



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:05 am BST

PDB ID : 6HZX  
Title : Protein-aromatic foldamer complex crystal structure  
Authors : Post, S.; Langlois d'Estaintot, B.; Fischer, L.; Granier, T.; Huc, I.  
Deposited on : 2018-10-24  
Resolution : 2.91 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

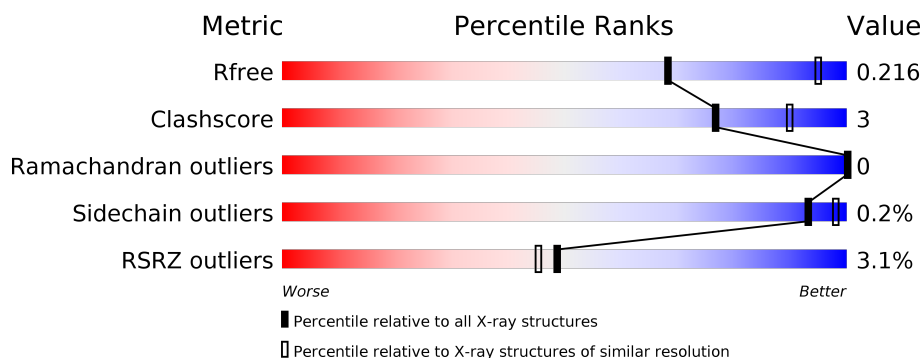
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	257	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	B	257	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 4687 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.

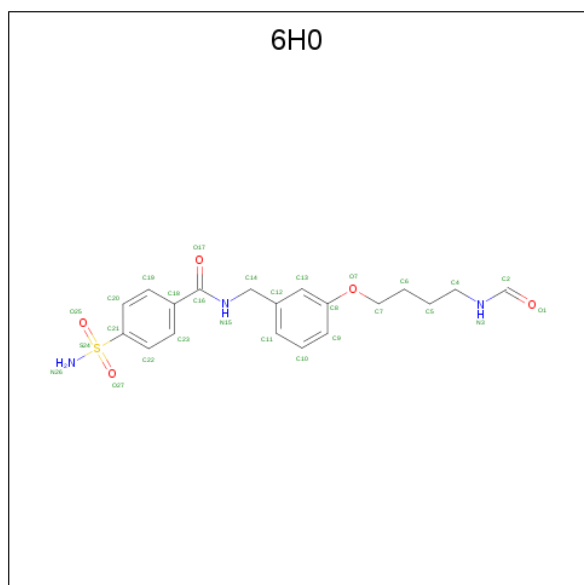
- Molecule 1 is a protein called Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1994	1278	339	375	2			
1	B	257	Total	C	N	O	S	0	0	0
			2002	1284	340	376	2			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

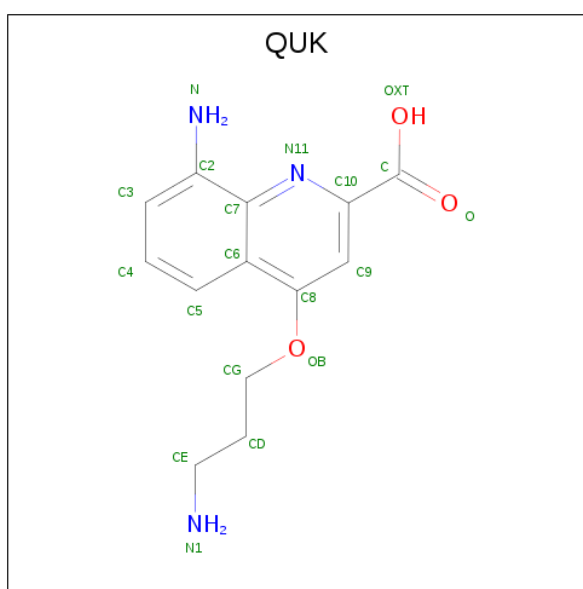
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is {N}-[[3-(4-formamidobutoxy)phenyl]methyl]-4-sulfamoyl-benzamide (three-letter code: 6H0) (formula: C<sub>19</sub>H<sub>23</sub>N<sub>3</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
3	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
3	B	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
3	B	1	Total	C	N	O	S	0	0
			28	19	3	5	1		

- Molecule 4 is 8-azanyl-4-(3-azanylpropoxy)quinoline-2-carboxylic acid (three-letter code: QUK) (formula: C<sub>13</sub>H<sub>15</sub>N<sub>3</sub>O<sub>3</sub>).



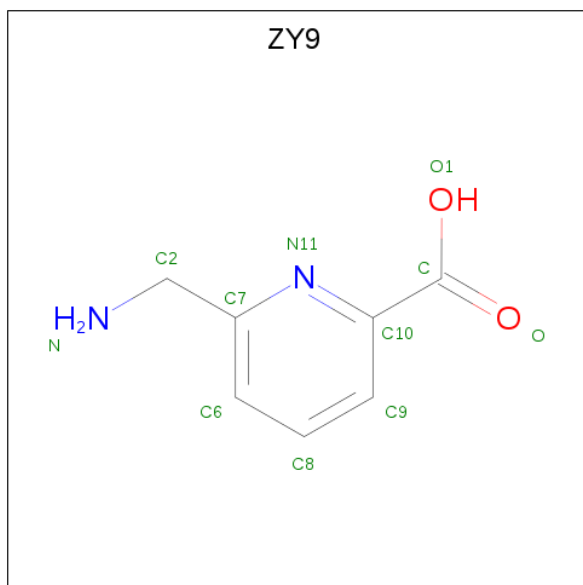
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	10	2	2		
4	A	1	Total	C	N	O	0	0
			19	13	3	3		
4	A	1	Total	C	N	O	0	0
			18	13	3	2		
4	A	1	Total	C	N	O	0	0
			19	13	3	3		
4	B	1	Total	C	N	O	0	0
			14	10	2	2		
4	B	1	Total	C	N	O	0	0
			19	13	3	3		
4	B	1	Total	C	N	O	0	0
			18	13	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			19	13	3	3		

- Molecule 5 is 6-(aminomethyl)pyridine-2-carboxylic acid (three-letter code: ZY9) (formula:  $C_7H_8N_2O_2$ ).



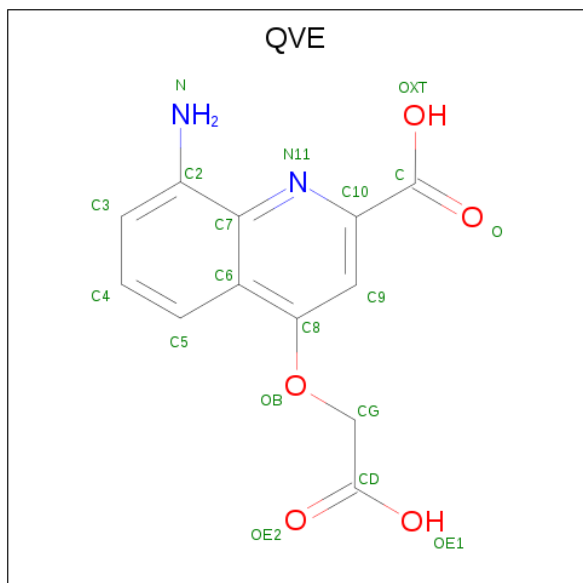
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	7	2	1		
5	A	1	Total	C	N	O	0	0
			10	7	2	1		
5	A	1	Total	C	N	O	0	0
			10	7	2	1		
5	A	1	Total	C	N	O	0	0
			10	7	2	1		
5	A	1	Total	C	N	O	0	0
			10	7	2	1		
5	B	1	Total	C	N	O	0	0
			10	7	2	1		
5	B	1	Total	C	N	O	0	0
			10	7	2	1		
5	B	1	Total	C	N	O	0	0
			10	7	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			10	7	2	1		
5	B	1	Total	C	N	O	0	0
			10	7	2	1		

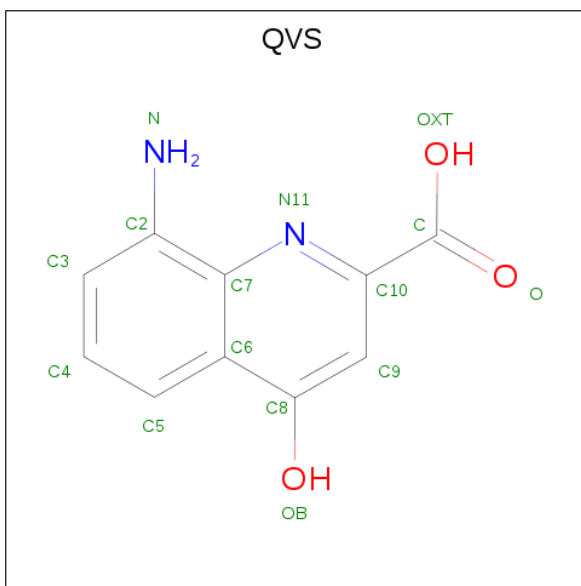
- Molecule 6 is 8-azanyl-4-(2-hydroxy-2-oxoethoxy)quinoline-2-carboxylic acid (three-letter code: QVE) (formula:  $C_{12}H_{10}N_2O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			18	12	2	4		
6	A	1	Total	C	N	O	0	0
			18	12	2	4		
6	A	1	Total	C	N	O	0	0
			18	12	2	4		
6	A	1	Total	C	N	O	0	0
			18	12	2	4		
6	B	1	Total	C	N	O	0	0
			18	12	2	4		
6	B	1	Total	C	N	O	0	0
			18	12	2	4		
6	B	1	Total	C	N	O	0	0
			18	12	2	4		
6	B	1	Total	C	N	O	0	0
			18	12	2	4		

