



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 11:52 AM BST

PDB ID : 6X9F  
Title : Pseudomonas aeruginosa MurC with AZ8074  
Authors : Horanyi, P.S.; Mayclin, S.J.; Durand-Reville, T.F.; Lorimer, D.D.; Edwards, T.E.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2020-06-02  
Resolution : 2.35 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](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 : 2.13  
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

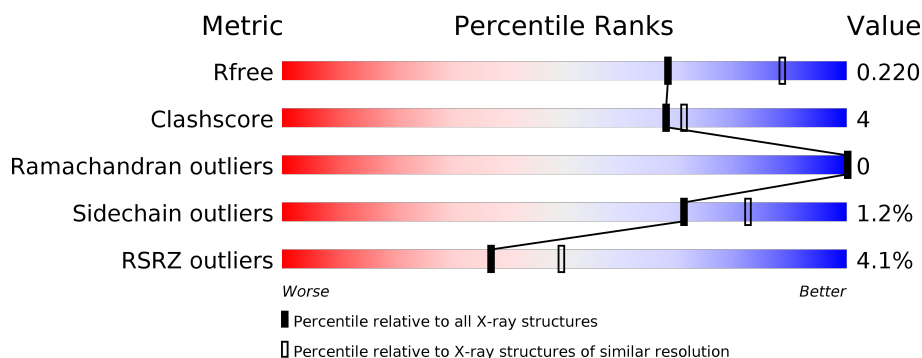
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	466	<div> <div>2%</div> <div>58% 7% 35%</div> </div>
1	B	466	<div> <div>4%</div> <div>58% 7% 35%</div> </div>
1	C	466	<div> <div>4%</div> <div>59% 6% 35%</div> </div>
1	D	466	<div> <div>3%</div> <div>59% 6% 35%</div> </div>
1	E	466	<div> <div>2%</div> <div>59% 6% 35%</div> </div>
1	F	466	<div> <div>%</div> <div>60% 5% 35%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	466	
1	H	466	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	C	502	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18978 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.

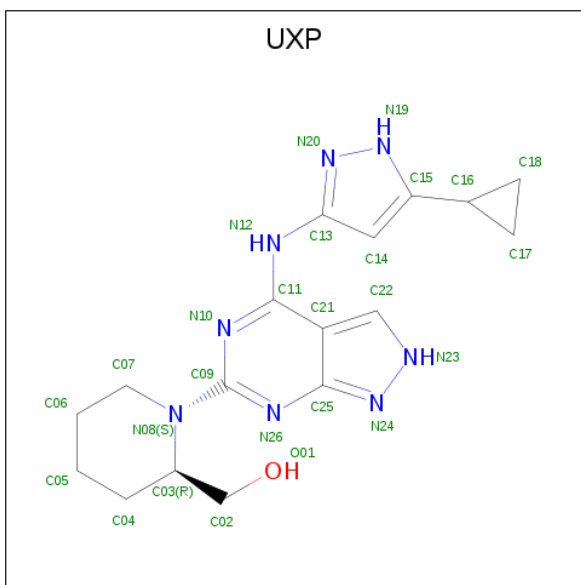
- Molecule 1 is a protein called UDP-N-acetylmuramate--L-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	3	0
			2240	1416	393	422	9			
1	B	304	Total	C	N	O	S	0	4	0
			2270	1434	399	427	10			
1	C	305	Total	C	N	O	S	0	2	0
			2242	1414	393	426	9			
1	D	304	Total	C	N	O	S	0	1	0
			2233	1409	393	422	9			
1	E	304	Total	C	N	O	S	0	3	0
			2255	1426	395	425	9			
1	F	305	Total	C	N	O	S	0	2	0
			2259	1424	399	427	9			
1	G	304	Total	C	N	O	S	0	1	0
			2243	1416	397	421	9			
1	H	304	Total	C	N	O	S	0	3	0
			2257	1427	395	426	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	HIS	-	expression tag	UNP Q9HW02
B	8	HIS	-	expression tag	UNP Q9HW02
C	8	HIS	-	expression tag	UNP Q9HW02
D	8	HIS	-	expression tag	UNP Q9HW02
E	8	HIS	-	expression tag	UNP Q9HW02
F	8	HIS	-	expression tag	UNP Q9HW02
G	8	HIS	-	expression tag	UNP Q9HW02
H	8	HIS	-	expression tag	UNP Q9HW02

- Molecule 2 is [(2R)-1-{4-[(5-cyclopropyl-1H-pyrazol-3-yl)amino]-2H-pyrazolo[3,4-d]pyrimidin-6-yl}piperidin-2-yl]methanol (three-letter code: UXP) (formula: C<sub>17</sub>H<sub>22</sub>N<sub>8</sub>O) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	17	8	1		
2	B	1	Total	C	N	O	0	0
			26	17	8	1		
2	C	1	Total	C	N	O	0	0
			26	17	8	1		
2	D	1	Total	C	N	O	0	0
			26	17	8	1		
2	E	1	Total	C	N	O	0	0
			26	17	8	1		
2	F	1	Total	C	N	O	0	0
			26	17	8	1		
2	G	1	Total	C	N	O	0	0
			26	17	8	1		
2	H	1	Total	C	N	O	0	0
			26	17	8	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	E	1	Total	C	O	S	0	0
			4	2	1	1		
4	E	1	Total	C	O	S	0	0
			4	2	1	1		
4	F	1	Total	C	O	S	0	0
			4	2	1	1		
4	G	1	Total	C	O	S	0	0
			4	2	1	1		
4	H	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



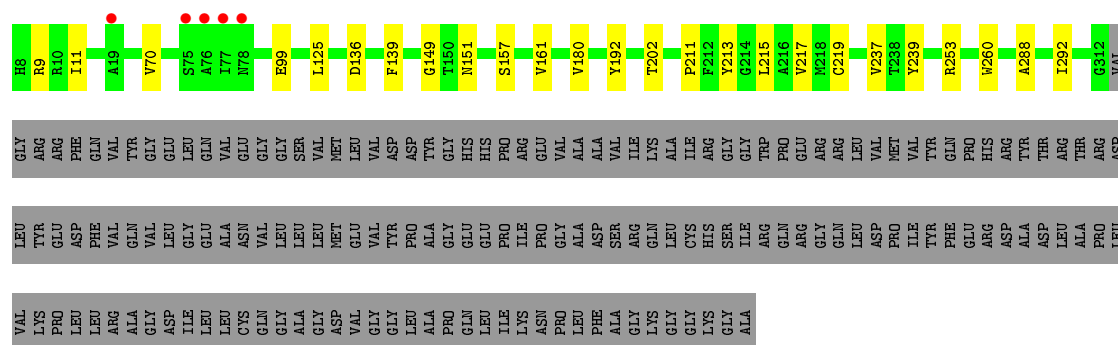
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0

- Molecule 6 is water.

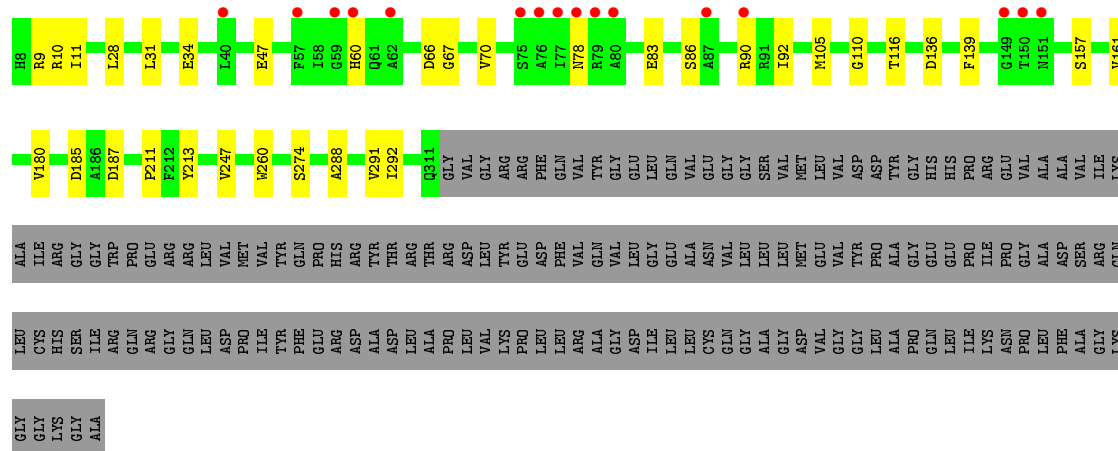
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	76	Total O 76 76	0	0
6	B	73	Total O 73 73	0	0
6	C	70	Total O 70 70	0	0
6	D	73	Total O 73 73	0	0
6	E	79	Total O 79 79	0	0
6	F	66	Total O 66 66	0	0
6	G	65	Total O 65 65	0	0
6	H	84	Total O 84 84	0	0



