



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:26 AM UTC

PDB ID : 4Z3O / pdb_00004z3o
Title : Quinolone(Moxifloxacin)-DNA cleavage complex of topoisomerase IV from *S. pneumoniae*
Authors : Laponogov, I.; Veselkov, D.A.; Pan, X.-S.; Selvarajah, J.; Crevel, I.M.-T.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2015-03-31
Resolution : 3.44 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

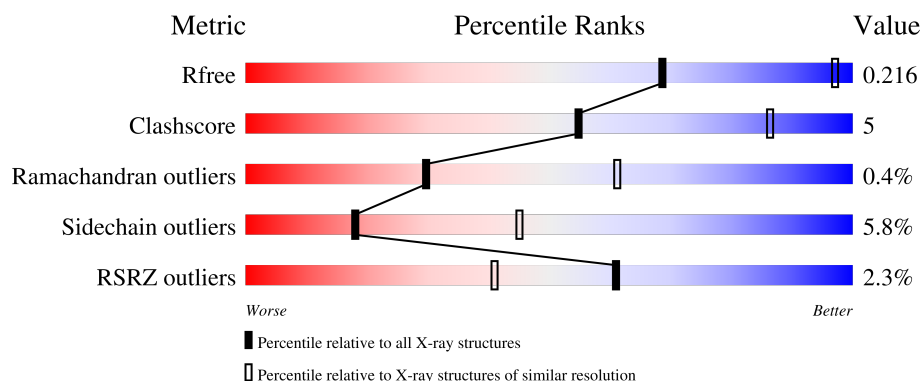
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

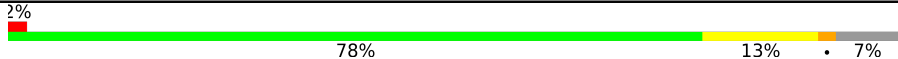
The reported resolution of this entry is 3.44 Å.

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	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)

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	742	
1	B	742	
2	E	7	
3	F	11	

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Mol	Chain	Length	Quality of chain
4	G	7	
5	H	11	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11053 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 DNA topoisomerase 4 subunit B,ParE30-ParC55 fused topo IV from *S. pneumoniae*.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	689	Total	C	N	O	S	0	0	0
			5136	3252	895	971	18			
1	B	689	Total	C	N	O	S	0	0	0
			5111	3241	885	967	18			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	403	MET	-	expression tag	UNP Q59961
A	460	ILE	VAL	engineered mutation	UNP Q59961
A	996	ALA	-	linker	UNP Q59961
A	997	THR	-	linker	UNP Q59961
A	998	VAL	-	linker	UNP Q59961
A	999	PHE	-	linker	UNP Q59961
A	1000	HIS	-	linker	UNP Q59961
A	1001	MET	-	linker	UNP Q59961
A	1002	SER	-	linker	UNP Q59961
A	1257	THR	ILE	engineered mutation	UNP P72525
A	1485	THR	-	expression tag	UNP P72525
A	1486	ALA	-	expression tag	UNP P72525
A	1487	LYS	-	expression tag	UNP P72525
A	1488	ALA	-	expression tag	UNP P72525
A	1489	LEU	-	expression tag	UNP P72525
A	1490	GLU	-	expression tag	UNP P72525
A	1491	HIS	-	expression tag	UNP P72525
A	1492	HIS	-	expression tag	UNP P72525
A	1493	HIS	-	expression tag	UNP P72525
A	1494	HIS	-	expression tag	UNP P72525
A	1495	HIS	-	expression tag	UNP P72525
A	1496	HIS	-	expression tag	UNP P72525
B	403	MET	-	expression tag	UNP Q59961
B	460	ILE	VAL	engineered mutation	UNP Q59961

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Chain	Residue	Modelled	Actual	Comment	Reference
B	996	ALA	-	linker	UNP Q59961
B	997	THR	-	linker	UNP Q59961
B	998	VAL	-	linker	UNP Q59961
B	999	PHE	-	linker	UNP Q59961
B	1000	HIS	-	linker	UNP Q59961
B	1001	MET	-	linker	UNP Q59961
B	1002	SER	-	linker	UNP Q59961
B	1257	THR	ILE	engineered mutation	UNP P72525
B	1485	THR	-	expression tag	UNP P72525
B	1486	ALA	-	expression tag	UNP P72525
B	1487	LYS	-	expression tag	UNP P72525
B	1488	ALA	-	expression tag	UNP P72525
B	1489	LEU	-	expression tag	UNP P72525
B	1490	GLU	-	expression tag	UNP P72525
B	1491	HIS	-	expression tag	UNP P72525
B	1492	HIS	-	expression tag	UNP P72525
B	1493	HIS	-	expression tag	UNP P72525
B	1494	HIS	-	expression tag	UNP P72525
B	1495	HIS	-	expression tag	UNP P72525
B	1496	HIS	-	expression tag	UNP P72525

