



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 12:08 pm BST

PDB ID : 4Z53
Title : Quinolone(Trovaflaxacin)-DNA cleavage complex of topoisomerase IV from *S. pneumoniae*
Authors : Laponogov, I.; Veselkov, D.A.; Pan, X.-S.; Selvarajah, J.; Crevel, I.M.-T.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2015-04-02
Resolution : 3.26 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

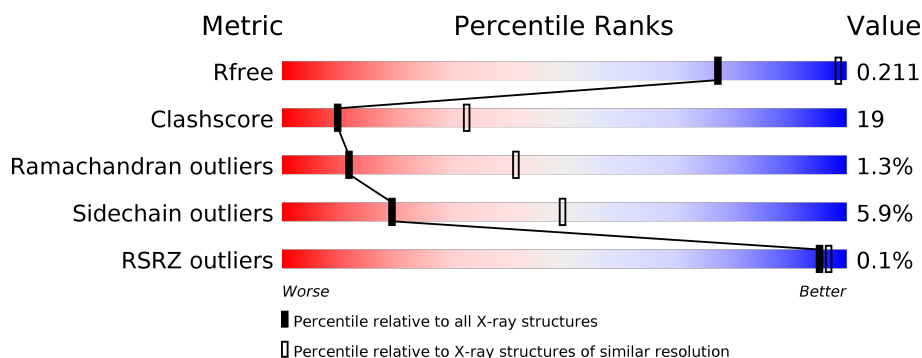
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 on 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	<div> <div>67%</div> <div>22%</div> <div>• 7%</div> </div>
1	B	742	<div> <div>66%</div> <div>25%</div> <div>• 6%</div> </div>
2	E	7	<div> <div>14%</div> <div>86%</div> </div>
3	F	11	<div> <div>36%</div> <div>64%</div> </div>
4	G	7	<div> <div>29%</div> <div>71%</div> </div>
5	H	11	<div> <div>9%</div> <div>91%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11112 atoms, of which 28 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	690	Total	C	N	O	S	0	0	0
			5138	3258	892	969	19			
1	B	695	Total	C	N	O	S	0	0	0
			5148	3265	887	978	18			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	403	MET	-	expression tag	UNP Q59961
A	460	ILE	VAL	engineered mutation	UNP Q59961
A	996	ALA	-	linker	UNP Q59961
A	997	THR	-	linker	UNP Q59961
A	998	VAL	-	linker	UNP Q59961
A	999	PHE	-	linker	UNP Q59961
A	1000	HIS	-	linker	UNP Q59961
A	1001	MET	-	linker	UNP Q59961
A	1002	SER	-	linker	UNP Q59961
A	1257	THR	ILE	engineered mutation	UNP P72525
A	1485	THR	-	expression tag	UNP P72525
A	1486	ALA	-	expression tag	UNP P72525
A	1487	LYS	-	expression tag	UNP P72525
A	1488	ALA	-	expression tag	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	-	expression tag	UNP Q59961
B	460	ILE	VAL	engineered mutation	UNP Q59961

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Chain	Residue	Modelled	Actual	Comment	Reference
B	996	ALA	-	linker	UNP Q59961
B	997	THR	-	linker	UNP Q59961
B	998	VAL	-	linker	UNP Q59961
B	999	PHE	-	linker	UNP Q59961
B	1000	HIS	-	linker	UNP Q59961
B	1001	MET	-	linker	UNP Q59961
B	1002	SER	-	linker	UNP Q59961
B	1257	THR	ILE	engineered mutation	UNP P72525
B	1485	THR	-	expression tag	UNP P72525
B	1486	ALA	-	expression tag	UNP P72525
B	1487	LYS	-	expression tag	UNP P72525
B	1488	ALA	-	expression tag	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 E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	P	0	0	0
			140	69	27	38	6			

- Molecule 3 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	11	Total	C	N	O	P	0	0	0
			225	108	39	67	11			

- Molecule 4 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	7	Total	C	N	O	P	0	0	0
			139	68	25	40	6			

