1: DNA topoisomerase 4 subunit A

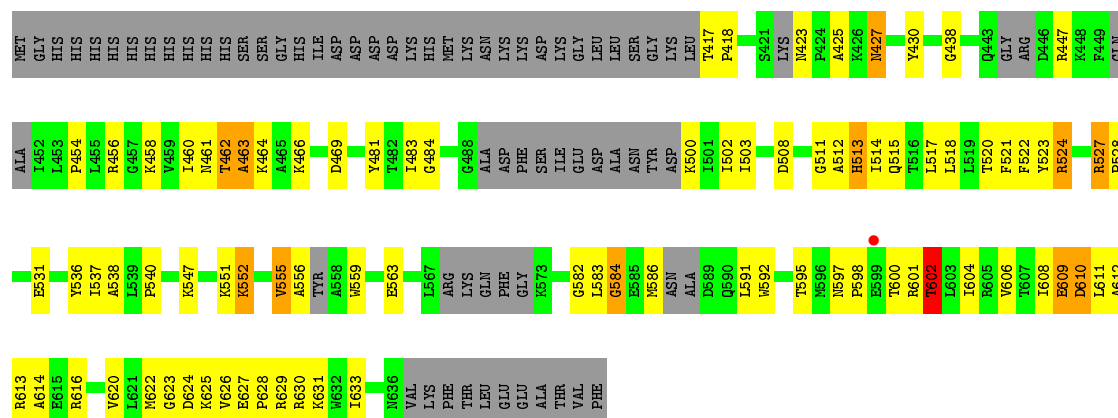






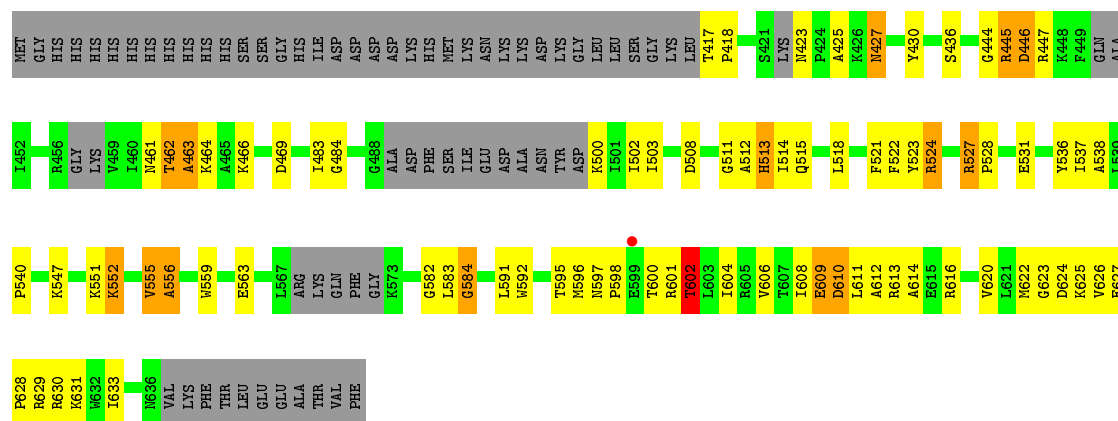
• Molecule 2: DNA topoisomerase 4 subunit B

Chain C: 41% 27% 27%



• Molecule 2: DNA topoisomerase 4 subunit B

Chain D: 44% 25% 5% 26%

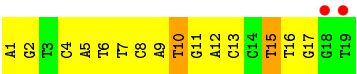


• Molecule 3: DNA (5'-D(P\*AP\*CP\*CP\*AP\*AP\*GP\*GP\*TP\*CP\*AP\*TP\*GP\*AP\*AP\*T)-3')

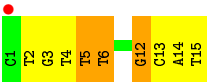
Chain E: 7% 33% 60% 7%



• Molecule 4: DNA (5'-D(P\*AP\*GP\*TP\*CP\*AP\*TP\*TP\*CP\*AP\*TP\*GP\*AP\*CP\*CP\*TP\*T P\*GP\*GP\*T)-3')



