Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2024 – 10:21 am BST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

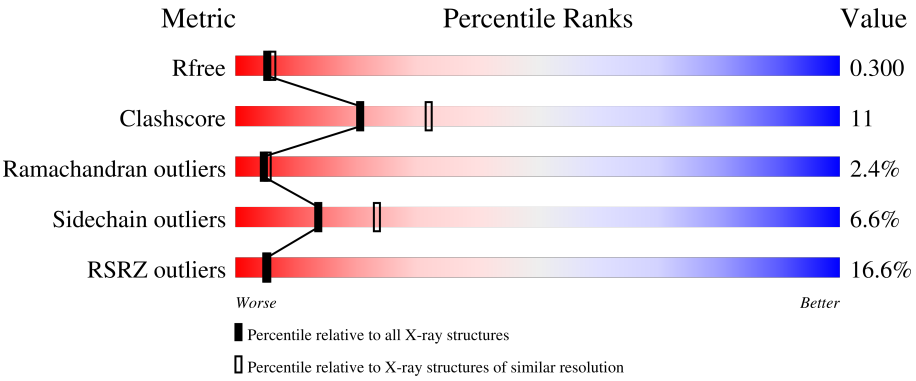
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	18% 73% 21%
1	B	742	14% 71% 23%
2	E	7	14% 43% 29% 29%
3	F	11	9% 55% 36% 9%

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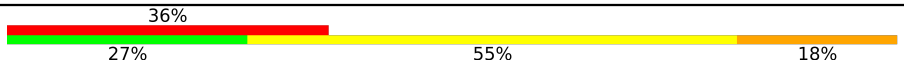
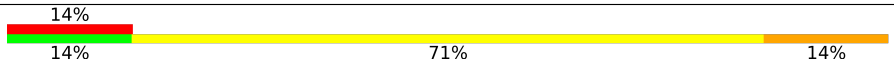
Mol	Chain	Length	Quality of chain
4	H	11	
5	G	7	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 24995 atoms, of which 12198 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA topoisomerase (ATP-hydrolyzing),DNA topoisomerase 4 subunit A.

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

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	403	MET	-	initiating methionine	UNP J0V1V8
A	404	LYS	-	expression tag	UNP J0V1V8
A	405	ASN	-	expression tag	UNP J0V1V8
A	406	LYS	-	expression tag	UNP J0V1V8
A	407	LYS	-	expression tag	UNP J0V1V8
A	408	ASP	-	expression tag	UNP J0V1V8
A	409	LYS	-	expression tag	UNP J0V1V8
A	410	GLY	-	expression tag	UNP J0V1V8
A	411	LEU	-	expression tag	UNP J0V1V8
A	648	HIS	-	linker	UNP J0V1V8
A	1257	THR	ILE	conflict	UNP P72525
A	1489	LEU	-	expression tag	UNP P72525
A	1490	GLU	-	expression tag	UNP P72525
A	1491	HIS	-	expression tag	UNP P72525
A	1492	HIS	-	expression tag	UNP P72525
A	1493	HIS	-	expression tag	UNP P72525
A	1494	HIS	-	expression tag	UNP P72525
A	1495	HIS	-	expression tag	UNP P72525
A	1496	HIS	-	expression tag	UNP P72525
B	403	MET	-	initiating methionine	UNP J0V1V8
B	404	LYS	-	expression tag	UNP J0V1V8
B	405	ASN	-	expression tag	UNP J0V1V8
B	406	LYS	-	expression tag	UNP J0V1V8
B	407	LYS	-	expression tag	UNP J0V1V8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	408	ASP	-	expression tag	UNP J0V1V8
B	409	LYS	-	expression tag	UNP J0V1V8
B	410	GLY	-	expression tag	UNP J0V1V8
B	411	LEU	-	expression tag	UNP J0V1V8
B	648	HIS	-	linker	UNP J0V1V8
B	1257	THR	ILE	conflict	UNP P72525
B	1489	LEU	-	expression tag	UNP P72525
B	1490	GLU	-	expression tag	UNP P72525
B	1491	HIS	-	expression tag	UNP P72525
B	1492	HIS	-	expression tag	UNP P72525
B	1493	HIS	-	expression tag	UNP P72525
B	1494	HIS	-	expression tag	UNP P72525
B	1495	HIS	-	expression tag	UNP P72525
B	1496	HIS	-	expression tag	UNP P72525

- Molecule 2 is a DNA chain called DNA (5'-D(*T)-R(P*G)-D(P*T)-R(P*GP*GP*A)-D(P*T)-3').

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

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

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

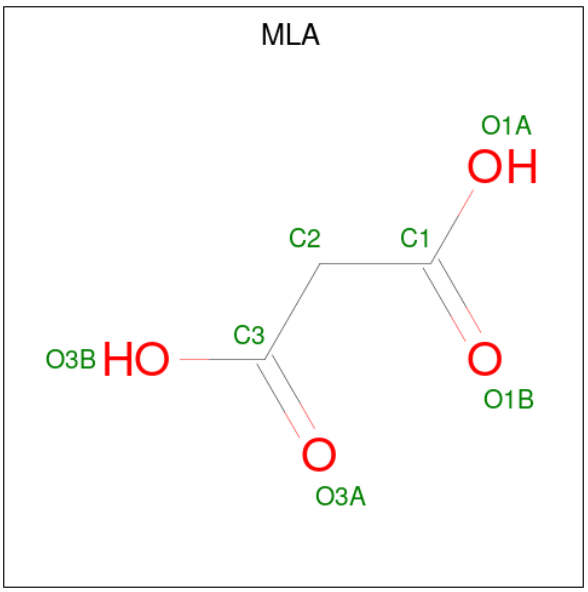
- Molecule 4 is a DNA chain called DNA/RNA (5'-R(P*AP*AP*CP*CP*G)-D(P*T)-R(P*A)-D(P*TP*T)-R(P*AP*C)-3').

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

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

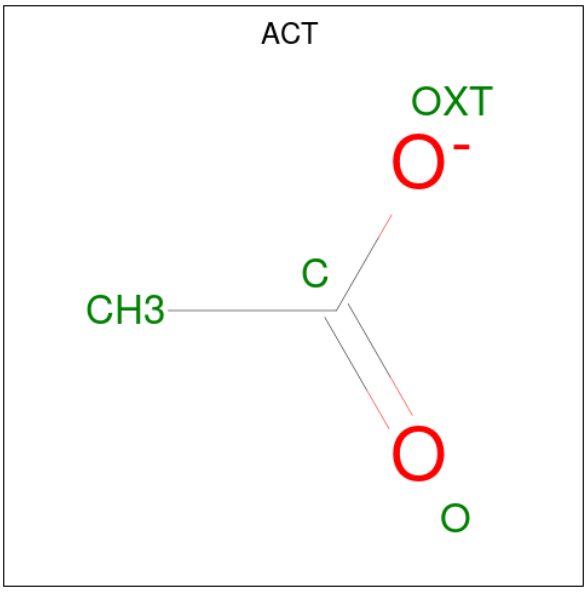
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
5	G	7	221	69	80	27	39	6	1	0	0

- Molecule 6 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



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

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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

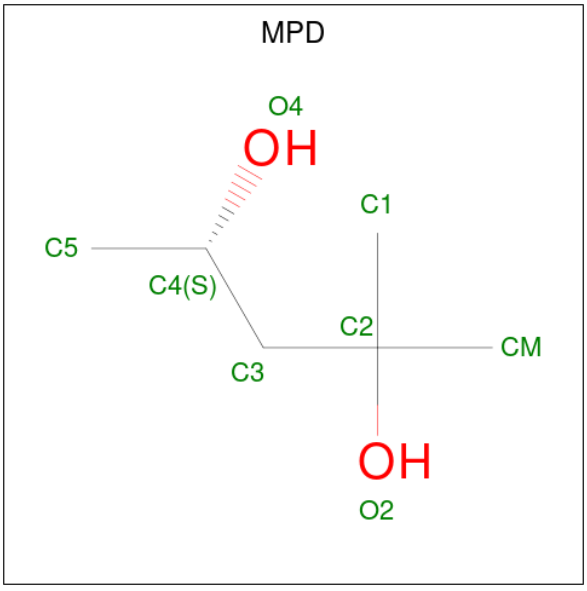
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

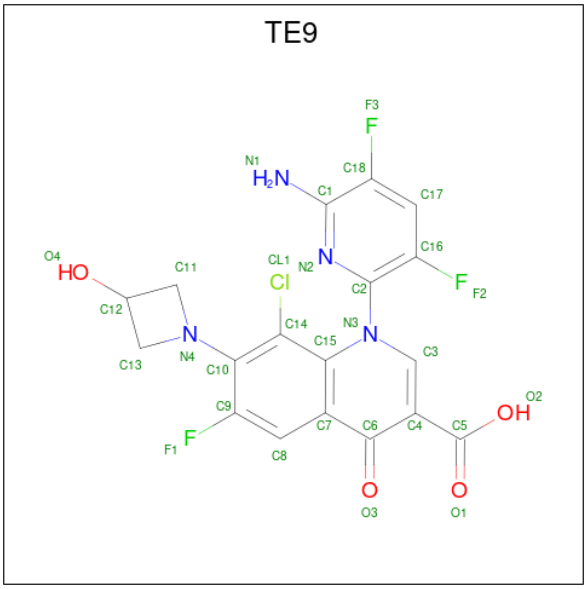
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Cl 1 1	0	0
9	B	1	Total Cl 1 1	0	0

- Molecule 10 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 11 is delafloxacin (three-letter code: TE9) (formula: $C_{18}H_{12}ClF_3N_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 12 is water.