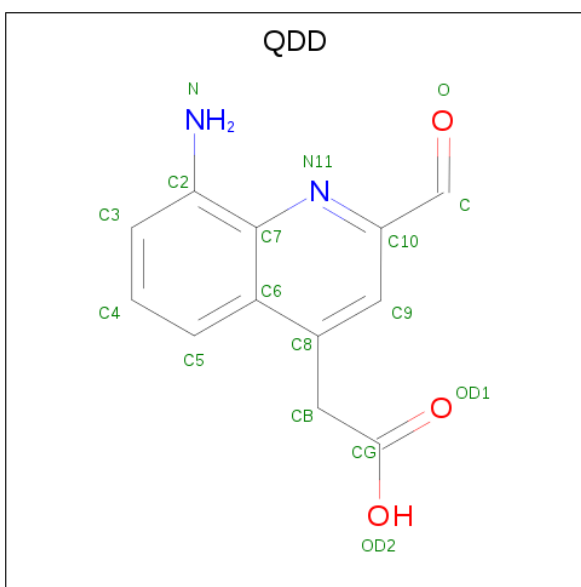
- Molecule 7 is 8-azanyl-4-oxidanyl-quinoline-2-carboxylic acid (three-letter code: QVS)

(formula:  $C_{10}H_8N_2O_3$ ).



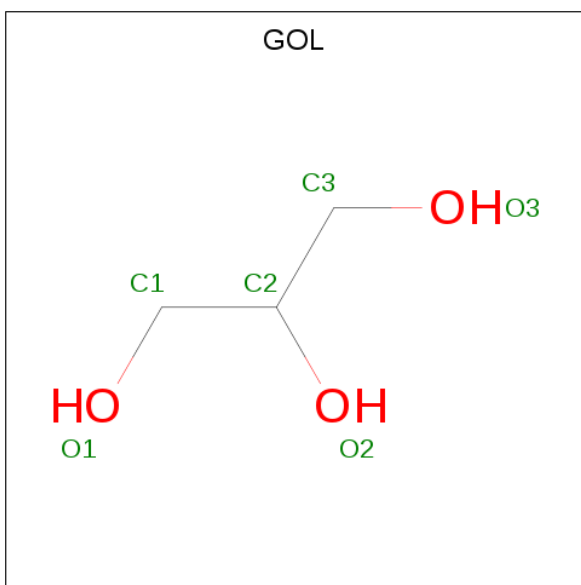
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	10	2	2		
7	A	1	Total	C	N	O	0	0
			14	10	2	2		
7	B	1	Total	C	N	O	0	0
			14	10	2	2		
7	B	1	Total	C	N	O	0	0
			14	10	2	2		

- Molecule 8 is 2-(8-azany-2-methanoyl-quinolin-4-yl)ethanoic acid (three-letter code: QDD) (formula:  $C_{12}H_{10}N_2O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			17	12	2	3		
8	A	1	Total	C	N	O	0	0
			17	12	2	3		
8	B	1	Total	C	N	O	0	0
			17	12	2	3		
8	B	1	Total	C	N	O	0	0
			17	12	2	3		

- Molecule 9 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
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		

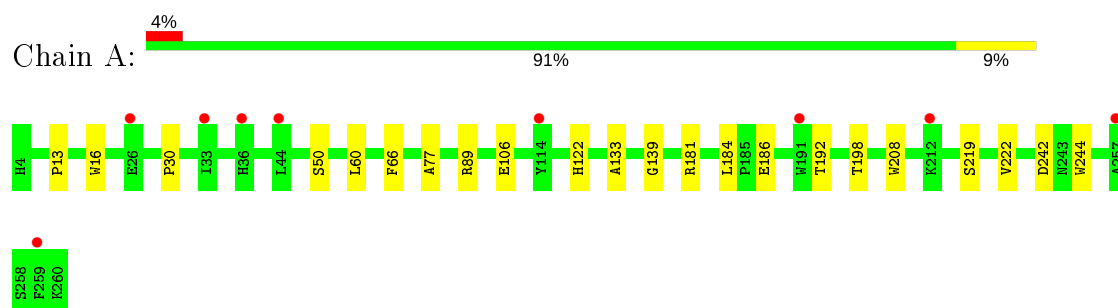
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	10	Total	O	0	0
			10	10		
10	B	15	Total	O	0	0
			15	15		

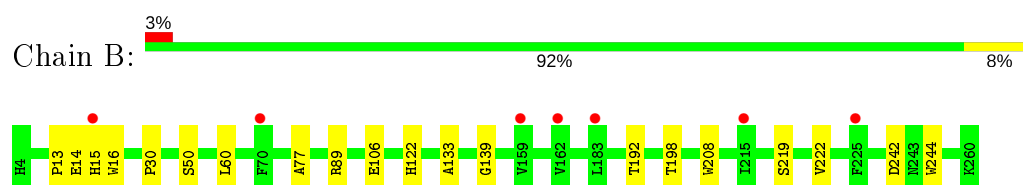
### 3 Residue-property plots [i](#)

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: Carbonic anhydrase 2



- Molecule 1: Carbonic anhydrase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.64Å 82.64Å 106.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.73 – 2.91 44.73 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.73-2.91) 99.5 (44.73-2.91)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.171 , 0.210 0.177 , 0.216	Depositor DCC
$R_{free}$ test set	785 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtriage
Anisotropy	0.847	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4687	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: GOL, ZN, QVE, QDD, 6H0, QUK, ZY9, QVS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.63	0/2054	0.74	0/2803
1	B	0.64	0/2063	0.73	0/2814
All	All	0.63	0/4117	0.73	0/5617

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	1994	0	1874	13	0
1	B	2002	0	1887	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	56	0	0	1	0
3	B	56	0	0	1	0
4	A	70	0	0	0	0
4	B	70	0	0	0	0
5	A	60	0	0	0	0
5	B	60	0	0	0	0
6	A	72	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	72	0	0	0	0
7	A	28	0	0	0	0
7	B	28	0	0	0	0
8	A	34	0	0	0	0
8	B	34	0	0	0	0
9	A	12	0	16	0	0
9	B	12	0	16	0	0
10	A	10	0	0	0	0
10	B	15	0	0	0	0
All	All	4687	0	3793	25	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 3.

