WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2024 – 10:16 am BST

PDB ID : 8QMB

Title : Nucleant-assisted 2.0 A resolution structure of the Streptococcus pneumoniae topoisomerase IV-V18mer DNA complex with the novel fluoroquinolone Delafloxacin

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Deposited on : 2023-09-21

Resolution : 2.00 Å(reported)

The following versions of software and data (see references ①) 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	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1　Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
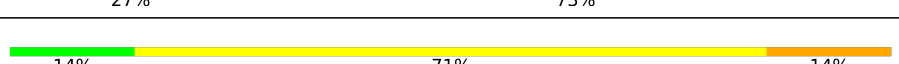
The reported resolution of this entry is 2.00 Å.

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.
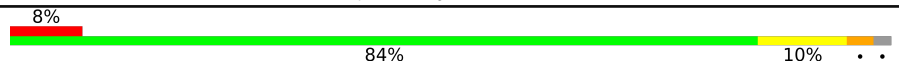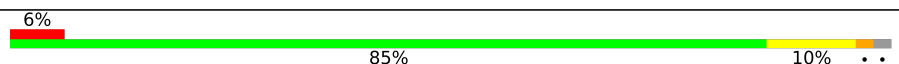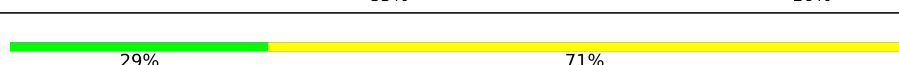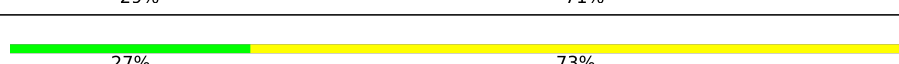
Metric	Percentile Ranks	Value
Rfree		0.206
Clashscore		3
Ramachandran outliers		0.8%
Sidechain outliers		5.2%
RSRZ outliers		6.7%

Worse　　　　　　　　　　　　　　　　*Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
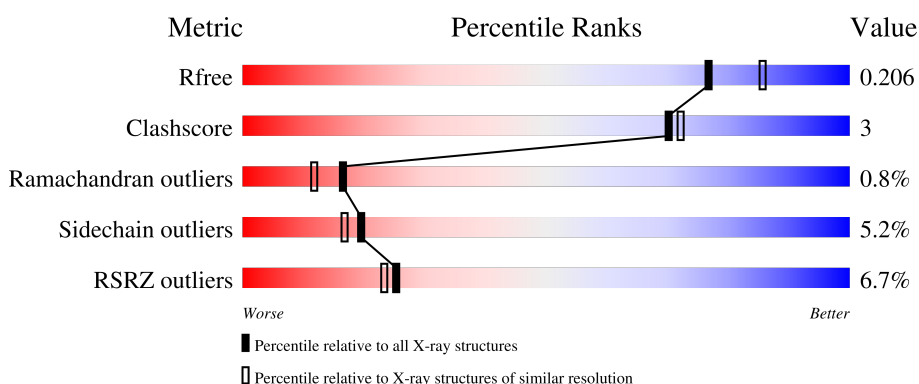
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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 <=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	8%　　84%　　10%　· ·
1	B	742	6%　　85%　　10%　· ·
2	E	7	29%　　71%
3	F	11	27%　　73%
4	G	7	14%　　71%　　14%

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Mol	Chain	Length	Quality of chain
5	H	11	55%　　　　　　　　　　　45%

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 225	C 70	H 81	N 26	O 42	P 6	10	0	0

- 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 349	C 107	H 125	N 40	O 66	P 11	10	0	0

- 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 221	C 69	H 80	N 27	O 39	P 6	7	0	0

- 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 348	C 107	H 125	N 40	O 65	P 11	10	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).
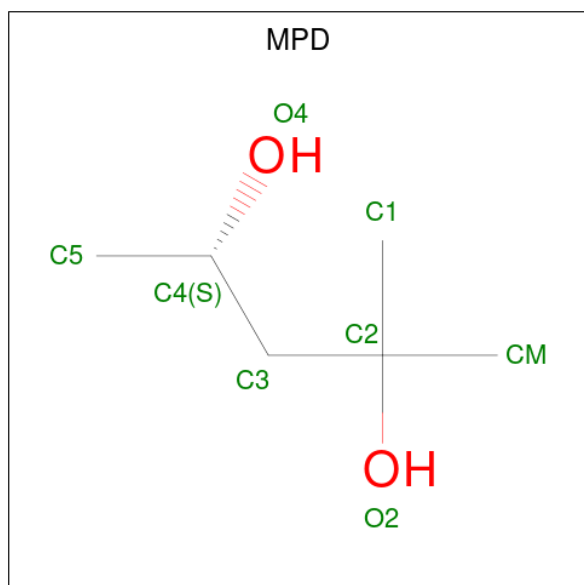
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 22	C 6	H 14	O 2	2	0
8	A	1	Total 22	C 6	H 14	O 2	2	0
8	B	1	Total 22	C 6	H 14	O 2	2	0

- Molecule 9 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).

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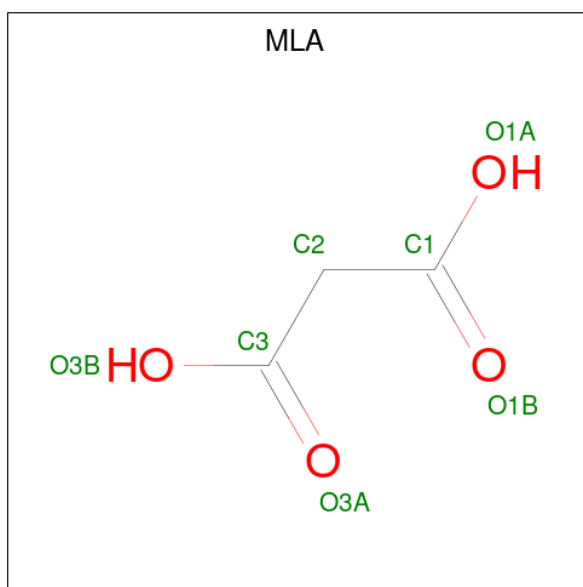
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			9	3	2	4		
9	A	1	Total	C	H	O	0	0
			9	3	2	4		

• Molecule 10 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

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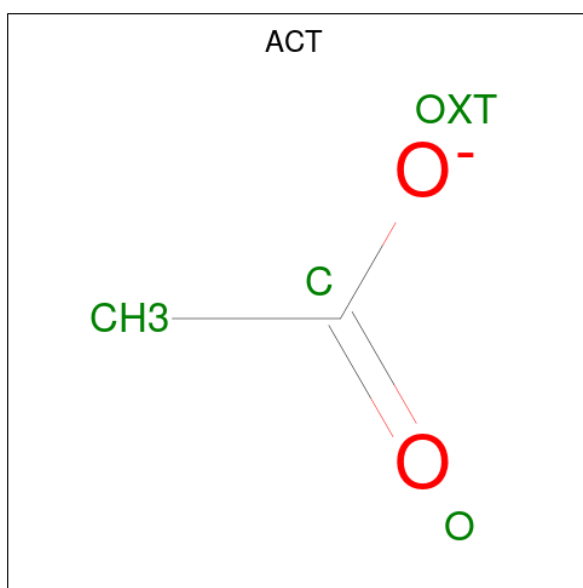
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	3	0
			7	2	3	2		
10	A	1	Total	C	H	O	3	0
			7	2	3	2		

