



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 06:43 PM UTC

PDB ID : 8FE2 / pdb\_00008fe2  
Title : Structure of J-PKAc chimera complexed with Aplithianine A  
Authors : Du, L.; Wilson, B.A.P.; Li, N.; Dalilian, M.; Wang, D.; Martinez Fiesco, J.A.;  
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Deposited on : 2022-12-05  
Resolution : 2.34 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

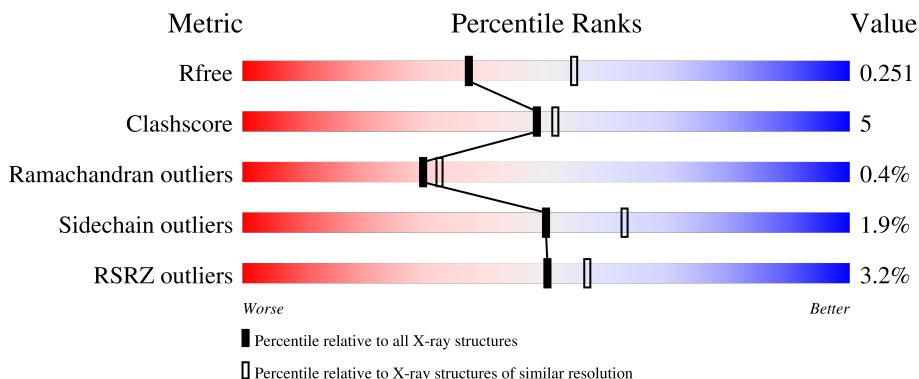
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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))
$R_{free}$	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 % 86% 13%
1	B	405	 5% 81% 17% ..
2	I	20	 10% 85% 10% 5%
2	J	20	 90% 5% 5%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7057 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.

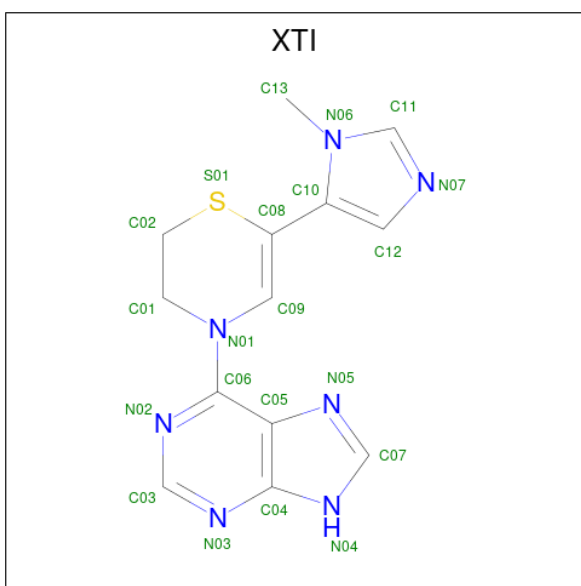
- Molecule 1 is a protein called DnaJ homolog subfamily B member 1, cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	403	Total	C	N	O	P	S	0	0	0
			3347	2154	568	614	3	8			
1	B	400	Total	C	N	O	P	S	0	0	0
			3323	2137	564	611	3	8			

- Molecule 2 is a protein called cAMP-dependent protein kinase inhibitor alpha.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
2	I	20	Total	C	N	O	0	0	0
			156	94	32	30			
2	J	19	Total	C	N	O	0	0	0
			148	90	31	27			

- Molecule 3 is 6-[(6M)-6-(1-methyl-1H-imidazol-5-yl)-2,3-dihydro-4H-1,4-thiazin-4-yl]-9H-purine (CCD ID: XTI) (formula: C<sub>13</sub>H<sub>13</sub>N<sub>7</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			21	13	7	1		
3	B	1	Total	C	N	S	0	0
			21	13	7	1		

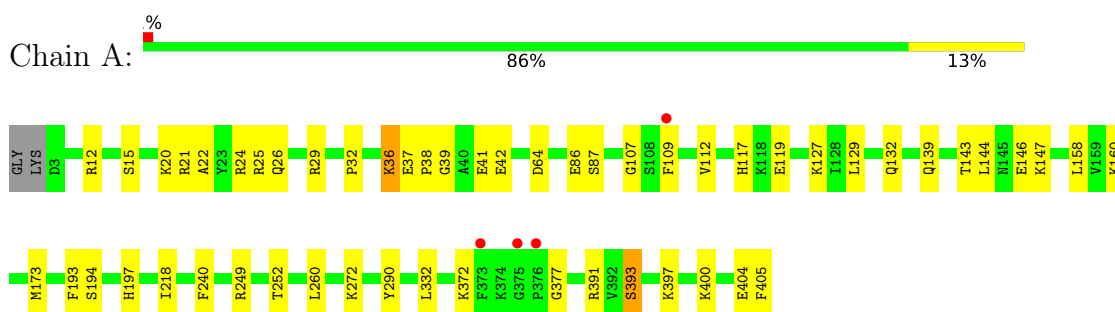
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	15	Total	O	0	0
			15	15		
4	J	2	Total	O	0	0
			2	2		

