



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 03:46 pm BST

PDB ID : 5UIL  
Title : X-ray structure of the FdtF N-formyltransferase from *Salmonella enterica* O60  
in complex with TDP-Fuc3N and tetrahydrofolate  
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.

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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

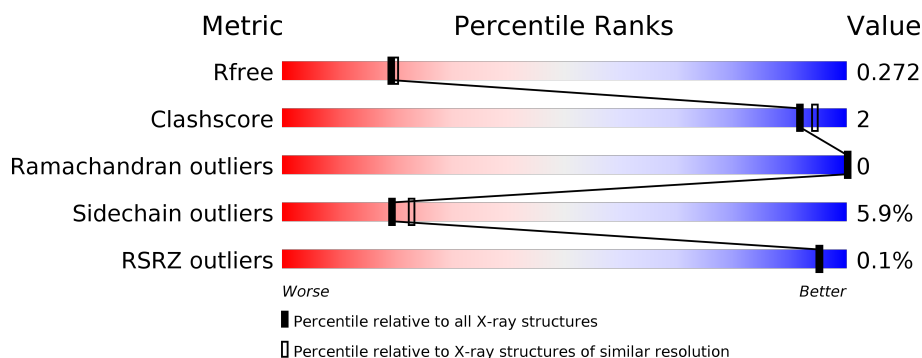
# 1 Overall quality at a glance

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	
1	B	405	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7000 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.

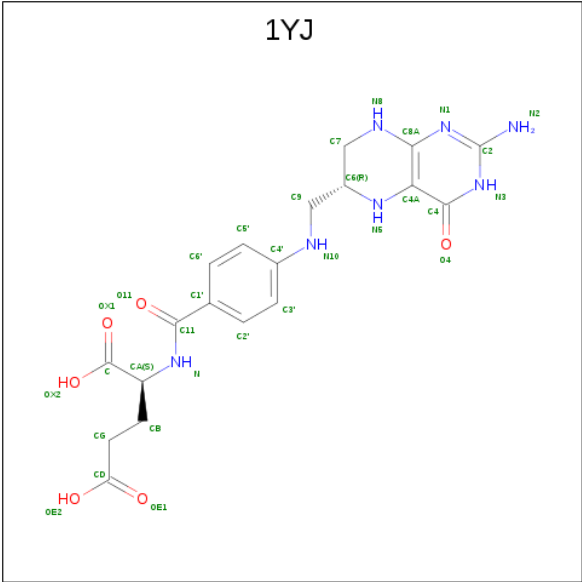
- Molecule 1 is a protein called Formyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	1	0
			3236	2101	513	609	13			
1	B	398	Total	C	N	O	S	0	1	0
			3240	2103	514	611	12			

There are 16 discrepancies between the modelled and reference sequences:

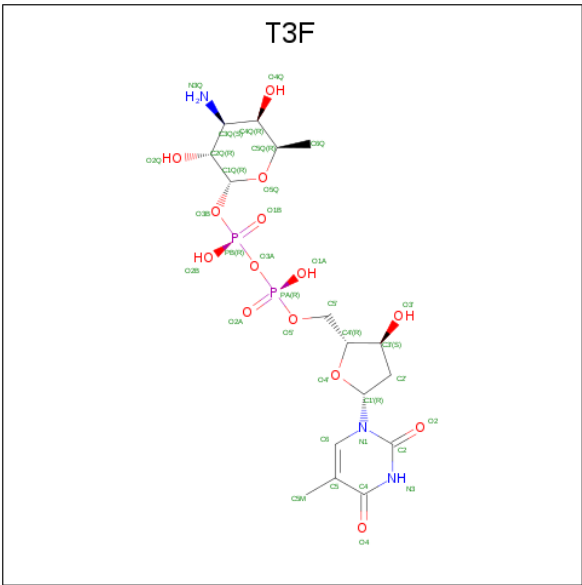
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP U3GK13
A	-5	GLY	-	expression tag	UNP U3GK13
A	-4	GLY	-	expression tag	UNP U3GK13
A	-3	GLY	-	expression tag	UNP U3GK13
A	-2	GLY	-	expression tag	UNP U3GK13
A	-1	GLY	-	expression tag	UNP U3GK13
A	0	HIS	-	expression tag	UNP U3GK13
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 N-[4-({[(6R)-2-amino-4-oxo-3,4,5,6,7,8-hexahydropteridin-6-yl]methyl}amino)benzoyl]-L-glutamic acid (three-letter code: 1YJ) (formula: C<sub>19</sub>H<sub>23</sub>N<sub>7</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	19	7	6		
2	B	1	Total	C	N	O	0	0
			32	19	7	6		

- Molecule 3 is (3R,4S,5R,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: T3F) (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
3	A	1	Total	C	N	O	P	0	0
			35	16	3	14	2		

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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


- Molecule 5 is water.

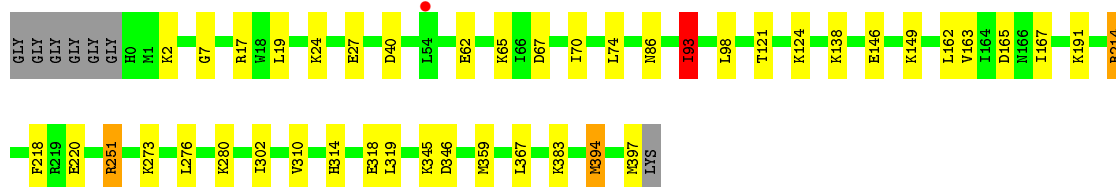
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	154	Total	O	0	0
			154	154		
5	B	162	Total	O	0	0
			162	162		

### 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.

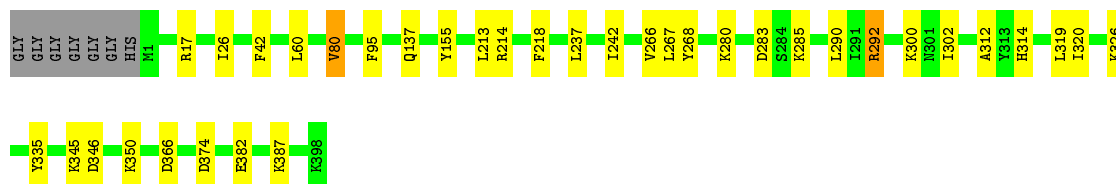
- Molecule 1: Formyltransferase

Chain A:  87% 10% ..