All (25) 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:219:SER:HA	1:B:222:VAL:HG12	1.92	0.52
1:A:219:SER:HA	1:A:222:VAL:HG12	1.92	0.51
1:A:50:SER:O	1:A:77:ALA:HA	2.11	0.50
1:A:242:ASP:HA	1:A:244:TRP:CD1	2.47	0.50
1:A:60:LEU:HD12	1:A:60:LEU:O	2.13	0.48
1:B:242:ASP:HA	1:B:244:TRP:CD1	2.48	0.48
1:B:89:ARG:O	1:B:122:HIS:HA	2.13	0.48
1:B:198:THR:OG1	3:B:302:6H0:N26	2.47	0.48
1:A:89:ARG:O	1:A:122:HIS:HA	2.13	0.48
1:A:198:THR:OG1	3:A:302:6H0:N26	2.48	0.47
1:B:14:GLU:HG2	1:B:15:HIS:CD2	2.50	0.47
1:A:60:LEU:HD12	1:A:60:LEU:C	2.36	0.46
1:B:50:SER:O	1:B:77:ALA:HA	2.17	0.45
1:B:60:LEU:O	1:B:60:LEU:HD12	2.16	0.45
1:A:192:THR:HA	1:A:208:TRP:O	2.17	0.45
1:B:192:THR:HA	1:B:208:TRP:O	2.17	0.44
1:B:13:PRO:HA	1:B:16:TRP:CD2	2.53	0.43
1:A:181:ARG:HA	1:A:184:LEU:HD12	2.01	0.43
1:B:60:LEU:HD12	1:B:60:LEU:C	2.38	0.42
1:A:30:PRO:HG3	1:A:106:GLU:HB3	2.02	0.42
1:A:13:PRO:HA	1:A:16:TRP:CD2	2.55	0.41
1:A:60:LEU:O	1:A:66:PHE:HA	2.20	0.41
1:B:133:ALA:O	1:B:139:GLY:HA3	2.20	0.41
1:A:133:ALA:O	1:A:139:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:PRO:HG3	1:B:106:GLU:HB3	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	255/257 (99%)	243 (95%)	12 (5%)	0	100	100
1	B	255/257 (99%)	243 (95%)	12 (5%)	0	100	100
All	All	510/514 (99%)	486 (95%)	24 (5%)	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	208/222 (94%)	207 (100%)	1 (0%)	88	96
1	B	210/222 (95%)	210 (100%)	0	100	100
All	All	418/444 (94%)	417 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 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
5	ZY9	A	309	8,6	10,10,11	4.19	2 (20%)	11,12,14	2.62	4 (36%)
4	QUK	B	321	6	17,20,20	0.80	0	20,27,27	2.18	5 (25%)
5	ZY9	B	314	4,6	10,10,11	4.37	2 (20%)	11,12,14	2.22	4 (36%)
5	ZY9	B	304	4,6	10,10,11	4.18	2 (20%)	11,12,14	2.40	4 (36%)
5	ZY9	A	304	4,6	10,10,11	4.31	2 (20%)	11,12,14	2.26	4 (36%)
7	QVS	B	316	5,6	15,15,16	2.36	2 (13%)	19,21,23	2.37	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ZY9	A	307	8,7	10,10,11	4.38	2 (20%)	11,12,14	2.14	5 (45%)
5	ZY9	B	309	8,6	10,10,11	4.23	2 (20%)	11,12,14	2.45	4 (36%)
6	QVE	B	315	5,7	16,19,20	2.37	1 (6%)	20,26,28	2.23	6 (30%)
8	QDD	B	308	5	15,18,18	1.85	3 (20%)	19,25,25	2.80	5 (26%)
6	QVE	B	320	5,4	16,19,20	1.94	1 (6%)	20,26,28	2.56	8 (40%)
3	6H0	A	312	4	29,29,29	2.33	5 (17%)	37,38,38	1.63	5 (13%)
8	QDD	A	318	5	15,18,18	2.13	3 (20%)	19,25,25	2.32	5 (26%)
8	QDD	A	308	5	15,18,18	2.16	2 (13%)	19,25,25	2.68	6 (31%)
4	QUK	B	313	3,5	19,19,20	2.08	2 (10%)	22,25,27	4.70	11 (50%)
5	ZY9	A	319	8,6	10,10,11	3.57	2 (20%)	11,12,14	2.29	4 (36%)
4	QUK	A	311	6	17,20,20	0.70	0	20,27,27	1.91	5 (25%)
7	QVS	A	306	5,6	15,15,16	2.55	1 (6%)	19,21,23	2.25	5 (26%)
9	GOL	B	322	-	5,5,5	0.11	0	5,5,5	0.31	0
3	6H0	B	302	2,4	29,29,29	1.97	5 (17%)	37,38,38	1.49	4 (10%)
9	GOL	B	323	-	5,5,5	0.09	0	5,5,5	0.29	0
5	ZY9	B	307	8,7	10,10,11	3.74	2 (20%)	11,12,14	2.22	5 (45%)
4	QUK	B	311	6	17,20,20	0.77	0	20,27,27	1.92	4 (20%)
6	QVE	A	305	5,7	16,19,20	2.11	1 (6%)	20,26,28	2.25	6 (30%)
6	QVE	A	320	5,4	16,19,20	2.10	1 (6%)	20,26,28	2.49	5 (25%)
5	ZY9	B	319	8,6	10,10,11	3.36	2 (20%)	11,12,14	2.31	6 (54%)
5	ZY9	B	317	8,7	10,10,11	4.40	2 (20%)	11,12,14	2.24	4 (36%)
5	ZY9	A	317	8,7	10,10,11	4.36	2 (20%)	11,12,14	1.86	4 (36%)
5	ZY9	A	314	4,6	10,10,11	4.47	2 (20%)	11,12,14	1.92	4 (36%)
6	QVE	A	310	5,4	16,19,20	2.11	1 (6%)	20,26,28	2.14	6 (30%)
9	GOL	A	322	-	5,5,5	0.10	0	5,5,5	0.26	0
6	QVE	A	315	5,7	16,19,20	2.57	1 (6%)	20,26,28	2.03	4 (20%)
9	GOL	A	323	-	5,5,5	0.12	0	5,5,5	0.39	0
4	QUK	B	303	3,5	15,15,20	2.35	1 (6%)	19,21,27	2.42	5 (26%)
7	QVS	B	306	5,6	15,15,16	2.48	1 (6%)	19,21,23	2.16	5 (26%)
4	QUK	A	313	3,5	19,19,20	2.06	2 (10%)	22,25,27	4.59	11 (50%)
4	QUK	A	321	6	17,20,20	0.80	0	20,27,27	1.80	3 (15%)
6	QVE	B	310	5,4	16,19,20	1.67	2 (12%)	20,26,28	2.25	5 (25%)
8	QDD	B	318	5	15,18,18	1.83	2 (13%)	19,25,25	2.35	4 (21%)
6	QVE	B	305	5,7	16,19,20	2.36	1 (6%)	20,26,28	1.98	5 (25%)
7	QVS	A	316	5,6	15,15,16	2.34	1 (6%)	19,21,23	2.37	5 (26%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	6H0	B	312	4	29,29,29	2.18	5 (17%)	37,38,38	1.47	5 (13%)
3	6H0	A	302	2,4	29,29,29	2.12	5 (17%)	37,38,38	1.32	6 (16%)
4	QUK	A	303	3,5	15,15,20	1.91	2 (13%)	19,21,27	2.95	6 (31%)

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
5	ZY9	A	309	8,6	-	2/4/4/6	0/1/1/1
4	QUK	B	321	6	-	0/5/9/9	0/2/2/2
5	ZY9	B	314	4,6	-	0/4/4/6	0/1/1/1
5	ZY9	B	304	4,6	-	0/4/4/6	0/1/1/1
5	ZY9	A	304	4,6	-	0/4/4/6	0/1/1/1
7	QVS	B	316	5,6	-	0/2/2/4	0/2/2/2
5	ZY9	A	307	8,7	-	0/4/4/6	0/1/1/1
5	ZY9	B	309	8,6	-	2/4/4/6	0/1/1/1
6	QVE	B	315	5,7	-	3/5/7/9	0/2/2/2
8	QDD	B	308	5	-	2/4/6/6	0/2/2/2
6	QVE	B	320	5,4	-	2/5/7/9	0/2/2/2
3	6H0	A	312	4	-	6/23/23/23	0/2/2/2
8	QDD	A	318	5	-	2/4/6/6	0/2/2/2
8	QDD	A	308	5	-	0/4/6/6	0/2/2/2
4	QUK	B	313	3,5	-	2/7/7/9	0/2/2/2
5	ZY9	A	319	8,6	-	0/4/4/6	0/1/1/1
4	QUK	A	311	6	-	1/5/9/9	0/2/2/2
7	QVS	A	306	5,6	-	2/2/2/4	0/2/2/2
9	GOL	B	322	-	-	2/4/4/4	-
3	6H0	B	302	2,4	-	8/23/23/23	0/2/2/2
9	GOL	B	323	-	-	0/4/4/4	-
5	ZY9	B	307	8,7	-	0/4/4/6	0/1/1/1
4	QUK	B	311	6	-	2/5/9/9	0/2/2/2
6	QVE	A	305	5,7	-	3/5/7/9	0/2/2/2
6	QVE	A	320	5,4	-	3/5/7/9	0/2/2/2
5	ZY9	B	319	8,6	-	1/4/4/6	0/1/1/1
5	ZY9	B	317	8,7	-	0/4/4/6	0/1/1/1
5	ZY9	A	317	8,7	-	0/4/4/6	0/1/1/1
5	ZY9	A	314	4,6	-	0/4/4/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	QVE	A	310	5,4	-	2/5/7/9	0/2/2/2
9	GOL	A	322	-	-	0/4/4/4	-
6	QVE	A	315	5,7	-	2/5/7/9	0/2/2/2
9	GOL	A	323	-	-	1/4/4/4	-
4	QUK	B	303	3,5	-	0/2/2/9	0/2/2/2
7	QVS	B	306	5,6	-	1/2/2/4	0/2/2/2
4	QUK	A	313	3,5	-	3/7/7/9	0/2/2/2
4	QUK	A	321	6	-	1/5/9/9	0/2/2/2
6	QVE	B	310	5,4	-	0/5/7/9	0/2/2/2
8	QDD	B	318	5	-	2/4/6/6	0/2/2/2
6	QVE	B	305	5,7	-	0/5/7/9	0/2/2/2
7	QVS	A	316	5,6	-	2/2/2/4	0/2/2/2
3	6H0	B	312	4	-	6/23/23/23	0/2/2/2
3	6H0	A	302	2,4	-	8/23/23/23	0/2/2/2
4	QUK	A	303	3,5	-	0/2/2/9	0/2/2/2

