



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 05:31 AM UTC

PDB ID : 8QMB / pdb_00008qmb
Title : Nucleant-assisted 2.0 Å resolution structure of the Streptococcus pneumoniae topoisomerase IV-V18mer DNA complex with the 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 : 2.00 Å(reported)

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

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

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

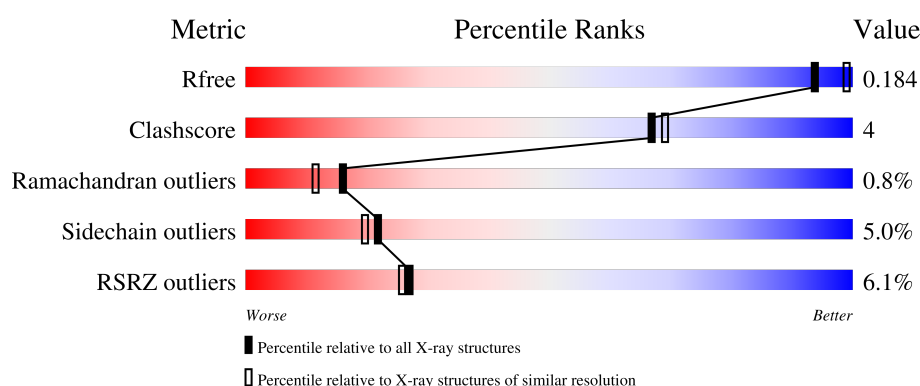
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	7% 83% 10% ...
1	B	742	5% 84% 11% ...
2	E	7	86% 14%
3	F	11	64% 36%
4	G	7	43% 43% 14%

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Mol	Chain	Length	Quality of chain
5	H	11	 73% 27%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ACT	B	1506	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 25726 atoms, of which 12251 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,DNA topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	724	Total 11665	C 3651	H 5885	N 1007	O 1097	S 25	117	4	0
1	B	724	Total 11637	C 3646	H 5867	N 1001	O 1099	S 24	117	3	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	403	MET	-	initiating methionine	UNP Q59961
A	460	ILE	VAL	variant	UNP Q59961
A	644	ALA	THR	variant	UNP Q59961
A	648	HIS	-	linker	UNP Q59961
A	1257	THR	ILE	variant	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 Q59961
B	460	ILE	VAL	variant	UNP Q59961
B	644	ALA	THR	variant	UNP Q59961
B	648	HIS	-	linker	UNP Q59961
B	1257	THR	ILE	variant	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1495	HIS	-	expression tag	UNP P72525
B	1496	HIS	-	expression tag	UNP P72525

- 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	H	N	O	P	10	0	0
			225	70	81	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	H	N	O	P	10	0	0
			349	107	125	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	H	N	O	P	7	0	0
			221	69	80	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	H	N	O	P	10	0	0
			348	107	125	40	65	11			

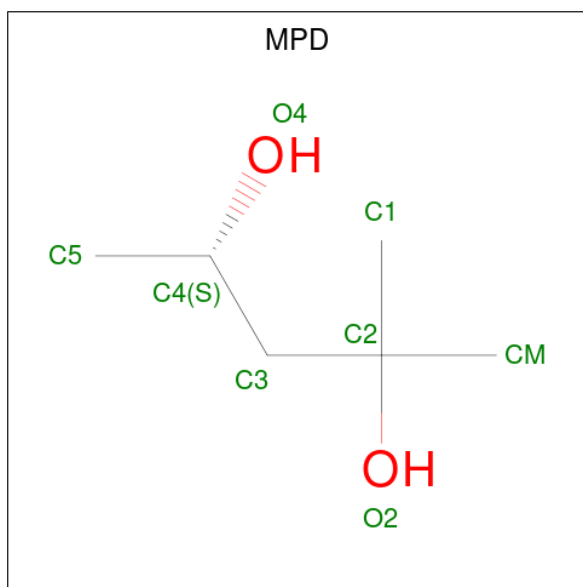
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

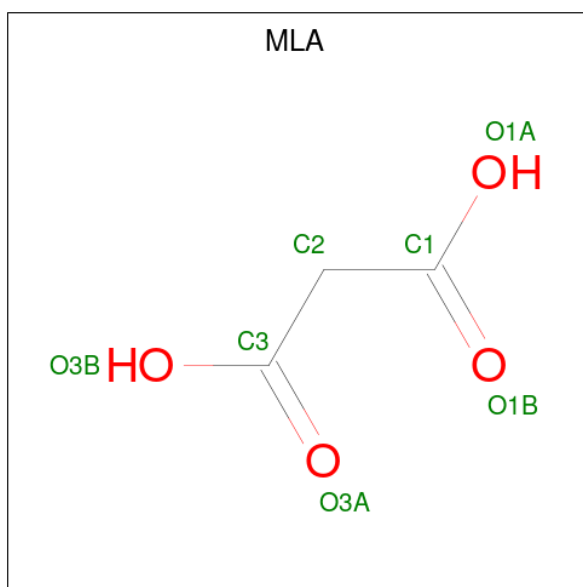
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0
7	B	1	Total Cl 1 1	0	0