- Molecule 1: Formyltransferase

Chain B:  89% 8% •



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.67Å 72.81Å 191.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 68.07 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-2.20) 93.6 (68.07-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, $R_{free}$	0.202 , 0.270 0.208 , 0.272	Depositor DCC
$R_{free}$ test set	2367 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 26.8	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	0.93	EDS
Total number of atoms	7000	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: T3F, NA, 1YJ

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	0.62	0/3305	0.88	6/4458 (0.1%)
1	B	0.64	0/3309	0.83	2/4462 (0.0%)
All	All	0.63	0/6614	0.85	8/8920 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ARG	NE-CZ-NH1	8.85	124.73	120.30
1	A	214	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	165	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	93	ILE	CG1-CB-CG2	-5.48	99.34	111.40
1	A	251	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	B	366	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	214	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	A	40	ASP	CB-CG-OD1	5.10	122.89	118.30

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	3236	0	3270	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3240	0	3280	10	0
2	A	32	0	21	0	0
2	B	32	0	21	1	0
3	A	70	0	50	0	0
3	B	70	0	50	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	154	0	0	1	0
5	B	162	0	0	1	0
All	All	7000	0	6692	22	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.

All (22) 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:A:67:ASP:OD1	1:A:86:ASN:ND2	2.31	0.62
1:A:149:LYS:NZ	5:A:501:HOH:O	2.34	0.59
1:A:276:LEU:HD22	1:A:310:VAL:HG21	1.88	0.55
1:A:93:ILE:HD13	1:A:163:VAL:HG22	1.90	0.54
1:B:213:LEU:HD11	1:B:267:LEU:HD22	1.90	0.53
1:A:19:LEU:HD21	1:A:167:ILE:HD13	1.92	0.52
1:A:7:GLY:HA3	1:A:74:LEU:O	2.13	0.48
1:B:312:ALA:HA	1:B:320:ILE:HD11	1.96	0.46
1:B:280:LYS:HG2	1:B:314:HIS:CE1	2.51	0.46
1:B:300:LYS:HE3	5:B:568:HOH:O	2.16	0.45
2:B:401:1YJ:H3	2:B:401:1YJ:H7	1.54	0.43
1:A:98:LEU:HD12	1:A:121:THR:HG21	2.01	0.43
1:B:237:LEU:HD21	1:B:266:VAL:CG2	2.48	0.43
1:B:268:TYR:CE1	1:B:292:ARG:HG3	2.54	0.43
1:B:42:PHE:HA	1:B:335:TYR:CE1	2.55	0.42
1:A:146:GLU:O	1:A:214:ARG:HD2	2.20	0.42
1:A:280:LYS:HG2	1:A:314:HIS:CE1	2.55	0.42
1:A:394:MET:HE2	1:A:397:MET:HG3	2.03	0.41
1:B:95:PHE:CD2	1:B:155:TYR:HB3	2.56	0.41
1:A:394:MET:CE	1:A:397:MET:HG3	2.50	0.41
1:B:283:ASP:OD2	1:B:285:LYS:HE2	2.21	0.40
1:B:60:LEU:HD11	1:B:80:VAL:HG22	2.04	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	397/405 (98%)	382 (96%)	15 (4%)	0	100	100
1	B	397/405 (98%)	374 (94%)	23 (6%)	0	100	100
All	All	794/810 (98%)	756 (95%)	38 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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%)	333 (93%)	25 (7%)	15	16
1	B	359/359 (100%)	342 (95%)	17 (5%)	26	33
All	All	717/718 (100%)	675 (94%)	42 (6%)	19	23

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	17	ARG
1	A	24	LYS
1	A	27	GLU
1	A	62	GLU
1	A	65	LYS
1	A	70	ILE
1	A	93	ILE

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Mol	Chain	Res	Type
1	A	124	LYS
1	A	138	LYS
1	A	162	LEU
1	A	191	LYS
1	A	218	PHE
1	A	220	GLU
1	A	251	ARG
1	A	273	LYS
1	A	302	ILE
1	A	318	GLU
1	A	319	LEU
1	A	345	LYS
1	A	346	ASP
1	A	359	MET
1	A	367	LEU
1	A	383	LYS
1	A	394	MET
1	B	17	ARG
1	B	26	ILE
1	B	80	VAL
1	B	137	GLN
1	B	218	PHE
1	B	242	ILE
1	B	290	LEU
1	B	292	ARG
1	B	302	ILE
1	B	319	LEU
1	B	326	LYS
1	B	345	LYS
1	B	346	ASP
1	B	350	LYS
1	B	374	ASP
1	B	382	GLU
1	B	387	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	B	92	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, 4 are monoatomic - leaving 6 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$
3	T3F	A	403	-	31,37,37	0.93	1 (3%)	42,57,57	1.60	5 (11%)
3	T3F	B	402	-	31,37,37	1.00	2 (6%)	42,57,57	1.76	4 (9%)
3	T3F	B	403	-	31,37,37	0.91	1 (3%)	42,57,57	2.03	8 (19%)
3	T3F	A	402	-	31,37,37	0.90	1 (3%)	42,57,57	1.58	3 (7%)
2	1YJ	A	401	-	26,34,34	1.15	1 (3%)	31,47,47	2.26	10 (32%)
2	1YJ	B	401	-	26,34,34	1.01	1 (3%)	31,47,47	2.01	7 (22%)

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
3	T3F	A	403	-	-	3/18/53/53	0/3/3/3
3	T3F	B	402	-	-	1/18/53/53	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	T3F	B	403	-	-	2/18/53/53	0/3/3/3
3	T3F	A	402	-	-	1/18/53/53	0/3/3/3
2	1YJ	A	401	-	-	3/16/31/31	0/3/3/3
2	1YJ	B	401	-	-	3/16/31/31	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	1YJ	O4-C4	4.63	1.36	1.24
2	B	401	1YJ	O4-C4	4.38	1.35	1.24
3	B	403	T3F	C4-C5	3.61	1.49	1.41
3	A	403	T3F	C4-C5	3.21	1.48	1.41
3	B	402	T3F	C4-C5	3.13	1.48	1.41
3	A	402	T3F	C4-C5	3.12	1.48	1.41
3	B	402	T3F	C3Q-N3Q	-2.41	1.43	1.47