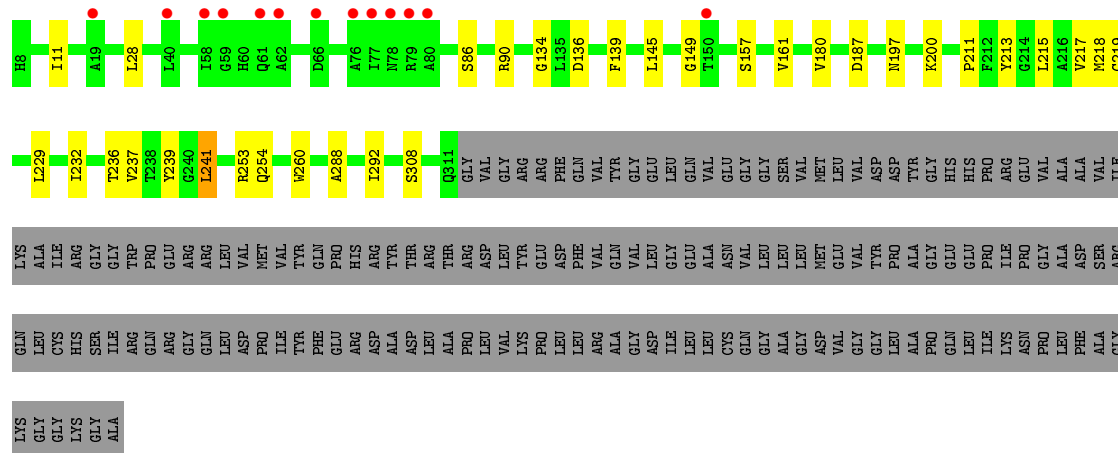




• Molecule 1: UDP-N-acetylmuramate--L-alanine ligase



• Molecule 1: UDP-N-acetylmuramate--L-alanine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	284.69Å 109.05Å 108.20Å 90.00° 112.26° 90.00°	Depositor
Resolution (Å)	47.67 – 2.35 47.67 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.67-2.35) 89.5 (47.67-2.35)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.34Å)	Xtriage
Refinement program	PHENIX PHENIX (dev_2733: ???)	Depositor
R, $R_{free}$	0.183 , 0.218 0.184 , 0.220	Depositor DCC
$R_{free}$ test set	2006 reflections (1.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.008 for -h-k-l,l,k 0.010 for -h+k-l,-l,-k 0.038 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.5984e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: DMS, EDO, UXP, CL

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	0.39	0/2288	0.55	0/3117
1	B	0.38	0/2321	0.57	0/3159
1	C	0.39	0/2287	0.57	0/3116
1	D	0.38	0/2275	0.56	0/3101
1	E	0.40	0/2303	0.59	0/3137
1	F	0.40	0/2301	0.59	0/3134
1	G	0.39	0/2285	0.56	0/3112
1	H	0.39	0/2305	0.57	0/3141
All	All	0.39	0/18365	0.57	0/25017

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	2240	0	2194	20	0
1	B	2270	0	2254	21	0
1	C	2242	0	2190	15	0
1	D	2233	0	2184	14	0
1	E	2255	0	2227	16	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2259	0	2218	14	0
1	G	2243	0	2214	19	0
1	H	2257	0	2229	18	0
2	A	26	0	0	0	0
2	B	26	0	0	0	0
2	C	26	0	0	0	0
2	D	26	0	0	0	0
2	E	26	0	0	0	0
2	F	26	0	0	0	0
2	G	26	0	0	0	0
2	H	26	0	0	0	0
3	A	20	0	30	0	0
3	B	24	0	36	5	0
3	C	20	0	30	0	0
3	D	16	0	24	1	0
3	E	16	0	24	1	0
3	F	12	0	18	1	0
3	G	8	0	12	0	0
3	H	12	0	18	1	0
4	A	4	0	6	1	0
4	B	20	0	30	3	0
4	D	8	0	12	1	0
4	E	8	0	12	1	0
4	F	4	0	6	0	0
4	G	4	0	6	1	0
4	H	4	0	6	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	76	0	0	2	0
6	B	73	0	0	1	0
6	C	70	0	0	0	0
6	D	73	0	0	1	0
6	E	79	0	0	1	0
6	F	66	0	0	1	0
6	G	65	0	0	1	0
6	H	84	0	0	2	0
All	All	18978	0	17980	139	0

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

The worst 5 of 139 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:C:258:ARG:NH1	1:C:274:SER:OG	2.25	0.69
1:B:19:ALA:O	3:B:507:EDO:H11	1.94	0.67
1:A:9:ARG:HH21	1:A:34:GLU:HG3	1.59	0.66
1:B:23:GLY:H	3:B:507:EDO:H12	1.61	0.65
1:F:99:GLU:HG2	3:F:503:EDO:H11	1.80	0.63

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	305/466 (66%)	296 (97%)	9 (3%)	0	100	100
1	B	306/466 (66%)	302 (99%)	4 (1%)	0	100	100
1	C	305/466 (66%)	299 (98%)	6 (2%)	0	100	100
1	D	303/466 (65%)	294 (97%)	9 (3%)	0	100	100
1	E	305/466 (66%)	294 (96%)	11 (4%)	0	100	100
1	F	305/466 (66%)	297 (97%)	8 (3%)	0	100	100
1	G	303/466 (65%)	298 (98%)	5 (2%)	0	100	100
1	H	305/466 (66%)	299 (98%)	6 (2%)	0	100	100
All	All	2437/3728 (65%)	2379 (98%)	58 (2%)	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	225/368 (61%)	222 (99%)	3 (1%)	69	80
1	B	234/368 (64%)	231 (99%)	3 (1%)	69	80
1	C	226/368 (61%)	225 (100%)	1 (0%)	91	95
1	D	225/368 (61%)	222 (99%)	3 (1%)	69	80
1	E	230/368 (62%)	227 (99%)	3 (1%)	69	80
1	F	229/368 (62%)	228 (100%)	1 (0%)	91	95
1	G	228/368 (62%)	225 (99%)	3 (1%)	69	80
1	H	231/368 (63%)	227 (98%)	4 (2%)	60	72
All	All	1828/2944 (62%)	1807 (99%)	21 (1%)	71	84

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	187	ASP
1	E	145	LEU
1	H	145	LEU
1	D	145	LEU
1	H	187	ASP

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

Mol	Chain	Res	Type
1	E	61	GLN
1	G	109	HIS

### 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](#)

Of 58 ligands modelled in this entry, 5 are monoatomic - leaving 53 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
4	DMS	B	508	-	3,3,3	0.70	0	3,3,3	0.93	0
3	EDO	G	502	-	3,3,3	0.44	0	2,2,2	0.46	0
3	EDO	A	503	-	3,3,3	0.49	0	2,2,2	0.36	0
3	EDO	E	502	-	3,3,3	0.55	0	2,2,2	0.20	0
3	EDO	D	505	-	3,3,3	0.45	0	2,2,2	0.31	0
3	EDO	E	503	-	3,3,3	0.43	0	2,2,2	0.41	0
2	UXP	E	501	-	29,30,30	3.38	7 (24%)	27,43,43	2.15	10 (37%)
3	EDO	F	504	-	3,3,3	0.47	0	2,2,2	0.43	0
3	EDO	G	503	-	3,3,3	0.51	0	2,2,2	0.35	0
3	EDO	H	503	-	3,3,3	0.52	0	2,2,2	0.34	0
3	EDO	D	504	-	3,3,3	0.38	0	2,2,2	0.61	0
4	DMS	A	507	-	3,3,3	0.59	0	3,3,3	0.54	0
3	EDO	C	505	-	3,3,3	0.52	0	2,2,2	0.33	0
3	EDO	E	505	-	3,3,3	0.57	0	2,2,2	0.09	0
2	UXP	F	501	-	29,30,30	3.37	7 (24%)	27,43,43	2.17	11 (40%)
3	EDO	D	502	-	3,3,3	0.40	0	2,2,2	0.50	0
3	EDO	A	502	-	3,3,3	0.51	0	2,2,2	0.34	0
3	EDO	B	502	-	3,3,3	0.49	0	2,2,2	0.51	0
2	UXP	A	501	-	29,30,30	3.39	7 (24%)	27,43,43	2.18	10 (37%)
4	DMS	H	505	-	3,3,3	0.59	0	3,3,3	0.67	0
3	EDO	C	503	-	3,3,3	0.36	0	2,2,2	0.91	0
4	DMS	B	509	-	3,3,3	0.60	0	3,3,3	0.51	0
3	EDO	H	504	-	3,3,3	0.52	0	2,2,2	0.32	0
3	EDO	E	504	-	3,3,3	0.52	0	2,2,2	0.15	0
3	EDO	A	504	-	3,3,3	0.44	0	2,2,2	0.46	0
4	DMS	G	504	-	3,3,3	0.73	0	3,3,3	0.39	0
3	EDO	C	502	-	3,3,3	0.53	0	2,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	UXP	H	501	-	29,30,30	3.33	7 (24%)	27,43,43	2.10	9 (33%)
4	DMS	F	505	-	3,3,3	0.67	0	3,3,3	0.75	0
3	EDO	B	506	-	3,3,3	0.50	0	2,2,2	0.31	0
4	DMS	D	506	-	3,3,3	0.63	0	3,3,3	0.79	0
2	UXP	G	501	-	29,30,30	3.44	8 (27%)	27,43,43	2.13	11 (40%)
3	EDO	C	504	-	3,3,3	0.40	0	2,2,2	0.54	0
3	EDO	B	503	-	3,3,3	0.47	0	2,2,2	0.56	0
2	UXP	B	501	-	29,30,30	3.32	7 (24%)	27,43,43	2.47	10 (37%)
4	DMS	E	507	-	3,3,3	0.66	0	3,3,3	0.66	0
3	EDO	B	507	-	3,3,3	0.42	0	2,2,2	0.43	0
3	EDO	D	503	-	3,3,3	0.49	0	2,2,2	0.28	0
2	UXP	D	501	-	29,30,30	3.46	7 (24%)	27,43,43	1.97	10 (37%)
4	DMS	B	510	-	3,3,3	0.67	0	3,3,3	0.59	0
3	EDO	C	506	-	3,3,3	0.60	0	2,2,2	0.12	0
3	EDO	A	506	-	3,3,3	0.49	0	2,2,2	0.40	0
3	EDO	F	502	-	3,3,3	0.40	0	2,2,2	0.57	0
4	DMS	E	506	-	3,3,3	0.74	0	3,3,3	0.28	0
3	EDO	B	505	-	3,3,3	0.65	0	2,2,2	0.13	0
3	EDO	B	504	-	3,3,3	0.47	0	2,2,2	0.31	0
4	DMS	D	507	-	3,3,3	0.56	0	3,3,3	0.54	0
3	EDO	H	502	-	3,3,3	0.36	0	2,2,2	0.55	0
2	UXP	C	501	-	29,30,30	3.32	7 (24%)	27,43,43	2.24	12 (44%)
4	DMS	B	511	-	3,3,3	0.66	0	3,3,3	0.60	0
3	EDO	F	503	-	3,3,3	0.47	0	2,2,2	0.28	0
3	EDO	A	505	-	3,3,3	0.49	0	2,2,2	0.27	0
4	DMS	B	512	-	3,3,3	0.66	0	3,3,3	0.61	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
3	EDO	G	502	-	-	0/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	E	502	-	-	0/1/1/1	-
3	EDO	D	505	-	-	1/1/1/1	-
3	EDO	E	503	-	-	0/1/1/1	-
2	UXP	E	501	-	-	4/12/27/27	0/5/5/5
3	EDO	F	504	-	-	1/1/1/1	-
3	EDO	G	503	-	-	0/1/1/1	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	H	503	-	-	0/1/1/1	-
3	EDO	D	504	-	-	0/1/1/1	-
3	EDO	C	505	-	-	1/1/1/1	-
3	EDO	E	505	-	-	0/1/1/1	-
2	UXP	F	501	-	-	3/12/27/27	0/5/5/5
3	EDO	D	502	-	-	0/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	B	502	-	-	1/1/1/1	-
2	UXP	A	501	-	-	3/12/27/27	0/5/5/5
3	EDO	C	503	-	-	1/1/1/1	-
3	EDO	H	504	-	-	1/1/1/1	-
3	EDO	E	504	-	-	0/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	C	502	-	-	0/1/1/1	-
2	UXP	H	501	-	-	4/12/27/27	0/5/5/5
3	EDO	B	506	-	-	1/1/1/1	-
2	UXP	G	501	-	-	2/12/27/27	0/5/5/5
3	EDO	C	504	-	-	0/1/1/1	-
3	EDO	B	503	-	-	1/1/1/1	-
2	UXP	B	501	-	-	2/12/27/27	0/5/5/5
3	EDO	B	507	-	-	1/1/1/1	-
3	EDO	D	503	-	-	1/1/1/1	-
2	UXP	D	501	-	-	4/12/27/27	0/5/5/5
3	EDO	C	506	-	-	1/1/1/1	-
3	EDO	A	506	-	-	0/1/1/1	-
3	EDO	F	502	-	-	0/1/1/1	-
3	EDO	B	505	-	-	1/1/1/1	-
3	EDO	B	504	-	-	0/1/1/1	-
3	EDO	H	502	-	-	0/1/1/1	-
2	UXP	C	501	-	-	4/12/27/27	0/5/5/5
3	EDO	F	503	-	-	0/1/1/1	-
3	EDO	A	505	-	-	0/1/1/1	-