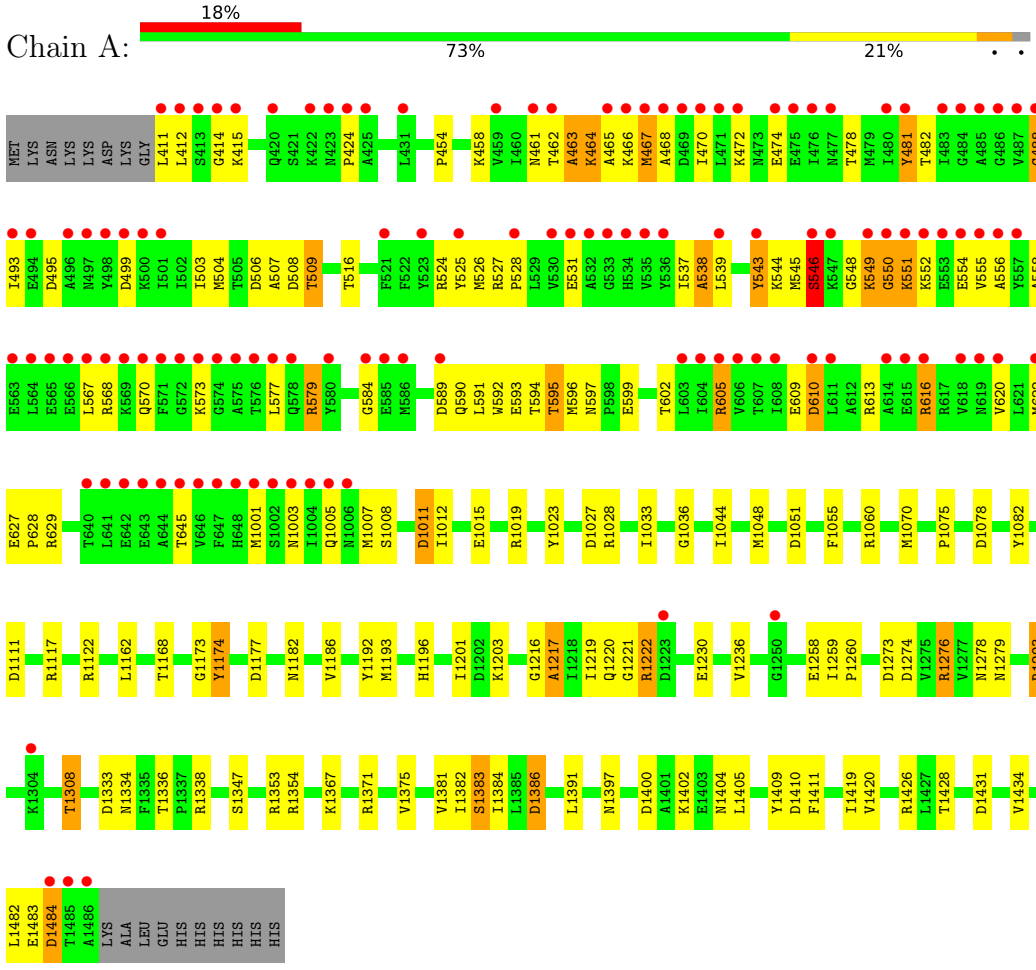
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	193	Total	O	0	0
			193	193		
12	B	199	Total	O	0	0
			199	199		
12	E	8	Total	O	0	0
			8	8		
12	F	9	Total	O	0	0
			9	9		
12	H	10	Total	O	0	0
			10	10		
12	G	7	Total	O	0	0
			7	7		

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.

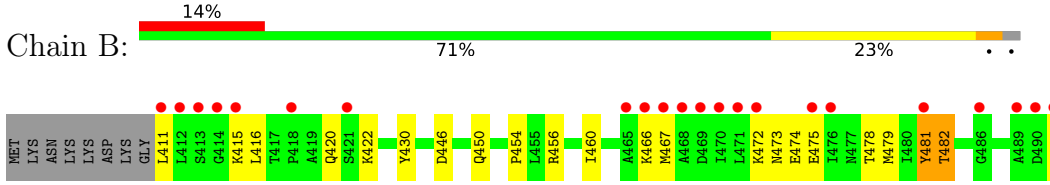
• Molecule 1: DNA topoisomerase (ATP-hydrolyzing),DNA topoisomerase 4 subunit A

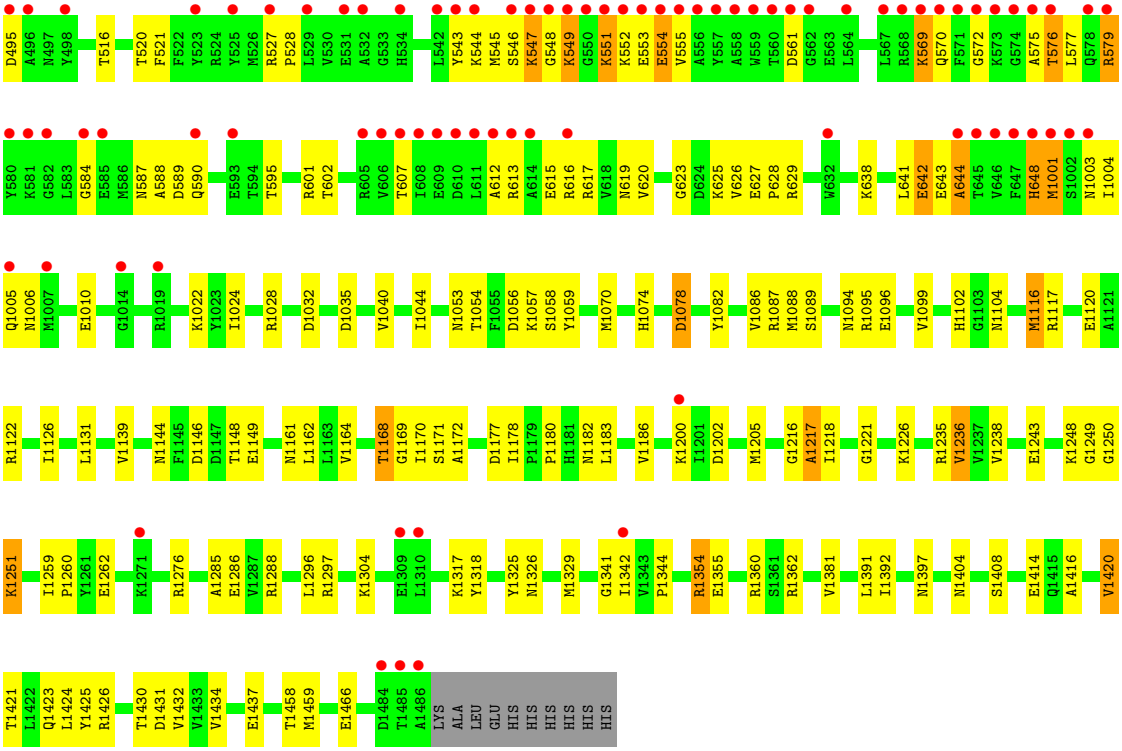
Chain A:



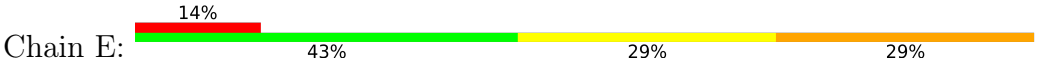
• Molecule 1: DNA topoisomerase (ATP-hydrolyzing),DNA topoisomerase 4 subunit A

Chain B:

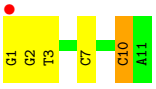




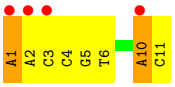
• Molecule 2: DNA (5'-D(*T)-R(P*G)-D(P*T)-R(P*GP*GP*A)-D(P*T)-3')



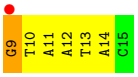
• Molecule 3: DNA/RNA (5'-R(P*GP*G)-D(P*TP*T)-R(P*A)-D(P*T)-R(P*CP*CP*AP*CP*A)-3')



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



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


G9
T10
A11
A12
T13
A14
C15

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.14Å 157.14Å 211.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.86 – 2.40 64.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	50.9 (64.86-2.40) 50.9 (64.86-2.40)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0352, PDB-REDO	Depositor
R, R_{free}	0.241 , 0.299 0.241 , 0.300	Depositor DCC
R_{free} test set	3069 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 23.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	24995	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

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

[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: MPD, ACT, CL, MG, TE9, MLA

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	0.37	0/5880	0.70	0/7927
1	B	0.36	0/5858	0.68	0/7900
2	E	0.81	0/161	1.40	4/248 (1.6%)
3	F	0.89	0/250	1.52	7/383 (1.8%)
4	H	0.73	0/249	1.55	8/381 (2.1%)
5	G	0.78	0/158	1.51	2/242 (0.8%)
All	All	0.41	0/12556	0.78	21/17081 (0.1%)

