



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2020 – 12:04 pm BST

PDB ID : 5UIM  
Title : X-ray structure of the FdtF N-formyltransferase from salmonella enteric O60  
in complex with folinic acid and TDP-Qui3N  
Authors : Woodford, C.R.; Thoden, J.B.; Holden, H.M.  
Deposited on : 2017-01-14  
Resolution : 2.20 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](mailto: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

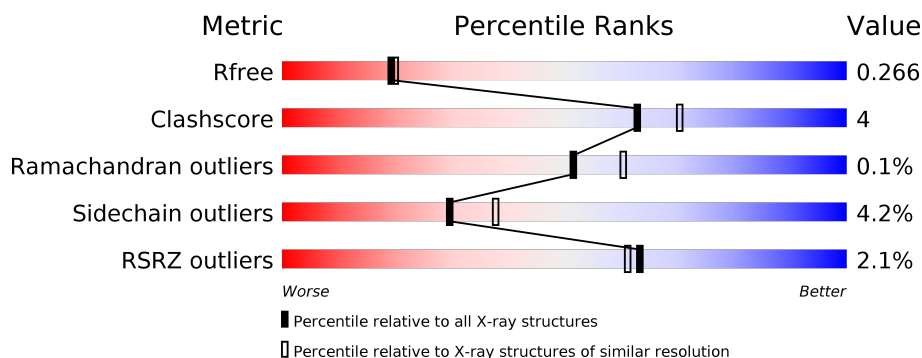
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	405	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>
1	B	405	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6878 atoms, of which 0 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.

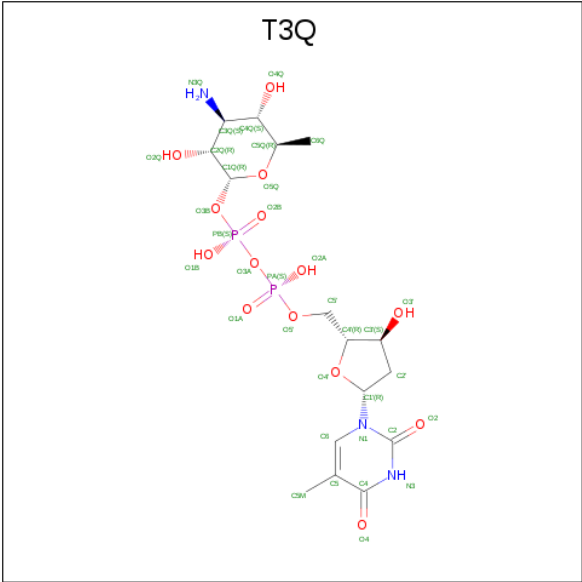
- Molecule 1 is a protein called Formyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3237	2101	514	610	12			
1	B	397	Total	C	N	O	S	0	3	0
			3242	2106	514	610	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP U3GK13
A	-5	GLY	-	expression tag	UNP U3GK13
A	-4	GLY	-	expression tag	UNP U3GK13
A	-3	GLY	-	expression tag	UNP U3GK13
A	-2	GLY	-	expression tag	UNP U3GK13
A	-1	GLY	-	expression tag	UNP U3GK13
A	0	HIS	-	expression tag	UNP U3GK13
A	395	ALA	GLU	engineered mutation	UNP U3GK13
B	-6	GLY	-	expression tag	UNP U3GK13
B	-5	GLY	-	expression tag	UNP U3GK13
B	-4	GLY	-	expression tag	UNP U3GK13
B	-3	GLY	-	expression tag	UNP U3GK13
B	-2	GLY	-	expression tag	UNP U3GK13
B	-1	GLY	-	expression tag	UNP U3GK13
B	0	HIS	-	expression tag	UNP U3GK13
B	395	ALA	GLU	engineered mutation	UNP U3GK13

- Molecule 2 is [(3R,4S,5S,6R)-4-amino-3,5-dihydroxy-6-methyloxan-2-yl][hydroxy-[[[(2R,3S,5R)-3-hydroxy-5-(5-methyl-2,4-dioxypyrimidin-1-yl)oxolan-2-yl]methoxy]phosphoryl]hydrogen phosphate (three-letter code: T3Q) (formula: C<sub>16</sub>H<sub>27</sub>N<sub>3</sub>O<sub>14</sub>P<sub>2</sub>).

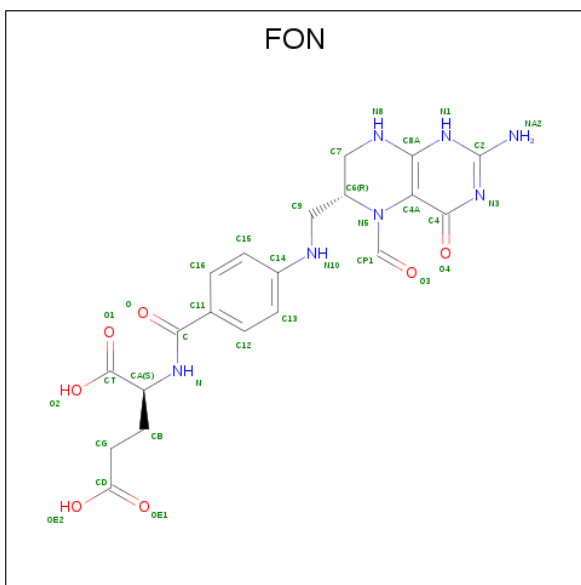


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			35	16	3	14	2		
2	A	1	Total	C	N	O	P	0	0
			35	16	3	14	2		
2	B	1	Total	C	N	O	P	0	0
			35	16	3	14	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

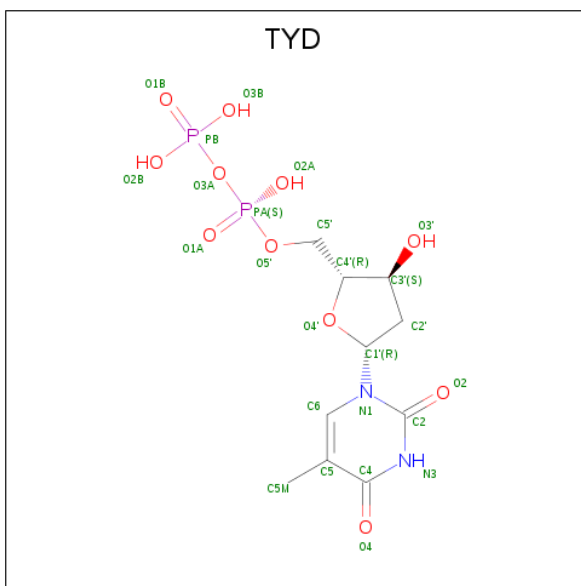
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Na	0	0
			2	2		
3	A	2	Total	Na	0	0
			2	2		

