



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 05:18 PM EST

PDB ID : 6WAA
Title : K. pneumoniae Topoisomerase IV (ParE-ParC) in complex with DNA and compound 34 (7-[(1S,5R)-1-amino-3-azabicyclo[3.1.0]hexan-3-yl]-4-(aminomethyl)-1-cyclopropyl-3,6-difluoro-8-methylquinolin-2(1H)-one)
Authors : Noeske, J.; Shu, W.; Bellamacina, C.
Deposited on : 2020-03-24
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

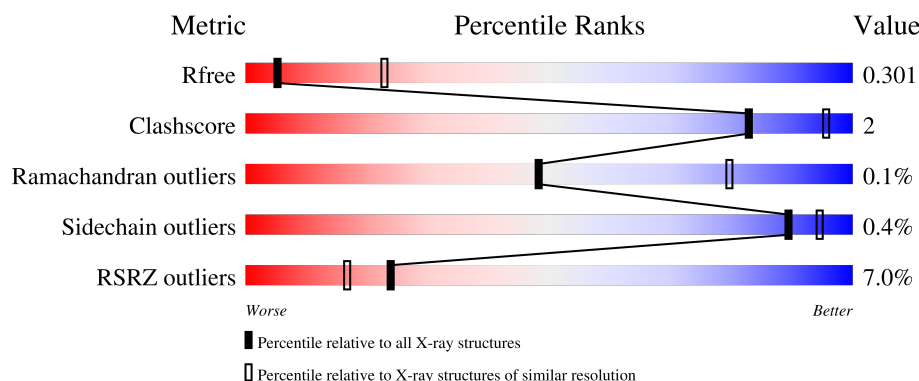
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	743	
1	D	743	
1	F	743	
1	H	743	

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Mol	Chain	Length	Quality of chain
2	I	11	 82%18%
2	L	11	 73%18%9%
2	M	11	 82%18%
2	P	11	 82%18%
3	J	15	 73%20%7%
3	K	15	 7%87%7%7%
3	N	15	 80%20%
3	O	15	 67%20%13%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 39965 atoms, of which 18474 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 (ATP-hydrolyzing) chimera.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	B	702	Total	C	H	N	O	P	S	0	0	0
			10037	3269	4832	929	981	1	25			
1	D	637	Total	C	H	N	O	P	S	0	0	0
			7767	2655	3494	782	819	1	16			
1	F	707	Total	C	H	N	O	P	S	0	0	0
			10011	3273	4801	927	984	1	25			
1	H	656	Total	C	H	N	O	P	S	0	0	0
			8865	2960	4190	830	864	1	20			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	389	MET	-	initiating methionine	UNP A0A377Y395
B	999	GLU	-	linker	UNP A0A377Y395
B	1000	PHE	-	linker	UNP A0A377Y395
B	1255	THR	SER	variant	UNP A0A377XIN8
B	1491	LEU	-	expression tag	UNP A0A377XIN8
B	1492	GLU	-	expression tag	UNP A0A377XIN8
B	1493	HIS	-	expression tag	UNP A0A377XIN8
B	1494	HIS	-	expression tag	UNP A0A377XIN8
B	1495	HIS	-	expression tag	UNP A0A377XIN8
B	1496	HIS	-	expression tag	UNP A0A377XIN8
B	1497	HIS	-	expression tag	UNP A0A377XIN8
B	1498	HIS	-	expression tag	UNP A0A377XIN8
D	389	MET	-	initiating methionine	UNP A0A377Y395
D	999	GLU	-	linker	UNP A0A377Y395
D	1000	PHE	-	linker	UNP A0A377Y395
D	1255	THR	SER	variant	UNP A0A377XIN8
D	1491	LEU	-	expression tag	UNP A0A377XIN8
D	1492	GLU	-	expression tag	UNP A0A377XIN8
D	1493	HIS	-	expression tag	UNP A0A377XIN8
D	1494	HIS	-	expression tag	UNP A0A377XIN8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1495	HIS	-	expression tag	UNP A0A377XIN8
D	1496	HIS	-	expression tag	UNP A0A377XIN8
D	1497	HIS	-	expression tag	UNP A0A377XIN8
D	1498	HIS	-	expression tag	UNP A0A377XIN8
F	389	MET	-	initiating methionine	UNP A0A377Y395
F	999	GLU	-	linker	UNP A0A377Y395
F	1000	PHE	-	linker	UNP A0A377Y395
F	1255	THR	SER	variant	UNP A0A377XIN8
F	1491	LEU	-	expression tag	UNP A0A377XIN8
F	1492	GLU	-	expression tag	UNP A0A377XIN8
F	1493	HIS	-	expression tag	UNP A0A377XIN8
F	1494	HIS	-	expression tag	UNP A0A377XIN8
F	1495	HIS	-	expression tag	UNP A0A377XIN8
F	1496	HIS	-	expression tag	UNP A0A377XIN8
F	1497	HIS	-	expression tag	UNP A0A377XIN8
F	1498	HIS	-	expression tag	UNP A0A377XIN8
H	389	MET	-	initiating methionine	UNP A0A377Y395
H	999	GLU	-	linker	UNP A0A377Y395
H	1000	PHE	-	linker	UNP A0A377Y395
H	1255	THR	SER	variant	UNP A0A377XIN8
H	1491	LEU	-	expression tag	UNP A0A377XIN8
H	1492	GLU	-	expression tag	UNP A0A377XIN8
H	1493	HIS	-	expression tag	UNP A0A377XIN8
H	1494	HIS	-	expression tag	UNP A0A377XIN8
H	1495	HIS	-	expression tag	UNP A0A377XIN8
H	1496	HIS	-	expression tag	UNP A0A377XIN8
H	1497	HIS	-	expression tag	UNP A0A377XIN8
H	1498	HIS	-	expression tag	UNP A0A377XIN8

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

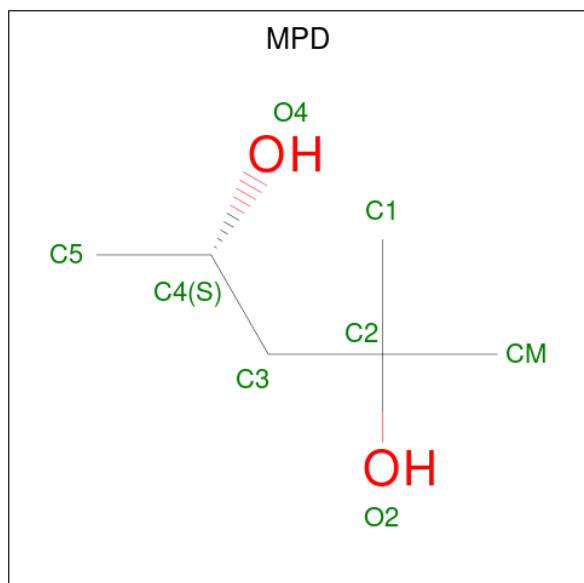
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	I	9	Total	C	H	N	O	P	0	0	0
			289	89	104	31	56	9			
2	L	10	Total	C	H	N	O	P	0	0	0
			321	99	116	33	63	10			
2	M	11	Total	C	H	N	O	P	0	0	0
			353	109	128	35	70	11			
2	P	9	Total	C	H	N	O	P	0	0	0
			289	89	104	31	56	9			