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	T3F	C4-N3-C2	9.36	123.05	115.14
3	B	402	T3F	C4-N3-C2	9.00	122.74	115.14
3	A	402	T3F	C4-N3-C2	7.49	121.46	115.14
3	A	403	T3F	C4-N3-C2	7.21	121.23	115.14
2	A	401	1YJ	CB-CA-N	-6.42	100.84	110.19
2	A	401	1YJ	C4-C4A-C8A	6.27	120.14	114.57
2	B	401	1YJ	C4-C4A-C8A	4.86	118.89	114.57
2	B	401	1YJ	CA-N-C11	4.51	128.15	122.34
2	B	401	1YJ	C4-C4A-N5	4.50	122.90	119.12
2	B	401	1YJ	CB-CG-CD	-4.15	104.68	113.59
3	B	403	T3F	O3A-PB-O3B	-4.03	94.36	102.48
3	B	403	T3F	O5Q-C1Q-C2Q	3.39	117.52	110.35
2	A	401	1YJ	CA-N-C11	3.35	126.65	122.34
2	A	401	1YJ	CB-CG-CD	-3.29	106.52	113.59
2	A	401	1YJ	C9-C6-C7	3.26	118.74	112.64
2	B	401	1YJ	C4-N3-C2	2.95	120.61	115.93
3	B	403	T3F	C6Q-C5Q-C4Q	-2.62	108.24	113.07
3	B	402	T3F	PA-O3A-PB	-2.60	123.90	132.83
2	A	401	1YJ	C4-N3-C2	2.59	120.05	115.93
2	A	401	1YJ	N2-C2-N3	2.56	121.24	117.25
3	B	403	T3F	C5Q-C4Q-C3Q	2.56	114.39	110.51
3	A	402	T3F	O3A-PB-O3B	-2.49	97.47	102.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	T3F	O3B-C1Q-C2Q	-2.38	104.02	108.38
3	B	402	T3F	O1A-PA-O2A	2.38	124.00	112.24
3	B	402	T3F	O5Q-C5Q-C6Q	2.34	111.76	106.70
2	B	401	1YJ	C9-N10-C4'	2.27	128.01	122.14
2	A	401	1YJ	C2-N1-C8A	2.26	119.61	114.54
3	B	403	T3F	O2B-PB-O3B	-2.26	97.85	106.78
2	A	401	1YJ	C3'-C4'-N10	-2.26	116.30	120.97
3	B	403	T3F	O2B-PB-O1B	2.20	123.10	112.24
2	A	401	1YJ	N3-C2-N1	-2.19	121.98	125.42
3	A	403	T3F	O1A-PA-O2A	2.13	122.75	112.24
3	A	403	T3F	C6Q-C5Q-C4Q	-2.12	109.15	113.07
3	A	403	T3F	O2B-PB-O1B	2.12	122.71	112.24
2	B	401	1YJ	C2-N1-C8A	2.11	119.27	114.54
3	A	403	T3F	O5Q-C1Q-C2Q	2.09	114.78	110.35
3	A	402	T3F	C1Q-C2Q-C3Q	2.01	113.09	110.40

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	T3F	O4'-C1'-N1-C6
3	B	403	T3F	O4'-C1'-N1-C6
3	A	402	T3F	O4'-C1'-N1-C6
2	A	401	1YJ	C7-C6-C9-N10
2	A	401	1YJ	N5-C6-C9-N10
2	B	401	1YJ	C7-C6-C9-N10
2	B	401	1YJ	N5-C6-C9-N10
2	A	401	1YJ	C-CA-N-C11
3	A	403	T3F	PB-O3A-PA-O5'
3	B	403	T3F	PB-O3A-PA-O5'
2	B	401	1YJ	N-CA-CB-CG
3	A	403	T3F	PB-O3A-PA-O2A
3	A	403	T3F	PA-O3A-PB-O1B

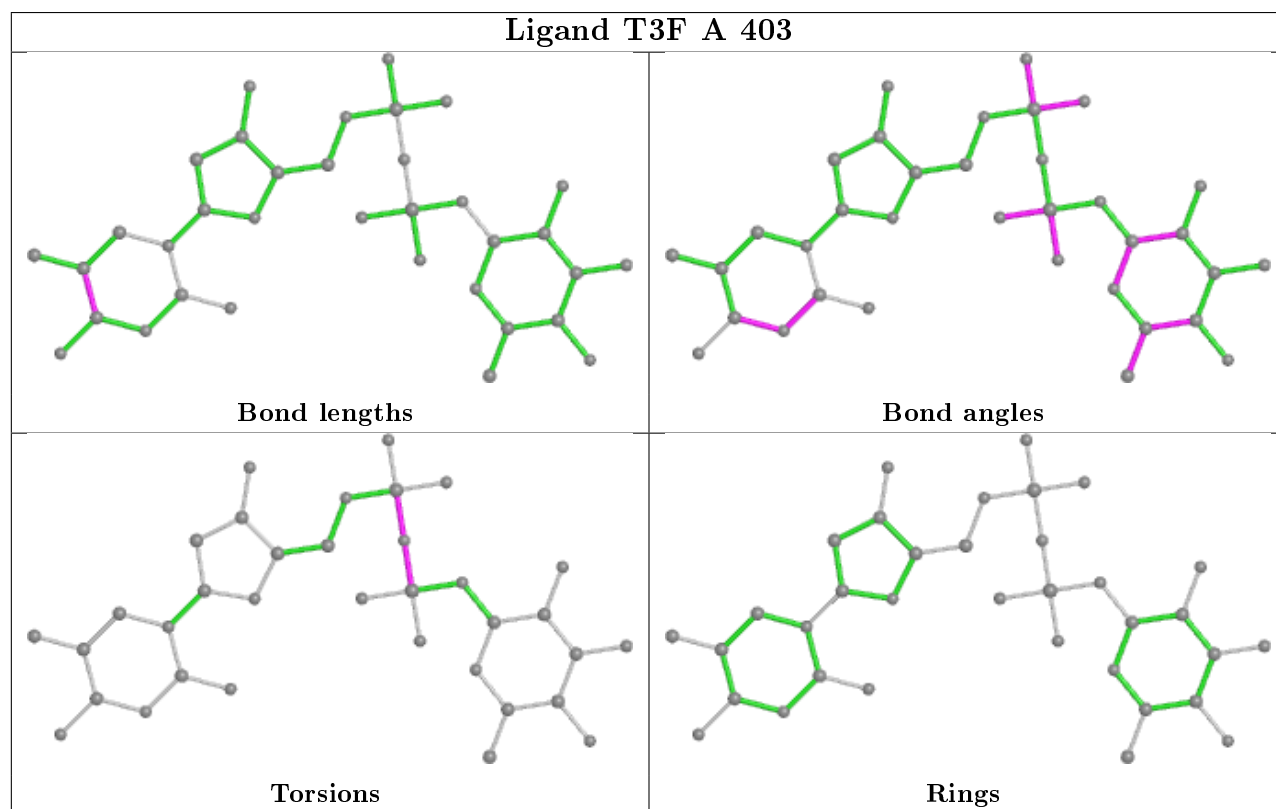
There are no ring outliers.

