



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 28, 2024 – 05:01 pm GMT

PDB ID : 5CDQ
Title : 2.95Å structure of Moxifloxacin with S.aureus DNA gyrase and DNA
Authors : Bax, B.D.; Srikannathasan, V.; Chan, P.F.
Deposited on : 2015-07-04
Resolution : 2.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

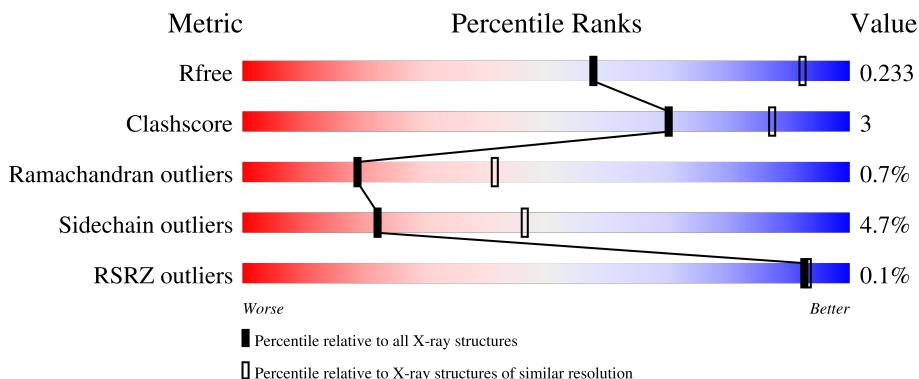
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	164625	1044 (2.98-2.94)
Clashscore	180529	1097 (2.98-2.94)
Ramachandran outliers	177936	1049 (2.98-2.94)
Sidechain outliers	177891	1049 (2.98-2.94)
RSRZ outliers	164620	1044 (2.98-2.94)

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	481	90% 9% .
1	C	481	91% 9%
1	R	481	89% 11%
1	T	481	90% 10% .
2	B	193	87% 12% ..

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Mol	Chain	Length	Quality of chain
2	D	193	 78% 20% ..
2	S	193	 83% 16% .
2	U	193	 81% 15% ..
3	E	20	 90% 10%
3	F	20	 5% 85% 15%
3	V	20	 75% 20% 5%
3	W	20	 80% 15% 5%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 23073 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 gyrase subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	481	Total 3767	C 2343	N 680	O 727	P 1	S 16	0	2	0
1	C	481	Total 3790	C 2357	N 689	O 727	P 1	S 16	0	2	0
1	R	481	Total 3804	C 2366	N 692	O 729	P 1	S 16	0	2	0
1	T	481	Total 3764	C 2343	N 679	O 726	P 1	S 15	0	2	0

- Molecule 2 is a protein called DNA gyrase subunit B,DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	191	Total 1468	C 923	N 251	O 285	S 9	0	0	0
2	D	190	Total 1429	C 895	N 248	O 279	S 7	0	0	0
2	S	193	Total 1499	C 943	N 260	O 287	S 9	0	0	0
2	U	192	Total 1454	C 915	N 251	O 279	S 9	0	0	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	THR	deletion	UNP P66937
B	?	-	GLN	deletion	UNP P66937
B	?	-	GLY	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLN	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	VAL	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	ASN	deletion	UNP P66937
B	?	-	ASP	deletion	UNP P66937
B	?	-	ARG	deletion	UNP P66937
B	?	-	GLU	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	ASP	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	SER	deletion	UNP P66937
B	?	-	GLU	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	ASN	deletion	UNP P66937
B	?	-	PRO	deletion	UNP P66937
B	?	-	THR	deletion	UNP P66937
B	?	-	PRO	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	TRP	deletion	UNP P66937
B	?	-	SER	deletion	UNP P66937
B	?	-	ILE	deletion	UNP P66937
B	544	THR	ALA	linker	UNP P66937
B	545	GLY	ARG	linker	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	TYR	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	THR	deletion	UNP P66937
D	?	-	GLN	deletion	UNP P66937
D	?	-	GLY	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	GLN	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	TYR	deletion	UNP P66937
D	?	-	TYR	deletion	UNP P66937
D	?	-	VAL	deletion	UNP P66937
D	?	-	TYR	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASN	deletion	UNP P66937
D	?	-	ASP	deletion	UNP P66937
D	?	-	ARG	deletion	UNP P66937
D	?	-	GLU	deletion	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	ASP	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	SER	deletion	UNP P66937
D	?	-	GLU	deletion	UNP P66937
D	?	-	LEU	deletion	UNP P66937
D	?	-	ASN	deletion	UNP P66937
D	?	-	PRO	deletion	UNP P66937
D	?	-	THR	deletion	UNP P66937
D	?	-	PRO	deletion	UNP P66937
D	?	-	LYS	deletion	UNP P66937
D	?	-	TRP	deletion	UNP P66937
D	?	-	SER	deletion	UNP P66937
D	?	-	ILE	deletion	UNP P66937
D	544	THR	ALA	linker	UNP P66937
D	545	GLY	ARG	linker	UNP P66937
S	?	-	LEU	deletion	UNP P66937
S	?	-	TYR	deletion	UNP P66937
S	?	-	LYS	deletion	UNP P66937
S	?	-	LEU	deletion	UNP P66937
S	?	-	THR	deletion	UNP P66937
S	?	-	GLN	deletion	UNP P66937
S	?	-	GLY	deletion	UNP P66937
S	?	-	LYS	deletion	UNP P66937
S	?	-	GLN	deletion	UNP P66937
S	?	-	LYS	deletion	UNP P66937
S	?	-	TYR	deletion	UNP P66937
S	?	-	TYR	deletion	UNP P66937
S	?	-	VAL	deletion	UNP P66937
S	?	-	TYR	deletion	UNP P66937
S	?	-	ASN	deletion	UNP P66937
S	?	-	ASP	deletion	UNP P66937
S	?	-	ARG	deletion	UNP P66937
S	?	-	GLU	deletion	UNP P66937
S	?	-	LEU	deletion	UNP P66937
S	?	-	ASP	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
S	?	-	LYS	deletion	UNP P66937
S	?	-	LEU	deletion	UNP P66937
S	?	-	LYS	deletion	UNP P66937
S	?	-	SER	deletion	UNP P66937
S	?	-	GLU	deletion	UNP P66937
S	?	-	LEU	deletion	UNP P66937
S	?	-	ASN	deletion	UNP P66937
S	?	-	PRO	deletion	UNP P66937
S	?	-	THR	deletion	UNP P66937
S	?	-	PRO	deletion	UNP P66937
S	?	-	LYS	deletion	UNP P66937
S	?	-	TRP	deletion	UNP P66937
S	?	-	SER	deletion	UNP P66937
S	?	-	ILE	deletion	UNP P66937
S	544	THR	ALA	linker	UNP P66937
S	545	GLY	ARG	linker	UNP P66937
U	?	-	LEU	deletion	UNP P66937
U	?	-	TYR	deletion	UNP P66937
U	?	-	LYS	deletion	UNP P66937
U	?	-	LEU	deletion	UNP P66937
U	?	-	THR	deletion	UNP P66937
U	?	-	GLN	deletion	UNP P66937
U	?	-	GLY	deletion	UNP P66937
U	?	-	LYS	deletion	UNP P66937
U	?	-	GLN	deletion	UNP P66937
U	?	-	LYS	deletion	UNP P66937
U	?	-	TYR	deletion	UNP P66937
U	?	-	TYR	deletion	UNP P66937
U	?	-	VAL	deletion	UNP P66937
U	?	-	TYR	deletion	UNP P66937
U	?	-	ASN	deletion	UNP P66937
U	?	-	ASP	deletion	UNP P66937
U	?	-	ARG	deletion	UNP P66937
U	?	-	GLU	deletion	UNP P66937
U	?	-	LEU	deletion	UNP P66937
U	?	-	ASP	deletion	UNP P66937
U	?	-	LYS	deletion	UNP P66937
U	?	-	LEU	deletion	UNP P66937
U	?	-	LYS	deletion	UNP P66937
U	?	-	SER	deletion	UNP P66937
U	?	-	GLU	deletion	UNP P66937
U	?	-	LEU	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
U	?	-	ASN	deletion	UNP P66937
U	?	-	PRO	deletion	UNP P66937
U	?	-	THR	deletion	UNP P66937
U	?	-	PRO	deletion	UNP P66937
U	?	-	LYS	deletion	UNP P66937
U	?	-	TRP	deletion	UNP P66937
U	?	-	SER	deletion	UNP P66937
U	?	-	ILE	deletion	UNP P66937
U	544	THR	ALA	linker	UNP P66937
U	545	GLY	ARG	linker	UNP P66937