- Molecule 2 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	P	0	0	0
			140	69	27	38	6			

- Molecule 3 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	11	Total	C	N	O	P	0	0	0
			225	108	39	67	11			

- Molecule 4 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	7	Total	C	N	O	P	0	0	0
			139	68	25	40	6			

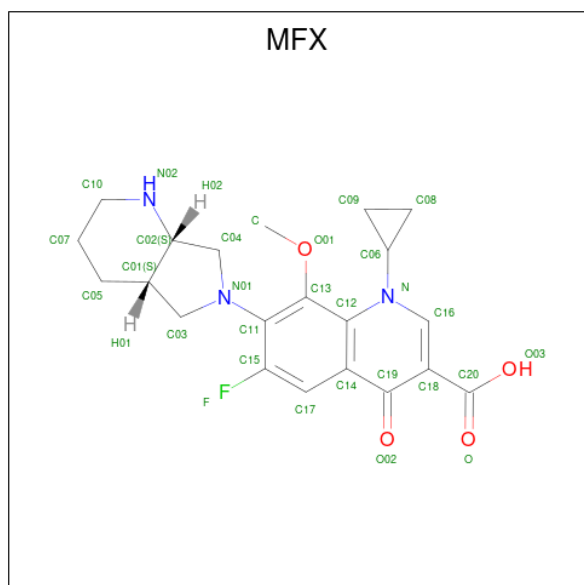
- Molecule 5 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	11	Total	C	N	O	P	0	0	0
			226	107	43	65	11			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		
6	B	2	Total	Mg	0	0
			2	2		

- 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 (CCD ID: MFX) (formula: C₂₁H₂₄FN₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	F	1	Total	C	F	N	O	0	0
			29	21	1	3	4		
7	H	1	Total	C	F	N	O	0	0
			29	21	1	3	4		

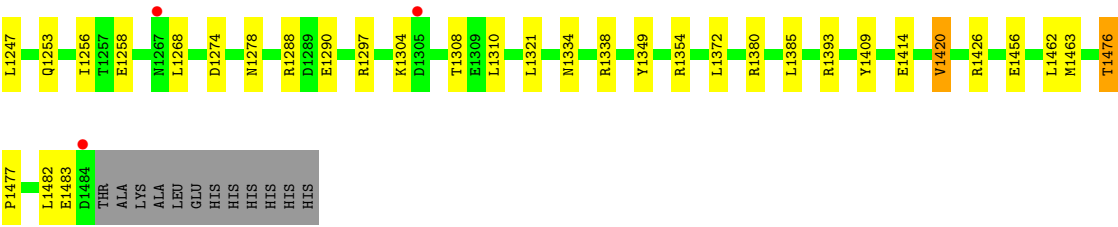
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	5	Total	O	0	0
			5	5		

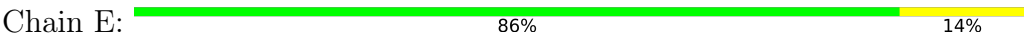
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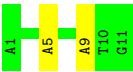
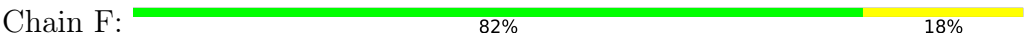
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	8	Total	O	0	0
			8	8		
8	F	1	Total	O	0	0
			1	1		



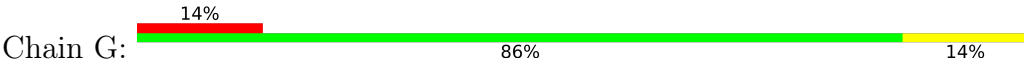
• Molecule 2: E-site DNA



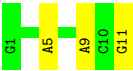
• Molecule 3: E-site DNA



• Molecule 4: E-site DNA



• Molecule 5: E-site DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.76Å 157.76Å 211.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.34 – 3.44 70.34 – 3.44	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.34-3.44) 97.4 (70.34-3.44)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.182 , 0.212 0.185 , 0.216	Depositor DCC
R_{free} test set	2566 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	85.7	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 72.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11053	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.28	0/5222	0.73	0/7098
1	B	0.27	0/5198	0.72	0/7067
2	E	0.08	0/157	0.51	0/241
3	F	0.12	0/251	0.59	0/385
4	G	0.08	0/155	0.51	0/238
5	H	0.11	0/253	0.57	0/388
All	All	0.27	0/11236	0.71	0/15417

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5136	0	4805	55	0
1	B	5111	0	4782	45	0
2	E	140	0	78	1	0
3	F	225	0	126	3	0
4	G	139	0	78	1	0
5	H	226	0	124	5	0
6	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	2	0	0	0	0
7	F	29	0	23	3	0
7	H	29	0	23	2	0
8	A	5	0	0	0	0
8	B	8	0	0	0	0
8	F	1	0	0	0	0
All	All	11053	0	10039	101	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 5.

