



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 01:13 PM UTC

PDB ID : 9GEF / pdb_00009gef
Title : Experimental localization of metal-binding sites reveals the role of metal ions in the delafloxacin-stabilized *Streptococcus pneumoniae* topoisomerase IV DNA cleavage complex
Authors : Wang, B.; Najmudin, S.; Pan, X.-S.; Mykhaylyk, V.; Orr, C.; Wagner, A.; Govada, L.; Chayen, N.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2024-08-08
Resolution : 2.62 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](#) ①) were used in the production of this report:

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

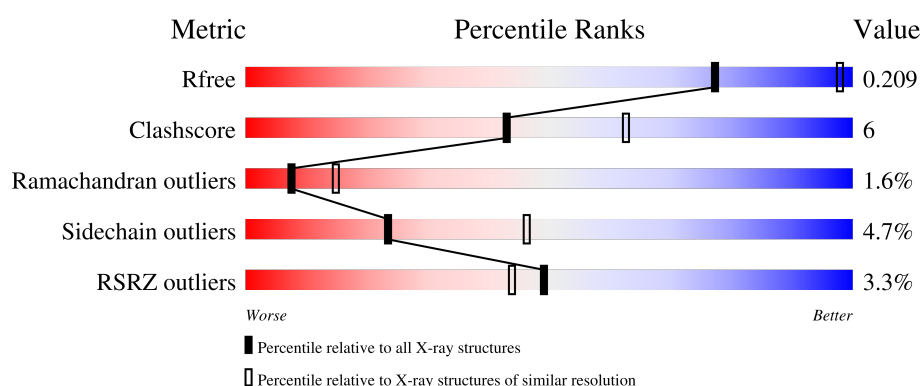
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	723	5% 81% 14% .
1	B	723	2% 84% 13% .
2	E	7	14% 86% 14%
3	F	11	73% 27%
4	G	7	57% 43%

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Mol	Chain	Length	Quality of chain
5	H	11	 82%18%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 12454 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 (ATP-HYDROLYZING),DNA TOPOISOMERASE 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	723	Total	C	N	O	S	0	0	0
			5752	3633	999	1096	24			
1	B	723	Total	C	N	O	S	0	0	0
			5752	3633	999	1096	24			

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*TP*GP*GP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	P	0	0	0
			144	70	26	42	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	11	Total	C	N	O	P	0	0	0
			224	107	40	66	11			

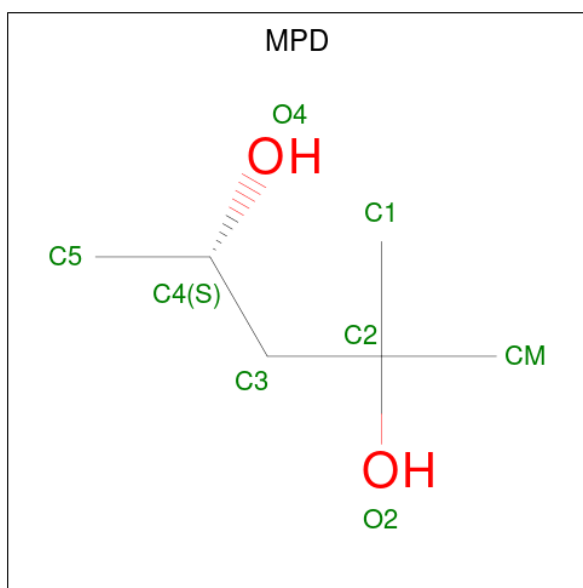
- Molecule 4 is a DNA chain called DNA (5'-D(*GP*TP*AP*AP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	7	Total	C	N	O	P	0	0	0
			141	69	27	39	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	11	Total	C	N	O	P	0	0	0
			223	107	40	65	11			

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Mg	0	0
			2	2		
7	B	1	Total	Mg	0	0
			1	1		
7	H	1	Total	Mg	0	0
			1	1		