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

- Molecule 11 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).
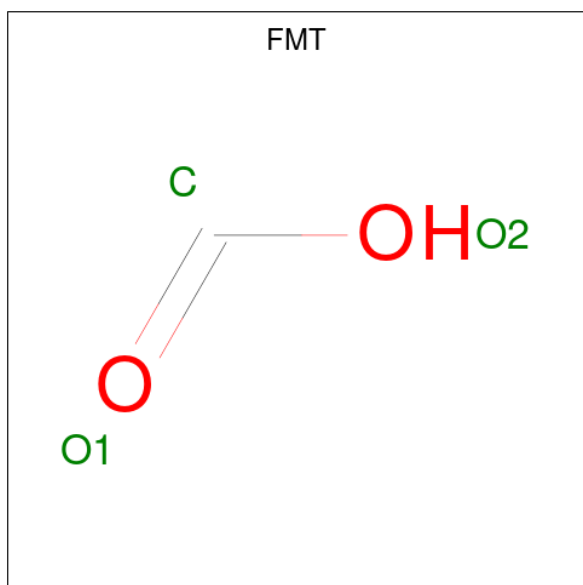
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total 5	C 1	H 2	O 2	1	0
11	A	1	Total 5	C 1	H 2	O 2	1	0
11	B	1	Total 5	C 1	H 2	O 2	1	0
11	B	1	Total 5	C 1	H 2	O 2	1	0

- Molecule 12 is delafloxacin (three-letter code: TE9) (formula: $C_{18}H_{12}ClF_3N_4O_4$) (labeled as "Ligand of Interest" by depositor).
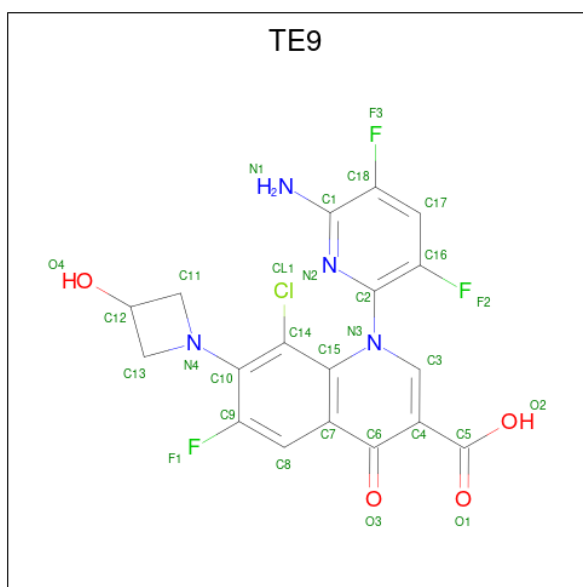
TE9

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 ⓘ

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.
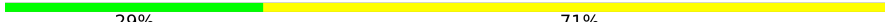
- Molecule 1: DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A
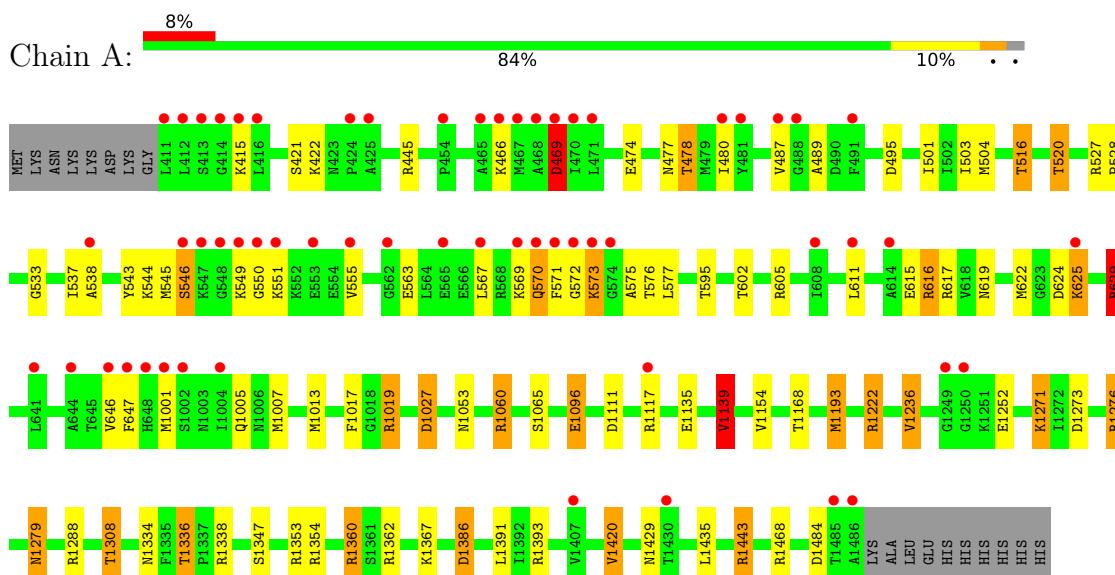
- Molecule 1: DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A
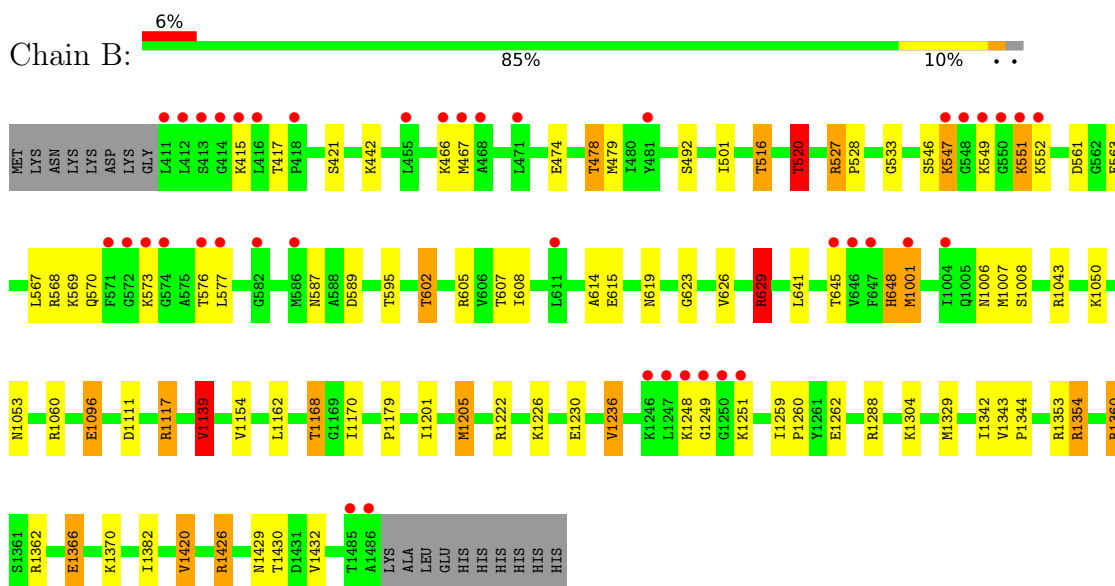
- Molecule 2: DNA (5'-D(TP*GP*TP*GP*GP*AP*T)-3')

Chain E:

29%　　　　　　　　　　　　　71%

T9 G10 T11 G12 G13 A14 T15

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

Chain F:

27%　　　　　　　　　　　　73%

G1 G2 T3 T4 A5 C8 A9 C10 A11
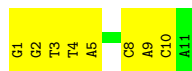
• Molecule 4: DNA (5'-D(GP*TP*AP*AP*TP*AP*C)-3')

Chain G:

14%　　　　　　　71%　　　　　　14%

G9 T10 A11 A12 T13 A14 C15
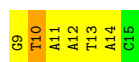
• Molecule 5: DNA (5'-D(P*AP*AP*CP*CP*GP*TP*AP*TP*TP*AP*C)-3')

Chain H:

55%　　　　　　　　　45%

A1 G5 T6 A7 T8 T9 A10 C11

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) 56.8 (83.63-2.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.169　,　0.206 0.169　,　0.206	Depositor DCC
R_{free} test set	10196 reflections (5.02%)	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 , 43.0	EDS
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.34$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: TE9, MG, CL, MPD, ACT, MLA, FMT