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

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

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	10	DA	P-O3'-C3'	-8.23	109.82	119.70
4	H	3	DC	P-O3'-C3'	-8.07	110.02	119.70
4	H	4	DC	P-O3'-C3'	-7.73	110.43	119.70
4	H	5	DG	P-O3'-C3'	-6.85	111.48	119.70
3	F	1	DG	O4'-C1'-N9	6.70	112.69	108.00
3	F	3	DT	O4'-C4'-C3'	-6.51	101.90	104.50
4	H	1	DA	O4'-C1'-N9	6.41	112.49	108.00
3	F	3	DT	C4'-C3'-C2'	-6.38	97.36	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2	DG	P-O3'-C3'	-6.33	112.11	119.70
2	E	14	DA	P-O3'-C3'	-6.14	112.33	119.70
5	G	9	DG	C1'-O4'-C4'	-6.10	104.00	110.10
3	F	1	DG	O4'-C1'-C2'	-5.96	101.13	105.90
4	H	5	DG	C8-N9-C1'	5.86	134.62	127.00
5	G	9	DG	P-O3'-C3'	5.79	126.64	119.70
2	E	11	DT	O5'-P-OP2	-5.72	100.55	105.70
4	H	5	DG	C4-N9-C1'	-5.62	119.19	126.50
2	E	12	DG	P-O3'-C3'	-5.56	113.03	119.70
2	E	12	DG	C8-N9-C1'	5.53	134.19	127.00
3	F	1	DG	C1'-O4'-C4'	-5.49	104.61	110.10
3	F	10	DC	C1'-O4'-C4'	-5.46	104.64	110.10
4	H	2	DA	P-O3'-C3'	-5.24	113.41	119.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1276	ARG	Sidechain
1	A	1353	ARG	Sidechain
1	A	1426	ARG	Sidechain
1	A	537	ILE	Peptide
1	A	550	GLY	Peptide
1	A	551	LYS	Peptide
1	B	1117	ARG	Sidechain
1	B	1354	ARG	Sidechain

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	5882	5871	121	0
1	B	5761	5859	5848	133	0
2	E	144	81	82	6	0
3	F	224	125	125	2	0
4	H	223	125	125	6	0
5	G	141	80	81	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	14	4	4	1	0
7	A	8	6	6	0	0
8	A	3	0	0	0	0
8	B	3	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	B	8	14	14	3	0
11	F	30	11	0	4	0
11	H	30	11	0	4	0
12	A	193	0	0	26	0
12	B	199	0	0	20	0
12	E	8	0	0	1	0
12	F	9	0	0	1	0
12	G	7	0	0	0	0
12	H	10	0	0	0	0
All	All	12797	12198	12156	270	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 11.