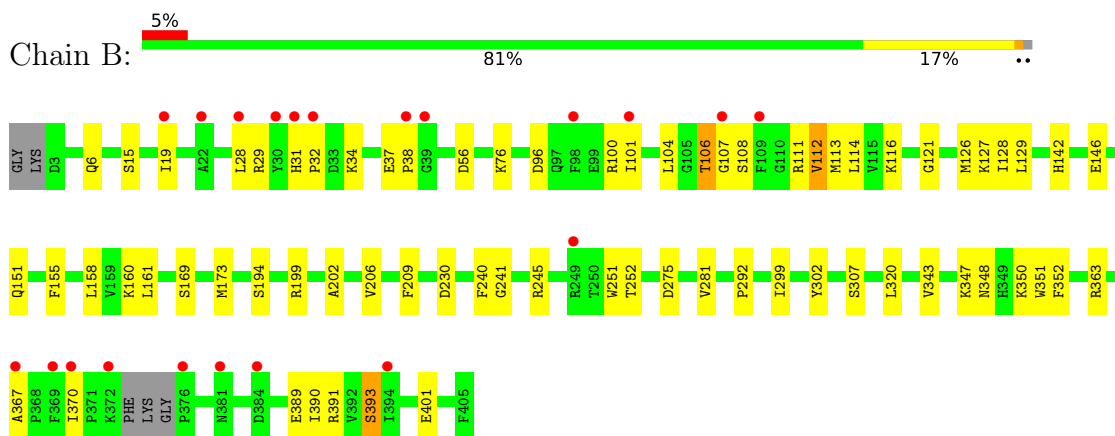
### 3 Residue-property plots [i](#)

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.

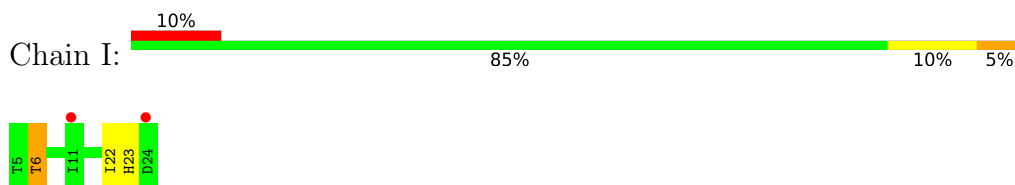
- Molecule 1: DnaJ homolog subfamily B member 1, cAMP-dependent protein kinase catalytic subunit alpha



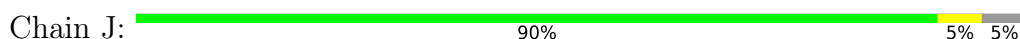
- Molecule 1: DnaJ homolog subfamily B member 1, cAMP-dependent protein kinase catalytic subunit alpha



- Molecule 2: cAMP-dependent protein kinase inhibitor alpha



- Molecule 2: cAMP-dependent protein kinase inhibitor alpha





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.63Å 171.78Å 61.48Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	43.62 – 2.34 43.62 – 2.34	Depositor EDS
% Data completeness (in resolution range)	96.8 (43.62-2.34) 93.4 (43.62-2.34)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.196 , 0.251 0.196 , 0.251	Depositor DCC
$R_{free}$ test set	1972 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtrriage
Anisotropy	0.259	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.066 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: XTI, SEP, TPO

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	0.37	0/3398	0.52	0/4571
1	B	0.34	0/3372	0.52	0/4535
2	I	0.32	0/158	0.59	0/212
2	J	0.36	0/150	0.52	0/201
All	All	0.35	0/7078	0.52	0/9519

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	3347	0	3301	37	0
1	B	3323	0	3276	42	0
2	I	156	0	146	2	0
2	J	148	0	142	1	0
3	A	21	0	0	2	0
3	B	21	0	0	1	0
4	A	24	0	0	0	0
4	B	15	0	0	1	0
4	J	2	0	0	0	0
All	All	7057	0	6865	76	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 5.

