



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:32 pm BST

PDB ID : 6D2L  
Title : Crystal structure of human CARM1 with (S)-SKI-72  
Authors : DONG, A.; ZENG, H.; WALKER, J.R.; Hutchinson, A.; Seitova, A.; LUO, M.; CAI, X.C.; KE, W.; WANG, J.; SHI, C.; ZHENG, W.; LEE, J.P.; IBANEZ, G.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.M.; BROWN, P.J.; WU, H.; Structural Genomics Consortium (SGC)  
Deposited on : 2018-04-13  
Resolution : 2.00 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

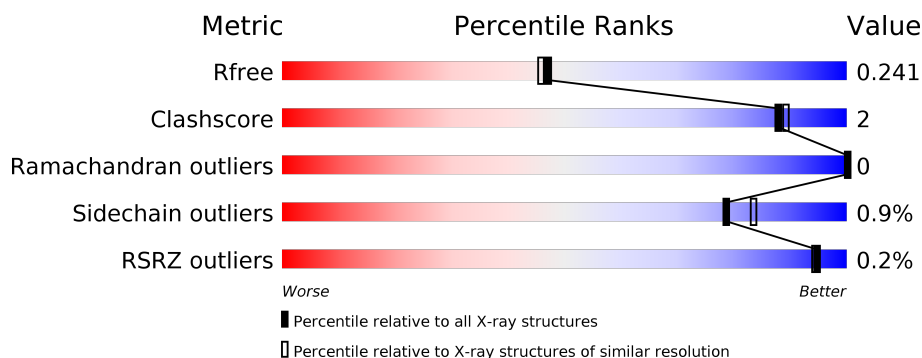
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	344	<div> <div>93%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> <div>• •</div> </div>
1	B	344	<div> <div>91%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> <div>5% •</div> </div>
1	C	344	<div> <div>92%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> <div>• •</div> </div>
1	D	344	<div> <div>92%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> <div>• •</div> </div>
1	E	344	<div> <div>89%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> <div>6% •</div> </div>
1	F	344	<div> <div>90%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> <div>5% 5%</div> </div>

## 2 Entry composition [i](#)

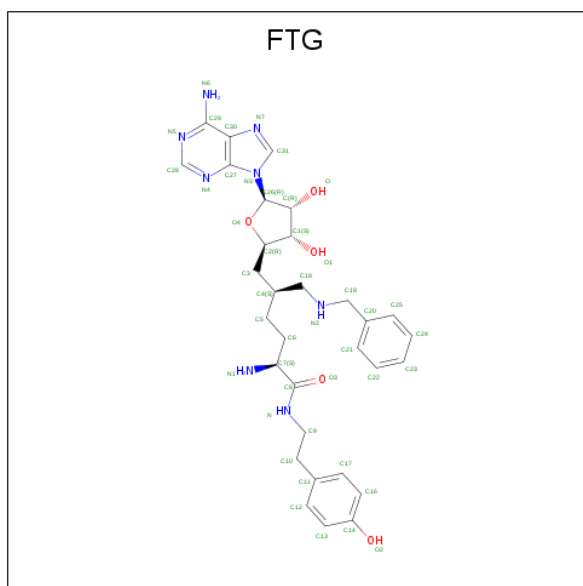
There are 6 unique types of molecules in this entry. The entry contains 16868 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Histone-arginine methyltransferase CARM1.

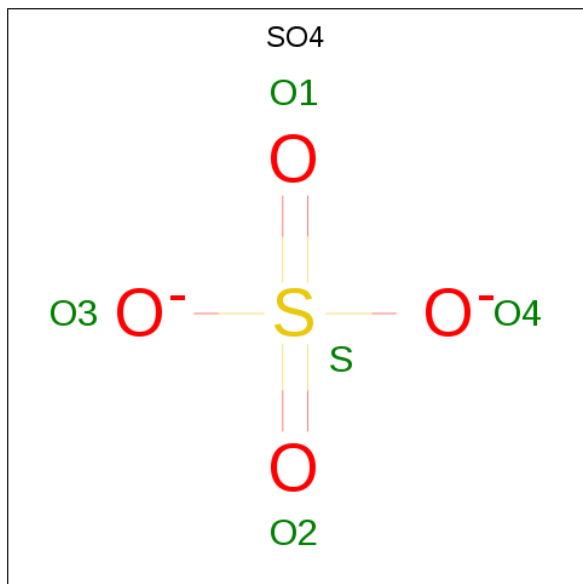
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	6	0
			2663	1725	436	487	15			
1	B	330	Total	C	N	O	S	0	8	0
			2666	1730	434	485	17			
1	C	330	Total	C	N	O	S	0	5	0
			2640	1712	427	485	16			
1	D	329	Total	C	N	O	S	0	5	0
			2634	1709	430	479	16			
1	E	329	Total	C	N	O	S	0	2	0
			2602	1688	423	476	15			
1	F	328	Total	C	N	O	S	0	2	0
			2614	1696	427	476	15			

- Molecule 2 is (2S,5S)-2-amino-6-[(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxy tetrahydrofuran-2-yl]-5-[(benzylamino)methyl]-N-[2-(4-hydroxyphenyl)ethyl]hexanamide (three-letter code: FTG) (formula: C<sub>31</sub>H<sub>40</sub>N<sub>8</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			44	31	8	5		
2	B	1	Total	C	N	O	0	0
			44	31	8	5		
2	C	1	Total	C	N	O	0	0
			39	27	8	4		
2	D	1	Total	C	N	O	0	0
			44	31	8	5		
2	E	1	Total	C	N	O	0	0
			38	26	8	4		
2	F	1	Total	C	N	O	0	0
			44	31	8	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	X	0	0
			1	1		
5	C	1	Total	X	0	0
			1	1		
5	F	1	Total	X	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	150	Total	O	0	1
			151	151		
6	B	166	Total	O	0	1
			167	167		
6	C	119	Total	O	0	1
			120	120		
6	D	110	Total	O	0	1
			111	111		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	103	Total 104	O 104	0	1
6	F	113	Total 113	O 113	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.

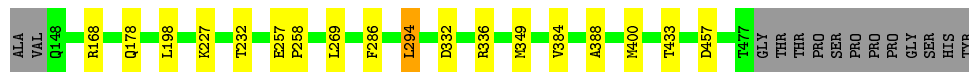
- Molecule 1: Histone-arginine methyltransferase CARM1

Chain A:  93%



- Molecule 1: Histone-arginine methyltransferase CARM1

Chain B:  91% 5%



- Molecule 1: Histone-arginine methyltransferase CARM1

Chain C:  92%




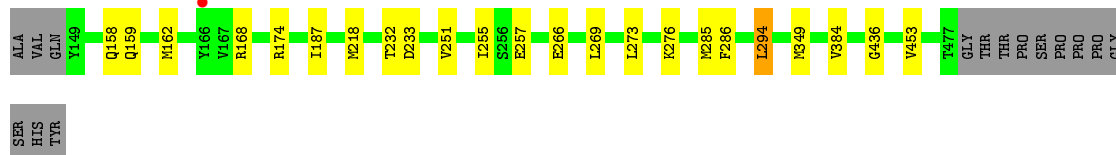
- Molecule 1: Histone-arginine methyltransferase CARM1