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

CP*GP*TP*AP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	J	14	Total	C	H	N	O	P	0	0	0
			426	137	143	55	78	13			
3	K	15	Total	C	H	N	O	P	0	0	0
			471	147	167	60	83	14			
3	N	15	Total	C	H	N	O	P	0	0	0
			471	147	167	60	83	14			
3	O	13	Total	C	H	N	O	P	0	0	0
			406	127	144	50	73	12			

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

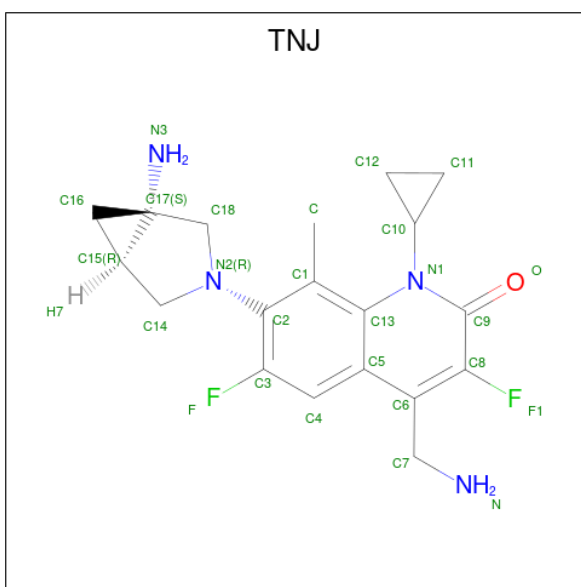
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	Mg 2	0	0
5	D	1	Total 1	Mg 1	0	0
5	F	3	Total 3	Mg 3	0	0
5	H	1	Total 1	Mg 1	0	0
5	I	1	Total 1	Mg 1	0	0
5	L	1	Total 1	Mg 1	0	0
5	M	1	Total 1	Mg 1	0	0
5	O	1	Total 1	Mg 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Cl 1	0	0
6	H	1	Total 1	Cl 1	0	0

- Molecule 7 is 7-[(1S,5R)-1-amino-3-azabicyclo[3.1.0]hexan-3-yl]-4-(aminomethyl)-1-cyclopropyl-3,6-difluoro-8-methylquinolin-2(1H)-one (three-letter code: TNJ) (formula: C₁₉H₂₂F₂N₄O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	J	1	Total	C	F	N	O	0	0
			26	19	2	4	1		
7	J	1	Total	C	F	N	O	0	0
			26	19	2	4	1		
7	N	1	Total	C	F	N	O	0	0
			26	19	2	4	1		
7	N	1	Total	C	F	N	O	0	0
			26	19	2	4	1		

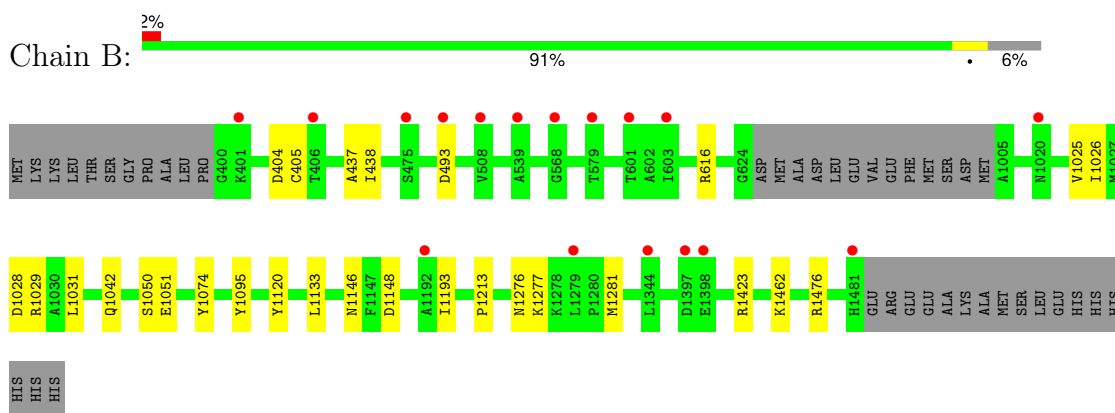
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	O	0	0
			1	1		
8	D	3	Total	O	0	0
			3	3		
8	F	4	Total	O	0	0
			4	4		
8	H	1	Total	O	0	0
			1	1		
8	N	1	Total	O	0	0
			1	1		

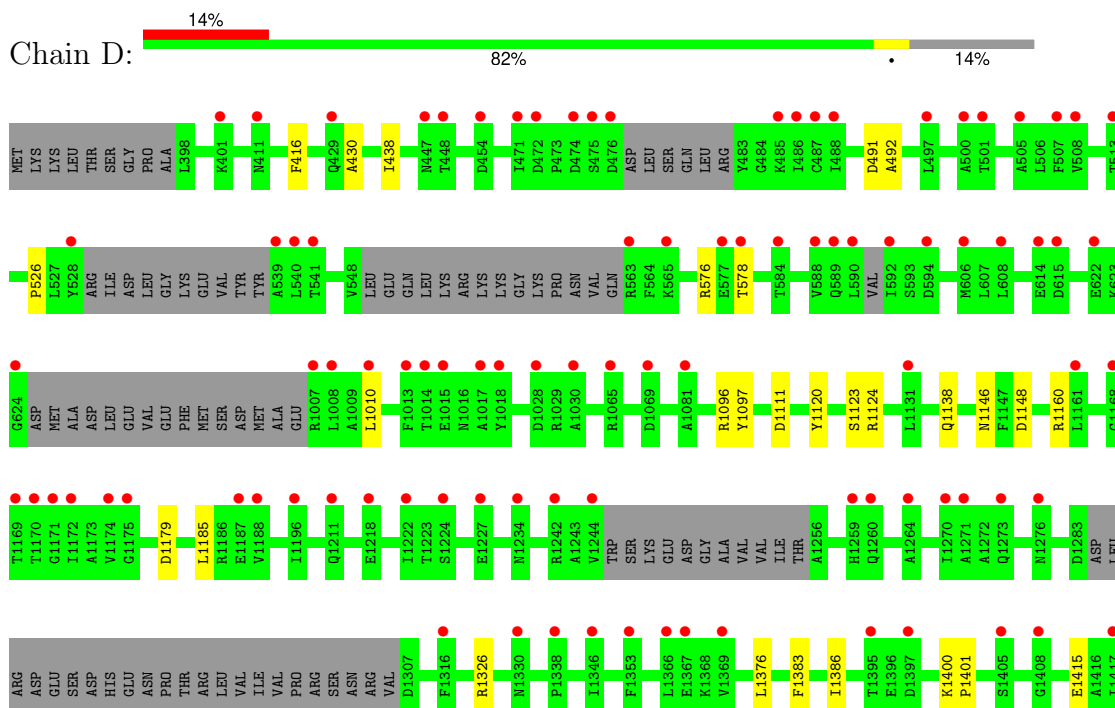
3 Residue-property plots [i](#)