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	20	Total 392	C 186	N 73	O 114	P 19	0	0	0
3	F	20	Total 389	C 187	N 73	O 111	P 18	0	0	0
3	V	20	Total 392	C 186	N 73	O 114	P 19	0	0	0
3	W	20	Total 391	C 188	N 73	O 112	P 18	0	0	0

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

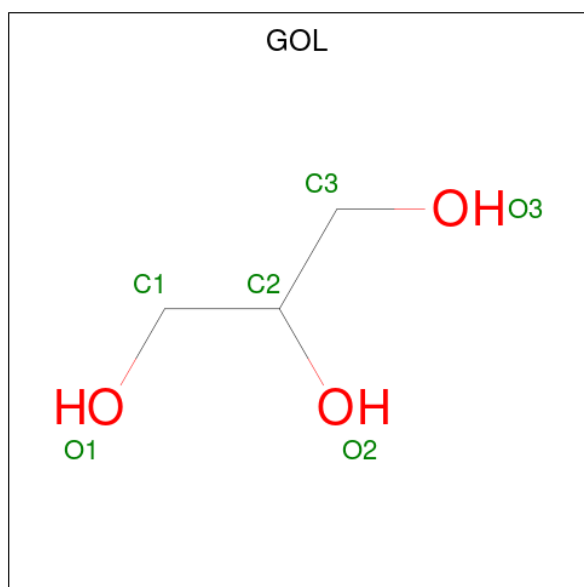
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Mg 2	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	2	Total 2	Mg 2	0	0
4	D	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	R	1	Total 1	Mg 1	0	0
4	S	1	Total 1	Mg 1	0	0

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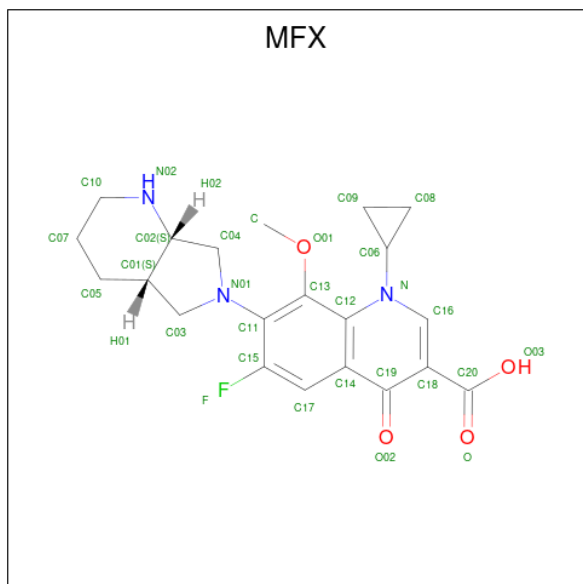
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	T	2	Total	Mg	0	0
			2	2		
4	U	1	Total	Mg	0	0
			1	1		
4	W	2	Total	Mg	0	0
			2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	R	1	Total	C	O	0	0
			6	3	3		
5	T	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 1-cyclopropyl-6-fluoro-8-methoxy-7-[(4a*S*,7a*S*)-octahydro-6*H*-pyrrolo[3,4-*b*]pyridin-6-yl]-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (three-letter code: MFX) (formula: C₂₁H₂₄FN₃O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	N			O
6	E	1	Total	C	F	N	O	0	0
			29	21	1	3	4		
6	F	1	Total	C	F	N	O	0	0
			29	21	1	3	4		
6	F	1	Total	C	F	N	O	0	0
			29	21	1	3	4		
6	V	1	Total	C	F	N	O	0	0
			29	21	1	3	4		
6	W	1	Total	C	F	N	O	0	0
			29	21	1	3	4		
6	W	1	Total	C	F	N	O	0	0
			29	21	1	3	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	42	Total	O	0	0
			42	42		
7	B	21	Total	O	0	0
			21	21		
7	C	41	Total	O	0	0
			41	41		
7	D	5	Total	O	0	0
			5	5		

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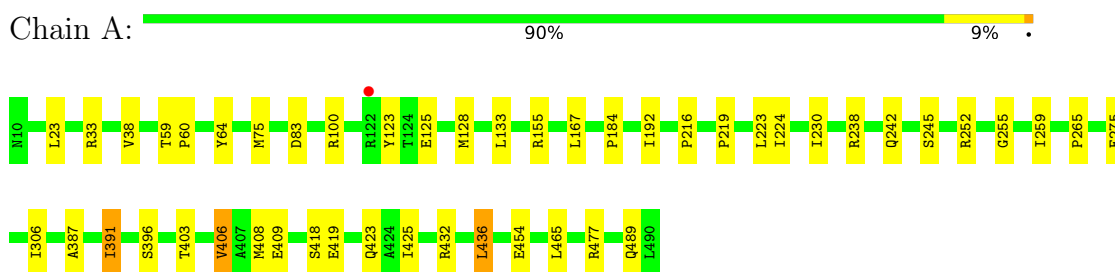
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	21	Total O 21 21	0	0
7	F	17	Total O 17 17	0	0
7	R	59	Total O 59 59	0	0
7	S	20	Total O 20 20	0	0
7	T	37	Total O 37 37	0	0
7	U	10	Total O 10 10	0	0
7	V	12	Total O 12 12	0	0
7	W	13	Total O 13 13	0	0

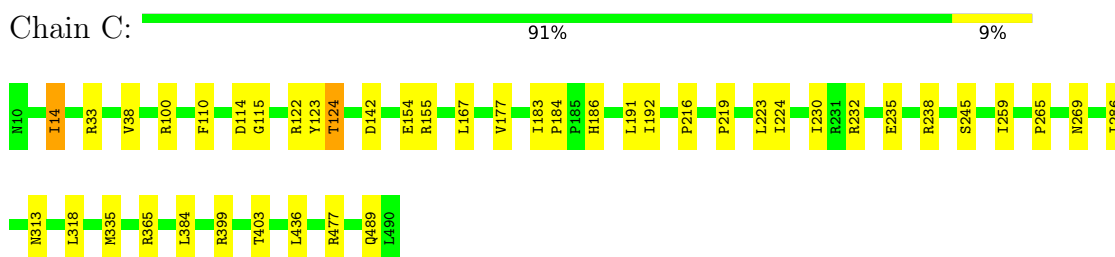
3 Residue-property plots [i](#)

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.

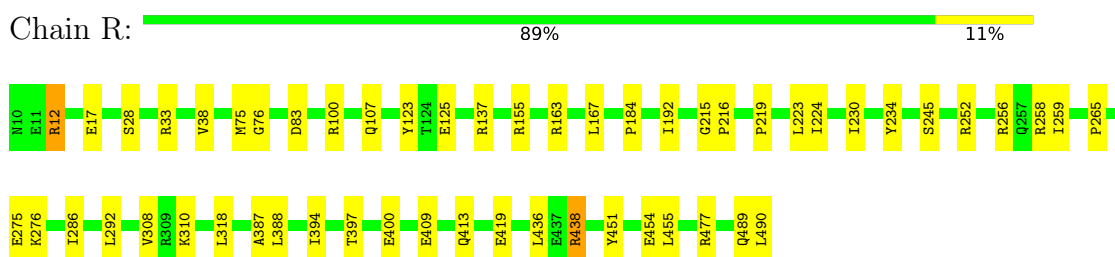
- Molecule 1: DNA gyrase subunit A



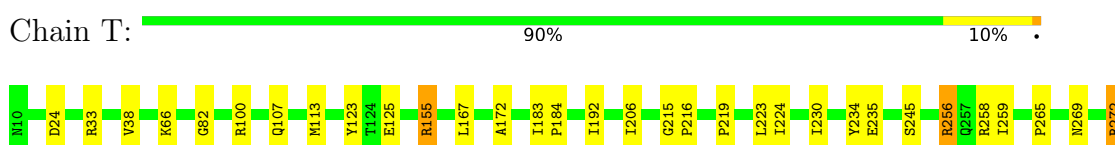
- Molecule 1: DNA gyrase subunit A



- Molecule 1: DNA gyrase subunit A

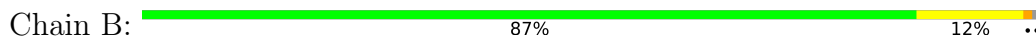


- Molecule 1: DNA gyrase subunit A

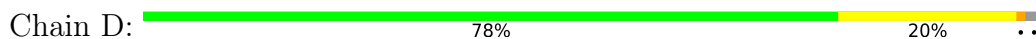




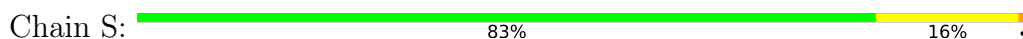
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