Chain D:  92%

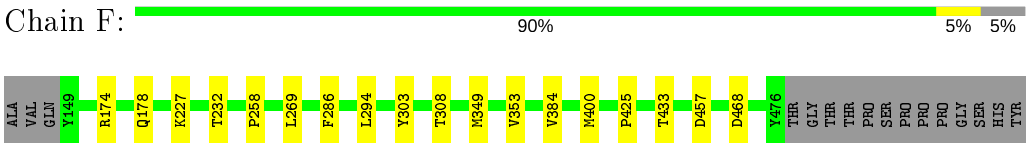


- Molecule 1: Histone-arginine methyltransferase CARM1

Chain E:  89% 6%



● Molecule 1: Histone-arginine methyltransferase CARM1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.60 Å 155.64 Å 95.34 Å 90.00° 101.04° 90.00°	Depositor
Resolution (Å)	50.01 – 2.00 49.64 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.01-2.00) 96.1 (49.64-1.99)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 1.98 Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, $R_{free}$	0.187 , 0.236 0.194 , 0.241	Depositor DCC
$R_{free}$ test set	1412 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.6	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	0.95	EDS
Total number of atoms	16868	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: UNX, GOL, SO4, FTG

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	0.46	0/2736	0.63	0/3714
1	B	0.47	0/2737	0.66	0/3716
1	C	0.46	0/2712	0.64	0/3686
1	D	0.45	0/2706	0.62	0/3677
1	E	0.43	0/2670	0.61	0/3629
1	F	0.47	0/2685	0.65	0/3645
All	All	0.46	0/16246	0.64	0/22067

There are no bond length outliers.

There are no bond angle outliers.

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	2663	0	2566	8	0
1	B	2666	0	2566	13	0
1	C	2640	0	2541	8	0
1	D	2634	0	2532	10	0
1	E	2602	0	2496	15	0
1	F	2614	0	2529	9	0
2	A	44	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	0	0	0
2	C	39	0	0	1	0
2	D	44	0	0	0	0
2	E	38	0	0	1	0
2	F	44	0	0	0	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
3	F	5	0	0	0	0
4	A	12	0	16	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
6	A	151	0	0	3	0
6	B	167	0	0	1	0
6	C	120	0	0	1	0
6	D	111	0	0	1	0
6	E	104	0	0	1	0
6	F	113	0	0	1	0
All	All	16868	0	15246	63	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 (63) 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:349[A]:MET:HE3	1:B:384:VAL:HG22	1.61	0.82
1:B:349[A]:MET:CE	1:B:384:VAL:HG22	2.12	0.78
1:A:349[A]:MET:CE	1:A:384:VAL:HG22	2.17	0.73
1:E:349[MET:HE3	1:E:384:VAL:HG22	1.72	0.70
1:A:349[A]:MET:HE3	1:A:384:VAL:HG22	1.73	0.69
1:F:349[A]:MET:CE	1:F:384:VAL:HG22	2.21	0.69
1:E:349:MET:CE	1:E:384:VAL:HG22	2.25	0.66
1:D:349[A]:MET:CE	1:D:384:VAL:HG22	2.26	0.65
1:E:349:MET:HE1	1:E:384:VAL:HA	1.78	0.64
1:B:178:GLN:OE1	1:B:400:MET:SD	2.55	0.63
1:E:159:GLN:HG3	1:E:218:MET:SD	2.43	0.59
1:D:349[A]:MET:HE3	1:D:384:VAL:HG22	1.85	0.58
1:B:349[A]:MET:HE1	1:B:384:VAL:HA	1.86	0.57
1:C:178:GLN:OE1	1:C:400:MET:SD	2.64	0.55
1:D:264:PHE:CE2	1:D:292[A]:VAL:HG21	2.43	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349[A]:MET:HE3	1:F:384:VAL:HG22	1.90	0.54
1:C:159:GLN:HG3	1:C:218:MET:SD	2.48	0.53
1:A:276:LYS:HD3	1:A:285:MET:SD	2.48	0.53
1:B:227:LYS:HG2	1:B:232:THR:HG21	1.90	0.52
1:E:276:LYS:HD3	1:E:285:MET:SD	2.50	0.52
1:F:227:LYS:HA	1:F:232:THR:HG23	1.91	0.51
1:E:158:GLN:HG3	1:E:162:MET:HE2	1.92	0.51
1:B:168[B]:ARG:NE	1:B:257:GLU:OE2	2.36	0.50
1:E:168[B]:ARG:NE	1:E:257:GLU:OE2	2.34	0.50
1:D:187:ILE:HG22	1:D:251:VAL:HG12	1.94	0.49
1:D:433:THR:HG23	6:D:2118:HOH:O	2.11	0.49
1:F:178:GLN:OE1	1:F:400:MET:SD	2.71	0.49
1:A:174[B]:ARG:HD2	6:A:601:HOH:O	2.13	0.47
1:A:294:LEU:HA	1:A:388:ALA:O	2.15	0.47
1:C:266:GLU:OE2	2:C:501:FTG:N	2.48	0.47
1:B:227:LYS:HG2	1:B:232:THR:CG2	2.44	0.47
1:A:174[B]:ARG:NH2	6:A:601:HOH:O	2.22	0.46
1:B:332:ASP:O	1:B:336:ARG:HG3	2.15	0.46
1:F:174:ARG:NH1	6:F:607:HOH:O	2.47	0.46
1:D:292[B]:VAL:CG2	1:D:355:TYR:HB3	2.46	0.46
1:B:258:PRO:HB2	1:B:269:LEU:HD23	1.99	0.45
1:C:276:LYS:HD3	1:C:285:MET:SD	2.56	0.45
1:C:349[A]:MET:SD	1:C:384:VAL:HG22	2.57	0.45
1:B:294:LEU:N	1:B:294:LEU:HD23	2.32	0.45
1:A:294:LEU:HD23	1:A:294:LEU:N	2.33	0.44
1:C:249:GLU:HG3	6:C:641:HOH:O	2.17	0.44
1:E:269:LEU:O	1:E:273:LEU:HG	2.18	0.44
1:D:349[A]:MET:HE1	1:D:384:VAL:HA	2.00	0.44
1:E:255:ILE:HG22	1:E:286:PHE:HB2	2.00	0.43
1:E:187:ILE:HG22	1:E:251:VAL:HG12	2.01	0.43
1:E:294:LEU:HD23	1:E:294:LEU:N	2.34	0.43
1:D:168[A]:ARG:C	1:D:168[A]:ARG:HD2	2.39	0.43
1:E:233:ASP:N	1:E:233:ASP:OD1	2.51	0.43
1:C:294:LEU:HA	1:C:388:ALA:O	2.19	0.42
1:F:258:PRO:HB2	1:F:269:LEU:HD23	2.01	0.42
1:E:436:GLY:HA3	1:E:453:VAL:O	2.20	0.42
1:E:174:ARG:HG3	6:E:2179:HOH:O	2.19	0.41
1:B:198:LEU:HD12	6:B:2102:HOH:O	2.20	0.41
1:C:265:ASN:O	1:C:266:GLU:HB2	2.20	0.41
1:B:433[A]:THR:OG1	1:B:457:ASP:HB2	2.20	0.41
1:D:241:LYS:O	1:D:245:VAL:HG13	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:705:HOH:O	1:F:178:GLN:HG2	2.20	0.41
1:F:433:THR:OG1	1:F:457:ASP:HB2	2.20	0.41
1:B:294:LEU:HA	1:B:388:ALA:O	2.21	0.41
1:E:266:GLU:OE2	2:E:2000:FTG:N	2.53	0.41
1:D:263:LEU:HD23	1:D:292[A]:VAL:HG22	2.03	0.40
1:A:187:ILE:HG22	1:A:251:VAL:HG12	2.02	0.40
1:F:303:TYR:CZ	1:F:425:PRO:HD3	2.57	0.40