1 monomer is involved in 1 short contact:

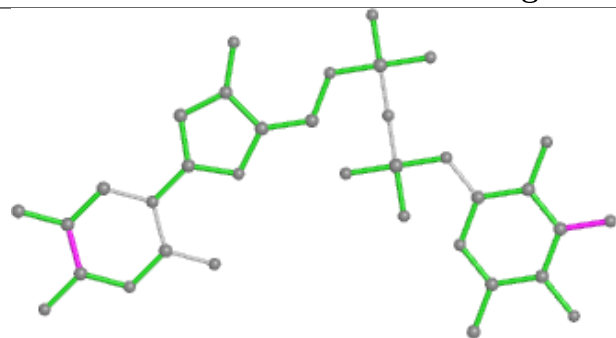
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	1YJ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

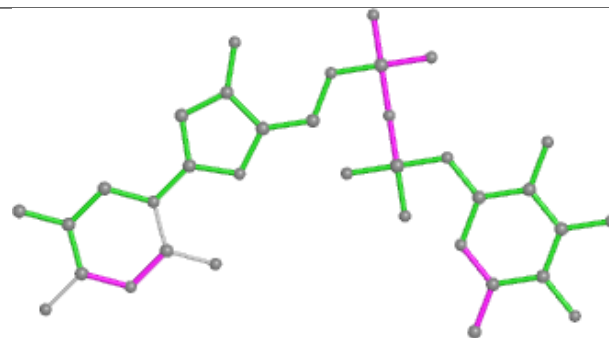
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