All (270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:101:TE9:CL1	11:H:101:TE9:N2	2.25	1.05
1:B:623:GLY:O	1:B:629:ARG:NH2	1.94	0.99
11:F:101:TE9:CL1	11:F:101:TE9:N2	2.33	0.98
1:B:1001:MET:HB3	1:B:1005:GLN:HE21	1.26	0.98
11:F:101:TE9:CL1	11:F:101:TE9:C2	2.54	0.93
11:H:101:TE9:CL1	11:H:101:TE9:C2	2.57	0.89
1:A:528:PRO:HA	12:A:1620:HOH:O	1.75	0.87
1:A:623:GLY:O	1:A:629:ARG:NH2	2.09	0.84
1:B:1408:SER:HB2	12:B:1602:HOH:O	1.76	0.84
1:B:1430:THR:HG22	10:B:1501:MPD:H52	1.61	0.81
1:A:1443[A]:ARG:NH1	6:A:1502:MLA:O1A	2.14	0.81
5:G:10:DT:H2"	5:G:11:DA:O5'	1.88	0.73
1:B:1202:ASP:OD1	1:B:1226:LYS:HE3	1.91	0.70
1:A:545:MET:HB3	1:A:567:LEU:HD23	1.74	0.69
1:B:555:VAL:HA	12:B:1725:HOH:O	1.91	0.69
1:A:531:GLU:HB2	12:A:1620:HOH:O	1.94	0.68
1:B:1054:THR:OG1	1:B:1056:ASP:OD1	2.12	0.68
1:A:1055:PHE:HA	1:A:1122:ARG:HD2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:SER:HB3	1:A:554:GLU:HB3	1.75	0.66
1:B:1423:GLN:NE2	1:B:1425:TYR:HE2	1.94	0.66
1:B:1003:ASN:HB3	1:B:1004:ILE:HD12	1.77	0.65
1:B:1286:GLU:OE1	1:B:1288:ARG:NH1	2.30	0.65
1:B:612:ALA:HA	12:B:1701:HOH:O	1.96	0.65
2:E:9:DT:H5"	2:E:9:DT:H6	1.62	0.65
11:H:101:TE9:CL1	11:H:101:TE9:C13	2.82	0.64
1:A:461:ASN:HD21	1:A:622[B]:MET:HB3	1.62	0.64
1:B:527:ARG:N	1:B:528:PRO:HD2	2.13	0.64
1:B:1423:GLN:HE21	1:B:1425:TYR:HE2	1.44	0.64
1:B:1010:GLU:HA	12:B:1735:HOH:O	1.98	0.64
1:B:1243:GLU:HB3	12:B:1714:HOH:O	1.98	0.64
1:A:1391:LEU:HD21	1:A:1404:ASN:HB2	1.79	0.63
1:A:1431:ASP:OD2	1:A:1434:VAL:HG23	1.99	0.63
1:A:1070:MET:HE1	1:A:1078:ASP:HB3	1.81	0.63
1:B:615:GLU:O	1:B:619:ASN:ND2	2.31	0.63
1:A:463:ALA:HB2	12:A:1627:HOH:O	1.98	0.63
1:B:1341:GLY:O	1:B:1344:PRO:HD2	1.99	0.63
2:E:9:DT:H6	2:E:9:DT:C5'	2.12	0.63
1:A:1308:THR:HB	12:A:1736:HOH:O	1.98	0.62
1:A:1044:ILE:O	1:A:1048:MET:HG3	1.99	0.61
1:B:1001:MET:CB	1:B:1005:GLN:HE21	2.09	0.60
11:F:101:TE9:CL1	11:F:101:TE9:C13	2.87	0.60
11:H:101:TE9:CL1	11:H:101:TE9:C1	2.87	0.60
1:A:584:GLY:HA2	12:A:1770:HOH:O	2.02	0.60
1:A:528:PRO:CA	12:A:1620:HOH:O	2.41	0.60
1:A:609:GLU:O	1:A:610:ASP:CB	2.50	0.59
1:B:1216:GLY:O	1:B:1217:ALA:HB3	2.03	0.59
1:B:1004:ILE:HD12	1:B:1004:ILE:H	1.68	0.59
1:B:1326:ASN:ND2	4:H:11:DC:H4'	2.17	0.58
1:A:1420:VAL:HG13	1:B:1425:TYR:HB3	1.83	0.58
1:B:1024[A]:ILE:HD11	1:B:1172:ALA:HB2	1.84	0.58
1:B:607:THR:HG21	1:B:1006:ASN:HD22	1.68	0.58
1:B:548:GLY:HA2	1:B:551:LYS:CG	2.34	0.58
1:A:590:GLN:HG3	12:A:1735:HOH:O	2.04	0.58
1:A:616:ARG:O	1:A:620:VAL:HG12	2.03	0.57
1:B:1360:ARG:HD3	12:B:1691:HOH:O	2.03	0.57
1:B:1296:LEU:HD23	1:B:1297:ARG:N	2.20	0.57
1:B:548:GLY:HA2	1:B:551:LYS:HG3	1.86	0.57
1:A:592:TRP:HA	1:A:596:MET:HB2	1.87	0.57
1:A:1411:PHE:HZ	12:A:1700:HOH:O	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:12:DA:H2'	5:G:12:DA:O5'	2.05	0.57
1:B:587:ASN:O	1:B:589:ASP:N	2.38	0.56
1:B:1362:ARG:HD3	12:B:1674:HOH:O	2.05	0.56
1:A:609:GLU:O	1:A:610:ASP:HB2	2.05	0.56
2:E:12:DG:H8	12:E:103:HOH:O	1.88	0.56
1:B:584:GLY:HA2	12:B:1765:HOH:O	2.04	0.56
1:B:1205:MET:HE1	1:B:1226:LYS:HA	1.86	0.56
1:A:579:ARG:HH11	1:A:579:ARG:HB3	1.70	0.56
1:A:1173:GLY:O	1:A:1174:TYR:CG	2.59	0.56
1:A:1293:ARG:HG2	1:A:1293:ARG:HH11	1.71	0.55
1:B:613:ARG:HG2	1:B:613:ARG:HH11	1.71	0.55
1:A:1383:SER:HB2	12:A:1673:HOH:O	2.06	0.55
1:A:531:GLU:CB	12:A:1620:HOH:O	2.50	0.55
11:F:101:TE9:CL1	11:F:101:TE9:C1	2.92	0.55
1:A:1274:ASP:O	1:A:1278:ASN:ND2	2.40	0.55
1:B:491:PHE:CD2	1:B:528:PRO:HG2	2.42	0.55
1:B:638:LYS:CG	1:B:641:LEU:HD23	2.37	0.54
1:B:1004:ILE:HD12	1:B:1004:ILE:N	2.23	0.54
1:A:506:ASP:C	1:A:508:ASP:H	2.11	0.54
1:A:1293:ARG:HD3	1:B:589:ASP:OD1	2.08	0.54
1:B:1326:ASN:HD21	4:H:11:DC:H4'	1.71	0.54
1:B:415:LYS:O	1:B:454:PRO:HD2	2.07	0.54
1:A:594:THR:OG1	1:A:595:THR:HG22	2.08	0.53
1:A:1308:THR:HG23	12:A:1723:HOH:O	2.08	0.53
1:A:1222:ARG:HH11	1:A:1484:ASP:CG	2.12	0.53
1:B:1235:ARG:HB2	12:B:1630:HOH:O	2.08	0.53
1:A:1117:ARG:NH1	12:A:1603:HOH:O	2.37	0.53
1:B:1168:THR:HG22	12:B:1692:HOH:O	2.07	0.53
1:A:1371:ARG:O	1:A:1375:VAL:HG23	2.09	0.53
4:H:10:DA:H61	5:G:10:DT:H3	1.57	0.52
1:B:627:GLU:N	1:B:628:PRO:HD2	2.24	0.52
1:B:1431:ASP:CG	1:B:1434:VAL:HG23	2.28	0.52
1:A:1182:ASN:O	1:A:1186:VAL:HG23	2.10	0.52
1:B:1216:GLY:O	1:B:1217:ALA:CB	2.57	0.52
1:A:503:ILE:O	1:A:538:ALA:HB2	2.10	0.52
1:B:1170:ILE:HD11	5:G:11:DA:C2	2.45	0.52
1:B:1205:MET:CE	1:B:1226:LYS:HA	2.40	0.52
1:B:615:GLU:HG3	1:B:619:ASN:HD21	1.74	0.51
1:B:1035:ASP:O	1:B:1161:ASN:HB3	2.11	0.51
1:A:1001:MET:HG3	1:A:1005:GLN:HE21	1.75	0.51
1:A:1381:VAL:HA	12:A:1700:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:MET:HA	1:A:538:ALA:HB2	1.92	0.51
1:A:1296:LEU:HD23	1:A:1297:ARG:N	2.26	0.51
1:B:626:VAL:HG11	4:H:10:DA:OP2	2.11	0.51
1:B:1391:LEU:HD11	1:B:1404:ASN:HB3	1.93	0.51
12:B:1617:HOH:O	4:H:1:DA:H8	1.94	0.51
1:B:1001:MET:HB3	1:B:1005:GLN:NE2	2.10	0.50
1:A:1333:ASP:OD2	1:A:1338:ARG:NH1	2.43	0.50
1:A:1384:ILE:HD13	1:A:1409:TYR:CD1	2.47	0.50
1:B:641:LEU:O	1:B:1022:LYS:NZ	2.44	0.50
1:A:524:ARG:O	1:A:525:TYR:CD1	2.65	0.50
1:B:1182:ASN:O	1:B:1186:VAL:HG23	2.11	0.50
1:A:597:ASN:ND2	1:A:599:GLU:HB2	2.27	0.50
1:A:1334:ASN:O	1:A:1336:THR:HG23	2.12	0.50
1:B:1218:ILE:O	1:B:1238:VAL:HA	2.10	0.50
1:B:1458:THR:HA	12:B:1671:HOH:O	2.11	0.50
1:B:602:THR:HG21	1:B:648:HIS:NE2	2.26	0.50
5:G:9:DG:H4'	5:G:10:DT:O5'	2.12	0.50
1:A:465:ALA:O	1:A:470:ILE:HD11	2.11	0.50
1:B:547:LYS:HB3	1:B:575:ALA:HB2	1.94	0.49
1:B:1088:MET:HA	1:B:1094:ASN:ND2	2.27	0.49
1:B:1354:ARG:HG3	1:B:1459:MET:CE	2.41	0.49
1:A:1400:ASP:OD2	1:A:1404:ASN:ND2	2.37	0.49
1:B:1144:ASN:ND2	1:B:1149:GLU:HB3	2.26	0.49
1:A:488:GLY:O	1:A:489:ALA:CB	2.61	0.49
1:B:416:LEU:HD22	1:B:482:THR:HG23	1.95	0.49
1:A:1173:GLY:O	1:A:1174:TYR:CD2	2.66	0.49
1:A:490:ASP:OD1	1:A:490:ASP:N	2.45	0.49
1:B:1082:TYR:O	1:B:1086:VAL:HG23	2.13	0.49
1:B:1087:ARG:HG2	1:B:1087:ARG:HH11	1.76	0.49
1:B:1317:LYS:HD3	1:B:1318:TYR:CE2	2.48	0.49
1:B:1028:ARG:CZ	5:G:14:DA:H4'	2.43	0.49
1:B:547:LYS:HG2	1:B:554:GLU:HG3	1.95	0.49
1:B:1146:ASP:OD1	1:B:1148:THR:HG23	2.13	0.49
1:A:568:ARG:HG2	1:A:568:ARG:HH11	1.78	0.48
1:A:1273:ASP:OD1	1:A:1276:ARG:NH1	2.46	0.48
1:B:638:LYS:HG3	1:B:641:LEU:HD23	1.95	0.48
1:A:543:TYR:HB3	1:A:577:LEU:HD11	1.94	0.48
1:A:1011:ASP:OD1	1:A:1011:ASP:N	2.45	0.48
1:A:467:MET:O	1:A:468:ALA:HB3	2.12	0.48
1:B:1205:MET:HE1	1:B:1226:LYS:CA	2.43	0.48
1:A:1028:ARG:CZ	2:E:14:DA:H4'	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:GLU:HA	12:A:1658:HOH:O	2.14	0.48
1:A:1259:ILE:HB	1:A:1260:PRO:CD	2.44	0.48
1:B:1420:VAL:HG12	1:B:1421:THR:HG23	1.96	0.48
1:B:1397:ASN:HB2	12:B:1652:HOH:O	2.14	0.47
1:A:463:ALA:CB	12:A:1627:HOH:O	2.57	0.47
1:A:546:SER:HB3	1:A:554:GLU:CB	2.44	0.47
1:B:460:ILE:HA	4:H:6:DT:O3'	2.14	0.47
1:B:1249:GLY:O	1:B:1304:LYS:HE2	2.14	0.47
1:A:478:THR:O	1:A:482:THR:OG1	2.32	0.47
1:B:1262:GLU:HG3	5:G:11:DA:H4'	1.96	0.47
1:A:414:GLY:HA3	1:A:454:PRO:O	2.15	0.47
1:B:1057:LYS:O	1:B:1122:ARG:NH1	2.45	0.47
1:B:1355:GLU:HA	1:B:1355:GLU:OE1	2.13	0.47
12:B:1779:HOH:O	5:G:9:DG:H5'	2.15	0.47
1:A:464:LYS:O	1:A:465:ALA:C	2.52	0.47
1:B:1096:GLU:HG2	1:B:1126:ILE:HD13	1.97	0.47
1:B:1164:VAL:HG21	1:B:1183:LEU:HD12	1.97	0.47
1:B:1262:GLU:CG	5:G:11:DA:H4'	2.45	0.47
1:B:1354:ARG:HG3	1:B:1459:MET:HE1	1.97	0.47
1:B:643:GLU:O	1:B:644:ALA:C	2.53	0.47
1:B:1259:ILE:HB	1:B:1260:PRO:CD	2.45	0.47
5:G:12:DA:H4'	5:G:13:DT:OP1	2.15	0.47
1:A:509:THR:HB	12:A:1791:HOH:O	2.15	0.47
1:B:446:ASP:O	1:B:450:GLN:HB2	2.14	0.47
1:A:605:ARG:HH11	1:A:605:ARG:CB	2.28	0.46
1:B:1056:ASP:OD1	1:B:1056:ASP:N	2.48	0.46
1:B:579:ARG:HB3	1:B:579:ARG:HH11	1.80	0.46
1:A:531:GLU:CG	12:A:1620:HOH:O	2.64	0.46
1:A:1216:GLY:O	1:A:1217:ALA:HB3	2.16	0.46
1:A:1354:ARG:HG3	1:A:1459:MET:HE2	1.97	0.46
1:A:1419:ILE:O	1:B:1424:LEU:HD12	2.15	0.46
1:A:461:ASN:O	1:A:465:ALA:HB3	2.15	0.46
1:B:1178:ILE:HG12	1:B:1329:MET:HG2	1.97	0.46
1:A:627:GLU:N	1:A:628:PRO:CD	2.78	0.46
1:B:1095:ARG:HG3	1:B:1095:ARG:HH11	1.81	0.46
1:B:1082:TYR:CD1	1:B:1116:MET:HB3	2.51	0.46
1:A:1382:ILE:HG22	12:A:1663:HOH:O	2.16	0.46
1:B:475:GLU:O	1:B:479:MET:HG3	2.16	0.46
1:B:1326:ASN:HB2	12:B:1655:HOH:O	2.15	0.46
1:A:1201:ILE:HG13	1:A:1230:GLU:HG3	1.97	0.45
1:A:591:LEU:HD12	1:A:595:THR:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1200:LYS:HB2	12:B:1616:HOH:O	2.16	0.45
1:A:548:GLY:O	1:A:549:LYS:HB3	2.16	0.45
1:B:638:LYS:HG2	1:B:641:LEU:HD23	1.97	0.45
1:B:1040:VAL:O	1:B:1044:ILE:HG13	2.16	0.45
1:B:1040:VAL:HG23	1:B:1074:HIS:CD2	2.51	0.45
5:G:10:DT:H2'	5:G:11:DA:C8	2.52	0.45
1:A:474:GLU:O	1:A:478:THR:HG23	2.16	0.45
1:A:1381:VAL:O	1:A:1382:ILE:C	2.55	0.45
1:B:1426:ARG:O	10:B:1501:MPD:H31	2.17	0.45
1:B:547:LYS:HG3	1:B:572:GLY:HA3	1.98	0.45
1:A:1431:ASP:HB2	12:A:1745:HOH:O	2.16	0.45
2:E:9:DT:C5'	2:E:9:DT:C6	2.97	0.45
1:A:463:ALA:O	1:A:464:LYS:C	2.55	0.44
1:B:1169:GLY:C	1:B:1170:ILE:HG13	2.38	0.44
1:A:1386:ASP:OD1	1:A:1386:ASP:N	2.47	0.44
1:A:481:TYR:CD1	1:A:481:TYR:C	2.91	0.44
1:B:642:GLU:C	1:B:643:GLU:HG3	2.38	0.44
1:A:610:ASP:OD2	1:A:613:ARG:HD3	2.18	0.44
1:A:1192:TYR:CE1	1:A:1196:HIS:CE1	3.06	0.44
1:B:1408:SER:CB	12:B:1602:HOH:O	2.52	0.44
1:A:595:THR:O	1:A:595:THR:OG1	2.32	0.44
1:A:1102:HIS:CE1	1:B:590:GLN:HE22	2.35	0.44
1:A:1036:GLY:HA2	1:A:1162:LEU:HD13	1.99	0.43
1:B:1416:ALA:O	1:B:1420:VAL:HB	2.18	0.43
1:B:545:MET:HA	1:B:576:THR:O	2.18	0.43
1:B:617:ARG:HA	12:B:1627:HOH:O	2.18	0.43
1:B:1236:VAL:HG12	1:B:1325:TYR:HB3	2.00	0.43
1:A:626:VAL:HG11	3:F:10:DC:OP2	2.19	0.43
1:A:527:ARG:N	1:A:528:PRO:CD	2.81	0.43
1:B:460:ILE:HD12	1:B:473:ASN:ND2	2.33	0.43
1:B:1276:ARG:HD2	1:B:1285:ALA:O	2.17	0.43
1:A:1023:TYR:HE2	1:A:1028:ARG:HH21	1.66	0.43
1:A:1193:MET:CE	1:A:1347:SER:HB3	2.49	0.43
1:A:625:LYS:HB2	1:A:628:PRO:HD2	2.01	0.42
1:B:411:LEU:O	1:B:456:ARG:NH1	2.51	0.42
1:B:430:TYR:OH	1:B:601:ARG:NH1	2.52	0.42
1:B:1089:SER:HA	1:B:1099:VAL:O	2.19	0.42
1:B:1426:ARG:HD2	10:B:1501:MPD:HM3	2.00	0.42
1:A:1333:ASP:O	1:A:1334:ASN:C	2.58	0.42
1:A:1397:ASN:HB2	12:A:1633:HOH:O	2.19	0.42
1:B:474:GLU:O	1:B:478:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1004:ILE:HG22	1:B:1005:GLN:N	2.35	0.42
1:B:1360:ARG:HH22	1:B:1466:GLU:CD	2.23	0.42
1:A:556:ALA:HB3	1:A:567:LEU:HD21	2.01	0.42
1:A:1060:ARG:HD3	12:A:1744:HOH:O	2.20	0.42
1:A:1060:ARG:NH2	12:A:1621:HOH:O	2.53	0.42
1:A:1015:GLU:O	1:A:1019[A]:ARG:HB2	2.20	0.42
1:B:544:LYS:O	1:B:577:LEU:HA	2.20	0.42
1:B:481:TYR:C	1:B:481:TYR:CD1	2.93	0.42
1:B:1177:ASP:HB3	1:B:1325:TYR:OH	2.20	0.42
1:A:458:LYS:HD3	1:A:458:LYS:HA	1.93	0.42
1:B:527:ARG:N	1:B:528:PRO:CD	2.81	0.42
1:B:1095:ARG:HB2	1:B:1180:PRO:HB3	2.02	0.42
1:A:1033:ILE:HA	1:A:1162:LEU:HD22	2.02	0.41
1:B:520:THR:O	1:B:521:PHE:C	2.59	0.41
1:A:543:TYR:HB2	1:A:558:ALA:HB3	2.03	0.41
1:A:545:MET:O	1:A:546:SER:HB2	2.21	0.41
1:A:1028:ARG:NH1	2:E:14:DA:H4'	2.34	0.41
1:B:1001:MET:H	1:B:1005:GLN:NE2	2.18	0.41
1:B:1250:GLY:O	1:B:1251:LYS:O	2.38	0.41
1:A:589:ASP:HB2	12:A:1735:HOH:O	2.21	0.41
1:A:1220:GLN:HG2	1:A:1483:GLU:HB2	2.03	0.41
1:A:544:LYS:O	1:A:577:LEU:HD12	2.20	0.41
1:A:579:ARG:HB3	12:A:1616:HOH:O	2.21	0.41
1:B:625:LYS:HB3	1:B:628:PRO:CG	2.50	0.41
1:B:1414:GLU:HG2	12:B:1787:HOH:O	2.20	0.41
1:A:1051:ASP:HB3	1:A:1060:ARG:HH12	1.86	0.41
1:A:1308:THR:CG2	12:A:1723:HOH:O	2.66	0.41
1:A:1402:LYS:O	1:A:1405:LEU:HB2	2.21	0.41
1:B:543:TYR:HB3	1:B:577:LEU:HD21	2.01	0.41
1:B:616:ARG:O	1:B:620:VAL:HG12	2.21	0.41
1:B:1078:ASP:CG	12:B:1704:HOH:O	2.59	0.41
1:B:1205:MET:HE1	1:B:1226:LYS:CB	2.50	0.41
1:A:1082:TYR:O	1:A:1086:VAL:HG23	2.20	0.41
1:A:548:GLY:O	1:A:549:LYS:CB	2.69	0.40
1:A:1007:MET:HE2	1:A:1012:ILE:CD1	2.51	0.40
1:A:1391:LEU:HD23	1:A:1391:LEU:C	2.42	0.40
1:A:1428:THR:HG22	1:B:1392:ILE:O	2.22	0.40
1:A:1008:SER:HB2	12:A:1778:HOH:O	2.20	0.40
1:B:625:LYS:HE2	1:B:625:LYS:HA	2.02	0.40
1:A:597:ASN:HD21	1:A:599:GLU:HB2	1.87	0.40
1:A:1203:LYS:HA	1:A:1203:LYS:HD2	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1296:LEU:HD23	1:B:1296:LEU:C	2.42	0.40
1:A:626:VAL:O	1:A:629:ARG:HB3	2.22	0.40
1:A:1219:ILE:HB	1:A:1482:LEU:HD23	2.03	0.40
1:B:1070:MET:HE1	1:B:1078:ASP:HB3	2.03	0.40
1:B:1459:MET:C	1:B:1459:MET:SD	3.00	0.40
3:F:7:DC:H1'	12:F:203:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	725/742 (98%)	657 (91%)	49 (7%)	19 (3%)	4	4
1	B	723/742 (97%)	660 (91%)	47 (6%)	16 (2%)	5	6
All	All	1448/1484 (98%)	1317 (91%)	96 (7%)	35 (2%)	5	5