• Molecule 5: DNA (5'-D(P\*CP\*TP\*GP\*TP\*TP\*TP\*TP\*AP\*CP\*GP\*TP\*GP\*CP\*AP\*T)-3' )



• Molecule 6: DNA (5'-D(P\*GP\*AP\*CP\*TP\*AP\*TP\*GP\*CP\*AP\*CP\*GP\*TP\*AP\*AP\*AP\*AP\*CP\*AP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.60Å 121.60Å 178.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.07 – 4.00 34.07 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.07-4.00) 89.8 (34.07-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.239 , 0.289 0.233 , 0.285	Depositor DCC
$R_{free}$ test set	4398 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	168.4	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 210.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.428 for -h,-k,l 0.049 for h,-h-k,-l 0.046 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8498	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MFX

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	0.44	1/2516 (0.0%)	0.55	2/3479 (0.1%)
1	B	0.43	1/2471 (0.0%)	0.52	1/3419 (0.0%)
2	C	0.36	0/1042	0.53	0/1438
2	D	0.37	0/1064	0.51	0/1471
3	E	0.55	0/344	1.45	1/527 (0.2%)
4	F	0.57	0/426	1.39	3/652 (0.5%)
5	G	0.53	0/332	1.54	5/507 (1.0%)
6	H	0.54	0/438	1.43	4/672 (0.6%)
All	All	0.44	2/8633 (0.0%)	0.80	16/12165 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	429	ASN	CB-CG	5.83	1.64	1.51
1	A	429	ASN	CB-CG	5.64	1.64	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	12	DG	O4'-C4'-C3'	-14.72	97.17	106.00
3	E	12	DG	O4'-C4'-C3'	-14.03	97.58	106.00
6	H	8	DC	O4'-C4'-C3'	-7.72	101.37	106.00
6	H	10	DC	C1'-O4'-C4'	-7.53	102.57	110.10
5	G	12	DG	C4'-C3'-C2'	-6.69	97.08	103.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2482	0	1460	150	0
1	B	2439	0	1420	143	0
2	C	1040	0	602	66	0
2	D	1059	0	608	70	0
3	E	306	0	160	19	0
4	F	381	0	196	27	0
5	G	298	0	152	13	0
6	H	389	0	204	31	0
7	F	29	23	24	10	0
7	H	29	23	24	8	0
All	All	8452	46	4850	504	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 38.

The worst 5 of 504 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:A:471:LYS:O	1:A:475:ALA:HB2	1.20	1.35
1:B:471:LYS:O	1:B:475:ALA:HB2	1.19	1.30
1:B:124:SER:O	1:B:127:ALA:HB3	1.35	1.23
1:A:124:SER:O	1:A:127:ALA:HB3	1.36	1.19
1:A:471:LYS:O	1:A:475:ALA:CB	1.95	1.15

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	421/496 (85%)	278 (66%)	97 (23%)	46 (11%)	0	7
1	B	416/496 (84%)	276 (66%)	95 (23%)	45 (11%)	0	7
2	C	180/268 (67%)	114 (63%)	42 (23%)	24 (13%)	0	4
2	D	187/268 (70%)	122 (65%)	42 (22%)	23 (12%)	0	5
All	All	1204/1528 (79%)	790 (66%)	276 (23%)	138 (12%)	0	6

5 of 138 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	61	LYS
1	A	125	GLU
1	A	129	TYR
1	A	133	ASP

### 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	76/431 (18%)	66 (87%)	10 (13%)	4	21
1	B	71/431 (16%)	61 (86%)	10 (14%)	3	19
2	C	24/224 (11%)	21 (88%)	3 (12%)	4	22
2	D	24/224 (11%)	21 (88%)	3 (12%)	4	22
All	All	195/1310 (15%)	169 (87%)	26 (13%)	4	21

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	49	ASN
1	B	335	PHE
2	D	527	ARG
1	B	87	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	334	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	ASN
1	B	334	ASN
1	B	72	ASN
1	A	76	HIS
1	B	49	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MFX	F	0	-	24,33,33	4.92	8 (33%)	26,50,50	2.22	6 (23%)
7	MFX	H	0	-	24,33,33	4.95	8 (33%)	26,50,50	2.07	7 (26%)