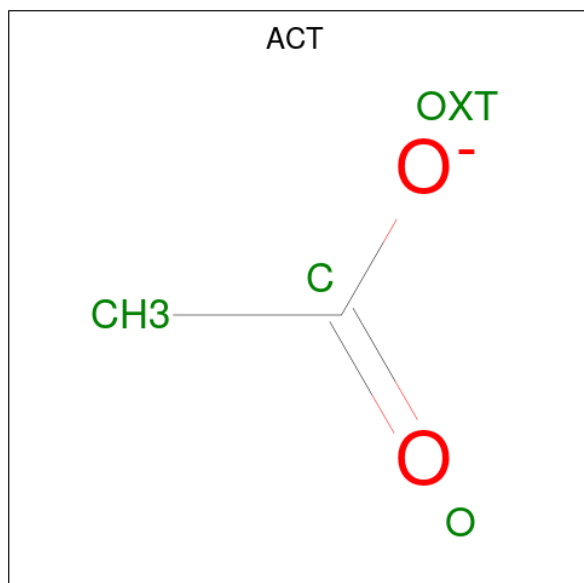
- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	K	0	0
			3	3		
8	B	5	Total	K	0	0
			5	5		

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

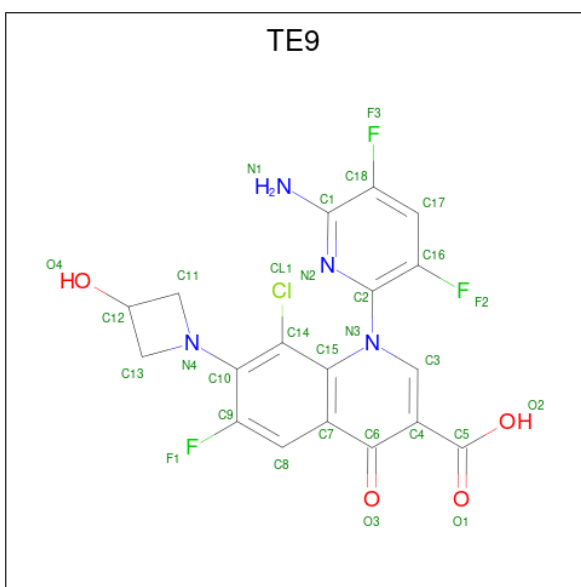
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		
9	B	1	Total	Cl	0	0
			1	1		

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			4	2	2		

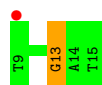
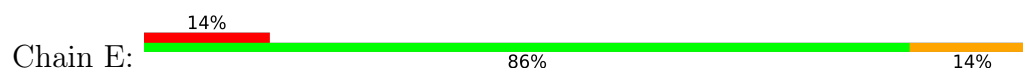
- Molecule 11 is delafloxacin (CCD ID: TE9) (formula: C₁₈H₁₂ClF₃N₄O₄).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	F	1	Total 30	C 18	Cl 1	F 3	N 4	O 4	0	0
11	H	1	Total 30	C 18	Cl 1	F 3	N 4	O 4	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	47	Total	O	0	0
			47	47		
12	B	45	Total	O	0	0
			45	45		
12	E	3	Total	O	0	0
			3	3		
12	F	6	Total	O	0	0
			6	6		
12	G	2	Total	O	0	0
			2	2		
12	H	5	Total	O	0	0
			5	5		



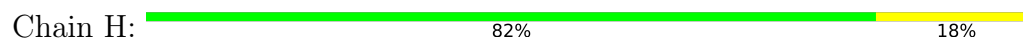
- Molecule 3: DNA (5'-D(P*GP*GP*TP*TP*AP*TP*CP*CP*AP*CP*A)-3')



- Molecule 4: DNA (5'-D(*GP*TP*AP*AP*TP*AP*C)-3')



- Molecule 5: DNA (5'-D(P*AP*AP*CP*CP*GP*TP*AP*TP*TP*AP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.53Å 158.53Å 210.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.39 – 2.62 79.39 – 2.62	Depositor EDS
% Data completeness (in resolution range)	69.5 (79.39-2.62) 69.5 (79.39-2.62)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.62Å)	Xtriage
Refinement program	PDB-REDO 8.11, PHENIX 4.4.7	Depositor
R, R_{free}	0.180 , 0.208 0.189 , 0.209	Depositor DCC
R_{free} test set	1109 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12454	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: MPD, K, TE9, MG, CL, ACT