All (101) 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:1380:ARG:NH1	1:A:1409:TYR:O	2.23	0.71
1:B:520:THR:HG21	1:B:622:MET:HG3	1.73	0.70
1:A:1350:ILE:HA	1:A:1463:MET:HE1	1.74	0.69
1:B:1288:ARG:NH1	1:B:1290:GLU:OE2	2.26	0.68
1:B:592:TRP:HA	1:B:596:MET:HB2	1.74	0.68
1:B:1290:GLU:OE1	1:B:1297:ARG:NH1	2.27	0.67
1:A:520:THR:HG21	1:A:622:MET:HG3	1.75	0.67
1:B:623:GLY:O	1:B:629:ARG:NH2	2.29	0.65
1:A:1077:GLY:HA2	1:B:1117:ARG:HD3	1.78	0.64
1:A:623:GLY:O	1:A:629:ARG:NH2	2.31	0.63
1:A:1024:ILE:HD12	1:A:1028:ARG:HE	1.64	0.62
1:B:1220:GLN:HG2	1:B:1483:GLU:HB2	1.84	0.58
1:A:592:TRP:HA	1:A:596:MET:HB2	1.84	0.58
1:A:1288:ARG:NH1	1:A:1290:GLU:OE2	2.33	0.57
1:A:1382:ILE:HD12	1:A:1432:VAL:HG23	1.85	0.57
1:A:1371:ARG:HG2	1:A:1442:LEU:HD11	1.87	0.56
1:A:1386:ASP:OD1	1:B:1393:ARG:NH2	2.38	0.56
1:A:1104:ASN:HB3	1:A:1114:ALA:HB2	1.87	0.56
1:A:1040:VAL:HG11	4:G:13:DC:H5'	1.89	0.54
1:A:1028:ARG:HH11	1:A:1028:ARG:HG3	1.72	0.54
1:A:1044:ILE:HG12	1:A:1069:ILE:HD13	1.90	0.54
1:B:1256:ILE:HD13	1:B:1321:LEU:HD21	1.90	0.54
1:B:1070:MET:HE1	1:B:1078:ASP:HB3	1.90	0.54
1:B:537:ILE:HB	1:B:604:ILE:HB	1.91	0.53
1:B:1219:ILE:HB	1:B:1482:LEU:HD23	1.90	0.53
1:A:1235:ARG:NH2	5:H:11:DG:O3'	2.38	0.53
1:B:1054:THR:OG1	1:B:1056:ASP:OD1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1380:ARG:NH2	1:B:1409:TYR:O	2.40	0.53
1:A:1051:ASP:O	1:A:1060:ARG:NH2	2.42	0.52
1:B:544:LYS:O	1:B:578:GLN:N	2.43	0.52
1:A:1219:ILE:HB	1:A:1482:LEU:HD23	1.92	0.52
5:H:5:DA:N3	7:H:101:MFX:H03	2.25	0.52
1:A:591:LEU:HD23	1:A:595:THR:HG23	1.93	0.51
1:A:591:LEU:HD22	1:A:596:MET:HG3	1.93	0.51
1:A:626:VAL:HG11	5:H:9:DA:H3'	1.92	0.50
1:B:1171:SER:OG	1:B:1172:ALA:N	2.43	0.50
1:B:1274:ASP:O	1:B:1278:ASN:ND2	2.37	0.50
1:B:1247:LEU:HD11	1:B:1253:GLN:HB2	1.93	0.49
1:A:1070:MET:HE1	1:A:1078:ASP:HB3	1.95	0.49
1:A:1020:TYR:O	1:A:1024:ILE:HG12	2.12	0.49
1:B:1169:GLY:HA2	1:B:1176:THR:HG22	1.95	0.49
1:A:1211:PRO:O	1:A:1478:ARG:NH2	2.44	0.49
1:B:462:THR:HG21	1:B:521:PHE:HD2	1.78	0.49
1:B:1044:ILE:HG12	1:B:1069:ILE:HD13	1.95	0.49
1:A:1340:VAL:HB	1:A:1344:PRO:HG2	1.95	0.48
1:A:458:LYS:HG2	1:A:514:ILE:HD11	1.95	0.48
1:A:1315:LEU:O	1:A:1319:THR:OG1	2.23	0.48
1:A:1168:THR:HA	1:A:1169:GLY:HA3	1.65	0.47
1:B:1096:GLU:HG2	1:B:1126:ILE:HD13	1.97	0.47
1:A:639:PHE:HA	1:A:1022:LYS:HE3	1.96	0.46
1:A:1161:ASN:OD1	1:A:1165:ASN:ND2	2.46	0.46
1:B:1241:LYS:HB3	1:B:1258:GLU:HB2	1.96	0.46
1:A:1235:ARG:HH21	5:H:11:DG:HO3'	1.63	0.46