All (76) 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:155:PHE:H	1:B:160:LYS:HZ1	1.21	0.86
1:A:132:GLN:NE2	1:A:397:LYS:HD2	2.03	0.73
1:B:116:LYS:HE3	1:B:121:GLY:HA2	1.71	0.71
1:B:343:VAL:HG22	1:B:347:LYS:HD2	1.73	0.70
1:B:6:GLN:OE1	1:B:348:ASN:ND2	2.25	0.69
1:A:218:ILE:HG12	1:A:272:LYS:HG3	1.75	0.68
1:B:158:LEU:HD22	1:B:240:PHE:HZ	1.61	0.65
1:B:104:LEU:HD21	1:B:114:LEU:HB2	1.78	0.65
1:B:350:LYS:H	1:B:350:LYS:HE2	1.62	0.65
1:A:158:LEU:HD22	1:A:240:PHE:HZ	1.64	0.63
1:A:400:LYS:HE2	1:B:251:TRP:CG	2.35	0.62
1:A:117:HIS:CE1	1:A:119:GLU:HB2	2.39	0.57
1:A:147:LYS:HA	1:A:173:MET:HE3	1.86	0.56
1:A:160:LYS:HA	1:A:160:LYS:HE3	1.88	0.56
1:B:127:LYS:HD3	1:B:173:MET:HE3	1.88	0.55
1:B:202:ALA:O	1:B:206:VAL:HG23	2.06	0.55
1:A:112:VAL:HG21	3:A:501:XTI:C10	2.37	0.54
1:B:76:LYS:NZ	4:B:602:HOH:O	2.39	0.54
1:B:155:PHE:H	1:B:160:LYS:NZ	2.01	0.54
1:B:230:ASP:OD2	1:B:363:ARG:NH2	2.35	0.54
1:B:350:LYS:H	1:B:350:LYS:CE	2.20	0.53
1:B:391:ARG:NH2	1:B:393:SEP:O2P	2.31	0.53
1:A:20:LYS:O	1:A:24:ARG:HG3	2.10	0.52
1:A:41:GLU:HG2	1:A:42:GLU:OE1	2.10	0.51
1:B:112:VAL:HG11	3:B:501:XTI:C08	2.41	0.51
1:A:139:GLN:O	1:A:143:THR:HG23	2.11	0.51
1:B:100:ARG:HG3	1:B:100:ARG:HH11	1.76	0.50
1:A:391:ARG:HH21	1:A:393:SEP:P	2.35	0.50
1:B:15:SER:O	1:B:19:ILE:HG13	2.13	0.49
1:A:193:PHE:HB3	1:A:197:HIS:HB3	1.95	0.48
1:A:332:LEU:HD23	1:A:332:LEU:HA	1.55	0.48
1:B:146:GLU:HG3	1:B:240:PHE:HB2	1.96	0.48
1:B:37:GLU:HG3	1:B:38:PRO:HD2	1.96	0.47
1:A:36:LYS:HE2	1:A:36:LYS:HA	1.97	0.47
1:B:367:ALA:HB3	1:B:370:ILE:CD1	2.45	0.47
1:A:39:GLY:HA2	1:A:42:GLU:CD	2.40	0.46
1:B:401:GLU:OE1	1:B:401:GLU:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HD22	1:A:404:GLU:HG2	1.98	0.46
1:B:128:ILE:C	1:B:129:LEU:HD23	2.41	0.45
1:B:389:GLU:CD	1:B:390:ILE:H	2.24	0.45
1:A:109:PHE:CD1	1:A:109:PHE:N	2.83	0.45
1:A:32:PRO:HB3	1:A:36:LYS:NZ	2.31	0.45
1:B:100:ARG:HG3	1:B:100:ARG:NH1	2.32	0.45
1:B:151:GLN:HB3	1:B:161:LEU:HD23	1.98	0.45
1:B:28:LEU:HD12	1:B:29:ARG:N	2.32	0.45
1:A:12:ARG:HH22	1:A:64:ASP:HA	1.81	0.45
1:A:21:ARG:HG2	1:A:22:ALA:N	2.32	0.44
1:B:155:PHE:N	1:B:160:LYS:HZ1	2.03	0.44
1:A:39:GLY:O	1:A:42:GLU:HG2	2.17	0.44
1:A:107:GLY:HA3	1:A:109:PHE:CE1	2.53	0.44
1:A:117:HIS:HE1	1:A:119:GLU:HB2	1.80	0.44
1:B:209:PHE:CE2	1:B:275:ASP:HB3	2.52	0.44
1:A:391:ARG:NH2	1:A:393:SEP:O1P	2.51	0.44
1:A:290:TYR:CZ	2:I:6:THR:HB	2.52	0.44
1:A:26:GLN:OE1	1:A:29:ARG:NH1	2.51	0.44
1:B:111:ARG:HD3	1:B:113:MET:HE3	1.99	0.43
1:A:127:LYS:NZ	1:A:146:GLU:OE2	2.51	0.43
1:B:199:ARG:HG3	1:B:352:PHE:CE1	2.54	0.43
1:A:37:GLU:HB3	1:A:38:PRO:HD2	2.00	0.42
1:B:302:TYR:OH	2:J:22:ILE:HD13	2.19	0.42
1:B:126:MET:HG2	1:B:128:ILE:CD1	2.49	0.42
1:B:367:ALA:HB3	1:B:370:ILE:HD13	2.01	0.42
1:A:112:VAL:HG21	3:A:501:XTI:C08	2.49	0.42
1:B:31:HIS:CG	1:B:32:PRO:HD2	2.55	0.42
1:B:142:HIS:HB3	1:B:241:GLY:O	2.19	0.42
1:A:109:PHE:HB2	1:A:129:LEU:HD22	2.02	0.42
1:A:147:LYS:HG3	1:A:405:PHE:CE2	2.55	0.41
1:A:372:LYS:HD2	1:A:372:LYS:HA	1.70	0.41
1:A:86:GLU:OE2	1:B:245:ARG:NH2	2.44	0.41
1:B:281:VAL:HG13	1:B:292:PRO:HD2	2.02	0.41
1:A:400:LYS:HE2	1:B:251:TRP:CD2	2.55	0.41
1:B:106:THR:HG23	1:B:107:GLY:N	2.35	0.41
1:A:41:GLU:H	1:A:41:GLU:CD	2.28	0.41
1:B:56:ASP:C	1:B:56:ASP:OD1	2.64	0.41
1:B:320:LEU:HD13	1:B:351:TRP:CE2	2.56	0.41
1:A:260:LEU:HD11	2:I:22:ILE:HD11	2.02	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	398/405 (98%)	382 (96%)	15 (4%)	1 (0%)	36	41
1	B	393/405 (97%)	374 (95%)	17 (4%)	2 (0%)	24	26
2	I	18/20 (90%)	16 (89%)	2 (11%)	0	100	100
2	J	17/20 (85%)	17 (100%)	0	0	100	100
All	All	826/850 (97%)	789 (96%)	34 (4%)	3 (0%)	30	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	ILE
1	B	34	LYS
1	A	377	GLY