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ALA
1	A	549	LYS
1	A	610	ASP
1	B	569	LYS
1	B	588	ALA
1	B	1217	ALA
1	B	1251	LYS
1	A	464	LYS
1	A	488	GLY
1	A	526	MET
1	A	546	SER
1	A	1003	ASN

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Mol	Chain	Res	Type
1	A	1217	ALA
1	A	1410	ASP
1	B	466	LYS
1	B	552	LYS
1	B	553	GLU
1	B	554	GLU
1	B	570	GLN
1	B	644	ALA
1	A	424	PRO
1	A	463	ALA
1	A	507	ALA
1	A	1174	TYR
1	B	642	GLU
1	B	648	HIS
1	B	1059	TYR
1	A	467	MET
1	B	467	MET
1	A	538	ALA
1	B	549	LYS
1	A	1075	PRO
1	A	550	GLY
1	A	1221	GLY
1	B	1221	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	622/635 (98%)	578 (93%)	44 (7%)	12	20
1	B	620/635 (98%)	582 (94%)	38 (6%)	15	27
All	All	1242/1270 (98%)	1160 (93%)	82 (7%)	14	23

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	411	LEU
1	A	412	LEU
1	A	415	LYS
1	A	462	THR
1	A	466	LYS
1	A	472	LYS
1	A	481	TYR
1	A	490	ASP
1	A	492	SER
1	A	493	ILE
1	A	495	ASP
1	A	499	ASP
1	A	509	THR
1	A	516	THR
1	A	539	LEU
1	A	543	TYR
1	A	546	SER
1	A	551	LYS
1	A	552	LYS
1	A	555	VAL
1	A	570	GLN
1	A	573	LYS
1	A	579	ARG
1	A	593	GLU
1	A	595	THR
1	A	602	THR
1	A	605	ARG
1	A	616	ARG
1	A	645	THR
1	A	1011	ASP
1	A	1027	ASP
1	A	1102	HIS
1	A	1111	ASP
1	A	1168	THR
1	A	1177	ASP
1	A	1222	ARG
1	A	1236	VAL
1	A	1279	ASN
1	A	1293	ARG
1	A	1308	THR
1	A	1367	LYS
1	A	1383	SER
1	A	1386	ASP

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Mol	Chain	Res	Type
1	A	1484	ASP
1	B	420	GLN
1	B	422	LYS
1	B	472	LYS
1	B	481	TYR
1	B	482	THR
1	B	492	SER
1	B	495	ASP
1	B	516	THR
1	B	546	SER
1	B	547	LYS
1	B	549	LYS
1	B	551	LYS
1	B	561	ASP
1	B	569	LYS
1	B	576	THR
1	B	579	ARG
1	B	595	THR
1	B	1001	MET
1	B	1032	ASP
1	B	1053	ASN
1	B	1058	SER
1	B	1078	ASP
1	B	1102	HIS
1	B	1104	ASN
1	B	1116	MET
1	B	1120	GLU
1	B	1131	LEU
1	B	1139	VAL
1	B	1162	LEU
1	B	1168	THR
1	B	1171	SER
1	B	1236	VAL
1	B	1248	LYS
1	B	1342	ILE
1	B	1381	VAL
1	B	1420	VAL
1	B	1432	VAL
1	B	1437	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	ASN
1	A	477	ASN
1	A	1005	GLN
1	A	1102	HIS
1	A	1267	ASN
1	A	1278	ASN
1	B	473	ASN
1	B	515	GLN
1	B	578	GLN
1	B	587	ASN
1	B	619	ASN
1	B	1005	GLN
1	B	1006	ASN
1	B	1049	ASN
1	B	1053	ASN