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



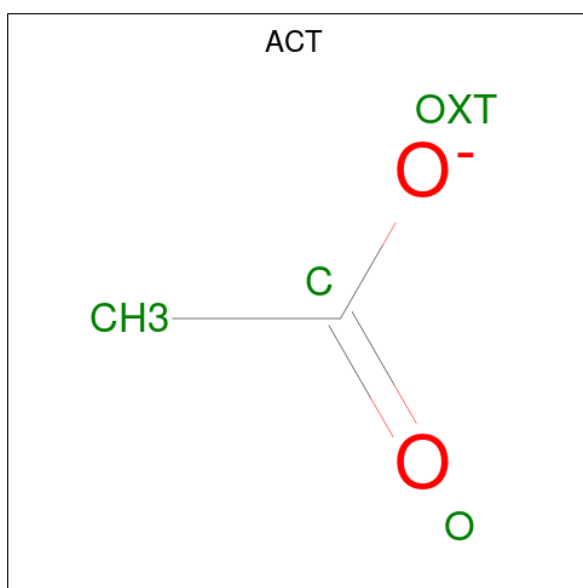
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H O 22 6 14 2	2	0
8	A	1	Total C H O 22 6 14 2	2	0
8	B	1	Total C H O 22 6 14 2	2	0

- Molecule 9 is MALONIC ACID (CCD ID: MLA) (formula: C₃H₄O₄).



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

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



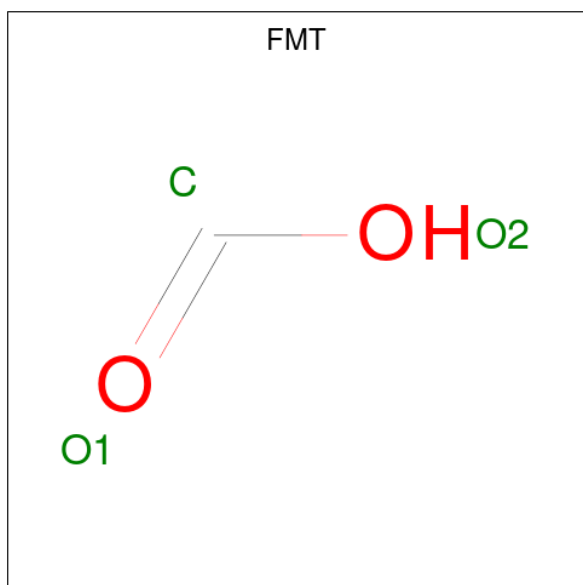
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	3	0
			7	2	3	2		
10	A	1	Total	C	H	O	3	0
			7	2	3	2		

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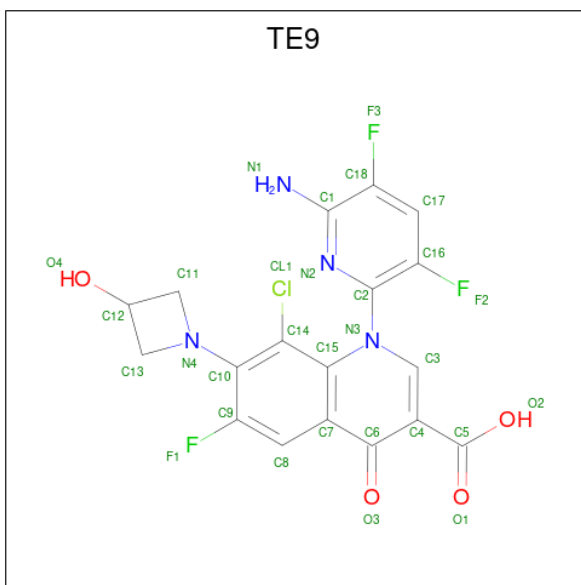
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	3	0
			7	2	3	2		
10	B	1	Total	C	H	O	3	0
			7	2	3	2		

- Molecule 11 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	H	O	1	0
			5	1	2	2		
11	A	1	Total	C	H	O	1	0
			5	1	2	2		
11	B	1	Total	C	H	O	1	0
			5	1	2	2		
11	B	1	Total	C	H	O	1	0
			5	1	2	2		

- Molecule 12 is delafloxacin (CCD ID: TE9) (formula: $\text{C}_{18}\text{H}_{12}\text{ClF}_3\text{N}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