1:A:1025:ILE:HG23	1:A:1030:LEU:HD12	1.97	0.46
1:A:1129:TYR:HB3	1:A:1158:ALA:HB3	1.98	0.46
1:B:1015:GLU:OE1	1:B:1016:ARG:NH1	2.49	0.46
1:B:1354:ARG:NE	1:B:1456:GLU:OE1	2.45	0.45
1:B:1028:ARG:NH1	2:E:14:DA:H4'	2.32	0.44
1:B:456:ARG:HB3	7:F:101:MFX:H	1.98	0.44
1:A:1307:ASN:ND2	1:A:1310:LEU:HB2	2.33	0.44
1:A:1425:TYR:HB3	1:B:1420:VAL:HG13	1.99	0.44
3:F:5:DA:N3	7:F:101:MFX:H03	2.33	0.44
1:A:1157:ALA:O	1:A:1353:ARG:HD3	2.18	0.44
1:A:1256:ILE:HD13	1:A:1321:LEU:HD21	1.99	0.44
1:B:626:VAL:HG11	3:F:9:DA:H3'	1.99	0.44
3:F:5:DA:C4	7:F:101:MFX:H03	2.52	0.43
1:A:513:HIS:HB2	1:A:1020:TYR:CD1	2.53	0.43
1:A:1459:MET:HE3	1:A:1459:MET:HB3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1358:LEU:O	1:A:1362:ARG:HG3	2.18	0.43
1:B:1095:ARG:HB2	1:B:1180:PRO:HB3	2.00	0.43
1:B:1463:MET:HE2	1:B:1463:MET:HB3	1.94	0.43
1:A:1049:ASN:HB2	1:A:1131:LEU:HD13	2.00	0.43
1:B:1191:VAL:HA	1:B:1194:ILE:HD12	2.00	0.43
1:B:1164:VAL:HG21	1:B:1183:LEU:HD23	2.01	0.43
1:A:1105:ASN:HA	1:A:1113:PRO:HB3	2.01	0.42
1:B:1168:THR:HA	1:B:1169:GLY:HA3	1.69	0.42
1:B:435:ASP:OD2	1:B:456:ARG:HG2	2.19	0.42
1:B:1426:ARG:HD3	1:B:1426:ARG:HA	1.91	0.42
1:A:1096:GLU:HG2	1:A:1126:ILE:HD13	2.02	0.42
1:A:1259:ILE:HD12	1:A:1263:ILE:HG22	2.01	0.42
1:B:1130:LEU:HD23	1:B:1157:ALA:HA	2.01	0.42
1:A:1423:GLN:H	1:A:1426:ARG:HH21	1.68	0.42
1:A:1240:SER:OG	1:A:1260:PRO:HD3	2.20	0.41
5:H:5:DA:C4	7:H:101:MFX:H03	2.55	0.41
1:A:416:LEU:HD12	1:A:453:LEU:HG	2.01	0.41
1:A:1070:MET:HA	1:A:1074:HIS:O	2.20	0.41
1:B:1022:LYS:O	1:B:1026:GLN:HG2	2.21	0.41
1:B:1084:ALA:O	1:B:1088:MET:HG3	2.21	0.41
1:B:580:TYR:CD2	1:B:586:MET:HE2	2.55	0.41
1:A:1178:ILE:HG12	1:A:1329:MET:HG2	2.01	0.41
1:A:1254:ILE:HB	1:A:1300:ILE:HB	2.03	0.41
1:A:1095:ARG:HA	1:A:1214:PRO:HB3	2.03	0.41
1:B:1027:ASP:C	1:B:1039:PRO:HG2	2.46	0.41
1:B:462:THR:HG21	1:B:521:PHE:CD2	2.56	0.41
1:A:423:ASN:C	1:A:425:ALA:H	2.29	0.40
1:B:1476:THR:HA	1:B:1477:PRO:HD3	1.95	0.40
1:A:1293:ARG:HH11	1:A:1293:ARG:HB3	1.86	0.40
1:A:516:THR:O	1:A:520:THR:HG23	2.22	0.40
1:A:1334:ASN:C	1:A:1336:THR:H	2.30	0.40
1:B:1038:LYS:NZ	1:B:1168:THR:O	2.49	0.40
1:B:1160:PRO:HG3	1:B:1349:TYR:CE2	2.57	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	681/742 (92%)	645 (95%)	34 (5%)	2 (0%)	36	66
1	B	681/742 (92%)	639 (94%)	39 (6%)	3 (0%)	30	61
All	All	1362/1484 (92%)	1284 (94%)	73 (5%)	5 (0%)	30	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1304	LYS
1	B	1169	GLY
1	A	1169	GLY
1	A	1329	MET
1	B	464	LYS