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	334/344 (97%)	326 (98%)	8 (2%)	0	100	100
1	B	336/344 (98%)	327 (97%)	9 (3%)	0	100	100
1	C	333/344 (97%)	322 (97%)	11 (3%)	0	100	100
1	D	332/344 (96%)	322 (97%)	10 (3%)	0	100	100
1	E	329/344 (96%)	317 (96%)	12 (4%)	0	100	100
1	F	328/344 (95%)	319 (97%)	9 (3%)	0	100	100
All	All	1992/2064 (96%)	1933 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	283/298 (95%)	282 (100%)	1 (0%)	91	93
1	B	278/298 (93%)	276 (99%)	2 (1%)	84	88
1	C	279/298 (94%)	277 (99%)	2 (1%)	84	88
1	D	276/298 (93%)	274 (99%)	2 (1%)	84	88
1	E	272/298 (91%)	270 (99%)	2 (1%)	84	88
1	F	275/298 (92%)	270 (98%)	5 (2%)	59	63
All	All	1663/1788 (93%)	1649 (99%)	14 (1%)	78	86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	294	LEU
1	B	286	PHE
1	B	294	LEU
1	C	294	LEU
1	C	447	SER
1	D	262	MET
1	D	294	LEU
1	E	232	THR
1	E	294	LEU
1	F	286	PHE
1	F	294	LEU
1	F	308	THR
1	F	353	VAL
1	F	468	ASP

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	319	HIS
1	B	380	HIS
1	C	158	GLN
1	C	180	HIS
1	D	159	GLN
1	E	159	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 3 are unknown - leaving 11 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	FTG	C	501	-	39,42,48	0.55	0	41,57,66	0.81	3 (7%)
4	GOL	A	504	-	5,5,5	0.32	0	5,5,5	0.34	0
2	FTG	B	2000	-	45,48,48	0.52	0	50,66,66	0.86	3 (6%)
3	SO4	A	502	-	4,4,4	0.38	0	6,6,6	0.19	0
4	GOL	A	503	-	5,5,5	0.24	0	5,5,5	0.36	0
3	SO4	C	502	-	4,4,4	0.40	0	6,6,6	0.20	0
2	FTG	F	501	-	45,48,48	0.58	0	50,66,66	0.77	3 (6%)
3	SO4	F	502	-	4,4,4	0.34	0	6,6,6	0.07	0
2	FTG	A	501	-	45,48,48	0.45	0	50,66,66	0.79	2 (4%)
2	FTG	E	2000	-	38,41,48	0.52	0	40,56,66	0.79	2 (5%)
2	FTG	D	2000	-	45,48,48	0.44	0	50,66,66	0.83	3 (6%)

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	FTG	C	501	-	-	1/24/44/45	0/4/4/5
4	GOL	A	504	-	-	2/4/4/4	-
2	FTG	B	2000	-	-	1/25/45/45	0/5/5/5
4	GOL	A	503	-	-	2/4/4/4	-
2	FTG	F	501	-	-	3/25/45/45	0/5/5/5
2	FTG	A	501	-	-	1/25/45/45	0/5/5/5
2	FTG	E	2000	-	-	0/23/43/45	0/4/4/5
2	FTG	D	2000	-	-	2/25/45/45	0/5/5/5

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FTG	C6-C7-N1	3.03	118.12	110.17
2	B	2000	FTG	C6-C7-N1	2.83	117.58	110.17
2	B	2000	FTG	C6-C7-C8	-2.57	105.30	110.85
2	B	2000	FTG	C30-C29-N6	2.56	124.24	120.35
2	D	2000	FTG	C6-C7-C8	-2.53	105.37	110.85
2	C	501	FTG	C6-C7-N1	2.37	116.39	110.17
2	C	501	FTG	C6-C7-C8	-2.36	105.75	110.85
2	A	501	FTG	C30-C29-N6	2.35	123.92	120.35
2	D	2000	FTG	C6-C7-N1	2.32	116.25	110.17
2	E	2000	FTG	C6-C7-N1	2.25	116.07	110.17
2	E	2000	FTG	C30-C29-N6	2.20	123.70	120.35
2	D	2000	FTG	C30-C29-N6	2.18	123.66	120.35
2	F	501	FTG	C30-C29-N6	2.11	123.55	120.35
2	C	501	FTG	C30-C29-N6	2.07	123.50	120.35
2	F	501	FTG	C8-C7-N1	2.05	117.30	109.40
2	F	501	FTG	C6-C7-C8	-2.04	106.44	110.85

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	GOL	O1-C1-C2-C3
2	D	2000	FTG	C11-C10-C9-N
2	F	501	FTG	C11-C10-C9-N
4	A	503	GOL	O1-C1-C2-O2
2	F	501	FTG	C2-C3-C4-C5
4	A	504	GOL	O1-C1-C2-O2
2	F	501	FTG	C5-C6-C7-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	D	2000	FTG	C5-C6-C7-C8
2	B	2000	FTG	C11-C10-C9-N
2	C	501	FTG	C11-C10-C9-N
2	A	501	FTG	C11-C10-C9-N
4	A	503	GOL	O1-C1-C2-C3

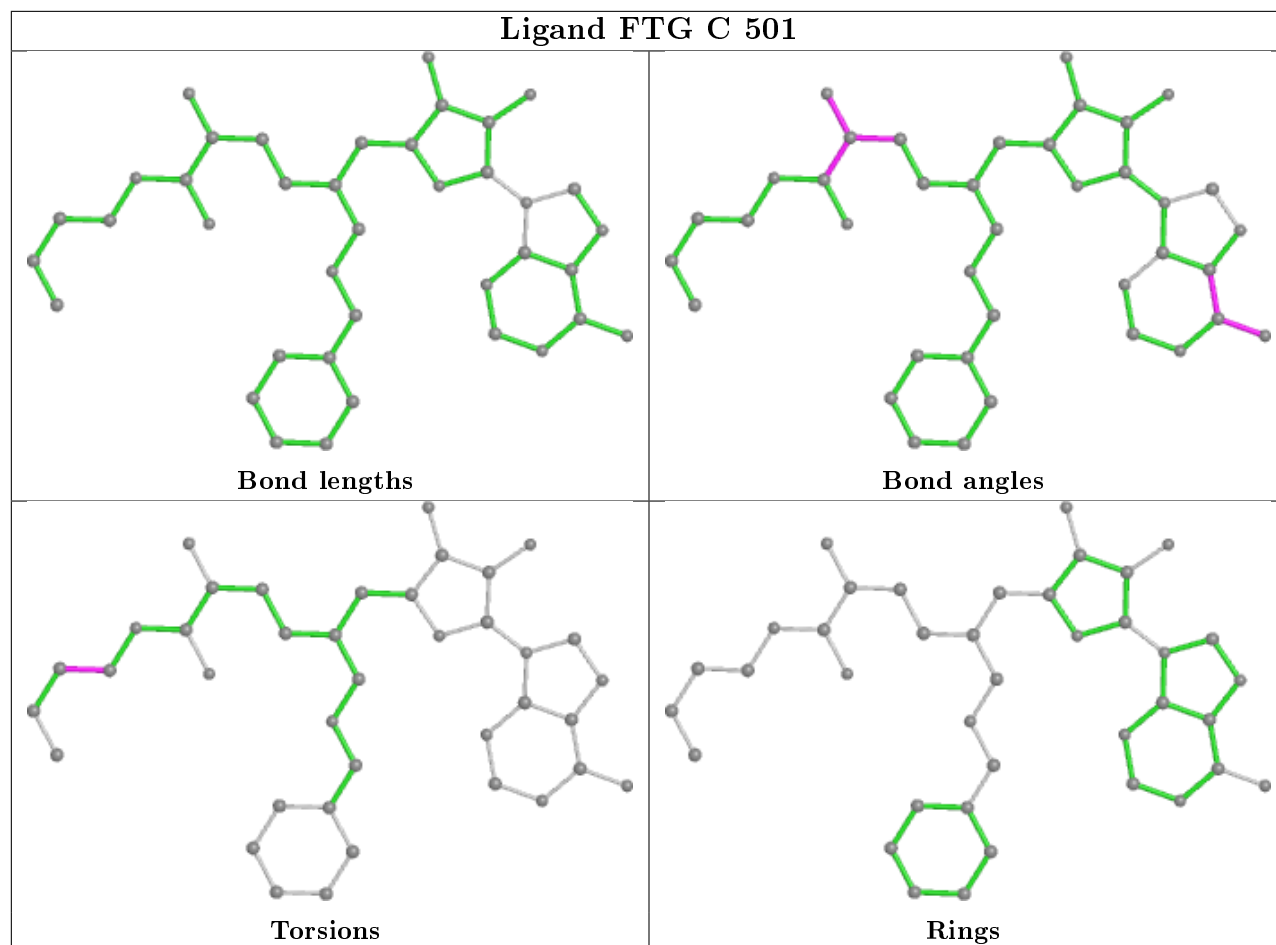
There are no ring outliers.

