



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 05:35 PM BST

PDB ID : 4NV1
Title : Crystal structure of a 4-N formyltransferase from Francisella tularensis
Authors : Thoden, J.B.; Zimmer, A.L.; Holden, H.M.
Deposited on : 2013-12-04
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

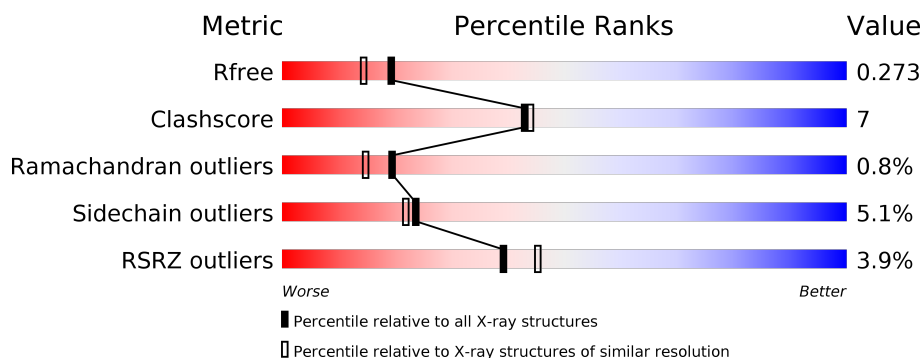
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	243	
1	B	243	
1	C	243	
1	D	243	
1	E	243	
1	F	243	

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Mol	Chain	Length	Quality of chain
1	G	243	<div><div></div><div>12%</div><div>72%</div><div>23%</div><div>•</div></div>
1	H	243	<div><div></div><div>2%</div><div>81%</div><div>16%</div><div>••</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16694 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	C	241	Total	C	N	O	S	0	0	0
			1960	1257	322	371	10			
1	D	240	Total	C	N	O	S	0	0	0
			1953	1254	321	368	10			
1	E	242	Total	C	N	O	S	0	2	0
			1980	1272	328	370	10			
1	F	240	Total	C	N	O	S	0	0	0
			1953	1254	321	368	10			
1	B	241	Total	C	N	O	S	0	0	0
			1959	1257	322	370	10			
1	A	240	Total	C	N	O	S	0	0	0
			1953	1254	321	368	10			
1	G	242	Total	C	N	O	S	0	0	0
			1967	1262	325	370	10			
1	H	241	Total	C	N	O	S	0	0	0
			1960	1257	322	371	10			

There are 16 discrepancies between the modelled and reference sequences:

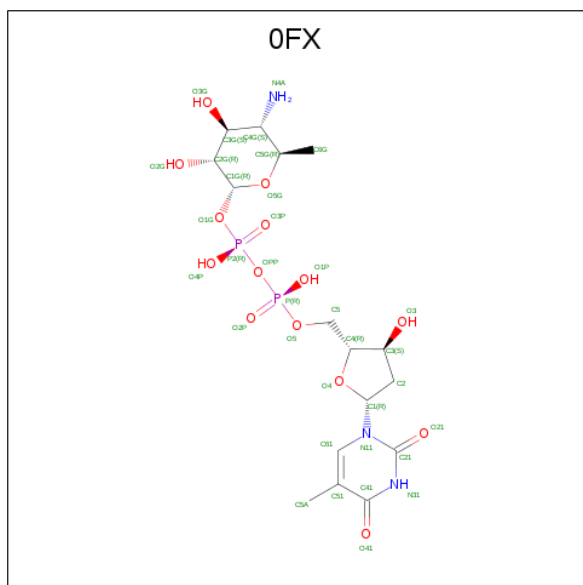
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP Q79RC8
C	0	HIS	-	EXPRESSION TAG	UNP Q79RC8
D	-1	GLY	-	EXPRESSION TAG	UNP Q79RC8
D	0	HIS	-	EXPRESSION TAG	UNP Q79RC8
E	-1	GLY	-	EXPRESSION TAG	UNP Q79RC8
E	0	HIS	-	EXPRESSION TAG	UNP Q79RC8
F	-1	GLY	-	EXPRESSION TAG	UNP Q79RC8
F	0	HIS	-	EXPRESSION TAG	UNP Q79RC8
B	-1	GLY	-	EXPRESSION TAG	UNP Q79RC8
B	0	HIS	-	EXPRESSION TAG	UNP Q79RC8
A	-1	GLY	-	EXPRESSION TAG	UNP Q79RC8
A	0	HIS	-	EXPRESSION TAG	UNP Q79RC8
G	-1	GLY	-	EXPRESSION TAG	UNP Q79RC8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	EXPRESSION TAG	UNP Q79RC8
H	-1	GLY	-	EXPRESSION TAG	UNP Q79RC8
H	0	HIS	-	EXPRESSION TAG	UNP Q79RC8

- Molecule 2 is dTDP-4-amino-4,6-dideoxyglucose (three-letter code: 0FX) (formula: $C_{16}H_{27}N_3O_{14}P_2$).



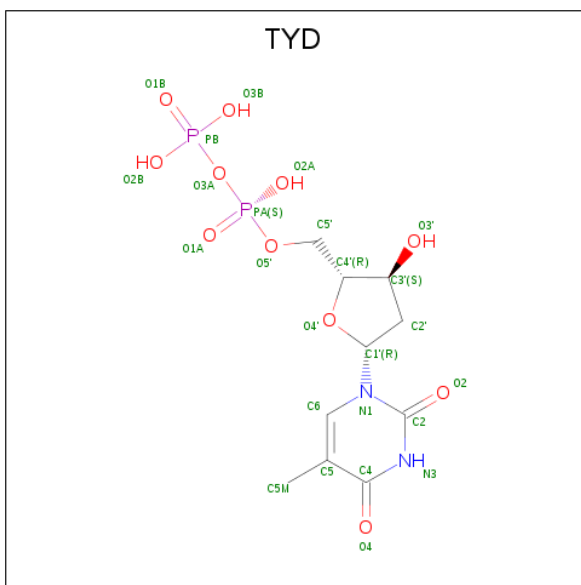
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			35	16	3	14	2		
2	E	1	Total	C	N	O	P	0	0
			35	16	3	14	2		
2	A	1	Total	C	N	O	P	0	0
			35	16	3	14	2		
2	G	1	Total	C	N	O	P	0	0
			35	16	3	14	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



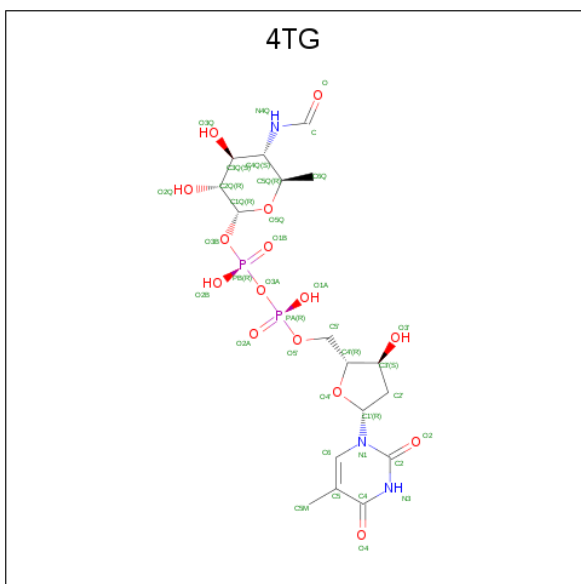
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula: $C_{10}H_{16}N_2O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total 25	C 10	N 2	O 11	P 2	0	0
4	F	1	Total 25	C 10	N 2	O 11	P 2	0	0
4	H	1	Total 25	C 10	N 2	O 11	P 2	0	0

- Molecule 5 is dTDP-4,6-dideoxy-4-formamido-glucose (three-letter code: 4TG) (formula: $\text{C}_{17}\text{H}_{27}\text{N}_3\text{O}_{15}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			37	17	3	15	2		