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	UXP	C15-N19	12.65	1.50	1.34
2	D	501	UXP	C15-N19	12.51	1.50	1.34
2	F	501	UXP	C15-N19	12.49	1.50	1.34
2	E	501	UXP	C15-N19	12.49	1.50	1.34
2	H	501	UXP	C15-N19	12.39	1.50	1.34

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	UXP	N12-C11-N10	-4.79	114.16	118.66
2	D	501	UXP	C04-C03-N08	4.54	116.19	109.98
2	A	501	UXP	C04-C03-N08	4.44	116.05	109.98
2	B	501	UXP	C04-C03-N08	4.29	115.85	109.98
2	C	501	UXP	C05-C04-C03	4.18	119.13	110.82

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	501	UXP	O01-C02-C03-C04
2	E	501	UXP	O01-C02-C03-N08
2	E	501	UXP	C14-C15-C16-C17
2	E	501	UXP	N19-C15-C16-C17
2	F	501	UXP	O01-C02-C03-C04

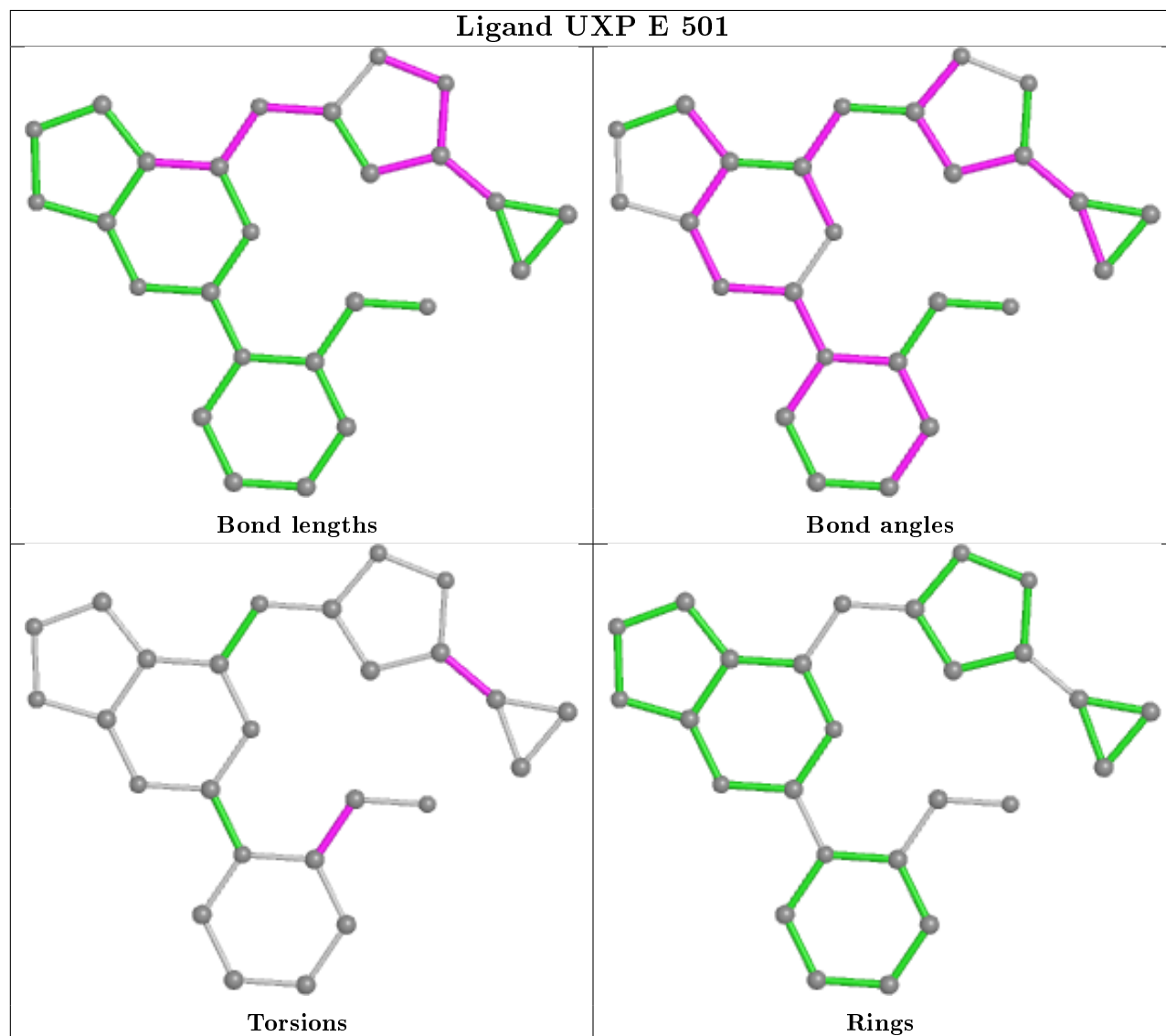
There are no ring outliers.

13 monomers are involved in 16 short contacts:

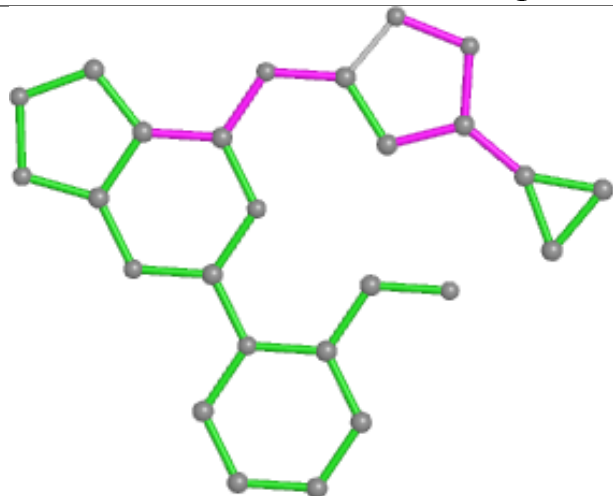
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	503	EDO	1	0
4	A	507	DMS	1	0
3	E	505	EDO	1	0
3	D	502	EDO	1	0
3	B	502	EDO	1	0
4	B	509	DMS	2	0
4	G	504	DMS	1	0
4	D	506	DMS	1	0
4	E	507	DMS	1	0
3	B	507	EDO	3	0
4	B	510	DMS	1	0
3	B	504	EDO	1	0
3	F	503	EDO	1	0