2 monomers are involved in 2 short contacts:

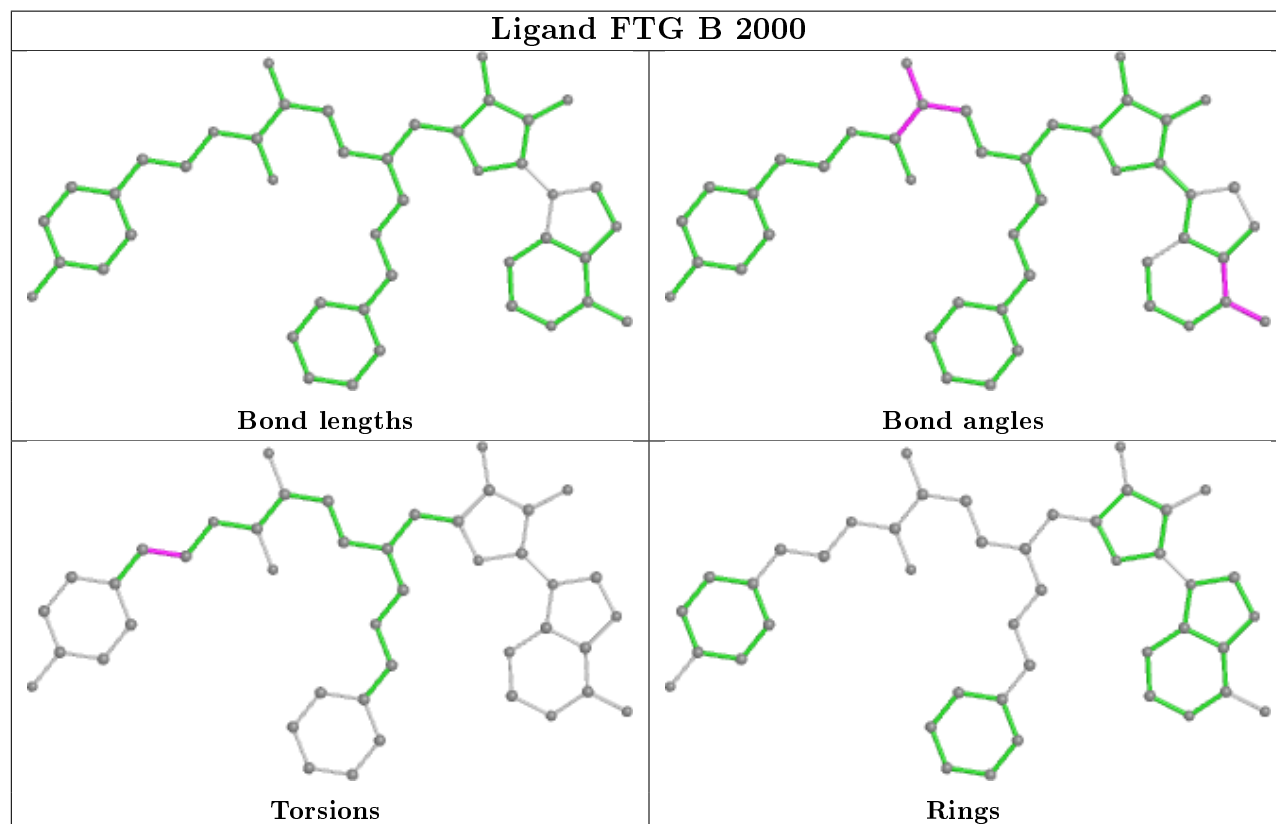
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	FTG	1	0
2	E	2000	FTG	1	0