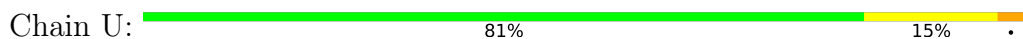
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



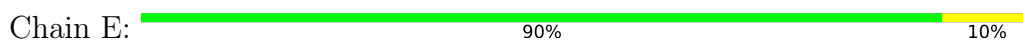
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



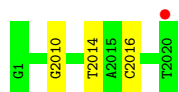
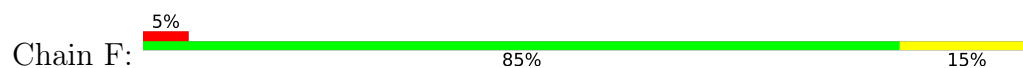
- Molecule 2: DNA gyrase subunit B,DNA gyrase subunit B



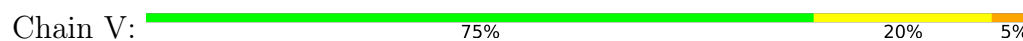
- Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*T*GP*GP*CP*CP*AP*TP*AP*CP*GP*CP*TP*T)-3')



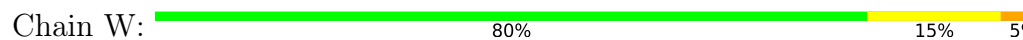
- Molecule 3: DNA (5'-D(P*GP*AP*GP*CP*GP*TP*AP*T*GP*GP*CP*CP*AP*TP*AP*CP*GP*CP*TP*T)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.93Å 170.55Å 125.67Å 90.00° 103.30° 90.00°	Depositor
Resolution (Å)	19.99 – 2.95 19.99 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.99-2.95) 98.4 (19.99-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.93Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.5	Depositor
R, R_{free}	0.174 , 0.218 0.190 , 0.233	Depositor DCC
R_{free} test set	3841 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 86.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23073	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.14% 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: PTR, GOL, MFX, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/3796	0.62	0/5123
1	C	0.42	0/3820	0.62	0/5154
1	R	0.41	0/3834	0.61	0/5168
1	T	0.41	0/3794	0.62	0/5122
2	B	0.44	0/1492	0.66	0/2017
2	D	0.43	0/1452	0.67	0/1969
2	S	0.44	0/1524	0.65	0/2059
2	U	0.46	0/1478	0.67	0/2003
3	E	1.04	0/438	0.94	0/673
3	F	1.00	1/435 (0.2%)	0.96	1/669 (0.1%)
3	V	1.00	0/438	0.97	2/673 (0.3%)
3	W	1.05	1/437 (0.2%)	1.00	1/672 (0.1%)
All	All	0.50	2/22938 (0.0%)	0.67	4/31302 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	1	DG	C3'-O3'	6.79	1.52	1.44
3	F	2010	DG	O5'-C5'	-5.56	1.28	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	2014	DT	O4'-C4'-C3'	-6.10	102.06	104.50
3	V	2013	DA	O4'-C1'-N9	5.34	111.74	108.00
3	W	2014	DT	O4'-C4'-C3'	-5.27	102.39	104.50
3	F	2014	DT	O4'-C4'-C3'	-5.08	102.47	104.50

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	3767	0	3745	22	0
1	C	3790	0	3790	21	0
1	R	3804	0	3826	28	0
1	T	3764	0	3745	22	0
2	B	1468	0	1423	10	0
2	D	1429	0	1353	17	0
2	S	1499	0	1473	15	0
2	U	1454	0	1400	14	0
3	E	392	0	212	1	0
3	F	389	0	212	1	0
3	V	392	0	212	4	0
3	W	391	0	213	3	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	T	2	0	0	0	0
4	U	1	0	0	0	0
4	W	2	0	0	0	0
5	A	12	0	16	0	0
5	C	12	0	16	1	0
5	R	18	0	24	0	0
5	T	6	0	8	1	0
6	E	29	0	23	1	0
6	F	58	0	46	2	0
6	V	29	0	23	3	0
6	W	58	0	46	0	0
7	A	42	0	0	0	0
7	B	21	0	0	0	0
7	C	41	0	0	0	0
7	D	5	0	0	0	0
7	E	21	0	0	0	0
7	F	17	0	0	0	0
7	R	59	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	S	20	0	0	0	0
7	T	37	0	0	1	0
7	U	10	0	0	0	0
7	V	12	0	0	0	0
7	W	13	0	0	0	0
All	All	23073	0	21806	145	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 3.

The worst 5 of 145 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:T:313:ASN:HD22	1:T:316:VAL:HG23	1.41	0.85
2:D:460:LYS:HA	2:D:516:ILE:HD11	1.59	0.82
2:D:592:TRP:HA	2:D:596:MET:HB2	1.69	0.73
2:U:587:ASN:HB3	2:U:590:GLN:HB2	1.72	0.72
1:R:76:GLY:HA2	1:T:66[B]:LYS:HG3	1.72	0.71

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	480/481 (100%)	462 (96%)	15 (3%)	3 (1%)	22 46
1	C	480/481 (100%)	464 (97%)	14 (3%)	2 (0%)	30 54
1	R	480/481 (100%)	465 (97%)	14 (3%)	1 (0%)	44 67
1	T	480/481 (100%)	463 (96%)	15 (3%)	2 (0%)	30 54
2	B	189/193 (98%)	183 (97%)	4 (2%)	2 (1%)	12 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	188/193 (97%)	178 (95%)	7 (4%)	3 (2%)	8	22
2	S	191/193 (99%)	182 (95%)	7 (4%)	2 (1%)	13	33
2	U	190/193 (98%)	180 (95%)	5 (3%)	5 (3%)	4	13
All	All	2678/2696 (99%)	2577 (96%)	81 (3%)	20 (1%)	19	41

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	637	ALA
2	D	545	GLY
2	D	580	TYR
2	U	544	THR
1	A	33	ARG

5.3.2 Protein sidechains [i](#)

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	397/415 (96%)	383 (96%)	14 (4%)	31	56
1	C	401/415 (97%)	391 (98%)	10 (2%)	42	66
1	R	405/415 (98%)	392 (97%)	13 (3%)	34	59
1	T	396/415 (95%)	381 (96%)	15 (4%)	28	53
2	B	151/160 (94%)	143 (95%)	8 (5%)	19	42
2	D	141/160 (88%)	124 (88%)	17 (12%)	4	12
2	S	156/160 (98%)	143 (92%)	13 (8%)	9	24
2	U	147/160 (92%)	135 (92%)	12 (8%)	9	24
All	All	2194/2300 (95%)	2092 (95%)	102 (5%)	22	47

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	419	GLU

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Mol	Chain	Res	Type
2	S	607	LYS
2	U	601	ARG
1	R	438	ARG
2	S	479	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	T	320	ASN
1	T	450	ASN
2	U	605	GLN
2	U	587	ASN
1	C	354	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	PTR	A	123	3,1	15,16,17	1.93	3 (20%)	19,22,24	1.74	5 (26%)
1	PTR	C	123	3,1	15,16,17	1.10	1 (6%)	19,22,24	1.36	3 (15%)
1	PTR	R	123	3,1	15,16,17	2.08	2 (13%)	19,22,24	1.54	4 (21%)
1	PTR	T	123	3,1	15,16,17	0.87	0	19,22,24	1.66	3 (15%)

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
1	PTR	A	123	3,1	-	0/10/11/13	0/1/1/1
1	PTR	C	123	3,1	-	1/10/11/13	0/1/1/1
1	PTR	R	123	3,1	-	0/10/11/13	0/1/1/1
1	PTR	T	123	3,1	-	0/10/11/13	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	123	PTR	P-OH	-6.68	1.48	1.59
1	A	123	PTR	CE1-CZ	4.44	1.47	1.38
1	A	123	PTR	P-OH	-3.99	1.52	1.59
1	R	123	PTR	CE2-CZ	2.80	1.44	1.38
1	A	123	PTR	CE1-CD1	2.57	1.43	1.38