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

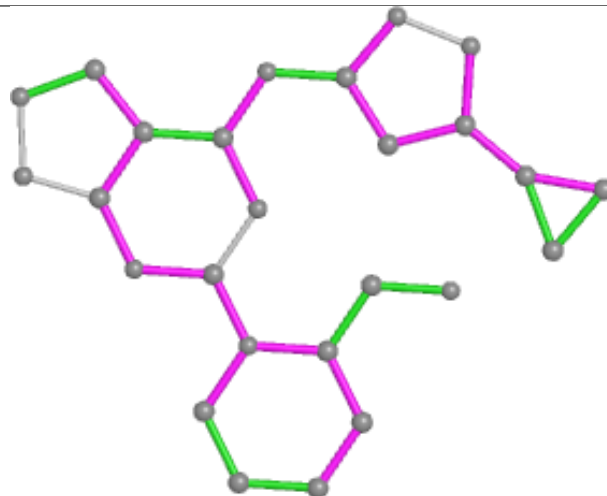
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



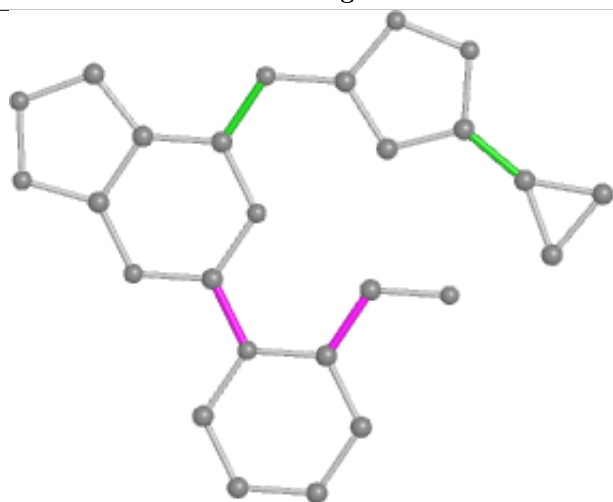
## Ligand UXP F 501



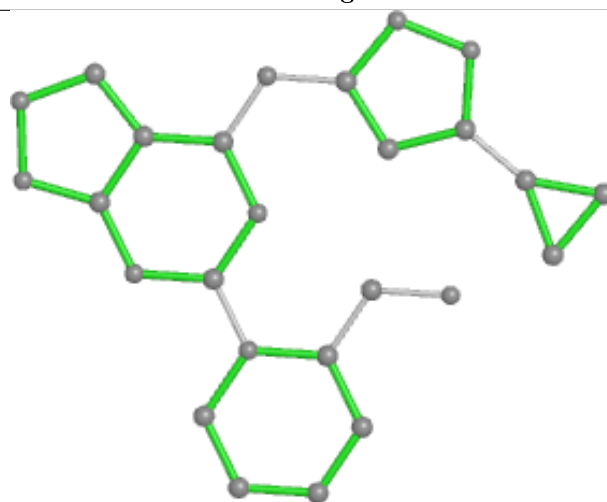
Bond lengths



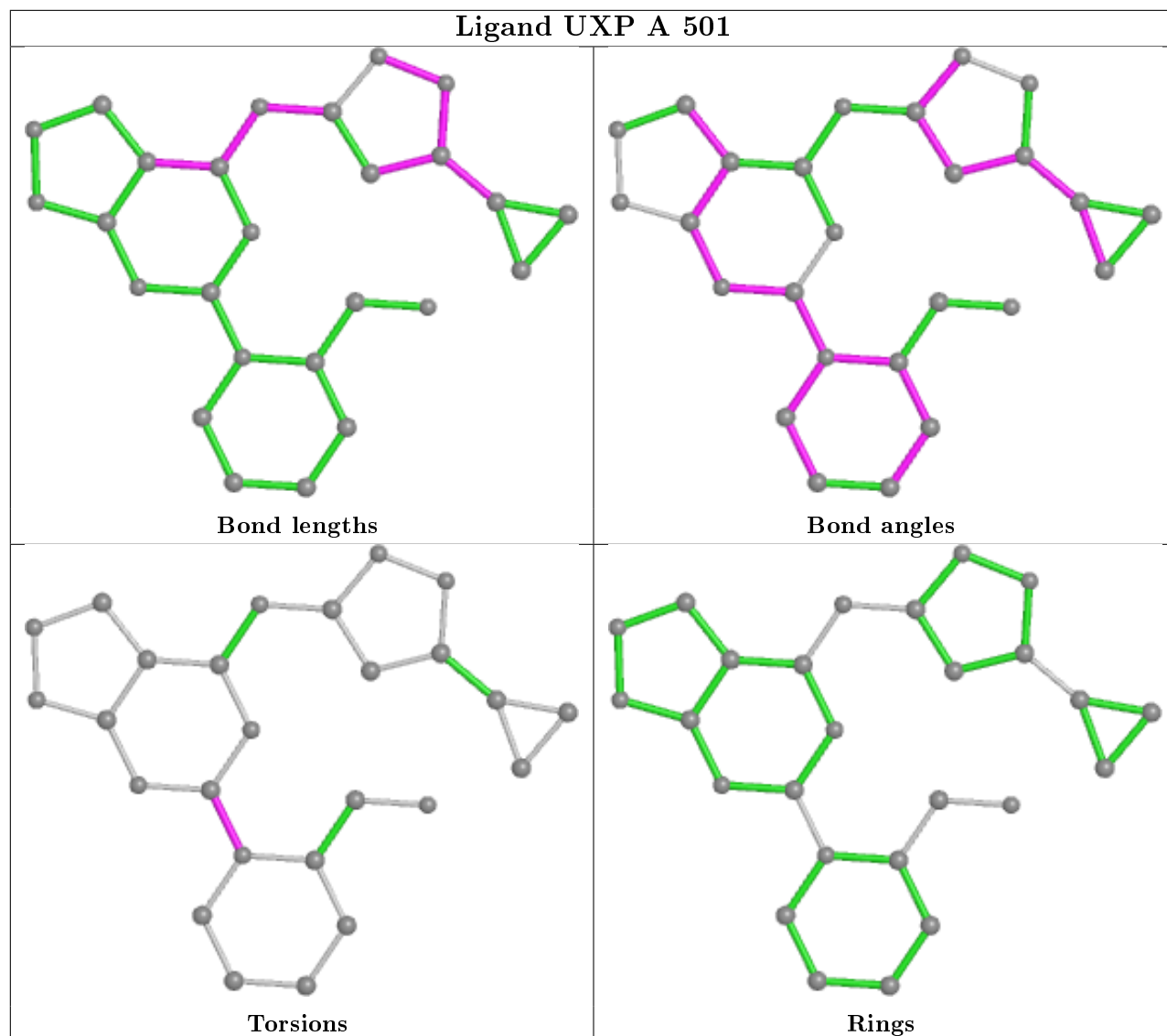
Bond angles



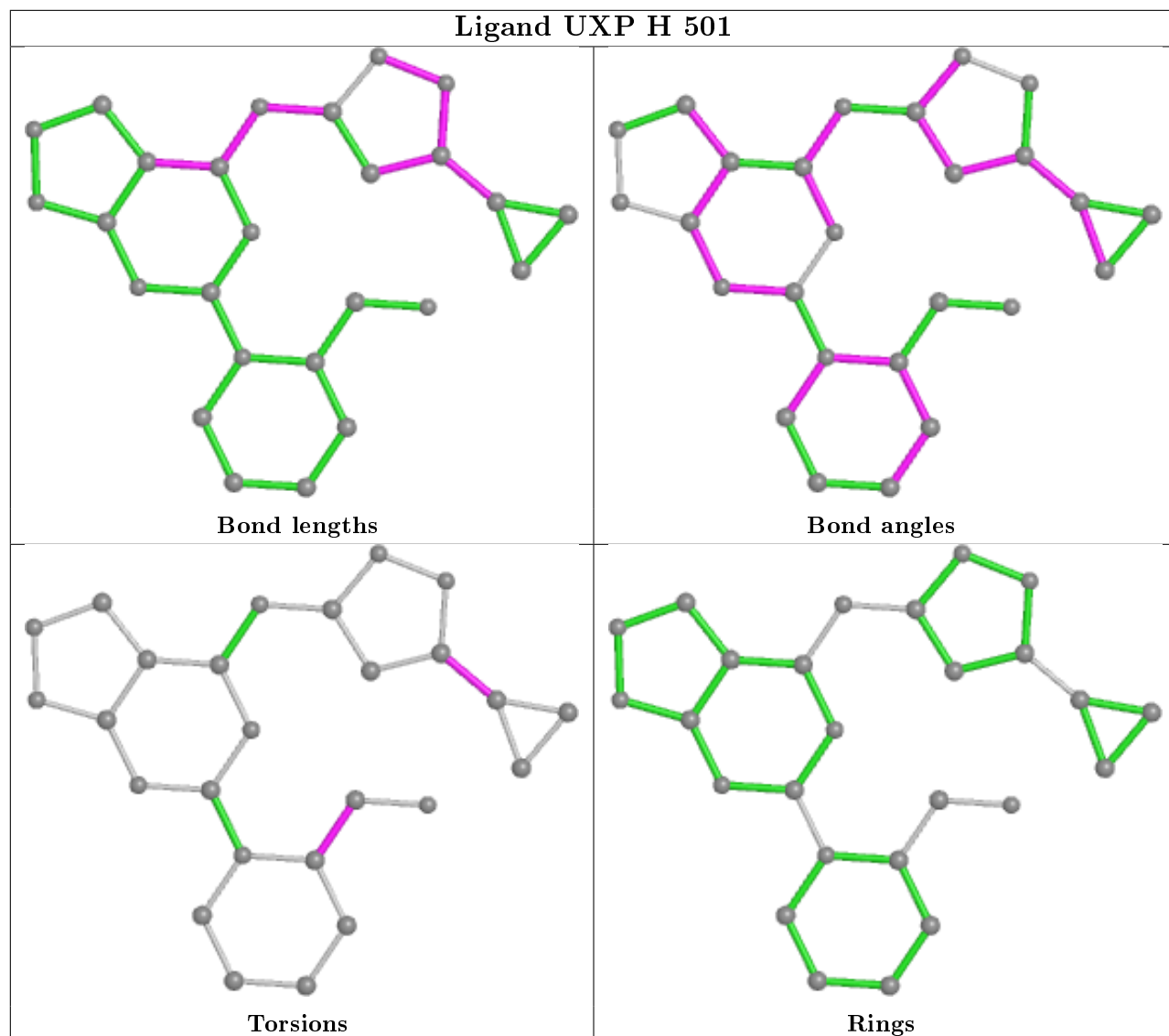
Torsions

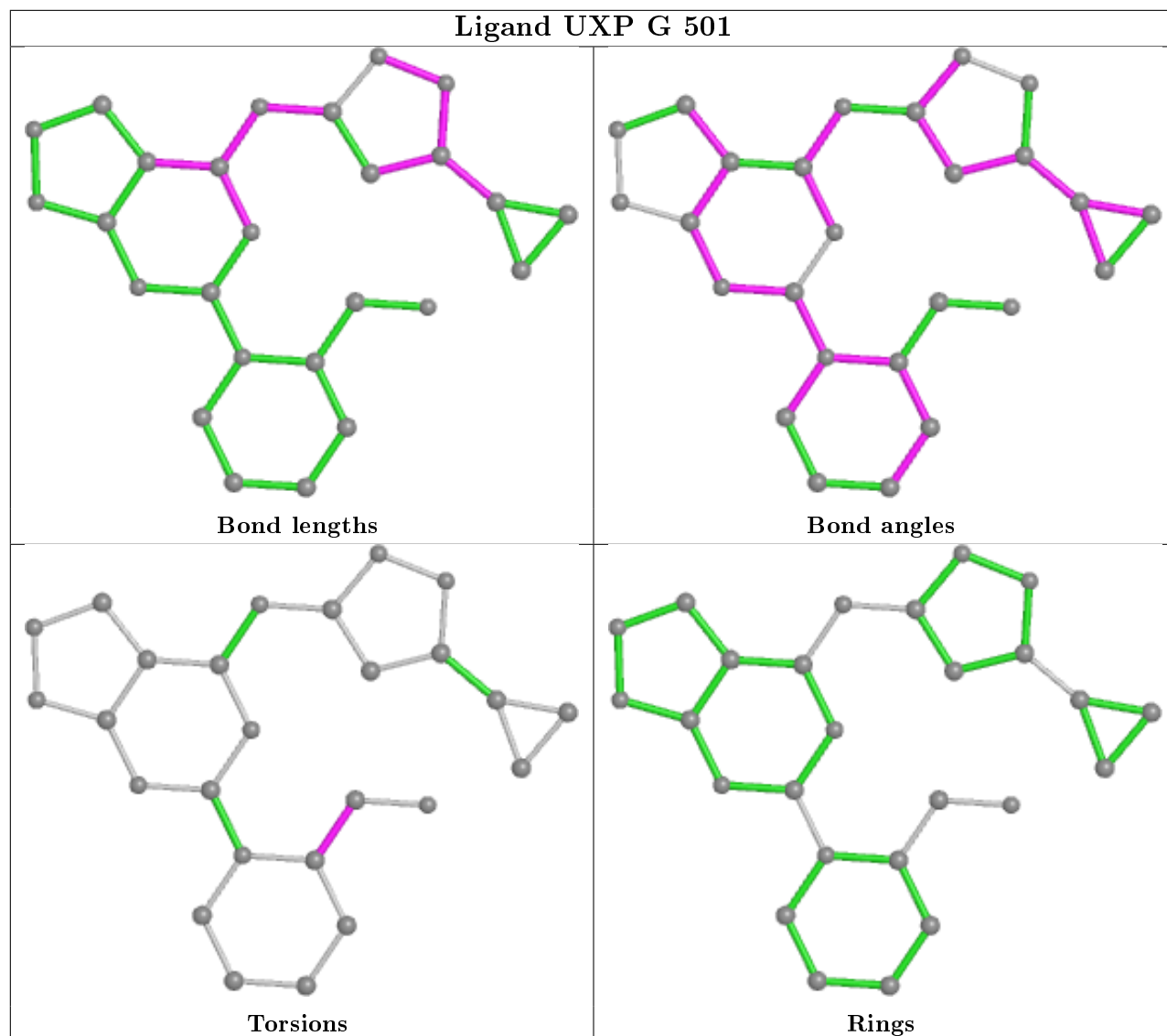


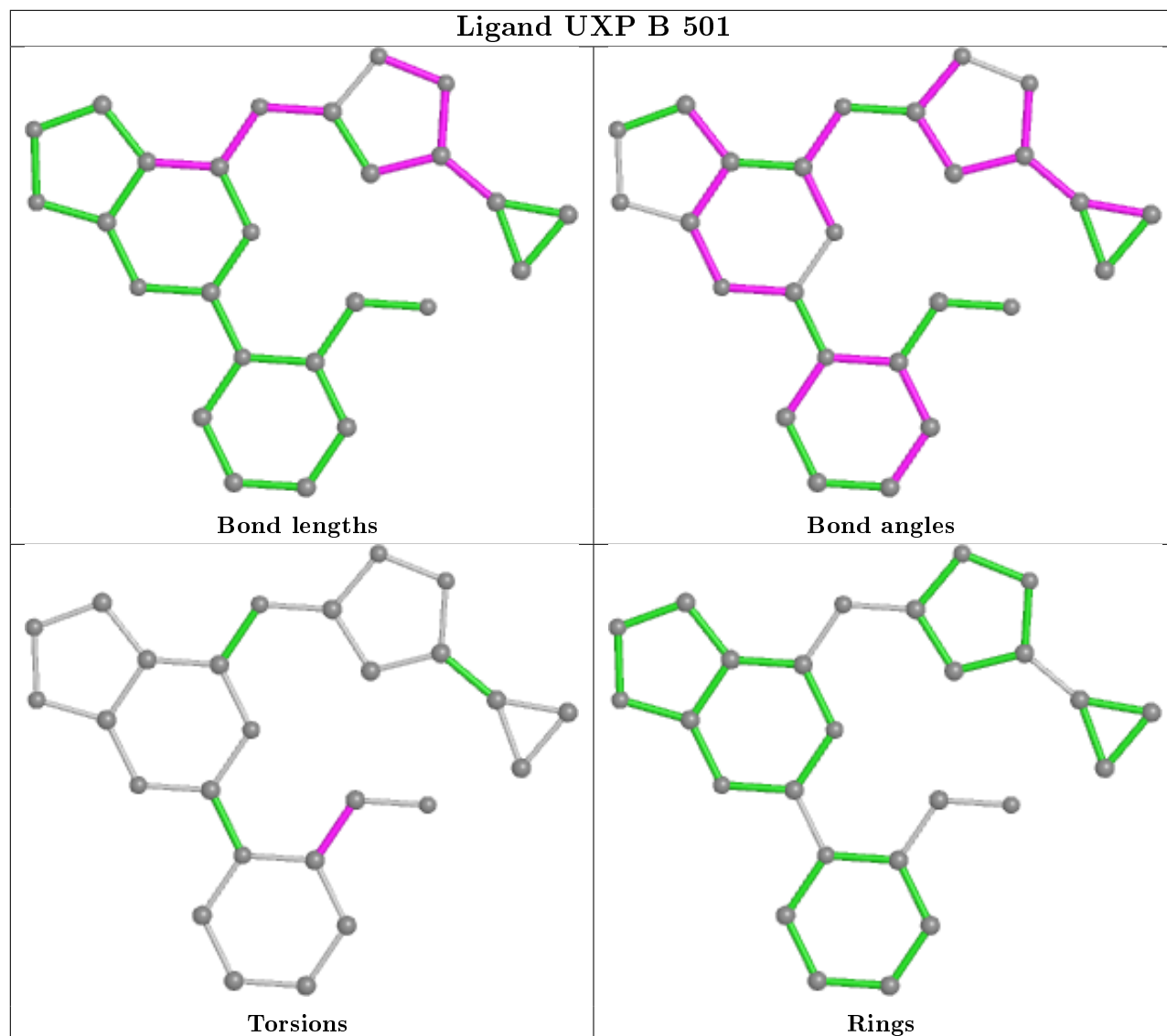
Rings

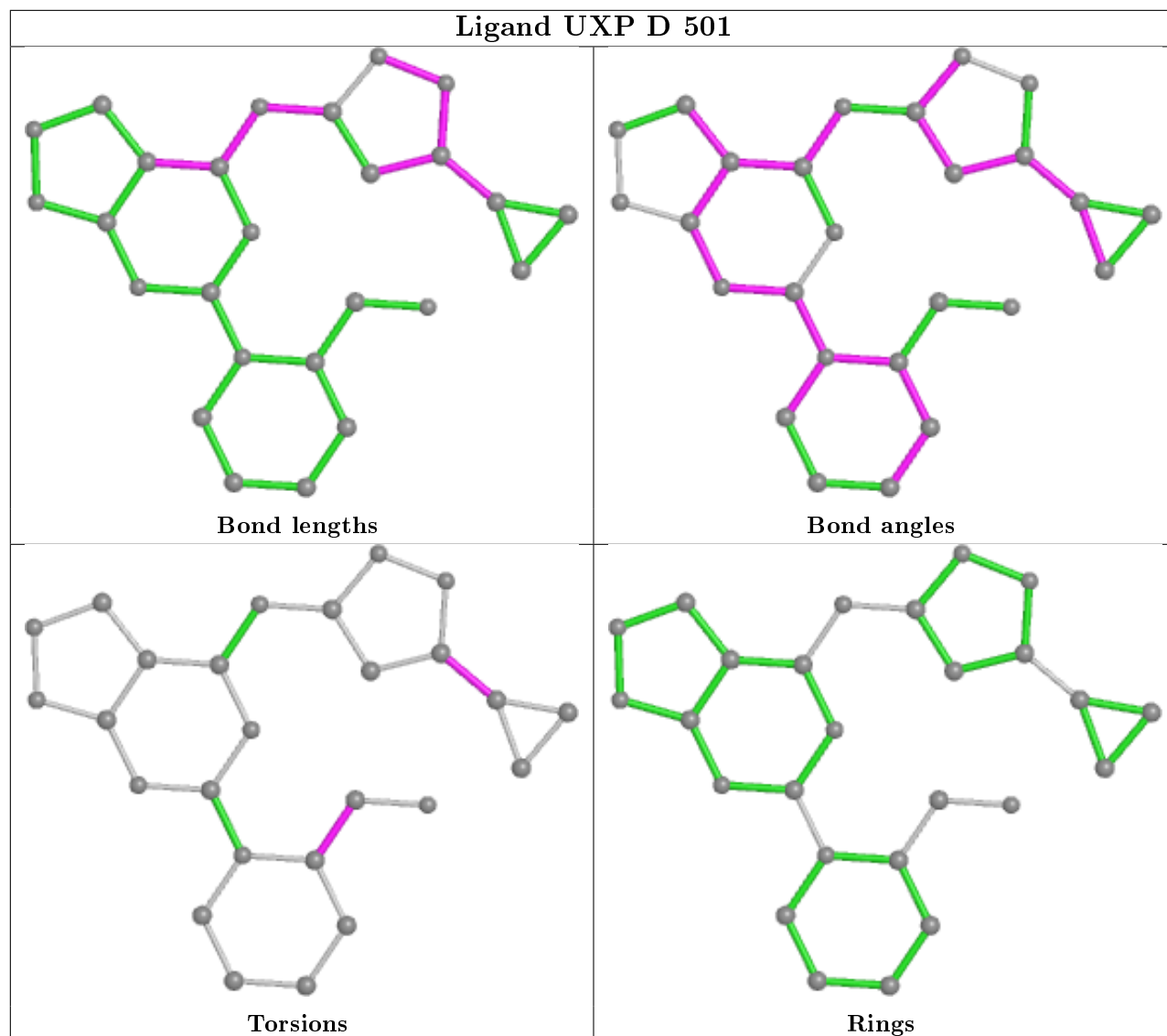


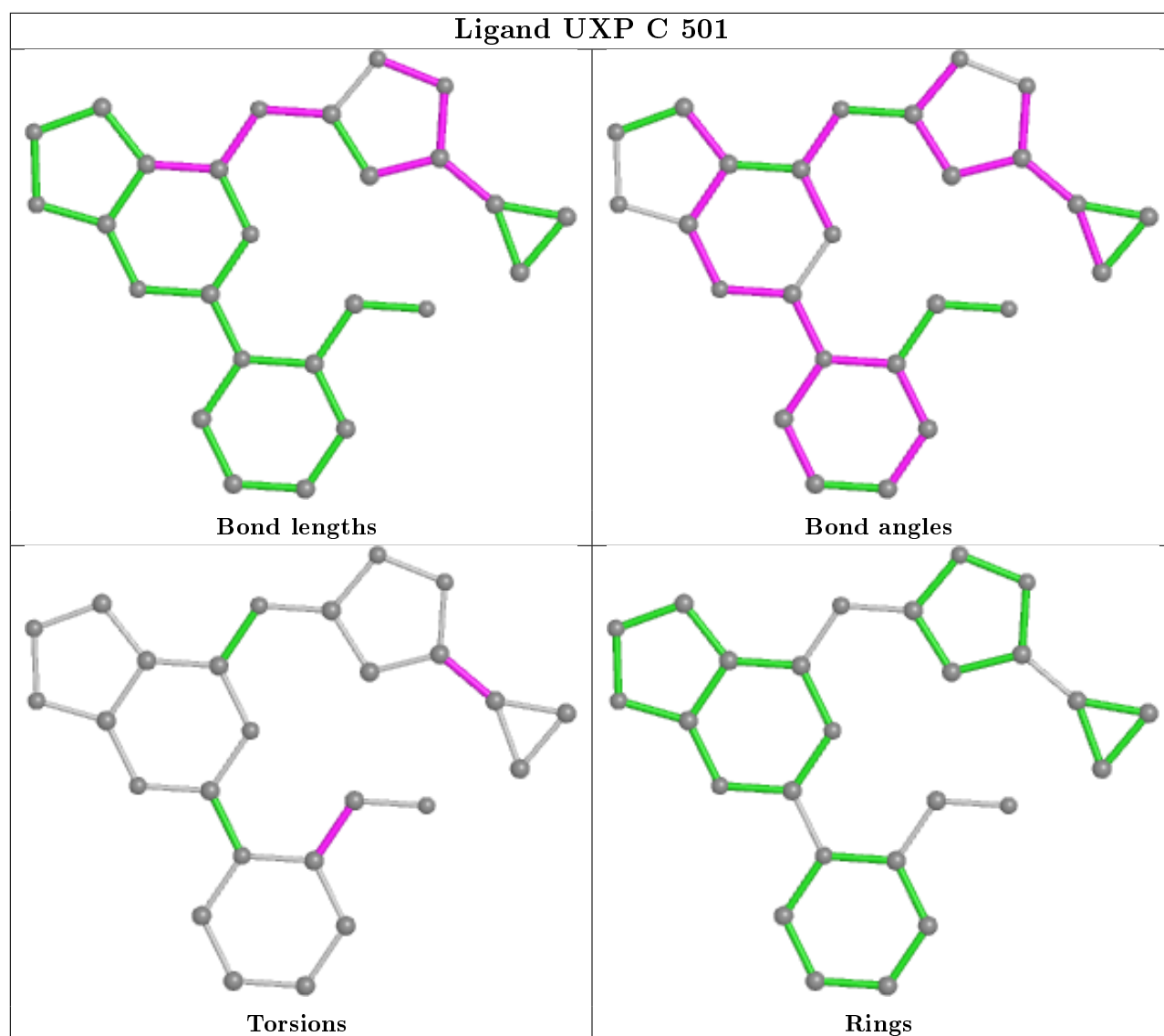












## 5.7 Other polymers [i](#)

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	304/466 (65%)	0.11	11 (3%) 42 55	31, 45, 82, 125	0
1	B	304/466 (65%)	0.21	17 (5%) 24 35	28, 42, 81, 124	0
1	C	305/466 (65%)	0.16	20 (6%) 18 26	30, 45, 84, 126	0
1	D	304/466 (65%)	0.03	12 (3%) 39 52	31, 45, 74, 112	0
1	E	304/466 (65%)	-0.00	7 (2%) 60 70	28, 41, 71, 113	0
1	F	305/466 (65%)	-0.03	5 (1%) 72 80	29, 44, 80, 128	0
1	G	304/466 (65%)	0.12	16 (5%) 26 38	31, 45, 82, 121	0