### 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	350/351 (100%)	345 (99%)	5 (1%)	59	71
1	B	348/351 (99%)	341 (98%)	7 (2%)	48	61
2	I	15/15 (100%)	13 (87%)	2 (13%)	4	3
2	J	14/15 (93%)	14 (100%)	0	100	100
All	All	727/732 (99%)	713 (98%)	14 (2%)	50	63

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

Mol	Chain	Res	Type
1	A	15	SER
1	A	25	ARG
1	A	36	LYS
1	A	87	SER
1	A	249	ARG
1	B	96	ASP
1	B	106	THR
1	B	108	SER
1	B	112	VAL
1	B	169	SER
1	B	299	ILE
1	B	307	SER
2	I	6	THR
2	I	23	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	139	GLN
1	A	232	GLN
1	A	381	ASN
1	B	94	HIS
1	B	154	ASN
1	B	329	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SEP	B	194	1	8,9,10	2.02	4 (50%)	7,12,14	2.59	1 (14%)
1	TPO	B	252	1	8,10,11	1.47	1 (12%)	10,14,16	1.80	2 (20%)
1	TPO	A	252	1	8,10,11	1.67	1 (12%)	10,14,16	1.61	2 (20%)
1	SEP	A	194	1	8,9,10	1.74	2 (25%)	7,12,14	1.27	1 (14%)
1	SEP	B	393	1	8,9,10	1.62	1 (12%)	7,12,14	1.41	1 (14%)
1	SEP	A	393	1	8,9,10	1.76	1 (12%)	7,12,14	1.51	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	B	194	1	-	3/6/8/10	-
1	TPO	B	252	1	-	1/9/11/13	-
1	TPO	A	252	1	-	1/9/11/13	-
1	SEP	A	194	1	-	1/6/8/10	-
1	SEP	B	393	1	-	3/6/8/10	-
1	SEP	A	393	1	-	5/6/8/10	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	SEP	P-O1P	3.97	1.62	1.50
1	A	393	SEP	P-O1P	3.88	1.62	1.50
1	A	194	SEP	P-O1P	3.79	1.62	1.50
1	B	393	SEP	P-O1P	3.59	1.61	1.50
1	A	252	TPO	P-O1P	3.36	1.60	1.50
1	B	252	TPO	P-O1P	3.20	1.60	1.50
1	B	194	SEP	P-O2P	2.42	1.63	1.54
1	B	194	SEP	P-O3P	2.15	1.62	1.54
1	B	194	SEP	P-OG	2.10	1.67	1.60
1	A	194	SEP	P-O3P	2.03	1.62	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	SEP	OG-CB-CA	5.93	113.91	108.14
1	B	252	TPO	P-OG1-CB	-4.13	112.12	123.33
1	A	252	TPO	P-OG1-CB	-3.94	112.61	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	SEP	OG-CB-CA	3.28	111.34	108.14
1	B	393	SEP	OG-CB-CA	2.91	110.97	108.14
1	B	252	TPO	CG2-CB-CA	-2.88	107.65	113.26
1	A	194	SEP	OG-CB-CA	2.64	110.71	108.14
1	A	252	TPO	CG2-CB-CA	-2.23	108.91	113.26