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	314	ZY9	C2-C7	-12.48	1.36	1.51
5	A	314	ZY9	C2-C7	-12.16	1.37	1.51
5	A	304	ZY9	C2-C7	-11.77	1.37	1.51
5	A	307	ZY9	C2-C7	-11.45	1.38	1.51
5	B	309	ZY9	C2-C7	-11.19	1.38	1.51
5	A	317	ZY9	C2-C7	-11.19	1.38	1.51
5	B	317	ZY9	C2-C7	-11.16	1.38	1.51
5	B	304	ZY9	C2-C7	-10.64	1.39	1.51
5	A	309	ZY9	C2-C7	-10.52	1.39	1.51
6	A	315	QVE	C10-C	-9.57	1.38	1.48
7	A	306	QVS	C10-C	-9.40	1.38	1.48
5	A	319	ZY9	C2-C7	-9.18	1.40	1.51
5	B	307	ZY9	C2-C7	-9.05	1.40	1.51
5	B	319	ZY9	C2-C7	-8.92	1.41	1.51
6	B	315	QVE	C10-C	-8.79	1.39	1.48
7	B	306	QVS	C10-C	-8.68	1.39	1.48
6	B	305	QVE	C10-C	-8.46	1.39	1.48
4	B	303	QUK	C10-C	-8.32	1.39	1.48
7	B	316	QVS	C10-C	-8.27	1.39	1.48
5	B	317	ZY9	C10-C	-8.10	1.40	1.48
7	A	316	QVS	C10-C	-8.09	1.40	1.48
5	A	309	ZY9	C10-C	-7.93	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	317	ZY9	C10-C	-7.89	1.40	1.48
5	A	307	ZY9	C10-C	-7.74	1.40	1.48
5	B	304	ZY9	C10-C	-7.74	1.40	1.48
6	A	305	QVE	C10-C	-7.63	1.40	1.48
6	A	310	QVE	C10-C	-7.53	1.40	1.48
4	B	313	QUK	C10-C	-7.41	1.40	1.48
6	A	320	QVE	C10-C	-7.35	1.40	1.48
5	B	307	ZY9	C10-C	-7.28	1.41	1.48
8	A	308	QDD	C10-C	-7.26	1.41	1.48
5	B	309	ZY9	C10-C	-7.20	1.41	1.48
5	A	314	ZY9	C10-C	-7.15	1.41	1.48
6	B	320	QVE	C10-C	-7.06	1.41	1.48
4	A	313	QUK	C10-C	-6.91	1.41	1.48
5	A	304	ZY9	C10-C	-6.62	1.41	1.48
8	A	318	QDD	C10-C	-6.59	1.41	1.48
3	A	312	6H0	C21-S24	6.51	1.87	1.77
3	A	302	6H0	C21-S24	-6.48	1.66	1.77
5	A	319	ZY9	C10-C	-6.38	1.41	1.48
4	A	303	QUK	C10-C	-6.28	1.42	1.48
5	B	314	ZY9	C10-C	-5.89	1.42	1.48
3	A	312	6H0	O27-S24	5.73	1.54	1.43
3	A	312	6H0	O25-S24	5.65	1.54	1.43
5	B	319	ZY9	C10-C	-5.63	1.42	1.48
8	B	308	QDD	C10-C	-5.61	1.42	1.48
3	B	312	6H0	O27-S24	5.59	1.54	1.43
3	B	302	6H0	C14-C12	-5.56	1.39	1.51
6	B	310	QVE	C10-C	-5.33	1.43	1.48
3	B	312	6H0	C21-S24	5.31	1.85	1.77
8	B	318	QDD	C10-C	-5.30	1.43	1.48
3	B	312	6H0	O25-S24	5.02	1.53	1.43
4	A	313	QUK	C10-N11	5.02	1.38	1.33
3	A	302	6H0	C14-C12	-4.84	1.40	1.51
3	B	302	6H0	O27-S24	4.76	1.52	1.43
3	B	312	6H0	C14-C12	-4.76	1.41	1.51
3	A	302	6H0	O25-S24	4.66	1.52	1.43
3	B	302	6H0	O25-S24	4.63	1.52	1.43
4	B	313	QUK	C10-N11	4.46	1.37	1.33
3	A	312	6H0	C14-C12	-4.42	1.41	1.51
3	B	302	6H0	C18-C16	-4.25	1.41	1.50
3	A	302	6H0	O27-S24	4.21	1.51	1.43
3	A	302	6H0	C18-C16	-4.06	1.41	1.50
3	B	312	6H0	C18-C16	-4.00	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	312	6H0	C18-C16	-3.90	1.42	1.50
3	B	302	6H0	C21-S24	-3.68	1.71	1.77
8	A	308	QDD	CB-C8	-2.84	1.41	1.52
8	A	318	QDD	C9-C8	2.69	1.42	1.37
8	B	308	QDD	CB-C8	-2.62	1.42	1.52
8	A	318	QDD	CB-C8	-2.57	1.42	1.52
8	B	318	QDD	CB-C8	-2.53	1.42	1.52
6	B	310	QVE	C10-N11	2.43	1.35	1.33
8	B	308	QDD	C9-C8	2.39	1.41	1.37
7	B	316	QVS	C10-N11	2.20	1.35	1.33
4	A	303	QUK	C10-N11	2.18	1.35	1.33