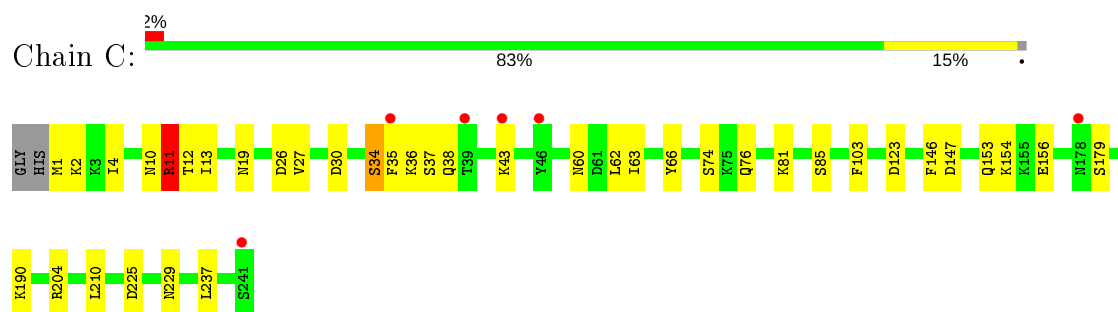
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	94	Total	O	0	0
			94	94		
6	D	104	Total	O	0	0
			104	104		
6	E	99	Total	O	0	0
			99	99		
6	F	101	Total	O	0	0
			101	101		
6	B	76	Total	O	0	0
			76	76		
6	A	115	Total	O	0	0
			115	115		
6	G	41	Total	O	0	0
			41	41		
6	H	102	Total	O	0	0
			102	102		

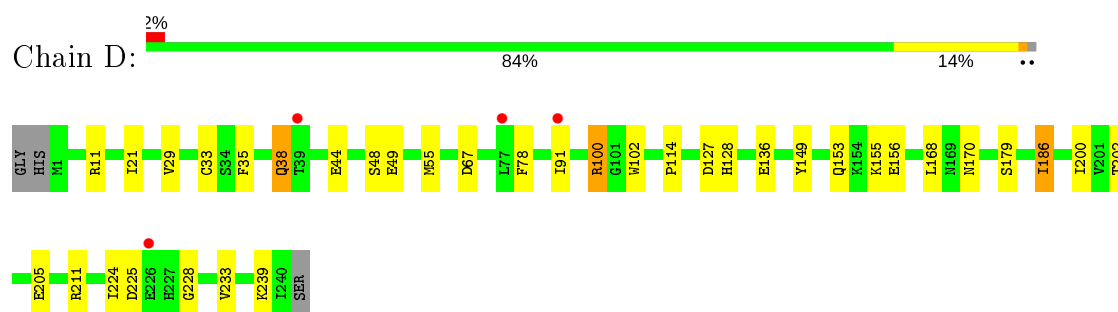
3 Residue-property plots [i](#)

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.

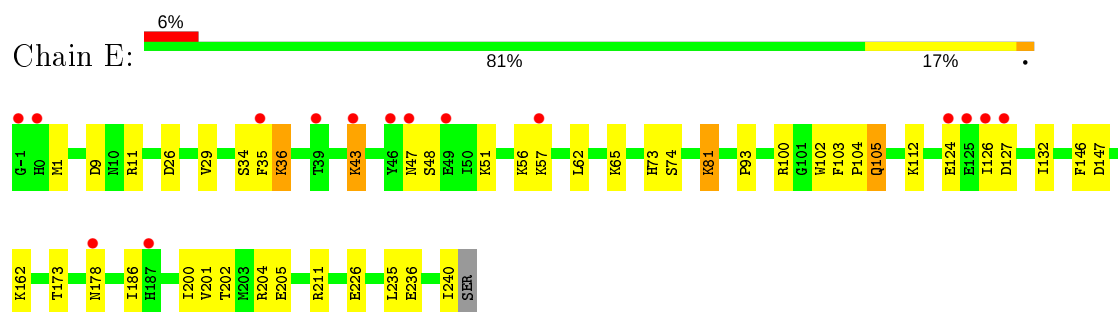
- Molecule 1: Formyltransferase



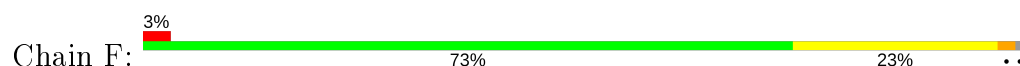
- Molecule 1: Formyltransferase



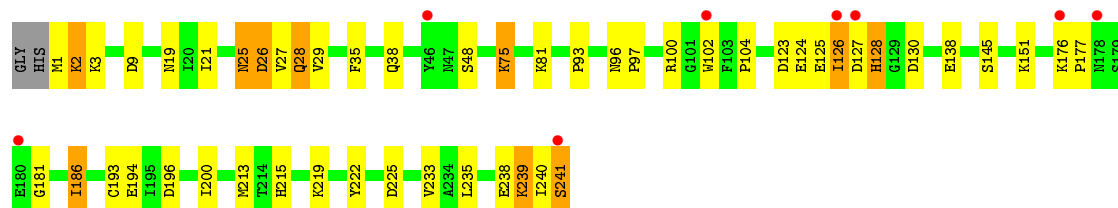
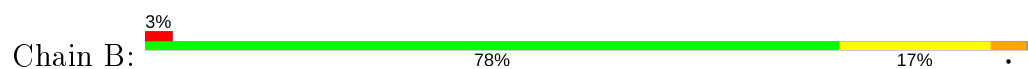
- Molecule 1: Formyltransferase



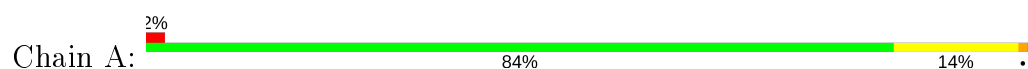
- Molecule 1: Formyltransferase



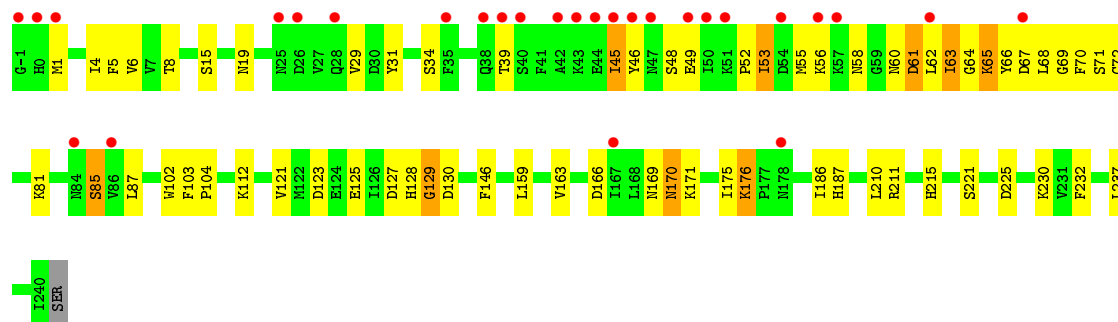
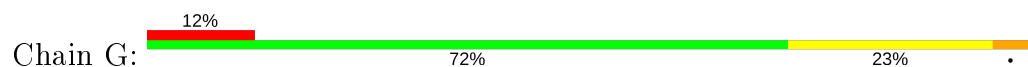
- Molecule 1: Formyltransferase



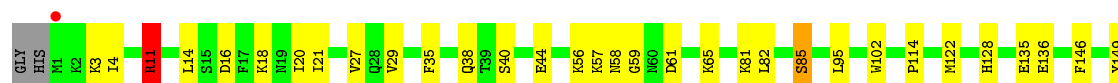
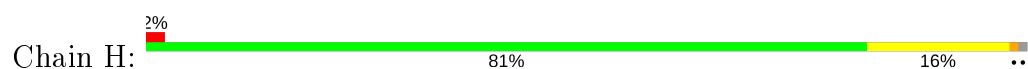
- Molecule 1: Formyltransferase



- Molecule 1: Formyltransferase



- Molecule 1: Formyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.94Å 80.06Å 109.85Å 71.72° 88.62° 89.78°	Depositor
Resolution (Å)	29.96 – 2.10 29.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.0 (29.96-2.10) 90.1 (29.94-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.29 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.191 , 0.270 0.198 , 0.273	Depositor DCC
R_{free} test set	6149 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.063 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16694	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: TYD, OFX, PO4, 4TG

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	0.63	0/1995	1.04	2/2692 (0.1%)
1	B	0.57	0/2001	1.06	3/2700 (0.1%)
1	C	0.66	0/2002	1.11	6/2700 (0.2%)
1	D	0.64	0/1995	1.05	7/2692 (0.3%)
1	E	0.66	0/2030	1.13	7/2738 (0.3%)
1	F	0.63	0/1995	1.02	3/2692 (0.1%)
1	G	0.53	0/2010	1.00	3/2712 (0.1%)
1	H	0.67	0/2002	1.07	5/2700 (0.2%)
All	All	0.63	0/16030	1.06	36/21626 (0.2%)