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

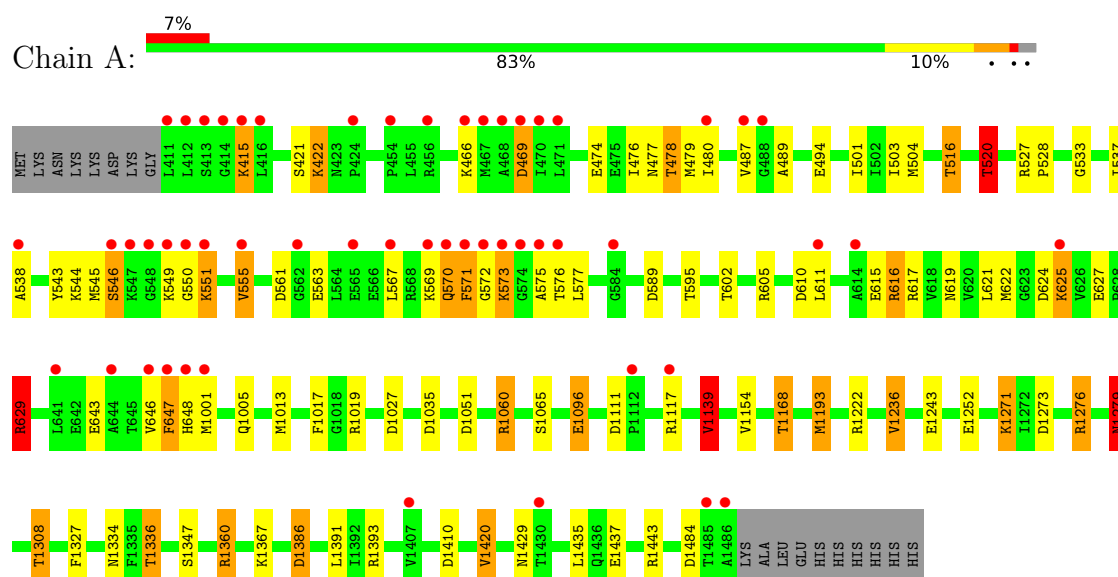
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	489	Total	O	0	0
			489	489		
13	B	510	Total	O	0	0
			510	510		
13	E	12	Total	O	0	0
			12	12		
13	F	20	Total	O	0	0
			20	20		
13	G	13	Total	O	0	0
			13	13		
13	H	15	Total	O	0	0
			15	15		

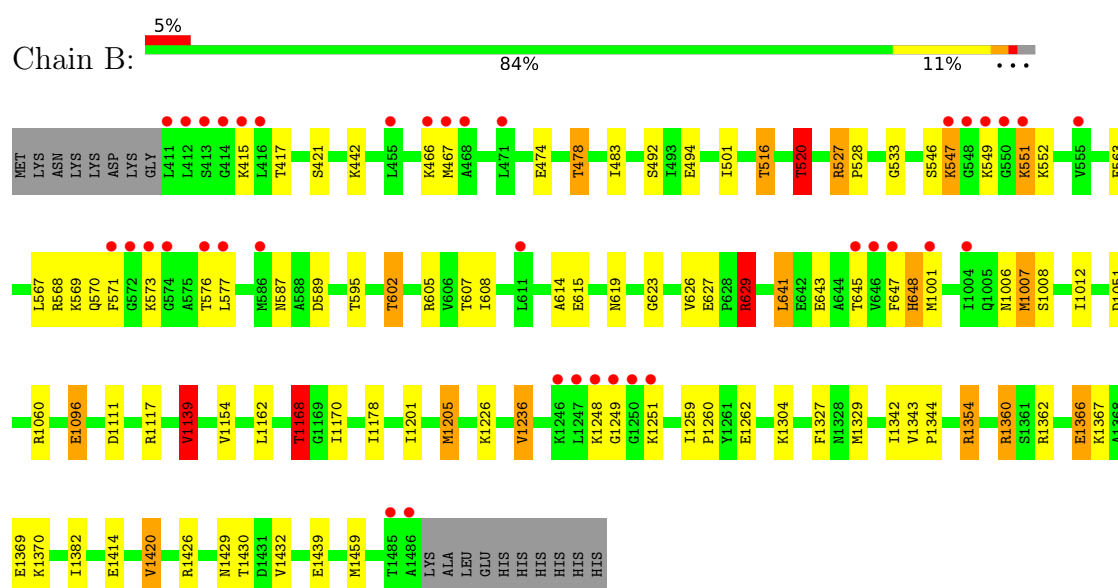
3 Residue-property plots [i](#)

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 topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A



- Molecule 1: DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A



- Molecule 2: DNA (5'-D(TP*GP*TP*GP*GP*AP*T)-3')

Chain E:  86% 14%

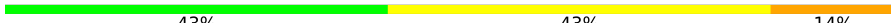


- Molecule 3: DNA (5'-D(P*GP*GP*TP*TP*AP*TP*CP*CP*AP*CP*A)-3')