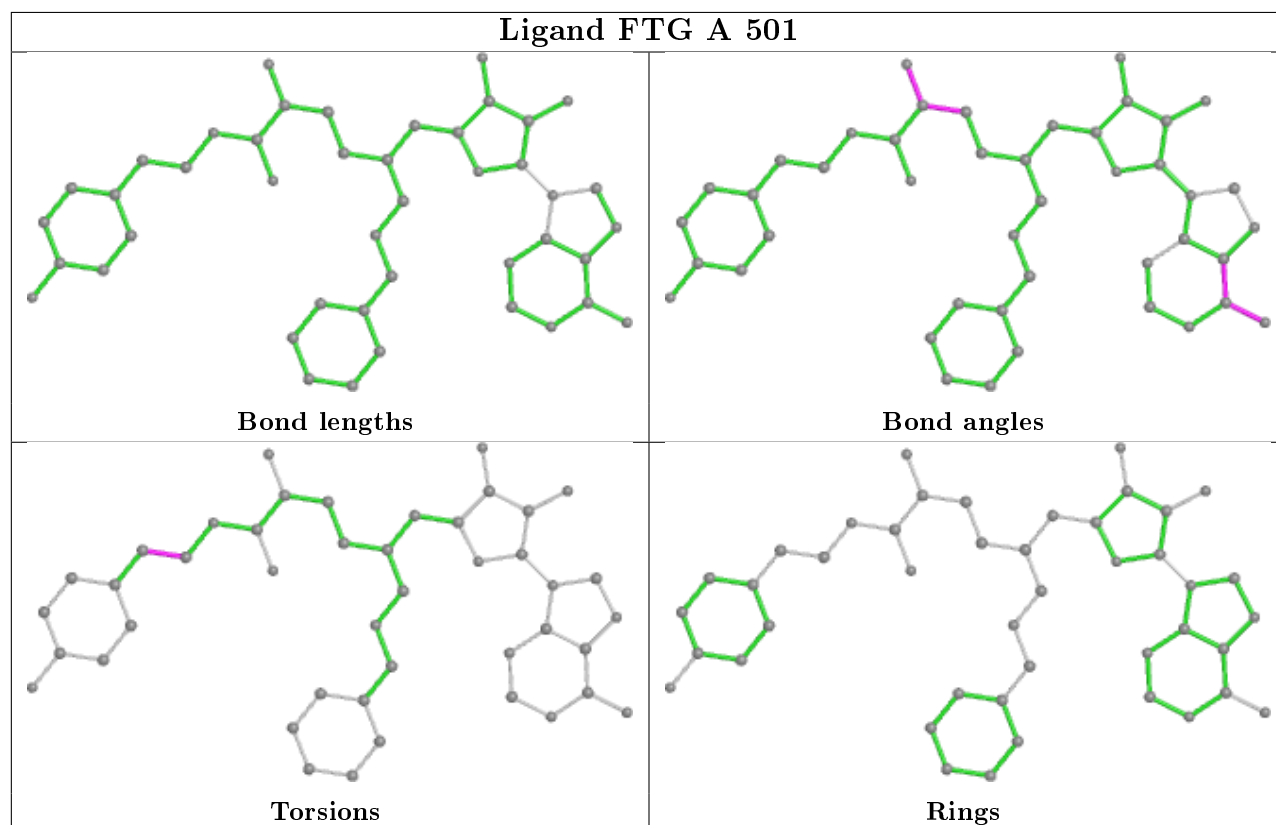
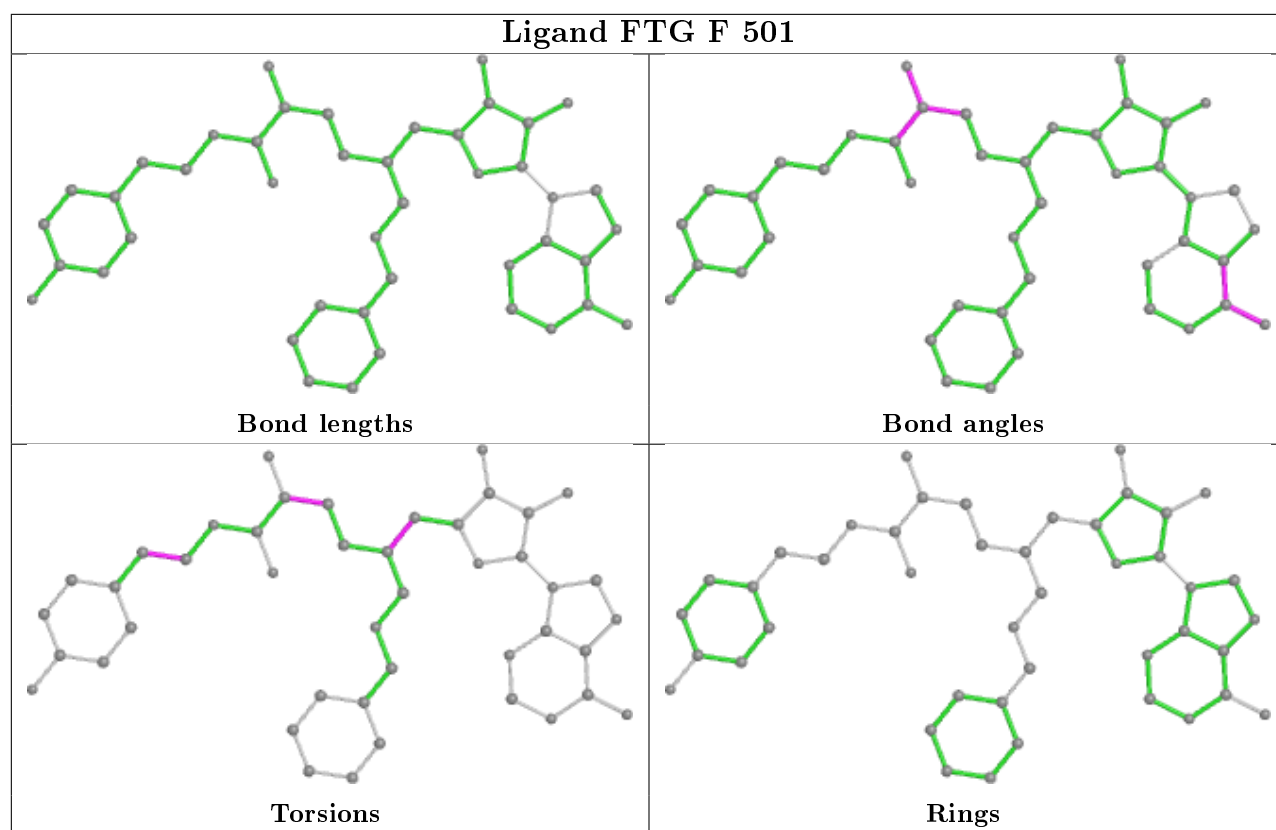
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