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
7	MFX	F	0	-	-	1/10/35/35	0/5/5/5
7	MFX	H	0	-	-	3/10/35/35	0/5/5/5

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	0	MFX	C13-C12	14.85	1.64	1.41
7	F	0	MFX	C13-C12	14.78	1.64	1.41
7	H	0	MFX	C17-C14	11.26	1.61	1.41
7	F	0	MFX	C17-C14	11.17	1.61	1.41
7	H	0	MFX	C14-C12	-9.56	1.33	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	0	MFX	C10-N02-C02	6.18	115.48	111.62
7	F	0	MFX	C17-C14-C12	5.42	120.66	118.48
7	H	0	MFX	C10-N02-C02	5.23	114.88	111.62
7	H	0	MFX	C17-C14-C12	4.94	120.47	118.48
7	F	0	MFX	C13-C11-C15	3.90	119.71	115.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	0	MFX	C13-C11-N01-C04
7	H	0	MFX	C15-C11-N01-C04
7	H	0	MFX	C13-C11-N01-C04
7	H	0	MFX	C13-C11-N01-C03

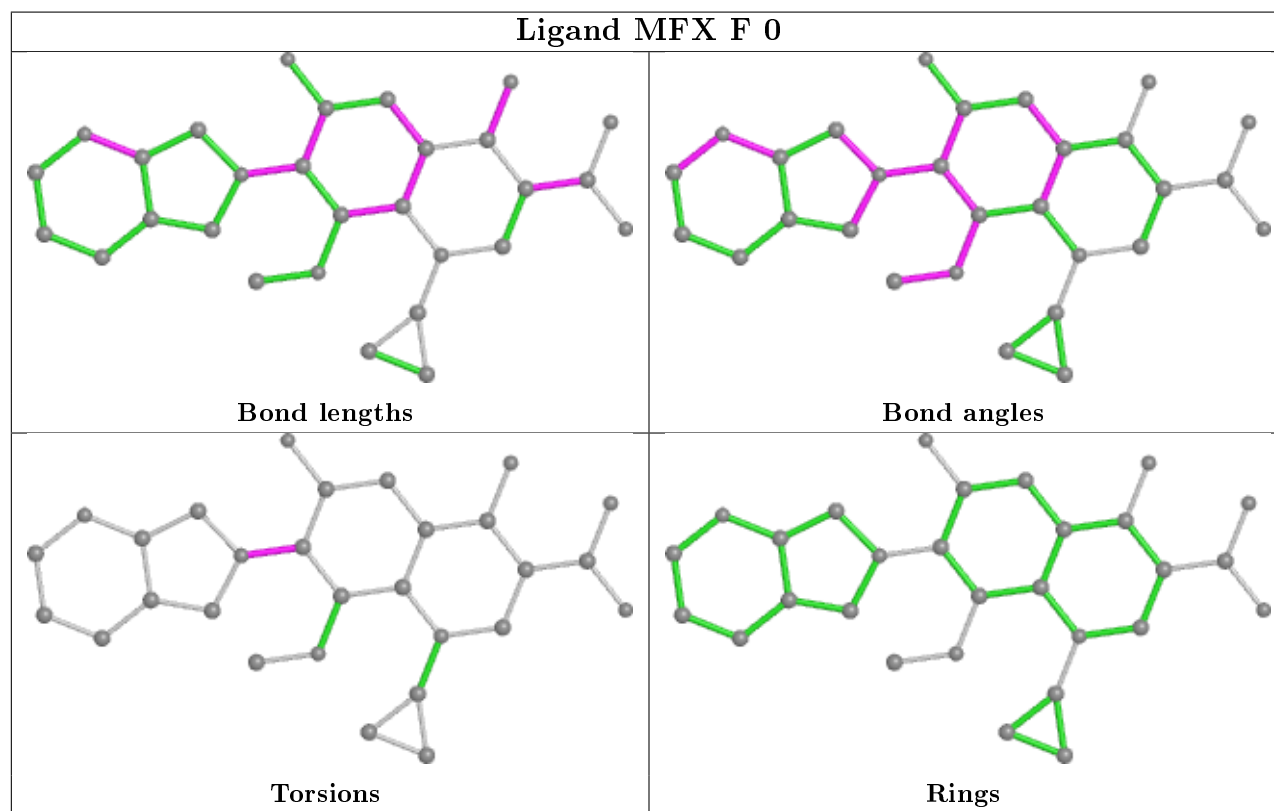
There are no ring outliers.