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	252	TPO	O-C-CA-CB
1	A	393	SEP	CB-OG-P-O2P
1	A	393	SEP	CB-OG-P-O3P
1	B	194	SEP	CB-OG-P-O1P
1	B	194	SEP	CB-OG-P-O2P
1	B	194	SEP	CB-OG-P-O3P
1	B	393	SEP	N-CA-CB-OG
1	A	393	SEP	CB-OG-P-O1P
1	B	393	SEP	CB-OG-P-O3P
1	A	393	SEP	CA-CB-OG-P
1	B	393	SEP	CA-CB-OG-P
1	A	194	SEP	N-CA-CB-OG
1	A	393	SEP	N-CA-CB-OG
1	B	252	TPO	CB-OG1-P-O3P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	393	SEP	1	0
1	A	393	SEP	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	XTI	B	501	-	23,24,24	3.08	11 (47%)	23,34,34	3.65	10 (43%)
3	XTI	A	501	-	23,24,24	2.96	12 (52%)	23,34,34	3.84	12 (52%)

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	XTI	B	501	-	-	0/3/18/18	0/4/4/4
3	XTI	A	501	-	-	0/3/18/18	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	XTI	C05-N05	8.05	1.53	1.39
3	B	501	XTI	C05-N05	7.64	1.53	1.39
3	A	501	XTI	C04-N04	-5.42	1.28	1.36
3	B	501	XTI	C10-C08	5.23	1.54	1.45
3	B	501	XTI	C04-N04	-5.04	1.29	1.36
3	A	501	XTI	C10-C08	4.62	1.53	1.45
3	B	501	XTI	C09-C08	4.56	1.43	1.35
3	A	501	XTI	C09-C08	3.86	1.42	1.35
3	B	501	XTI	C05-C04	3.67	1.45	1.39
3	B	501	XTI	C09-N01	3.52	1.39	1.34
3	B	501	XTI	C07-N04	-3.42	1.27	1.35
3	A	501	XTI	C07-N04	-3.40	1.27	1.35
3	A	501	XTI	C09-N01	3.19	1.38	1.34
3	A	501	XTI	C05-C04	3.14	1.44	1.39
3	B	501	XTI	C06-N01	2.91	1.45	1.39
3	B	501	XTI	C02-C01	2.85	1.60	1.51
3	A	501	XTI	C02-C01	2.82	1.60	1.51
3	A	501	XTI	C06-N01	2.35	1.44	1.39
3	B	501	XTI	C02-S01	2.28	1.88	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	XTI	C11-N06	2.23	1.41	1.35
3	A	501	XTI	C02-S01	2.20	1.88	1.80
3	A	501	XTI	C11-N06	2.08	1.41	1.35
3	A	501	XTI	C05-C06	-2.02	1.36	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	XTI	C04-N04-C07	13.38	118.90	106.43
3	B	501	XTI	C04-N04-C07	12.63	118.21	106.43
3	B	501	XTI	N06-C11-N07	-6.94	108.81	112.94
3	A	501	XTI	N06-C11-N07	-6.63	108.99	112.94
3	A	501	XTI	C12-C10-N06	4.58	107.32	105.25
3	B	501	XTI	C12-C10-N06	4.50	107.28	105.25
3	A	501	XTI	C06-C05-N05	4.08	139.94	133.43
3	B	501	XTI	C04-C05-N05	-3.84	105.34	110.67
3	A	501	XTI	C04-C05-N05	-3.70	105.54	110.67
3	B	501	XTI	C06-C05-N05	3.64	139.24	133.43
3	B	501	XTI	C03-N02-C06	3.06	119.31	111.83
3	A	501	XTI	C05-C06-N01	-2.96	120.13	123.80
3	A	501	XTI	C13-N06-C10	2.81	130.99	127.70
3	A	501	XTI	N04-C04-N03	2.69	131.04	126.69
3	A	501	XTI	C03-N02-C06	2.42	117.74	111.83
3	B	501	XTI	N04-C04-N03	2.32	130.45	126.69
3	B	501	XTI	C13-N06-C10	2.31	130.41	127.70
3	A	501	XTI	C13-N06-C11	-2.30	121.99	126.28
3	B	501	XTI	C12-N07-C11	2.28	108.23	105.24
3	B	501	XTI	C10-C12-N07	-2.15	108.66	110.92
3	A	501	XTI	N04-C07-N05	-2.04	110.77	113.87
3	A	501	XTI	C05-C04-N04	-2.02	102.98	105.67