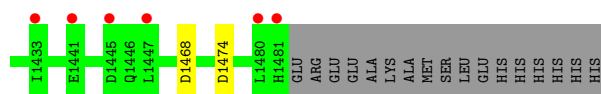
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA topoisomerase 4 subunit B,DNA topoisomerase (ATP-hydrolyzing) chimera



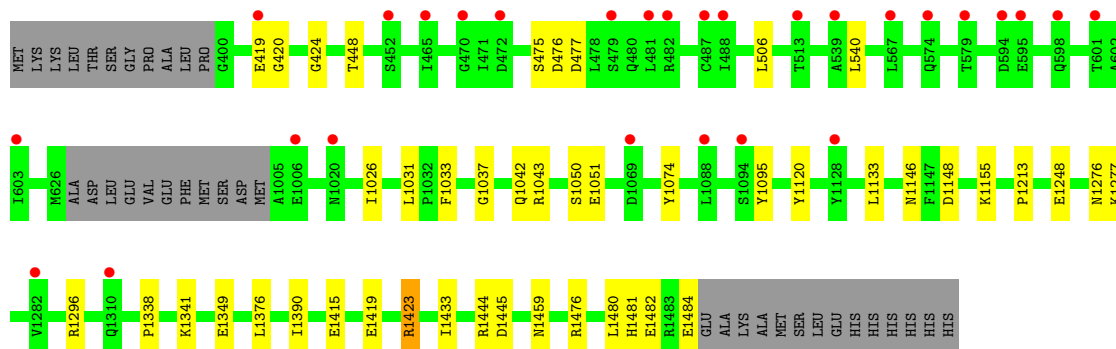
- Molecule 1: DNA topoisomerase 4 subunit B,DNA topoisomerase (ATP-hydrolyzing) chimera





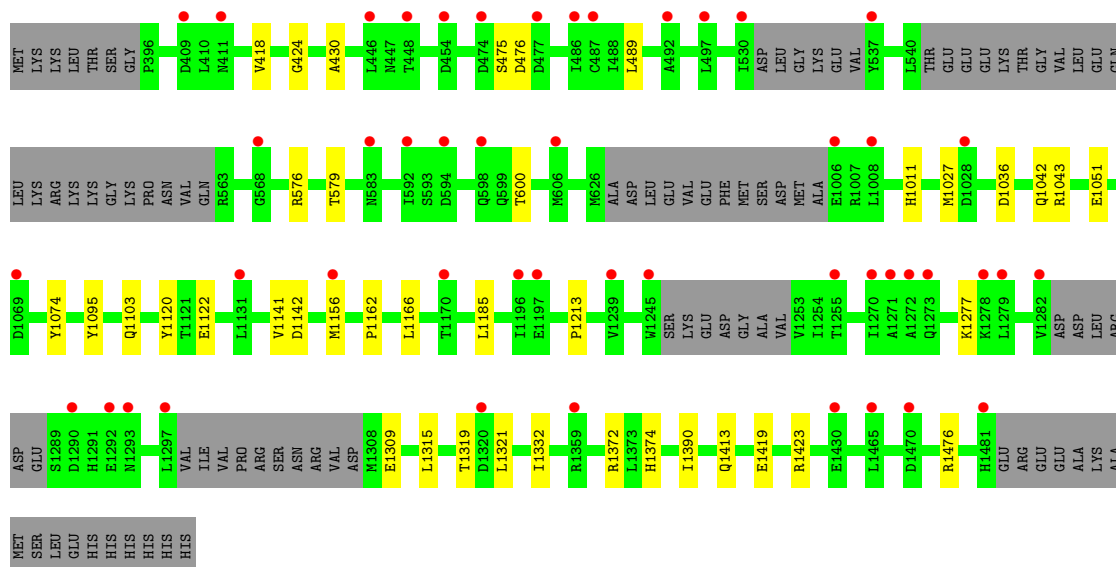
- Molecule 1: DNA topoisomerase 4 subunit B,DNA topoisomerase (ATP-hydrolyzing) chimera

Chain F: 4% 89% 6% 5%



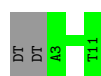
- Molecule 1: DNA topoisomerase 4 subunit B,DNA topoisomerase (ATP-hydrolyzing) chimera

Chain H: 6% 83% 5% 12%



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

Chain I: 82% 18%

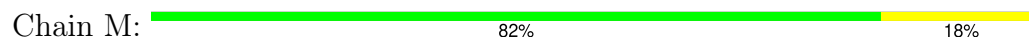


- Molecule 2: DNA (5'-D(*TP*TP*AP*CP*GP*TP*TP*GP*TP*AP*T)-3')

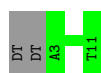
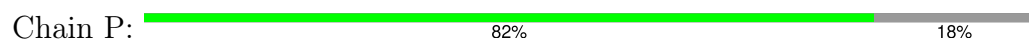
Chain L: 73% 18% 9%



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



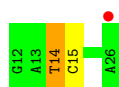
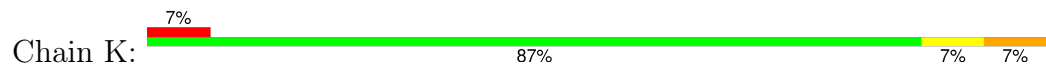
- Molecule 2: DNA (5'-D(*TP*TP*AP*CP*GP*TP*TP*GP*TP*AP*T)-3')



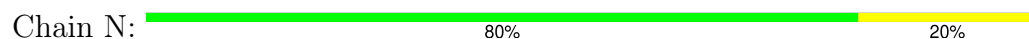
- Molecule 3: DNA (5'-D(*GP*AP*TP*CP*AP*TP*AP*CP*AP*AP*CP*GP*TP*AP*A)-3')



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.59Å 157.48Å 144.06Å 90.00° 94.93° 90.00°	Depositor
Resolution (Å)	82.08 – 3.20 82.08 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (82.08-3.20) 99.5 (82.08-3.20)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.274 , 0.301 0.274 , 0.301	Depositor DCC
R_{free} test set	3280 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	79.1	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 79.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	39965	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.60% 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, CL, PTR, TNJ, MPD