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	204	ARG	NE-CZ-NH2	9.65	125.12	120.30
1	G	211	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	C	225	ASP	CB-CG-OD1	8.89	126.30	118.30
1	E	204	ARG	NE-CZ-NH1	-7.47	116.57	120.30
1	D	211	ARG	NE-CZ-NH1	6.82	123.71	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	1953	0	1942	19	0
1	B	1959	0	1947	35	0
1	C	1960	0	1947	25	0
1	D	1953	0	1942	26	0
1	E	1980	0	1972	22	0
1	F	1953	0	1942	37	0
1	G	1967	0	1952	37	0
1	H	1960	0	1947	23	0
2	A	35	0	26	2	0
2	C	35	0	26	2	0
2	E	35	0	26	0	0
2	G	35	0	26	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	F	5	0	0	0	0
3	H	10	0	0	0	0
4	D	25	0	13	2	0
4	F	25	0	13	2	0
4	H	25	0	13	1	0
5	B	37	0	26	0	0
6	A	115	0	0	0	0
6	B	76	0	0	1	0
6	C	94	0	0	2	0
6	D	104	0	0	3	0
6	E	99	0	0	3	0
6	F	101	0	0	5	0
6	G	41	0	0	0	0
6	H	102	0	0	2	0
All	All	16694	0	15760	214	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 7.

The worst 5 of 214 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:11:ARG:NH2	1:F:44:GLU:OE1	2.12	0.83
1:B:138:GLU:O	1:B:151:LYS:NZ	2.12	0.80
1:E:147:ASP:O	6:E:429:HOH:O	2.01	0.78
1:H:235:LEU:HD23	1:H:237:LEU:HD11	1.65	0.77
1:C:103:PHE:CE2	2:C:301:OFX:H19	2.21	0.76

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	238/243 (98%)	228 (96%)	10 (4%)	0	100	100
1	B	239/243 (98%)	226 (95%)	12 (5%)	1 (0%)	34	32
1	C	239/243 (98%)	222 (93%)	16 (7%)	1 (0%)	34	32
1	D	238/243 (98%)	224 (94%)	14 (6%)	0	100	100
1	E	242/243 (100%)	228 (94%)	9 (4%)	5 (2%)	7	3
1	F	238/243 (98%)	225 (94%)	11 (5%)	2 (1%)	19	15
1	G	240/243 (99%)	220 (92%)	13 (5%)	7 (3%)	4	1
1	H	239/243 (98%)	226 (95%)	13 (5%)	0	100	100
All	All	1913/1944 (98%)	1799 (94%)	98 (5%)	16 (1%)	19	15

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	126	ILE
1	E	226	GLU
1	F	170	ASN
1	B	126	ILE
1	G	48	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	A	223/225 (99%)	213 (96%)	10 (4%)	27	27
1	B	224/225 (100%)	209 (93%)	15 (7%)	16	13
1	C	224/225 (100%)	214 (96%)	10 (4%)	27	27
1	D	223/225 (99%)	216 (97%)	7 (3%)	40	43
1	E	226/225 (100%)	214 (95%)	12 (5%)	22	20
1	F	223/225 (99%)	210 (94%)	13 (6%)	20	17
1	G	224/225 (100%)	208 (93%)	16 (7%)	14	11
1	H	224/225 (100%)	215 (96%)	9 (4%)	31	32
All	All	1791/1800 (100%)	1699 (95%)	92 (5%)	24	22

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	233	VAL
1	B	123	ASP
1	H	40	SER
1	B	1	MET
1	B	26	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	ASN
1	B	169	ASN
1	H	120	HIS
1	B	28	GLN
1	B	96	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands 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
3	PO4	C	302	-	4,4,4	1.04	0	6,6,6	0.62	0
2	0FX	G	301	-	30,37,37	0.84	1 (3%)	42,57,57	1.72	11 (26%)
5	4TG	B	301	-	32,39,39	1.23	2 (6%)	40,59,59	1.91	12 (30%)
3	PO4	B	302	-	4,4,4	0.88	0	6,6,6	1.40	1 (16%)
4	TYD	H	301	-	23,26,26	2.13	3 (13%)	33,40,40	2.47	16 (48%)
2	0FX	A	301	-	30,37,37	1.10	1 (3%)	42,57,57	1.98	14 (33%)
3	PO4	F	302	-	4,4,4	0.63	0	6,6,6	1.53	1 (16%)
2	0FX	C	301	-	30,37,37	1.00	2 (6%)	42,57,57	2.10	13 (30%)
2	0FX	E	301	-	30,37,37	1.18	2 (6%)	42,57,57	2.38	15 (35%)
4	TYD	D	301	-	23,26,26	2.55	3 (13%)	33,40,40	2.50	13 (39%)
3	PO4	H	302	-	4,4,4	0.81	0	6,6,6	0.61	0
4	TYD	F	301	-	23,26,26	2.40	3 (13%)	33,40,40	2.68	15 (45%)
3	PO4	H	303	-	4,4,4	0.73	0	6,6,6	0.68	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
2	0FX	G	301	-	-	5/18/53/53	0/3/3/3
5	4TG	B	301	-	-	3/21/56/56	0/3/3/3
2	0FX	A	301	-	-	2/18/53/53	0/3/3/3
2	0FX	C	301	-	-	3/18/53/53	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0FX	E	301	-	-	5/18/53/53	0/3/3/3
4	TYD	D	301	-	-	1/16/28/28	0/2/2/2
4	TYD	F	301	-	-	1/16/28/28	0/2/2/2
4	TYD	H	301	-	-	3/16/28/28	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	TYD	C6-N1	-10.69	1.33	1.46
4	F	301	TYD	C6-N1	-10.05	1.34	1.46
4	H	301	TYD	C6-N1	-8.59	1.36	1.46
2	A	301	0FX	O41-C41	5.18	1.37	1.24
2	E	301	0FX	O41-C41	4.93	1.36	1.24

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	0FX	OPP-P2-O1G	-7.20	87.97	102.48
4	F	301	TYD	C2'-C1'-N1	-7.12	106.91	115.61
2	E	301	0FX	O1G-C1G-C2G	-6.01	97.37	108.38
2	E	301	0FX	C41-N31-C21	5.65	119.92	115.14
4	D	301	TYD	C2'-C1'-N1	-5.55	108.83	115.61

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	301	0FX	P-OPP-P2-O1G
2	G	301	0FX	O5G-C1G-O1G-P2
5	B	301	4TG	C5'-O5'-PA-O2A
4	H	301	TYD	C5'-O5'-PA-O1A
4	H	301	TYD	C5'-O5'-PA-O2A

There are no ring outliers.

6 monomers are involved in 10 short contacts:

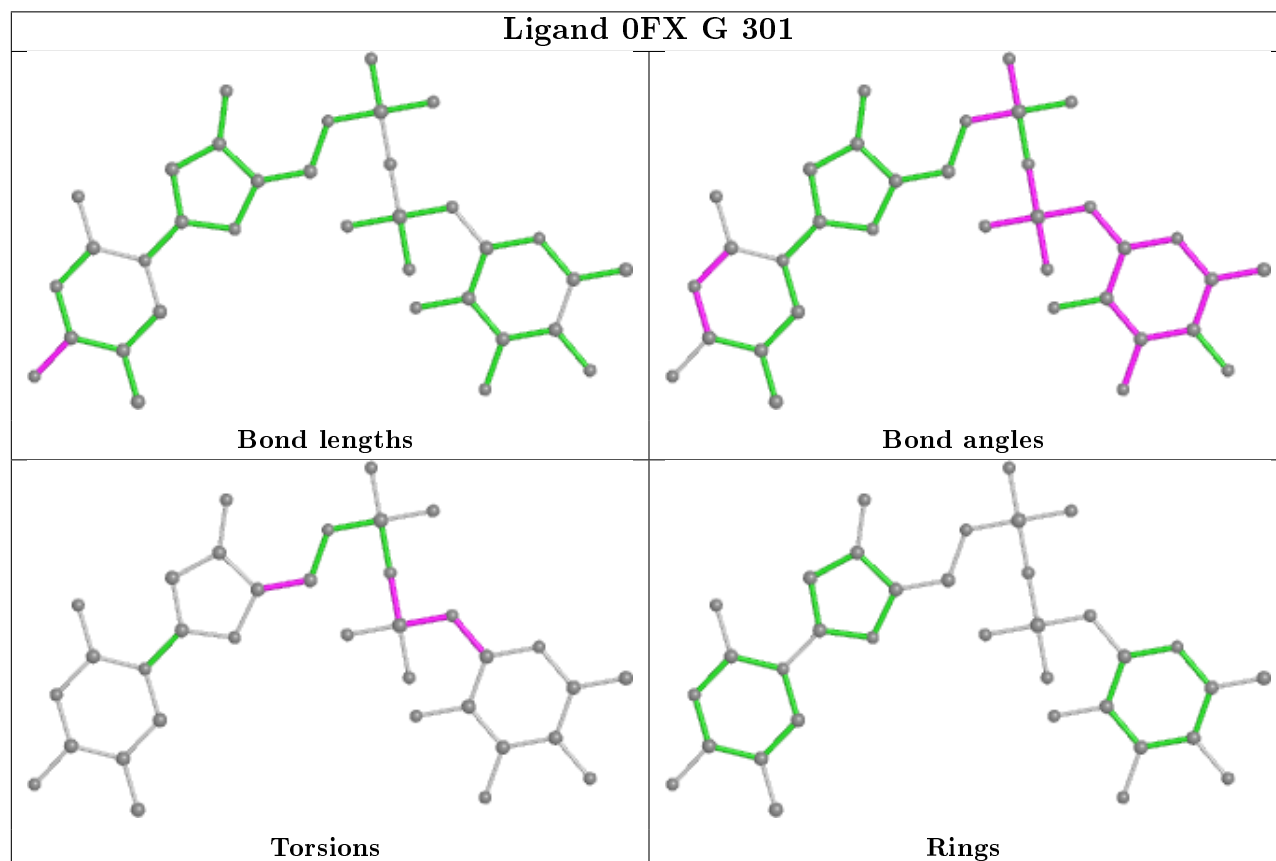
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	PO4	1	0
4	H	301	TYD	1	0
2	A	301	0FX	2	0

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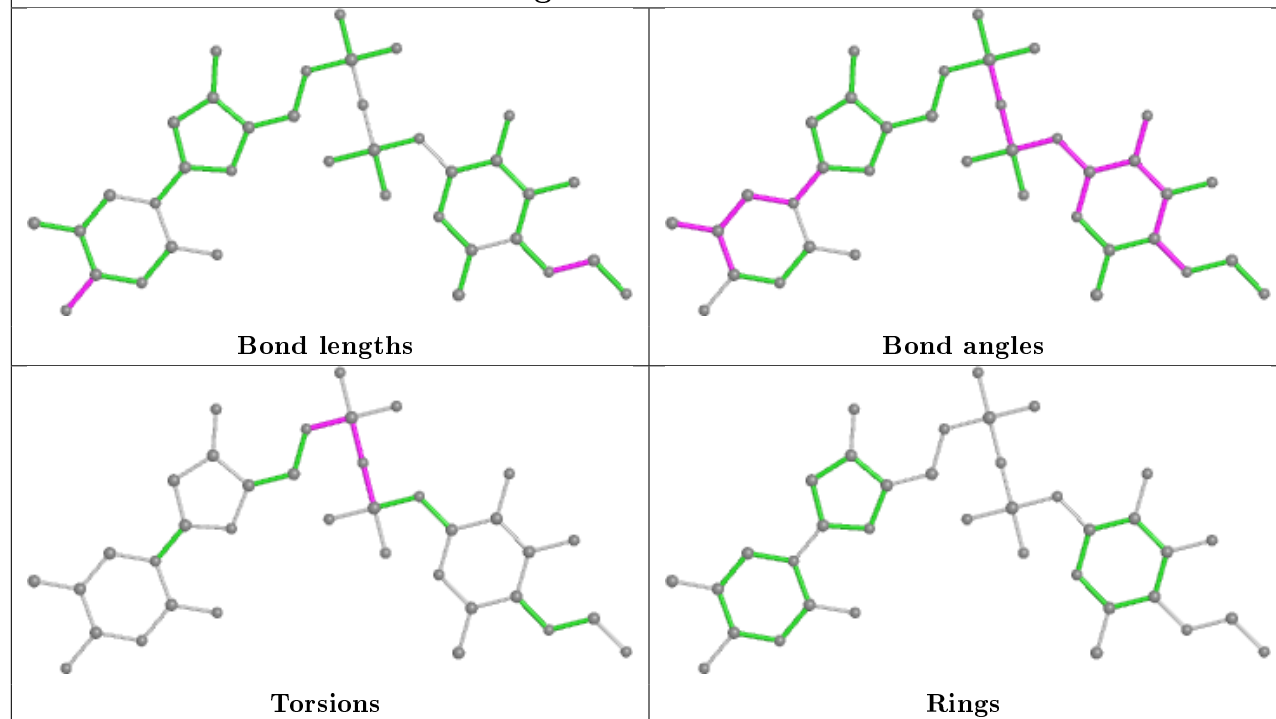
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	0FX	2	0
4	D	301	TYD	2	0
4	F	301	TYD	2	0

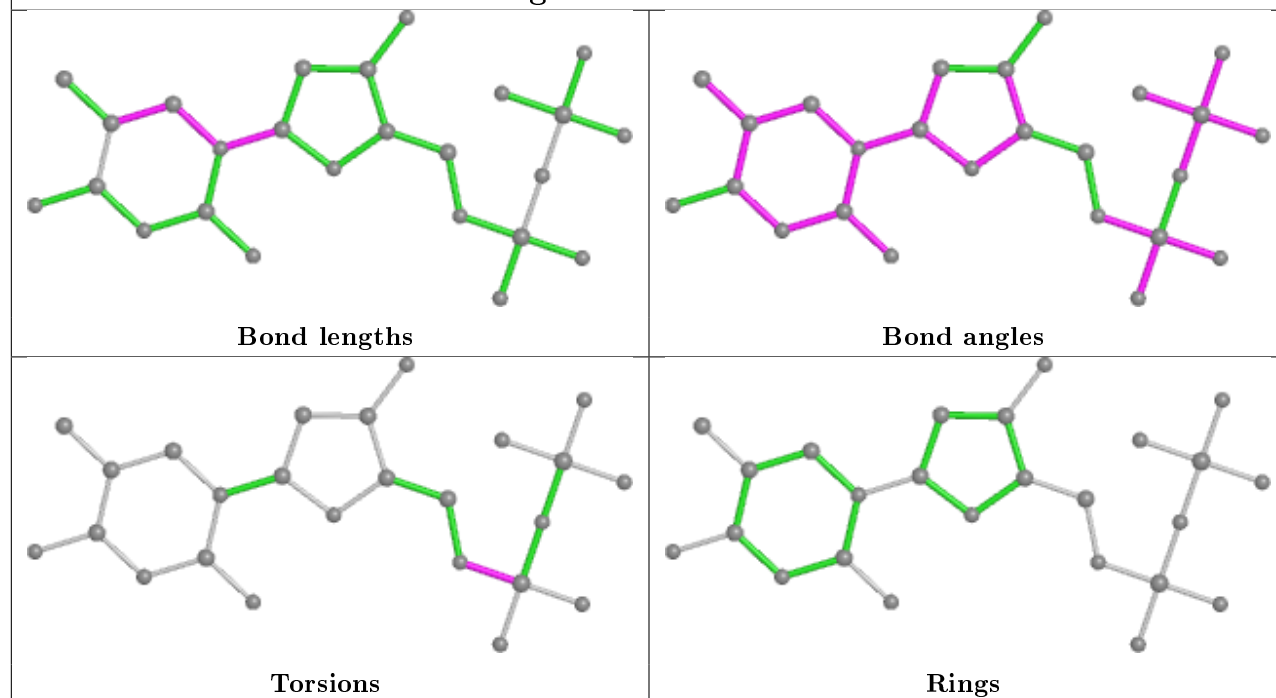
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