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	479/635 (75%)	447 (93%)	32 (7%)	15	41
1	B	477/635 (75%)	454 (95%)	23 (5%)	23	50
All	All	956/1270 (75%)	901 (94%)	55 (6%)	18	45

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	416	LEU

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Mol	Chain	Res	Type
1	A	429	LEU
1	A	453	LEU
1	A	524	ARG
1	A	591	LEU
1	A	595	THR
1	A	605	ARG
1	A	1009	LEU
1	A	1096	GLU
1	A	1102	HIS
1	A	1139	VAL
1	A	1162	LEU
1	A	1168	THR
1	A	1183	LEU
1	A	1208	LEU
1	A	1236	VAL
1	A	1263	ILE
1	A	1268	LEU
1	A	1279	ASN
1	A	1281	VAL
1	A	1293	ARG
1	A	1310	LEU
1	A	1338	ARG
1	A	1342	ILE
1	A	1366	GLU
1	A	1371	ARG
1	A	1385	LEU
1	A	1387	GLU
1	A	1414	GLU
1	A	1420	VAL
1	A	1432	VAL
1	A	1462	LEU
1	B	416	LEU
1	B	429	LEU
1	B	524	ARG
1	B	595	THR
1	B	1096	GLU
1	B	1102	HIS
1	B	1139	VAL
1	B	1162	LEU
1	B	1176	THR
1	B	1177	ASP
1	B	1208	LEU

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Mol	Chain	Res	Type
1	B	1236	VAL
1	B	1268	LEU
1	B	1308	THR
1	B	1310	LEU
1	B	1334	ASN
1	B	1338	ARG
1	B	1372	LEU
1	B	1385	LEU
1	B	1414	GLU
1	B	1420	VAL
1	B	1462	LEU
1	B	1476	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	534	HIS
1	A	1068	ASN
1	A	1253	GLN
1	A	1307	ASN
1	A	1324	ASN
1	B	1006	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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
7	MFX	F	101	6	33,33,33	2.18	8 (24%)	45,50,50	1.86	10 (22%)
7	MFX	H	101	6	33,33,33	2.20	9 (27%)	45,50,50	2.01	13 (28%)

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	101	6	-	4/14/35/35	0/5/5/5
7	MFX	H	101	6	-	4/14/35/35	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	101	MFX	O-C20	5.51	1.36	1.22
7	H	101	MFX	O-C20	5.45	1.36	1.22
7	H	101	MFX	C08-C06	4.79	1.59	1.48
7	F	101	MFX	C08-C06	4.74	1.59	1.48
7	H	101	MFX	C09-C06	4.57	1.58	1.48
7	F	101	MFX	C09-C06	4.40	1.58	1.48
7	H	101	MFX	F-C15	3.86	1.45	1.35
7	F	101	MFX	F-C15	3.75	1.45	1.35
7	F	101	MFX	C14-C19	-3.50	1.41	1.48
7	H	101	MFX	C14-C19	-3.46	1.41	1.48
7	F	101	MFX	C12-N	-3.06	1.35	1.40
7	H	101	MFX	C12-N	-2.94	1.35	1.40
7	H	101	MFX	C09-C08	2.87	1.59	1.48
7	F	101	MFX	C09-C08	2.87	1.59	1.48
7	F	101	MFX	O03-C20	-2.61	1.23	1.30
7	H	101	MFX	O03-C20	-2.52	1.23	1.30
7	H	101	MFX	C12-C13	2.00	1.43	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	101	MFX	C06-N-C16	-6.10	110.80	119.74
7	F	101	MFX	C06-N-C16	-5.50	111.67	119.74
7	H	101	MFX	C12-N-C06	5.15	127.74	122.35
7	H	101	MFX	C13-C11-C15	4.51	120.31	115.92
7	F	101	MFX	C12-N-C06	4.36	126.92	122.35
7	F	101	MFX	C13-C11-C15	4.33	120.14	115.92
7	H	101	MFX	C14-C12-C13	-3.47	116.42	120.32
7	F	101	MFX	C14-C12-C13	-3.42	116.47	120.32
7	F	101	MFX	O03-C20-O	-2.73	117.40	123.90
7	H	101	MFX	O03-C20-O	-2.70	117.47	123.90
7	H	101	MFX	C13-C12-N	2.67	126.03	123.05
7	H	101	MFX	C17-C15-C11	-2.64	119.41	123.34
7	F	101	MFX	C17-C15-C11	-2.60	119.48	123.34
7	H	101	MFX	C16-C18-C19	-2.55	118.07	119.94
7	H	101	MFX	C10-N02-C02	2.55	113.21	111.62
7	F	101	MFX	C16-C18-C19	-2.52	118.09	119.94
7	F	101	MFX	C13-C12-N	2.50	125.83	123.05
7	H	101	MFX	C-O01-C13	2.48	121.49	114.74
7	F	101	MFX	C-O01-C13	2.22	120.77	114.74
7	H	101	MFX	C08-C06-N	-2.22	115.36	118.87
7	H	101	MFX	F-C15-C11	2.13	121.80	118.28
7	F	101	MFX	F-C15-C11	2.11	121.76	118.28
7	H	101	MFX	C12-N-C16	2.03	121.46	119.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	101	MFX	C15-C11-N01-C04
7	H	101	MFX	C15-C11-N01-C04
7	F	101	MFX	C15-C11-N01-C03
7	H	101	MFX	C15-C11-N01-C03
7	F	101	MFX	C19-C18-C20-O03
7	F	101	MFX	C19-C18-C20-O
7	H	101	MFX	C19-C18-C20-O03
7	H	101	MFX	C19-C18-C20-O