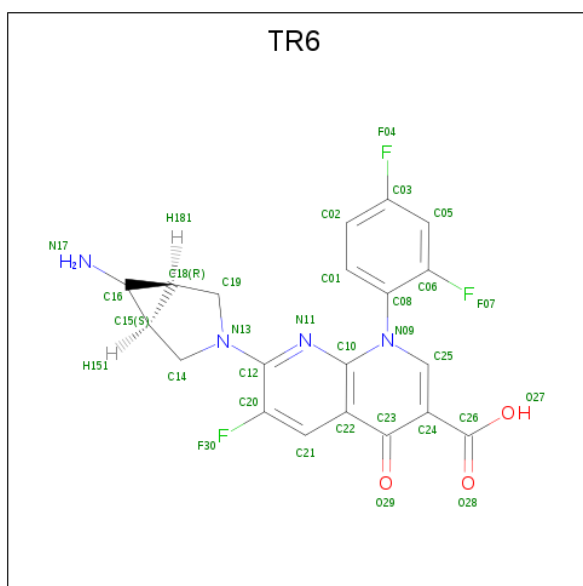
- Molecule 5 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	11	Total	C	N	O	P	0	0	0
			226	107	43	65	11			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Mg	0	0
			2	2		
6	A	2	Total	Mg	0	0
			2	2		

- Molecule 7 is Trovafloxacin (three-letter code: TR6) (formula: C₂₀H₁₅F₃N₄O₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	F	1	Total	C	F	H	N	O	0	0
			44	20	3	14	4	3		
7	H	1	Total	C	F	H	N	O	0	0
			44	20	3	14	4	3		

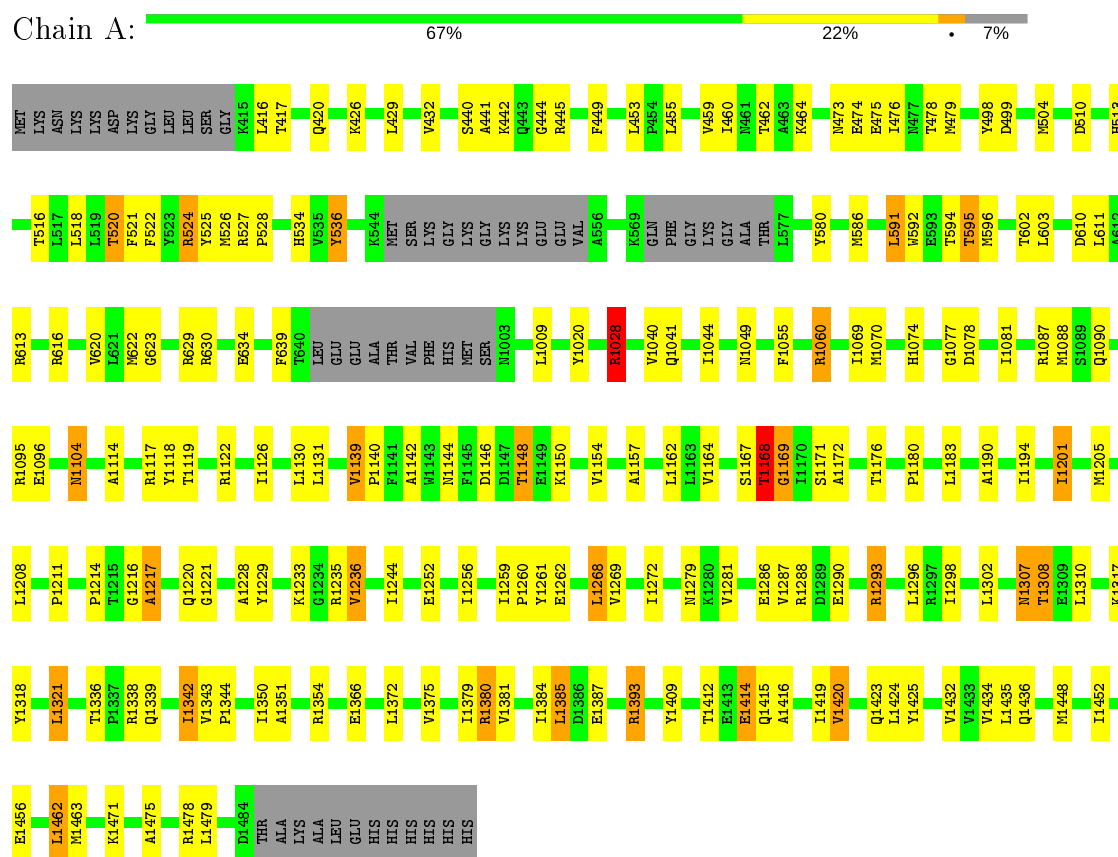
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	O	0	0
			3	3		
8	B	1	Total	O	0	0
			1	1		