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 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MLA	A	1501	-	6,6,6	1.25	0	7,7,7	1.08	0
10	MPD	B	1501	-	7,7,7	0.21	0	9,10,10	0.56	0
7	ACT	A	1503	-	3,3,3	0.98	0	3,3,3	1.10	0
7	ACT	A	1504	-	3,3,3	1.13	0	3,3,3	0.91	0
6	MLA	A	1502	-	6,6,6	1.29	0	7,7,7	1.06	0
11	TE9	H	101	8	31,33,33	1.15	3 (9%)	37,51,51	1.20	2 (5%)
11	TE9	F	101	8	31,33,33	1.09	3 (9%)	37,51,51	1.21	3 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MLA	A	1501	-	-	0/4/4/4	-
10	MPD	B	1501	-	-	0/5/5/5	-
11	TE9	F	101	8	-	3/11/20/20	0/4/4/4
6	MLA	A	1502	-	-	2/4/4/4	-
11	TE9	H	101	8	-	7/11/20/20	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	101	TE9	C2-C16	-2.90	1.39	1.42
11	H	101	TE9	C1-C18	2.52	1.42	1.40
11	F	101	TE9	C2-C16	-2.40	1.39	1.42
11	F	101	TE9	C1-C18	2.27	1.42	1.40
11	H	101	TE9	C3-N3	2.20	1.42	1.37
11	F	101	TE9	O1-C5	2.06	1.28	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	101	TE9	C17-C18-C1	-3.28	119.56	121.70
11	F	101	TE9	C17-C18-C1	-3.24	119.59	121.70
11	H	101	TE9	C4-C3-N3	-2.60	120.55	123.75
11	F	101	TE9	C4-C3-N3	-2.39	120.80	123.75
11	F	101	TE9	C1-N2-C2	2.10	122.34	116.99

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	101	TE9	C16-C2-N3-C15
11	F	101	TE9	N2-C2-N3-C3
11	H	101	TE9	C16-C2-N3-C15
11	H	101	TE9	N2-C2-N3-C3
11	H	101	TE9	C6-C4-C5-O2
6	A	1502	MLA	C1-C2-C3-O3A
6	A	1502	MLA	C1-C2-C3-O3B
11	H	101	TE9	C3-C4-C5-O2
11	H	101	TE9	C6-C4-C5-O1
11	H	101	TE9	C3-C4-C5-O1
11	F	101	TE9	N2-C2-N3-C15
11	H	101	TE9	N2-C2-N3-C15

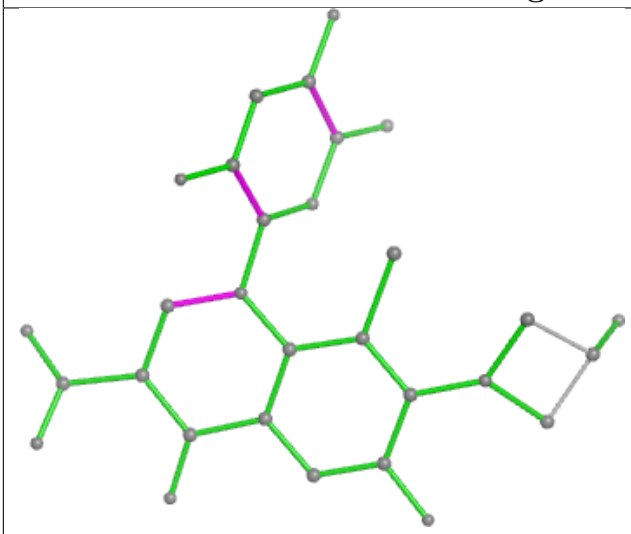
There are no ring outliers.

4 monomers are involved in 12 short contacts:

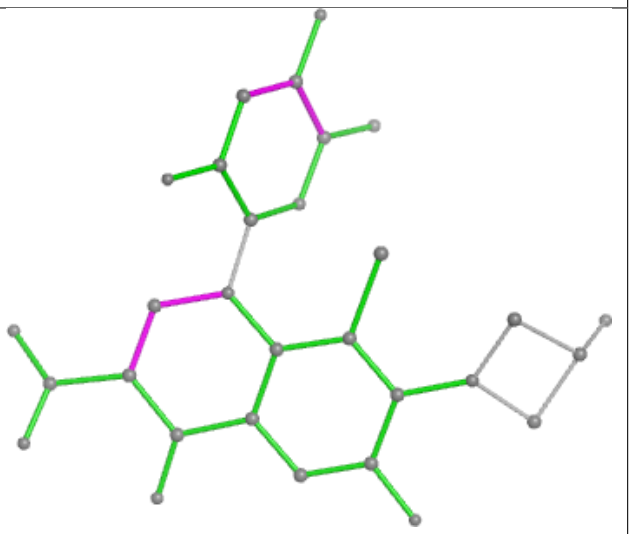
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1501	MPD	3	0
6	A	1502	MLA	1	0
11	H	101	TE9	4	0
11	F	101	TE9	4	0

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.