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	123	PTR	CB-CA-C	-4.62	102.81	111.47
1	R	123	PTR	CB-CA-C	-4.05	103.88	111.47
1	A	123	PTR	CB-CA-C	-3.87	104.22	111.47
1	C	123	PTR	CB-CA-C	-2.97	105.90	111.47
1	A	123	PTR	OH-CZ-CE1	2.83	127.66	119.23

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	123	PTR	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 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
6	MFX	W	2103	4	33,33,33	2.53	7 (21%)	46,50,50	3.08	16 (34%)
5	GOL	C	504	-	5,5,5	0.15	0	5,5,5	0.37	0
5	GOL	A	504	-	5,5,5	0.08	0	5,5,5	0.15	0
6	MFX	W	2101	4	33,33,33	2.37	7 (21%)	46,50,50	3.44	19 (41%)
5	GOL	R	4302	-	5,5,5	0.14	0	5,5,5	0.28	0
5	GOL	A	503	-	5,5,5	0.08	0	5,5,5	0.23	0
5	GOL	C	503	-	5,5,5	0.07	0	5,5,5	0.12	0
6	MFX	E	2101	4	33,33,33	2.43	7 (21%)	46,50,50	3.40	17 (36%)
6	MFX	V	2101	4	33,33,33	2.38	6 (18%)	46,50,50	3.34	14 (30%)
6	MFX	F	2101	4	33,33,33	2.33	6 (18%)	46,50,50	3.39	17 (36%)
6	MFX	F	2103	4	33,33,33	2.51	5 (15%)	46,50,50	3.46	16 (34%)
5	GOL	R	4303	-	5,5,5	0.10	0	5,5,5	0.30	0
5	GOL	R	4304	-	5,5,5	0.07	0	5,5,5	0.13	0
5	GOL	T	4503	-	5,5,5	0.10	0	5,5,5	0.19	0

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
6	MFX	W	2103	4	-	5/14/35/35	0/5/5/5
5	GOL	C	504	-	-	0/4/4/4	-
5	GOL	A	504	-	-	1/4/4/4	-
6	MFX	W	2101	4	-	1/14/35/35	0/5/5/5
5	GOL	R	4302	-	-	2/4/4/4	-
5	GOL	A	503	-	-	0/4/4/4	-
5	GOL	C	503	-	-	2/4/4/4	-
6	MFX	E	2101	4	-	2/14/35/35	0/5/5/5
6	MFX	V	2101	4	-	0/14/35/35	0/5/5/5
6	MFX	F	2101	4	-	1/14/35/35	0/5/5/5
6	MFX	F	2103	4	-	5/14/35/35	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	R	4303	-	-	0/4/4/4	-
5	GOL	R	4304	-	-	2/4/4/4	-
5	GOL	T	4503	-	-	0/4/4/4	-

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	2101	MFX	C14-C12	7.80	1.51	1.40
6	F	2103	MFX	C14-C12	7.77	1.51	1.40
6	E	2101	MFX	C14-C12	7.74	1.51	1.40
6	W	2103	MFX	C14-C12	7.38	1.50	1.40
6	F	2103	MFX	C12-C13	6.95	1.52	1.40

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	2101	MFX	C10-N02-C02	17.45	122.51	111.62
6	W	2101	MFX	C10-N02-C02	17.33	122.43	111.62
6	V	2101	MFX	C10-N02-C02	17.30	122.42	111.62
6	F	2101	MFX	C10-N02-C02	17.21	122.36	111.62
6	F	2103	MFX	C10-N02-C02	16.34	121.82	111.62

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	4302	GOL	O1-C1-C2-C3
5	C	503	GOL	O1-C1-C2-O2
6	W	2103	MFX	C09-C06-N-C12
5	C	503	GOL	O1-C1-C2-C3
5	R	4304	GOL	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 8 short contacts:

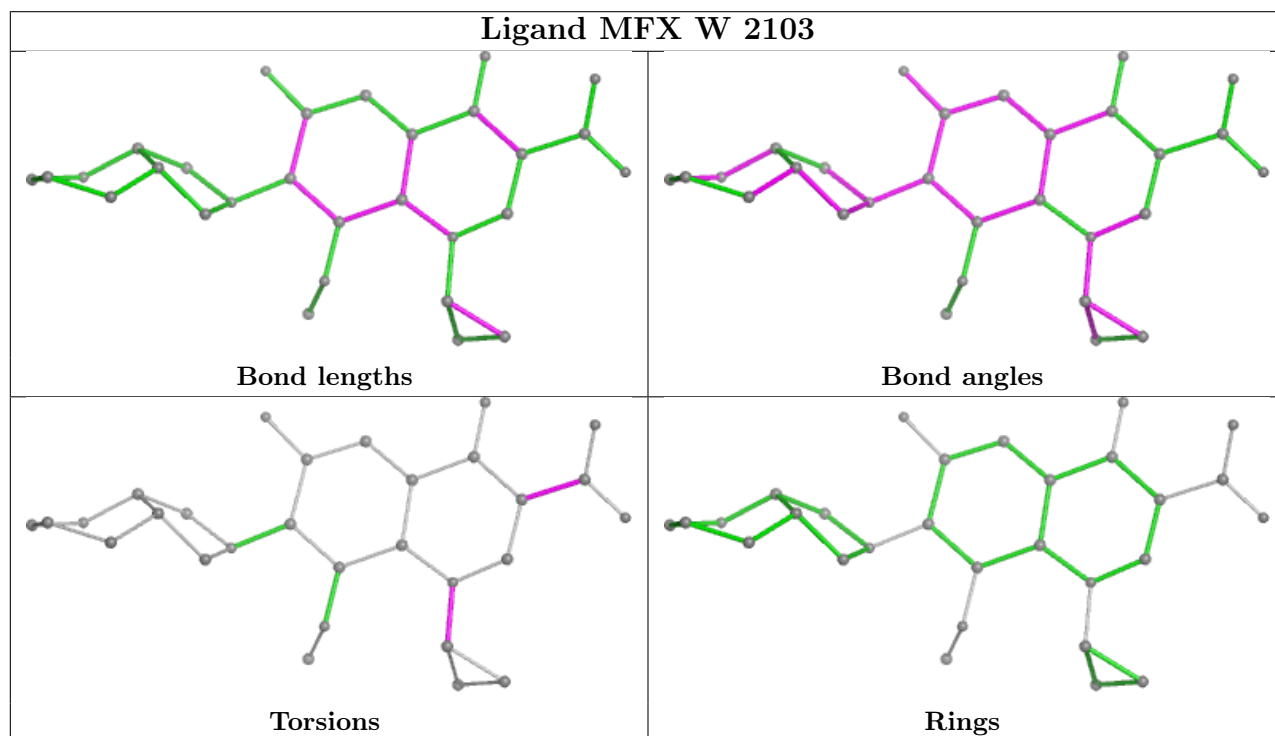
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	504	GOL	1	0
6	E	2101	MFX	1	0
6	V	2101	MFX	3	0
6	F	2101	MFX	1	0
6	F	2103	MFX	1	0