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	B	0.23	0/5276	0.40	0/7167
1	D	0.23	0/4325	0.39	0/5910
1	F	0.24	0/5282	0.40	0/7177
1	H	0.23	0/4739	0.40	0/6451
2	I	0.62	0/206	1.07	0/316
2	L	0.57	0/228	1.11	0/350
2	M	0.51	0/250	1.11	0/384
2	P	0.52	0/206	1.02	0/316
3	J	0.61	0/318	0.90	0/489
3	K	0.53	0/342	0.90	1/526 (0.2%)
3	N	0.50	0/342	0.88	0/526
3	O	0.53	0/294	0.89	0/452
All	All	0.28	0/21808	0.50	1/30064 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	14	DT	P-O3'-C3'	5.63	126.46	119.70

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	B	5205	4832	4848	13	0
1	D	4273	3494	3503	17	0
1	F	5210	4801	4801	25	0
1	H	4675	4190	4190	25	0
2	I	185	104	104	0	0
2	L	205	116	116	1	0
2	M	225	128	128	1	0
2	P	185	104	104	0	0
3	J	283	143	156	4	0
3	K	304	167	167	2	0
3	N	304	167	167	2	0
3	O	262	144	145	2	0
4	B	16	28	28	1	0
4	D	8	14	14	0	0
4	F	8	14	14	0	0
4	H	16	28	28	2	0
5	B	2	0	0	0	0
5	D	1	0	0	0	0
5	F	3	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	O	1	0	0	0	0
6	B	1	0	0	0	0
6	H	1	0	0	0	0
7	J	52	0	0	0	0
7	N	52	0	0	1	0
8	B	1	0	0	0	0
8	D	3	0	0	1	0
8	F	4	0	0	0	0
8	H	1	0	0	0	0
8	N	1	0	0	1	0
All	All	21491	18474	18513	87	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 2.

The worst 5 of 87 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:F:1043:ARG:NH1	1:F:1155:LYS:O	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1146:ASN:ND2	1:B:1148:ASP:OD1	2.15	0.79
1:H:1036:ASP:OD2	1:H:1043:ARG:NH1	2.20	0.74
1:H:489:LEU:HD22	1:H:579:THR:HG21	1.70	0.73
1:F:1419:GLU:OE2	1:H:1423:ARG:NH2	2.22	0.72

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	B	697/743 (94%)	679 (97%)	18 (3%)	0	100	100
1	D	620/743 (83%)	604 (97%)	16 (3%)	0	100	100
1	F	702/743 (94%)	679 (97%)	21 (3%)	2 (0%)	37	69
1	H	641/743 (86%)	623 (97%)	18 (3%)	0	100	100
All	All	2660/2972 (90%)	2585 (97%)	73 (3%)	2 (0%)	48	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	1481	HIS
1	F	475	SER

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	B	482/639 (75%)	479 (99%)	3 (1%)	84	92
1	D	314/639 (49%)	314 (100%)	0	100	100
1	F	472/639 (74%)	470 (100%)	2 (0%)	89	94
1	H	391/639 (61%)	390 (100%)	1 (0%)	91	96
All	All	1659/2556 (65%)	1653 (100%)	6 (0%)	89	94

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1423	ARG
1	F	1459	ASN
1	H	1277	LYS
1	B	1028	ASP
1	B	493	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	PTR	B	1120	3,1	15,16,17	1.26	1 (6%)	17,22,24	0.63	0
1	PTR	D	1120	3,1	15,16,17	1.24	1 (6%)	17,22,24	0.61	0
1	PTR	F	1120	1	15,16,17	1.35	1 (6%)	17,22,24	0.50	0
1	PTR	H	1120	3,1	15,16,17	1.36	1 (6%)	17,22,24	0.56	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
1	PTR	B	1120	3,1	-	1/10/11/13	0/1/1/1
1	PTR	D	1120	3,1	-	1/10/11/13	0/1/1/1
1	PTR	F	1120	1	-	0/10/11/13	0/1/1/1
1	PTR	H	1120	3,1	-	1/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1120	PTR	OH-CZ	-4.60	1.30	1.40
1	H	1120	PTR	OH-CZ	-4.52	1.30	1.40
1	F	1120	PTR	OH-CZ	-4.51	1.30	1.40
1	D	1120	PTR	OH-CZ	-4.45	1.30	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1120	PTR	CZ-OH-P-O2P
1	D	1120	PTR	CZ-OH-P-O2P
1	H	1120	PTR	CZ-OH-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 13 are monoatomic - leaving 10 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	$\# Z > 2$
4	MPD	H	1502	-	7,7,7	0.30	0	9,10,10	0.38	0
4	MPD	F	1501	-	7,7,7	0.33	0	9,10,10	0.26	0
4	MPD	B	1501	-	7,7,7	0.32	0	9,10,10	0.30	0
4	MPD	H	1501	-	7,7,7	0.29	0	9,10,10	0.28	0
7	TNJ	J	101	-	27,30,30	1.10	2 (7%)	30,49,49	1.28	2 (6%)
7	TNJ	N	102	-	27,30,30	1.12	2 (7%)	30,49,49	1.43	2 (6%)
7	TNJ	N	101	-	27,30,30	1.11	1 (3%)	30,49,49	1.22	3 (10%)
4	MPD	B	1502	-	7,7,7	0.33	0	9,10,10	0.18	0
7	TNJ	J	102	-	27,30,30	1.17	2 (7%)	30,49,49	1.49	2 (6%)
4	MPD	D	1501	-	7,7,7	0.33	0	9,10,10	0.20	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
4	MPD	H	1502	-	-	0/5/5/5	-
4	MPD	F	1501	-	-	0/5/5/5	-
4	MPD	B	1501	-	-	0/5/5/5	-
4	MPD	H	1501	-	-	0/5/5/5	-
7	TNJ	J	101	-	-	2/8/29/29	0/5/5/5
7	TNJ	N	102	-	-	2/8/29/29	0/5/5/5
7	TNJ	N	101	-	-	4/8/29/29	0/5/5/5
4	MPD	B	1502	-	-	0/5/5/5	-
7	TNJ	J	102	-	-	3/8/29/29	0/5/5/5
4	MPD	D	1501	-	-	0/5/5/5	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	102	TNJ	C14-N2	2.63	1.50	1.46
7	N	102	TNJ	C14-N2	2.52	1.50	1.46
7	J	101	TNJ	C14-N2	2.36	1.50	1.46
7	N	101	TNJ	C14-N2	2.28	1.50	1.46
7	J	102	TNJ	C18-N2	2.21	1.50	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	102	TNJ	C14-N2-C2	-4.99	115.59	123.36
7	N	102	TNJ	C14-N2-C2	-4.42	116.47	123.36
7	J	101	TNJ	C14-N2-C2	-3.94	117.23	123.36
7	N	101	TNJ	C14-N2-C2	-3.48	117.94	123.36
7	N	102	TNJ	C-C1-C2	-3.38	114.61	121.20