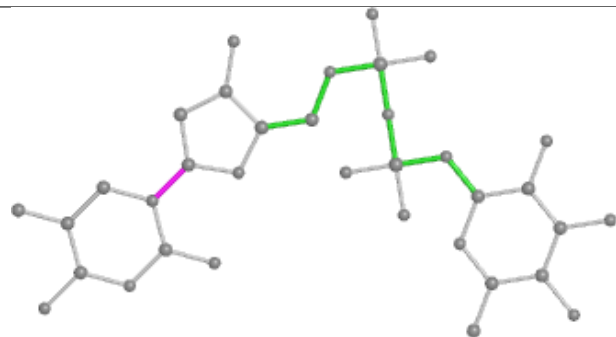
## Ligand T3F B 402



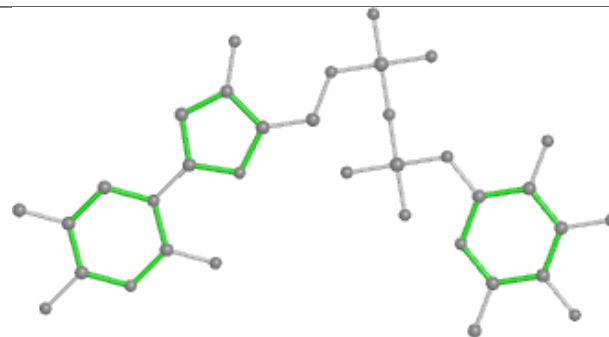
Bond lengths



Bond angles

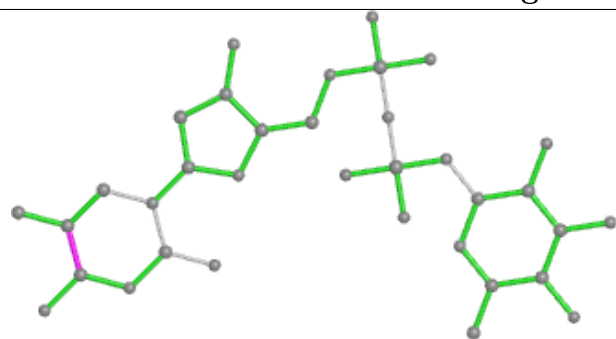


Torsions

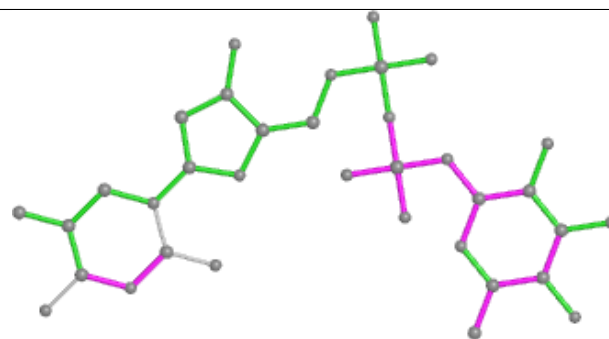


Rings

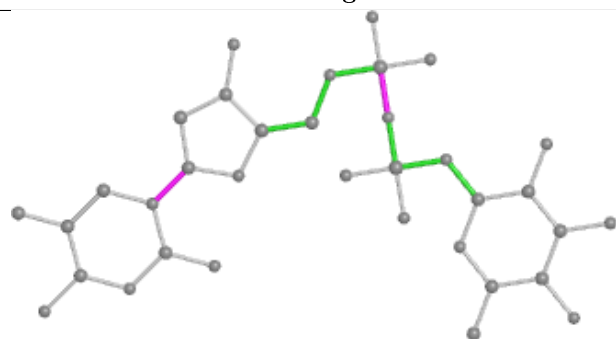
## Ligand T3F B 403



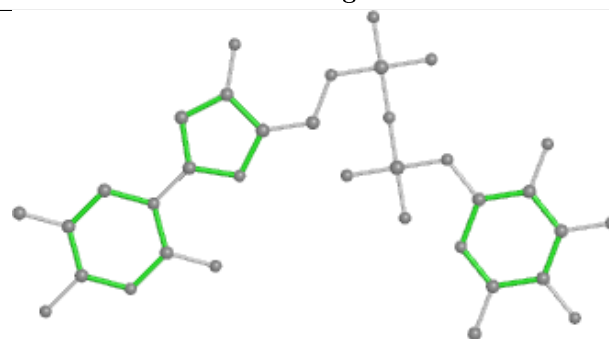
Bond lengths



Bond angles



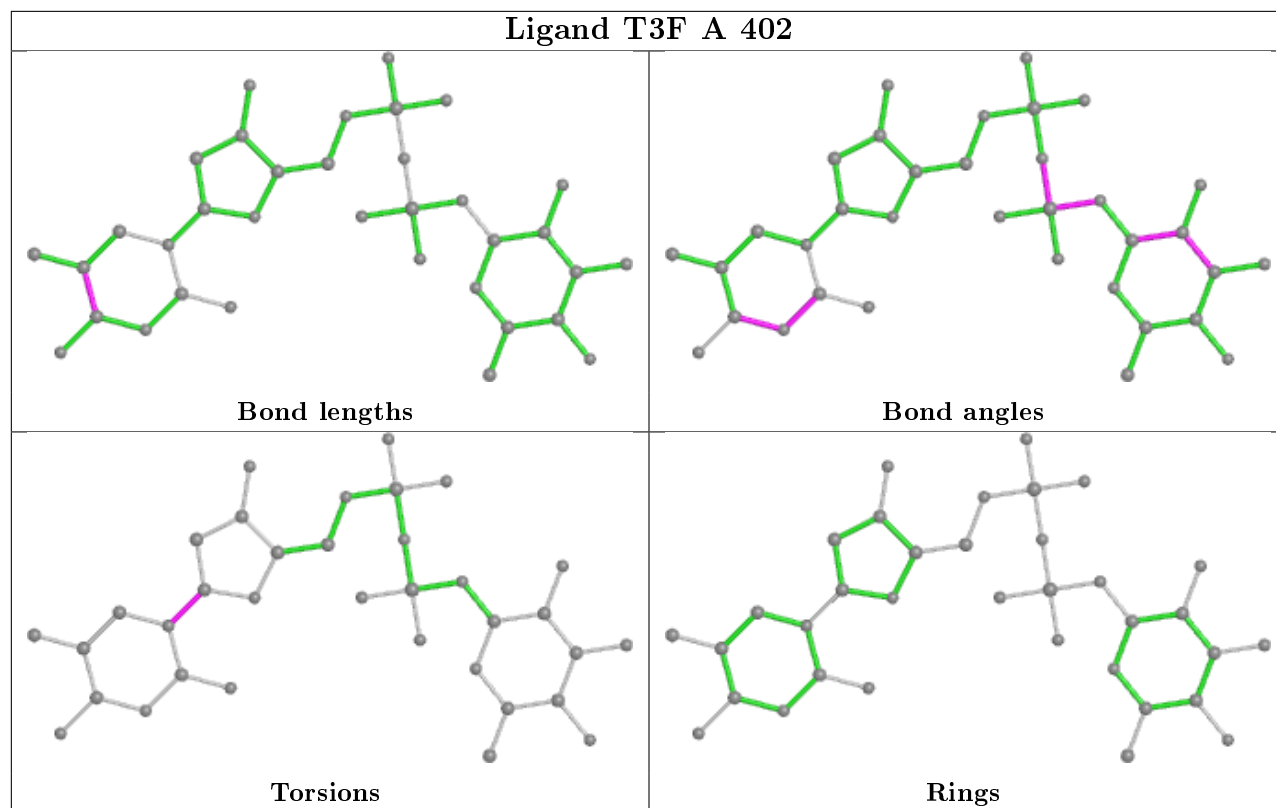
Torsions



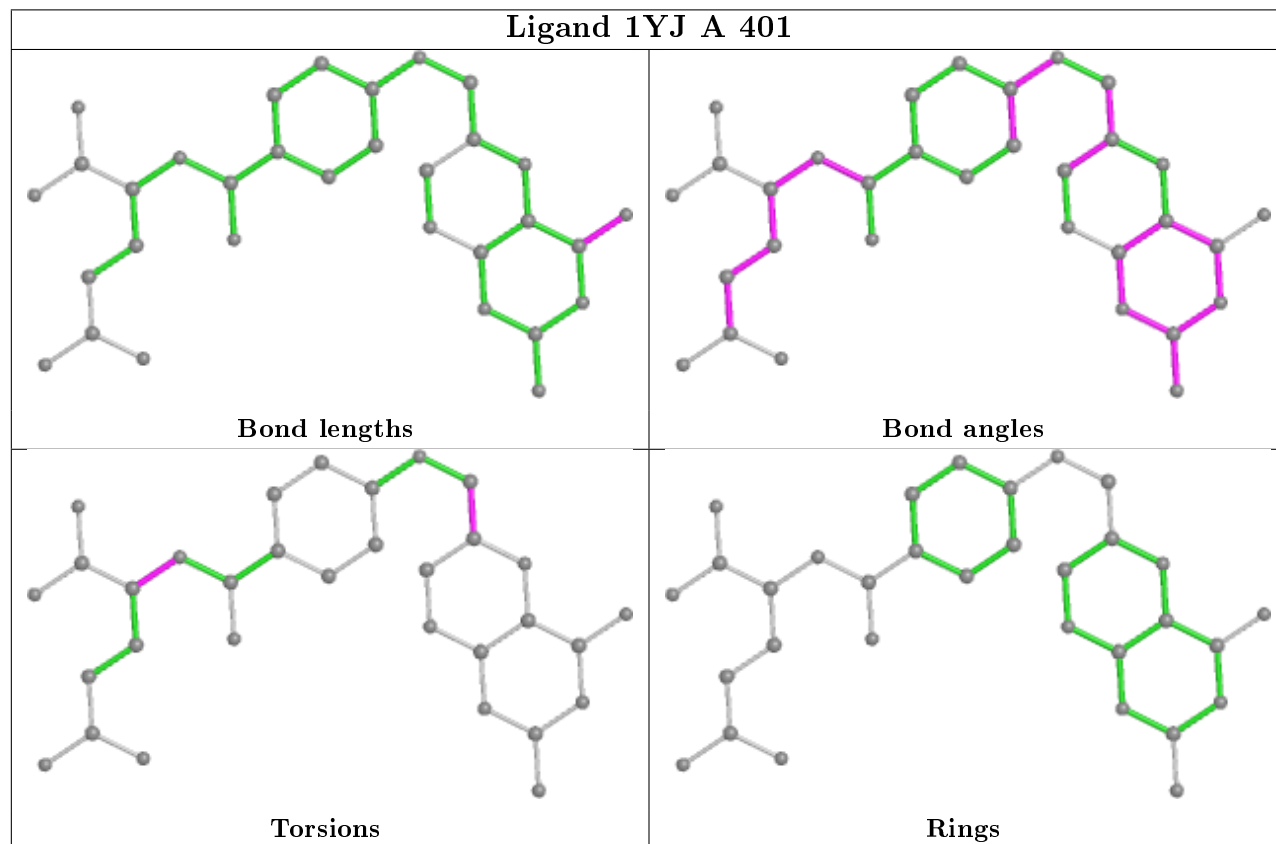
Rings

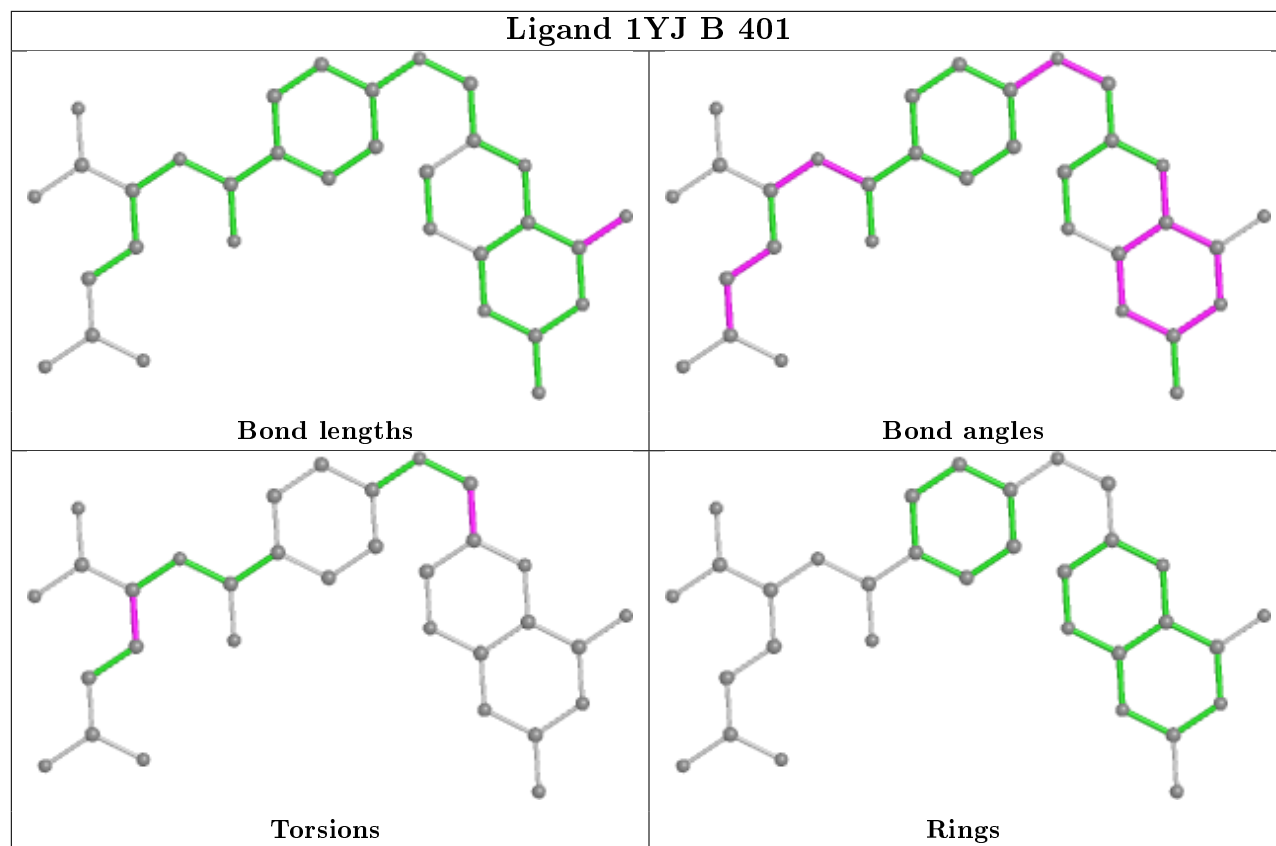


## Ligand T3F A 402



## Ligand 1YJ A 401





## 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, 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%)	-0.59	1 (0%) 94 93	12, 24, 46, 69	0
1	B	398/405 (98%)	-0.60	0 100 100	12, 21, 45, 63	0
All	All	796/810 (98%)	-0.59	1 (0%) 95 95	12, 23, 46, 69	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	LEU	2.9

### 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 carbohydrates 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<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(Å <sup>2</sup> )	Q<0.9
4	NA	A	405	1/1	0.90	0.17	38,38,38,38	0
4	NA	B	405	1/1	0.90	0.06	30,30,30,30	0
2	1YJ	A	401	32/32	0.92	0.14	25,31,59,69	0
2	1YJ	B	401	32/32	0.93	0.13	18,34,44,51	0