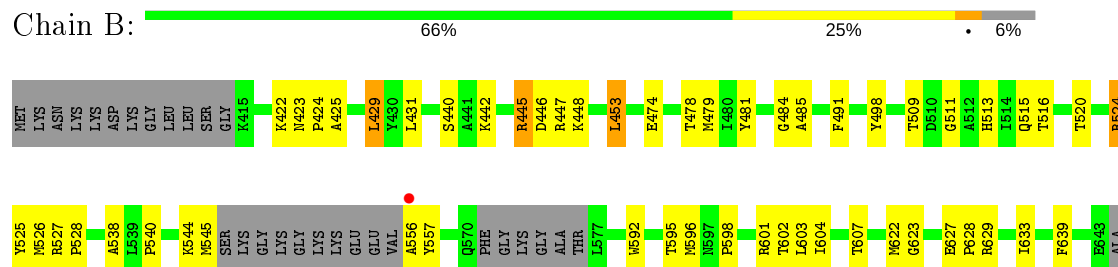
3 Residue-property plots

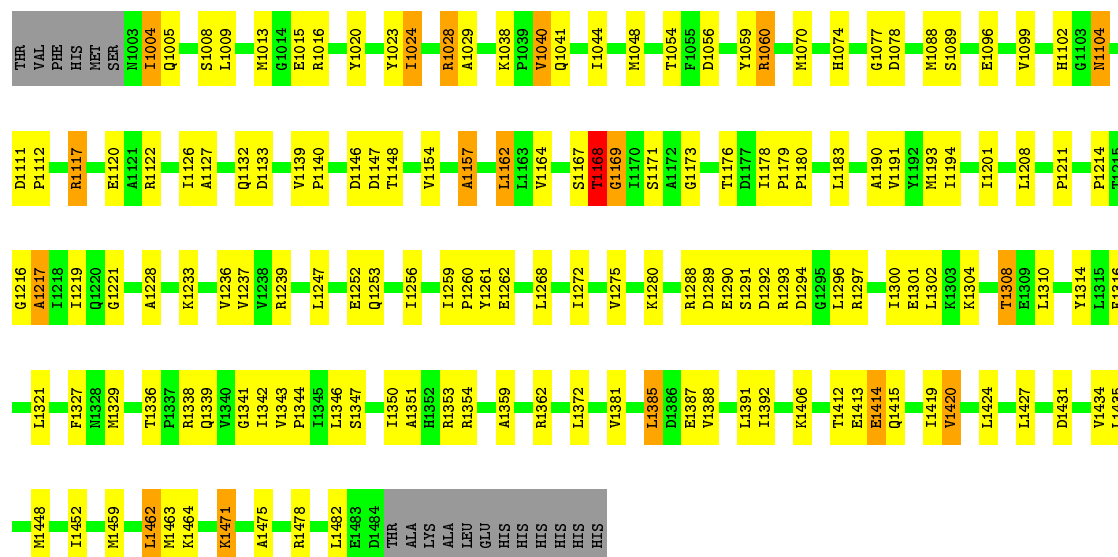
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

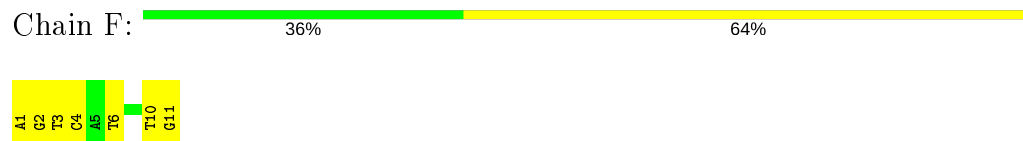




- Molecule 2: E-site DNA



- Molecule 3: E-site DNA



- Molecule 4: E-site DNA



- Molecule 5: E-site DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.83Å 157.83Å 210.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	73.90 – 3.26 73.90 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.9 (73.90-3.26) 95.0 (73.90-3.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.173 , 0.207 0.175 , 0.211	Depositor DCC
R_{free} test set	3039 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11112	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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, TR6