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	0.73	2/5846 (0.0%)	1.01	8/7882 (0.1%)
1	B	0.71	3/5846 (0.1%)	1.01	7/7882 (0.1%)
2	E	0.31	0/161	1.12	1/248 (0.4%)
3	F	0.36	0/250	1.09	1/383 (0.3%)
4	G	0.32	0/158	1.26	1/242 (0.4%)
5	H	0.34	0/249	1.00	0/381
All	All	0.70	5/12510 (0.0%)	1.02	18/17018 (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	13
1	B	0	15
All	All	0	28

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1448	MET	SD-CE	8.90	2.01	1.79
1	B	1193	MET	SD-CE	7.59	1.98	1.79
1	B	1007	MET	SD-CE	5.96	1.94	1.79
1	A	1048	MET	SD-CE	-5.83	1.65	1.79
1	B	1448	MET	SD-CE	5.04	1.92	1.79

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	624	ASP	CA-CB-CG	7.83	120.43	112.60
1	B	1305	ASP	CA-CB-CG	7.50	120.11	112.60
1	B	1432	VAL	N-CA-C	7.28	118.04	110.62
3	F	5	DA	P-O5'-C5'	-6.58	110.14	120.00
1	B	466	LYS	N-CA-C	6.35	120.88	111.04

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1060	ARG	Sidechain
1	A	447	ARG	Sidechain
1	A	579	ARG	Sidechain
1	A	605	ARG	Sidechain
1	A	613	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5752	0	5832	80	1
1	B	5752	0	5832	69	1
2	E	144	0	82	1	0
3	F	224	0	125	2	0
4	G	141	0	81	2	0
5	H	223	0	125	1	0
6	A	16	0	28	4	0
6	B	16	0	28	3	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	H	1	0	0	1	0
8	A	3	0	0	0	0
8	B	5	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	1	0
10	B	4	0	3	0	0
11	F	30	0	0	4	0
11	H	30	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	A	47	0	0	0	0
12	B	45	0	0	1	0
12	E	3	0	0	0	0
12	F	6	0	0	0	0
12	G	2	0	0	0	0
12	H	5	0	0	2	0
All	All	12454	0	12136	152	1

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 6.

The worst 5 of 152 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:1448:MET:SD	1:A:1448:MET:CE	2.01	1.48
11:H:101:TE9:CL1	11:H:101:TE9:N2	2.32	0.98
1:A:546:SER:O	1:A:554:GLU:HG2	1.71	0.91
11:F:101:TE9:CL1	11:F:101:TE9:N2	2.41	0.90
11:H:101:TE9:CL1	11:H:101:TE9:C2	2.58	0.88

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1393:ARG:NH2	1:B:1279:ASN:O[4_455]	2.15	0.05

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	721/723 (100%)	684 (95%)	24 (3%)	13 (2%)	6 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	721/723 (100%)	685 (95%)	26 (4%)	10 (1%)	9	17
All	All	1442/1446 (100%)	1369 (95%)	50 (4%)	23 (2%)	7	15

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	ALA
1	A	553	GLU
1	A	555	VAL
1	A	573	LYS
1	A	1003	ASN

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	619/619 (100%)	586 (95%)	33 (5%)	20	41
1	B	619/619 (100%)	594 (96%)	25 (4%)	28	53
All	All	1238/1238 (100%)	1180 (95%)	58 (5%)	23	46

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1302	LEU
1	B	1444	GLU
1	B	520	THR
1	B	1433	VAL
1	B	1268	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1196	HIS
1	B	1461	ASN

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Mol	Chain	Res	Type
1	B	1326	ASN
1	B	570	GLN
1	B	1132	GLN