1	H	304/466 (65%)	0.16	13 (4%) 35 47	27, 42, 78, 125	0
All	All	2434/3728 (65%)	0.09	101 (4%) 37 49	27, 44, 81, 128	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	77	ILE	6.4
1	G	80	ALA	6.4
1	F	76	ALA	5.3
1	C	77	ILE	5.2
1	C	76	ALA	4.9

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

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

### 6.3 Carbohydrates [i](#)

There are no 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, 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	EDO	E	505	4/4	0.60	0.25	76,76,77,80	0
3	EDO	E	502	4/4	0.66	0.24	72,75,75,76	0
3	EDO	C	506	4/4	0.66	0.23	54,57,61,62	0
3	EDO	B	505	4/4	0.74	0.32	63,64,66,66	0
3	EDO	C	502	4/4	0.75	0.49	79,79,82,85	0
3	EDO	F	504	4/4	0.77	0.30	66,68,73,76	0
3	EDO	G	503	4/4	0.77	0.30	65,72,78,81	0
3	EDO	A	504	4/4	0.78	0.34	73,73,74,74	0
3	EDO	C	505	4/4	0.81	0.24	59,61,63,66	0
3	EDO	H	503	4/4	0.82	0.47	67,76,82,89	0
3	EDO	B	502	4/4	0.83	0.40	65,66,67,70	0
3	EDO	B	506	4/4	0.83	0.32	63,69,75,77	0