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	101	TNJ	C3-C2-N2-C18
7	J	102	TNJ	C3-C2-N2-C18
7	N	101	TNJ	C3-C2-N2-C18
7	N	102	TNJ	C3-C2-N2-C18
7	N	101	TNJ	C11-C10-N1-C13

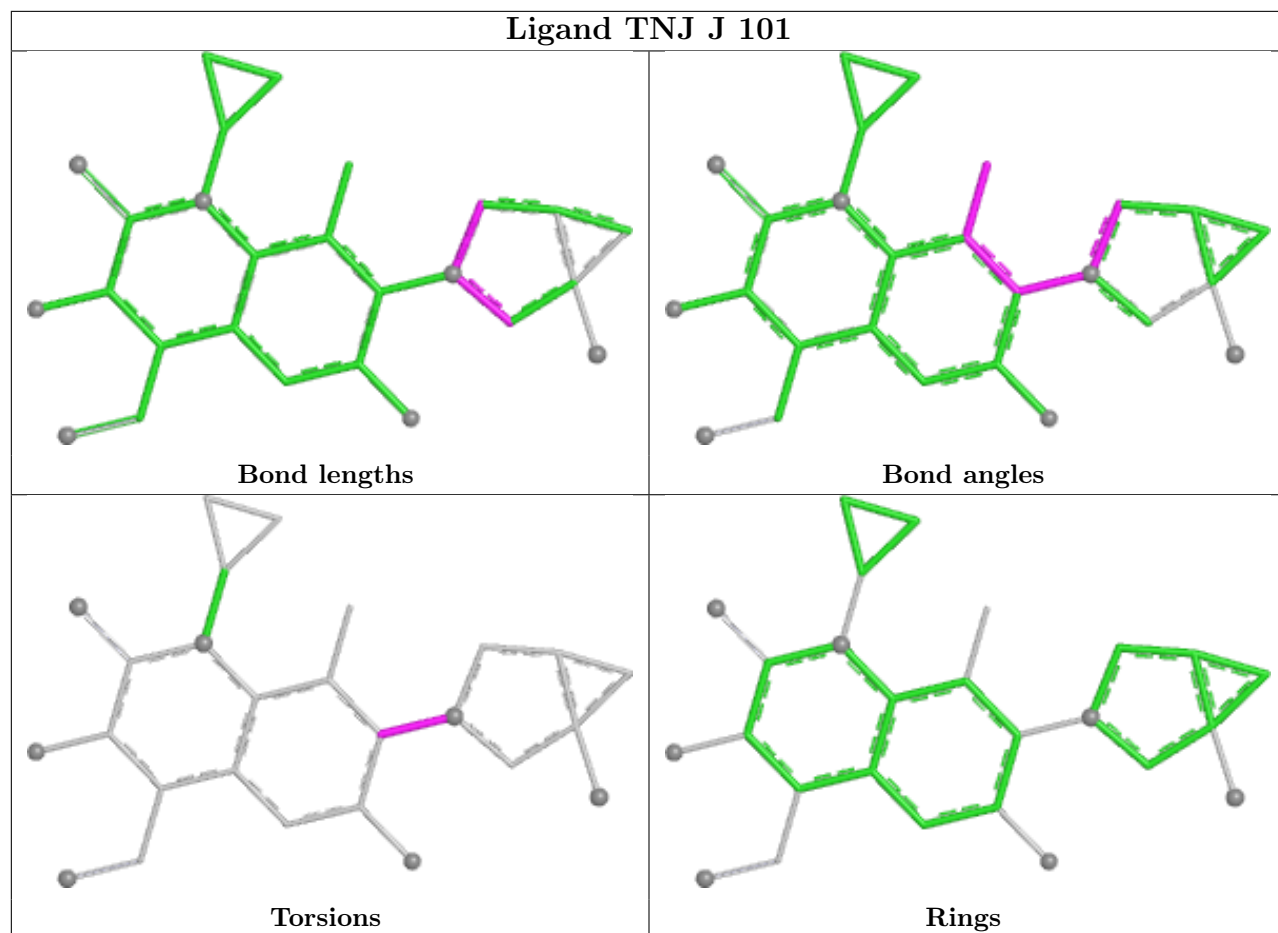
There are no ring outliers.

3 monomers are involved in 4 short contacts:

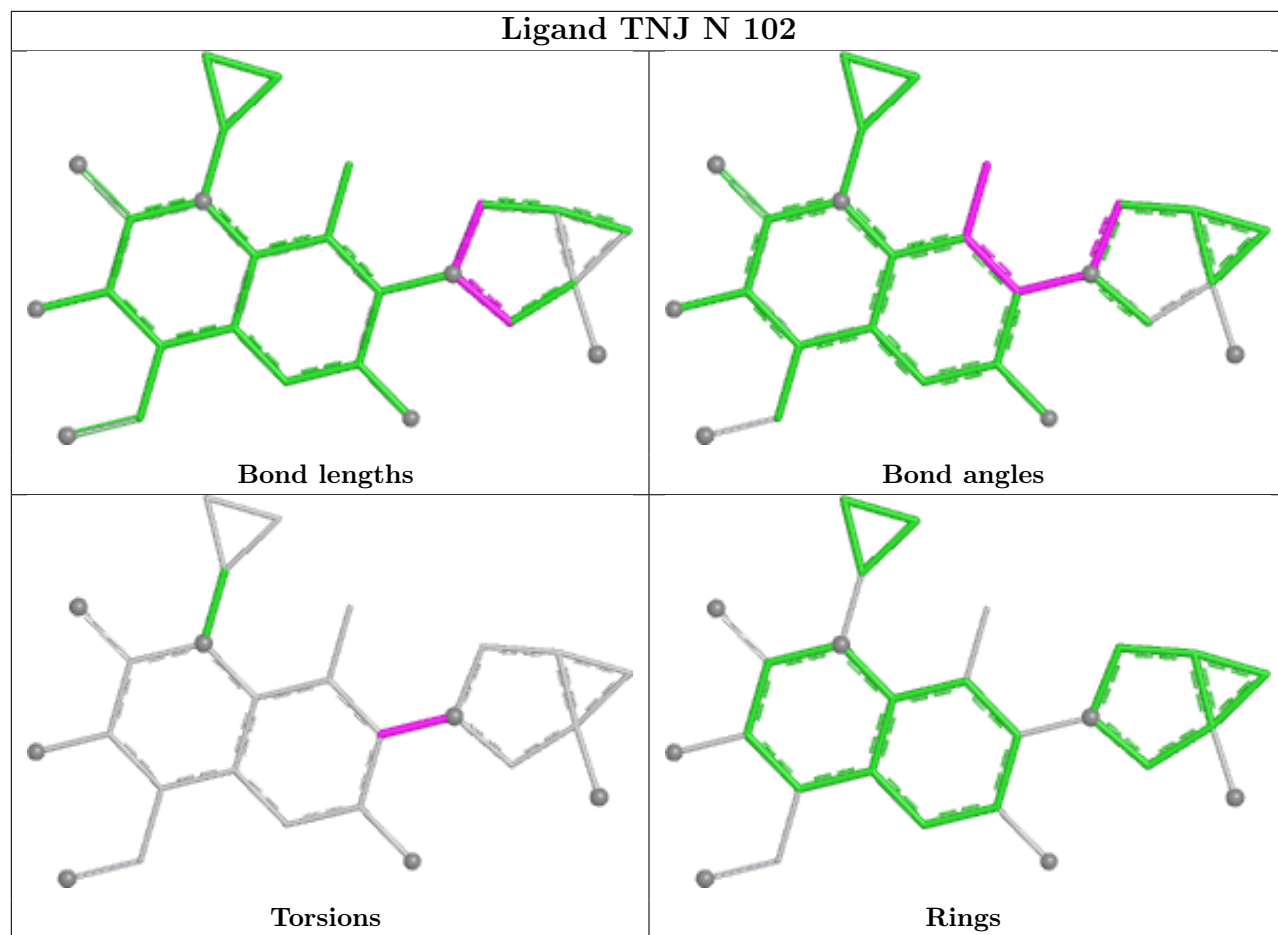
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1502	MPD	2	0
4	B	1501	MPD	1	0
7	N	102	TNJ	1	0