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	0.60	2/5884 (0.0%)	1.15	35/7932 (0.4%)
1	B	0.61	0/5876	1.14	30/7924 (0.4%)
2	E	1.37	0/161	1.99	8/248 (3.2%)
3	F	1.28	1/250 (0.4%)	2.34	20/383 (5.2%)
4	G	1.31	1/158 (0.6%)	2.29	10/242 (4.1%)
5	H	1.42	2/249 (0.8%)	2.19	12/381 (3.1%)
All	All	0.68	6/12578 (0.0%)	1.26	115/17110 (0.7%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1	DA	P-OP2	8.53	1.63	1.49
5	H	7	DA	C6-N1	5.85	1.39	1.35
1	A	1135	GLU	CD-OE1	5.65	1.31	1.25
4	G	13	DT	C5-C7	5.46	1.53	1.50
3	F	1	DG	P-OP1	5.18	1.57	1.49
1	A	1065	SER	CA-CB	-5.06	1.45	1.52

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1360	ARG	NE-CZ-NH1	16.78	128.69	120.30
1	B	629	ARG	NE-CZ-NH2	-15.27	112.66	120.30
1	A	629	ARG	NE-CZ-NH2	-13.70	113.45	120.30
1	A	1360	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	A	629	ARG	NE-CZ-NH1	11.50	126.05	120.30
3	F	8	DC	O5'-P-OP2	-10.68	96.09	105.70
4	G	13	DT	N3-C2-O2	-9.62	116.53	122.30
1	B	1360	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	B	1205	MET	CG-SD-CE	-9.41	85.15	100.20
1	B	1111	ASP	CB-CA-C	9.40	129.21	110.40
1	B	629	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	B	1001	MET	CG-SD-CE	9.27	115.04	100.20
1	B	1360	ARG	NE-CZ-NH2	-9.09	115.75	120.30
5	H	9	DT	N3-C4-O4	-8.85	114.59	119.90
5	H	7	DA	N1-C6-N6	8.71	123.82	118.60
1	B	1007	MET	CG-SD-CE	8.70	114.11	100.20
1	A	1111	ASP	CB-CA-C	8.57	127.54	110.40
3	F	4	DT	O4'-C4'-C3'	-8.27	101.04	106.00
5	H	7	DA	C5-C6-N6	-8.26	117.09	123.70
5	H	1	DA	O5'-P-OP2	7.98	120.27	110.70
4	G	14	DA	O5'-P-OP1	-7.84	98.65	105.70
3	F	3	DT	OP1-P-O3'	7.83	122.42	105.20
4	G	13	DT	N3-C4-O4	-7.75	115.25	119.90
3	F	1	DG	O5'-P-OP1	7.72	119.96	110.70
2	E	9	DT	OP2-P-O3'	7.68	122.10	105.20
4	G	10	DT	O5'-P-OP2	-7.48	98.97	105.70
3	F	3	DT	OP2-P-O3'	-7.47	88.77	105.20
1	B	1426	ARG	NE-CZ-NH2	-7.46	116.57	120.30
4	G	12	DA	O5'-P-OP1	7.39	119.57	110.70
3	F	3	DT	O5'-P-OP2	7.30	119.46	110.70
1	A	624	ASP	CB-CA-C	-7.28	95.85	110.40
1	B	1360	ARG	CD-NE-CZ	7.23	133.72	123.60
1	A	1193	MET	CG-SD-CE	-7.04	88.94	100.20
3	F	2	DG	O3'-P-O5'	-6.99	90.73	104.00
2	E	10	DG	O5'-P-OP2	-6.97	99.42	105.70
1	B	1096	GLU	N-CA-CB	-6.97	98.06	110.60
1	A	1362	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	A	629	ARG	CD-NE-CZ	6.90	133.26	123.60
3	F	10	DC	C1'-O4'-C4'	-6.89	103.21	110.10
3	F	8	DC	O4'-C4'-C3'	-6.84	101.76	104.50
2	E	11	DT	N3-C2-O2	-6.68	118.29	122.30
3	F	1	DG	O3'-P-O5'	-6.63	91.40	104.00
1	B	1353	ARG	NE-CZ-NH2	-6.57	117.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	5	DG	C4'-C3'-C2'	-6.52	97.23	103.10
3	F	1	DG	OP1-P-O3'	6.51	119.52	105.20
5	H	9	DT	O5'-P-OP2	-6.44	99.90	105.70
1	A	1096	GLU	N-CA-CB	-6.43	99.03	110.60
1	B	1117	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	629	ARG	CD-NE-CZ	6.35	132.49	123.60
5	H	10	DA	O3'-P-O5'	-6.24	92.15	104.00
1	B	1353	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	B	1354	ARG	NE-CZ-NH2	-6.21	117.20	120.30
5	H	9	DT	N3-C2-O2	-6.16	118.60	122.30
3	F	9	DA	N1-C6-N6	6.15	122.29	118.60
1	A	1236	VAL	N-CA-CB	-6.13	98.02	111.50
1	A	1060	ARG	CB-CA-C	6.12	122.65	110.40
5	H	9	DT	C5-C4-O4	6.10	129.17	124.90
1	A	1007	MET	CG-SD-CE	6.08	109.92	100.20
1	A	1443[A]	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	1443[B]	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	B	1236	VAL	N-CA-CB	-6.04	98.20	111.50
2	E	10	DG	OP2-P-O3'	6.04	118.48	105.20
1	A	1420	VAL	N-CA-CB	-6.00	98.30	111.50
1	A	1271	LYS	CB-CG-CD	5.95	127.06	111.60
3	F	5	DA	O4'-C4'-C3'	-5.85	102.16	104.50
1	A	1468	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	1043	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	616	ARG	CG-CD-NE	5.72	123.81	111.80
3	F	3	DT	P-O3'-C3'	5.71	126.55	119.70
4	G	10	DT	N3-C2-O2	-5.70	118.88	122.30
1	B	1420	VAL	N-CA-CB	-5.68	98.99	111.50
3	F	9	DA	O4'-C1'-N9	-5.68	104.03	108.00
1	B	1060	ARG	CB-CA-C	5.66	121.72	110.40
1	A	1027	ASP	CB-CG-OD1	-5.65	113.21	118.30
3	F	9	DA	C5-C6-N6	-5.63	119.19	123.70
3	F	5	DA	N1-C2-N3	-5.61	126.49	129.30
1	B	1117	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	1354	ARG	NE-CZ-NH1	5.58	123.09	120.30
3	F	9	DA	O5'-P-OP2	-5.58	100.68	105.70
4	G	9	DG	P-O3'-C3'	5.56	126.37	119.70
1	A	1360	ARG	CD-NE-CZ	5.54	131.35	123.60
1	A	625	LYS	N-CA-CB	5.52	120.54	110.60
1	A	469	ASP	N-CA-CB	5.50	120.51	110.60
1	A	1271	LYS	CD-CE-NZ	5.48	124.30	111.70
2	E	13	DG	C5-N7-C8	-5.47	101.57	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	9	DG	O4'-C1'-C2'	-5.39	101.58	105.90
2	E	11	DT	N3-C4-O4	-5.39	116.67	119.90
1	B	1050	LYS	CD-CE-NZ	5.38	124.08	111.70
1	A	1139	VAL	N-CA-CB	-5.36	99.70	111.50
1	A	1353	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	1468	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	1117	ARG	NH1-CZ-NH2	5.34	125.27	119.40
1	B	1139	VAL	N-CA-CB	-5.31	99.82	111.50
5	H	9	DT	O4'-C1'-N1	-5.29	104.29	108.00
1	B	1288	ARG	NE-CZ-NH1	5.29	122.94	120.30
3	F	4	DT	OP2-P-O3'	5.27	116.79	105.20
1	A	1367	LYS	N-CA-CB	5.23	120.02	110.60
4	G	9	DG	OP2-P-O3'	5.21	116.66	105.20
2	E	15	DT	O5'-P-OP1	5.21	116.95	110.70
1	A	1338	ARG	NE-CZ-NH1	5.20	122.90	120.30
3	F	4	DT	O4'-C1'-N1	5.19	111.63	108.00
1	A	1288	ARG	NE-CZ-NH1	5.17	122.88	120.30
5	H	1	DA	O4'-C1'-C2'	-5.15	101.78	105.90
1	A	625	LYS	CA-CB-CG	5.12	124.66	113.40
1	A	1019[A]	ARG	CG-CD-NE	5.09	122.50	111.80
1	A	1019[B]	ARG	CG-CD-NE	5.09	122.50	111.80
5	H	9	DT	C4-C5-C7	5.07	122.04	119.00
1	B	520	THR	N-CA-CB	5.07	119.93	110.30
1	B	568	ARG	CB-CA-C	-5.06	100.29	110.40
4	G	9	DG	N9-C1'-C2'	5.05	122.20	112.60
1	B	1262	GLU	CG-CD-OE1	-5.04	108.21	118.30
1	B	479	MET	CG-SD-CE	-5.04	92.14	100.20
1	B	1230	GLU	CG-CD-OE2	-5.03	108.24	118.30
1	A	445	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	E	13	DG	C4-C5-N7	5.00	112.80	110.80