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 21 ligands modelled in this entry, 14 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	$\# Z > 2$
11	TE9	H	101	7	32,33,33	1.23	4 (12%)	38,51,51	1.56	8 (21%)
6	MPD	B	1502	-	7,7,7	0.25	0	9,10,10	0.54	0
10	ACT	B	1510	-	3,3,3	1.30	0	3,3,3	0.83	0
6	MPD	A	1501	-	7,7,7	0.24	0	9,10,10	0.46	0
11	TE9	F	101	7	32,33,33	1.26	5 (15%)	38,51,51	1.45	7 (18%)
6	MPD	A	1508	-	7,7,7	0.13	0	9,10,10	0.35	0
6	MPD	B	1501	-	7,7,7	0.33	0	9,10,10	0.95	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
11	TE9	H	101	7	-	5/11/20/20	0/4/4/4
6	MPD	B	1502	-	-	4/5/5/5	-
6	MPD	A	1501	-	-	3/5/5/5	-
11	TE9	F	101	7	-	1/11/20/20	0/4/4/4
6	MPD	A	1508	-	-	1/5/5/5	-
6	MPD	B	1501	-	-	5/5/5/5	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	101	TE9	C10-C14	-3.15	1.35	1.40
11	F	101	TE9	C2-C16	-3.14	1.38	1.42
11	H	101	TE9	C2-C16	-3.04	1.38	1.42
11	F	101	TE9	C10-C14	-2.84	1.35	1.40
11	F	101	TE9	C11-C12	2.34	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	101	TE9	C17-C18-C1	-3.79	119.20	121.68
11	H	101	TE9	C4-C3-N3	-3.49	119.68	123.81
11	F	101	TE9	C13-N4-C11	-3.24	91.86	94.52
11	F	101	TE9	C4-C3-N3	-3.04	120.22	123.81
11	H	101	TE9	O1-C5-C4	-2.85	116.77	122.67

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

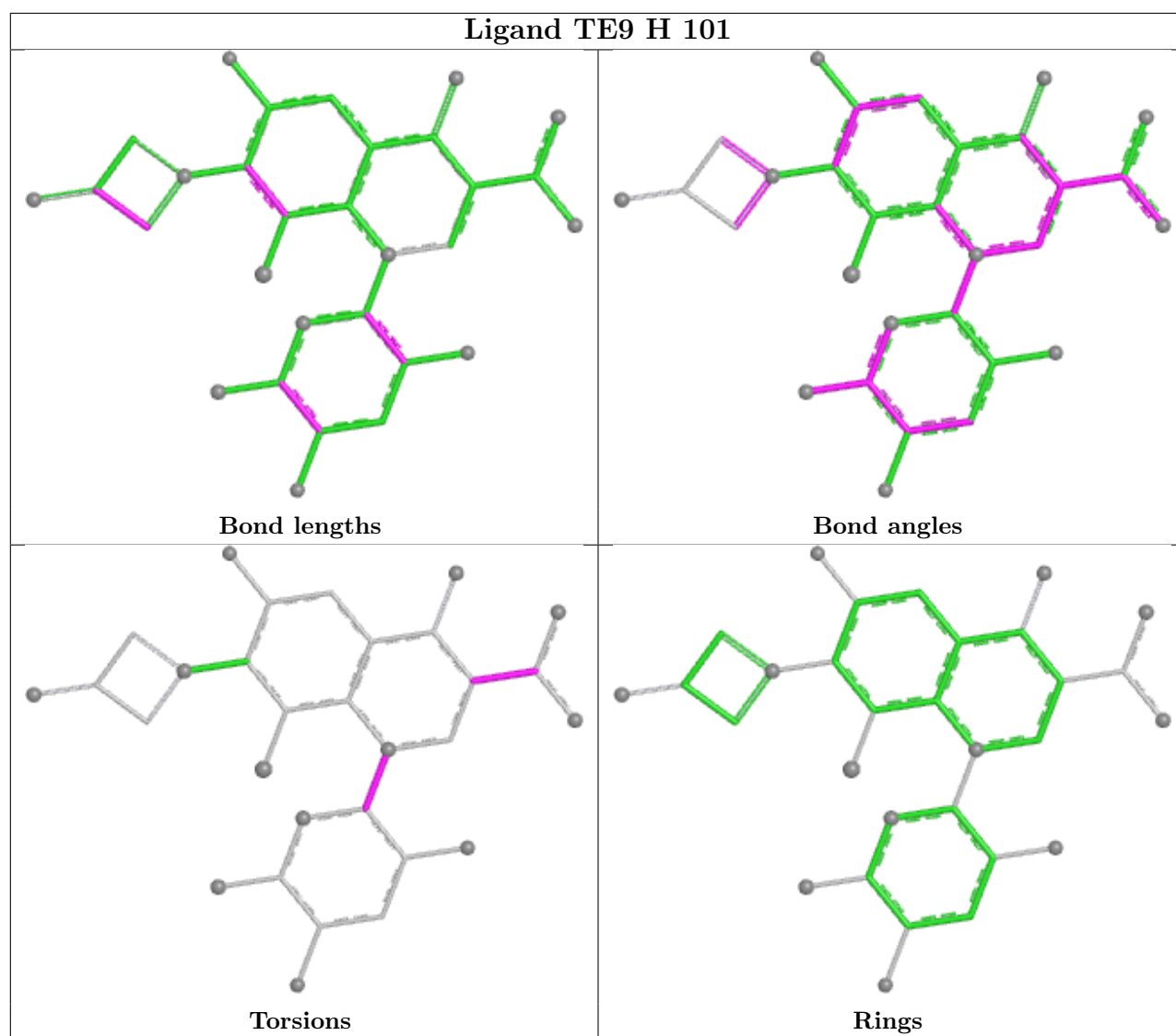
Mol	Chain	Res	Type	Atoms
6	B	1501	MPD	C1-C2-C3-C4
6	B	1501	MPD	O2-C2-C3-C4
11	F	101	TE9	N2-C2-N3-C3
11	H	101	TE9	N2-C2-N3-C3
11	H	101	TE9	C6-C4-C5-O1