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	313	QUK	C-C10-N11	11.85	126.27	114.66
4	A	313	QUK	C-C10-N11	11.48	125.92	114.66
8	B	308	QDD	C10-N11-C7	8.93	124.89	118.11
4	B	313	QUK	C9-C10-C	-8.89	113.54	121.23
4	A	313	QUK	C7-C2-N	8.81	134.86	118.07
6	B	320	QVE	C10-N11-C7	8.51	124.56	118.11
4	B	313	QUK	C7-C2-N	8.47	134.22	118.07
4	A	313	QUK	C9-C10-C	-8.14	114.19	121.23
6	A	320	QVE	C10-N11-C7	8.10	124.25	118.11
8	A	308	QDD	C10-N11-C7	7.92	124.11	118.11
6	A	305	QVE	C10-N11-C7	7.71	123.96	118.11
4	A	313	QUK	C2-C7-N11	7.63	126.19	118.64
4	B	313	QUK	C2-C7-N11	7.58	126.14	118.64
8	B	318	QDD	C10-N11-C7	7.52	123.81	118.11
4	A	303	QUK	C10-N11-C7	7.51	123.81	118.11
4	A	313	QUK	C3-C2-N	-7.08	106.21	120.36
4	B	313	QUK	C3-C2-N	-6.91	106.56	120.36
4	B	321	QUK	C10-N11-C7	6.90	123.56	118.26
8	A	318	QDD	C10-N11-C7	6.82	123.28	118.11
4	A	303	QUK	C-C10-N11	6.74	121.27	114.66
6	A	315	QVE	C10-N11-C7	6.52	123.05	118.11
6	B	310	QVE	C10-N11-C7	6.51	123.05	118.11
7	A	306	QVS	C10-N11-C7	6.47	123.02	118.11
7	B	316	QVS	C-C10-N11	6.33	120.86	114.66
6	B	315	QVE	C10-N11-C7	6.27	122.86	118.11
6	A	310	QVE	C10-N11-C7	6.25	122.85	118.11
4	A	311	QUK	C10-N11-C7	6.23	123.04	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	308	QDD	C-C10-N11	6.15	120.69	114.66
3	A	312	6H0	O25-S24-O27	-6.03	108.85	118.76
7	A	316	QVS	C-C10-N11	6.01	120.55	114.66
6	B	305	QVE	C10-N11-C7	5.85	122.55	118.11
8	A	308	QDD	C-C10-N11	5.80	120.35	114.66
4	B	311	QUK	C10-N11-C7	5.73	122.65	118.26
4	A	321	QUK	C10-N11-C7	5.49	122.47	118.26
7	B	316	QVS	C10-N11-C7	5.48	122.26	118.11
4	B	313	QUK	O-C-C10	-5.45	119.06	124.22
7	A	316	QVS	C10-N11-C7	5.45	122.24	118.11
7	B	306	QVS	C-C10-N11	5.34	119.89	114.66
3	B	312	6H0	O25-S24-O27	-5.33	110.00	118.76
4	B	303	QUK	C-C10-N11	5.28	119.83	114.66
4	A	303	QUK	OB-C8-C6	5.26	122.88	116.31
5	B	314	ZY9	O-C-C10	-5.18	119.31	124.22
5	B	304	ZY9	O-C-C10	-5.18	119.32	124.22
4	B	303	QUK	O-C-C10	-5.05	119.44	124.22
7	B	306	QVS	C10-N11-C7	5.05	121.94	118.11
5	A	309	ZY9	O-C-C10	-5.03	119.45	124.22
6	B	310	QVE	C-C10-N11	4.94	119.50	114.66
3	B	302	6H0	O25-S24-O27	-4.88	110.74	118.76
4	A	313	QUK	O-C-C10	-4.87	119.61	124.22
4	B	313	QUK	C10-N11-C7	4.58	121.58	118.11
8	A	318	QDD	C-C10-N11	4.57	119.14	114.66
5	B	309	ZY9	O-C-C10	-4.57	119.90	124.22
4	B	303	QUK	C10-N11-C7	4.54	121.55	118.11
5	A	304	ZY9	O-C-C10	-4.53	119.93	124.22
7	A	306	QVS	C-C10-N11	4.39	118.96	114.66
4	B	303	QUK	OB-C8-C6	4.38	121.78	116.31
8	B	318	QDD	C-C10-N11	4.26	118.84	114.66
6	A	320	QVE	O-C-C10	-4.17	120.27	124.22
4	A	313	QUK	C10-N11-C7	4.14	121.24	118.11
5	A	309	ZY9	C6-C7-N11	-4.13	117.17	122.41
5	A	314	ZY9	O-C-C10	-3.98	120.45	124.22
4	A	303	QUK	O-C-C10	-3.93	120.50	124.22
4	B	311	QUK	C9-C10-N11	-3.90	118.68	122.23
5	B	307	ZY9	C10-N11-C7	3.89	124.00	118.41
7	A	316	QVS	O-C-C10	-3.88	120.55	124.22
3	B	302	6H0	O1-C2-N3	-3.82	121.03	124.89
3	A	302	6H0	O27-S24-N26	3.81	113.01	107.36
5	A	319	ZY9	C6-C7-N11	-3.77	117.63	122.41
6	B	315	QVE	C3-C2-N	3.71	127.78	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	315	QVE	CG-OB-C8	-3.69	112.37	117.56
5	A	307	ZY9	O-C-C10	-3.67	120.74	124.22
5	A	319	ZY9	C10-N11-C7	3.67	123.69	118.41
5	A	304	ZY9	C2-C7-N11	3.63	122.06	115.89
3	A	312	6H0	O1-C2-N3	-3.63	121.22	124.89
6	B	305	QVE	CG-OB-C8	-3.63	112.46	117.56
5	A	309	ZY9	C10-N11-C7	3.61	123.61	118.41
3	A	302	6H0	O25-S24-O27	-3.61	112.82	118.76
5	B	309	ZY9	C6-C7-N11	-3.61	117.83	122.41
5	B	317	ZY9	O-C-C10	-3.60	120.81	124.22
7	B	316	QVS	O-C-C10	-3.58	120.83	124.22
5	B	304	ZY9	C2-C7-N11	3.58	121.98	115.89
5	B	317	ZY9	C10-N11-C7	3.52	123.48	118.41
5	B	319	ZY9	C10-N11-C7	3.52	123.47	118.41
5	B	309	ZY9	C2-C7-N11	3.50	121.84	115.89
4	B	321	QUK	C3-C2-N	3.47	127.31	120.36
4	B	321	QUK	C9-C10-N11	-3.41	119.12	122.23
5	A	307	ZY9	C10-N11-C7	3.41	123.32	118.41
5	A	319	ZY9	C2-C7-N11	3.39	121.65	115.89
5	B	317	ZY9	C6-C7-N11	-3.37	118.14	122.41
6	B	310	QVE	C3-C2-N	3.34	127.04	120.36
7	A	316	QVS	C3-C2-N	3.34	127.03	120.36
6	A	310	QVE	O-C-C10	-3.31	121.08	124.22
4	B	311	QUK	C3-C2-N	3.29	126.94	120.36
5	B	319	ZY9	O-C-C10	-3.27	121.13	124.22
5	A	319	ZY9	O-C-C10	-3.26	121.13	124.22
4	A	313	QUK	C5-C6-C8	-3.26	115.08	122.58
5	A	317	ZY9	O-C-C10	-3.25	121.14	124.22
6	A	310	QVE	C3-C2-N	3.24	126.85	120.36
6	B	315	QVE	O-C-C10	-3.21	121.19	124.22
5	B	309	ZY9	C10-N11-C7	3.16	122.96	118.41
8	A	308	QDD	O-C-C10	-3.16	121.23	124.22
8	B	318	QDD	C9-C10-C	3.16	123.96	121.23
6	B	320	QVE	C3-C2-N	3.15	126.66	120.36
7	B	306	QVS	C3-C2-N	3.14	126.65	120.36
5	B	317	ZY9	C2-C7-N11	3.14	121.23	115.89
6	B	320	QVE	C-C10-N11	3.14	117.74	114.66
6	A	320	QVE	C9-C10-C	3.13	123.94	121.23
6	B	320	QVE	O-C-C10	-3.13	121.25	124.22
5	B	307	ZY9	C6-C7-N11	-3.13	118.43	122.41
5	A	309	ZY9	C2-C7-N11	3.12	121.20	115.89
5	A	307	ZY9	C2-C7-N11	3.10	121.16	115.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	306	QVS	C3-C2-N	3.04	126.43	120.36
4	B	313	QUK	C5-C6-C8	-3.03	115.61	122.58
6	B	305	QVE	C3-C2-N	3.03	126.41	120.36
5	B	319	ZY9	C9-C10-N11	-3.02	118.14	122.47
5	B	319	ZY9	C2-C7-N11	3.00	120.99	115.89
7	B	316	QVS	C3-C2-N	2.97	126.30	120.36
4	A	311	QUK	C3-C2-N	2.97	126.29	120.36
5	A	304	ZY9	C10-N11-C7	2.96	122.67	118.41
5	B	307	ZY9	O-C-C10	-2.93	121.44	124.22
8	B	308	QDD	O-C-C10	-2.93	121.45	124.22
3	A	312	6H0	C8-C13-C12	2.92	122.95	119.73
6	B	310	QVE	O-C-C10	-2.91	121.47	124.22
7	B	306	QVS	O-C-C10	-2.89	121.49	124.22
5	B	307	ZY9	C2-C7-N11	2.88	120.79	115.89
6	A	320	QVE	C3-C2-N	2.87	126.10	120.36
3	A	302	6H0	O1-C2-N3	-2.86	122.00	124.89
6	A	305	QVE	C3-C2-N	2.85	126.05	120.36
6	A	315	QVE	O-C-C10	-2.84	121.53	124.22
4	A	321	QUK	C3-C2-N	2.83	126.02	120.36
3	B	312	6H0	O27-S24-C21	2.83	110.51	107.35
5	B	314	ZY9	C10-N11-C7	2.82	122.47	118.41
4	A	311	QUK	C9-C10-N11	-2.81	119.66	122.23
4	B	321	QUK	C7-C2-N	-2.80	112.72	118.07
3	B	312	6H0	O1-C2-N3	-2.80	122.06	124.89
6	A	310	QVE	C9-C10-C	2.80	123.64	121.23
5	B	314	ZY9	C9-C10-N11	-2.79	118.47	122.47
6	A	315	QVE	C3-C2-N	2.79	125.94	120.36
6	B	315	QVE	C-C10-N11	2.78	117.39	114.66
8	A	308	QDD	CG-CB-C8	-2.77	108.27	114.71
8	A	308	QDD	C3-C2-N	2.76	125.89	120.36
6	A	315	QVE	C-C10-N11	2.76	117.37	114.66
5	B	304	ZY9	C6-C7-N11	-2.74	118.94	122.41
5	B	307	ZY9	C9-C10-N11	-2.73	118.56	122.47
8	A	318	QDD	C3-C2-N	2.73	125.81	120.36
5	B	319	ZY9	C6-C7-N11	-2.69	118.99	122.41
4	A	321	QUK	CE-CD-CG	-2.66	104.12	113.61
4	B	313	QUK	CG-OB-C8	2.65	125.67	117.74
5	B	304	ZY9	C10-N11-C7	2.65	122.23	118.41
5	A	317	ZY9	C10-N11-C7	2.63	122.19	118.41
3	B	302	6H0	O27-S24-N26	2.62	111.25	107.36
5	B	319	ZY9	C9-C10-C	2.61	123.52	121.19
6	A	305	QVE	C9-C10-C	2.61	123.48	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	318	QDD	CG-CB-C8	-2.61	108.65	114.71
4	B	311	QUK	C7-C2-N	-2.58	113.14	118.07
7	B	306	QVS	C7-C2-N	-2.58	113.16	118.07
5	A	304	ZY9	C6-C7-N11	-2.56	119.16	122.41
3	B	302	6H0	O27-S24-C21	2.54	110.19	107.35
4	B	321	QUK	CE-CD-CG	-2.54	104.55	113.61
8	A	318	QDD	C9-C10-C	2.50	123.39	121.23
5	A	314	ZY9	C10-N11-C7	2.50	122.01	118.41
3	A	302	6H0	O25-S24-N26	-2.49	103.67	107.36
6	B	310	QVE	C7-C2-N	-2.48	113.34	118.07
4	B	313	QUK	C6-C7-N11	-2.48	117.67	122.78
6	B	305	QVE	C-C10-N11	2.47	117.09	114.66
6	A	305	QVE	C-C10-N11	2.47	117.08	114.66
6	A	305	QVE	O-C-C10	-2.46	121.89	124.22
5	A	307	ZY9	C9-C10-N11	-2.46	118.95	122.47
5	A	317	ZY9	C2-C7-N11	2.46	120.07	115.89
5	A	317	ZY9	C6-C7-N11	-2.46	119.29	122.41
4	A	313	QUK	C6-C7-N11	-2.46	117.71	122.78
7	A	316	QVS	C7-C2-N	-2.44	113.41	118.07
5	A	314	ZY9	C2-C7-N11	2.38	119.94	115.89
6	B	320	QVE	C7-C2-N	-2.36	113.57	118.07
5	B	314	ZY9	C2-C7-N11	2.36	119.89	115.89
6	A	310	QVE	C7-C2-N	-2.35	113.59	118.07
5	A	307	ZY9	C6-C7-N11	-2.32	119.47	122.41
6	B	305	QVE	C7-C2-N	-2.30	113.69	118.07
5	A	314	ZY9	C9-C10-N11	-2.28	119.20	122.47
7	A	306	QVS	OB-C8-C6	2.28	119.16	116.31
3	B	312	6H0	C12-C14-N15	-2.27	108.19	113.05
6	B	320	QVE	C9-C10-C	2.25	123.17	121.23
6	B	320	QVE	OB-CG-CD	-2.25	102.54	108.59
6	A	310	QVE	OB-CG-CD	-2.24	102.57	108.59
6	B	315	QVE	C7-C2-N	-2.23	113.81	118.07
4	A	303	QUK	C3-C2-N	2.23	124.81	120.36
4	A	311	QUK	C2-C7-N11	2.22	120.83	118.64
8	B	318	QDD	C3-C2-N	2.22	124.79	120.36
3	A	312	6H0	C12-C14-N15	-2.19	108.36	113.05
6	A	320	QVE	C7-C2-N	-2.17	113.92	118.07
8	B	308	QDD	C3-C2-N	2.16	124.68	120.36
4	B	303	QUK	C3-C2-N	2.15	124.67	120.36
7	A	306	QVS	O-C-C10	-2.13	122.20	124.22
3	A	302	6H0	C8-C13-C12	2.12	122.06	119.73
4	A	311	QUK	C7-C2-N	-2.12	114.03	118.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	312	6H0	C21-S24-N26	2.11	111.37	108.38
8	B	308	QDD	CG-CB-C8	-2.10	109.82	114.71
4	A	303	QUK	C8-C9-C10	2.09	121.09	119.05
3	A	302	6H0	O25-S24-C21	2.09	109.68	107.35
8	A	308	QDD	C7-C2-N	-2.08	114.10	118.07
4	B	313	QUK	OB-C8-C6	2.05	120.75	115.01
3	B	312	6H0	C8-C13-C12	2.03	121.96	119.73
4	A	313	QUK	CG-OB-C8	2.02	123.78	117.74
6	A	305	QVE	C7-C2-N	-2.01	114.23	118.07
6	B	320	QVE	C6-C7-N11	-2.01	118.63	122.78
4	A	313	QUK	C8-C6-C7	2.01	121.83	117.19