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1117	ARG	Sidechain
1	A	1276	ARG	Sidechain
1	A	1360	ARG	Sidechain
1	A	537	ILE	Peptide
1	A	545	MET	Peptide
1	A	549	LYS	Peptide
1	A	550	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	551	LYS	Peptide
1	A	572	GLY	Peptide
1	A	616	ARG	Sidechain
1	A	617	ARG	Sidechain
1	A	629	ARG	Sidechain
1	B	1117	ARG	Sidechain
1	B	1354	ARG	Sidechain
1	B	1360	ARG	Sidechain
1	B	1426	ARG	Sidechain
1	B	467	MET	Peptide
1	B	527	ARG	Sidechain
1	B	547	LYS	Peptide
1	B	549	LYS	Peptide
1	B	551	LYS	Peptide
1	B	629	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	5780	5885	5869	37	0
1	B	5770	5867	5848	35	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	H	30	11	0	3	0
13	A	489	0	0	5	0
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	80	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.

All (80) 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:B:1205:MET:HE1	1:B:1226:LYS:HA	1.56	0.87
1:A:569:LYS:O	13:A:1601:HOH:O	1.95	0.82
1:A:546:SER:HA	1:A:575:ALA:HB1	1.66	0.77
1:B:614:ALA:HB2	10:B:1506:ACT:CH3	2.18	0.74
12:F:101:TE9:CL1	12:F:101:TE9:C2	2.73	0.73
1:B:1008:SER:HB2	10:B:1506:ACT:OXT	1.89	0.72
1:B:474:GLU:O	1:B:478:THR:HG23	1.90	0.72
12:H:101:TE9:C2	12:H:101:TE9:CL1	2.74	0.72
1:A:1222:ARG:NH1	1:A:1484:ASP:OD1	2.25	0.69
1:B:608:ILE:HG23	10:B:1506:ACT:H3	1.72	0.69
1:B:614:ALA:HB2	10:B:1506:ACT:H2	1.74	0.69
7:B:1504:CL:CL	13:B:1966:HOH:O	2.47	0.68
1:B:623:GLY:O	1:B:629:ARG:NH2	2.23	0.67
1:A:474:GLU:O	1:A:478:THR:HG23	1.95	0.67
1:B:1382:ILE:HD11	8:B:1508:MPD:HM3	1.76	0.67
1:B:608:ILE:HA	10:B:1506:ACT:H1	1.78	0.65
12:F:101:TE9:CL1	12:F:101:TE9:C13	2.83	0.64
1:B:1362:ARG:HD3	13:B:1965:HOH:O	1.98	0.62
12:H:101:TE9:CL1	12:H:101:TE9:C13	2.86	0.61
12:H:101:TE9:CL1	12:H:101:TE9:N2	2.73	0.58
12:F:101:TE9:CL1	12:F:101:TE9:N2	2.74	0.58
1:A:1193:MET:CE	1:A:1347:SER:HB3	2.35	0.57
1:B:1170:ILE:HD11	4:G:11:DA:C2	2.41	0.56
1:A:1386:ASP:N	1:A:1386:ASP:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:MET:HE1	1:A:1347:SER:HB3	1.89	0.54
1:A:1334:ASN:O	1:A:1336:THR:HG23	2.08	0.54
1:A:1252:GLU:OE1	1:A:1308:THR:HG21	2.08	0.53
1:A:1001:MET:HG2	1:A:1005:GLN:HE21	1.73	0.53
1:A:520:THR:HG21	1:A:622[B]:MET:HG3	1.90	0.53
1:B:626:VAL:HG23	13:B:1647:HOH:O	2.10	0.51
1:B:1429:ASN:O	8:B:1508:MPD:HM1	2.11	0.51
1:B:1201:ILE:CG2	1:B:1205:MET:HE2	2.41	0.50
1:A:570:GLN:O	1:A:570:GLN:NE2	2.44	0.50
1:A:622[A]:MET:HE1	1:A:1017:PHE:CD1	2.46	0.49
1:A:1435:LEU:HD23	13:A:1658:HOH:O	2.13	0.49
1:A:1429:ASN:O	8:A:1505:MPD:HM1	2.13	0.48
1:A:503:ILE:O	1:A:538:ALA:HB2	2.14	0.47
1:A:1139:VAL:HG22	1:A:1154:VAL:HG13	1.96	0.47
1:B:1179:PRO:HD2	1:B:1329:MET:HE2	1.96	0.47
1:A:1391:LEU:C	1:A:1391:LEU:HD23	2.34	0.47
1:A:477:ASN:O	1:A:480:ILE:HG12	2.15	0.46
1:A:520:THR:HG22	1:A:1013:MET:CE	2.46	0.46
1:A:527:ARG:N	1:A:528:PRO:CD	2.80	0.45
1:A:1308:THR:HG23	13:A:1834:HOH:O	2.17	0.45
1:B:602:THR:HG21	1:B:648:HIS:NE2	2.32	0.45
1:B:615:GLU:O	1:B:619:ASN:ND2	2.50	0.44
1:A:1393:ARG:HD3	13:A:1845:HOH:O	2.17	0.44
1:B:1249:GLY:O	1:B:1304:LYS:HE2	2.17	0.44
1:B:527:ARG:N	1:B:528:PRO:CD	2.81	0.44
1:A:504:MET:HA	1:A:538:ALA:HB2	1.98	0.44
1:A:520:THR:HG21	1:A:622[A]:MET:HG3	1.99	0.44
1:B:1139:VAL:HG22	1:B:1154:VAL:HG13	2.00	0.44
11:A:1510:FMT:C	1:B:587:ASN:ND2	2.82	0.43
1:B:516:THR:O	1:B:520:THR:HG23	2.19	0.43
1:B:1168:THR:CG2	13:B:1847:HOH:O	2.67	0.43
1:B:417:THR:HG21	1:B:442:LYS:HG3	2.00	0.42
1:A:646:VAL:HG22	1:A:647:PHE:O	2.19	0.42
1:B:1259:ILE:HB	1:B:1260:PRO:CD	2.50	0.42
1:B:607:THR:CG2	1:B:1006:ASN:HD22	2.32	0.42
1:A:1273:ASP:OD1	1:A:1276:ARG:NH1	2.48	0.42
1:B:563:GLU:O	1:B:567:LEU:HD13	2.19	0.42
1:A:533:GLY:HA3	1:A:605:ARG:HD3	2.02	0.42
1:A:563:GLU:O	1:A:567:LEU:HD13	2.19	0.42
1:B:641:LEU:HD22	13:B:1622:HOH:O	2.20	0.42
1:A:543:TYR:HB3	1:A:577:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:THR:HG22	1:A:1013:MET:HE1	2.03	0.41
1:A:615:GLU:O	1:A:619:ASN:ND2	2.53	0.41
1:B:533:GLY:HA3	1:B:605:ARG:HD3	2.03	0.41
1:B:607:THR:HG21	1:B:1006:ASN:HD22	1.85	0.41
1:B:1168:THR:HG23	13:B:1847:HOH:O	2.21	0.41
1:B:1343:VAL:HB	1:B:1344:PRO:HD3	2.03	0.41
1:B:1366:GLU:OE1	1:B:1370:LYS:HE2	2.21	0.41
1:A:516:THR:O	1:A:520:THR:HG23	2.21	0.41
1:B:1201:ILE:HG22	1:B:1205:MET:CE	2.51	0.41
4:G:10:DT:H2"	4:G:11:DA:C8	2.55	0.41
1:A:611:LEU:HD23	1:A:611:LEU:O	2.21	0.40
1:A:1279:ASN:ND2	13:A:1633:HOH:O	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/742 (98%)	686 (94%)	35 (5%)	5 (1%)	19	14
1	B	725/742 (98%)	693 (96%)	25 (3%)	7 (1%)	13	8
All	All	1451/1484 (98%)	1379 (95%)	60 (4%)	12 (1%)	16	12