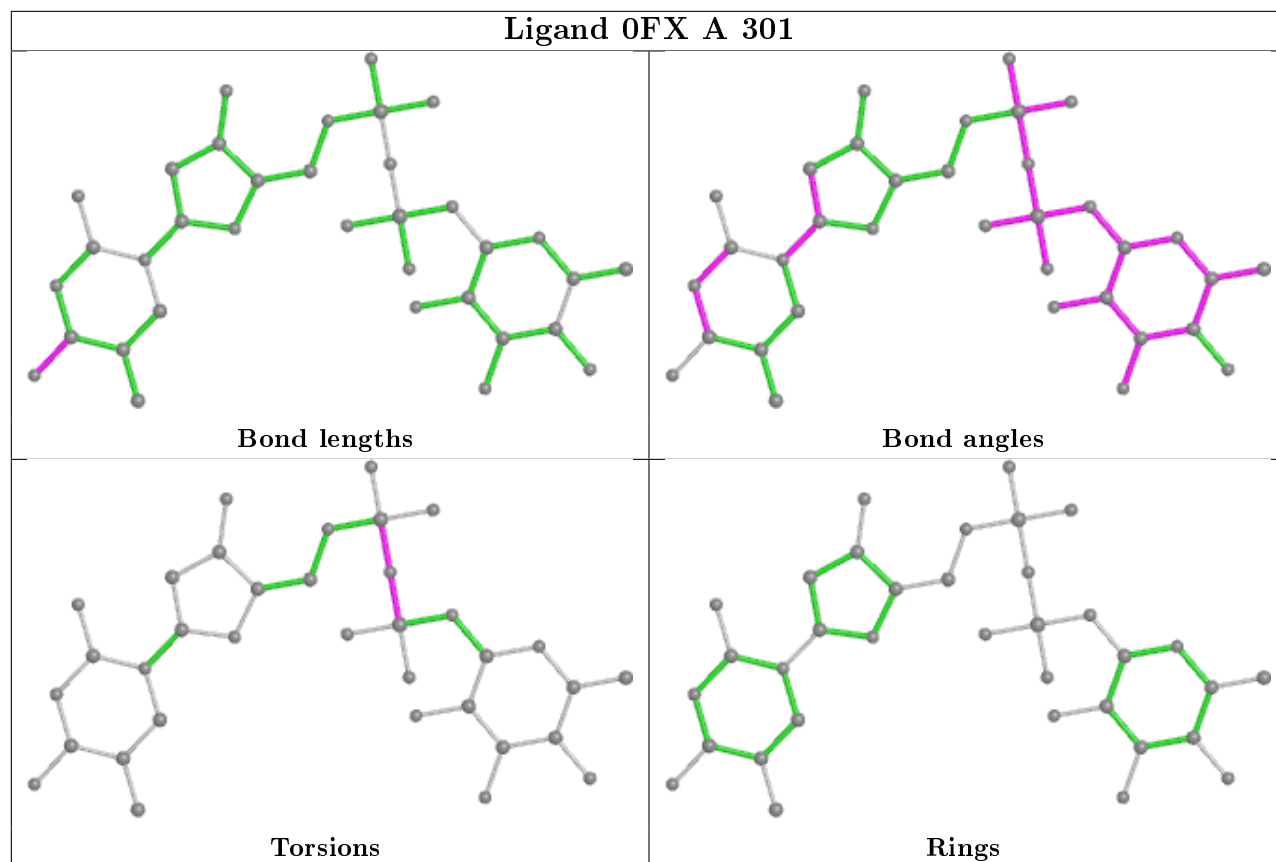
Ligand 4TG B 301



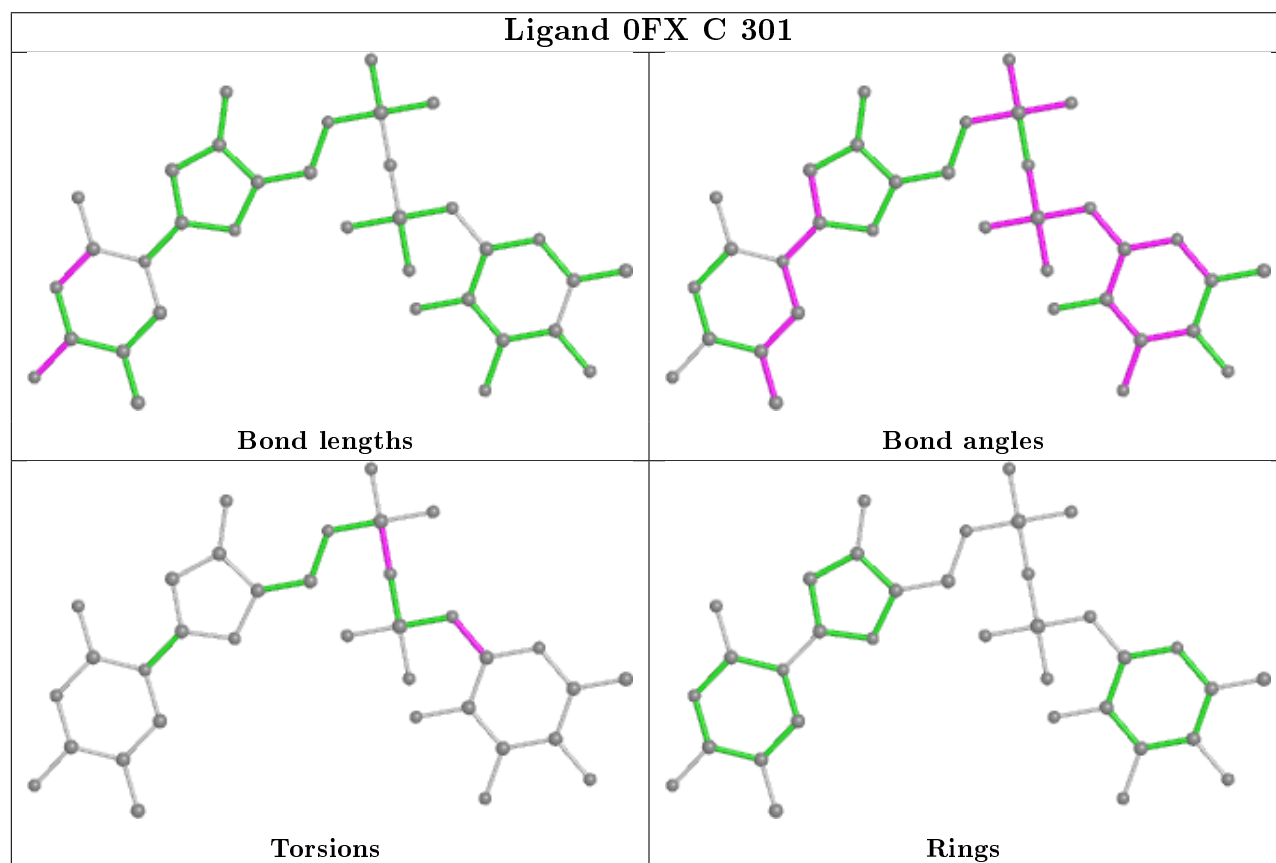
Ligand TYD H 301



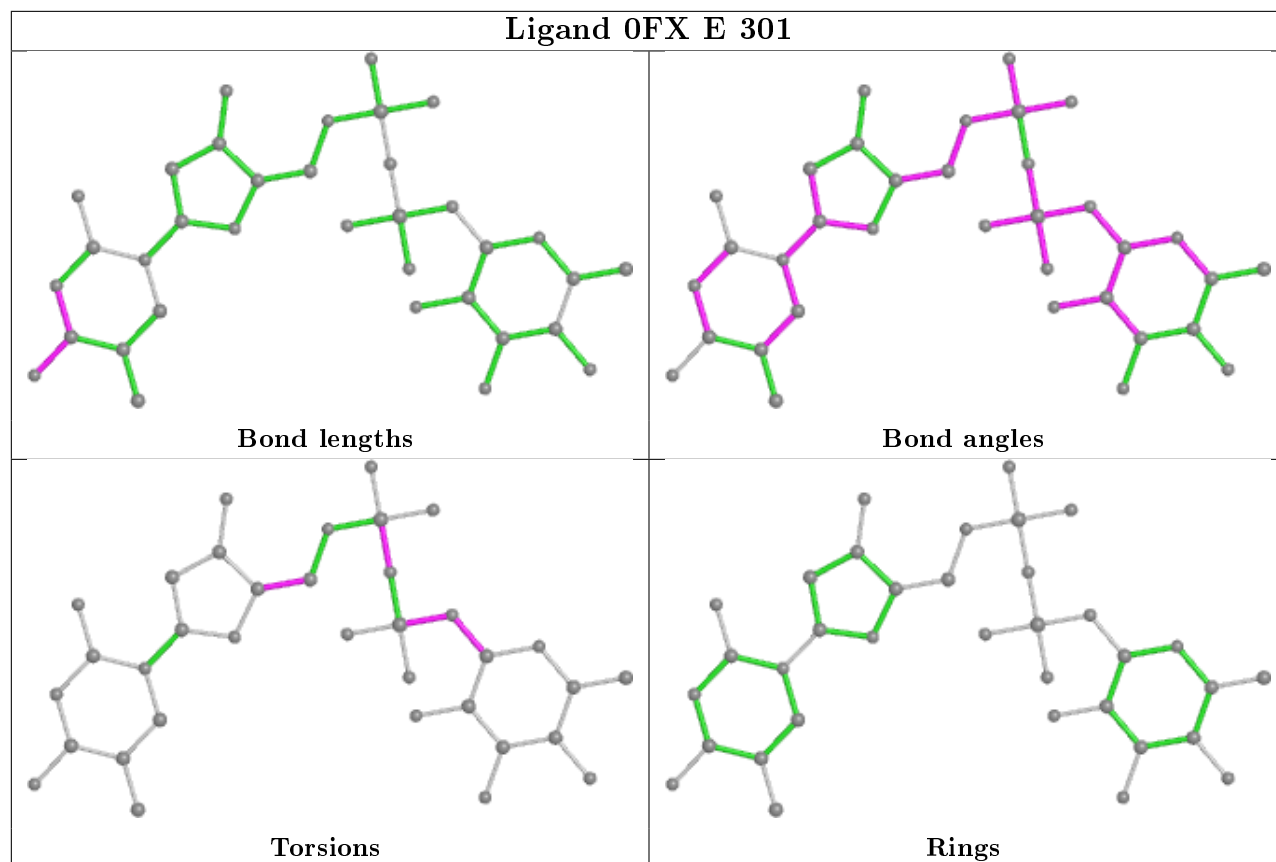
Ligand 0FX A 301



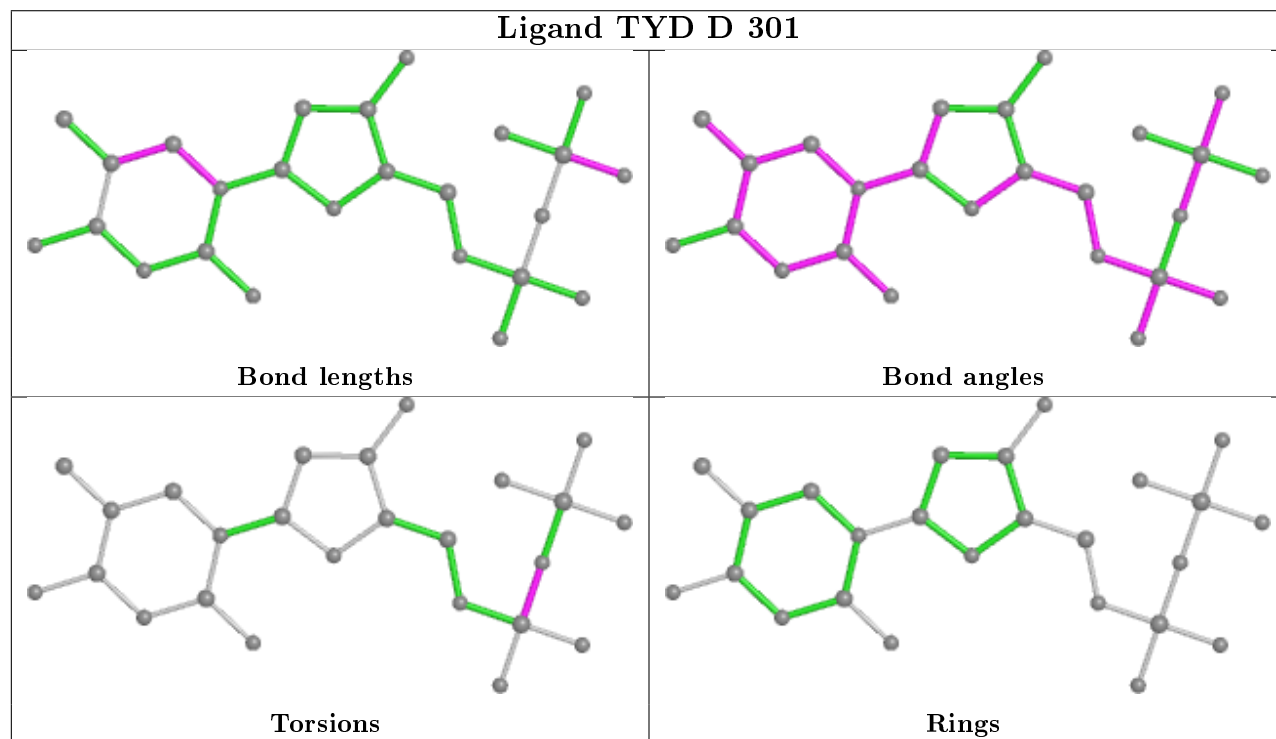
Ligand 0FX C 301

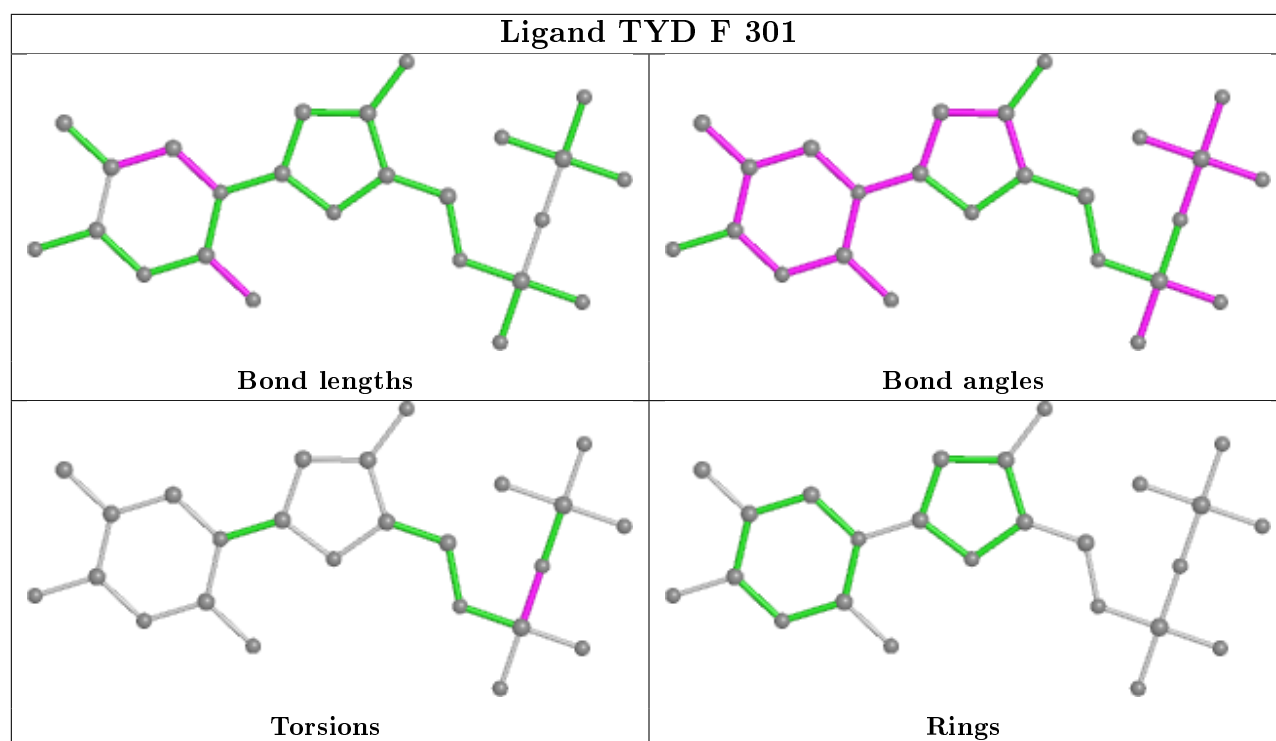


Ligand 0FX E 301



Ligand TYD D 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	240/243 (98%)	-0.03	4 (1%) 70 74	19, 32, 52, 76	0
1	B	241/243 (99%)	0.03	8 (3%) 46 53	25, 40, 70, 116	0
1	C	241/243 (99%)	-0.06	6 (2%) 57 62	18, 34, 61, 79	0
1	D	240/243 (98%)	-0.04	4 (1%) 70 74	18, 33, 57, 73	0
1	E	242/243 (99%)	0.03	15 (6%) 20 25	18, 33, 66, 109	0
1	F	240/243 (98%)	0.05	7 (2%) 51 57	21, 36, 66, 90	0
1	G	242/243 (99%)	0.55	28 (11%) 4 6	23, 51, 88, 103	0
1	H	241/243 (99%)	-0.02	4 (1%) 70 74	17, 32, 56, 72	0
All	All	1927/1944 (99%)	0.06	76 (3%) 39 45	17, 36, 70, 116	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	ILE	7.5
1	G	46	TYR	7.1
1	G	-1	GLY	6.8
1	E	46	TYR	5.6
1	E	-1	GLY	5.5

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 monosaccharides in this entry.