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	309	ZY9	O-C-C10-N11
5	A	309	ZY9	O-C-C10-C9
5	B	309	ZY9	O-C-C10-N11
5	B	309	ZY9	O-C-C10-C9
8	A	318	QDD	C9-C8-CB-CG
7	A	306	QVS	O-C-C10-C9
7	A	306	QVS	O-C-C10-N11
7	B	306	QVS	O-C-C10-C9
8	B	318	QDD	C9-C8-CB-CG
7	A	316	QVS	O-C-C10-C9
6	A	305	QVE	C6-C8-OB-CG
6	B	315	QVE	C9-C8-OB-CG
6	A	320	QVE	C6-C8-OB-CG
6	A	310	QVE	C6-C8-OB-CG
4	A	313	QUK	C6-C8-OB-CG
6	B	315	QVE	C6-C8-OB-CG
4	B	313	QUK	C6-C8-OB-CG
4	B	313	QUK	C9-C8-OB-CG
6	A	305	QVE	C9-C8-OB-CG
6	A	315	QVE	C6-C8-OB-CG
6	A	320	QVE	C9-C8-OB-CG
6	A	315	QVE	C9-C8-OB-CG
6	A	310	QVE	C9-C8-OB-CG
4	A	313	QUK	C9-C8-OB-CG
3	B	302	6H0	C5-C6-C7-O7
3	A	312	6H0	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
9	B	322	GOL	C1-C2-C3-O3
9	A	323	GOL	C1-C2-C3-O3
3	B	302	6H0	C9-C8-O7-C7
6	A	305	QVE	CD-CG-OB-C8
3	B	302	6H0	C13-C8-O7-C7
4	A	313	QUK	CG-CD-CE-N1
3	A	302	6H0	C20-C21-S24-N26
3	A	312	6H0	C6-C7-O7-C8
3	A	302	6H0	C9-C8-O7-C7
3	B	312	6H0	C5-C6-C7-O7
3	B	312	6H0	C6-C7-O7-C8
6	B	315	QVE	CD-CG-OB-C8
3	A	302	6H0	C13-C8-O7-C7
4	B	311	QUK	CE-CD-CG-OB
3	A	302	6H0	C20-C21-S24-O25
3	A	302	6H0	C22-C21-S24-O25
8	B	308	QDD	C9-C8-CB-CG
3	A	302	6H0	C22-C21-S24-N26
4	B	311	QUK	CG-CD-CE-N1
3	A	312	6H0	C9-C8-O7-C7
9	B	322	GOL	O2-C2-C3-O3
3	A	312	6H0	C13-C8-O7-C7
8	A	318	QDD	C6-C8-CB-CG
8	B	318	QDD	C6-C8-CB-CG
3	A	312	6H0	C5-C4-N3-C2
3	B	312	6H0	C5-C4-N3-C2
4	A	321	QUK	CE-CD-CG-OB
3	A	312	6H0	O1-C2-N3-C4
3	B	312	6H0	O1-C2-N3-C4
6	B	320	QVE	C6-C8-OB-CG
6	A	320	QVE	CD-CG-OB-C8
6	B	320	QVE	C9-C8-OB-CG
4	A	311	QUK	CG-CD-CE-N1
3	B	302	6H0	C20-C21-S24-O25
3	B	302	6H0	C22-C21-S24-O25
3	A	302	6H0	C5-C6-C7-O7
3	B	302	6H0	C5-C4-N3-C2
8	B	308	QDD	C6-C8-CB-CG
3	B	312	6H0	C9-C8-O7-C7
3	A	302	6H0	C5-C4-N3-C2
3	B	312	6H0	C13-C8-O7-C7
5	B	319	ZY9	O-C-C10-N11

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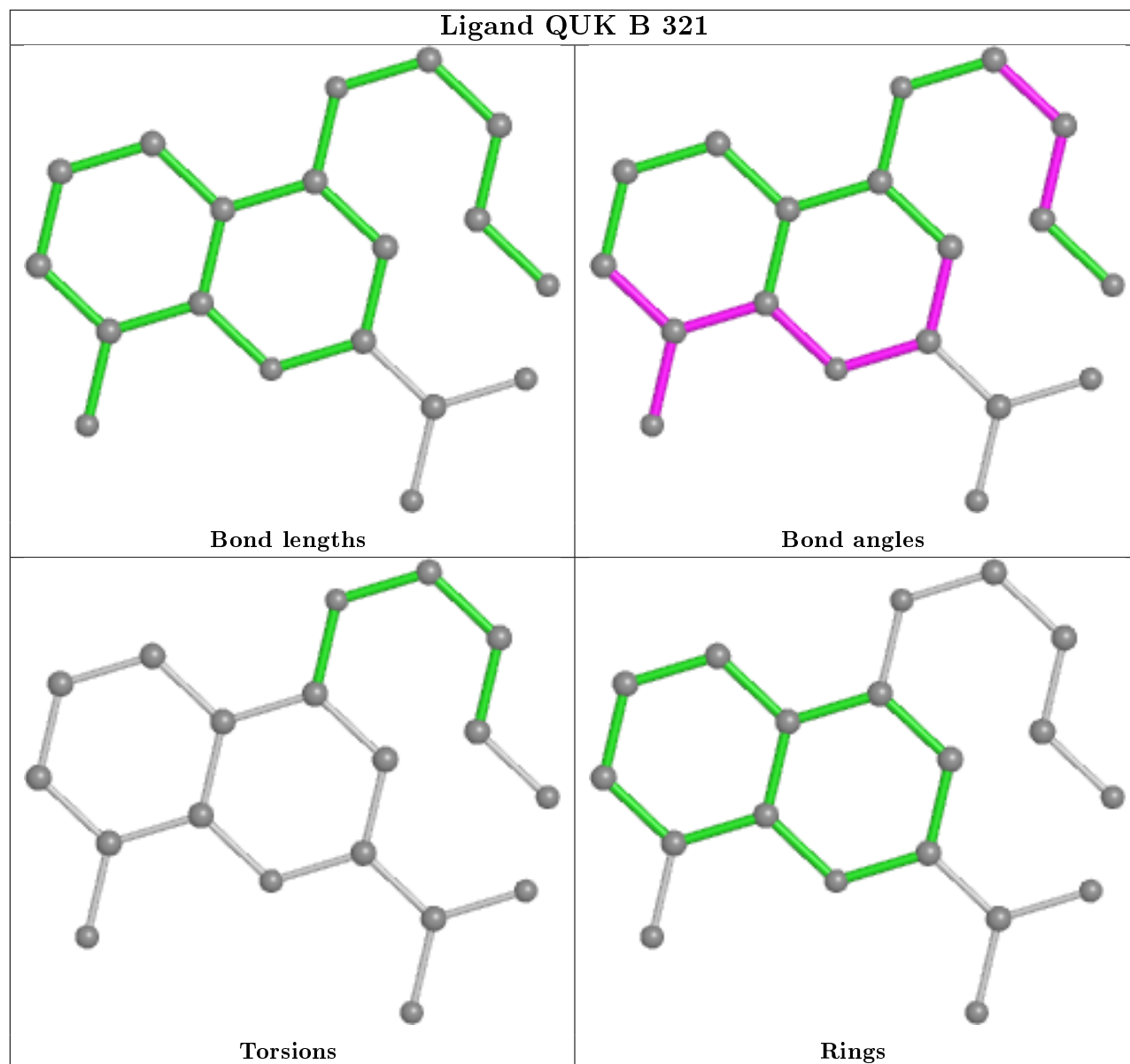
Mol	Chain	Res	Type	Atoms
7	A	316	QVS	O-C-C10-N11
3	B	302	6H0	C20-C21-S24-N26
3	B	302	6H0	C22-C21-S24-N26

There are no ring outliers.