- Molecule 4 is N-{[4-({[(6R)-2-amino-5-formyl-4-oxo-1,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)phenyl]carbonyl}-L-glutamic acid (three-letter code: FON) (formula: C<sub>20</sub>H<sub>23</sub>N<sub>7</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			34	20	7	7		

- Molecule 5 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula:  $C_{10}H_{16}N_2O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total K 1 1	0	0

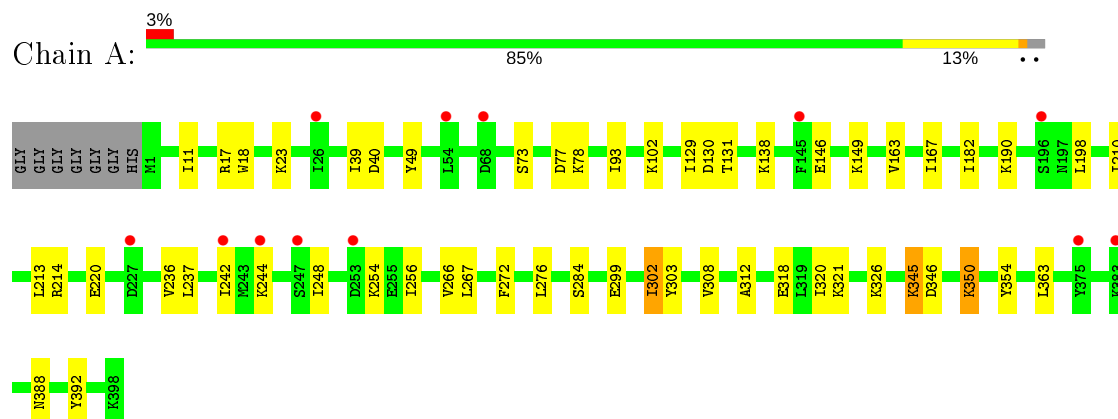
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	107	Total O 107 107	0	0
7	B	123	Total O 123 123	0	0

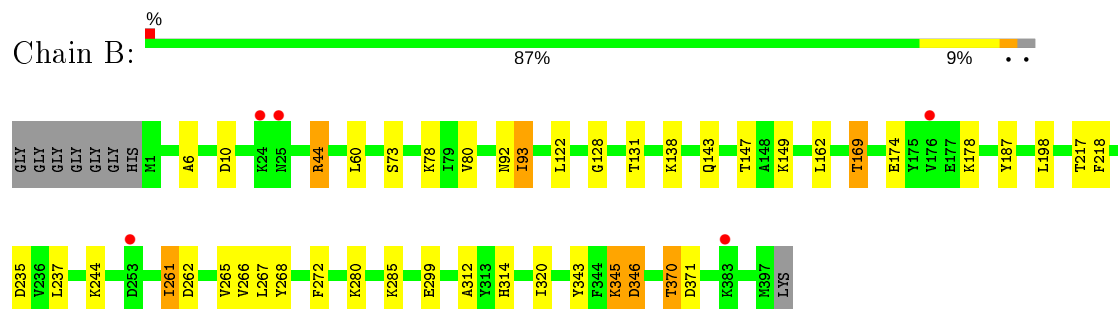
### 3 Residue-property plots [i](#)

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: Formyltransferase



#### • Molecule 1: Formyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.24Å 58.41Å 106.78Å 90.00° 96.04° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 28.79 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-2.20) 95.2 (28.79-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, $R_{free}$	0.195 , 0.264 0.201 , 0.266	Depositor DCC
$R_{free}$ test set	2149 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6878	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TYD, NA, K, FON, T3Q

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	0.68	0/3303	0.81	0/4454
1	B	0.68	0/3317	0.83	4/4474 (0.1%)
All	All	0.68	0/6620	0.82	4/8928 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	ASP	CB-CG-OD1	5.82	123.54	118.30
1	B	93	ILE	CG1-CB-CG2	-5.57	99.15	111.40
1	B	44	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	44	ARG	NE-CZ-NH2	-5.11	117.75	120.30