All (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
1	B	573	LYS

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Mol	Chain	Res	Type
1	B	648	HIS
1	B	1251	LYS
1	B	569	LYS
1	A	573	LYS
1	B	570	GLN
1	A	571	PHE

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%)	587 (94%)	35 (6%)	17	15
1	B	622/635 (98%)	592 (95%)	30 (5%)	21	19
All	All	1244/1270 (98%)	1179 (95%)	65 (5%)	19	17

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	415	LYS
1	A	421	SER
1	A	422	LYS
1	A	466	LYS
1	A	469	ASP
1	A	478	THR
1	A	487	VAL
1	A	495	ASP
1	A	501	ILE
1	A	516	THR
1	A	520	THR
1	A	544	LYS
1	A	555	VAL
1	A	570	GLN
1	A	573	LYS
1	A	576	THR
1	A	595	THR

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Mol	Chain	Res	Type
1	A	602	THR
1	A	625	LYS
1	A	1019[A]	ARG
1	A	1019[B]	ARG
1	A	1027	ASP
1	A	1053	ASN
1	A	1060	ARG
1	A	1096	GLU
1	A	1139	VAL
1	A	1168	THR
1	A	1222	ARG
1	A	1236	VAL
1	A	1271	LYS
1	A	1279	ASN
1	A	1308	THR
1	A	1336	THR
1	A	1386	ASP
1	A	1420	VAL
1	B	415	LYS
1	B	421	SER
1	B	478	THR
1	B	492	SER
1	B	501	ILE
1	B	516	THR
1	B	520	THR
1	B	546	SER
1	B	547	LYS
1	B	552	LYS
1	B	561	ASP
1	B	576	THR
1	B	577	LEU
1	B	589	ASP
1	B	595	THR
1	B	602	THR
1	B	645	THR
1	B	1001	MET
1	B	1053	ASN
1	B	1096	GLU
1	B	1139	VAL
1	B	1162	LEU
1	B	1168	THR
1	B	1222	ARG

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Mol	Chain	Res	Type
1	B	1236	VAL
1	B	1248	LYS
1	B	1342	ILE
1	B	1366	GLU
1	B	1420	VAL
1	B	1432	VAL

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

Mol	Chain	Res	Type
1	A	619	ASN
1	A	1005	GLN
1	B	587	ASN
1	B	619	ASN
1	B	1090	GLN
1	B	1461	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 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
10	ACT	A	1511	-	3,3,3	1.19	0	3,3,3	0.95	0
11	FMT	B	1509	-	2,2,2	2.02	1 (50%)	1,1,1	0.28	0
12	TE9	H	101	6	31,33,33	2.53	13 (41%)	37,51,51	3.25	17 (45%)
10	ACT	B	1506	-	3,3,3	1.00	0	3,3,3	0.72	0
9	MLA	A	1509	-	6,6,6	1.63	2 (33%)	7,7,7	0.80	0
8	MPD	A	1506	-	7,7,7	0.46	0	9,10,10	0.92	0
12	TE9	F	101	6	31,33,33	2.17	11 (35%)	37,51,51	3.15	18 (48%)
10	ACT	A	1508	-	3,3,3	1.63	0	3,3,3	0.47	0
9	MLA	A	1507	-	6,6,6	1.38	1 (16%)	7,7,7	1.51	1 (14%)
11	FMT	B	1507	-	2,2,2	1.42	1 (50%)	1,1,1	0.13	0
11	FMT	A	1512	-	2,2,2	1.19	0	1,1,1	0.05	0
11	FMT	A	1510	-	2,2,2	1.77	1 (50%)	1,1,1	0.06	0
10	ACT	B	1505	-	3,3,3	1.25	0	3,3,3	1.00	0
8	MPD	A	1505	-	7,7,7	0.37	0	9,10,10	0.70	0
8	MPD	B	1508	-	7,7,7	0.56	0	9,10,10	1.07	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
12	TE9	H	101	6	-	3/11/20/20	0/4/4/4
9	MLA	A	1509	-	-	2/4/4/4	-
8	MPD	A	1506	-	-	2/5/5/5	-
12	TE9	F	101	6	-	3/11/20/20	0/4/4/4
9	MLA	A	1507	-	-	2/4/4/4	-
8	MPD	A	1505	-	-	3/5/5/5	-
8	MPD	B	1508	-	-	0/5/5/5	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	101	TE9	C2-N2	6.56	1.42	1.34
12	F	101	TE9	C2-N2	5.90	1.41	1.34
12	H	101	TE9	C1-C18	5.69	1.45	1.40
12	F	101	TE9	C2-C16	-5.08	1.36	1.42
12	H	101	TE9	C11-N4	4.63	1.52	1.47
12	F	101	TE9	C13-N4	4.39	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	101	TE9	C13-N4	4.35	1.51	1.47
12	H	101	TE9	C2-C16	-4.21	1.37	1.42
12	F	101	TE9	O1-C5	3.54	1.32	1.22
12	H	101	TE9	C17-C16	3.41	1.43	1.37
12	H	101	TE9	O3-C6	3.20	1.30	1.23
11	B	1509	FMT	O2-C	2.82	1.42	1.28
12	H	101	TE9	C14-CL1	2.82	1.78	1.72
12	F	101	TE9	C17-C16	2.72	1.42	1.37
12	H	101	TE9	C1-N2	2.54	1.38	1.35
9	A	1507	MLA	O3B-C3	-2.54	1.22	1.30
11	A	1510	FMT	O2-C	2.50	1.41	1.28
12	H	101	TE9	F3-C18	2.48	1.41	1.35
12	F	101	TE9	C14-CL1	2.42	1.78	1.72
12	H	101	TE9	C3-N3	2.39	1.42	1.37
9	A	1509	MLA	O1B-C1	2.26	1.29	1.22
9	A	1509	MLA	O3B-C3	-2.19	1.23	1.30
12	F	101	TE9	F3-C18	2.17	1.41	1.35
12	H	101	TE9	C7-C15	2.14	1.43	1.40
12	H	101	TE9	C10-N4	2.13	1.46	1.40
12	F	101	TE9	C3-C4	2.05	1.43	1.38
12	F	101	TE9	O3-C6	2.04	1.27	1.23
12	F	101	TE9	C8-C9	2.03	1.41	1.37
12	F	101	TE9	C3-N3	2.02	1.41	1.37
11	B	1507	FMT	O2-C	2.01	1.38	1.28