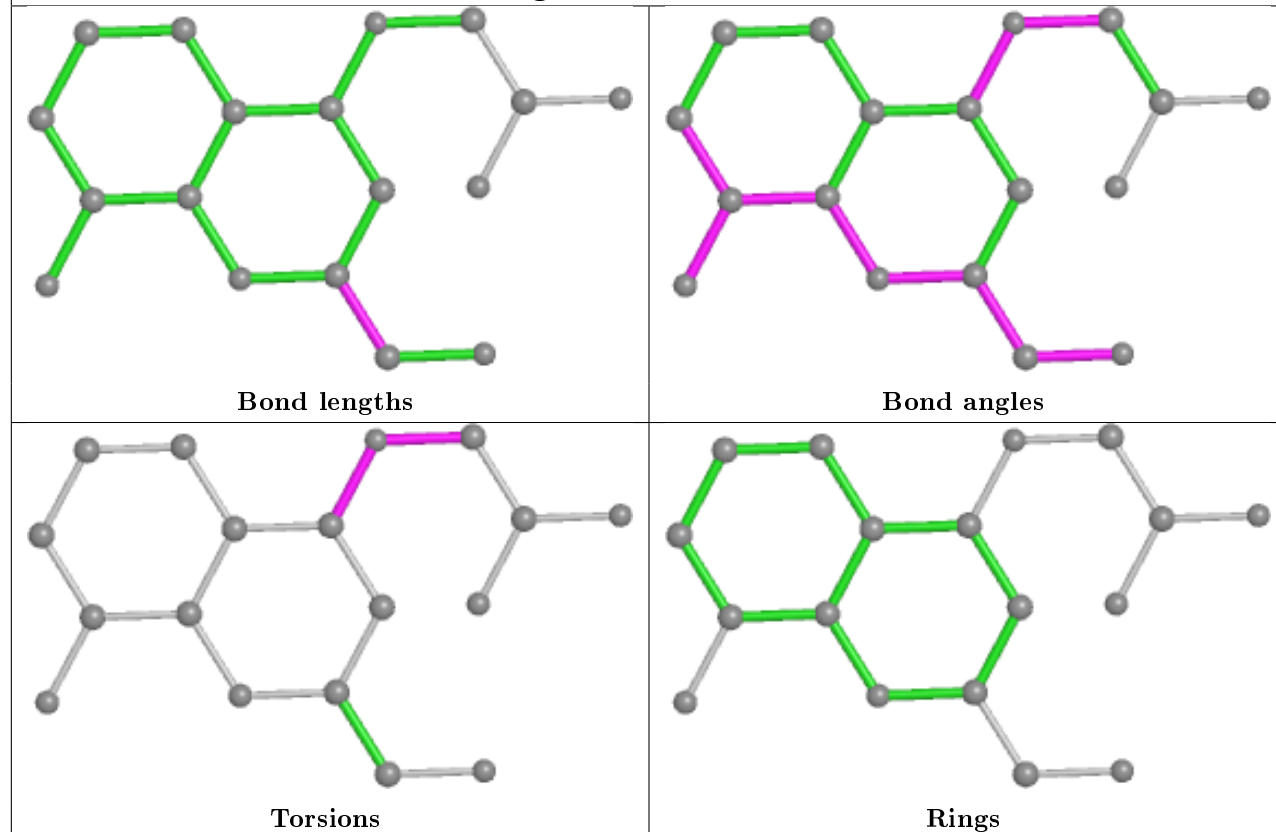
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	6H0	1	0
3	A	302	6H0	1	0

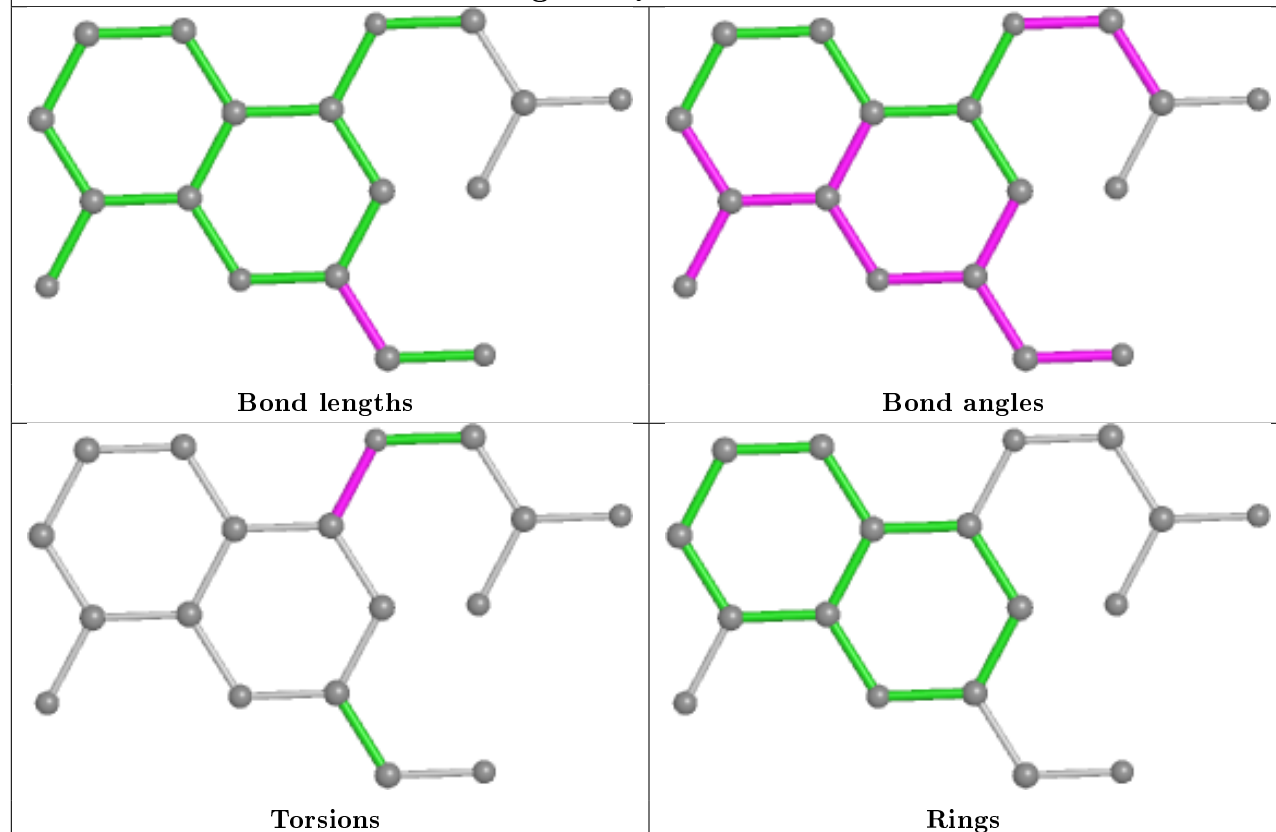
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

