



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 04:38 PM UTC

PDB ID : 8QMC / pdb_00008qmc
Title : High resolution structure of the Streptococcus pneumoniae topoisomerase IV-complex with the V-site 18mer dsDNA and novel fluoroquinolone Delafloxacin
Authors : Najmudin, S.; Pan, X.S.; Wang, B.; Chayen, N.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2023-09-21
Resolution : 2.40 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:

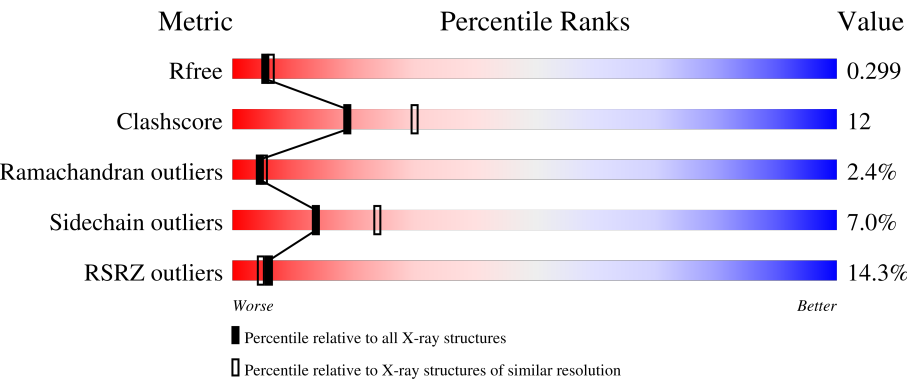
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	A	742	15% 71% 22% 5% .
1	B	742	12% 70% 25% . .
2	E	7	57% 29% 14%
3	F	11	9% 64% 36%

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Mol	Chain	Length	Quality of chain
4	H	11	27% 36% 55% 9%
5	G	7	14% 14% 86%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 24995 atoms, of which 12198 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 (ATP-hydrolyzing), DNA topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	724	Total 11662	C 3651	H 5882	N 1007	O 1097	S 25	325	3	0
1	B	724	Total 11620	C 3641	H 5859	N 1000	O 1096	S 24	321	1	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	403	MET	-	initiating methionine	UNP J0V1V8
A	404	LYS	-	expression tag	UNP J0V1V8
A	405	ASN	-	expression tag	UNP J0V1V8
A	406	LYS	-	expression tag	UNP J0V1V8
A	407	LYS	-	expression tag	UNP J0V1V8
A	408	ASP	-	expression tag	UNP J0V1V8
A	409	LYS	-	expression tag	UNP J0V1V8
A	410	GLY	-	expression tag	UNP J0V1V8
A	411	LEU	-	expression tag	UNP J0V1V8
A	648	HIS	-	linker	UNP J0V1V8
A	1257	THR	ILE	conflict	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	-	initiating methionine	UNP J0V1V8
B	404	LYS	-	expression tag	UNP J0V1V8
B	405	ASN	-	expression tag	UNP J0V1V8
B	406	LYS	-	expression tag	UNP J0V1V8
B	407	LYS	-	expression tag	UNP J0V1V8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	408	ASP	-	expression tag	UNP J0V1V8
B	409	LYS	-	expression tag	UNP J0V1V8
B	410	GLY	-	expression tag	UNP J0V1V8
B	411	LEU	-	expression tag	UNP J0V1V8
B	648	HIS	-	linker	UNP J0V1V8
B	1257	THR	ILE	conflict	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 DNA (5'-D(*T)-R(P*G)-D(P*T)-R(P*GP*GP*A)-D(P*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	7	Total	C	H	N	O	P	1	0	0
			225	70	81	26	42	6			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	11	Total	C	H	N	O	P	1	0	0
			349	107	125	40	66	11			