3	EDO	B	504	4/4	0.84	0.39	74,77,81,85	0
3	EDO	A	503	4/4	0.86	0.17	74,78,82,83	0
3	EDO	E	504	4/4	0.86	0.40	73,78,80,83	0
3	EDO	H	502	4/4	0.86	0.20	75,77,79,85	0
3	EDO	F	503	4/4	0.86	0.20	67,69,70,72	0
3	EDO	H	504	4/4	0.87	0.31	58,67,73,74	0
3	EDO	D	503	4/4	0.88	0.30	67,69,74,75	0
3	EDO	D	502	4/4	0.88	0.23	69,72,74,75	0
5	CL	E	508	1/1	0.88	0.55	123,123,123,123	0
3	EDO	A	506	4/4	0.89	0.14	60,61,64,66	0
4	DMS	D	507	4/4	0.89	0.20	80,83,88,94	0
5	CL	H	506	1/1	0.89	0.48	123,123,123,123	0
2	UXP	B	501	26/26	0.89	0.18	42,58,71,78	0
3	EDO	B	503	4/4	0.90	0.15	62,68,69,70	0
3	EDO	A	502	4/4	0.90	0.24	60,62,64,64	0
3	EDO	C	503	4/4	0.90	0.25	69,71,71,73	0
4	DMS	B	510	4/4	0.90	0.26	85,88,90,91	0
3	EDO	A	505	4/4	0.90	0.31	63,72,78,81	0
4	DMS	B	512	4/4	0.90	0.26	90,93,93,94	0
4	DMS	E	506	4/4	0.91	0.19	69,75,77,82	0
2	UXP	F	501	26/26	0.91	0.18	50,56,67,88	0
3	EDO	D	505	4/4	0.91	0.22	64,65,66,69	0
4	DMS	B	508	4/4	0.91	0.20	51,76,79,79	0
5	CL	G	505	1/1	0.92	0.20	85,85,85,85	0
2	UXP	D	501	26/26	0.92	0.18	44,60,77,104	0