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	101	TE9	C17-C18-C1	-10.06	115.14	121.70
12	F	101	TE9	C17-C18-C1	-9.62	115.43	121.70
12	H	101	TE9	F2-C16-C2	-8.89	111.39	119.92
12	F	101	TE9	C18-C1-N1	-8.49	114.51	121.47
12	H	101	TE9	C3-C4-C6	6.65	124.83	119.88
12	H	101	TE9	C4-C3-N3	-5.27	117.24	123.75
12	F	101	TE9	N1-C1-N2	4.77	123.77	117.03
12	H	101	TE9	O1-C5-C4	-4.71	112.11	122.46
12	F	101	TE9	F3-C18-C17	4.21	126.99	118.61
12	F	101	TE9	C16-C2-N2	-4.16	113.11	118.19
12	H	101	TE9	C18-C1-N1	-4.05	118.15	121.47
12	F	101	TE9	F2-C16-C2	-4.01	116.06	119.92
12	H	101	TE9	F2-C16-C17	3.78	126.12	118.61
12	F	101	TE9	O1-C5-C4	-3.72	114.30	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1507	MLA	C3-C2-C1	-3.32	101.23	112.87
12	F	101	TE9	C14-C15-N3	-3.32	118.53	123.42
12	H	101	TE9	F3-C18-C17	3.23	125.04	118.61
12	F	101	TE9	C4-C3-N3	-3.20	119.80	123.75
12	F	101	TE9	O3-C6-C4	-3.18	117.89	123.22
12	F	101	TE9	O2-C5-O1	3.14	130.80	123.61
12	F	101	TE9	O3-C6-C7	3.08	126.54	121.56
12	H	101	TE9	C18-C17-C16	2.94	122.31	117.10
12	F	101	TE9	C18-C17-C16	2.94	122.30	117.10
12	H	101	TE9	O3-C6-C7	2.82	126.12	121.56
12	H	101	TE9	N1-C1-N2	2.68	120.83	117.03
12	F	101	TE9	F1-C9-C8	2.66	123.91	118.61
12	F	101	TE9	C3-C4-C6	2.56	121.78	119.88
12	H	101	TE9	O3-C6-C4	-2.53	118.97	123.22
12	H	101	TE9	C16-C2-N2	-2.49	115.15	118.19
12	F	101	TE9	C1-N2-C2	2.42	123.16	116.99
12	H	101	TE9	O2-C5-O1	2.34	128.96	123.61
12	F	101	TE9	C7-C15-N3	2.34	120.75	118.40
12	H	101	TE9	C1-N2-C2	2.28	122.79	116.99
12	H	101	TE9	F1-C9-C10	-2.07	115.36	118.36
12	F	101	TE9	C17-C16-C2	2.07	123.06	121.73
12	H	101	TE9	C15-N3-C3	2.04	122.41	119.09

There are no chirality outliers.
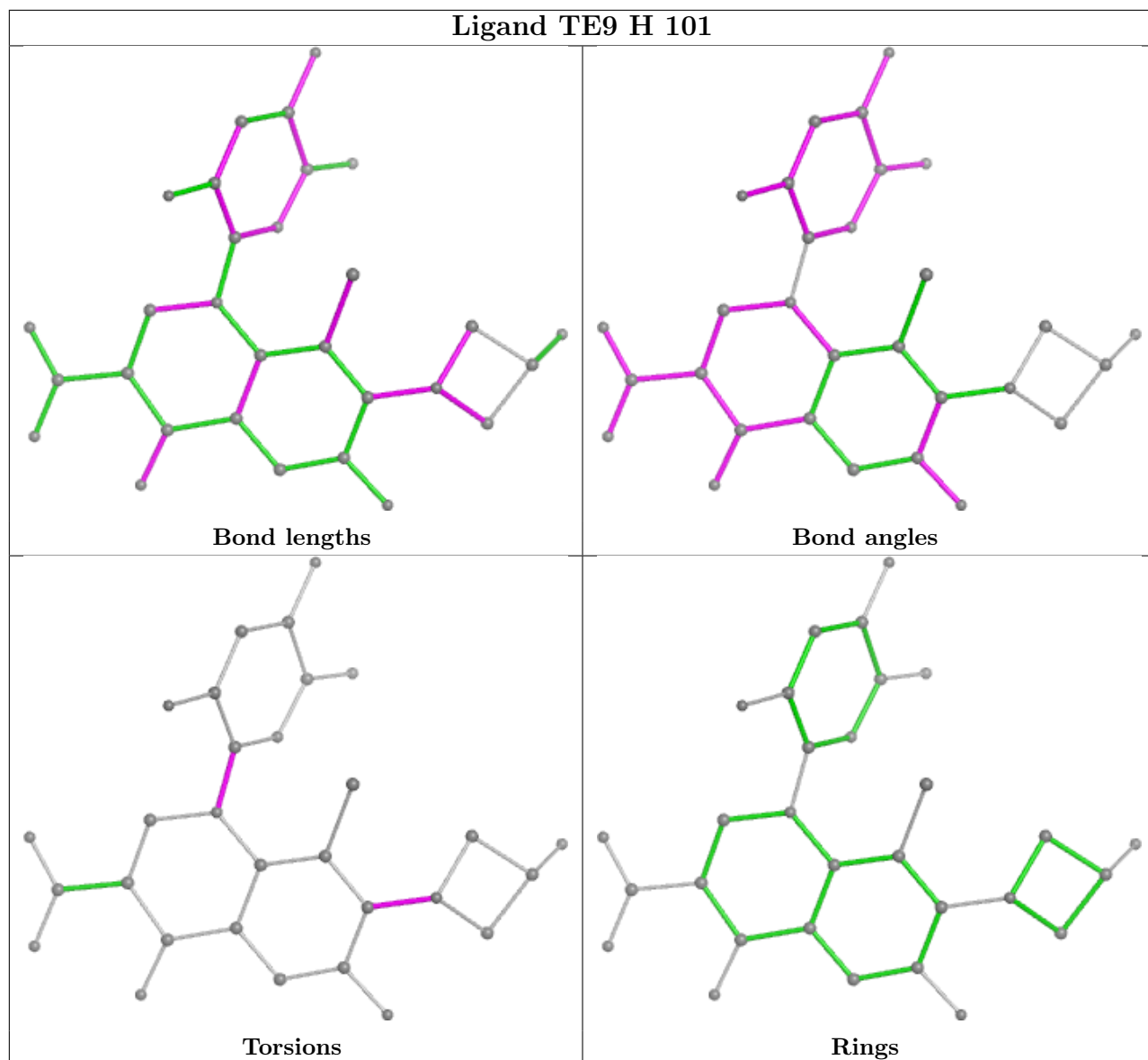
All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	101	TE9	C16-C2-N3-C15
12	F	101	TE9	N2-C2-N3-C3
12	H	101	TE9	C16-C2-N3-C15
12	H	101	TE9	N2-C2-N3-C3
9	A	1509	MLA	O1A-C1-C2-C3
9	A	1509	MLA	O1B-C1-C2-C3
9	A	1507	MLA	O1B-C1-C2-C3
12	F	101	TE9	C6-C4-C5-O1
9	A	1507	MLA	O1A-C1-C2-C3
8	A	1505	MPD	O2-C2-C3-C4
8	A	1506	MPD	O2-C2-C3-C4
12	H	101	TE9	C14-C10-N4-C11
8	A	1505	MPD	C2-C3-C4-C5
8	A	1506	MPD	C2-C3-C4-C5
8	A	1505	MPD	C2-C3-C4-O4

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	101	TE9	3	0
10	B	1506	ACT	5	0
12	F	101	TE9	3	0
9	A	1507	MLA	1	0
11	A	1510	FMT	1	0
8	A	1505	MPD	1	0
8	B	1508	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 then 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.