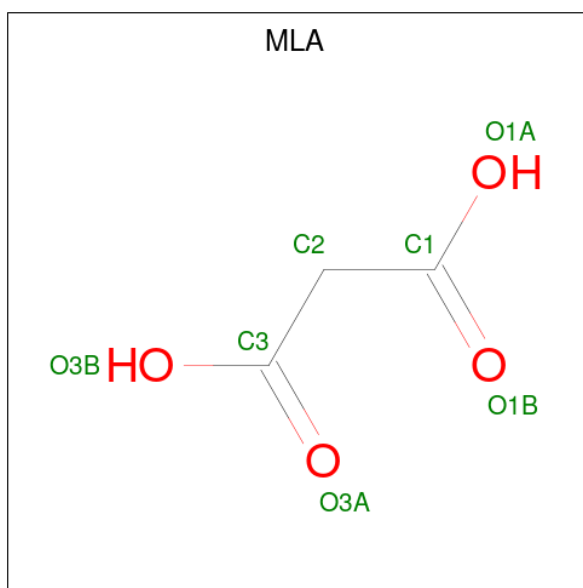
- Molecule 4 is a DNA chain called DNA/RNA (5'-R(P*AP*AP*CP*CP*G)-D(P*T)-R(P*A)-D(P*TP*T)-R(P*AP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	H	11	Total	C	H	N	O	P	1	0	0
			348	107	125	40	65	11			

- Molecule 5 is a DNA chain called DNA/RNA (5'-R(*G)-D(P*T)-R(P*AP*A)-D(P*T)-R(P*AP*C)-3').

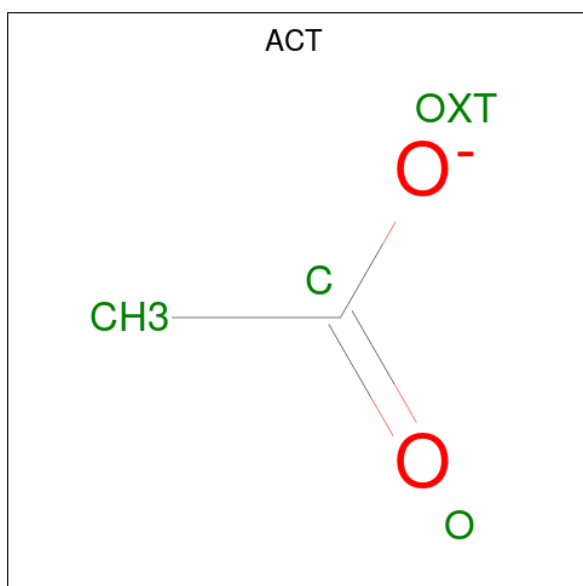
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	G	7	Total	C	H	N	O	P	1	0	0
			221	69	80	27	39	6			

- Molecule 6 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			9	3	2	4		
6	A	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			7	2	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			7	2	3	2		

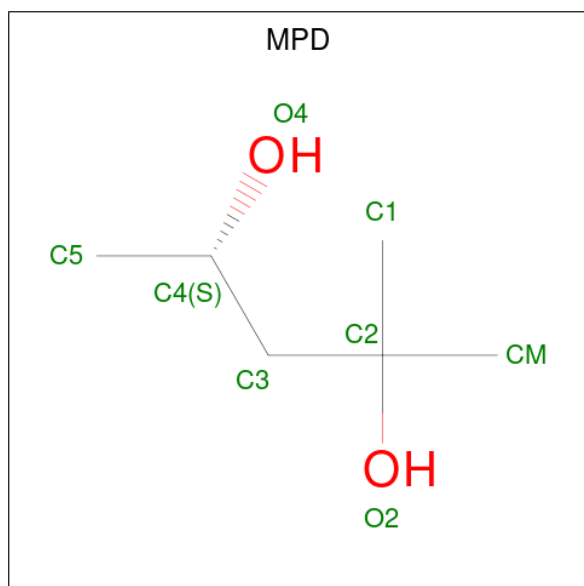
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	Mg	0	0
			3	3		
8	B	3	Total	Mg	0	0
			3	3		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		
9	B	1	Total	Cl	0	0
			1	1		