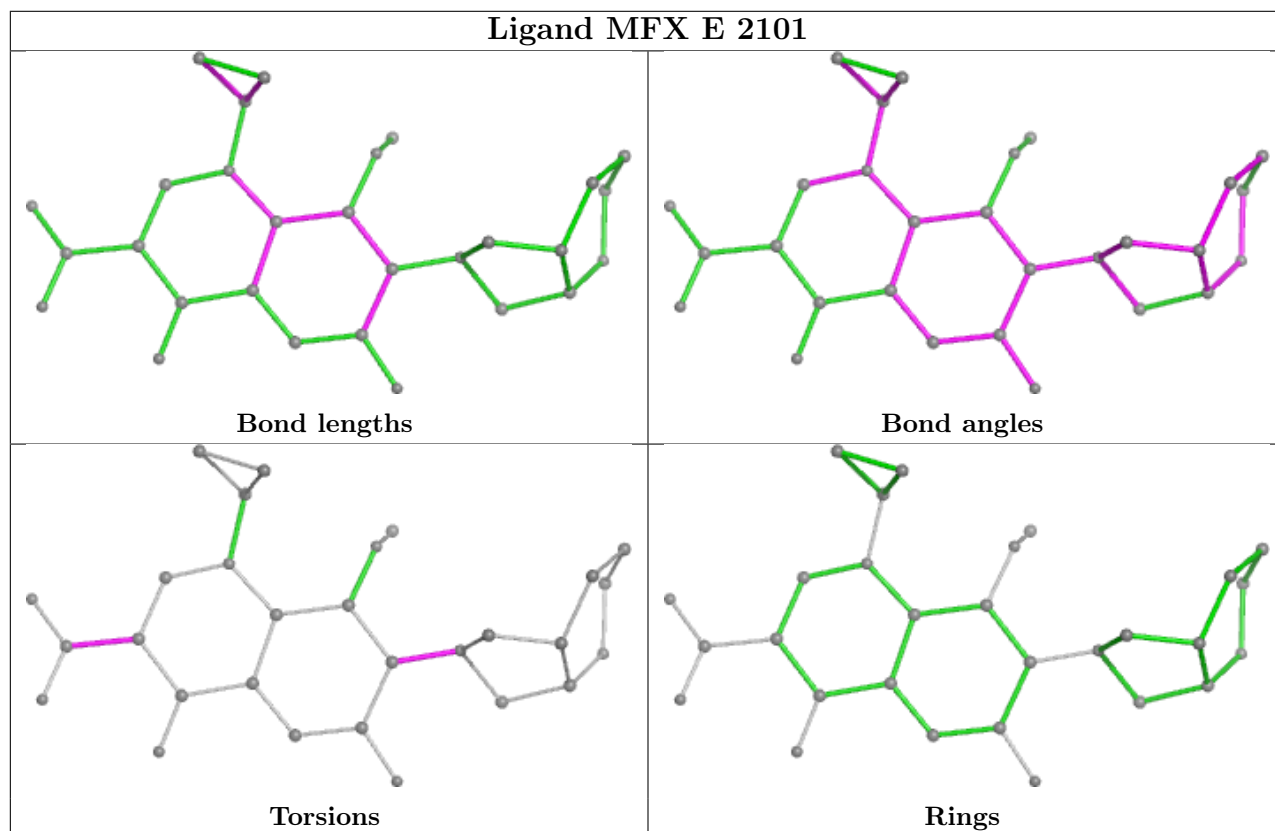
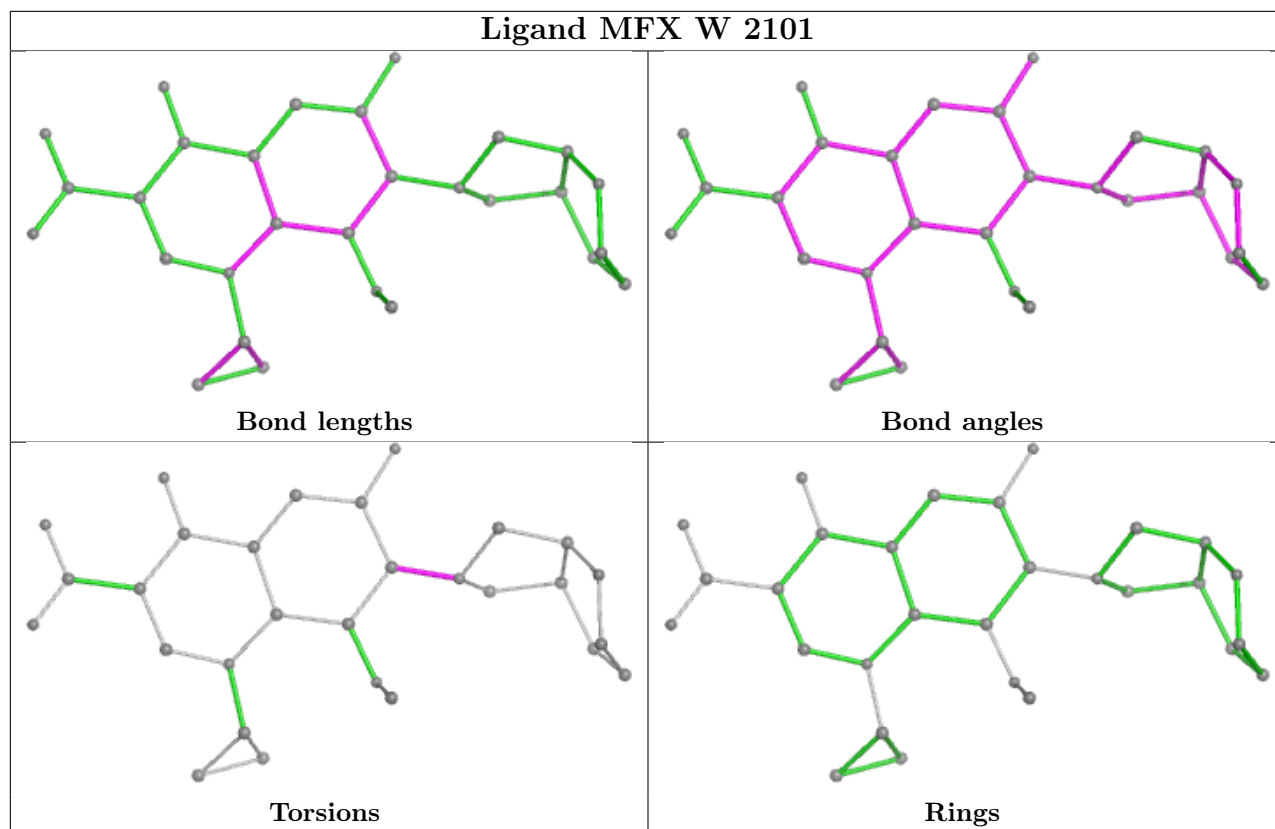
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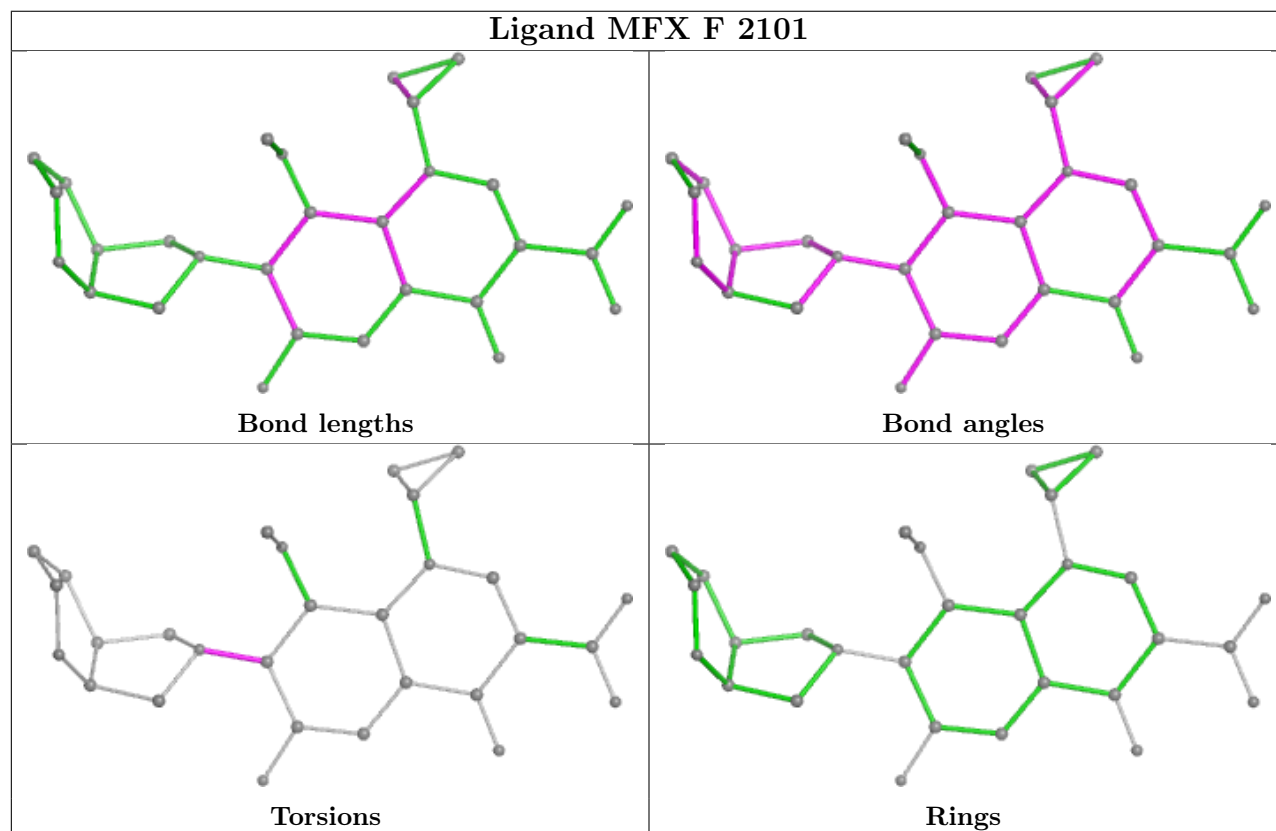
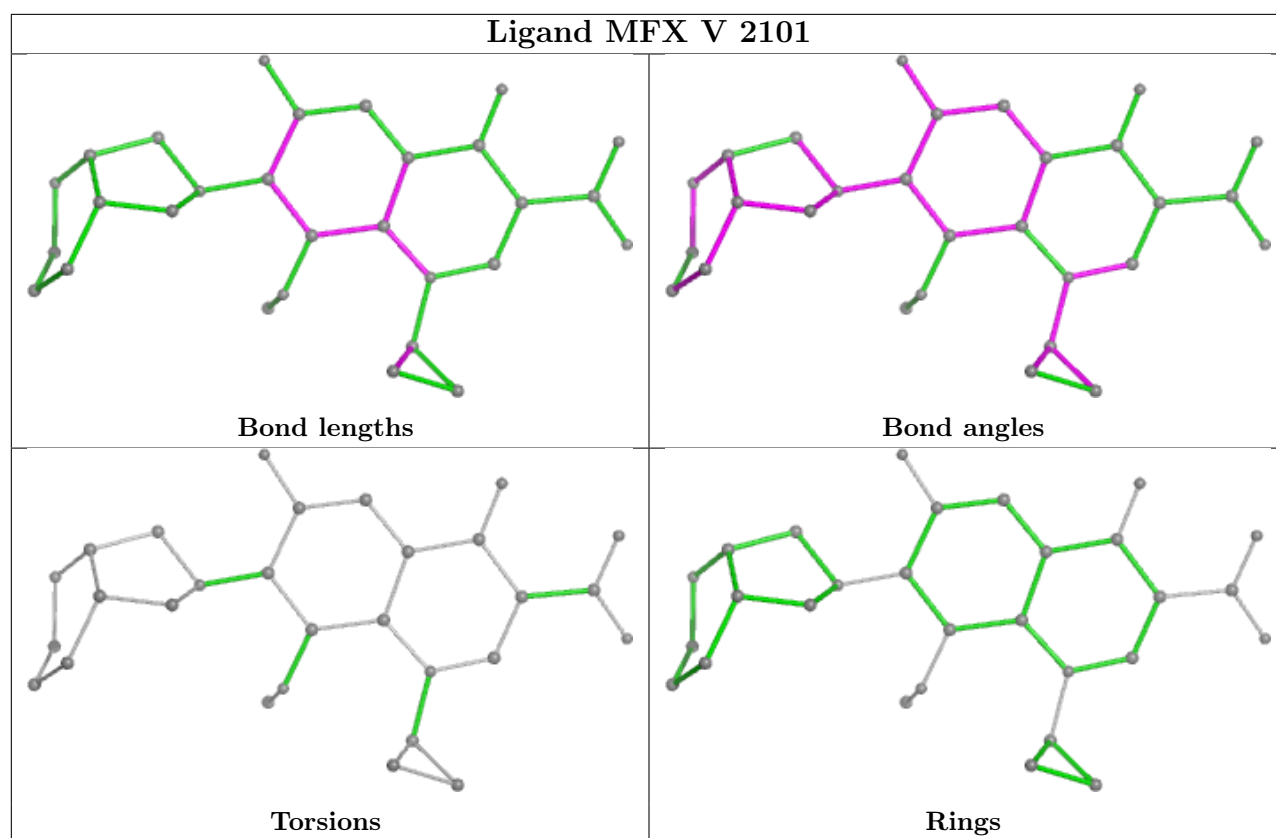
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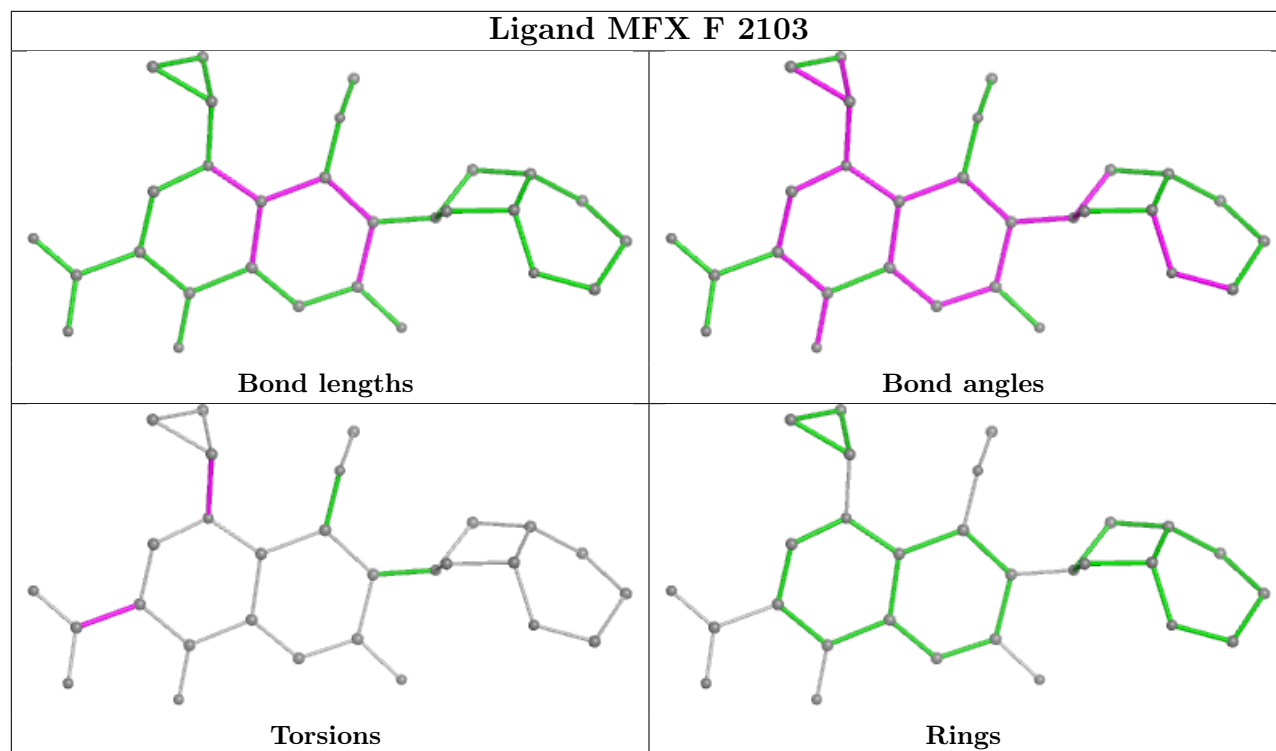
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	4503	GOL	1	0