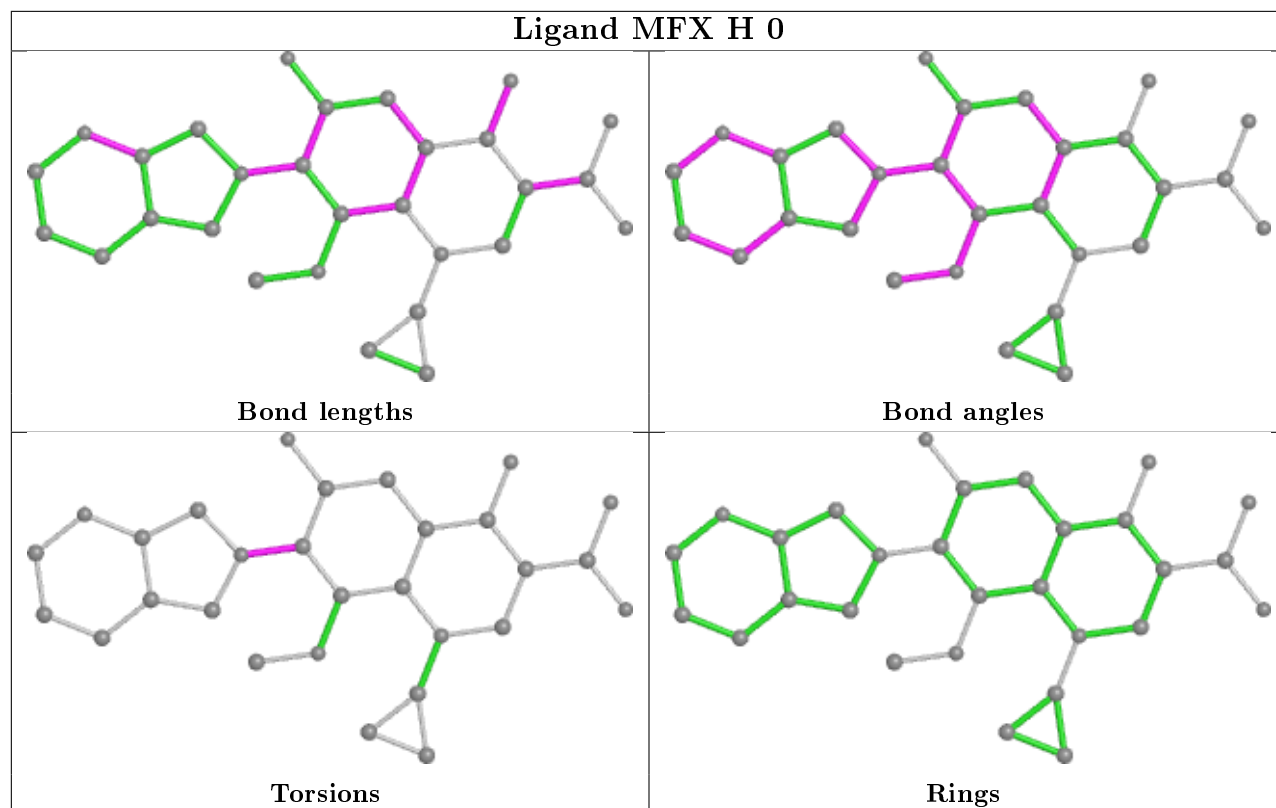
2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	0	MFX	10	0
7	H	0	MFX	8	0