There are no ring outliers.

2 monomers are involved in 5 short contacts:

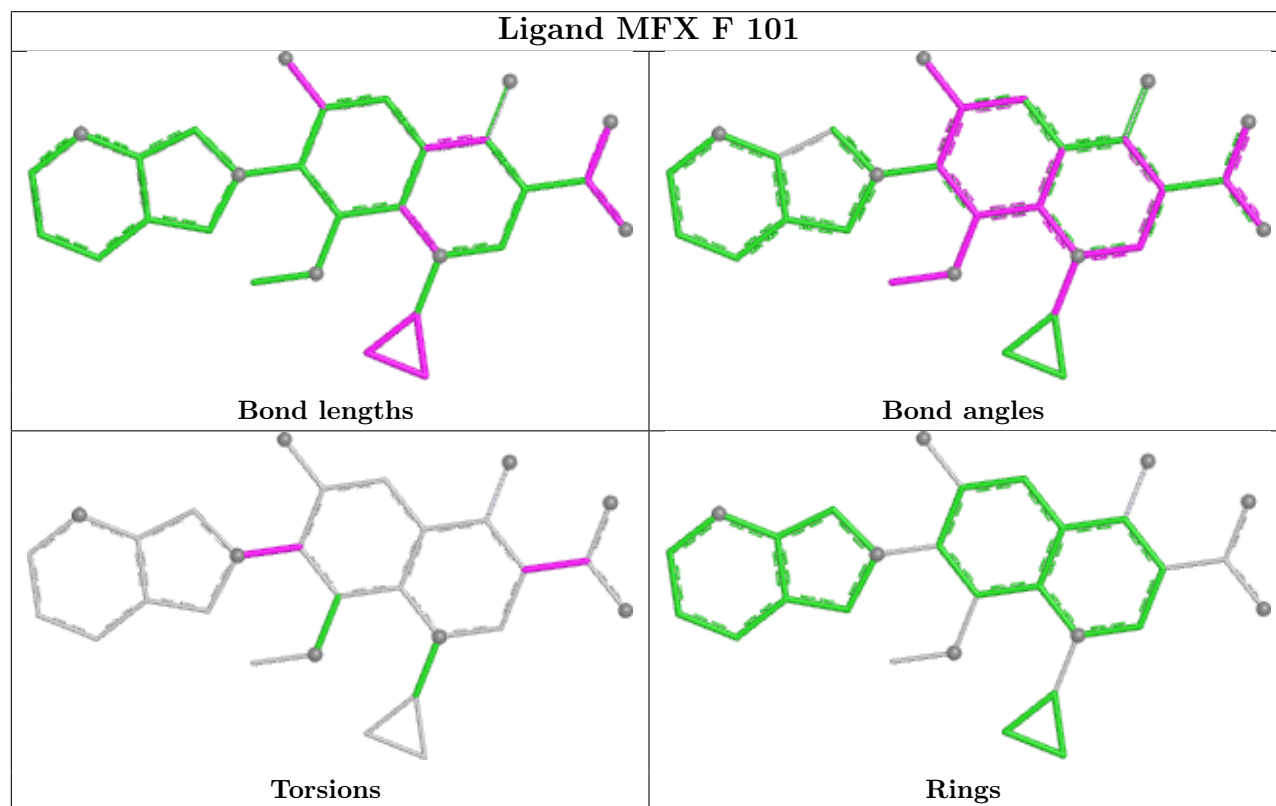
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	101	MFX	3	0