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.

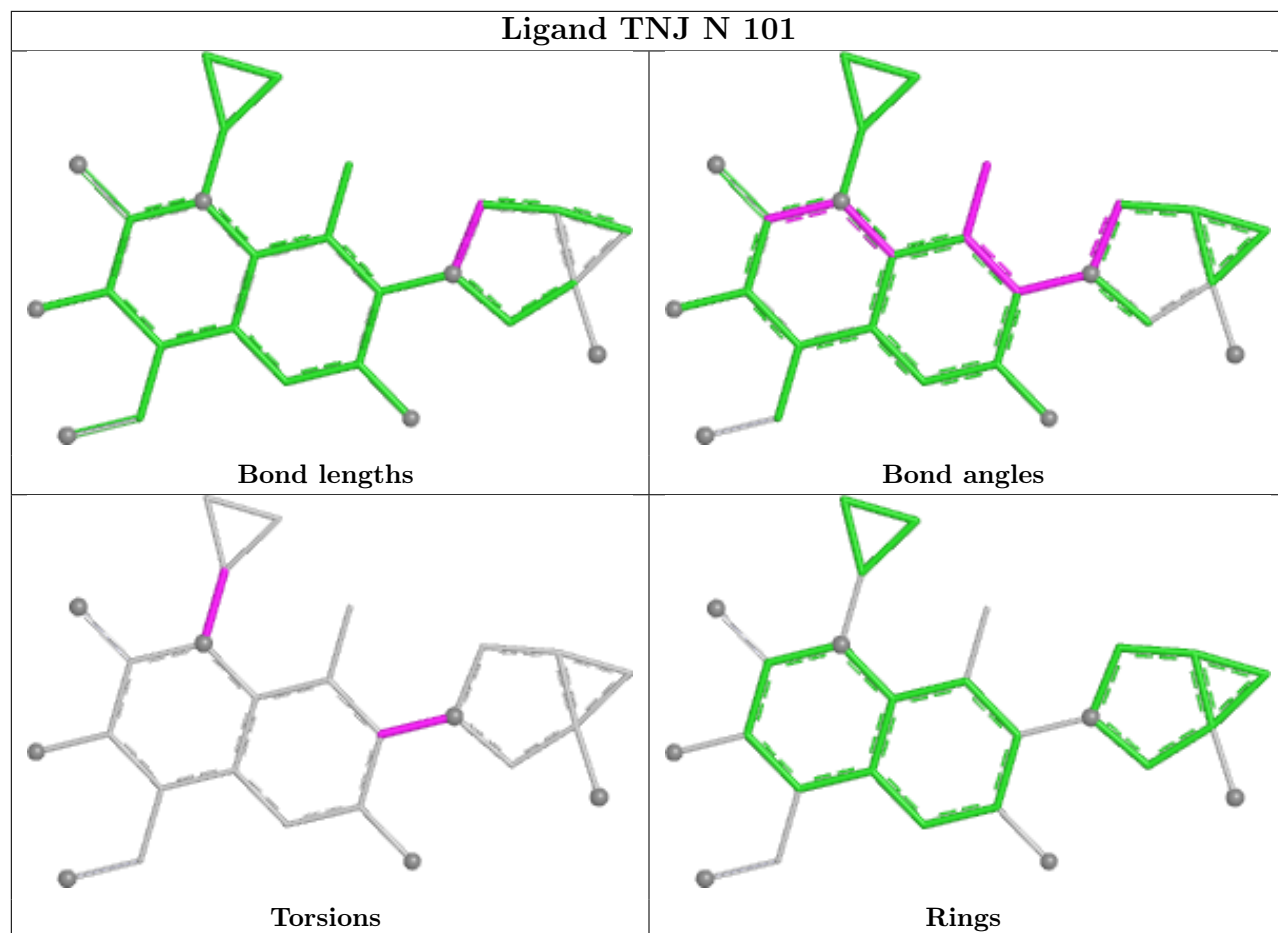
Ligand TNJ J 101

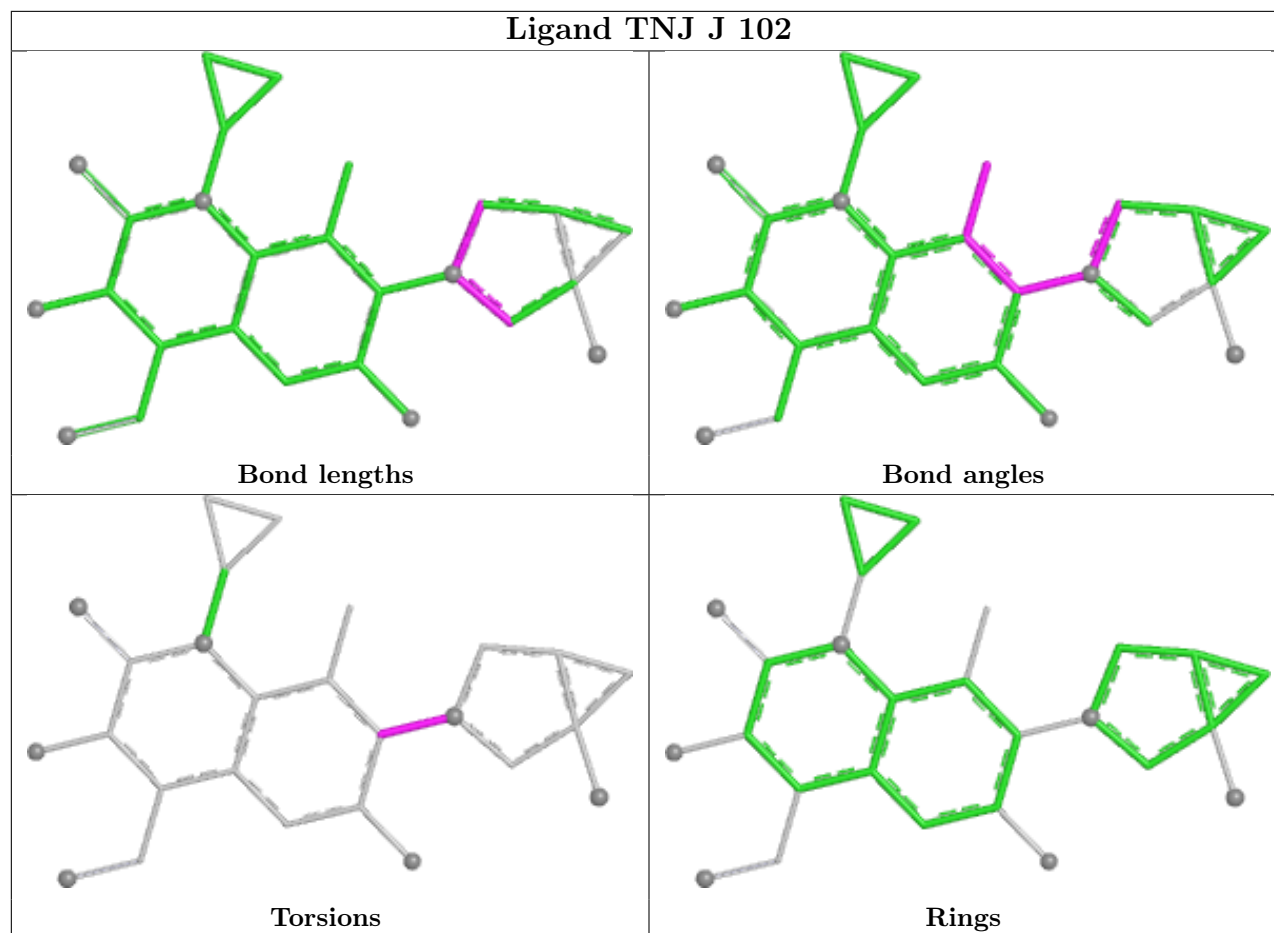


Ligand TNJ N 102



Ligand TNJ N 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	701/743 (94%)	0.36	17 (2%) 59 44	36, 71, 120, 148	0
1	D	636/743 (85%)	1.18	101 (15%) 6 4	74, 133, 173, 201	0
1	F	706/743 (95%)	0.37	28 (3%) 43 29	38, 70, 125, 154	0
1	H	655/743 (88%)	0.64	48 (7%) 22 16	48, 102, 156, 189	0
2	I	9/11 (81%)	0.30	0 100 100	59, 65, 137, 156	0
2	L	10/11 (90%)	0.72	0 100 100	105, 134, 221, 248	0
2	M	11/11 (100%)	0.19	0 100 100	52, 62, 114, 135	0
2	P	9/11 (81%)	0.24	0 100 100	83, 102, 155, 183	0
3	J	14/15 (93%)	0.30	0 100 100	62, 94, 114, 120	0
3	K	15/15 (100%)	1.01	1 (6%) 25 17	104, 128, 248, 251	0
3	N	15/15 (100%)	0.42	0 100 100	61, 78, 117, 124	0
3	O	13/15 (86%)	0.59	0 100 100	98, 112, 190, 212	0
All	All	2794/3076 (90%)	0.62	195 (6%) 24 17	36, 92, 157, 251	0

The worst 5 of 195 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	592	ILE	6.1
1	D	1408	GLY	4.7
1	D	1397	ASP	4.5
1	D	1316	PHE	4.4
1	D	1015	GLU	4.2

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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