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	0.23	0/5224	0.42	0/7102
1	B	0.23	0/5236	0.42	0/7123
2	E	0.51	0/157	1.08	0/241
3	F	0.48	0/251	1.22	3/385 (0.8%)
4	G	0.48	0/155	1.12	1/238 (0.4%)
5	H	0.47	0/253	1.04	0/388
All	All	0.26	0/11276	0.51	4/15477 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	6	DT	O4'-C4'-C3'	-7.99	101.21	106.00
3	F	6	DT	O4'-C1'-N1	5.38	111.77	108.00
4	G	11	DT	N3-C4-O4	5.27	123.06	119.90
3	F	10	DT	C1'-O4'-C4'	-5.01	105.09	110.10

There are no chirality outliers.

There are no planarity outliers.

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	5138	0	4821	196	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5148	0	4781	188	0
2	E	140	0	78	9	0
3	F	225	0	126	8	0
4	G	139	0	78	5	0
5	H	226	0	124	13	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	F	30	14	14	1	0
7	H	30	14	14	0	0
8	A	3	0	0	1	0
8	B	1	0	0	0	0
All	All	11084	28	10036	404	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 19.

The worst 5 of 404 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:545:MET:HB3	1:B:556:ALA:CB	1.69	1.21
1:B:545:MET:CB	1:B:556:ALA:HB3	1.71	1.20
1:B:1117:ARG:HH11	1:B:1117:ARG:HG2	1.05	1.17
1:A:1146:ASP:HB3	1:A:1148:THR:HG22	1.27	1.13
1:A:1293:ARG:HB3	1:A:1293:ARG:HH11	1.13	1.12

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	682/742 (92%)	630 (92%)	45 (7%)	7 (1%)	15 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	689/742 (93%)	627 (91%)	51 (7%)	11 (2%)	9	37
All	All	1371/1484 (92%)	1257 (92%)	96 (7%)	18 (1%)	12	41

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1307	ASN
1	B	1168	THR
1	B	1157	ALA
1	B	1293	ARG
1	A	1104	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	480/635 (76%)	450 (94%)	30 (6%)	18	47
1	B	474/635 (75%)	448 (94%)	26 (6%)	21	52
All	All	954/1270 (75%)	898 (94%)	56 (6%)	19	50

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1385	LEU
1	B	445	ARG
1	B	1385	LEU
1	A	1393	ARG
1	A	1420	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1253	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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
7	TR6	H	101	6	26,34,34	1.82	8 (30%)	31,53,53	1.79	8 (25%)
7	TR6	F	101	6	26,34,34	1.82	9 (34%)	31,53,53	1.96	9 (29%)

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
7	TR6	H	101	6	-	0/8/29/29	0/5/5/5
7	TR6	F	101	6	-	3/8/29/29	0/5/5/5

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	101	TR6	C24-C26	3.78	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	101	TR6	C24-C26	3.62	1.50	1.47
7	H	101	TR6	C12-N13	3.52	1.46	1.37
7	F	101	TR6	C12-N13	3.43	1.46	1.37
7	H	101	TR6	C12-N11	3.43	1.35	1.31

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	101	TR6	C25-N09-C10	4.81	122.64	118.14
7	F	101	TR6	C25-N09-C10	4.31	122.17	118.14
7	F	101	TR6	C21-C20-C12	-3.83	119.27	121.73
7	H	101	TR6	C21-C20-C12	-3.36	119.58	121.73
7	F	101	TR6	N11-C12-N13	-3.31	115.27	117.62

There are no chirality outliers.