Chain F:  64% 36%



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

Chain G:  43% 43% 14%



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

Chain H:  73% 27%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.22Å 157.22Å 211.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	83.63 – 2.00 83.63 – 2.00	Depositor EDS
% Data completeness (in resolution range)	56.8 (83.63-2.00) 56.6 (83.63-2.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.169 , 0.206 (Not available) , 0.184	Depositor DCC
R_{free} test set	5806 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25726	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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, MPD, CL, TE9, FMT, MLA, 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	0.78	1/5884 (0.0%)	1.37	42/7932 (0.5%)
1	B	0.79	0/5876	1.35	26/7924 (0.3%)
2	E	0.64	0/161	1.51	1/248 (0.4%)
3	F	0.71	0/250	1.72	6/383 (1.6%)
4	G	0.65	0/158	1.61	3/242 (1.2%)
5	H	0.83	1/249 (0.4%)	1.52	2/381 (0.5%)
All	All	0.78	2/12578 (0.0%)	1.38	80/17110 (0.5%)

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	12
1	B	0	10
All	All	0	22

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1	DA	P-OP2	7.50	1.63	1.48
1	A	1065	SER	CA-CB	-5.16	1.45	1.53

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1111	ASP	CB-CA-C	12.60	129.21	109.42
1	A	1111	ASP	CB-CA-C	11.54	127.54	109.42
3	F	2	DG	O3'-P-O5'	-8.85	90.73	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1236	VAL	N-CA-CB	-8.60	98.02	112.47
1	B	1236	VAL	N-CA-CB	-8.47	98.20	112.44

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	537	ILE	Peptide
1	A	545	MET	Peptide
1	A	549	LYS	Peptide
1	A	550	GLY	Peptide
1	A	551	LYS	Peptide

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	5780	5885	5869	43	0
1	B	5770	5867	5848	40	0
2	E	144	81	82	0	0
3	F	224	125	125	0	0
4	G	141	80	81	2	0
5	H	223	125	125	0	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	1	0
8	A	16	28	28	1	0
8	B	8	14	14	3	0
9	A	14	4	4	1	0
10	A	8	6	6	0	0
10	B	8	6	6	5	0
11	A	6	4	4	1	0
11	B	6	4	4	0	0
12	F	30	11	0	3	0
12	H	30	11	0	3	0
13	A	489	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	B	510	0	0	6	0
13	E	12	0	0	0	0
13	F	20	0	0	0	0
13	G	13	0	0	0	0
13	H	15	0	0	0	0
All	All	13475	12251	12196	91	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 4.

The worst 5 of 91 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:B:1430:THR:HG22	8:B:1508:MPD:HM2	1.47	0.95
1:A:1443[A]:ARG:NH1	9:A:1507:MLA:O1B	2.01	0.94
1:A:569:LYS:O	13:A:1601:HOH:O	1.95	0.82
1:A:621:LEU:HB3	1:A:622[A]:MET:HE2	1.65	0.78
1:A:546:SER:HA	1:A:575:ALA:HB1	1.66	0.77

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	726/742 (98%)	686 (94%)	35 (5%)	5 (1%)	18	14
1	B	725/742 (98%)	693 (96%)	25 (3%)	7 (1%)	12	8
All	All	1451/1484 (98%)	1379 (95%)	60 (4%)	12 (1%)	16	11

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	ASP
1	A	489	ALA
1	A	546	SER
1	B	466	LYS
1	B	551	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	622/635 (98%)	589 (95%)	33 (5%)	20	18
1	B	622/635 (98%)	592 (95%)	30 (5%)	23	21
All	All	1244/1270 (98%)	1181 (95%)	63 (5%)	22	19

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1279	ASN
1	B	1236	VAL
1	B	478	THR
1	B	1168	THR
1	B	1366	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	619	ASN
1	B	1053	ASN
1	B	1461	ASN
1	B	1182	ASN
1	B	1436	GLN