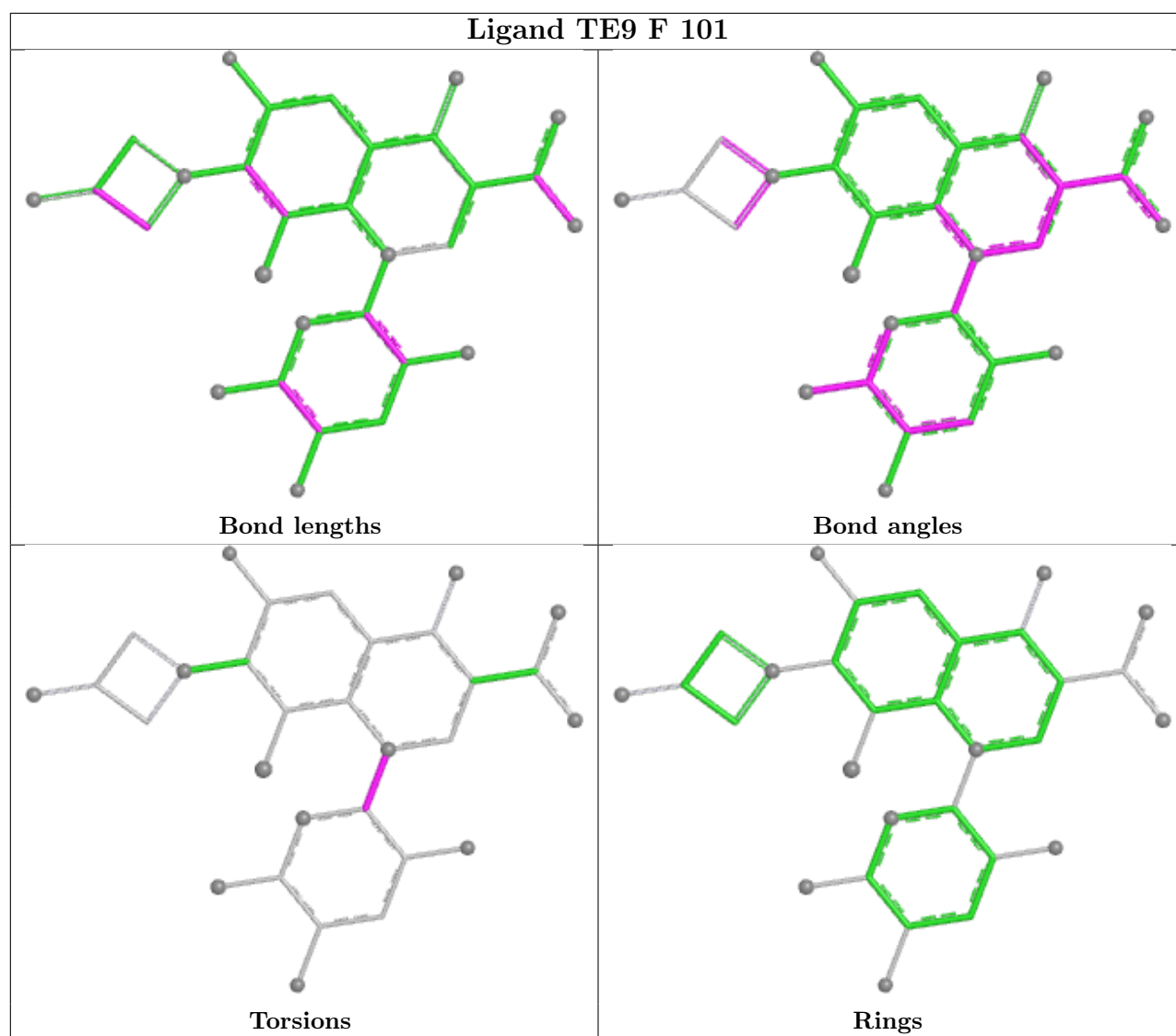
There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	H	101	TE9	5	0
6	A	1501	MPD	2	0
11	F	101	TE9	4	0
6	A	1508	MPD	2	0
6	B	1501	MPD	3	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	723/723 (100%)	-0.08	34 (4%) 36 31	24, 41, 87, 142	0
1	B	723/723 (100%)	-0.15	14 (1%) 66 62	23, 40, 87, 131	0
2	E	7/7 (100%)	0.16	1 (14%) 6 5	34, 36, 62, 84	0
3	F	11/11 (100%)	-0.02	0 100 100	42, 57, 68, 86	0
4	G	7/7 (100%)	-0.26	0 100 100	33, 35, 64, 82	0
5	H	11/11 (100%)	-0.09	0 100 100	41, 53, 66, 84	0
All	All	1482/1482 (100%)	-0.12	49 (3%) 49 44	23, 41, 87, 142	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	547	LYS	7.6
1	A	411	LEU	6.1
1	A	548	GLY	5.6
1	A	555	VAL	5.5
1	A	646	VAL	5.5