*Continued on next page...*

*Continued from previous page...*

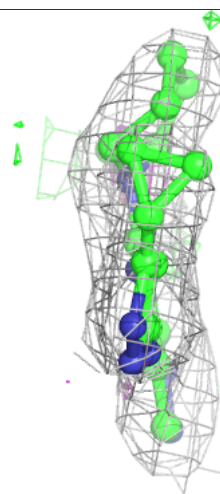
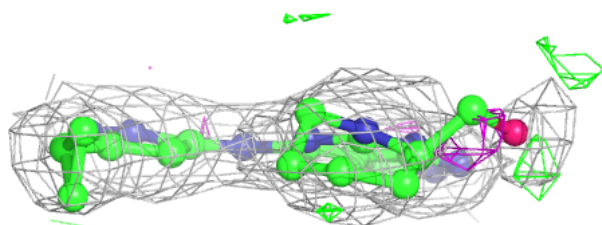
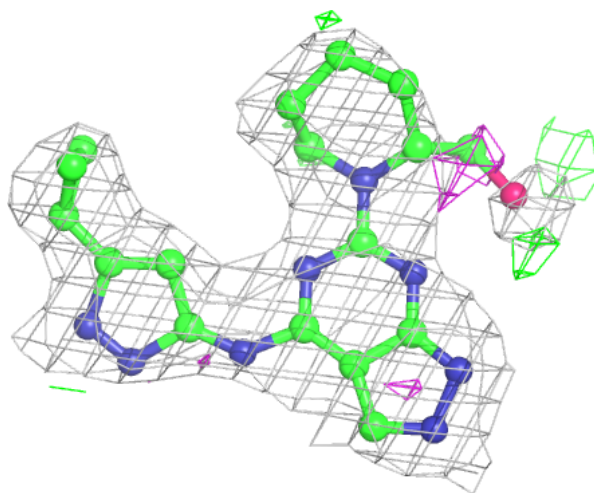
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	UXP	G	501	26/26	0.92	0.20	54,65,73,94	0
5	CL	F	506	1/1	0.92	0.34	98,98,98,98	0
2	UXP	C	501	26/26	0.92	0.15	49,59,70,89	0
4	DMS	G	504	4/4	0.92	0.17	69,72,74,79	0
3	EDO	D	504	4/4	0.92	0.28	52,52,55,58	0
4	DMS	E	507	4/4	0.92	0.20	92,94,94,95	0
4	DMS	H	505	4/4	0.93	0.17	66,76,78,80	0
2	UXP	E	501	26/26	0.93	0.16	46,57,68,92	0
5	CL	D	508	1/1	0.93	0.41	97,97,97,97	0
2	UXP	A	501	26/26	0.93	0.13	50,58,68,78	0
3	EDO	C	504	4/4	0.94	0.16	56,59,65,72	0
4	DMS	B	511	4/4	0.94	0.18	86,89,90,91	0
3	EDO	E	503	4/4	0.94	0.18	54,55,59,65	0
4	DMS	A	507	4/4	0.94	0.20	72,76,78,82	0
2	UXP	H	501	26/26	0.94	0.19	43,54,69,92	0
3	EDO	F	502	4/4	0.95	0.15	44,50,62,73	0
3	EDO	B	507	4/4	0.95	0.24	59,61,61,61	0
4	DMS	B	509	4/4	0.96	0.15	66,66,69,73	0
3	EDO	G	502	4/4	0.96	0.22	74,76,80,80	0
4	DMS	F	505	4/4	0.97	0.14	65,70,70,70	0
4	DMS	D	506	4/4	0.97	0.20	61,70,70,74	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.



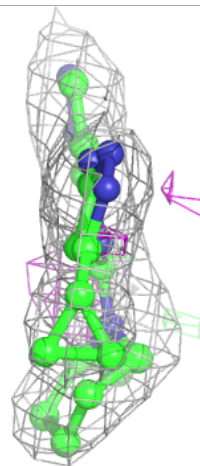
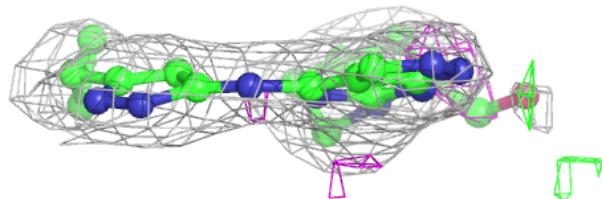
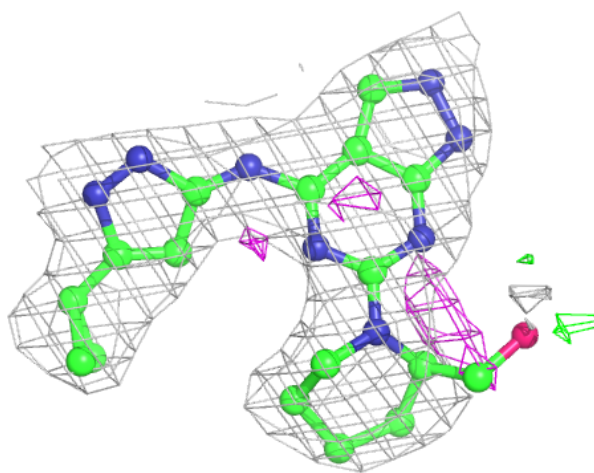
**Electron density around UXP B 501:**

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



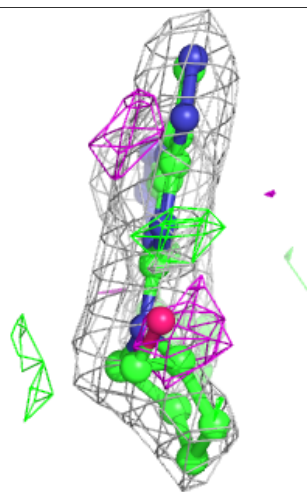
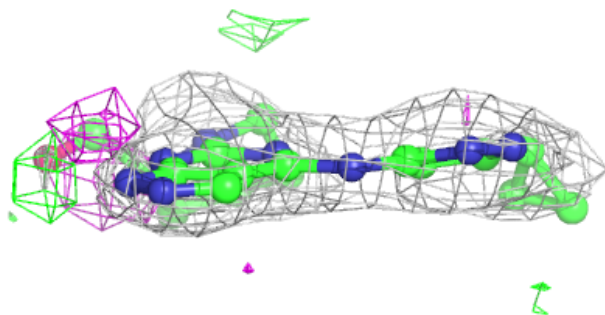
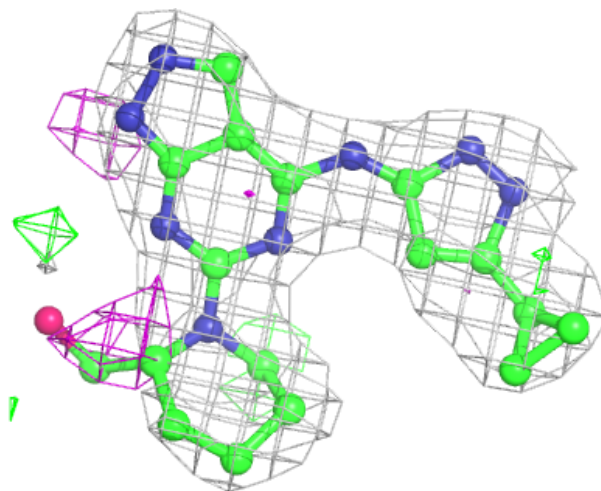
**Electron density around UXP F 501:**