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.









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, 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	480/481 (99%)	-0.79	1 (0%) 92 92	31, 84, 125, 146	2 (0%)
1	C	480/481 (99%)	-0.81	0 100 100	44, 82, 109, 147	2 (0%)
1	R	480/481 (99%)	-0.82	0 100 100	30, 75, 134, 176	2 (0%)
1	T	480/481 (99%)	-0.72	0 100 100	29, 87, 133, 163	2 (0%)
2	B	191/193 (98%)	-0.68	0 100 100	62, 90, 120, 129	0
2	D	190/193 (98%)	-0.32	0 100 100	80, 125, 166, 179	0
2	S	193/193 (100%)	-0.67	0 100 100	59, 94, 125, 142	0
2	U	192/193 (99%)	-0.43	0 100 100	81, 115, 152, 163	0
3	E	20/20 (100%)	-0.94	0 100 100	63, 81, 108, 112	0
3	F	20/20 (100%)	-0.87	1 (5%) 35 32	65, 86, 106, 115	0
3	V	20/20 (100%)	-0.89	0 100 100	67, 83, 111, 123	0
3	W	20/20 (100%)	-0.86	0 100 100	63, 89, 109, 113	0
All	All	2766/2776 (99%)	-0.72	2 (0%) 92 93	29, 88, 137, 179	8 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	2020	DT	2.7
1	A	122[A]	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
1	PTR	R	123	16/17	0.94	0.08	73,77,90,91	0
1	PTR	C	123	16/17	0.95	0.08	75,79,83,86	0
1	PTR	T	123	16/17	0.95	0.08	74,78,84,87	0
1	PTR	A	123	16/17	0.96	0.09	80,85,91,92	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.