All (3) torsion outliers are listed below:

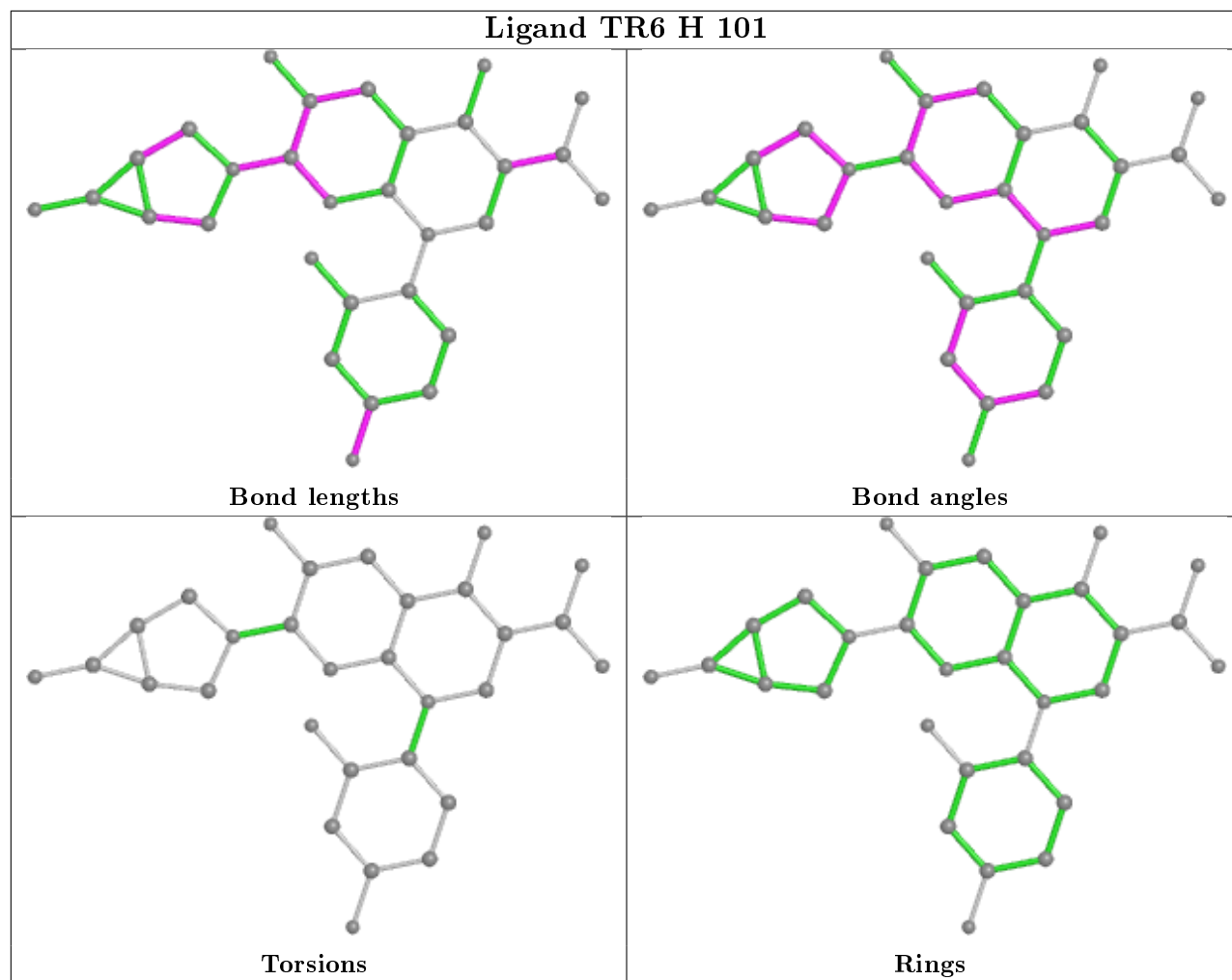
Mol	Chain	Res	Type	Atoms
7	F	101	TR6	C06-C08-N09-C10
7	F	101	TR6	C20-C12-N13-C14
7	F	101	TR6	N11-C12-N13-C14