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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	435/496 (87%)	-1.00	1 (0%) 95 93	91, 178, 258, 361	0
1	B	432/496 (87%)	-1.00	0 100 100	91, 178, 255, 355	0
2	C	196/268 (73%)	-0.88	1 (0%) 91 85	114, 180, 291, 395	0
2	D	199/268 (74%)	-0.87	1 (0%) 91 85	107, 182, 292, 386	0
3	E	15/15 (100%)	-0.03	1 (6%) 17 14	143, 263, 436, 512	0
4	F	19/19 (100%)	0.06	2 (10%) 6 6	148, 232, 469, 484	0
5	G	15/15 (100%)	-0.12	1 (6%) 17 14	141, 253, 368, 479	0
6	H	19/19 (100%)	0.04	2 (10%) 6 6	155, 209, 445, 475	0
All	All	1330/1596 (83%)	-0.91	9 (0%) 87 82	91, 181, 282, 512	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	19	DT	4.9
6	H	18	DA	3.3
4	F	18	DG	3.3
2	D	599	GLU	3.1
6	H	19	DG	2.8

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

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

### 6.3 Carbohydrates [i](#)

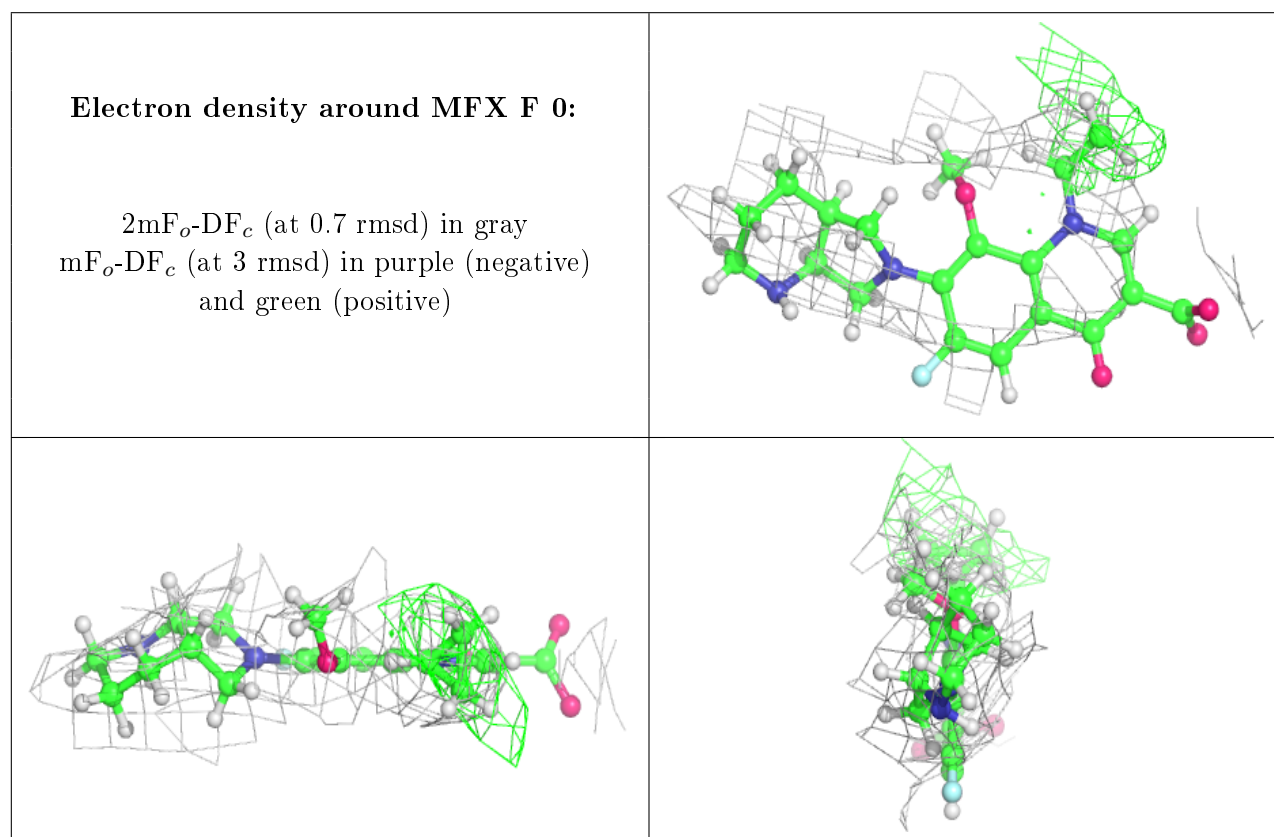
There are no carbohydrates in this entry.