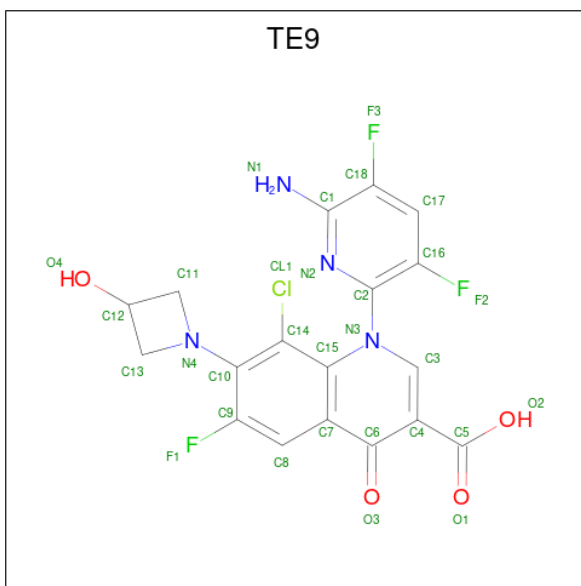
- Molecule 10 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	1	0
			22	6	14	2		

- Molecule 11 is delafloxacin (CCD ID: TE9) (formula: C₁₈H₁₂ClF₃N₄O₄) (labeled as "Ligand

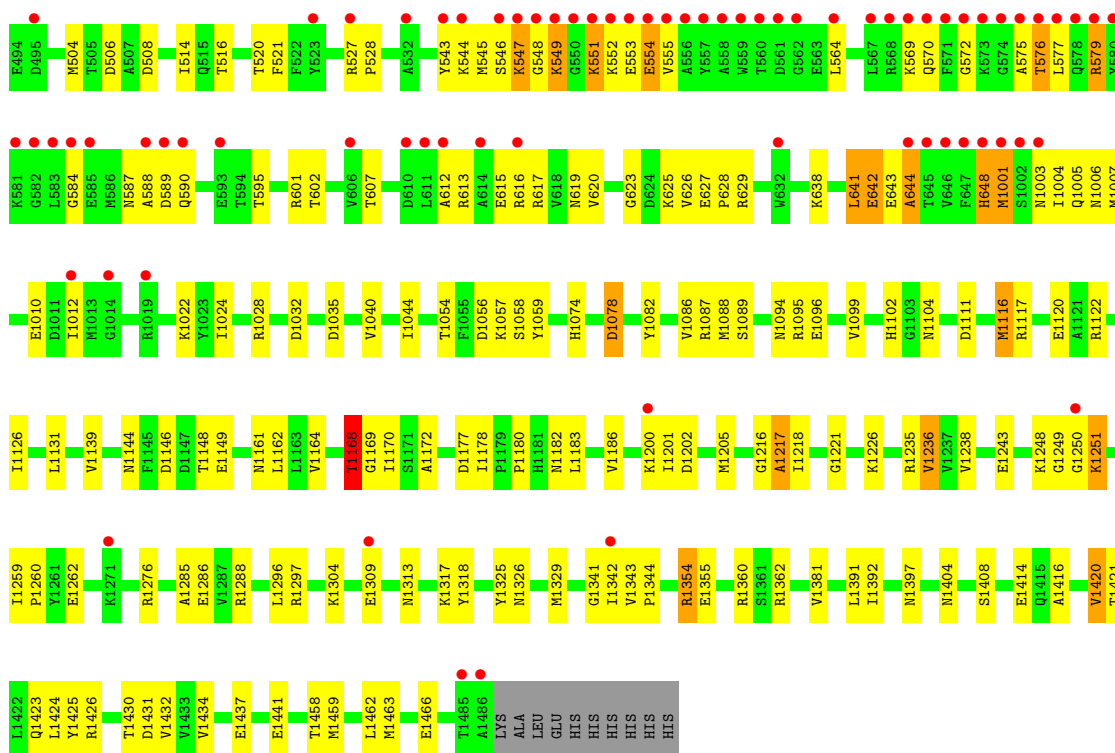
of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
11	F	1	Total	C	Cl	F	H	N	O	1	0
			41	18	1	3	11	4	4		
11	H	1	Total	C	Cl	F	H	N	O	1	0
			41	18	1	3	11	4	4		

- Molecule 12 is water.