1	PTR	D	1120	16/17	0.86	0.13	77,84,89,91	0
1	PTR	H	1120	16/17	0.89	0.13	68,77,82,85	0
1	PTR	B	1120	16/17	0.90	0.12	55,83,86,88	0
1	PTR	F	1120	16/17	0.91	0.12	57,76,78,79	0

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, 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
5	MG	H	1503	1/1	0.49	0.26	84,84,84,84	0
4	MPD	H	1502	8/8	0.58	0.23	12,12,69,69	0
4	MPD	B	1501	8/8	0.63	0.17	78,87,92,92	0
5	MG	D	1502	1/1	0.68	0.33	87,87,87,87	0
4	MPD	D	1501	8/8	0.78	0.24	82,85,93,96	0
5	MG	F	1503	1/1	0.79	0.26	64,64,64,64	0
5	MG	B	1504	1/1	0.80	0.25	71,71,71,71	0
4	MPD	F	1501	8/8	0.81	0.16	51,61,68,71	0
4	MPD	B	1502	8/8	0.81	0.16	12,12,76,76	0
5	MG	L	101	1/1	0.82	0.33	82,82,82,82	0
7	TNJ	J	102	26/26	0.82	0.17	121,122,122,123	0
4	MPD	H	1501	8/8	0.84	0.18	48,61,86,89	0
5	MG	F	1502	1/1	0.84	0.23	29,29,29,29	0
7	TNJ	J	101	26/26	0.85	0.15	72,77,83,83	0
7	TNJ	N	101	26/26	0.86	0.15	92,98,107,109	0
7	TNJ	N	102	26/26	0.88	0.14	74,78,84,86	0
5	MG	F	1504	1/1	0.89	0.26	30,30,30,30	0
5	MG	O	101	1/1	0.92	0.22	66,66,66,66	0
6	CL	B	1505	1/1	0.92	0.06	64,64,64,64	0
5	MG	I	101	1/1	0.93	0.29	39,39,39,39	0
5	MG	M	101	1/1	0.93	0.27	34,34,34,34	0
6	CL	H	1504	1/1	0.96	0.09	62,62,62,62	0