*Continued on next page...*

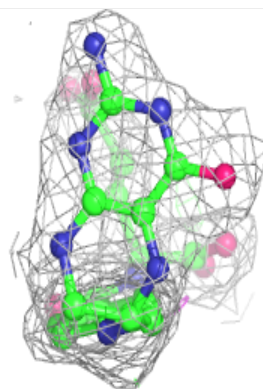
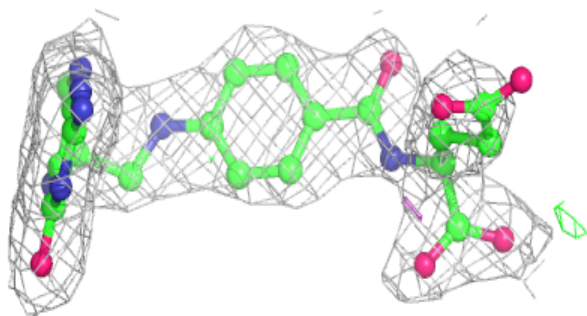
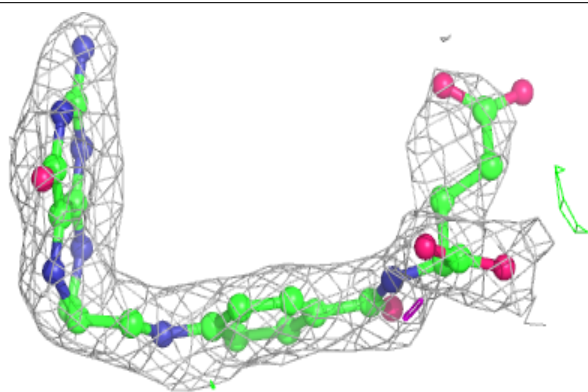
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	T3F	B	403	35/35	0.95	0.10	20,23,36,38	0
3	T3F	A	403	35/35	0.95	0.10	17,24,33,37	0
3	T3F	A	402	35/35	0.97	0.10	18,23,27,29	0
3	T3F	B	402	35/35	0.97	0.09	18,23,25,26	0
4	NA	B	404	1/1	0.97	0.06	23,23,23,23	0
4	NA	A	404	1/1	0.99	0.05	18,18,18,18	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.

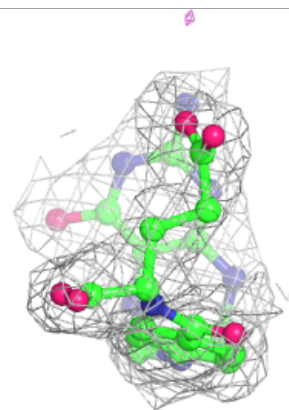
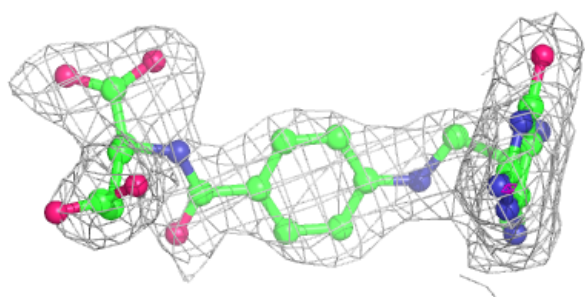
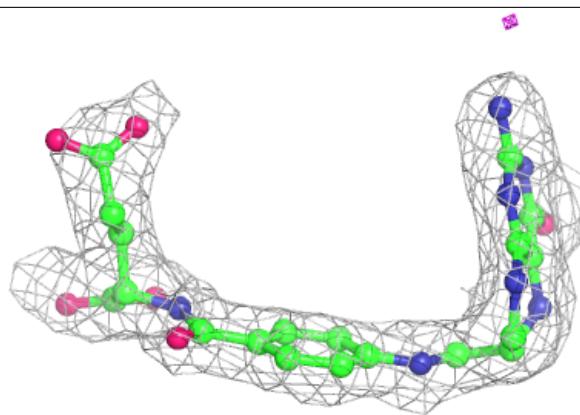
**Electron density around 1YJ A 401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

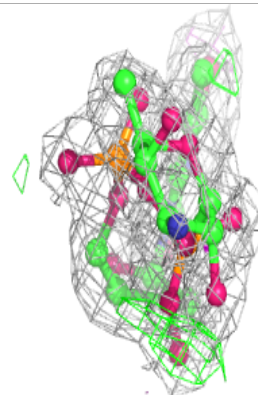
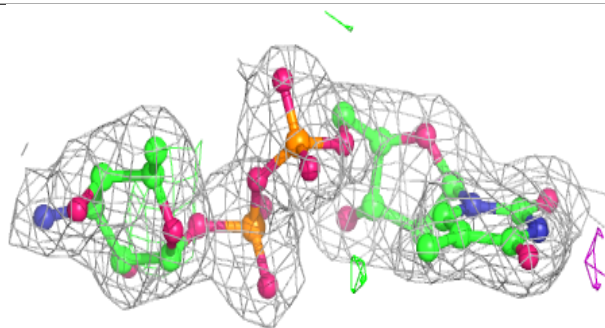
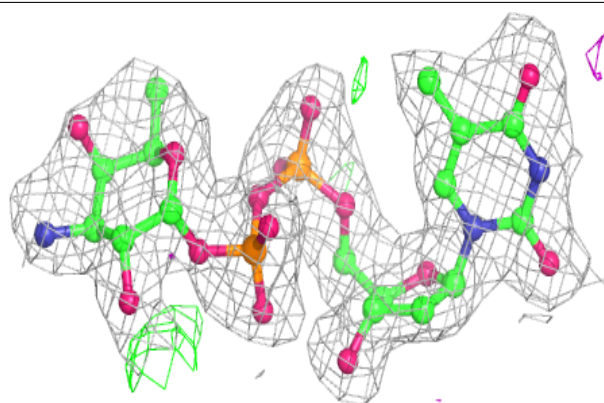