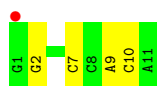
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	193	Total	O	0	0
			193	193		
12	B	199	Total	O	0	0
			199	199		
12	E	8	Total	O	0	0
			8	8		
12	F	9	Total	O	0	0
			9	9		
12	H	10	Total	O	0	0
			10	10		
12	G	7	Total	O	0	0
			7	7		



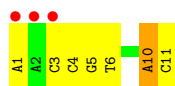
- Molecule 2: DNA (5'-D(*T)-R(P*G)-D(P*T)-R(P*GP*GP*A)-D(P*T)-3')



- Molecule 3: DNA/RNA (5'-R(P*GP*G)-D(P*TP*T)-R(P*A)-D(P*T)-R(P*CP*CP*AP*CP*A)-3')



- Molecule 4: DNA/RNA (5'-R(P*AP*AP*CP*CP*G)-D(P*T)-R(P*A)-D(P*TP*T)-R(P*AP*C)-3')



- Molecule 5: DNA/RNA (5'-R(*G)-D(P*T)-R(P*AP*A)-D(P*T)-R(P*AP*C)-3')



G9
T10
A11
A12
T13
A14
G15

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.14Å 157.14Å 211.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.86 – 2.40 64.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	50.9 (64.86-2.40) 50.9 (64.86-2.40)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0352, PDB-REDO	Depositor
R, R_{free}	0.241 , 0.299 0.241 , 0.299	Depositor DCC
R_{free} test set	3070 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 21.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	24995	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, MLA, ACT, TE9, CL, 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	0.54	0/5880	1.06	3/7927 (0.0%)
1	B	0.53	0/5858	1.03	5/7900 (0.1%)
2	E	0.54	0/161	1.22	1/248 (0.4%)
3	F	0.63	0/250	1.21	1/383 (0.3%)
4	H	0.53	0/249	1.30	6/381 (1.6%)
5	G	0.54	0/158	1.26	0/242
All	All	0.54	0/12556	1.06	16/17081 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	2
All	All	0	8

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	508	ASP	CA-CB-CG	8.93	121.53	112.60
4	H	10	DA	P-O3'-C3'	-6.92	109.82	120.20
1	B	1111	ASP	CB-CA-C	6.91	120.27	109.42
4	H	3	DC	P-O3'-C3'	-6.79	110.02	120.20
4	H	4	DC	P-O3'-C3'	-6.51	110.43	120.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1276	ARG	Sidechain
1	A	1353	ARG	Sidechain
1	A	537	ILE	Peptide
1	A	550	GLY	Peptide
1	A	551	LYS	Peptide

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	5780	5882	5871	136	0
1	B	5761	5859	5848	137	0
2	E	144	81	82	6	0
3	F	224	125	125	3	0
4	H	223	125	125	6	0
5	G	141	80	81	11	0
6	A	14	4	4	1	0
7	A	8	6	6	0	0
8	A	3	0	0	0	0
8	B	3	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	B	8	14	14	3	0
11	F	30	11	0	4	0
11	H	30	11	0	4	0
12	A	193	0	0	27	0
12	B	199	0	0	21	0
12	E	8	0	0	1	0
12	F	9	0	0	1	0
12	G	7	0	0	0	0
12	H	10	0	0	0	0
All	All	12797	12198	12156	289	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 12.

The worst 5 of 289 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)
11:H:101:TE9:CL1	11:H:101:TE9:N2	2.25	1.05
1:B:623:GLY:O	1:B:629:ARG:NH2	1.94	0.99
11:F:101:TE9:CL1	11:F:101:TE9:N2	2.33	0.98
1:B:1001:MET:HB3	1:B:1005:GLN:HE21	1.26	0.98
11:F:101:TE9:CL1	11:F:101:TE9:C2	2.54	0.93

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	725/742 (98%)	657 (91%)	49 (7%)	19 (3%)	4	4
1	B	723/742 (97%)	660 (91%)	47 (6%)	16 (2%)	5	6
All	All	1448/1484 (98%)	1317 (91%)	96 (7%)	35 (2%)	4	5

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ALA
1	A	549	LYS
1	A	610	ASP
1	B	569	LYS
1	B	588	ALA

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	622/635 (98%)	574 (92%)	48 (8%)	12	20
1	B	620/635 (98%)	580 (94%)	40 (6%)	15	27
All	All	1242/1270 (98%)	1154 (93%)	88 (7%)	14	23