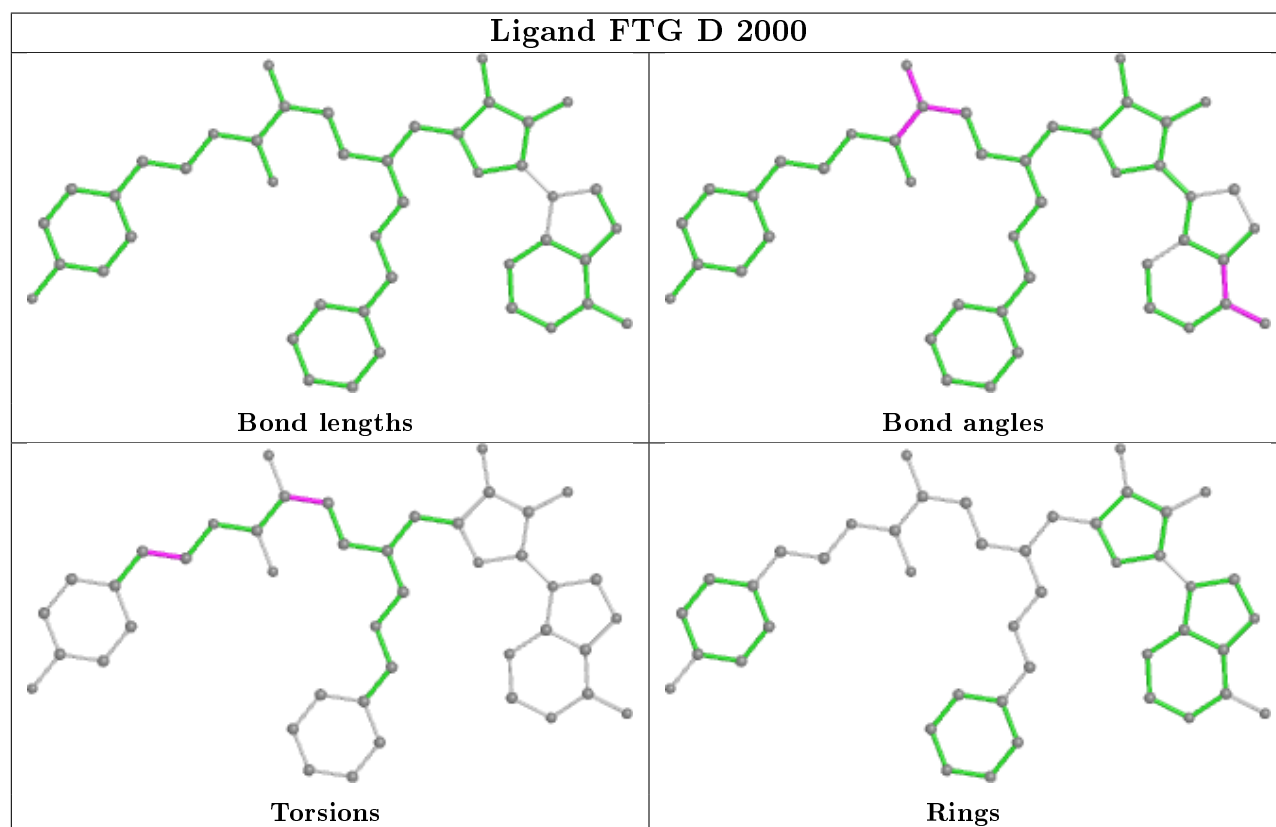
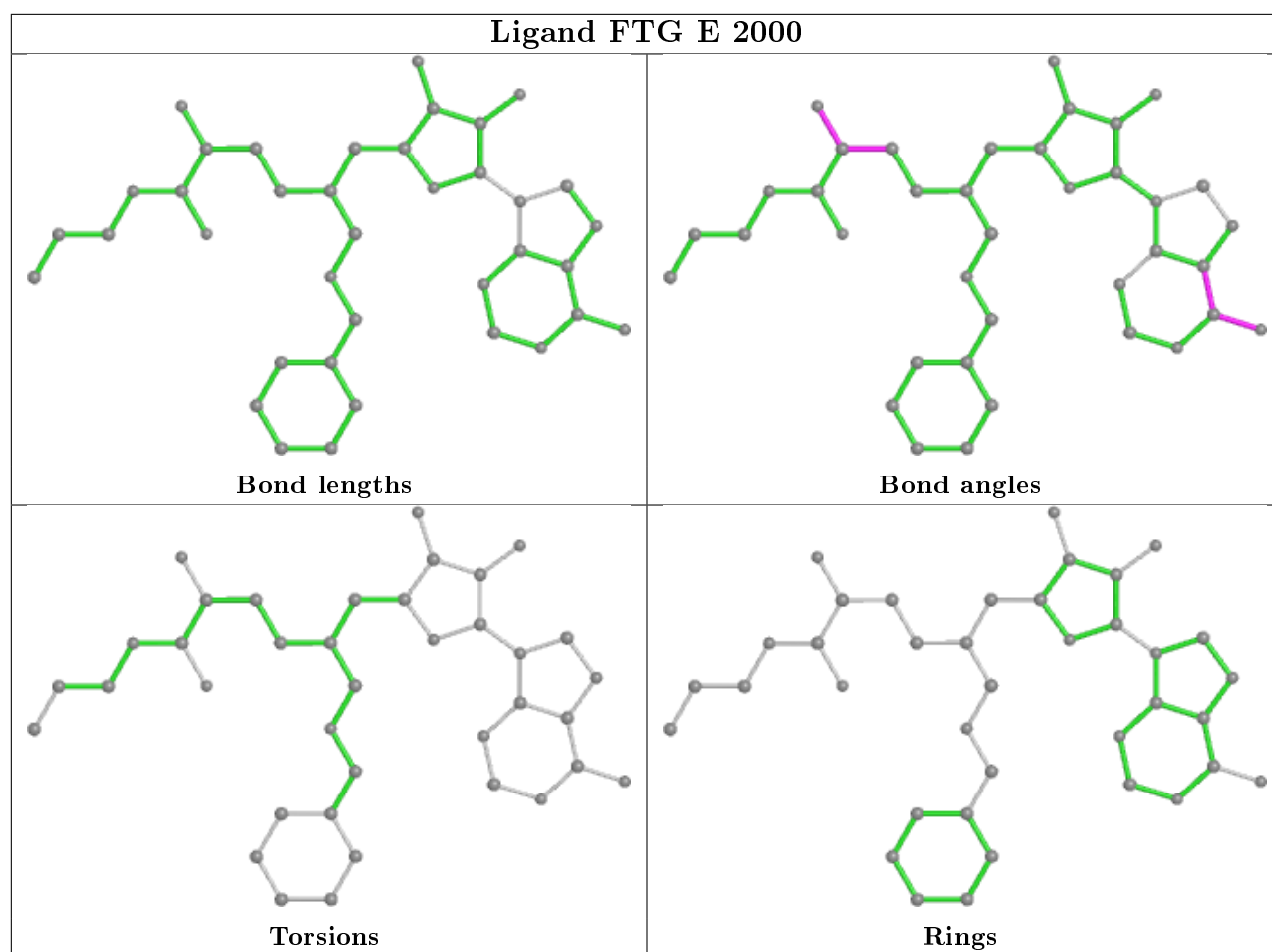
## Ligand FTG C 501



## Ligand FTG B 2000







## 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	330/344 (95%)	-0.52	1 (0%) 94 93	18, 26, 37, 71	0
1	B	330/344 (95%)	-0.59	0 100 100	17, 25, 37, 61	0
1	C	330/344 (95%)	-0.52	0 100 100	20, 28, 45, 61	0
1	D	329/344 (95%)	-0.37	1 (0%) 94 93	20, 31, 50, 71	0
1	E	329/344 (95%)	-0.41	1 (0%) 94 93	19, 35, 51, 73	0
1	F	328/344 (95%)	-0.39	0 100 100	18, 30, 44, 54	0
All	All	1976/2064 (95%)	-0.46	3 (0%) 95 94	17, 29, 46, 73	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	TYR	3.7
1	D	149	TYR	2.3
1	E	166	TYR	2.2

### 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,

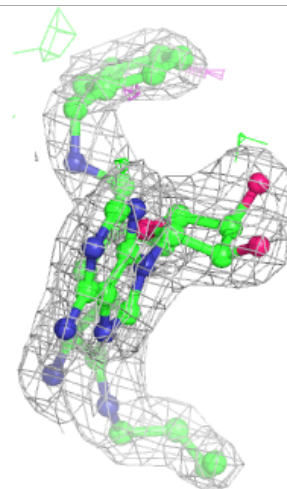
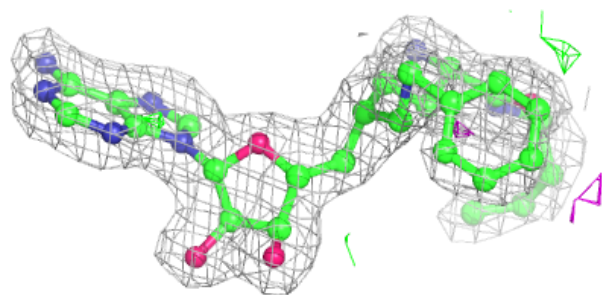
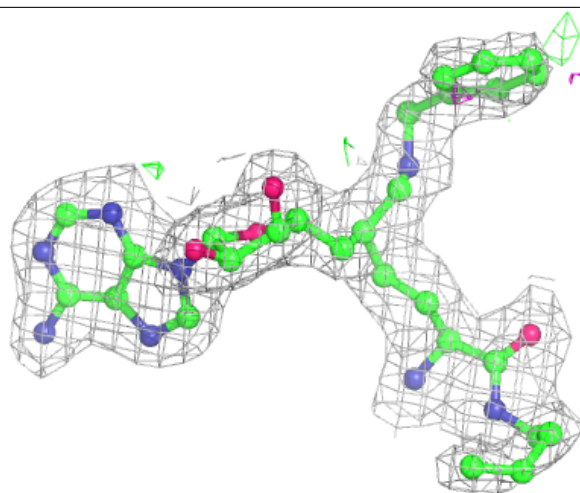
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	UNX	C	503	1/1	0.79	0.34	46,46,46,46	0
4	GOL	A	504	6/6	0.81	0.19	49,54,54,54	0
5	UNX	F	503	1/1	0.82	0.45	42,42,42,42	0
5	UNX	A	505	1/1	0.84	0.45	52,52,52,52	0
4	GOL	A	503	6/6	0.90	0.09	50,54,55,56	0
3	SO4	F	502	5/5	0.90	0.22	78,79,83,85	0
2	FTG	C	501	39/44	0.94	0.11	24,32,50,50	0
3	SO4	C	502	5/5	0.94	0.14	61,65,68,69	0
2	FTG	A	501	44/44	0.94	0.12	22,29,49,52	0
2	FTG	E	2000	38/44	0.94	0.12	31,35,62,64	0
2	FTG	B	2000	44/44	0.94	0.11	23,26,46,48	0
2	FTG	D	2000	44/44	0.94	0.12	21,30,49,53	0
3	SO4	A	502	5/5	0.95	0.16	65,66,68,73	0
2	FTG	F	501	44/44	0.95	0.13	21,31,49,53	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.