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	3237	0	3274	32	0
1	B	3242	0	3286	26	0
2	A	70	0	50	0	0
2	B	35	0	25	1	0
3	A	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
4	B	34	0	21	1	0
5	B	25	0	13	0	0
6	B	1	0	0	0	0
7	A	107	0	0	2	0
7	B	123	0	0	1	0
All	All	6878	0	6669	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (56) 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:237:LEU:HD21	1:B:266:VAL:CG2	2.17	0.75
1:B:128:GLY:HA3	1:B:131:THR:HB	1.74	0.67
1:A:131:THR:HG21	1:B:262:ASP:HB3	1.82	0.61
1:B:78[B]:LYS:NZ	7:B:502:HOH:O	2.32	0.61
1:A:237:LEU:HD21	1:A:266:VAL:CG2	2.34	0.57
1:B:343:TYR:OH	2:B:402:T3Q:O2A	2.20	0.56
1:A:302:ILE:HD13	1:A:303:TYR:CE1	2.41	0.56
1:B:60:LEU:HD11	1:B:80:VAL:HG22	1.87	0.54
1:A:18:TRP:CZ3	1:A:167:ILE:HG21	2.43	0.54
1:B:235:ASP:OD2	1:B:268:TYR:OH	2.15	0.54
1:A:248:ILE:HG23	1:A:256:ILE:HG23	1.89	0.54
1:A:102:LYS:NZ	1:A:131:THR:HG22	2.22	0.53
1:B:187:TYR:OH	4:B:401:FON:O2	2.21	0.53
1:A:312:ALA:HA	1:A:320:ILE:HD11	1.90	0.53
1:B:345:LYS:NZ	1:B:346:ASP:OD2	2.34	0.53
1:B:169:THR:HG22	1:B:174:GLU:O	2.11	0.51
1:B:312:ALA:HA	1:B:320:ILE:HD11	1.93	0.50
1:A:354:TYR:HB3	1:A:392:TYR:CE2	2.48	0.49
1:A:146:GLU:O	1:A:214:ARG:HD2	2.12	0.49
1:A:102:LYS:HE2	1:A:130:ASP:O	2.12	0.49
1:A:93:ILE:HD13	1:A:163:VAL:HG22	1.94	0.48
1:A:93:ILE:HD13	1:A:163:VAL:CG2	2.44	0.48
1:A:272:PHE:CE1	1:A:299:GLU:HB2	2.48	0.48
1:B:73:SER:CB	1:B:92:ASN:HD22	2.26	0.48
1:A:321:LYS:HG2	1:A:363:LEU:HD11	1.95	0.47
1:A:213:LEU:HD11	1:A:267:LEU:HD22	1.97	0.47
1:B:267:LEU:HD23	1:B:267:LEU:N	2.31	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LYS:HG2	1:B:314:HIS:CE1	2.51	0.46
1:A:11:ILE:HD11	1:A:93:ILE:HG21	1.98	0.45
1:A:77:ASP:OD2	1:A:78:LYS:HE3	2.16	0.45
1:B:265:VAL:HG12	1:B:267:LEU:HD23	1.96	0.45
1:A:182:ILE:HD12	1:A:182:ILE:H	1.82	0.45
1:B:237:LEU:HD11	1:B:266:VAL:HG22	1.99	0.44
1:A:210:ILE:HD12	1:A:236:VAL:HG22	1.99	0.44
1:B:261:ILE:HA	1:B:261:ILE:HD13	1.82	0.44
1:B:73:SER:HB3	1:B:92:ASN:HD22	1.82	0.44
1:B:370:THR:HG23	1:B:371:ASP:O	2.17	0.44
1:A:129:ILE:HD12	1:B:261:ILE:HD12	2.01	0.43
1:B:272:PHE:CE1	1:B:299:GLU:HB2	2.54	0.43
1:A:248:ILE:HG23	1:A:256:ILE:CG2	2.48	0.43
1:B:6:ALA:O	1:B:73:SER:HA	2.19	0.43
1:B:60:LEU:CD1	1:B:80:VAL:HG22	2.49	0.42
1:A:17:ARG:HG2	1:A:49:TYR:OH	2.20	0.42
1:A:302:ILE:CD1	1:A:303:TYR:CZ	3.02	0.42
1:A:236:VAL:HG12	1:A:237:LEU:O	2.19	0.42
1:A:237:LEU:HD21	1:A:266:VAL:HG21	2.01	0.42
1:A:149:LYS:HE2	1:A:220:GLU:OE1	2.20	0.41
1:A:345:LYS:C	1:A:345:LYS:HD2	2.40	0.41
1:B:93:ILE:CD1	1:B:122:LEU:HD13	2.50	0.41
1:A:149:LYS:HE2	7:A:560:HOH:O	2.20	0.41
1:A:284:SER:N	1:A:318:GLU:OE2	2.46	0.41
1:B:147:THR:HG21	1:B:217:THR:CG2	2.50	0.41
1:A:39:ILE:HG22	1:A:40:ASP:O	2.21	0.41
1:A:350:LYS:NZ	7:A:501:HOH:O	2.18	0.41
1:B:73:SER:OG	1:B:92:ASN:ND2	2.55	0.40
1:A:312:ALA:CA	1:A:320:ILE:HD11	2.49	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	396/405 (98%)	371 (94%)	25 (6%)	0	100	100
1	B	398/405 (98%)	377 (95%)	20 (5%)	1 (0%)	41	46
All	All	794/810 (98%)	748 (94%)	45 (6%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	261	ILE

### 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	358/359 (100%)	342 (96%)	16 (4%)	27	34
1	B	360/359 (100%)	346 (96%)	14 (4%)	32	41
All	All	718/718 (100%)	688 (96%)	30 (4%)	30	38

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	73	SER
1	A	138	LYS
1	A	190	LYS
1	A	198	LEU
1	A	242	ILE
1	A	244	LYS
1	A	254	LYS
1	A	276	LEU
1	A	302	ILE
1	A	308	VAL
1	A	326	LYS
1	A	345	LYS
1	A	346	ASP
1	A	350	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	388	ASN
1	B	44	ARG
1	B	138	LYS
1	B	143	GLN
1	B	149	LYS
1	B	162	LEU
1	B	169	THR
1	B	178	LYS
1	B	198	LEU
1	B	218	PHE
1	B	244	LYS
1	B	285	LYS
1	B	345	LYS
1	B	346	ASP
1	B	370	THR

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

Mol	Chain	Res	Type
1	A	92	ASN
1	A	143	GLN
1	A	329	ASN
1	B	88	ASN
1	B	92	ASN
1	B	197	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
2	T3Q	A	401	-	31,37,37	0.93	1 (3%)	42,57,57	1.66	7 (16%)
5	TYD	B	403	-	23,26,26	2.41	5 (21%)	33,40,40	1.91	8 (24%)
2	T3Q	B	402	-	31,37,37	1.09	3 (9%)	42,57,57	1.69	8 (19%)
2	T3Q	A	402	-	31,37,37	1.02	1 (3%)	42,57,57	1.64	7 (16%)
4	FON	B	401	-	28,36,36	1.59	3 (10%)	28,50,50	1.68	7 (25%)