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	551	LYS
1	B	1116	MET
1	B	576	THR
1	B	1012	ILE
1	B	1162	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	619	ASN
1	B	1006	ASN
1	B	1005	GLN
1	B	1053	ASN
1	A	1267	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	MLA	A	1501	-	6,6,6	1.28	0	7,7,7	1.12	0
10	MPD	B	1501	-	7,7,7	0.21	0	9,10,10	0.57	0
7	ACT	A	1503	-	3,3,3	1.04	0	3,3,3	1.09	0
11	TE9	F	101	8	32,33,33	1.10	3 (9%)	38,51,51	1.22	3 (7%)
7	ACT	A	1504	-	3,3,3	1.20	0	3,3,3	0.91	0
11	TE9	H	101	8	32,33,33	1.13	2 (6%)	38,51,51	1.21	2 (5%)
6	MLA	A	1502	-	6,6,6	1.32	0	7,7,7	1.09	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	MLA	A	1501	-	-	0/4/4/4	-
10	MPD	B	1501	-	-	0/5/5/5	-
11	TE9	F	101	8	-	3/11/20/20	0/4/4/4
11	TE9	H	101	8	-	6/11/20/20	0/4/4/4
6	MLA	A	1502	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	101	TE9	C2-C16	-2.83	1.39	1.42
11	H	101	TE9	C1-C18	2.51	1.42	1.39
11	F	101	TE9	C2-C16	-2.34	1.39	1.42
11	F	101	TE9	C1-C18	2.29	1.42	1.39
11	F	101	TE9	O1-C5	2.25	1.28	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	101	TE9	C17-C18-C1	-3.23	119.56	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	101	TE9	C17-C18-C1	-3.19	119.59	121.68
11	H	101	TE9	C4-C3-N3	-2.76	120.55	123.81
11	F	101	TE9	C4-C3-N3	-2.55	120.80	123.81
11	F	101	TE9	C1-N2-C2	2.10	122.34	116.99

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

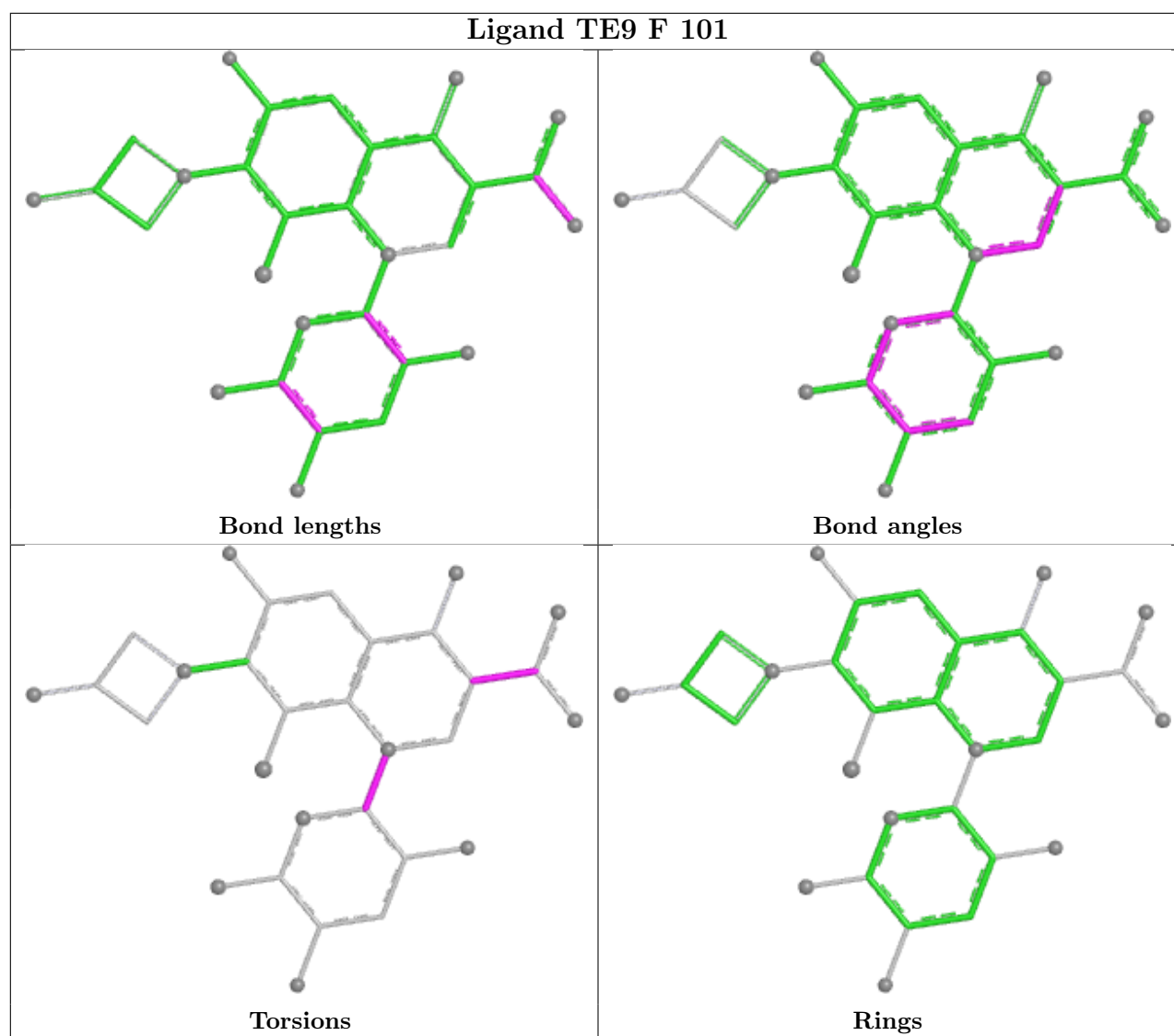
Mol	Chain	Res	Type	Atoms
11	F	101	TE9	N2-C2-N3-C3
11	H	101	TE9	N2-C2-N3-C3
6	A	1502	MLA	C1-C2-C3-O3A
11	H	101	TE9	C6-C4-C5-O2
6	A	1502	MLA	C1-C2-C3-O3B