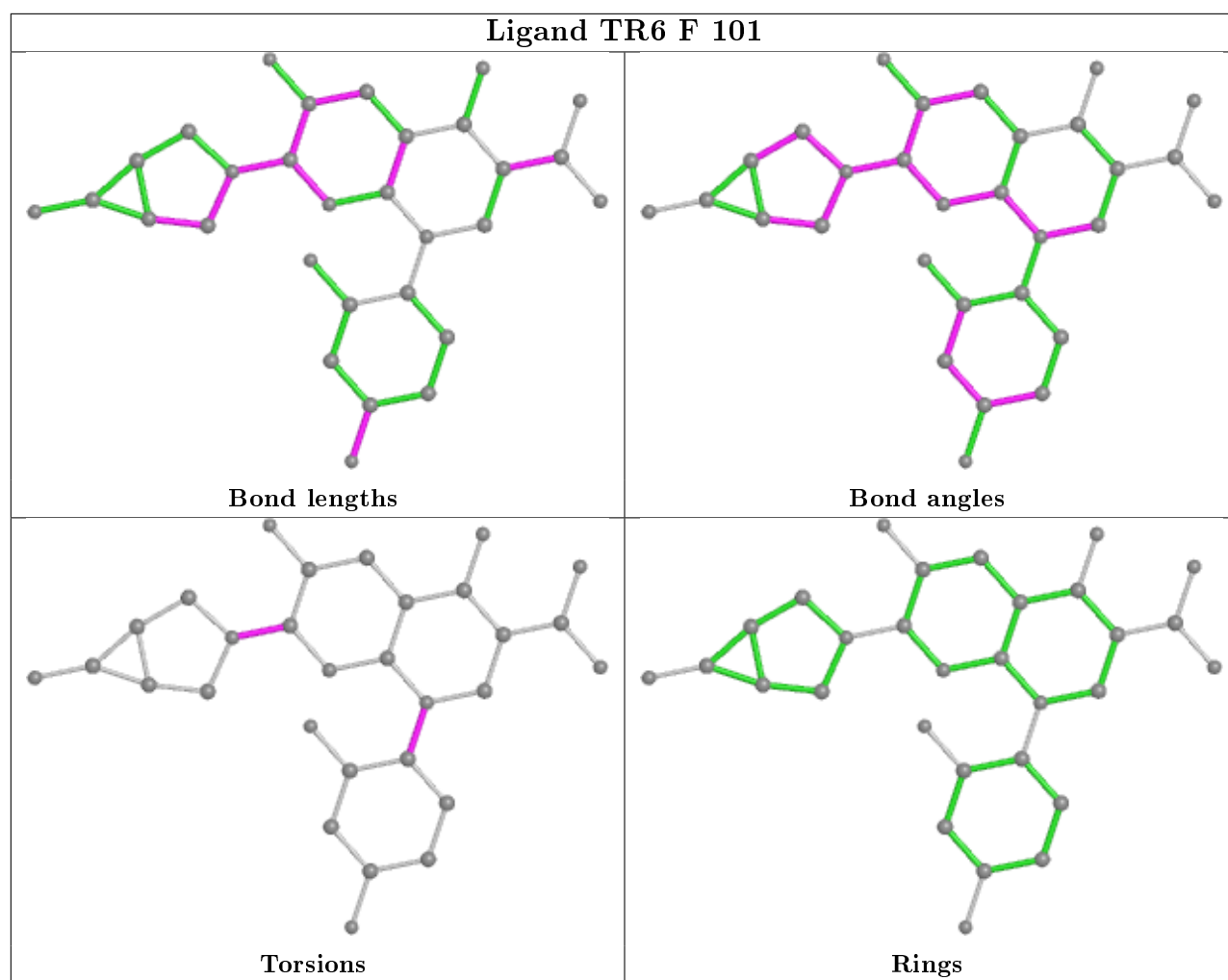
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	101	TR6	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 ⓘ

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	690/742 (92%)	-0.57	0 100 100	46, 79, 138, 173	0
1	B	695/742 (93%)	-0.60	1 (0%) 95 97	47, 77, 145, 184	0
2	E	7/7 (100%)	-0.49	0 100 100	79, 84, 108, 130	0
3	F	11/11 (100%)	-0.58	0 100 100	81, 99, 138, 144	0
4	G	7/7 (100%)	-0.41	0 100 100	72, 78, 106, 129	0
5	H	11/11 (100%)	-0.57	0 100 100	81, 97, 131, 140	0
All	All	1421/1520 (93%)	-0.58	1 (0%) 95 97	46, 79, 141, 184	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	556	ALA	2.4

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 carbohydrates in this entry.