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



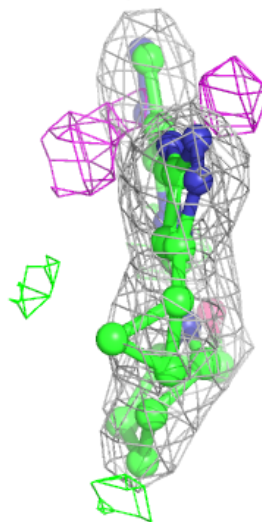
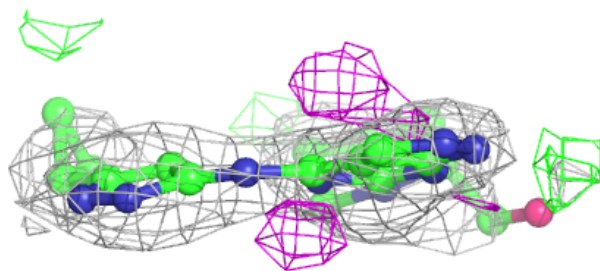
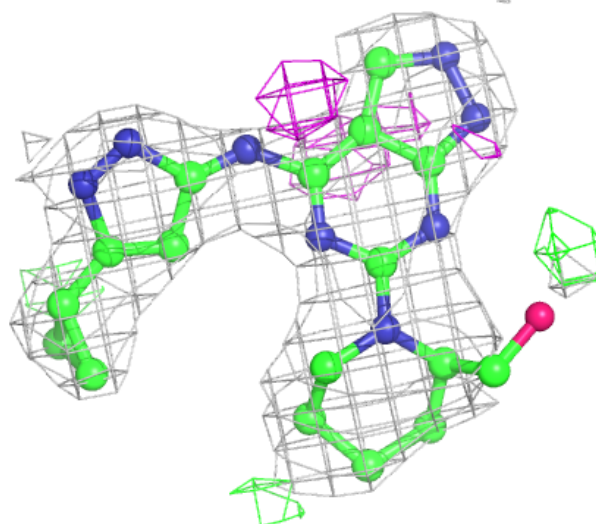
**Electron density around UXP D 501:**

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



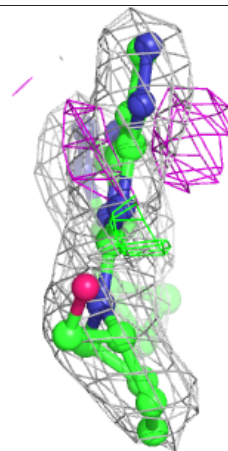
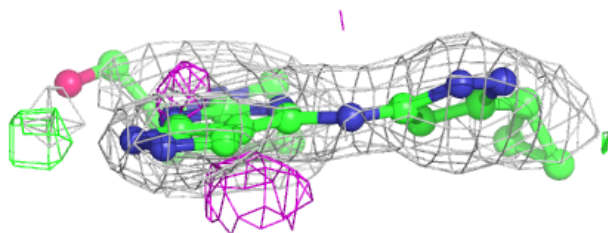
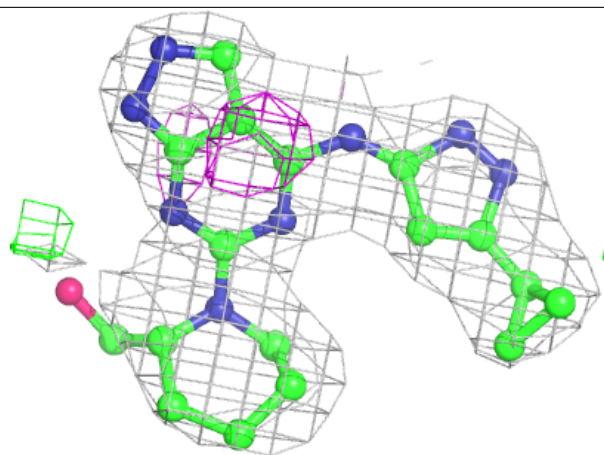
**Electron density around UXP G 501:**

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



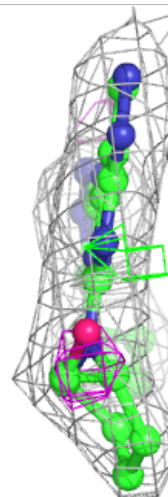
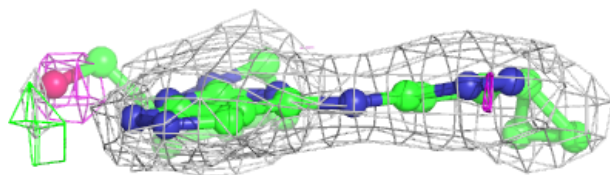
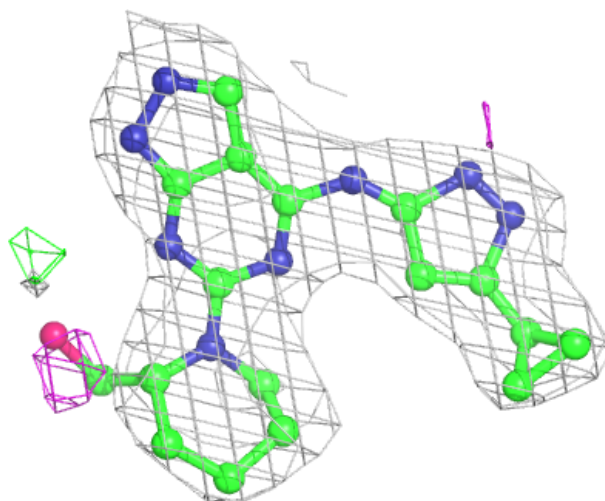
**Electron density around UXP C 501:**

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



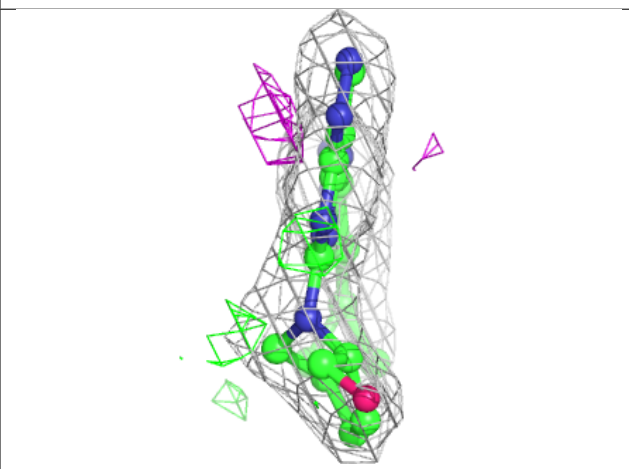
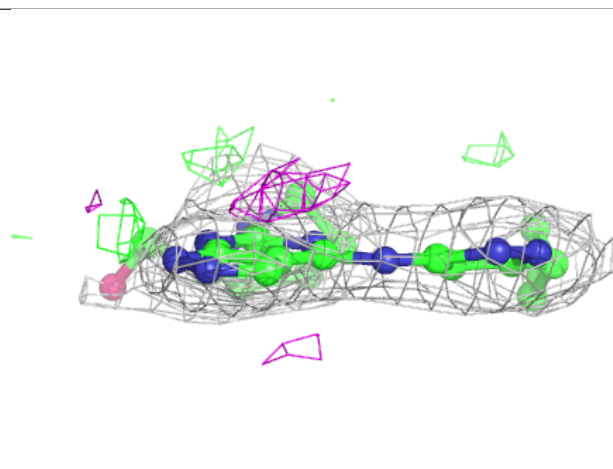
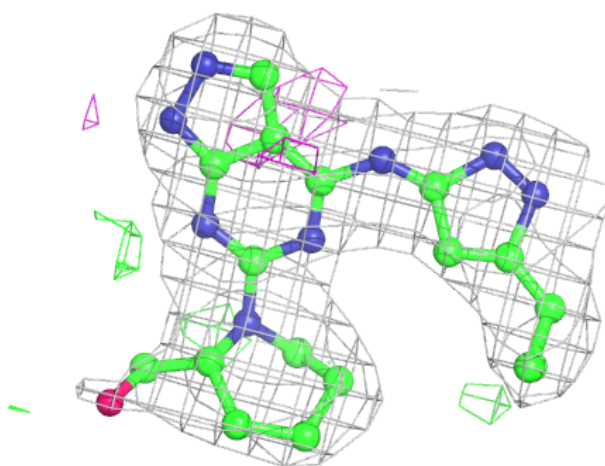
**Electron density around UXP E 501:**

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



**Electron density around UXP A 501:**

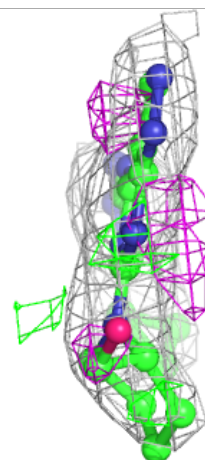
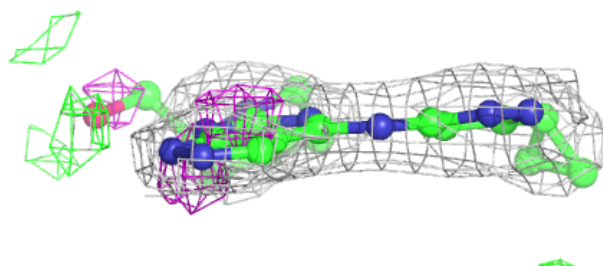
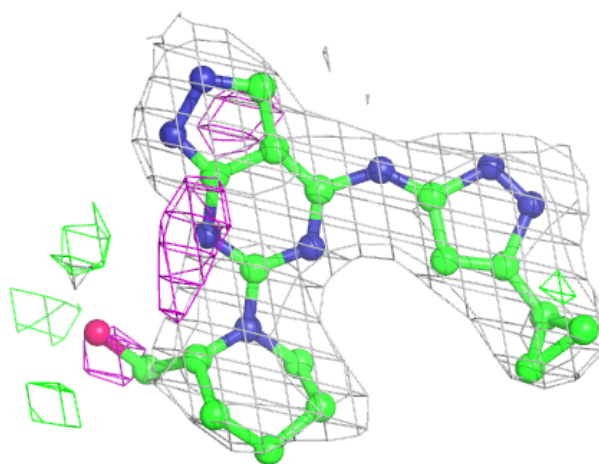
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around UXP H 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.