Full wwPDB X-ray Structure Validation Report

Ligand TE9 H 101

Ligand TE9 F 101

Bond lengths

Bond angles

Torsions

Rings
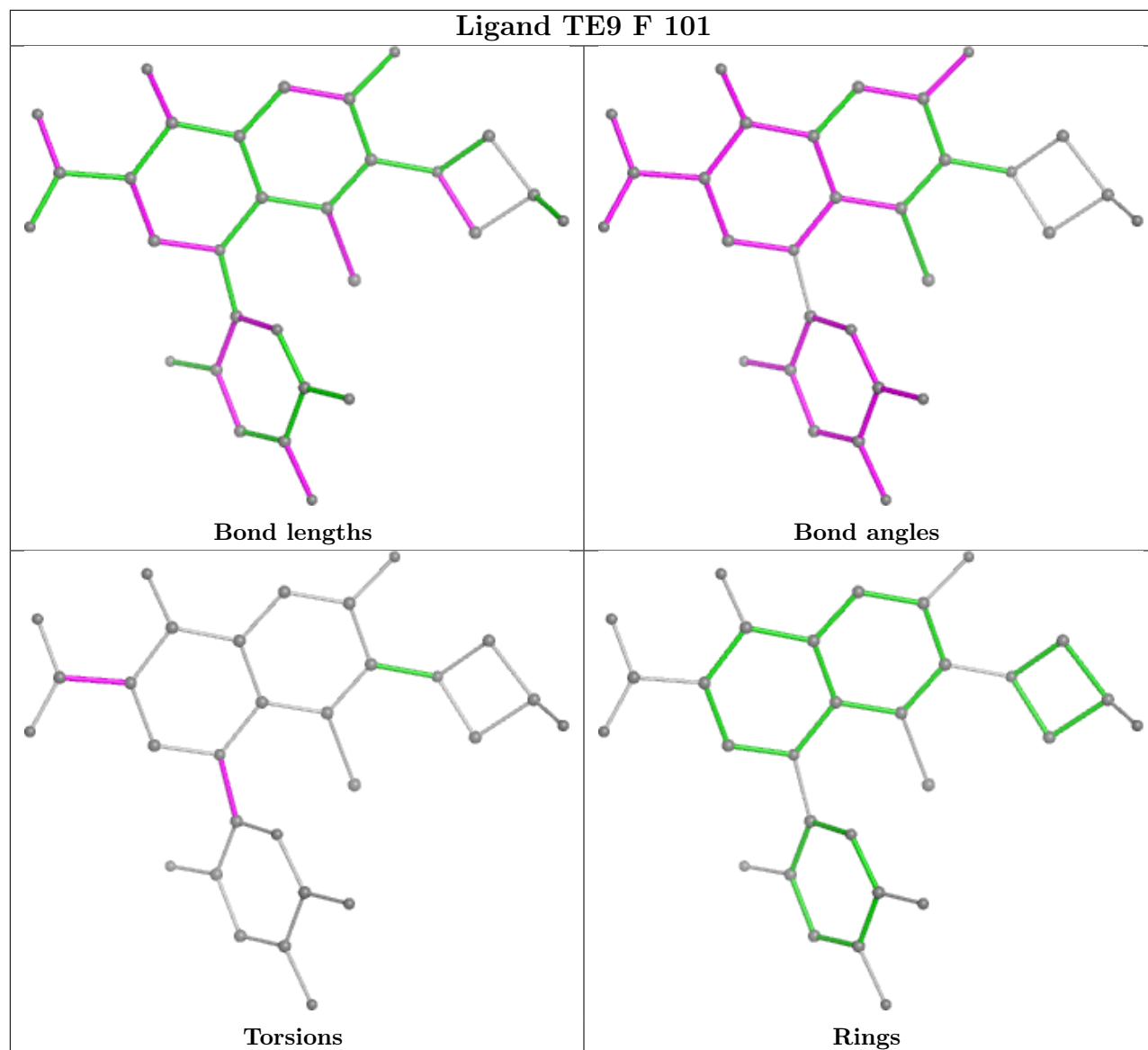
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	724/742 (97%)	0.18	58 (8%)	20	18	15, 41, 94, 157	3 (0%)
1	B	724/742 (97%)	0.08	41 (5%)	30	28	15, 39, 92, 140	2 (0%)
2	E	7/7 (100%)	-0.70	0	100	100	27, 30, 62, 79	0
3	F	11/11 (100%)	-0.72	0	100	100	34, 41, 56, 70	0
4	G	7/7 (100%)	-0.75	0	100	100	26, 31, 61, 84	0
5	H	11/11 (100%)	-0.64	0	100	100	34, 44, 59, 75	0
All	All	1484/1520 (97%)	0.11	99 (6%)	25	23	15, 40, 94, 157	5 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	647	PHE	7.2
1	A	411	LEU	6.5
1	A	1486	ALA	6.3
1	A	415	LYS	6.3
1	A	412	LEU	6.0
1	B	412	LEU	6.0
1	A	571	PHE	5.8
1	A	646	VAL	5.7
1	B	571	PHE	5.5
1	B	411	LEU	5.3
1	A	467	MET	5.2
1	B	414	GLY	5.1
1	A	414	GLY	4.8
1	B	1486	ALA	4.8
1	B	1248	LYS	4.3
1	A	471	LEU	4.1
1	A	555	VAL	4.1
1	B	645	THR	4.1
1	B	471	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	647	PHE	3.9
1	A	466	LYS	3.8
1	A	1001	MET	3.8
1	B	549	LYS	3.7
1	A	574	GLY	3.6
1	A	546	SER	3.6
1	A	550	GLY	3.5
1	B	548	GLY	3.4
1	A	1485	THR	3.4
1	A	547	LYS	3.4
1	B	550	GLY	3.4
1	B	611	LEU	3.3
1	B	415	LYS	3.3
1	A	413	SER	3.3
1	B	467	MET	3.3
1	A	538	ALA	3.2
1	A	424	PRO	3.2
1	B	1250	GLY	3.2
1	A	567	LEU	3.0
1	B	468	ALA	3.0
1	B	646	VAL	3.0
1	B	455	LEU	3.0
1	B	551	LYS	2.9
1	A	572	GLY	2.9
1	B	466	LYS	2.9
1	A	468	ALA	2.9
1	A	1430	THR	2.9
1	B	1249	GLY	2.9
1	A	487	VAL	2.9
1	A	614	ALA	2.8
1	A	1117	ARG	2.8
1	B	547	LYS	2.7
1	B	1004	ILE	2.7
1	A	562	GLY	2.7
1	A	480	ILE	2.7
1	A	454	PRO	2.7
1	B	413	SER	2.7
1	A	1004	ILE	2.7
1	A	551	LYS	2.6
1	A	491	PHE	2.6
1	B	576	THR	2.6
1	A	565	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	469	ASP	2.5
1	A	549	LYS	2.5
1	A	569	LYS	2.5
1	A	488	GLY	2.5
1	B	574	GLY	2.5
1	A	573	LYS	2.5
1	B	572	GLY	2.4
1	B	573	LYS	2.4
1	B	1251	LYS	2.4
1	A	481	TYR	2.4
1	A	1407	VAL	2.4
1	B	1001	MET	2.4
1	A	611	LEU	2.3
1	A	608	ILE	2.3
1	B	1247	LEU	2.3
1	A	641	LEU	2.3
1	B	577	LEU	2.3
1	A	625	LYS	2.2
1	A	570	GLN	2.2
1	A	644	ALA	2.2
1	A	1250	GLY	2.2
1	A	416	LEU	2.2
1	A	425	ALA	2.2
1	A	1002	SER	2.2
1	B	1246	LYS	2.1
1	A	648	HIS	2.1
1	A	1249	GLY	2.1
1	B	416	LEU	2.1
1	A	465	ALA	2.1
1	B	481	TYR	2.1
1	B	586	MET	2.1
1	B	582	GLY	2.1
1	A	553	GLU	2.1
1	A	548	GLY	2.0
1	B	1485	THR	2.0
1	A	470	ILE	2.0
1	B	418	PRO	2.0
1	B	552	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