5.3.3 RNA ⓘ

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 23 ligands modelled in this entry, 8 are monoatomic - leaving 15 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$
9	MLA	A	1507	-	6,6,6	1.41	1 (16%)	7,7,7	1.52	1 (14%)
11	FMT	B	1509	-	2,2,2	1.99	1 (50%)	1,1,1	0.29	0
10	ACT	B	1505	-	3,3,3	1.31	0	3,3,3	1.00	0
11	FMT	A	1510	-	2,2,2	1.74	1 (50%)	1,1,1	0.05	0
8	MPD	B	1508	-	7,7,7	0.60	0	9,10,10	1.08	0
11	FMT	B	1507	-	2,2,2	1.40	0	1,1,1	0.12	0
12	TE9	F	101	6	32,33,33	2.17	10 (31%)	38,51,51	3.27	18 (47%)
12	TE9	H	101	6	32,33,33	2.49	12 (37%)	38,51,51	3.44	17 (44%)
9	MLA	A	1509	-	6,6,6	1.66	2 (33%)	7,7,7	0.83	0
10	ACT	B	1506	-	3,3,3	1.06	0	3,3,3	0.73	0
11	FMT	A	1512	-	2,2,2	1.16	0	1,1,1	0.04	0
10	ACT	A	1511	-	3,3,3	1.25	0	3,3,3	0.95	0
10	ACT	A	1508	-	3,3,3	1.72	1 (33%)	3,3,3	0.48	0
8	MPD	A	1505	-	7,7,7	0.39	0	9,10,10	0.68	0
8	MPD	A	1506	-	7,7,7	0.44	0	9,10,10	0.91	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
9	MLA	A	1507	-	-	1/4/4/4	-
12	TE9	H	101	6	-	3/11/20/20	0/4/4/4
8	MPD	B	1508	-	-	0/5/5/5	-
12	TE9	F	101	6	-	4/11/20/20	0/4/4/4
9	MLA	A	1509	-	-	2/4/4/4	-
8	MPD	A	1505	-	-	5/5/5/5	-
8	MPD	A	1506	-	-	2/5/5/5	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	101	TE9	C2-N2	6.47	1.42	1.34
12	F	101	TE9	C2-N2	5.82	1.41	1.34
12	H	101	TE9	C1-C18	5.43	1.45	1.39
12	H	101	TE9	C11-N4	4.99	1.52	1.47
12	F	101	TE9	C2-C16	-4.99	1.36	1.42

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	101	TE9	C17-C18-C1	-9.99	115.14	121.68
12	F	101	TE9	C17-C18-C1	-9.56	115.43	121.68
12	F	101	TE9	C18-C1-N1	-9.04	114.51	121.52
12	H	101	TE9	F2-C16-C2	-8.93	111.39	119.87
12	H	101	TE9	C13-N4-C11	-6.88	88.86	94.52

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1505	MPD	C2-C3-C4-C5
12	F	101	TE9	N2-C2-N3-C3
12	H	101	TE9	N2-C2-N3-C3
9	A	1509	MLA	O1A-C1-C2-C3
9	A	1509	MLA	O1B-C1-C2-C3

There are no ring outliers.

7 monomers are involved in 17 short contacts:

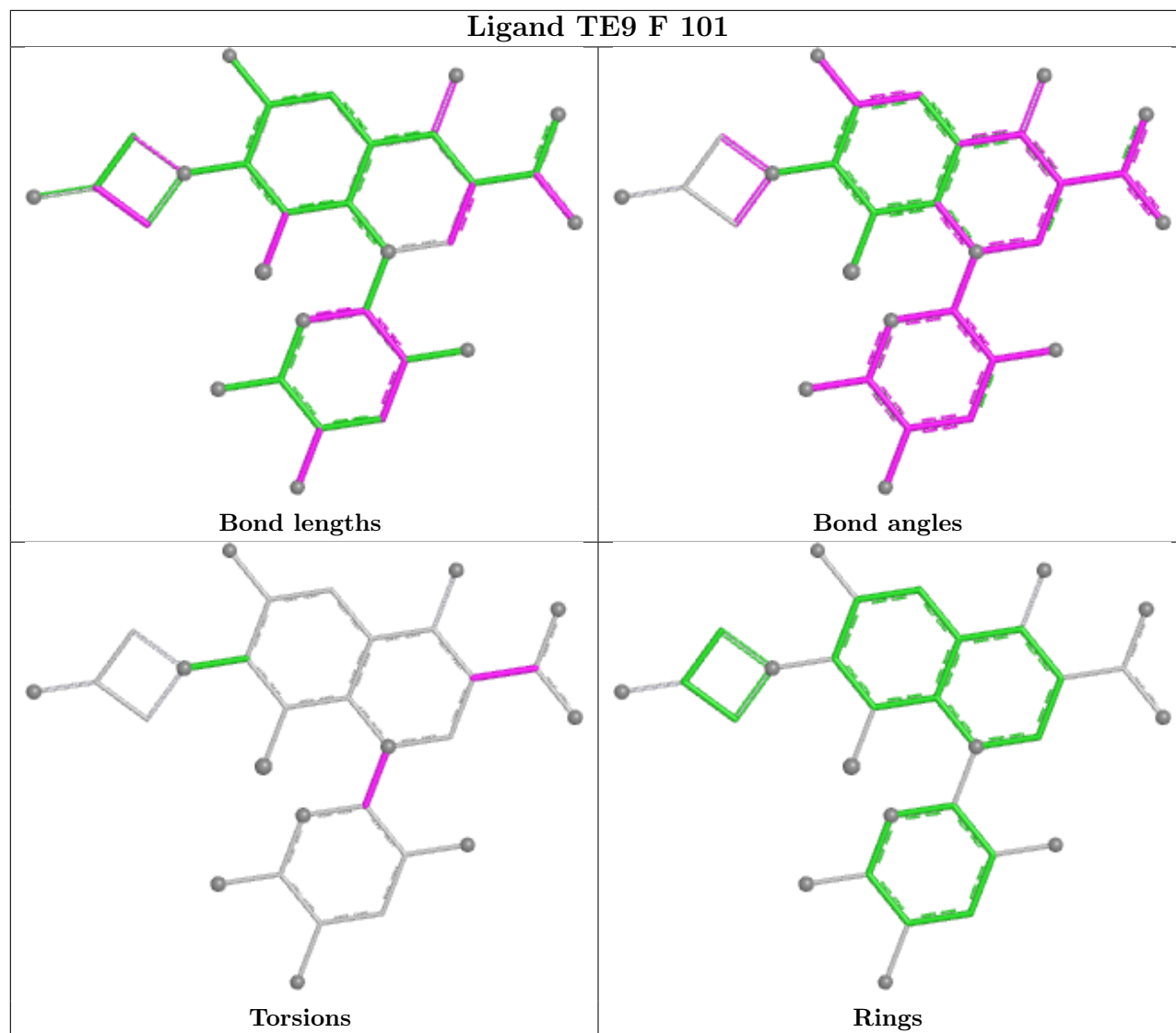
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1507	MLA	1	0