6.4 Ligands ⓘ

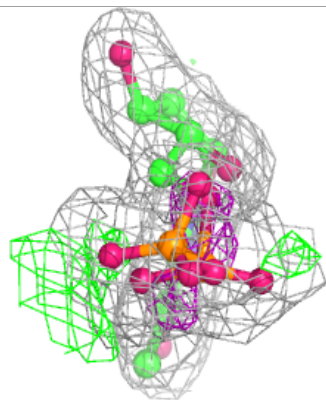
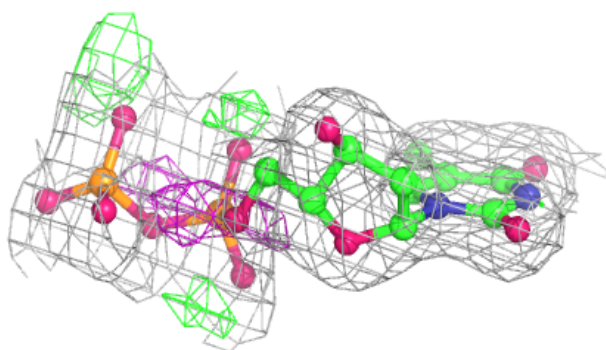
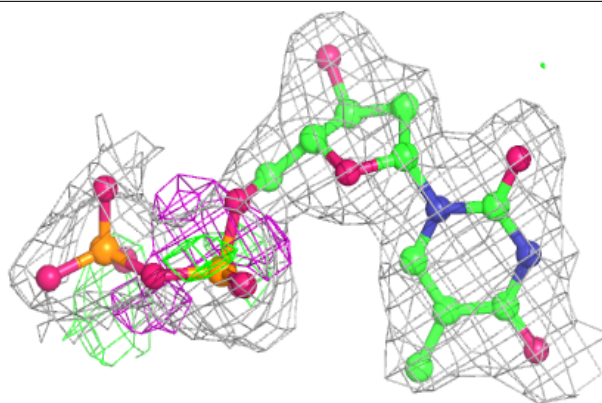
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TYD	H	301	25/25	0.88	0.12	20,29,71,80	0
4	TYD	D	301	25/25	0.91	0.11	28,36,51,65	0
4	TYD	F	301	25/25	0.91	0.12	23,35,62,64	0
3	PO4	F	302	5/5	0.92	0.13	46,59,61,64	0
2	0FX	A	301	35/35	0.93	0.11	26,49,66,67	0
2	0FX	G	301	35/35	0.94	0.12	30,40,58,63	0
3	PO4	H	302	5/5	0.94	0.16	57,59,69,84	0
2	0FX	C	301	35/35	0.94	0.12	25,35,52,55	0
3	PO4	H	303	5/5	0.94	0.12	41,51,66,67	0
3	PO4	B	302	5/5	0.95	0.14	47,49,59,60	0
2	0FX	E	301	35/35	0.95	0.10	24,37,47,53	0
3	PO4	C	302	5/5	0.97	0.09	42,45,53,56	0
5	4TG	B	301	37/37	0.97	0.08	30,37,50,58	0

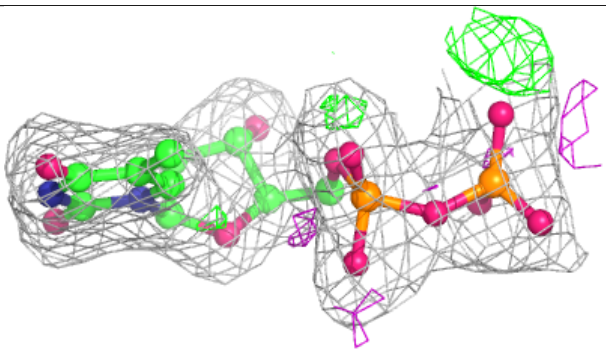
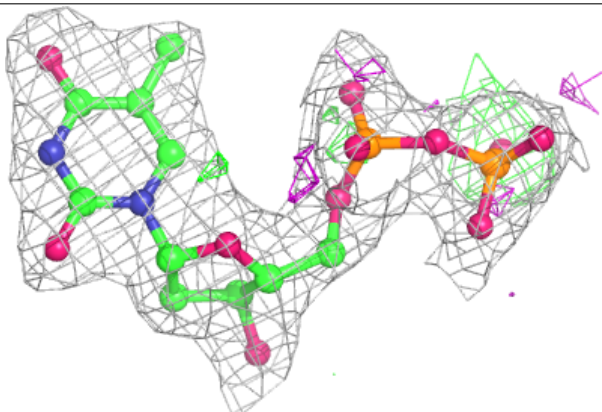
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TYD H 301:

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

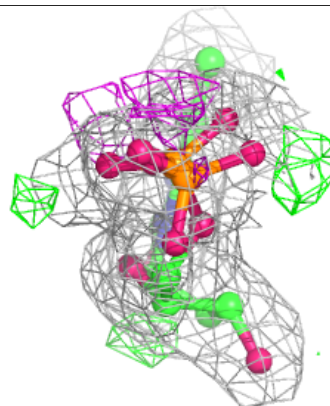
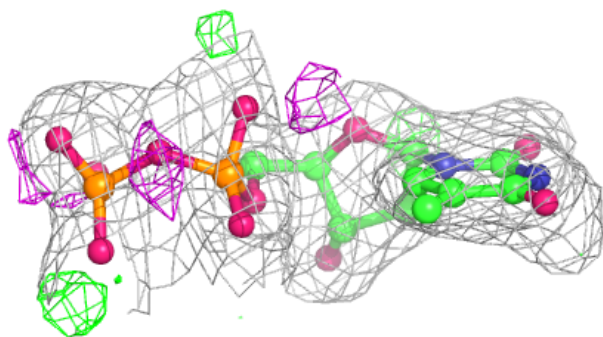
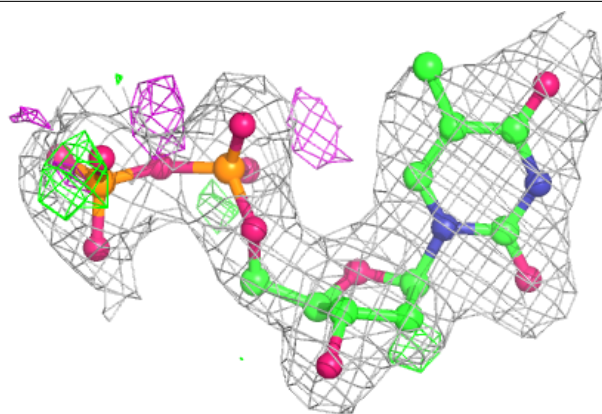
**Electron density around TYD D 301:**

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

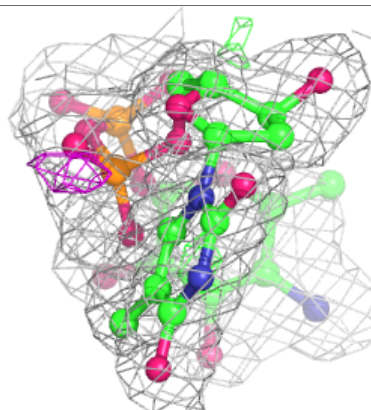
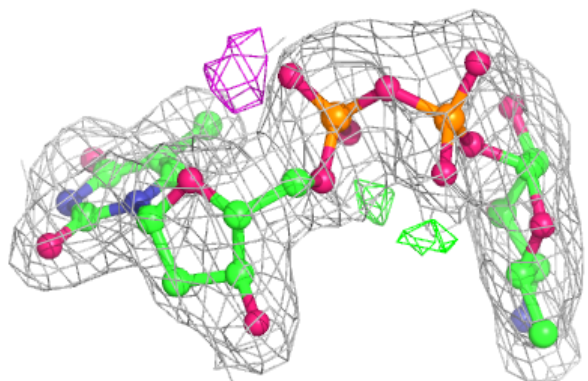
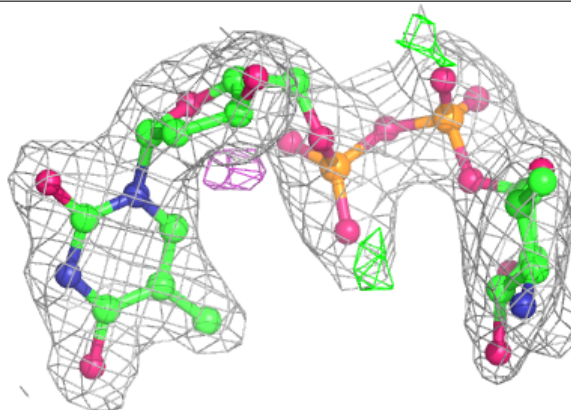