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
2	T3Q	A	401	-	-	3/18/53/53	0/3/3/3
5	TYD	B	403	-	-	2/16/28/28	0/2/2/2
2	T3Q	B	402	-	-	1/18/53/53	0/3/3/3
2	T3Q	A	402	-	-	1/18/53/53	0/3/3/3
4	FON	B	401	-	-	2/18/37/37	0/2/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	TYD	C6-N1	-9.13	1.35	1.46
4	B	401	FON	C4A-C8A	4.47	1.50	1.41
4	B	401	FON	C4-C4A	4.43	1.47	1.41
4	B	401	FON	CP1-N5	-4.19	1.29	1.35
5	B	403	TYD	C6-C5	-3.89	1.39	1.51
2	A	402	T3Q	C4-C5	3.58	1.49	1.41
5	B	403	TYD	C2-N1	3.49	1.40	1.35
2	B	402	T3Q	C4-C5	3.14	1.48	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	T3Q	C4-C5	3.14	1.48	1.41
5	B	403	TYD	C2-N3	-2.73	1.33	1.38
2	B	402	T3Q	C4Q-C3Q	-2.40	1.50	1.53
5	B	403	TYD	C1'-N1	2.17	1.48	1.45
2	B	402	T3Q	C2Q-C3Q	-2.13	1.50	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	T3Q	C4-N3-C2	6.86	120.93	115.14
2	A	402	T3Q	C4-N3-C2	6.47	120.60	115.14
2	B	402	T3Q	C4-N3-C2	6.21	120.39	115.14
5	B	403	TYD	C5-C6-N1	5.18	121.31	111.11
5	B	403	TYD	O4'-C1'-N1	-4.29	102.94	108.41
5	B	403	TYD	N3-C2-N1	4.28	121.19	116.65
4	B	401	FON	CB-CA-N	3.78	115.71	110.19
5	B	403	TYD	C5M-C5-C6	3.58	119.99	112.34
5	B	403	TYD	C4-N3-C2	-3.57	122.49	126.86
4	B	401	FON	C4-N3-C2	3.26	121.10	115.93
2	A	401	T3Q	O4Q-C4Q-C5Q	3.22	116.81	109.67
2	B	402	T3Q	PB-O3A-PA	-3.22	121.78	132.83
4	B	401	FON	C2-N1-C8A	2.99	121.24	114.54
2	A	402	T3Q	O5Q-C1Q-O3B	2.93	115.20	111.36
4	B	401	FON	CB-CG-CD	-2.90	107.36	113.59
2	B	402	T3Q	O2Q-C2Q-C3Q	-2.88	105.05	110.22
2	A	402	T3Q	PB-O3A-PA	-2.78	123.29	132.83
2	B	402	T3Q	O1B-PB-O2B	2.63	125.24	112.24
2	A	402	T3Q	O5Q-C5Q-C6Q	2.56	112.22	106.70
4	B	401	FON	O3-CP1-N5	-2.54	121.69	125.36
2	A	401	T3Q	O5Q-C1Q-C2Q	2.49	115.63	110.35
2	A	402	T3Q	O2A-PA-O1A	2.48	124.48	112.24
2	A	402	T3Q	O1B-PB-O2B	2.45	124.35	112.24
4	B	401	FON	C4A-N5-C6	-2.42	115.02	119.31
2	B	402	T3Q	C5M-C5-C6	2.38	123.70	118.68
2	B	402	T3Q	C5-C6-N1	-2.37	119.64	122.19
2	A	401	T3Q	O3A-PB-O3B	-2.19	98.08	102.48
2	B	402	T3Q	O4Q-C4Q-C3Q	-2.18	106.31	110.22
4	B	401	FON	C4A-C4-N3	-2.16	118.69	123.14
5	B	403	TYD	O2B-PB-O3A	-2.14	97.47	104.64
2	A	401	T3Q	O3B-PB-O2B	-2.12	101.52	109.47
2	A	401	T3Q	O3B-C1Q-C2Q	-2.12	104.50	108.38
2	B	402	T3Q	O2A-PA-O1A	2.07	122.48	112.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	403	TYD	C6-C5-C4	2.06	117.43	111.53
2	A	402	T3Q	C1Q-C2Q-C3Q	-2.06	107.64	110.40
5	B	403	TYD	O2-C2-N3	-2.05	117.69	121.50
2	A	401	T3Q	O2A-PA-O1A	2.02	122.25	112.24

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	FON	CT-CA-N-C
2	A	401	T3Q	O4'-C1'-N1-C6
2	B	402	T3Q	O4'-C1'-N1-C6
2	A	402	T3Q	O4'-C1'-N1-C6
4	B	401	FON	CB-CA-N-C
2	A	401	T3Q	PB-O3A-PA-O5'
5	B	403	TYD	C5'-O5'-PA-O2A
2	A	401	T3Q	C1Q-O3B-PB-O1B
5	B	403	TYD	C5'-O5'-PA-O3A

There are no ring outliers.

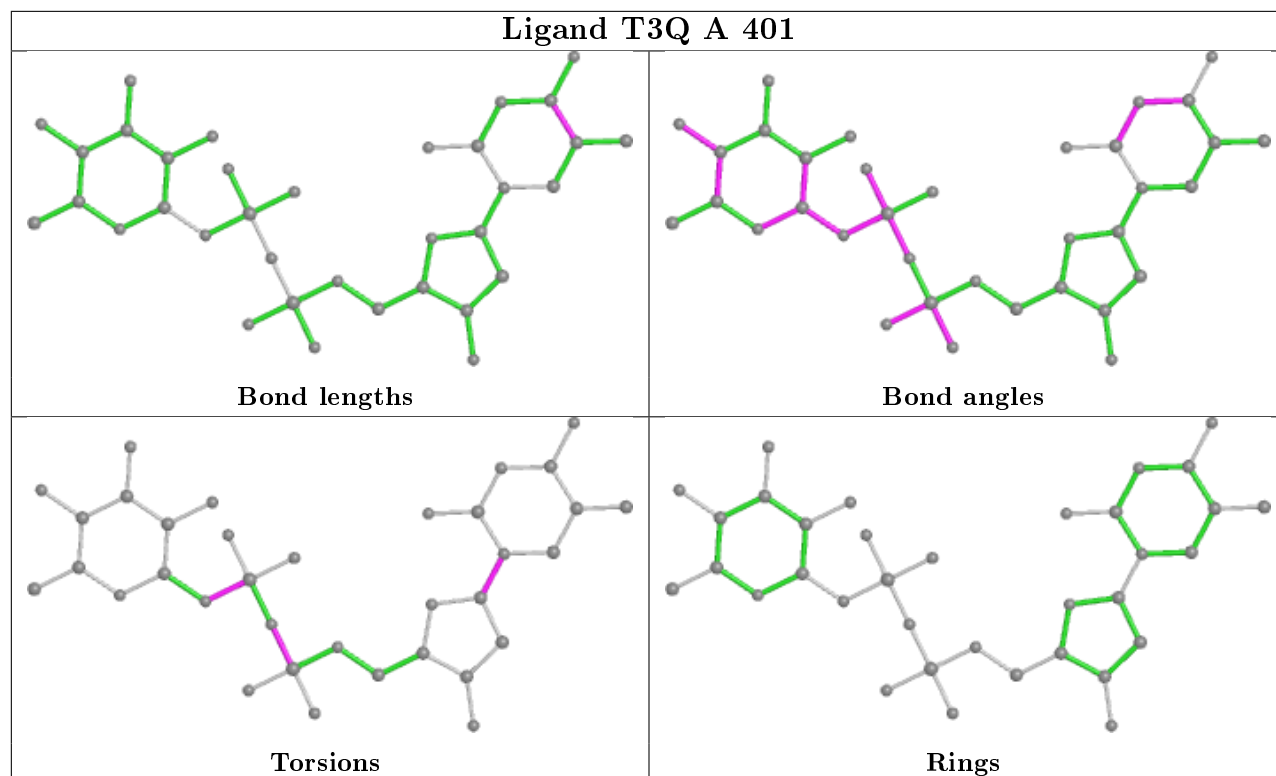
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	T3Q	1	0
4	B	401	FON	1	0