**Electron density around 1YJ B 401:**

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

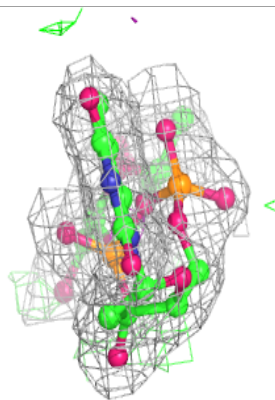
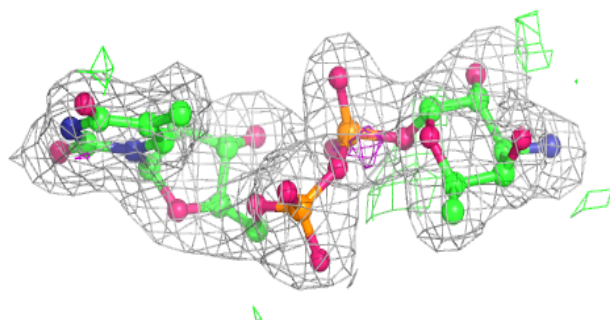
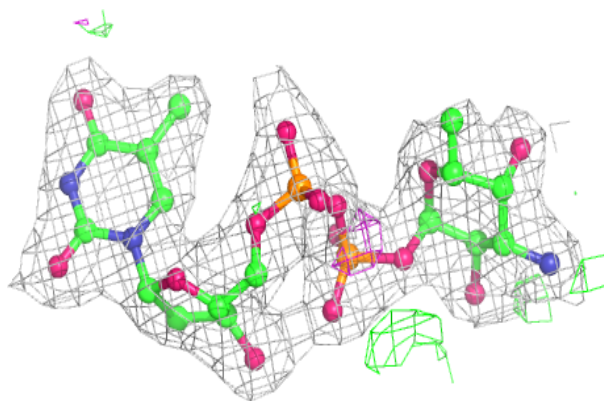
**Electron density around T3F B 403:**

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

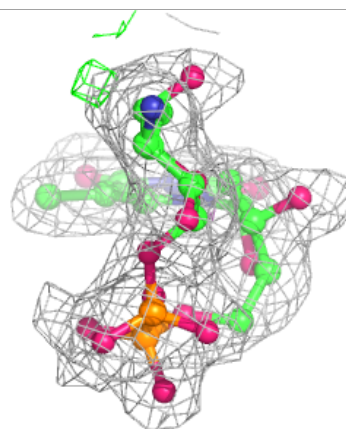
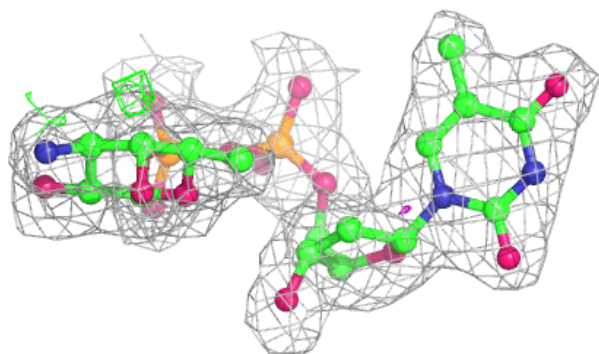
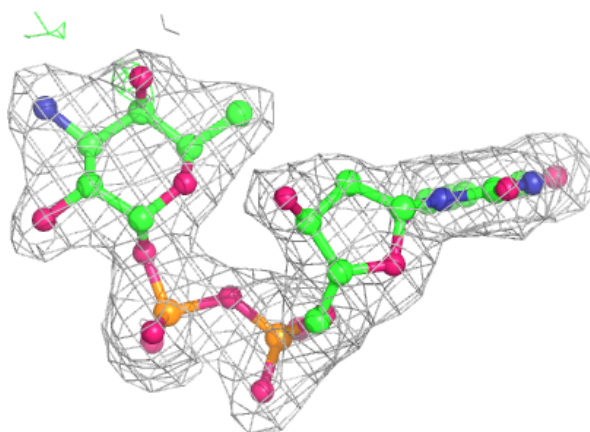


**Electron density around T3F A 403:**

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

**Electron density around T3F A 402:**

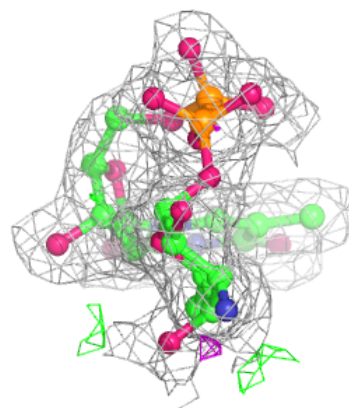
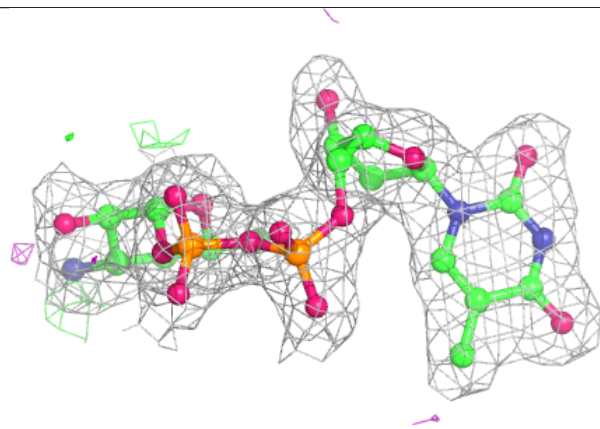
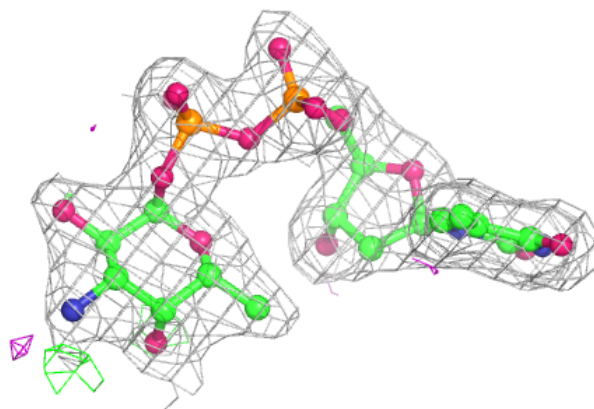
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around T3F 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.