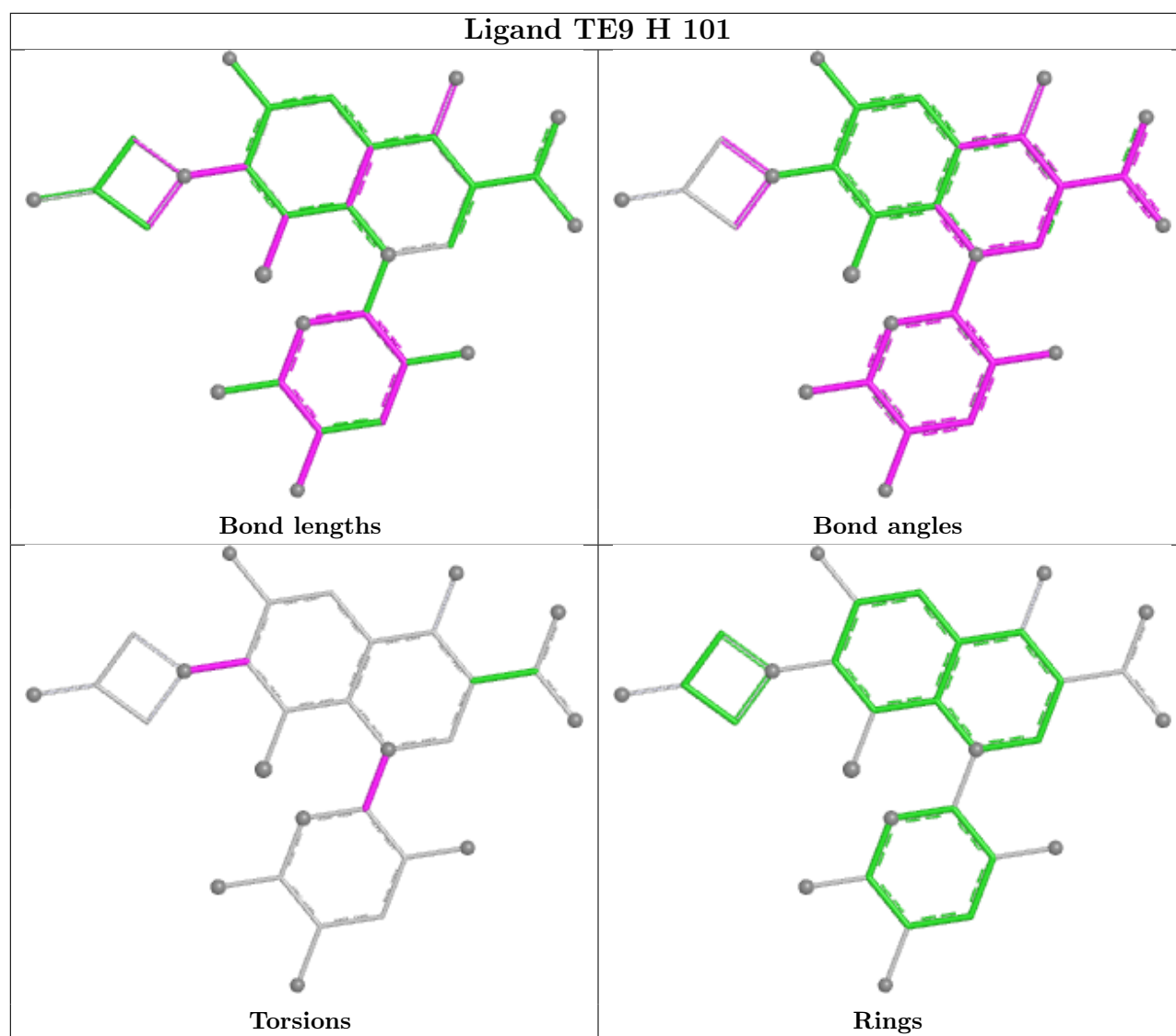
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1510	FMT	1	0
8	B	1508	MPD	3	0
12	F	101	TE9	3	0
12	H	101	TE9	3	0
10	B	1506	ACT	5	0
8	A	1505	MPD	1	0