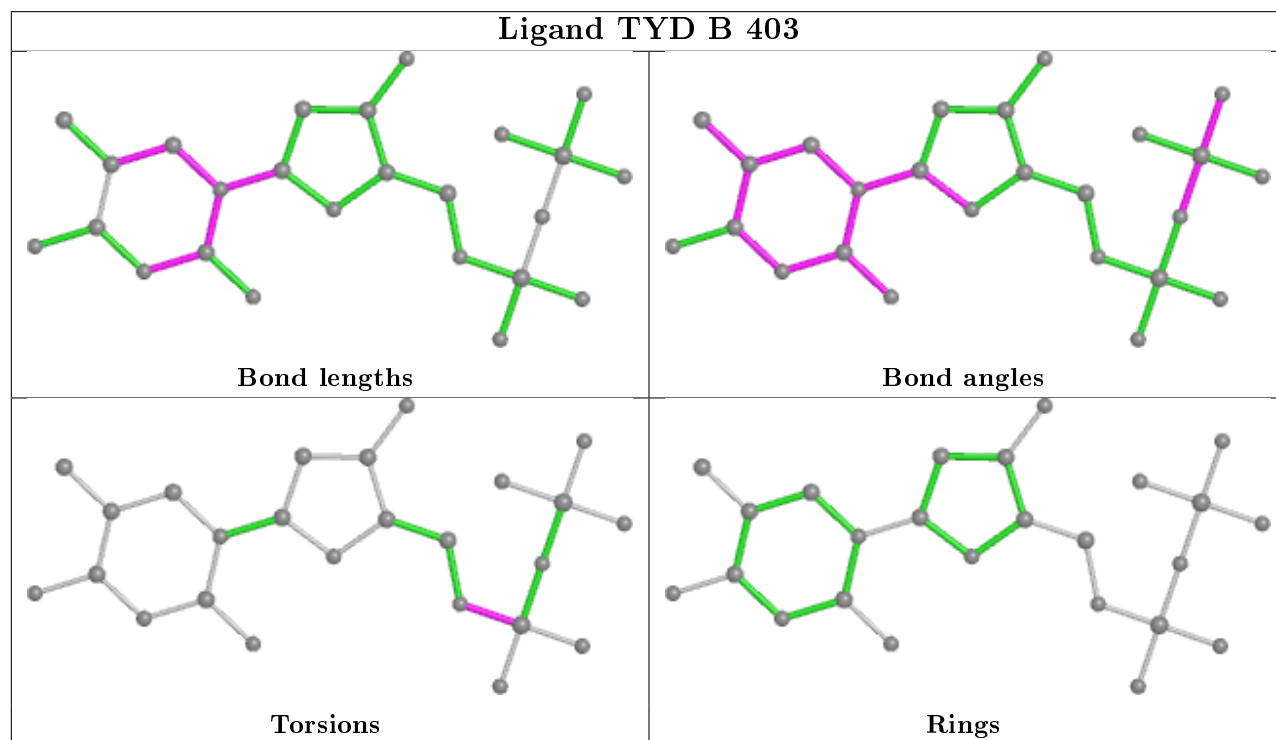
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

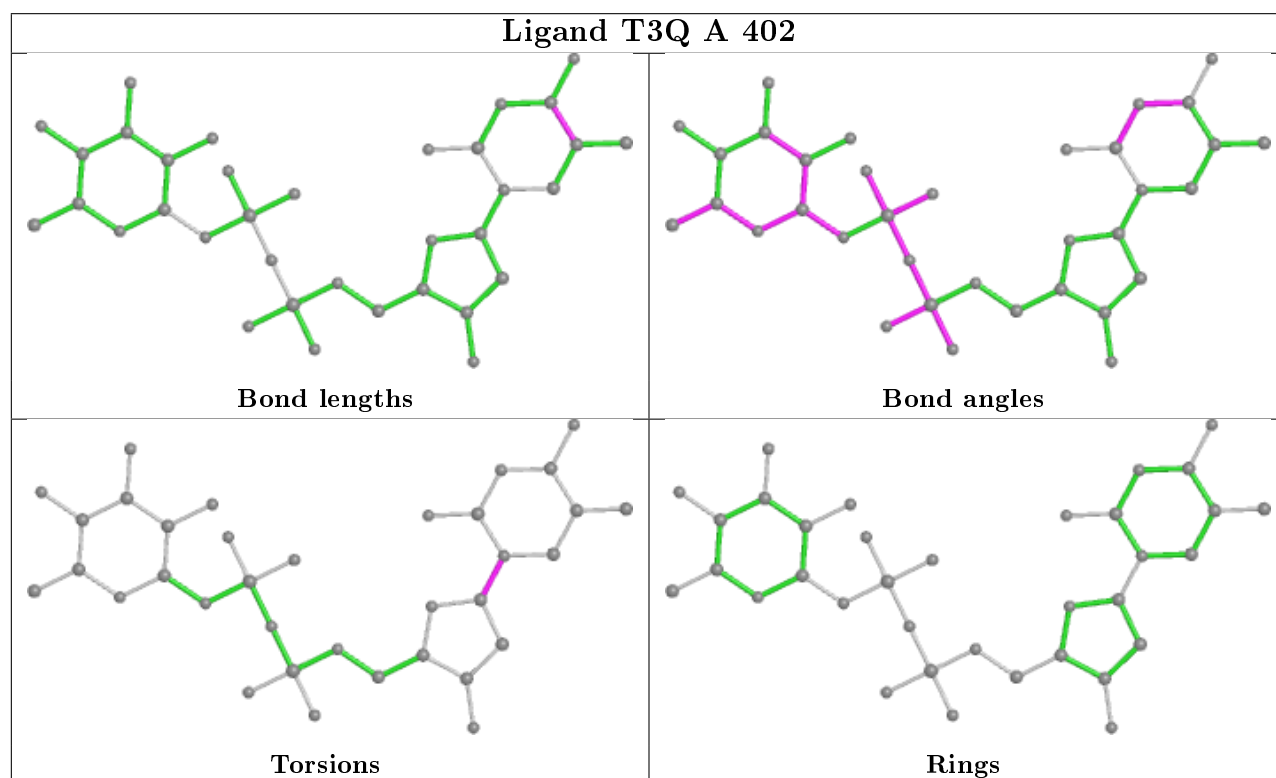
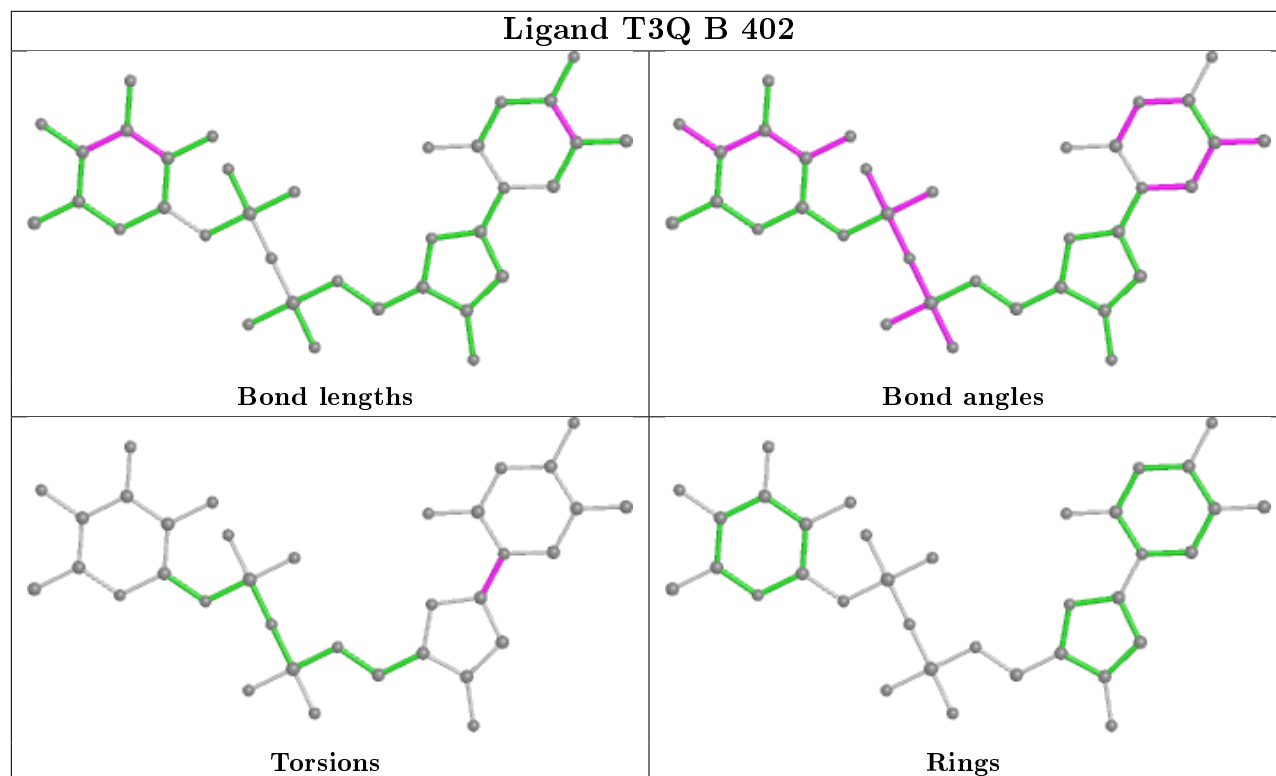