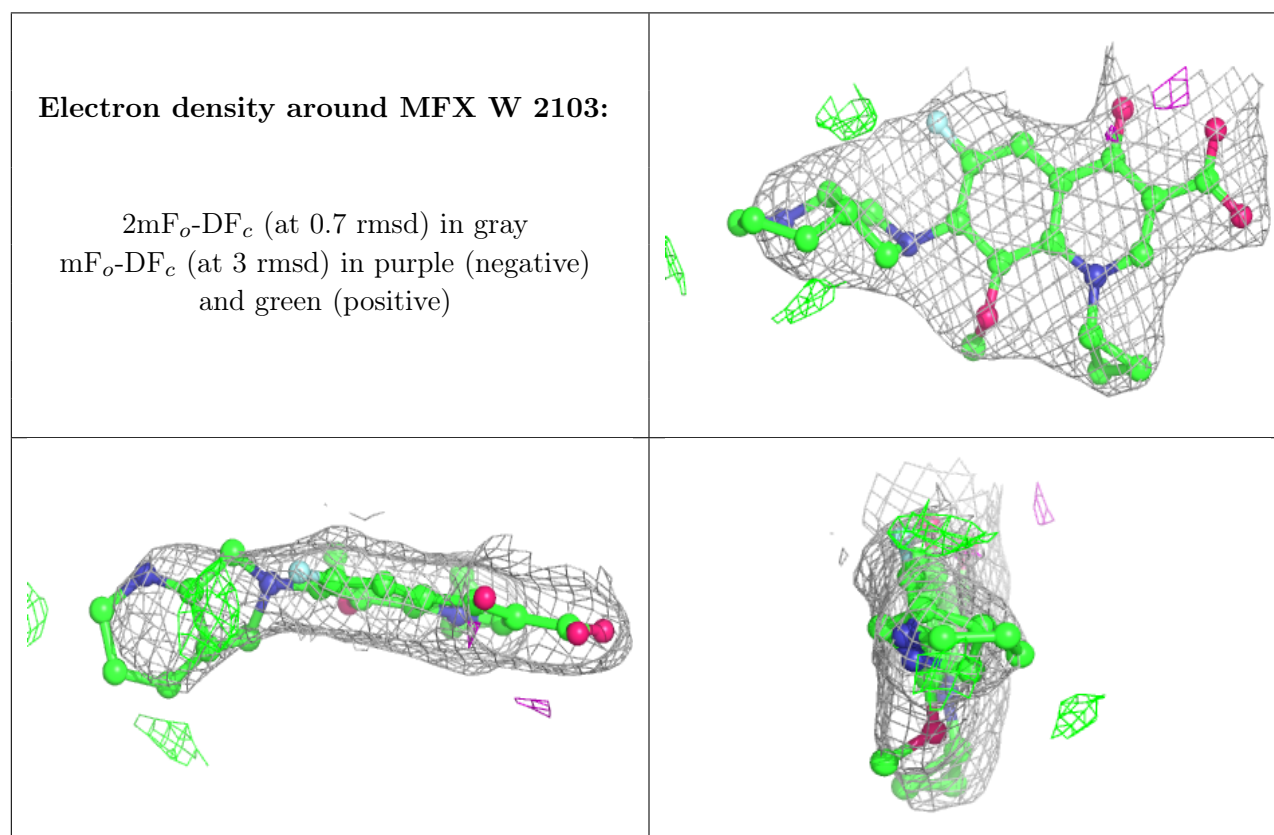
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	R	4302	6/6	0.70	0.13	79,85,86,87	0
5	GOL	T	4503	6/6	0.75	0.10	92,96,98,99	0
5	GOL	C	503	6/6	0.77	0.11	102,103,103,103	0
5	GOL	R	4304	6/6	0.82	0.10	97,100,100,101	0
5	GOL	R	4303	6/6	0.84	0.18	116,123,125,126	0
5	GOL	A	504	6/6	0.85	0.10	85,85,86,87	0
4	MG	A	502	1/1	0.88	0.05	84,84,84,84	0
5	GOL	C	504	6/6	0.89	0.12	97,98,99,100	0
4	MG	T	4502	1/1	0.90	0.07	79,79,79,79	0
5	GOL	A	503	6/6	0.91	0.06	80,80,82,83	0
6	MFX	W	2103	29/29	0.92	0.09	61,71,90,91	0
4	MG	W	2104	1/1	0.93	0.27	75,75,75,75	0
4	MG	C	502	1/1	0.93	0.06	66,66,66,66	0
6	MFX	F	2101	29/29	0.94	0.09	86,90,100,101	0
6	MFX	V	2101	29/29	0.95	0.08	59,68,74,75	0
6	MFX	W	2101	29/29	0.95	0.08	76,80,91,92	0
6	MFX	F	2103	29/29	0.95	0.06	66,72,82,82	0
6	MFX	E	2101	29/29	0.96	0.08	61,67,75,77	0
4	MG	B	1001	1/1	0.98	0.07	42,42,42,42	0
4	MG	A	501	1/1	0.99	0.05	76,76,76,76	0
4	MG	F	2102	1/1	0.99	0.05	69,69,69,69	0
4	MG	R	4301	1/1	0.99	0.04	73,73,73,73	0
4	MG	T	4501	1/1	0.99	0.03	83,83,83,83	0
4	MG	C	501	1/1	0.99	0.03	94,94,94,94	0
4	MG	W	2102	1/1	1.00	0.03	55,55,55,55	0

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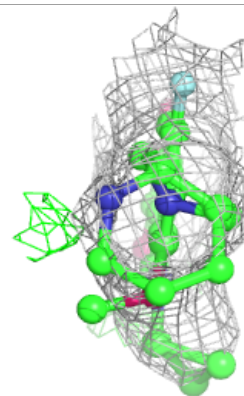
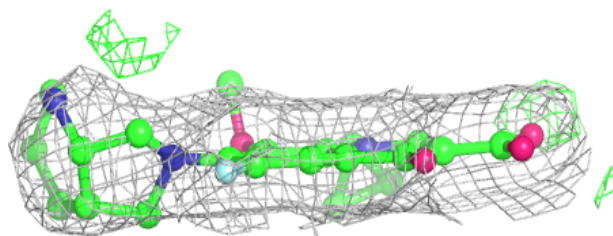
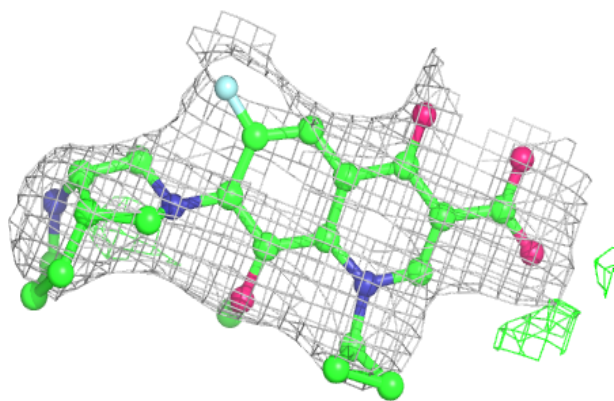
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	D	1001	1/1	1.00	0.06	66,66,66,66	0
4	MG	S	1001	1/1	1.00	0.06	52,52,52,52	0
4	MG	U	1001	1/1	1.00	0.04	52,52,52,52	0

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.