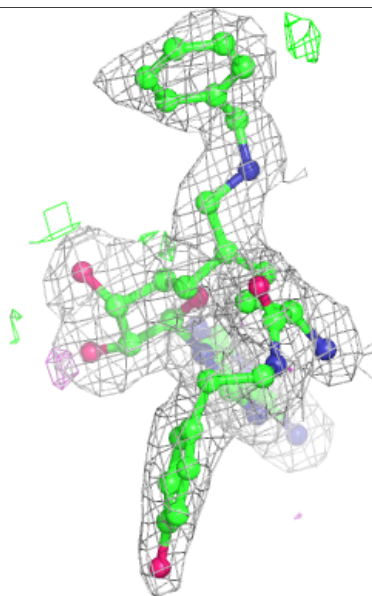
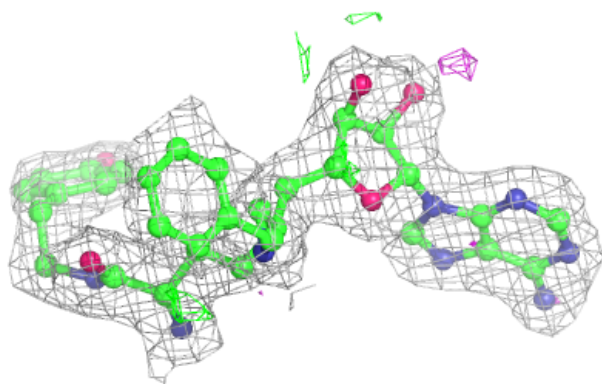
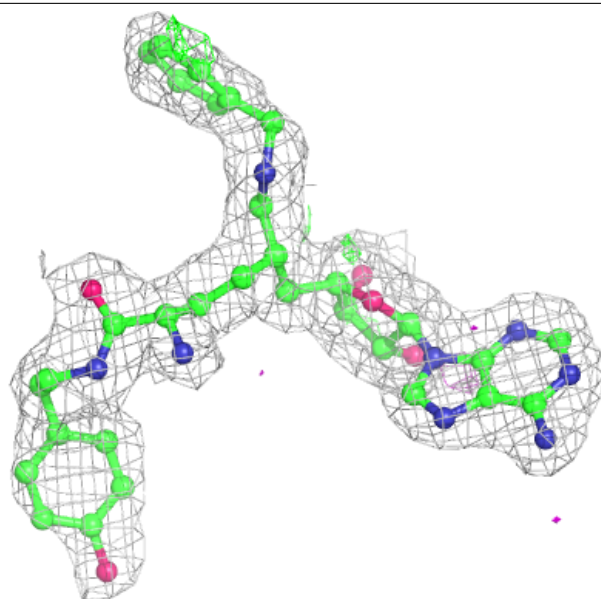
**Electron density around FTG C 501:**

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



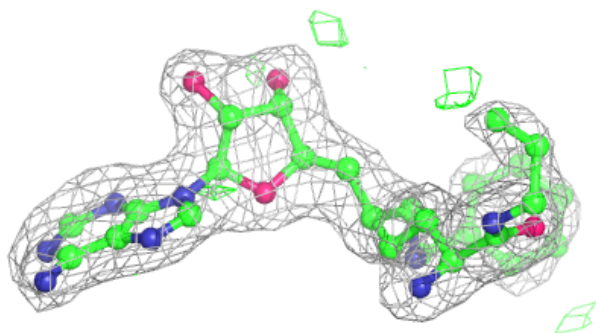
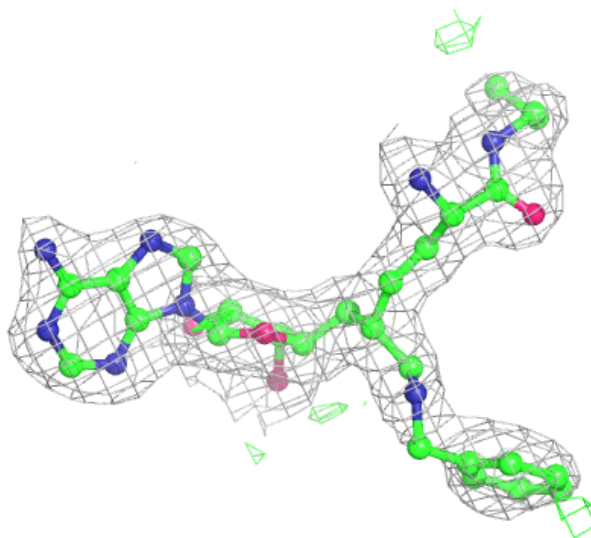
**Electron density around FTG A 501:**