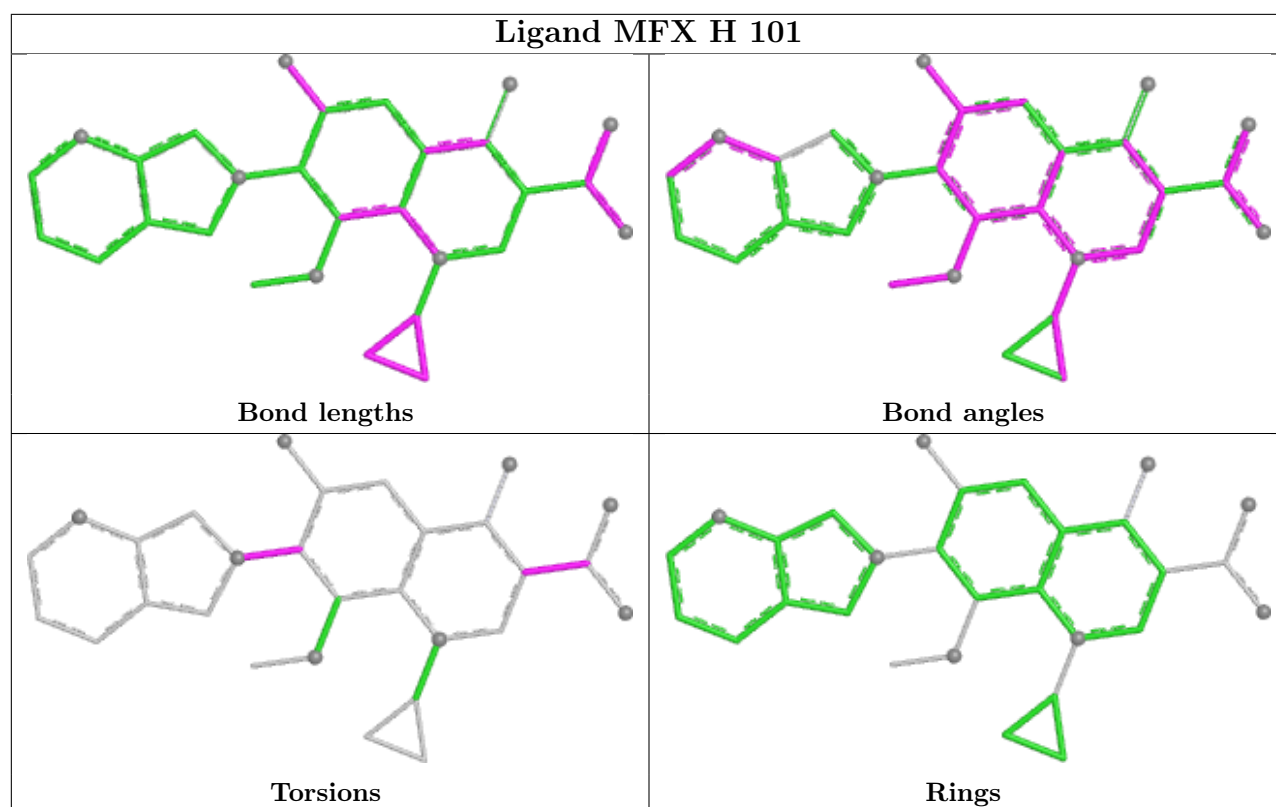
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	101	MFX	2	0