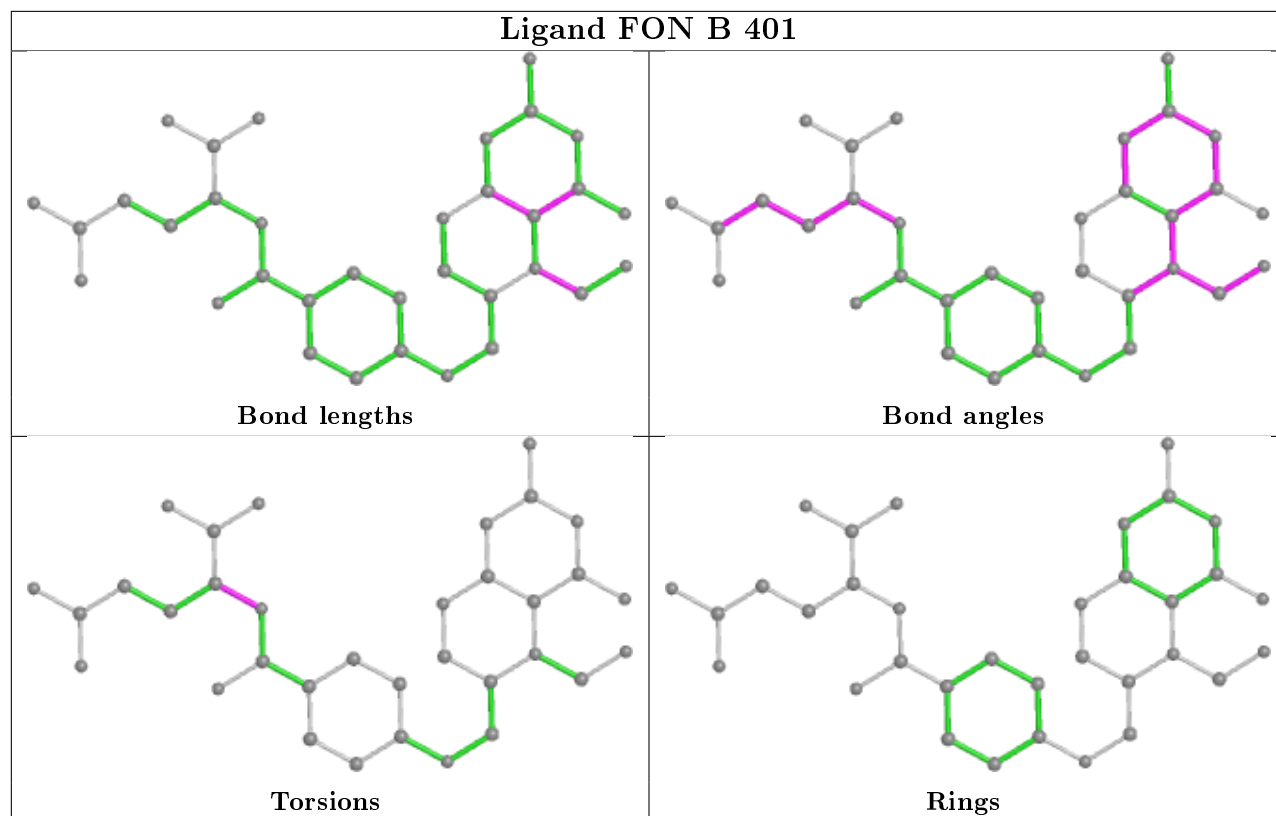
## Ligand T3Q A 401



## Ligand TYD B 403







## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	398/405 (98%)	-0.12	12 (3%) 50 48	16, 32, 61, 87	0
1	B	397/405 (98%)	-0.36	5 (1%) 77 75	16, 26, 50, 68	0
All	All	795/810 (98%)	-0.24	17 (2%) 63 61	16, 29, 55, 87	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383	LYS	3.5
1	A	244	LYS	3.4
1	B	253	ASP	3.3
1	A	196	SER	3.2
1	A	253	ASP	3.1
1	A	242	ILE	3.0
1	A	227	ASP	2.7
1	A	247	SER	2.7
1	B	24	LYS	2.7
1	A	54	LEU	2.6
1	B	176	VAL	2.4
1	A	26	ILE	2.3
1	B	25	ASN	2.3
1	A	375	TYR	2.3
1	A	145	PHE	2.2
1	A	68	ASP	2.2
1	B	383	LYS	2.1