There are no chirality outliers.

There are no torsion outliers.

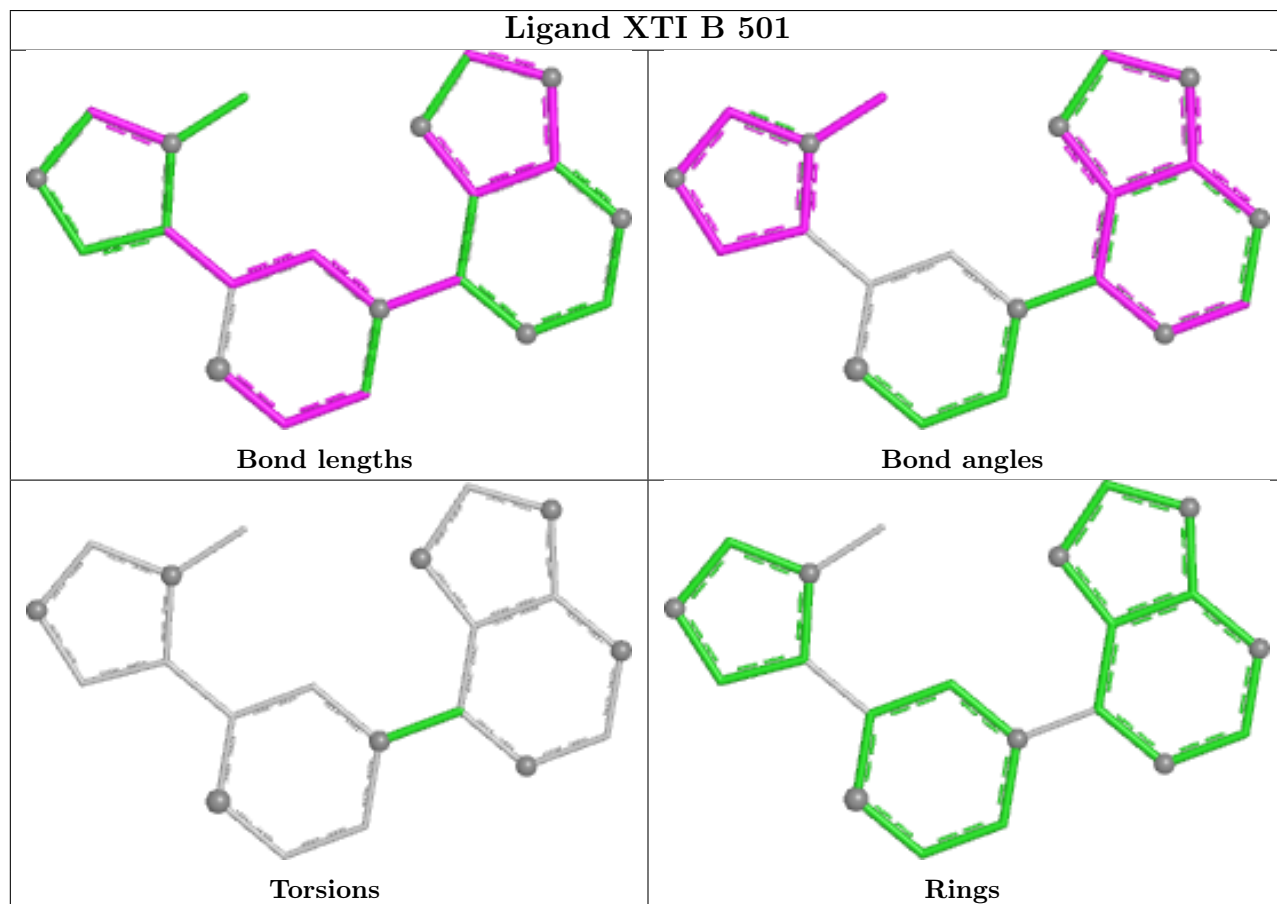
There are no ring outliers.