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%)	0.09	53 (7%)	21 19	15, 41, 94, 157	3 (0%)
1	B	724/742 (97%)	0.05	38 (5%)	33 31	15, 39, 92, 140	2 (0%)
2	E	7/7 (100%)	-0.64	0	100 100	27, 30, 62, 79	0
3	F	11/11 (100%)	-0.67	0	100 100	34, 41, 56, 70	0
4	G	7/7 (100%)	-0.67	0	100 100	26, 31, 61, 84	0
5	H	11/11 (100%)	-0.58	0	100 100	34, 44, 59, 75	0
All	All	1484/1520 (97%)	0.05	91 (6%)	27 26	15, 40, 94, 157	5 (0%)

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	647	PHE	7.7
1	A	411	LEU	6.9
1	A	1486	ALA	6.6
1	A	412	LEU	6.2
1	A	646	VAL	6.0

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 ⓘ

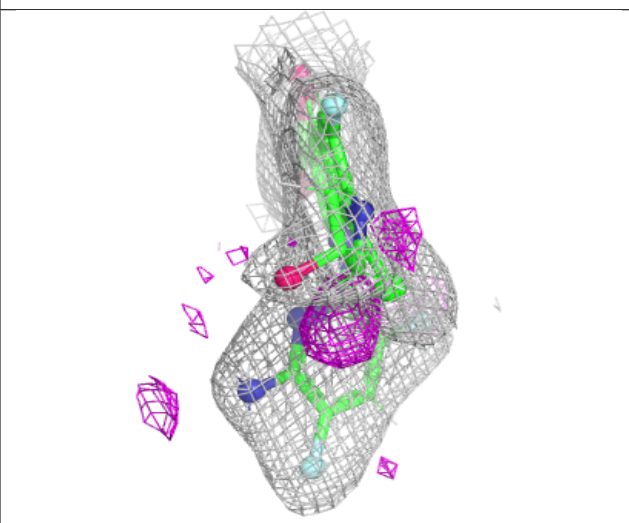
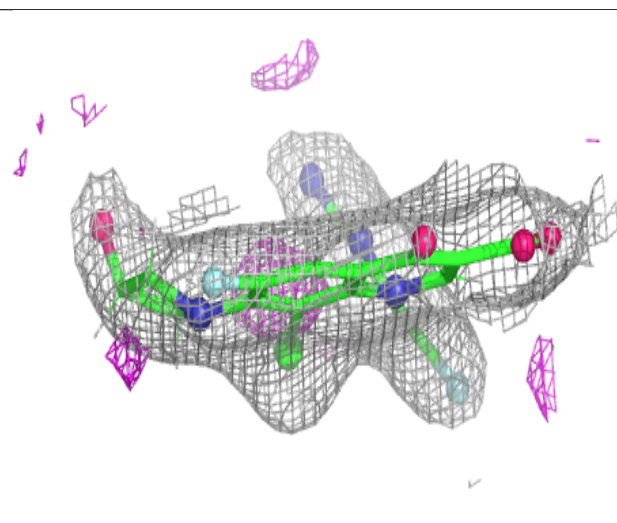
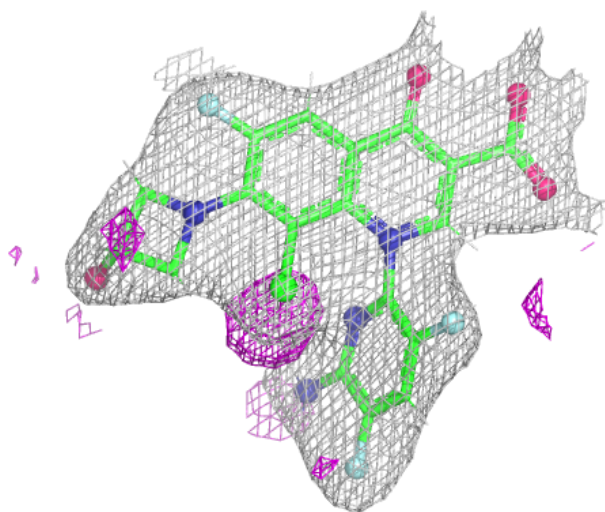
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	1508	4/4	0.83	0.25	30,30,56,64	3
11	FMT	B	1507	3/3	0.83	0.19	30,55,71,74	1
10	ACT	B	1505	4/4	0.87	0.20	30,30,60,68	3
10	ACT	A	1511	4/4	0.88	0.16	30,30,64,66	3
8	MPD	A	1506	8/8	0.91	0.15	30,71,80,84	2
11	FMT	B	1509	3/3	0.91	0.14	30,42,53,63	1
10	ACT	B	1506	4/4	0.92	0.15	30,30,75,106	3
8	MPD	B	1508	8/8	0.93	0.14	30,42,51,58	2
11	FMT	A	1512	3/3	0.93	0.11	30,36,48,67	1
9	MLA	A	1507	7/7	0.94	0.10	46,60,61,63	0
7	CL	A	1504	1/1	0.95	0.07	58,58,58,58	0
8	MPD	A	1505	8/8	0.95	0.14	30,62,65,75	2
6	MG	A	1501	1/1	0.96	0.07	50,50,50,50	0
9	MLA	A	1509	7/7	0.96	0.08	49,60,66,66	0
11	FMT	A	1510	3/3	0.96	0.14	30,33,48,57	1
6	MG	B	1501	1/1	0.97	0.04	50,50,50,50	0
7	CL	B	1504	1/1	0.97	0.10	68,68,68,68	0
6	MG	B	1502	1/1	0.97	0.06	32,32,32,32	0
12	TE9	F	101	30/30	0.97	0.06	25,34,44,55	1
12	TE9	H	101	30/30	0.97	0.05	29,36,44,48	1
6	MG	A	1502	1/1	0.99	0.03	17,17,17,17	0
6	MG	B	1503	1/1	1.00	0.04	33,33,33,33	0
6	MG	A	1503	1/1	1.00	0.01	40,40,40,40	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.