### 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 ⓘ

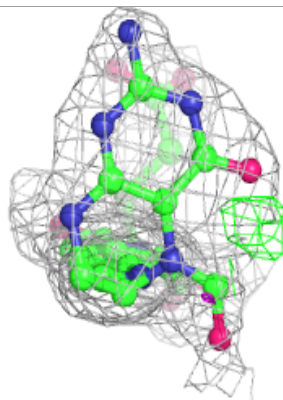
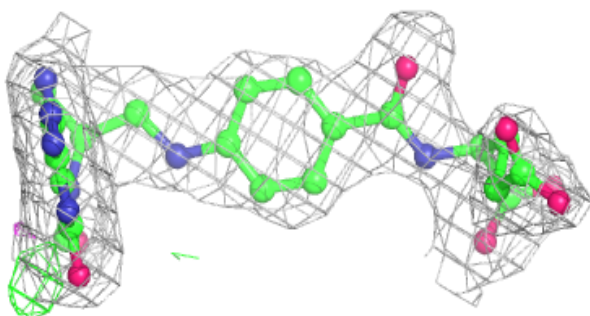
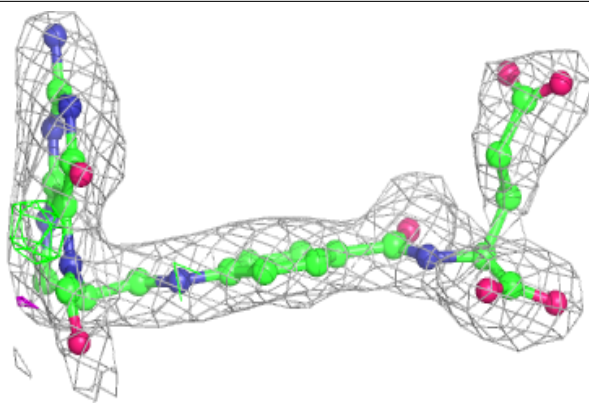
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FON	B	401	34/34	0.89	0.15	27,34,56,58	0
3	NA	A	404	1/1	0.92	0.06	42,42,42,42	0
5	TYD	B	403	25/25	0.94	0.12	18,22,64,75	0
2	T3Q	A	401	35/35	0.95	0.10	24,34,45,46	0
3	NA	A	403	1/1	0.96	0.07	28,28,28,28	0
3	NA	B	404	1/1	0.96	0.13	26,26,26,26	0
2	T3Q	B	402	35/35	0.97	0.09	21,27,31,32	0
2	T3Q	A	402	35/35	0.97	0.10	23,29,35,37	0
3	NA	B	406	1/1	0.98	0.14	33,33,33,33	0
6	K	B	405	1/1	0.98	0.05	22,22,22,22	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.

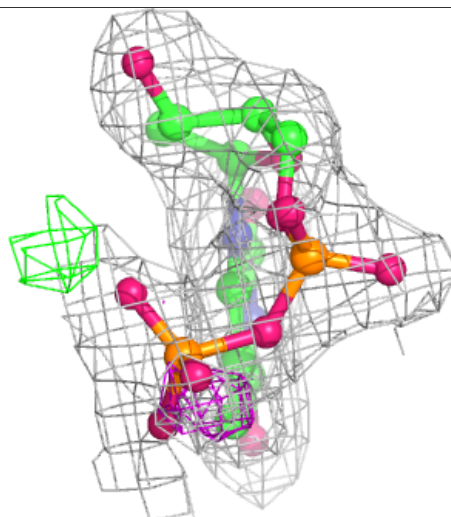
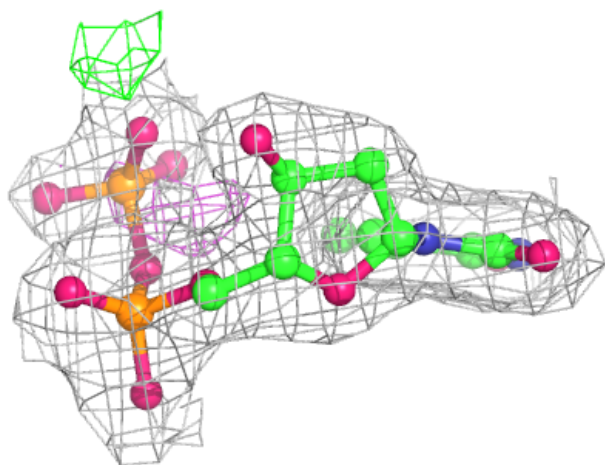
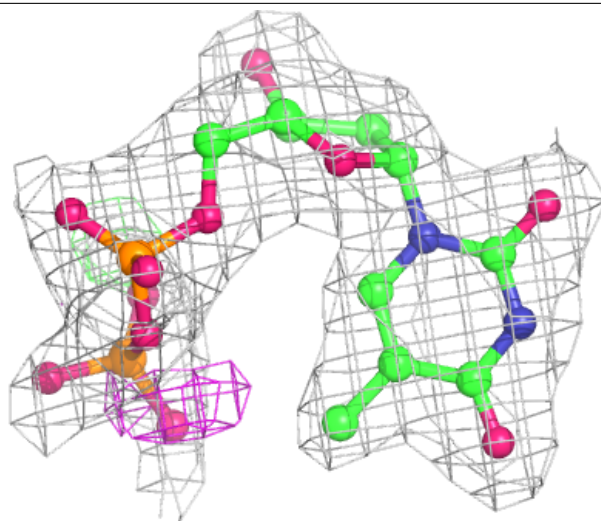
**Electron density around FON B 401:**