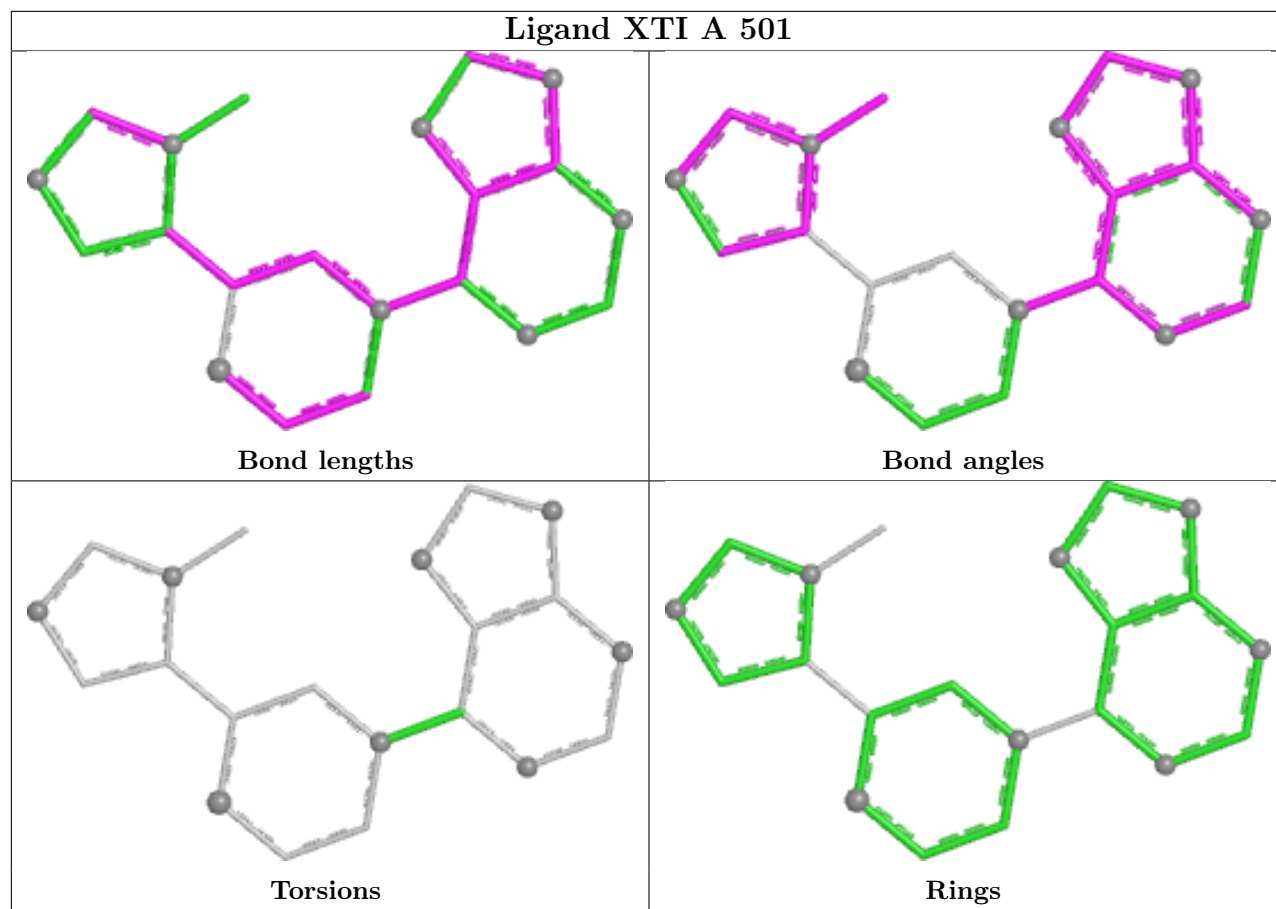
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	XTI	1	0
3	A	501	XTI	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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	400/405 (98%)	0.12	4 (1%) 79 82	34, 52, 80, 98	0
1	B	397/405 (98%)	0.47	21 (5%) 32 37	36, 58, 92, 109	0
2	I	20/20 (100%)	0.81	2 (10%) 12 15	48, 63, 79, 79	0
2	J	19/20 (95%)	0.09	0 100 100	45, 53, 57, 65	0
All	All	836/850 (98%)	0.30	27 (3%) 50 57	34, 55, 87, 109	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	PHE	4.6
1	A	109	PHE	3.6
1	A	376	PRO	3.1
1	B	39	GLY	2.9
1	B	376	PRO	2.9
1	B	32	PRO	2.7
1	B	30	TYR	2.6
1	B	28	LEU	2.6
1	B	19	ILE	2.6
1	B	38	PRO	2.4
1	B	107	GLY	2.3
1	B	381	ASN	2.3
1	B	101	ILE	2.3
1	B	249	ARG	2.3
1	B	372	LYS	2.3
2	I	11	ILE	2.3
1	B	367	ALA	2.2
1	B	394	ILE	2.2
1	B	109	PHE	2.2
1	B	384	ASP	2.2
2	I	24	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	98	PHE	2.1
1	A	375	GLY	2.1
1	B	369	PHE	2.1
1	B	370	ILE	2.0
1	B	22	ALA	2.0
1	B	31	HIS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	SEP	B	194	10/11	0.81	0.16	55,66,82,94	0
1	SEP	A	194	10/11	0.87	0.10	50,57,73,73	0
1	SEP	A	393	10/11	0.92	0.07	68,73,79,82	0
1	SEP	B	393	10/11	0.93	0.08	78,80,82,91	0
1	TPO	B	252	11/12	0.96	0.09	41,43,48,52	0
1	TPO	A	252	11/12	0.98	0.06	38,42,45,46	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