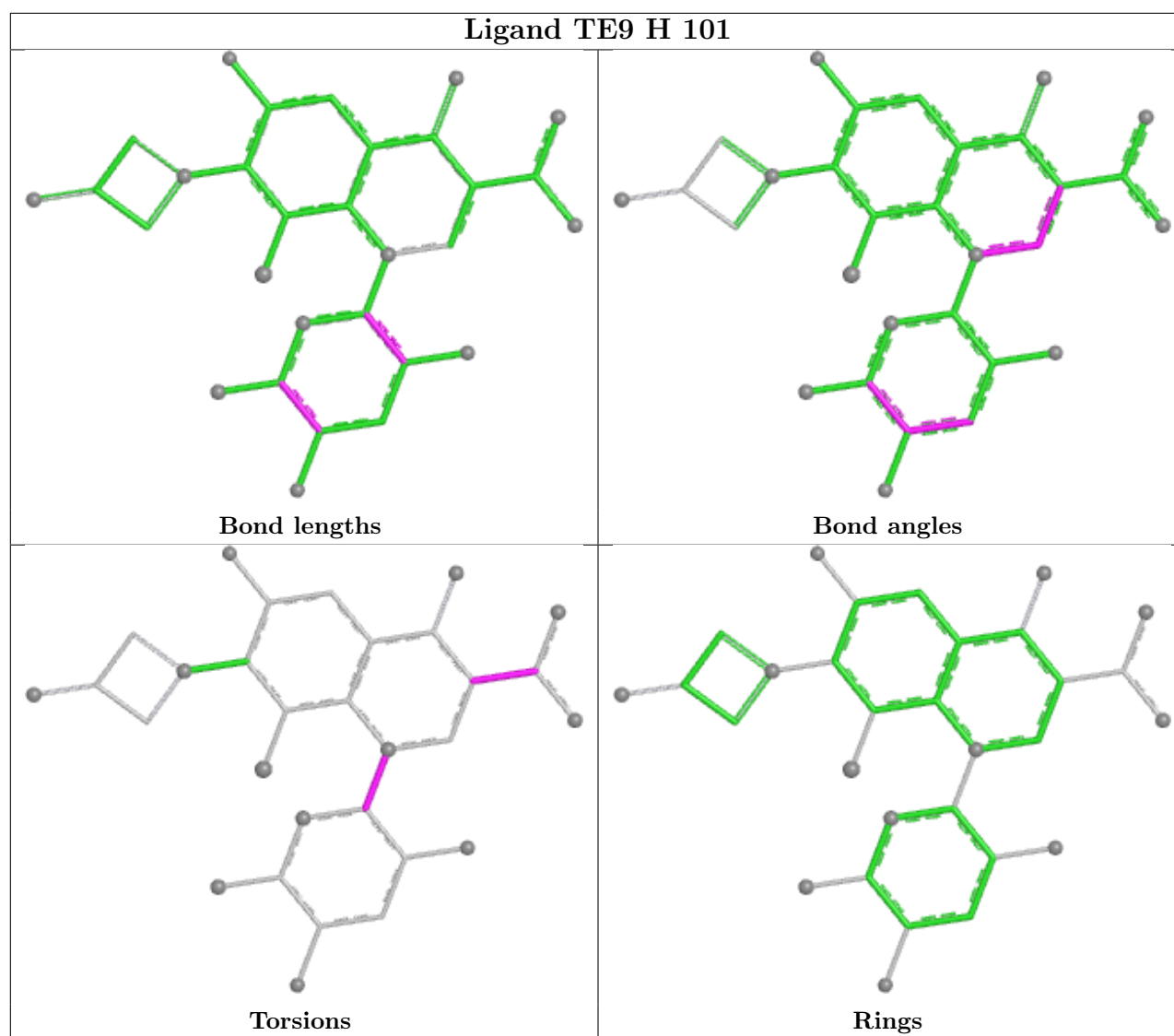
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1501	MPD	3	0
11	F	101	TE9	4	0
11	H	101	TE9	4	0
6	A	1502	MLA	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	724/742 (97%)	0.77	115 (15%) 5 4	6, 21, 65, 93	3 (0%)
1	B	724/742 (97%)	0.60	92 (12%) 8 6	6, 19, 57, 87	1 (0%)
2	E	7/7 (100%)	0.36	0 100 100	16, 16, 36, 52	0
3	F	11/11 (100%)	0.77	1 (9%) 15 12	20, 28, 51, 55	0
4	H	11/11 (100%)	1.39	3 (27%) 1 1	37, 47, 64, 65	0
5	G	7/7 (100%)	0.11	1 (14%) 6 5	12, 14, 36, 54	0
All	All	1484/1520 (97%)	0.69	212 (14%) 6 5	6, 21, 61, 93	4 (0%)