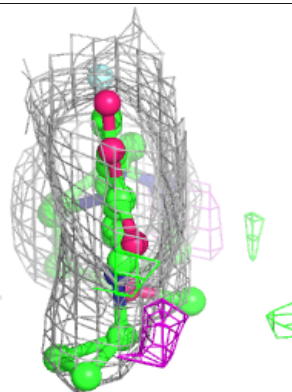
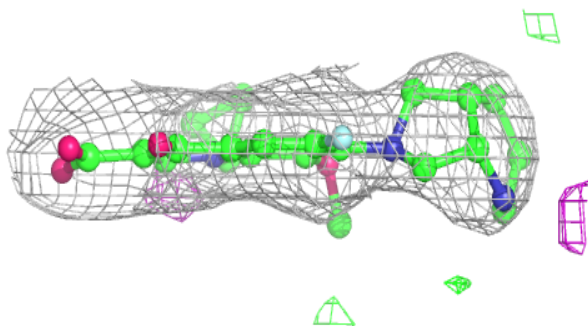
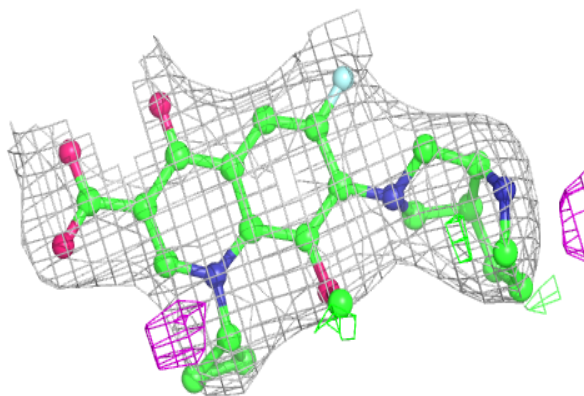


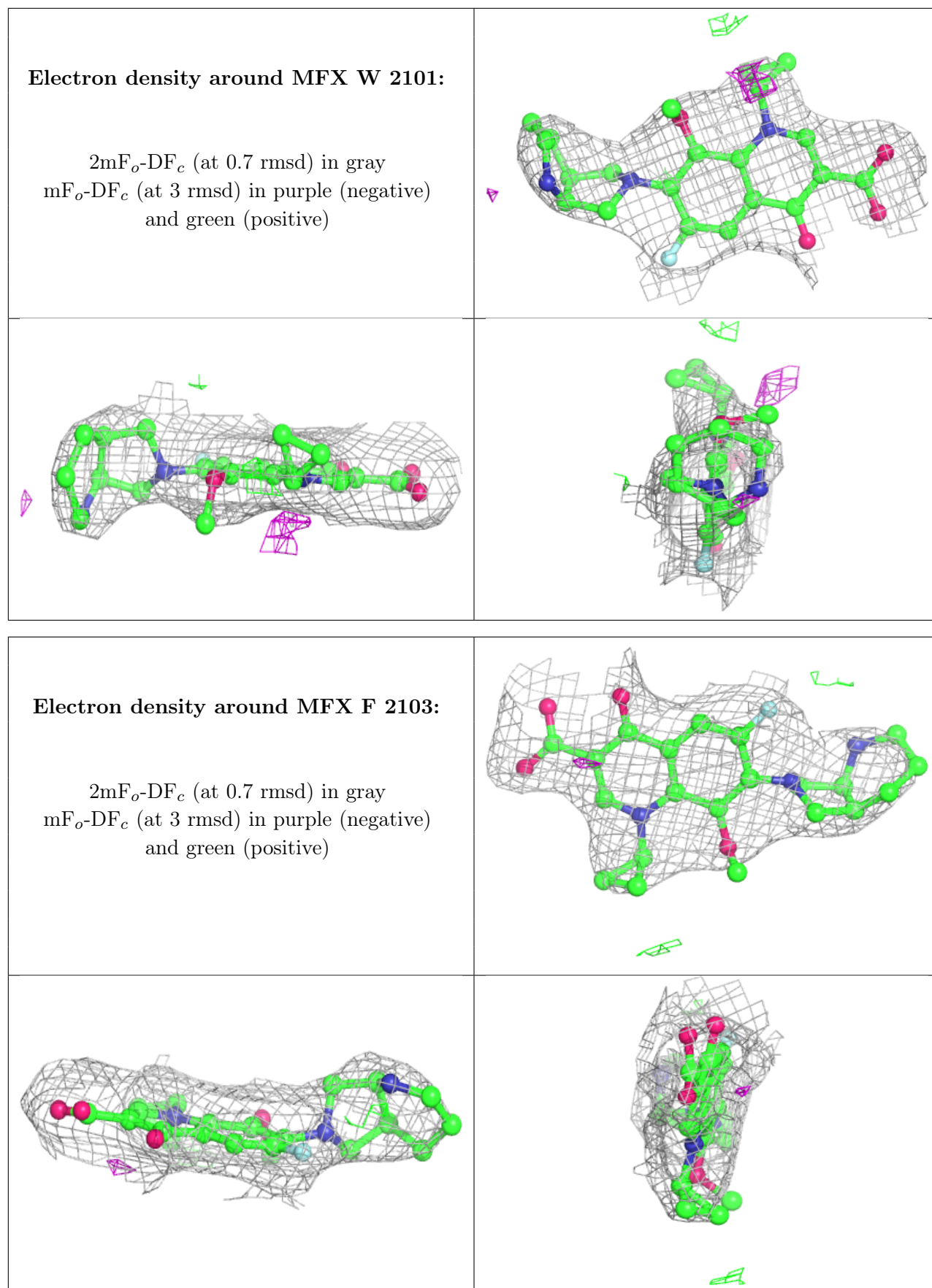
Electron density around MFX F 2101:

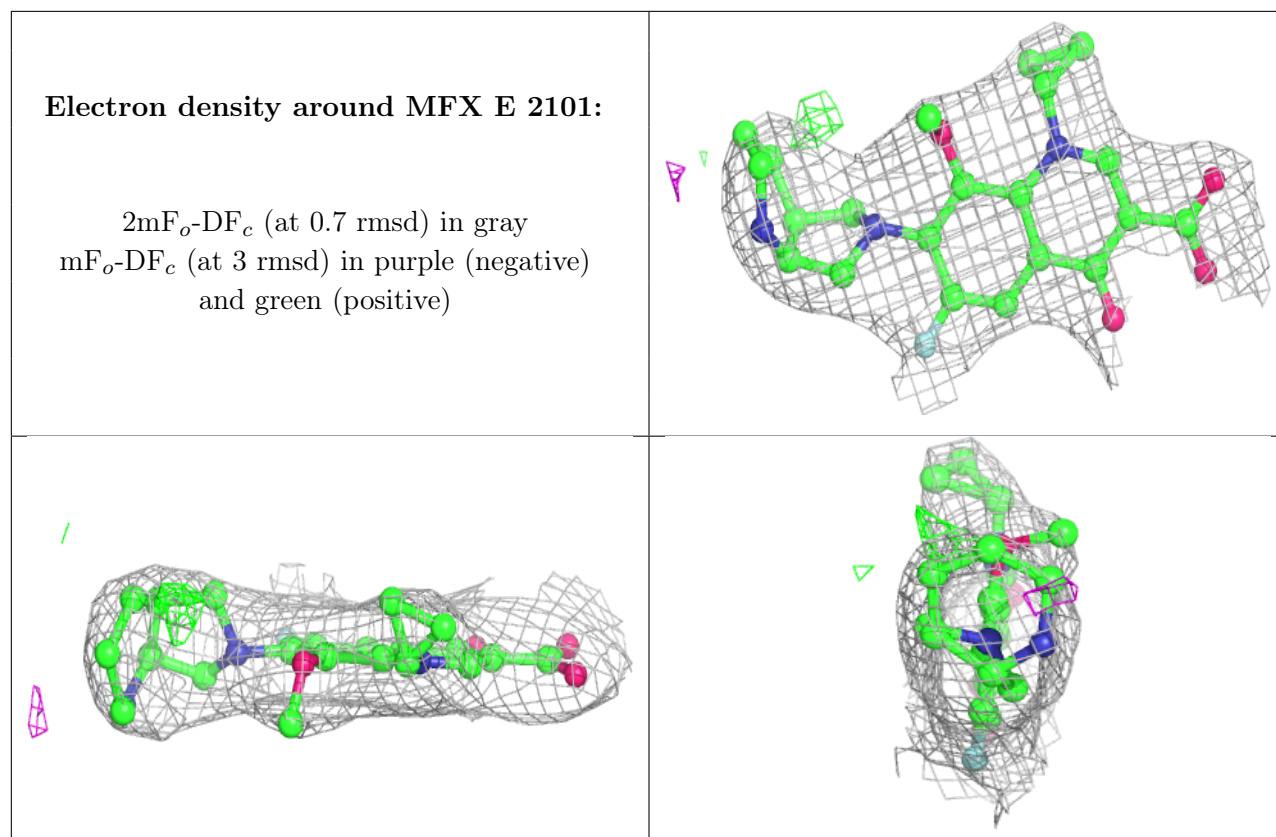
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around MFX V 2101:**

$2mF_o-DF_c$ (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.