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

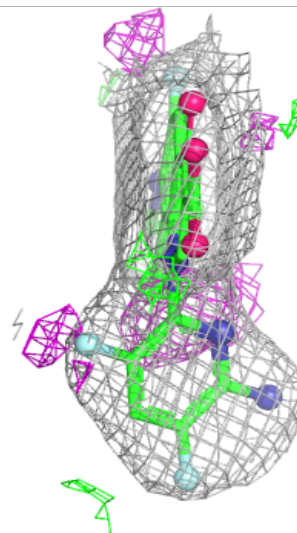
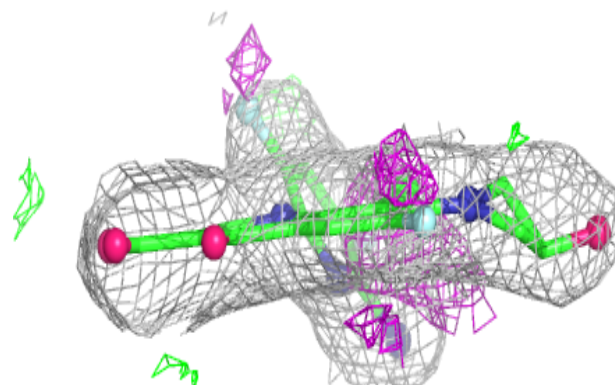
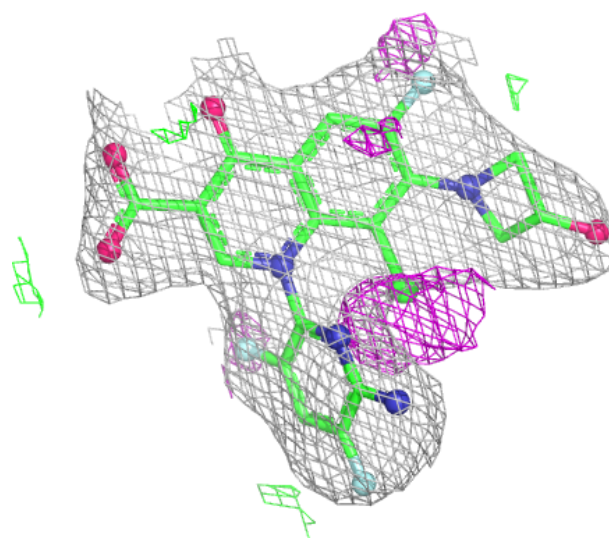
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	ACT	B	1510	4/4	0.74	0.21	45,53,55,56	0
6	MPD	B	1501	8/8	0.83	0.18	48,52,57,58	0
6	MPD	A	1501	8/8	0.84	0.20	47,53,63,70	0
8	K	B	1507	1/1	0.89	0.21	79,79,79,79	0
8	K	A	1505	1/1	0.89	0.21	67,67,67,67	0
6	MPD	A	1508	8/8	0.90	0.13	43,51,54,54	0
8	K	B	1505	1/1	0.91	0.11	68,68,68,68	0
9	CL	B	1509	1/1	0.92	0.11	76,76,76,76	0
6	MPD	B	1502	8/8	0.94	0.13	44,45,51,54	0
9	CL	A	1507	1/1	0.94	0.09	75,75,75,75	0
8	K	B	1504	1/1	0.95	0.15	45,45,45,45	0
8	K	B	1506	1/1	0.95	0.08	68,68,68,68	0
11	TE9	F	101	30/30	0.95	0.08	32,38,45,87	0
11	TE9	H	101	30/30	0.95	0.07	31,35,42,83	0
8	K	A	1504	1/1	0.96	0.19	39,39,39,39	0
7	MG	A	1502	1/1	0.96	0.07	45,45,45,45	0
8	K	A	1506	1/1	0.96	0.15	34,34,34,34	0
7	MG	H	102	1/1	0.96	0.05	54,54,54,54	0
8	K	B	1508	1/1	0.97	0.17	29,29,29,29	0
7	MG	A	1503	1/1	0.99	0.04	21,21,21,21	0
7	MG	B	1503	1/1	1.00	0.03	22,22,22,22	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.