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



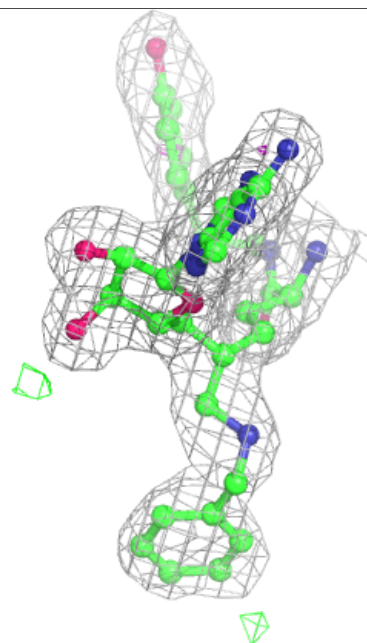
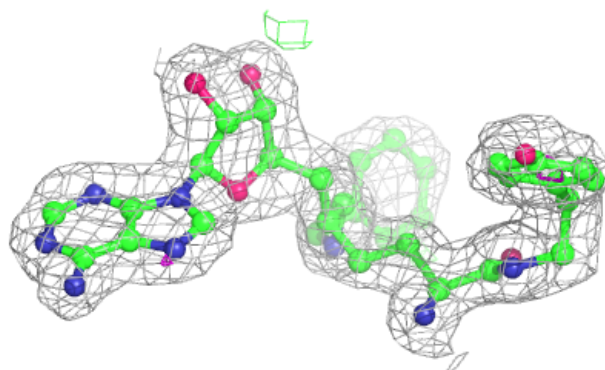
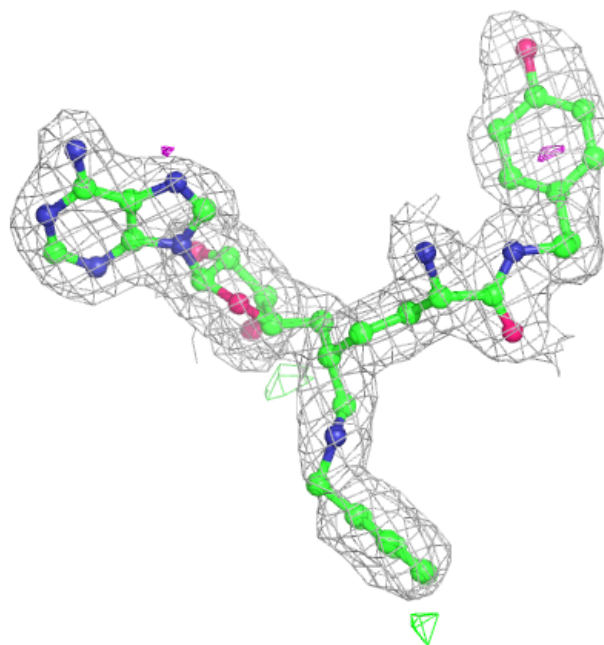
**Electron density around FTG E 2000:**

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



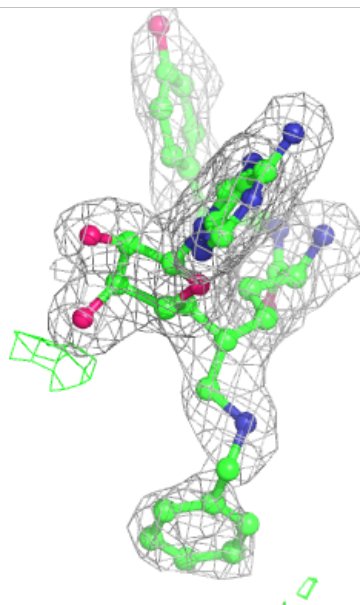
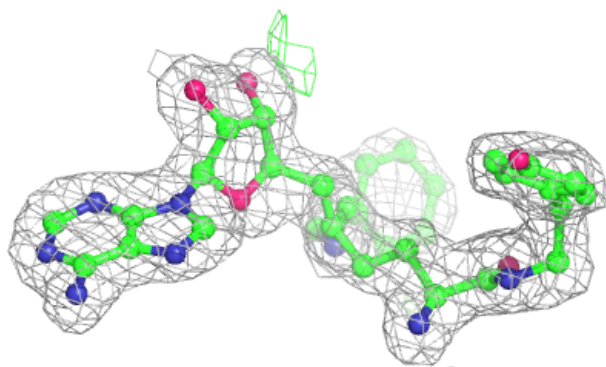
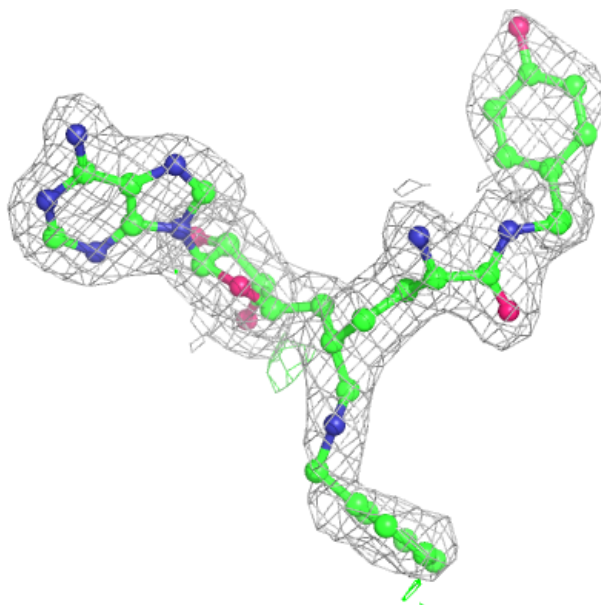
**Electron density around FTG B 2000:**

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



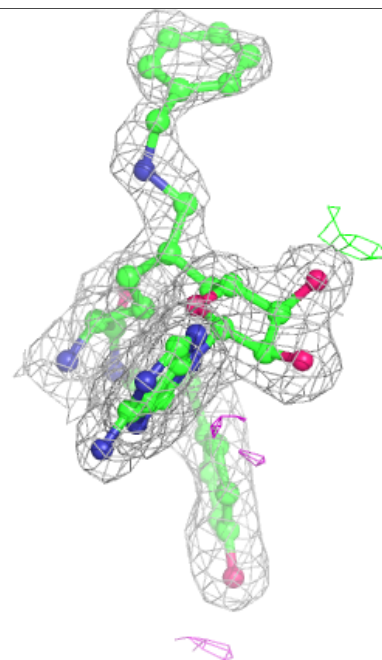
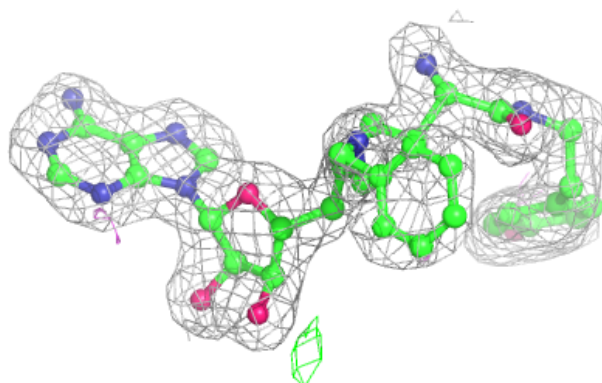
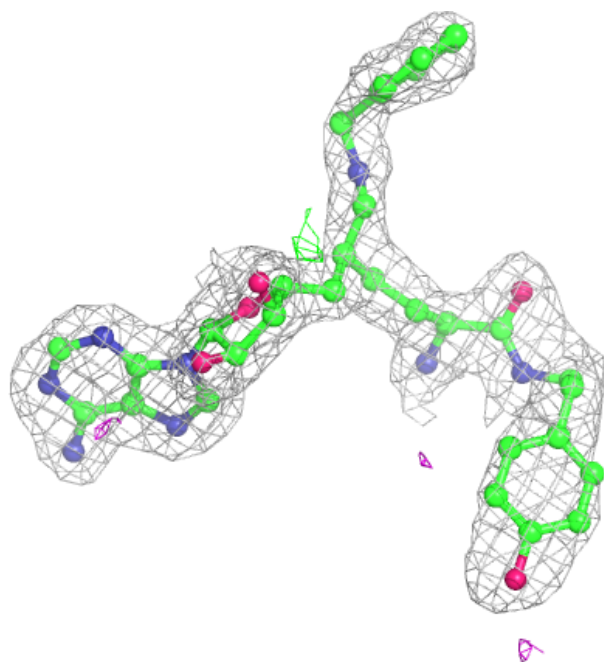
**Electron density around FTG D 2000:**

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



**Electron density around FTG F 501:**

$2mF_o - DF_c$  (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.