6.4 Ligands ⓘ

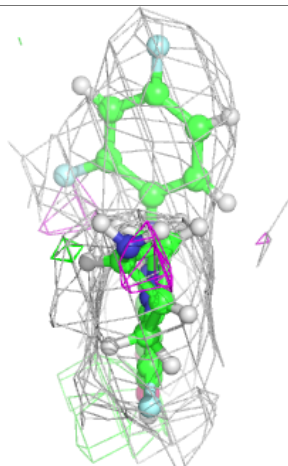
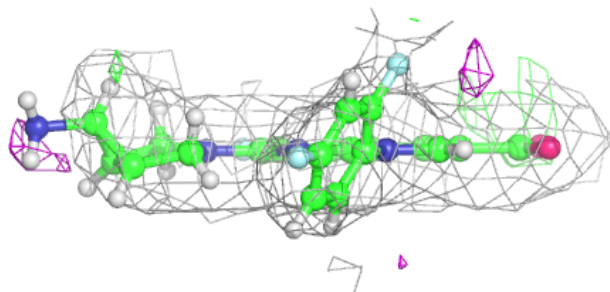
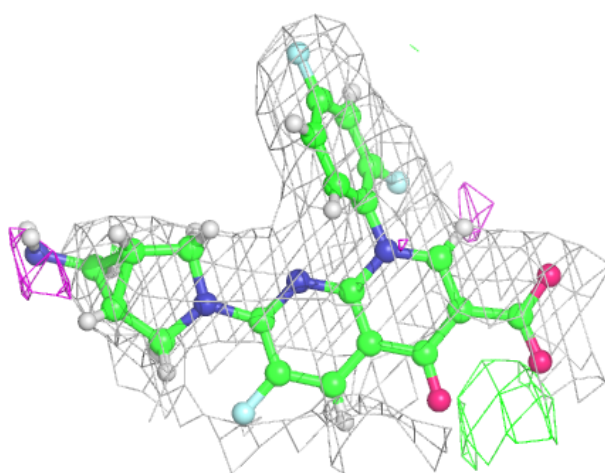
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	B	1502	1/1	0.32	0.29	84,84,84,84	0
6	MG	A	1502	1/1	0.69	0.33	90,90,90,90	0
6	MG	A	1501	1/1	0.92	0.37	92,92,92,92	0
7	TR6	H	101	30/30	0.94	0.19	95,120,141,165	0
7	TR6	F	101	30/30	0.95	0.20	84,109,134,154	0
6	MG	B	1501	1/1	0.95	0.45	101,101,101,101	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.

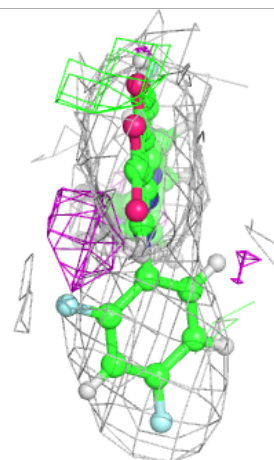
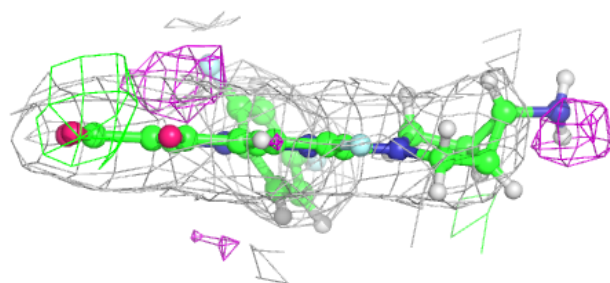
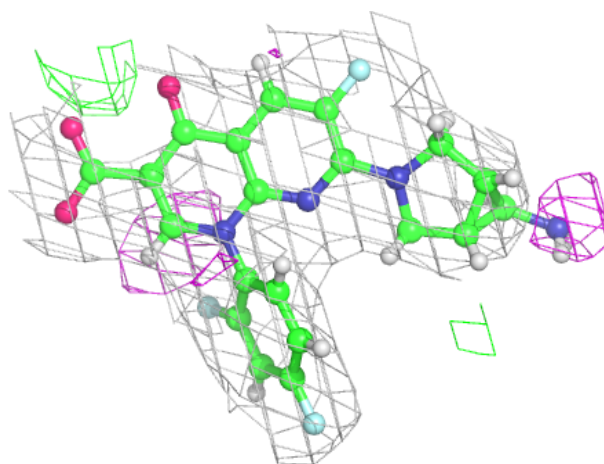
Electron density around TR6 H 101:

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 TR6 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.