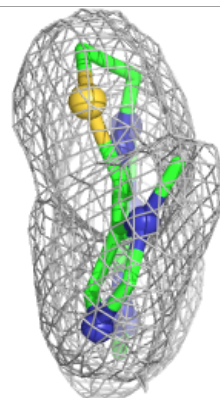
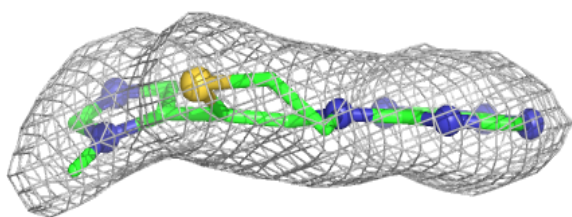
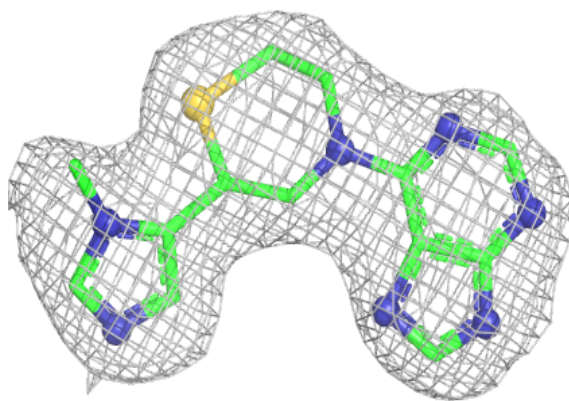
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	XTI	B	501	21/21	0.93	0.10	59,64,66,71	0
3	XTI	A	501	21/21	0.96	0.08	48,53,59,61	0

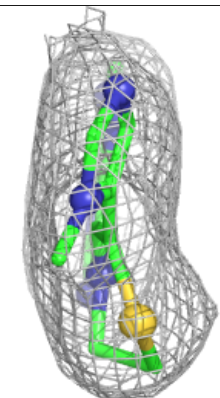
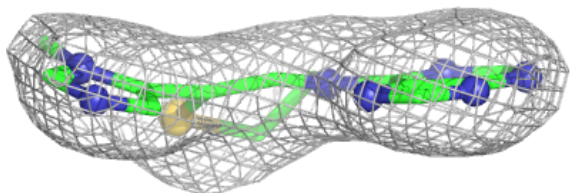
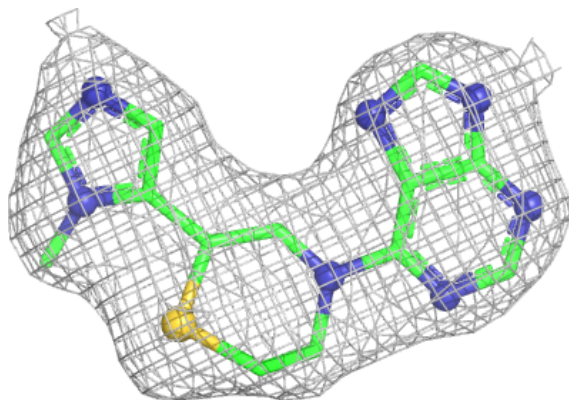
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around XTI B 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 XTI 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.