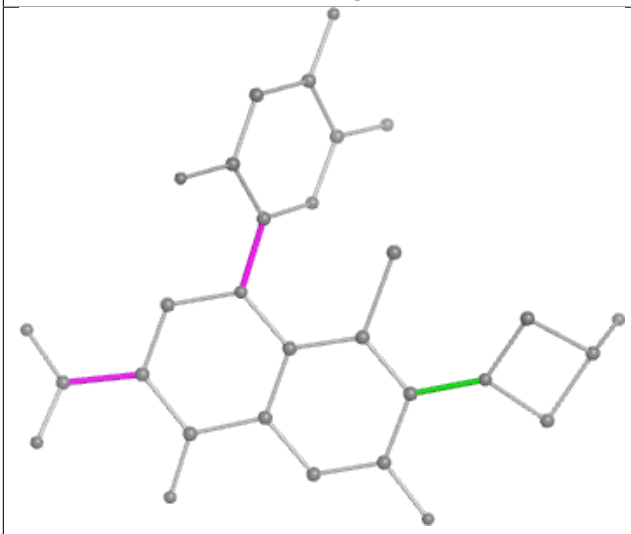
Ligand TE9 H 101



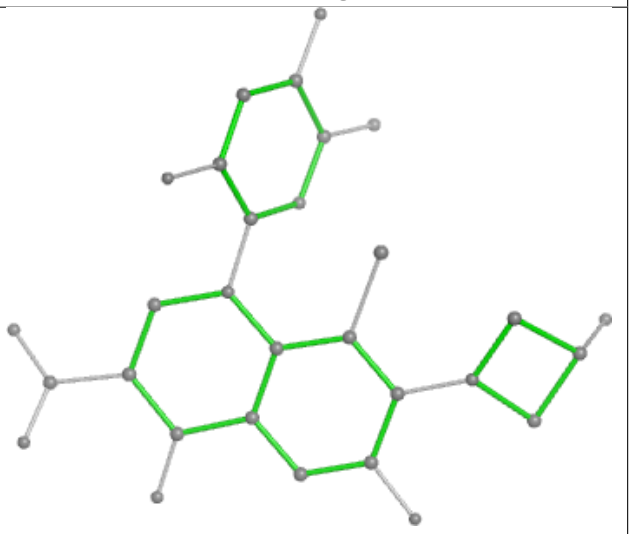
Bond lengths



Bond angles

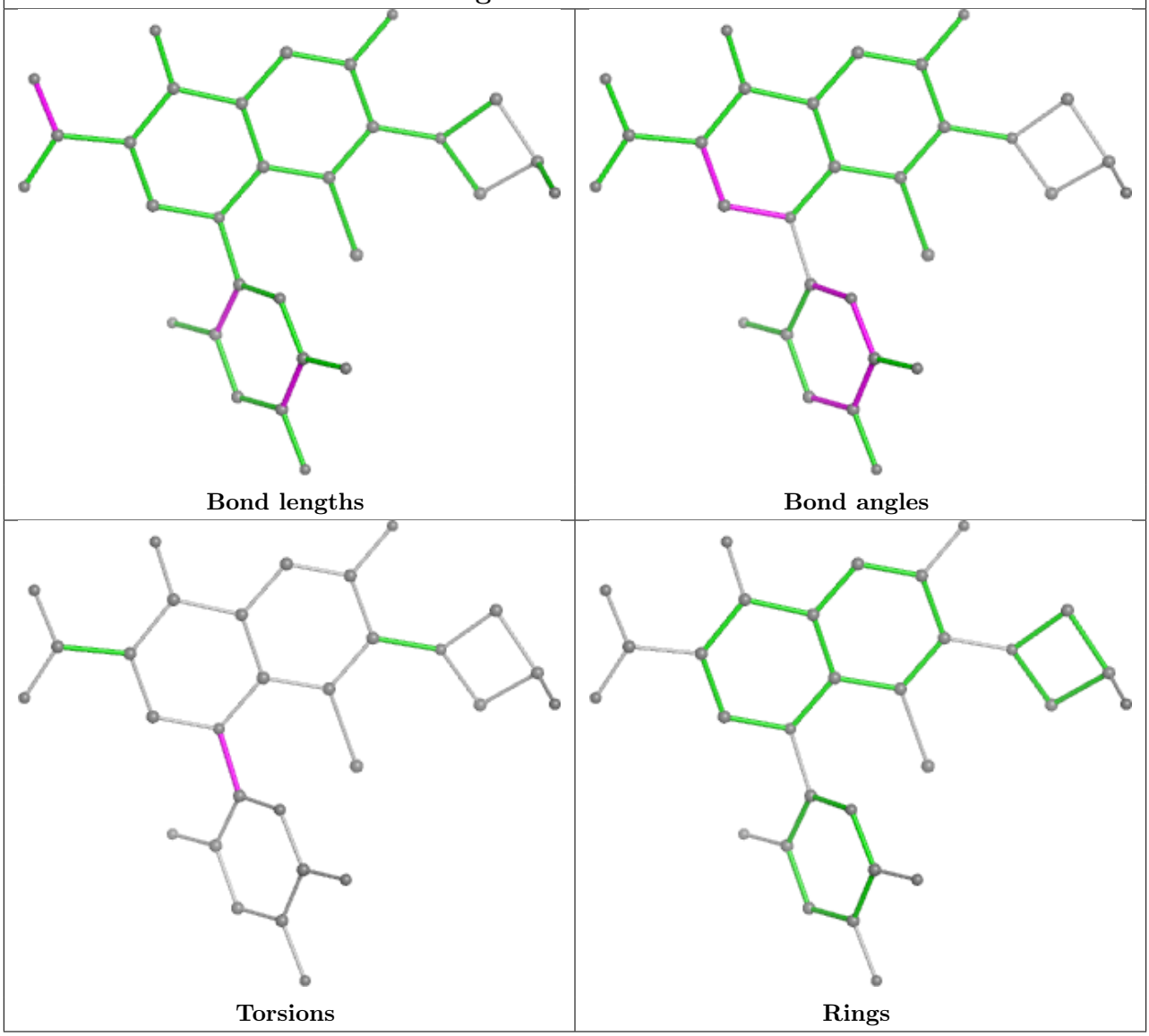


Torsions



Rings

Ligand TE9 F 101



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

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, 95^{th} 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%)	0.81	133 (18%) 4 4	6, 21, 65, 93	3 (0%)
1	B	724/742 (97%)	0.61	107 (14%) 7 6	6, 19, 57, 87	1 (0%)
2	E	7/7 (100%)	0.45	1 (14%) 7 6	16, 16, 36, 52	0
3	F	11/11 (100%)	0.71	1 (9%) 16 14	20, 28, 51, 55	0
4	H	11/11 (100%)	1.56	4 (36%) 1 1	37, 47, 64, 65	0
5	G	7/7 (100%)	0.15	1 (14%) 7 6	12, 14, 36, 54	0
All	All	1484/1520 (97%)	0.72	247 (16%) 5 5	6, 21, 61, 93	4 (0%)

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	644	ALA	8.6
1	A	571	PHE	8.3
1	B	555	VAL	8.2
1	B	572	GLY	7.8
1	A	574	GLY	7.8
1	B	644	ALA	7.6
1	A	647	PHE	7.5
1	A	646	VAL	7.5
1	B	571	PHE	7.5
1	A	551	LYS	7.3
1	B	646	VAL	6.8
1	A	572	GLY	6.6
1	B	549	LYS	6.6
1	B	1001	MET	6.5
1	B	550	GLY	6.4
1	B	570	GLN	6.3
1	B	647	PHE	6.1
1	A	466	LYS	5.9
1	A	567	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	553	GLU	5.9
1	B	552	LYS	5.6
1	B	551	LYS	5.6
1	B	645	THR	5.6
1	A	570	GLN	5.5
1	A	645	THR	5.5
1	A	549	LYS	5.4
1	A	411	LEU	5.2
1	A	1002	SER	5.1
1	A	471	LEU	5.0
1	A	565	GLU	5.0
1	A	468	ALA	5.0
1	A	641	LEU	5.0
1	A	484	GLY	4.9
1	B	569	LYS	4.8
1	B	574	GLY	4.8
1	A	576	THR	4.8
1	A	564	LEU	4.7
1	A	553	GLU	4.7
1	A	425	ALA	4.7
1	B	548	GLY	4.6
1	A	415	LYS	4.6
1	A	550	GLY	4.6
1	B	466	LYS	4.5
1	A	1485	THR	4.5
1	A	547	LYS	4.5
1	B	584	GLY	4.5
1	A	1003	ASN	4.4
1	A	424	PRO	4.4
1	A	1486	ALA	4.4
1	A	562	GLY	4.4
1	B	411	LEU	4.4
1	A	1001	MET	4.4
1	A	578	GLN	4.4
1	A	488	GLY	4.3
1	B	468	ALA	4.3
1	A	560	THR	4.3
1	B	611	LEU	4.3
1	A	525	TYR	4.3
1	B	575	ALA	4.2
1	A	467	MET	4.2
1	A	554	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	648	HIS	4.2
1	B	413	SER	4.2
1	B	414	GLY	4.2
1	A	493	ILE	4.2
1	B	556	ALA	4.2
1	B	1003	ASN	4.1
1	A	573	LYS	4.1
1	B	554	GLU	4.1
1	A	575	ALA	4.1
1	A	568	ARG	4.1
1	A	607	THR	4.1
1	A	469	ASP	4.0
1	B	489	ALA	4.0
1	A	465	ALA	4.0
1	A	605	ARG	3.9
1	A	533	GLY	3.9
1	A	496	ALA	3.9
1	B	412	LEU	3.9
1	A	481	TYR	3.9
1	A	485	ALA	3.8
1	B	523	TYR	3.8
1	B	471	LEU	3.7
1	B	576	THR	3.7
1	A	423	ASN	3.7
1	B	1485	THR	3.7
1	B	573	LYS	3.7
1	A	556	ALA	3.7
1	A	555	VAL	3.6
1	B	557	TYR	3.6
1	B	1486	ALA	3.6
1	A	611	LEU	3.6
1	A	643	GLU	3.6
1	A	616	ARG	3.6
1	B	612	ALA	3.5
1	A	476	ILE	3.5
1	A	569	LYS	3.5
1	A	606	VAL	3.4
1	B	1002	SER	3.4
1	A	648	HIS	3.4
1	A	422	LYS	3.4
1	A	470	ILE	3.4
1	B	581	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	557	TYR	3.3
1	A	614	ALA	3.3
1	A	642	GLU	3.3
1	A	412	LEU	3.3
1	A	534	HIS	3.2
1	B	467	MET	3.2
1	A	1484	ASP	3.2
1	B	486	GLY	3.2
1	A	608	ILE	3.2
1	A	543	TYR	3.2
1	A	497	ASN	3.2
1	A	480	ILE	3.1
1	A	615	GLU	3.1
1	B	472	LYS	3.1
1	B	562	GLY	3.1
1	A	487	VAL	3.1
1	A	523	TYR	3.1
1	B	579	ARG	3.1
1	B	491	PHE	3.1
1	A	561	ASP	3.1
1	A	559	TRP	3.1
1	A	472	LYS	3.1
1	B	614	ALA	3.0
1	A	1005	GLN	3.0
1	A	414	GLY	3.0
1	A	546	SER	3.0
1	A	552	LYS	3.0
1	A	585	GLU	2.9
1	B	415	LYS	2.9
1	A	491	PHE	2.9
1	B	559	TRP	2.9
1	A	584	GLY	2.9
1	A	622[A]	MET	2.9
1	B	421	SER	2.9
1	A	563	GLU	2.9
1	A	490	ASP	2.9
1	B	465	ALA	2.9
1	A	494	GLU	2.8
1	B	610	ASP	2.8
1	B	593	GLU	2.8
1	A	580	TYR	2.8
1	A	625	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	489	ALA	2.8
1	B	564	LEU	2.8
1	B	493	ILE	2.8
5	G	9	DG	2.8
1	B	492	SER	2.8
1	A	1004	ILE	2.8
1	B	582	GLY	2.8
1	B	606	VAL	2.8
1	B	547	LYS	2.7
1	A	499	ASP	2.7
1	B	495	ASP	2.7
1	A	577	LEU	2.7
1	B	568	ARG	2.7
1	A	531	GLU	2.7
1	A	1295	GLY	2.7
1	B	546	SER	2.7
1	A	603	LEU	2.6
1	B	558	ALA	2.6
1	B	578	GLN	2.6
1	B	590	GLN	2.6
4	H	3	DC	2.6
1	B	544	LYS	2.6
1	B	543	TYR	2.6
1	B	1014	GLY	2.6
1	B	616	ARG	2.6
1	B	567	LEU	2.5
1	B	607	THR	2.5
1	B	418	PRO	2.5
1	A	475	GLU	2.5
1	B	1309	GLU	2.5
1	B	469	ASP	2.5
1	A	500	LYS	2.5
1	A	539	LEU	2.5
1	B	529	LEU	2.5
1	B	560	THR	2.5
4	H	2	DA	2.4
4	H	10	DA	2.4
1	A	566	GLU	2.4
1	B	475	GLU	2.4
1	A	589	ASP	2.4
1	B	481	TYR	2.4
1	B	498	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	618	VAL	2.4
1	A	532	ALA	2.4
1	B	561	ASP	2.4
1	B	580	TYR	2.3
1	B	1200	LYS	2.3
1	B	532	ALA	2.3
1	B	1271	LYS	2.3
1	B	494	GLU	2.3
1	B	476	ILE	2.3
1	A	413	SER	2.3
1	A	610	ASP	2.3
1	B	585	GLU	2.3
1	A	420	GLN	2.3
1	A	1250	GLY	2.3
1	A	474	GLU	2.3
1	A	477	ASN	2.2
1	A	619	ASN	2.2
1	A	483	ILE	2.2
1	A	462	THR	2.2
1	B	613	ARG	2.2
1	A	1006	ASN	2.2
1	B	609	GLU	2.2
1	A	604	ILE	2.2
1	B	534	HIS	2.2
1	A	431	LEU	2.2
1	A	521	PHE	2.2
1	B	1484	ASP	2.2
1	A	640	THR	2.2
1	B	531	GLU	2.2
1	A	1304	LYS	2.2
2	E	9	DT	2.2
1	B	525	TYR	2.1
1	A	586	MET	2.1
1	B	605	ARG	2.1
1	A	1223	ASP	2.1
1	B	470	ILE	2.1
1	A	459	VAL	2.1
1	A	620	VAL	2.1
1	B	1005	GLN	2.1
1	A	461	ASN	2.1
1	A	501	ILE	2.1
1	B	608	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	536	TYR	2.1
4	H	1	DA	2.1
1	B	1342	ILE	2.1
1	A	535	VAL	2.1
1	B	496	ALA	2.1
1	B	1019	ARG	2.1
1	A	486	GLY	2.1
1	A	498	TYR	2.1
1	A	492	SER	2.1
1	B	542	LEU	2.0
1	B	1310	LEU	2.0
1	B	632	TRP	2.0
1	A	528	PRO	2.0
1	B	490	ASP	2.0
1	A	530	VAL	2.0
1	B	1007	MET	2.0
3	F	1	DG	2.0
1	B	527	ARG	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
8	MG	B	1504	1/1	0.77	0.11	9,9,9,9	0
6	MLA	A	1502	7/7	0.79	0.14	24,26,28,28	0
8	MG	B	1502	1/1	0.81	0.10	15,15,15,15	0
7	ACT	A	1504	4/4	0.83	0.13	22,22,23,23	0
9	CL	A	1508	1/1	0.86	0.14	17,17,17,17	0