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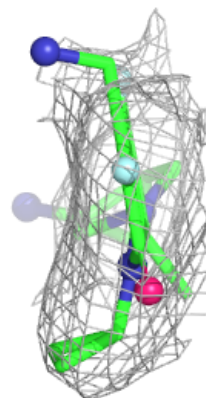
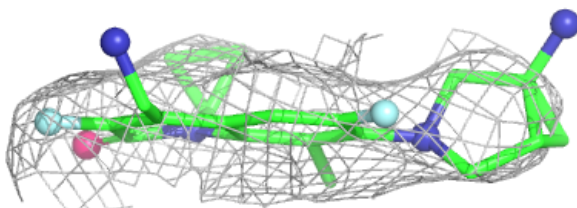
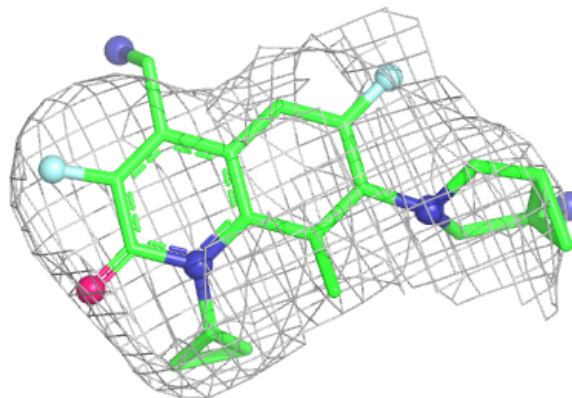
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	B	1503	1/1	0.97	0.22	35,35,35,35	0

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.

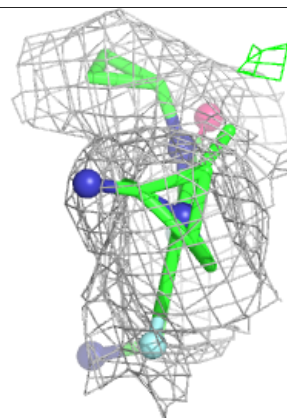
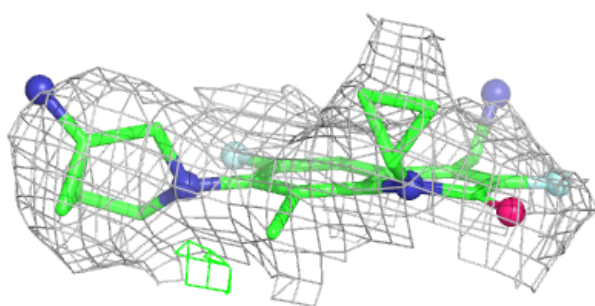
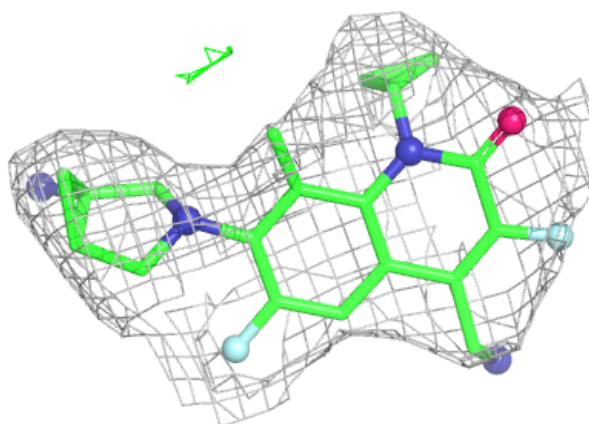
Electron density around TNJ J 102:

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

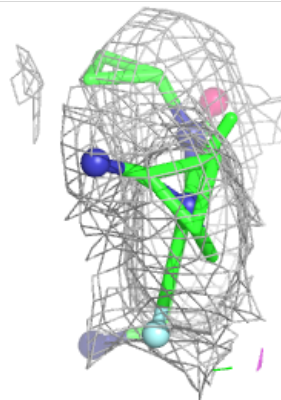
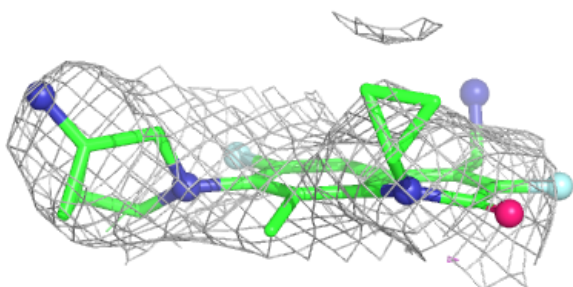
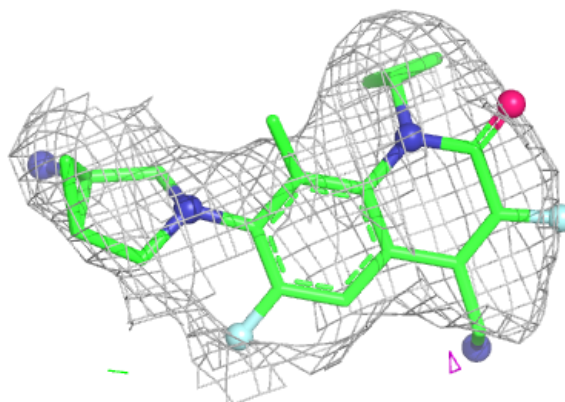


Electron density around TNJ J 101:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

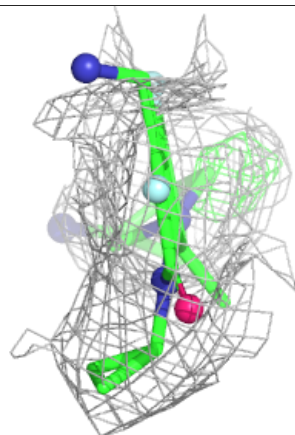
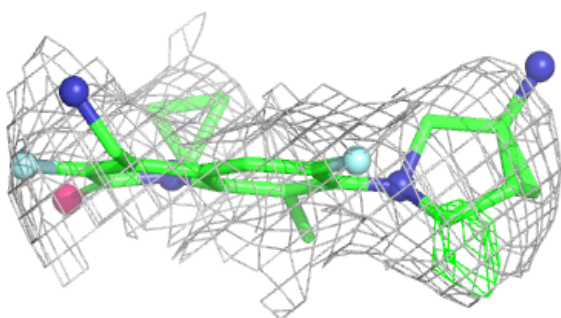
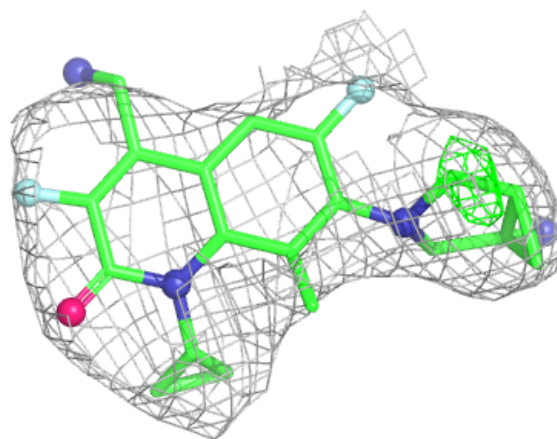
**Electron density around TNJ N 101:**

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



Electron density around TNJ N 102:

$2mF_o - DF_c$ (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.