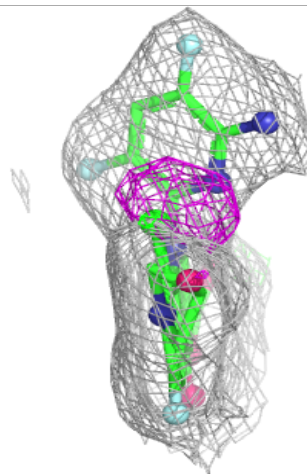
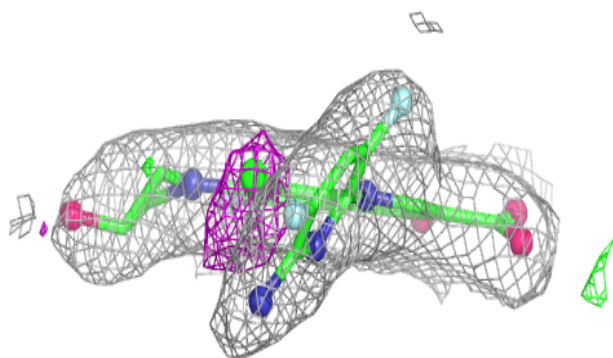
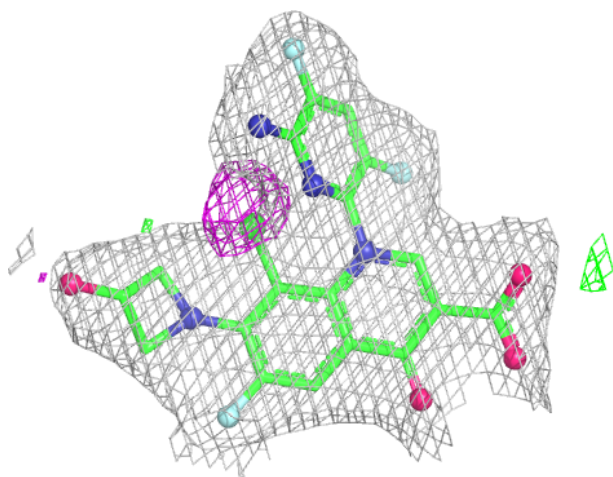
Electron density around TE9 F 101:

$2mF_o-DF_c$ (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.