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



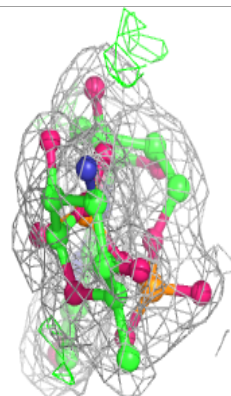
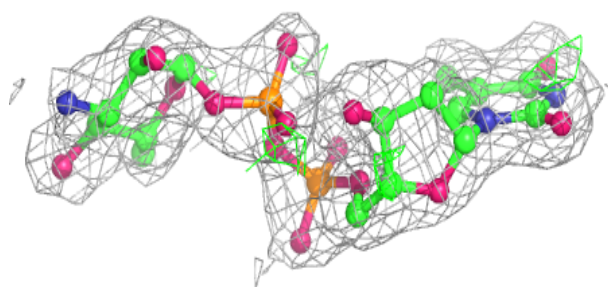
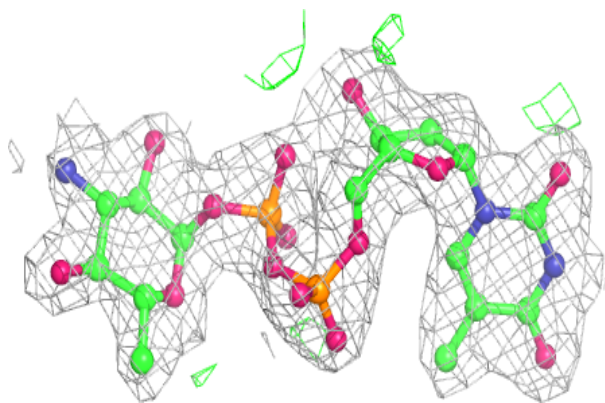
**Electron density around TYD B 403:**

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

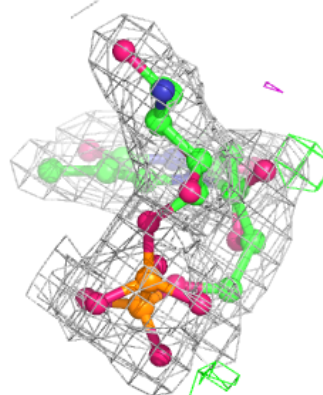
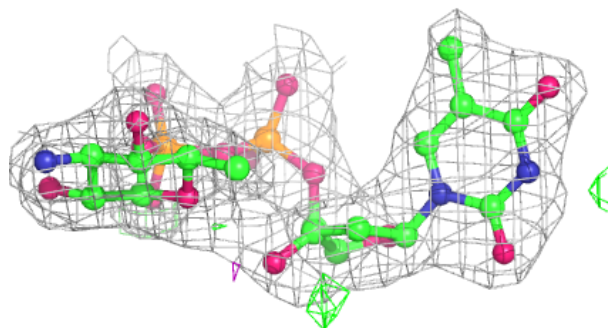
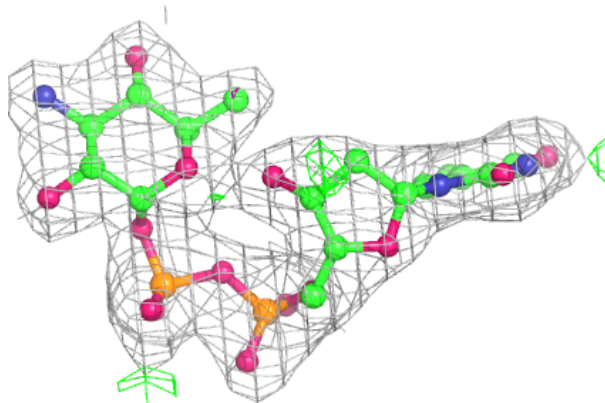


**Electron density around T3Q A 401:**

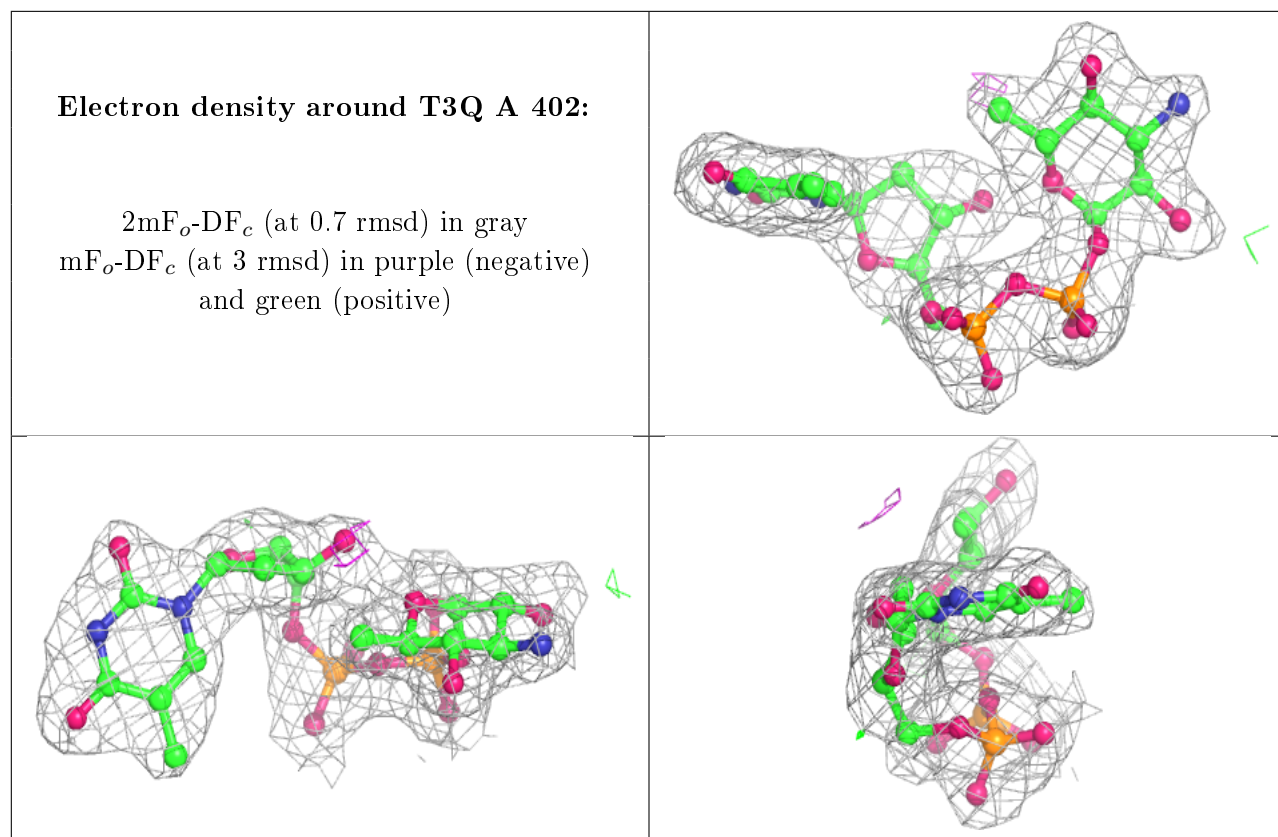
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around T3Q B 402:**

$2mF_o-DF_c$  (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.