Electron density around TYD F 301:

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

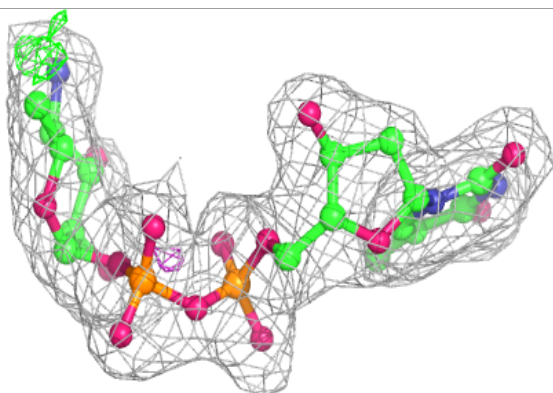
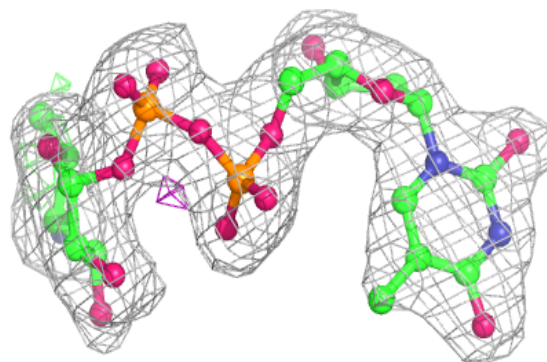
**Electron density around OFX A 301:**

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

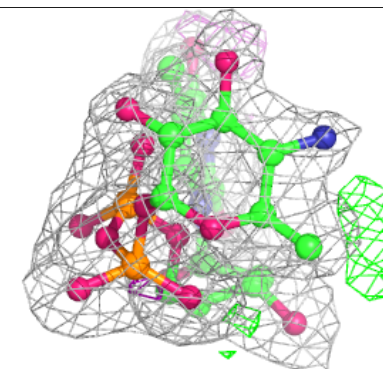
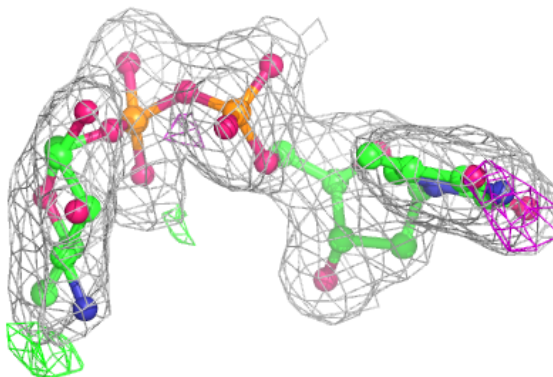
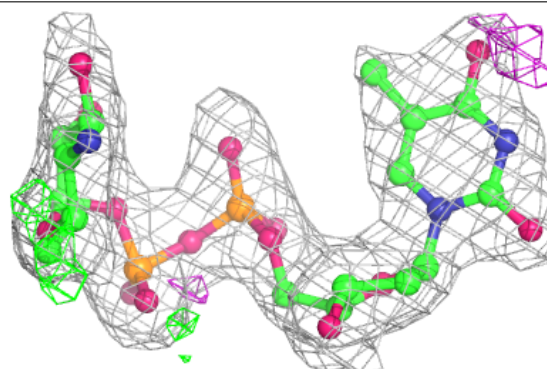


Electron density around 0FX G 301:

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

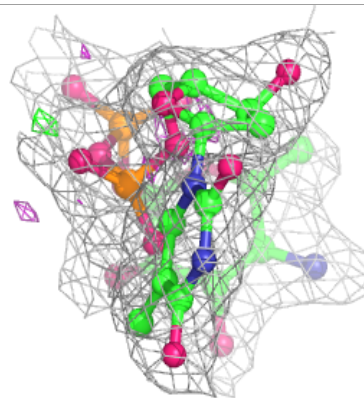
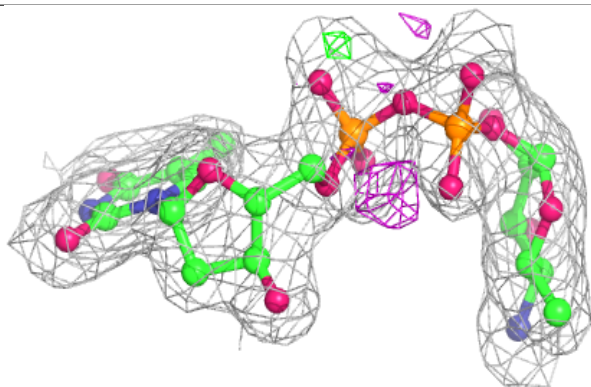
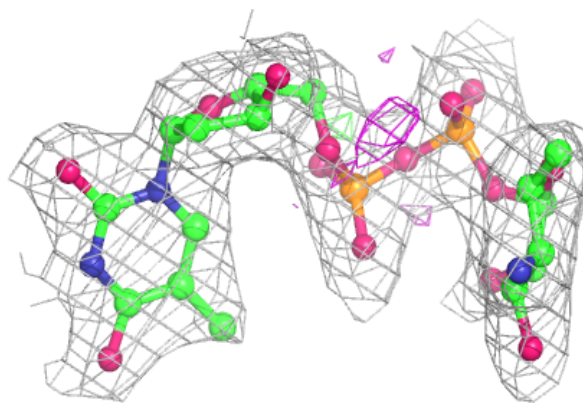
**Electron density around 0FX C 301:**

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and green (positive)

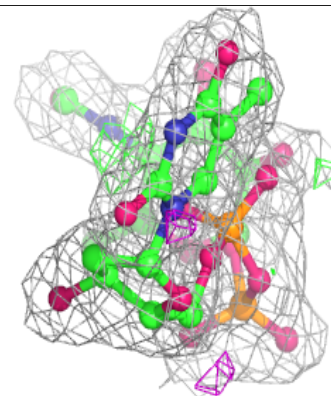
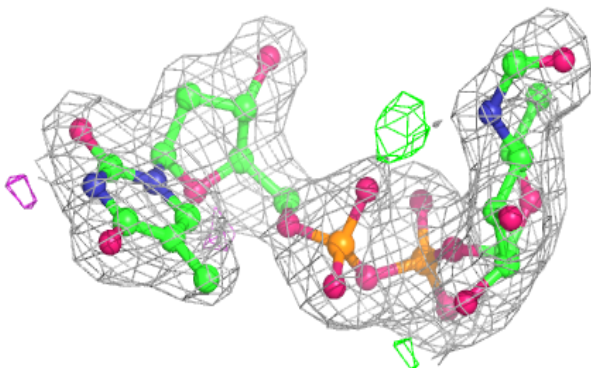
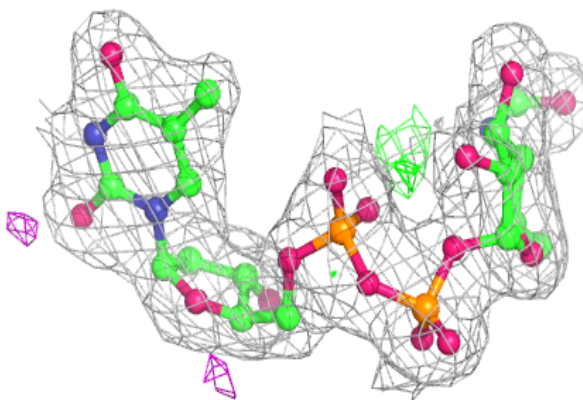


Electron density around 0FX E 301:

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

**Electron density around 4TG B 301:**

$2mF_o-DF_c$ (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.