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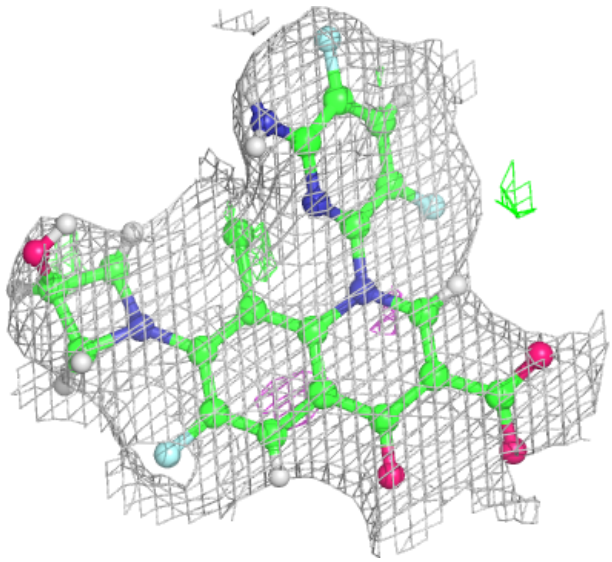
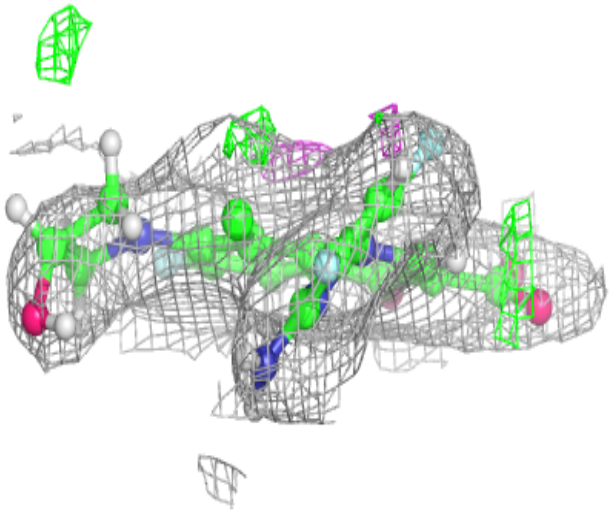
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	TE9	H	101	30/30	0.88	0.15	30,42,45,45	1
11	TE9	F	101	30/30	0.89	0.12	22,25,29,30	1
6	MLA	A	1501	7/7	0.89	0.11	23,23,24,24	0
8	MG	A	1507	1/1	0.90	0.06	17,17,17,17	0
9	CL	B	1505	1/1	0.91	0.06	15,15,15,15	0
8	MG	A	1505	1/1	0.91	0.04	11,11,11,11	0
8	MG	A	1506	1/1	0.91	0.12	8,8,8,8	0
7	ACT	A	1503	4/4	0.93	0.11	13,13,13,14	0
10	MPD	B	1501	8/8	0.94	0.11	11,12,14,30	1
8	MG	B	1503	1/1	0.96	0.07	12,12,12,12	0

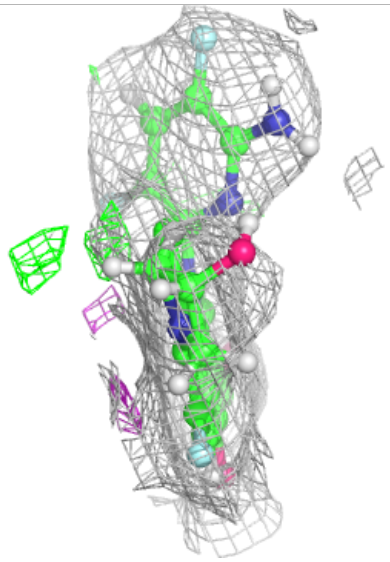
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TE9 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)

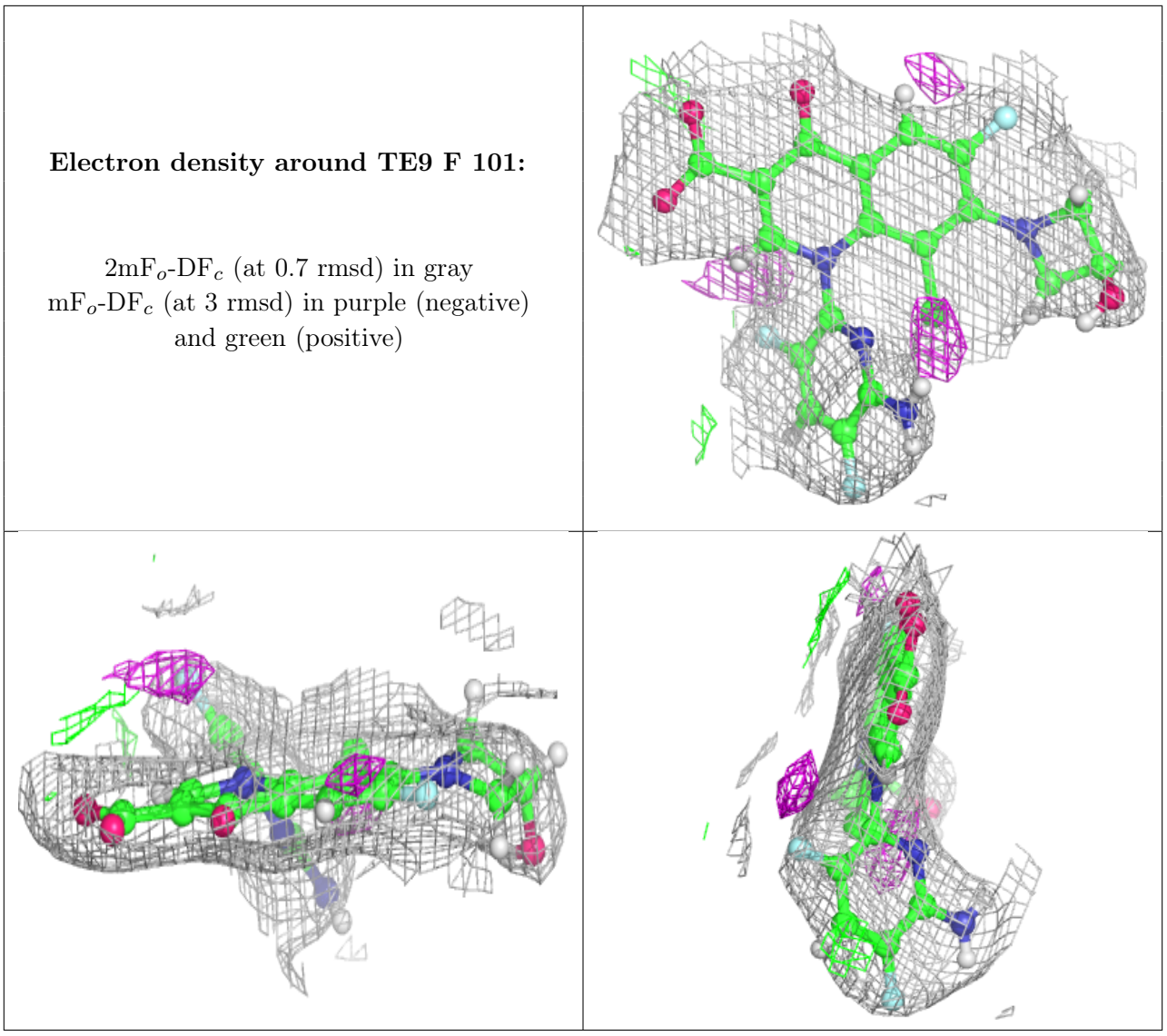






Electron density around TE9 F 101:

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



6.5 Other polymers (i)

There are no such residues in this entry.