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





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	689/742 (92%)	-0.11	17 (2%) 58 39	47, 86, 145, 174	0
1	B	689/742 (92%)	-0.16	15 (2%) 62 42	46, 82, 146, 171	0
2	E	7/7 (100%)	0.01	0 100 100	88, 89, 126, 139	0
3	F	11/11 (100%)	0.15	0 100 100	89, 107, 155, 156	0
4	G	7/7 (100%)	0.67	1 (14%) 6 6	94, 99, 123, 172	0
5	H	11/11 (100%)	0.06	0 100 100	100, 116, 148, 161	0
All	All	1414/1520 (93%)	-0.13	33 (2%) 61 41	46, 85, 147, 174	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	584	GLY	6.2
1	A	586	MET	5.4
1	B	1484	ASP	5.1
1	A	1484	ASP	4.9
1	A	469	ASP	4.5
4	G	9	DC	4.0
1	B	585	GLU	3.8
1	B	469	ASP	3.8
1	B	602	THR	3.6
1	B	640	THR	3.3
1	A	492	SER	3.2
1	A	585	GLU	3.1
1	A	544	LYS	2.7
1	A	589	ASP	2.7
1	B	589	ASP	2.7
1	A	495	ASP	2.5
1	A	1294	ASP	2.5
1	B	467	MET	2.4
1	B	1305	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	522	PHE	2.4
1	A	609	GLU	2.4
1	A	640	THR	2.3
1	A	1174	TYR	2.3
1	B	613	ARG	2.3
1	B	587	ASN	2.2
1	B	1267	ASN	2.2
1	B	624	ASP	2.2
1	A	1243	GLU	2.2
1	B	522	PHE	2.1
1	B	1112	PRO	2.1
1	A	415	LYS	2.1
1	A	1168	THR	2.1
1	A	578	GLN	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.

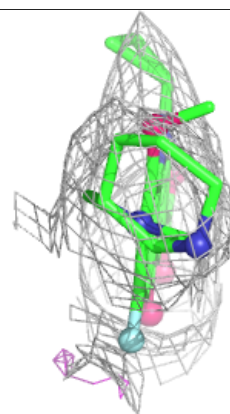
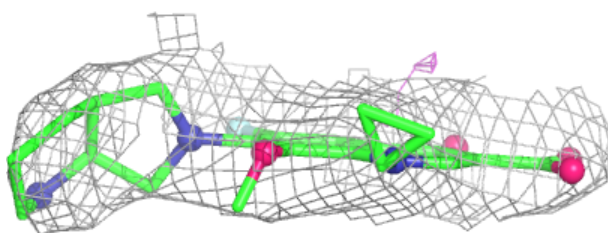
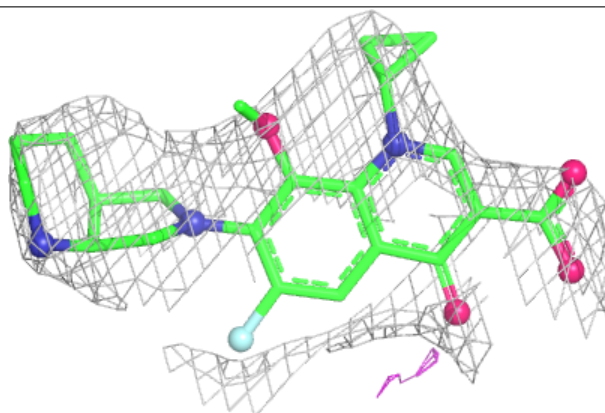
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	B	1501	1/1	0.83	0.29	73,73,73,73	0
6	MG	A	1501	1/1	0.84	0.29	83,83,83,83	0
7	MFX	H	101	29/29	0.91	0.12	93,126,142,180	0
7	MFX	F	101	29/29	0.94	0.11	74,108,137,167	0
6	MG	A	1502	1/1	0.94	0.09	100,100,100,100	0
6	MG	B	1502	1/1	0.95	0.11	83,83,83,83	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.

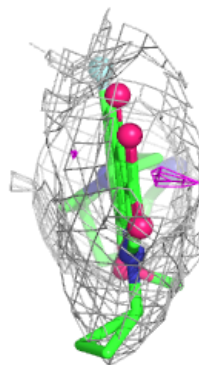
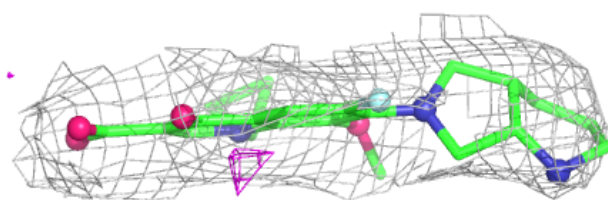
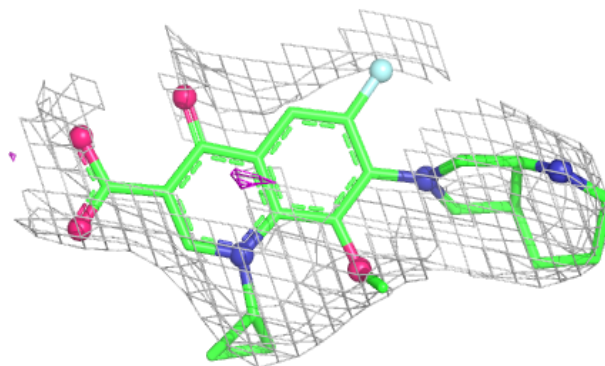
Electron density around MFX H 101:

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



Electron density around MFX F 101:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.