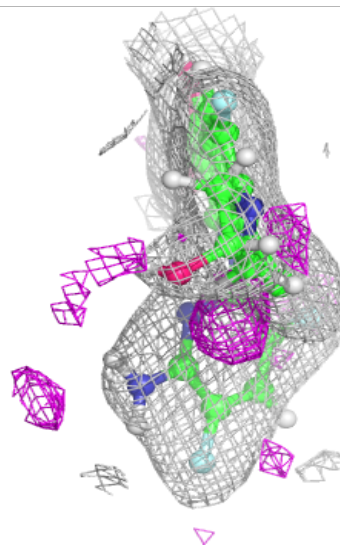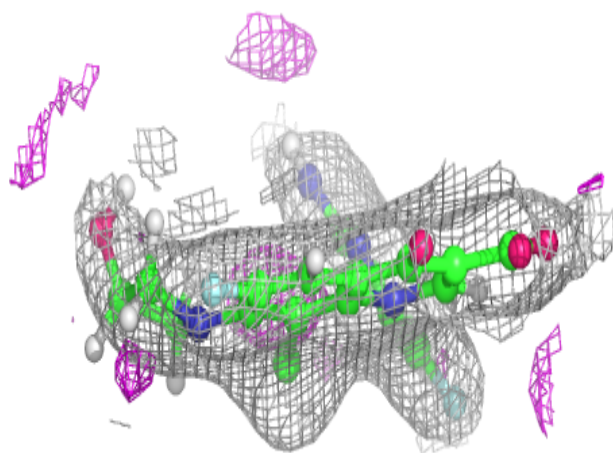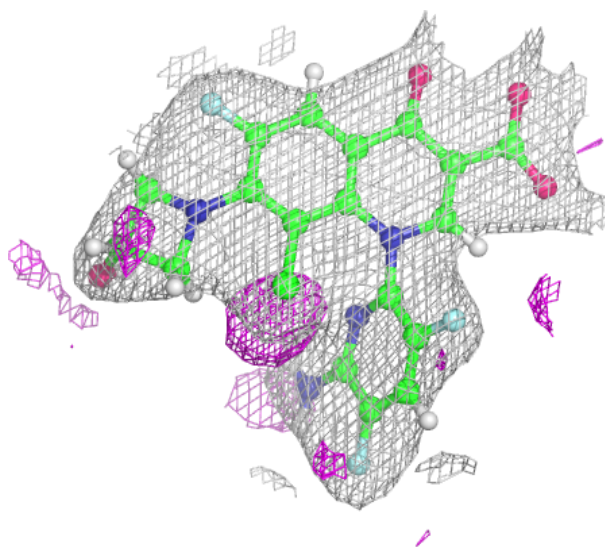There are no monosaccharides in this entry.

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.
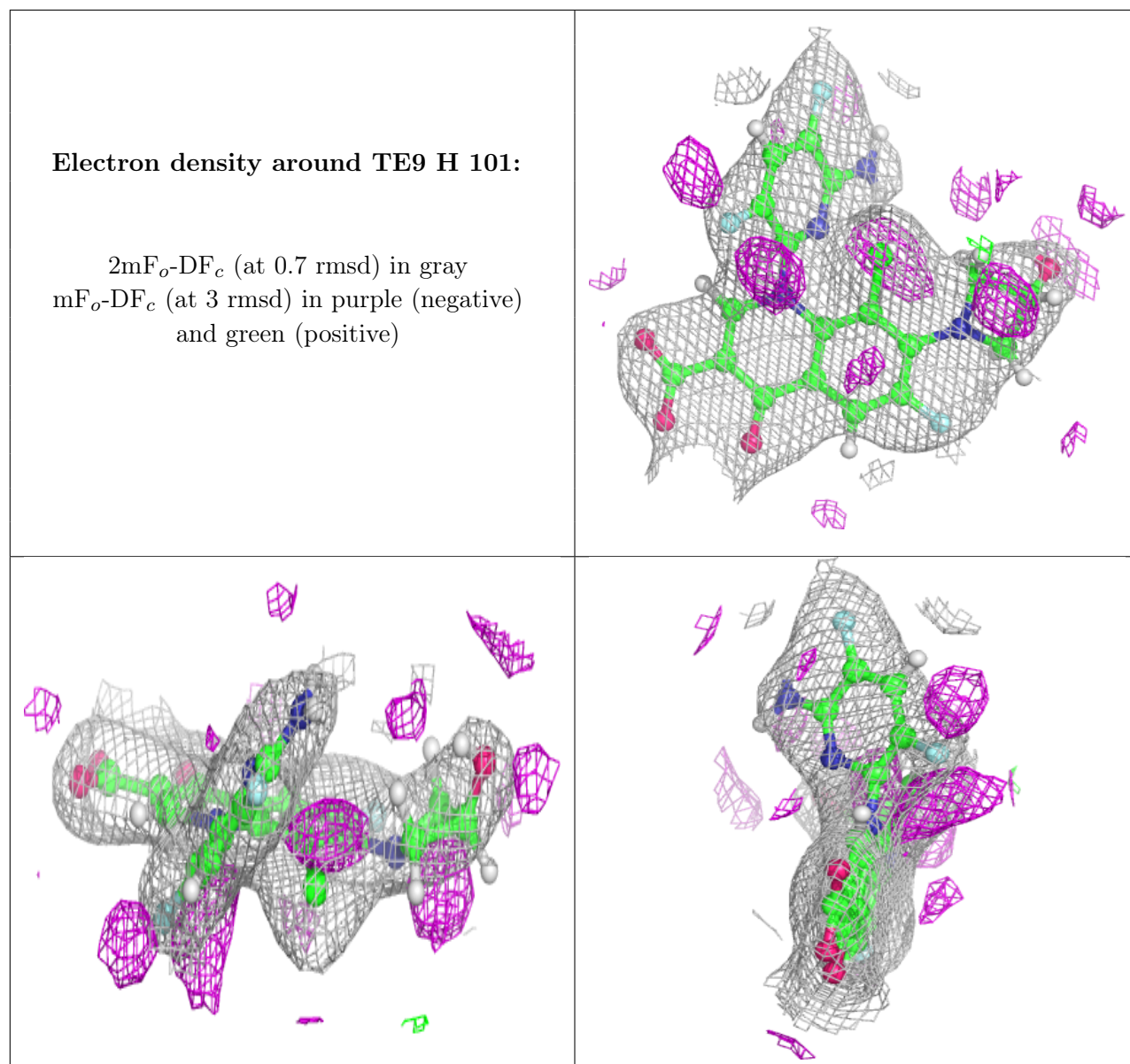
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
10	ACT	A	1508	4/4	0.82	0.26	30,30,56,64	3
10	ACT	B	1505	4/4	0.83	0.21	30,30,60,68	3
11	FMT	B	1507	3/3	0.83	0.20	30,55,71,74	1
10	ACT	A	1511	4/4	0.88	0.17	30,30,64,66	3
10	ACT	B	1506	4/4	0.90	0.18	30,30,75,106	3
11	FMT	B	1509	3/3	0.90	0.14	30,42,53,63	1
8	MPD	A	1506	8/8	0.92	0.15	30,71,80,84	2
11	FMT	A	1512	3/3	0.92	0.12	30,36,48,67	1
9	MLA	A	1507	7/7	0.93	0.11	46,60,61,63	0
9	MLA	A	1509	7/7	0.93	0.10	49,60,66,66	0
8	MPD	B	1508	8/8	0.93	0.14	30,42,51,58	2
7	CL	A	1504	1/1	0.94	0.08	58,58,58,58	0
8	MPD	A	1505	8/8	0.96	0.14	30,62,65,75	2
6	MG	B	1502	1/1	0.96	0.06	32,32,32,32	0
6	MG	A	1501	1/1	0.96	0.07	50,50,50,50	0
11	FMT	A	1510	3/3	0.97	0.13	30,33,48,57	1
7	CL	B	1504	1/1	0.97	0.11	68,68,68,68	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	B	1501	1/1	0.98	0.04	50,50,50,50	0
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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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 ⓘ

There are no such residues in this entry.