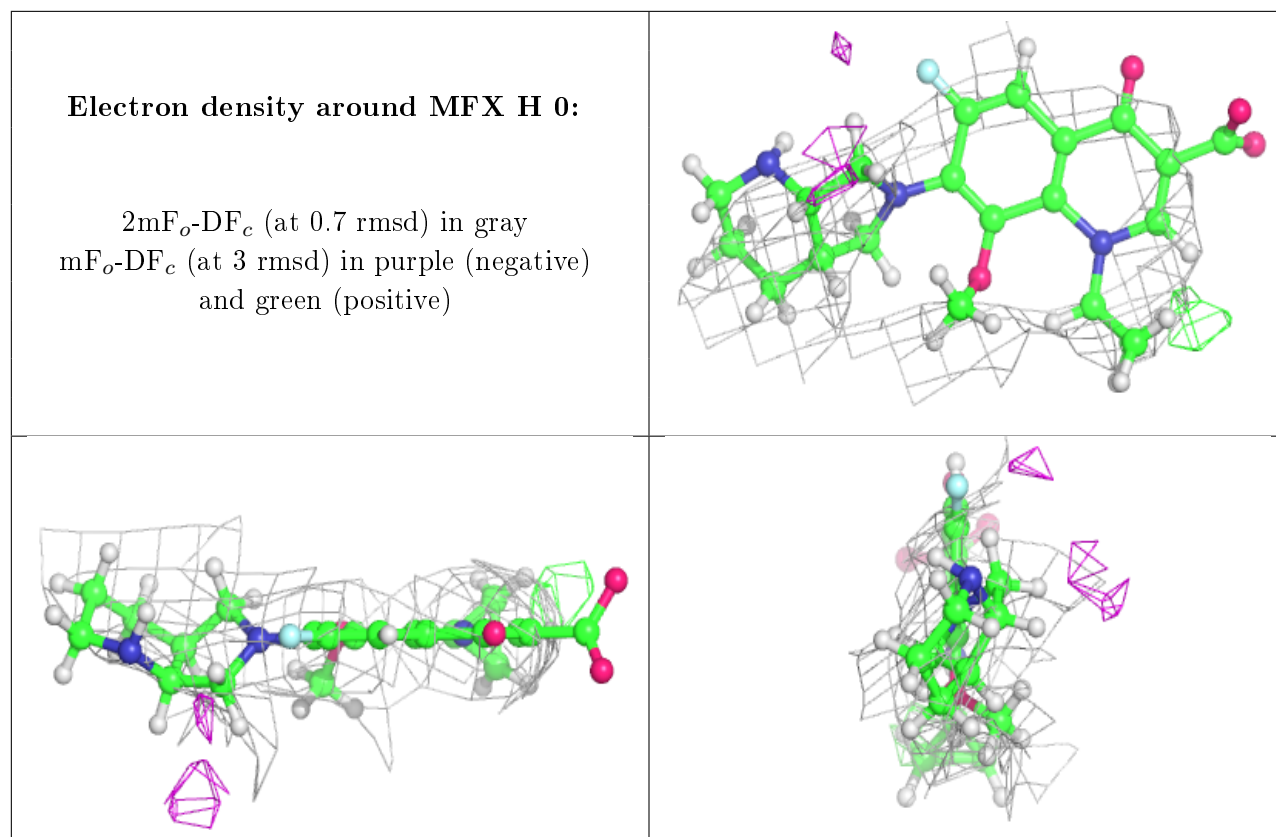
## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	MFX	F	0	29/29	0.83	0.29	229,278,346,350	0
7	MFX	H	0	29/29	0.84	0.31	224,270,369,415	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.