The worst 5 of 212 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	555	VAL	8.5
1	A	644	ALA	8.1
1	A	646	VAL	8.0
1	B	571	PHE	7.7
1	B	644	ALA	7.6

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

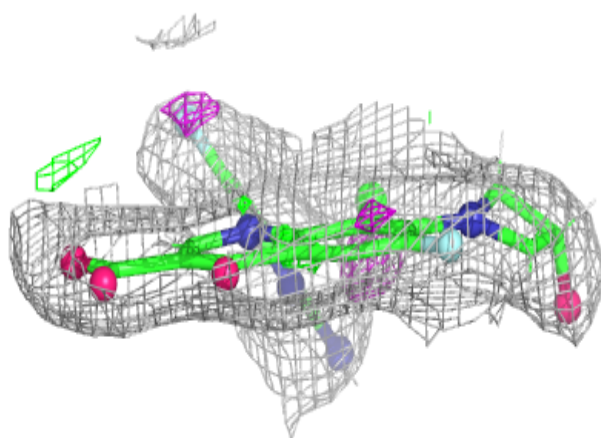
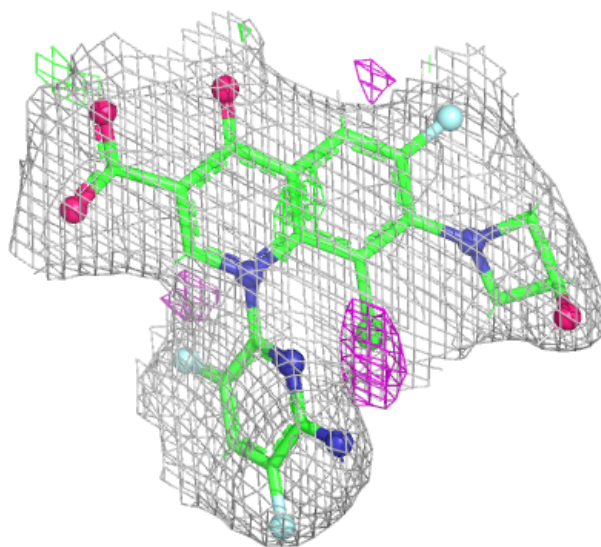
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MLA	A	1502	7/7	0.81	0.14	24,26,28,28	0
7	ACT	A	1504	4/4	0.81	0.14	22,22,23,23	0
8	MG	B	1502	1/1	0.81	0.10	15,15,15,15	0
8	MG	B	1504	1/1	0.84	0.10	9,9,9,9	0
9	CL	A	1508	1/1	0.84	0.15	17,17,17,17	0
6	MLA	A	1501	7/7	0.88	0.11	23,23,24,24	0
11	TE9	F	101	30/30	0.89	0.13	22,25,29,30	1
11	TE9	H	101	30/30	0.89	0.14	30,42,45,45	1
8	MG	A	1505	1/1	0.90	0.05	11,11,11,11	0
9	CL	B	1505	1/1	0.90	0.06	15,15,15,15	0
8	MG	A	1507	1/1	0.91	0.07	17,17,17,17	0
7	ACT	A	1503	4/4	0.92	0.12	13,13,13,14	0
8	MG	A	1506	1/1	0.93	0.11	8,8,8,8	0
10	MPD	B	1501	8/8	0.93	0.11	11,12,14,30	1
8	MG	B	1503	1/1	0.96	0.08	12,12,12,12	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.

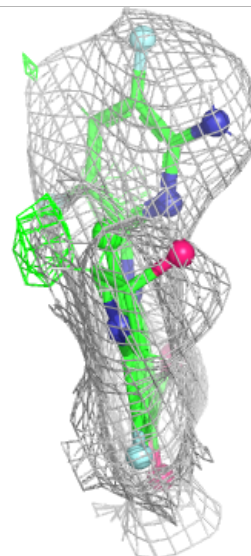
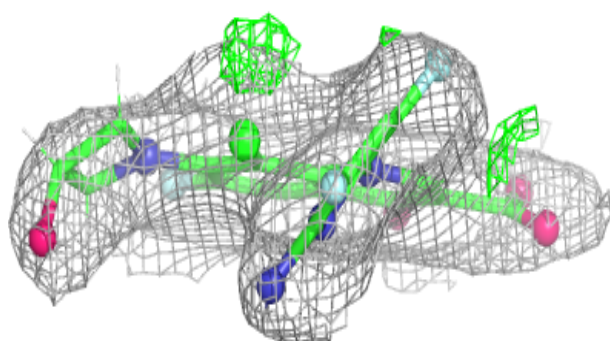
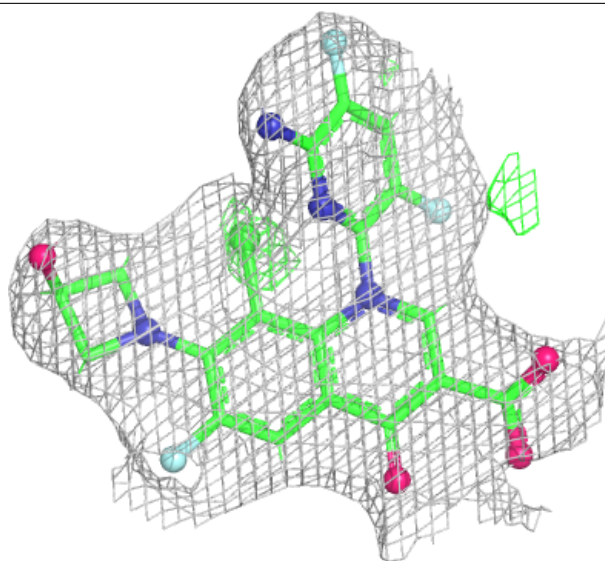
Electron density around TE9 F 101:

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



Electron density around TE9 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.