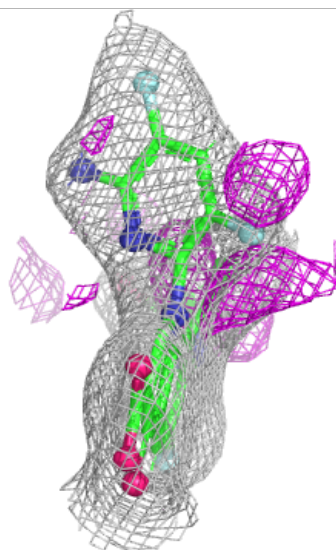
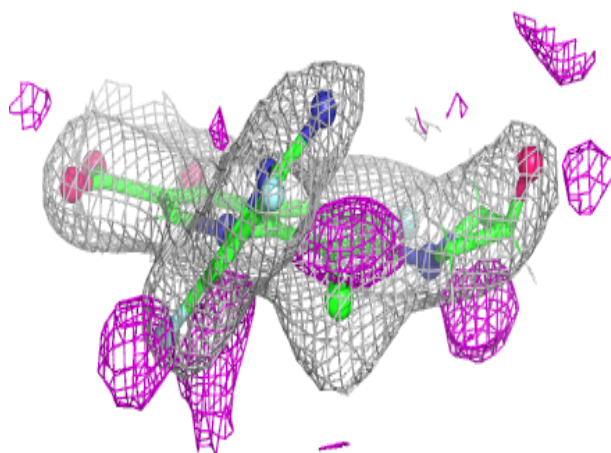
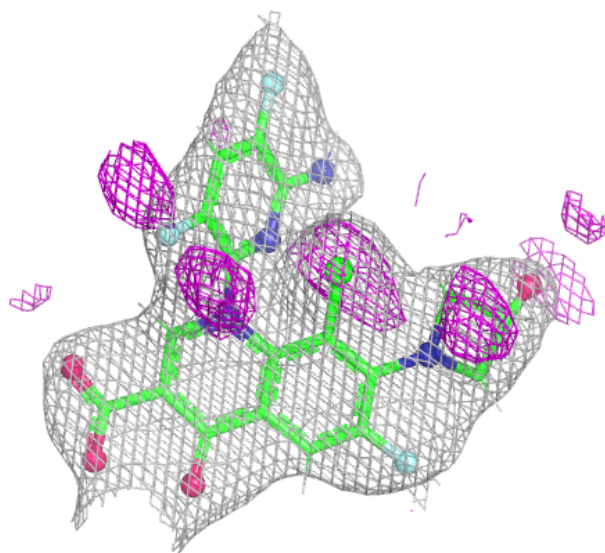
Electron density around TE9 F 101:

$2mF_o-DF_c$ (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.