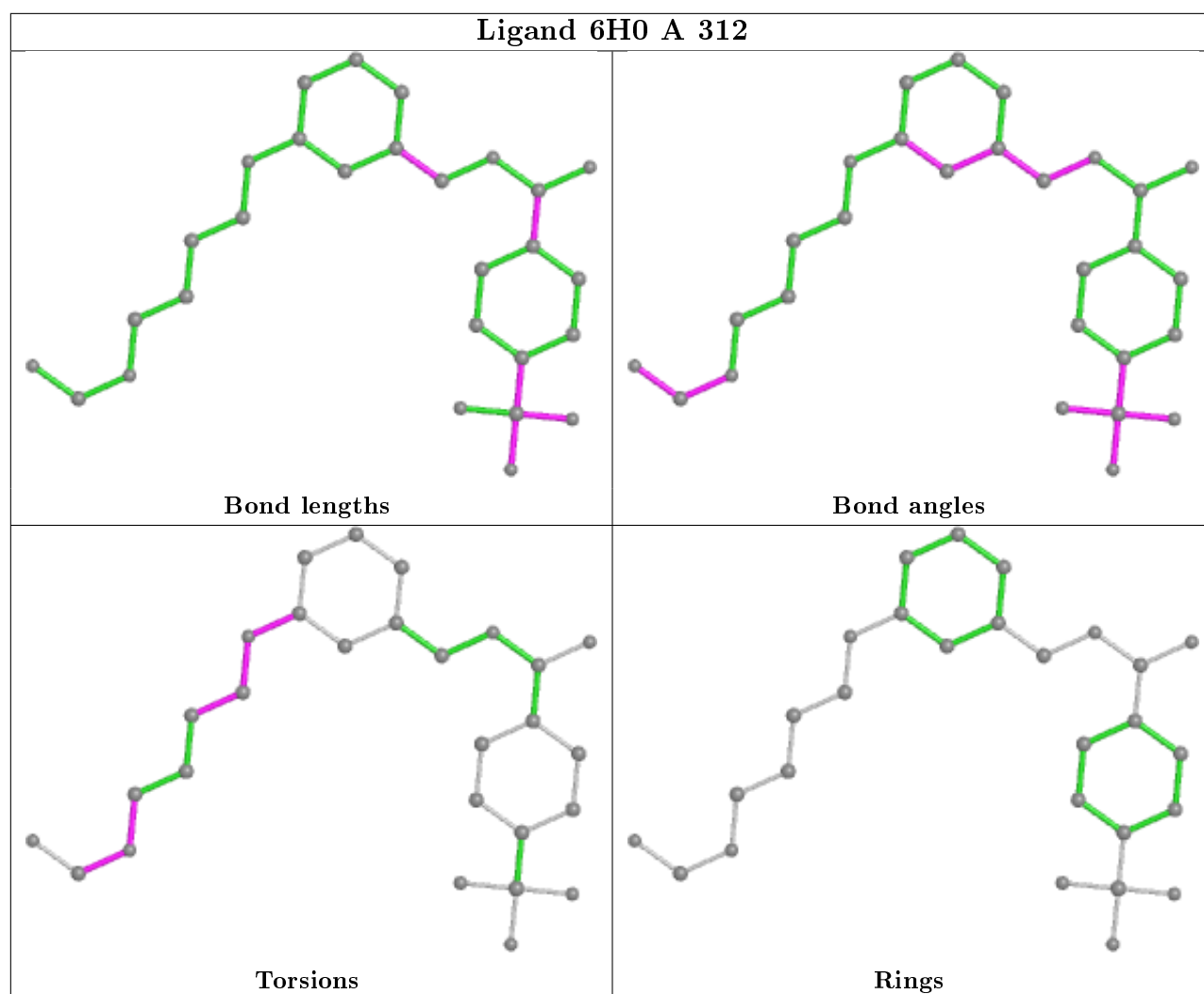


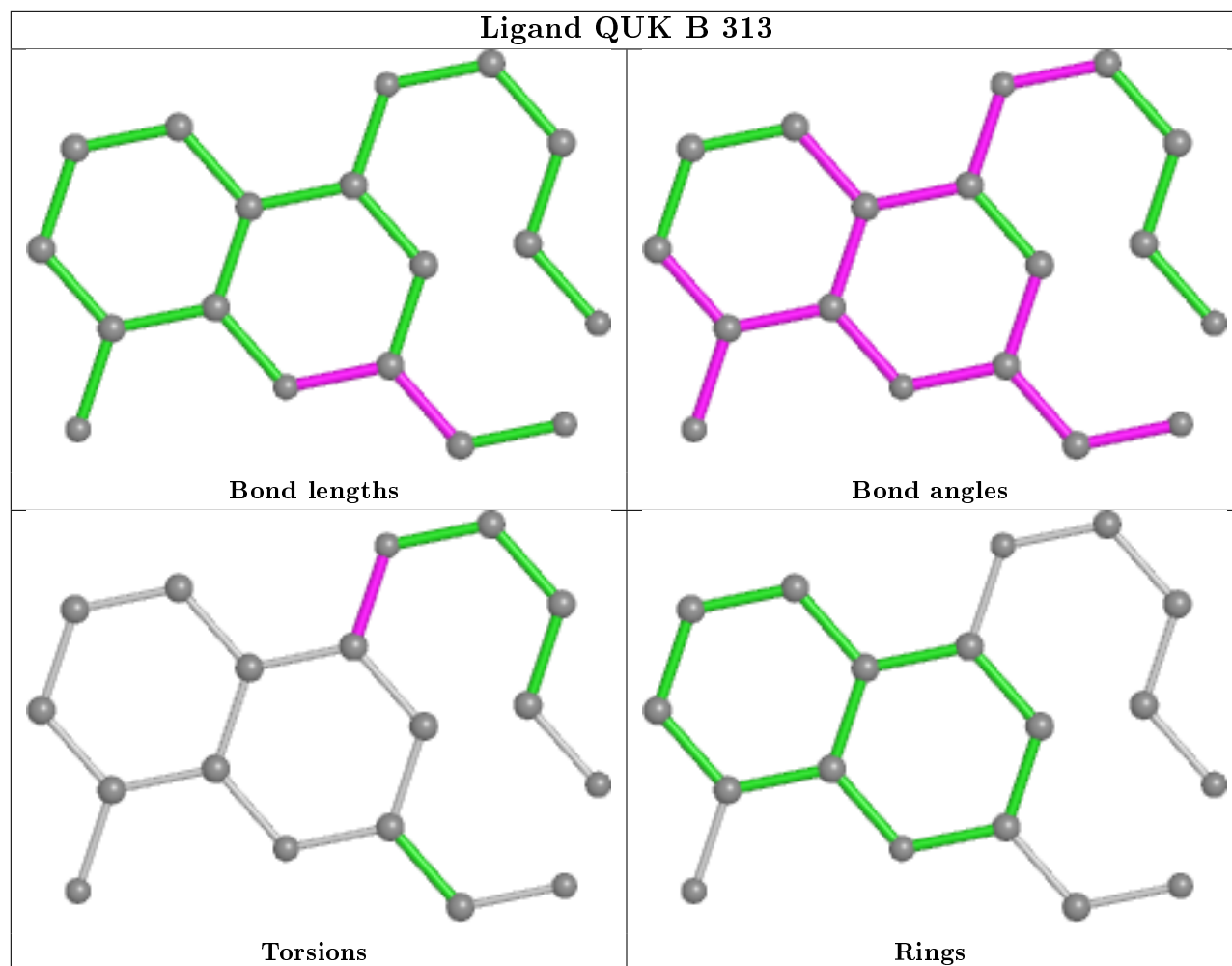
## Ligand QVE B 315

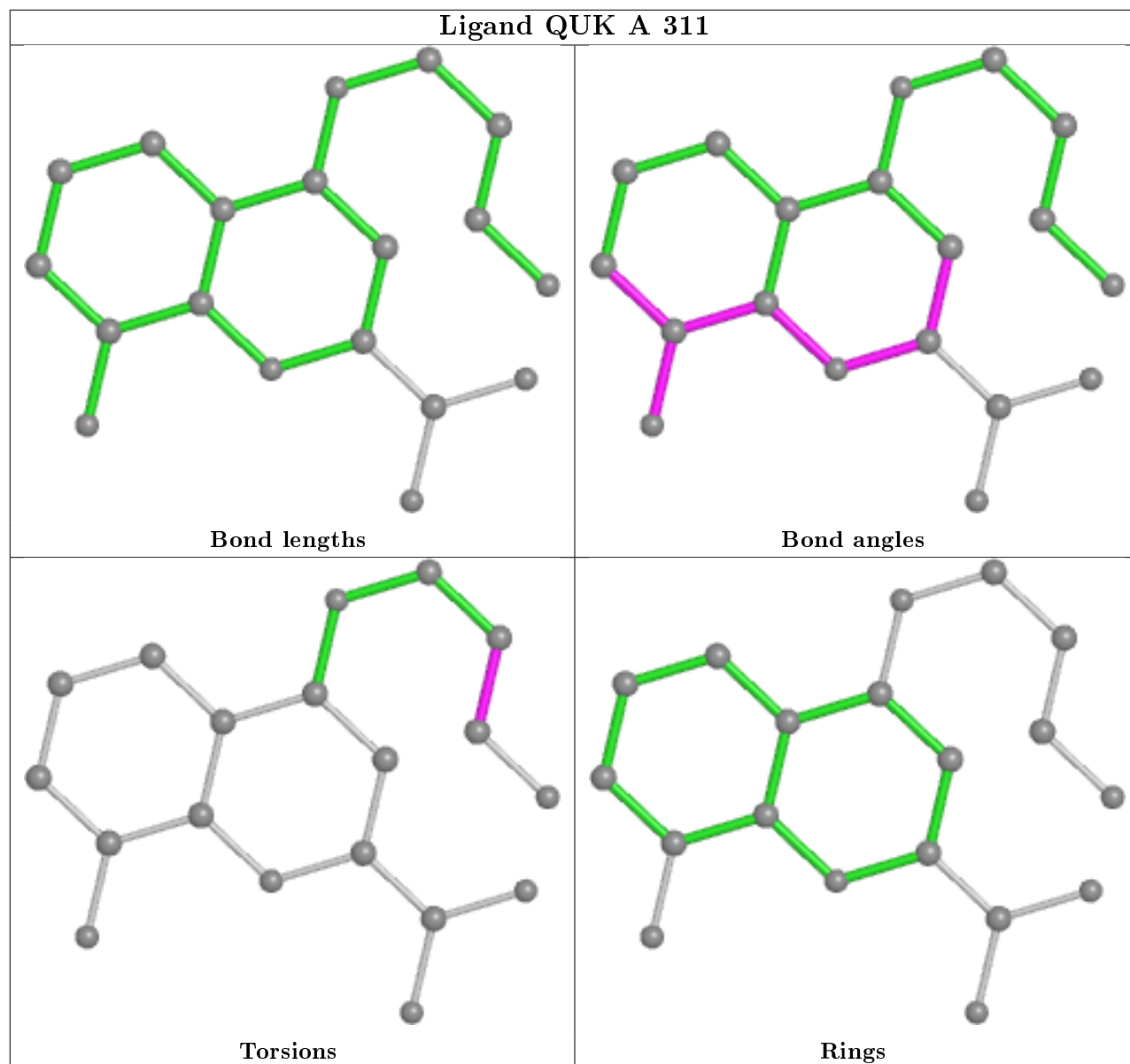


## Ligand QVE B 320

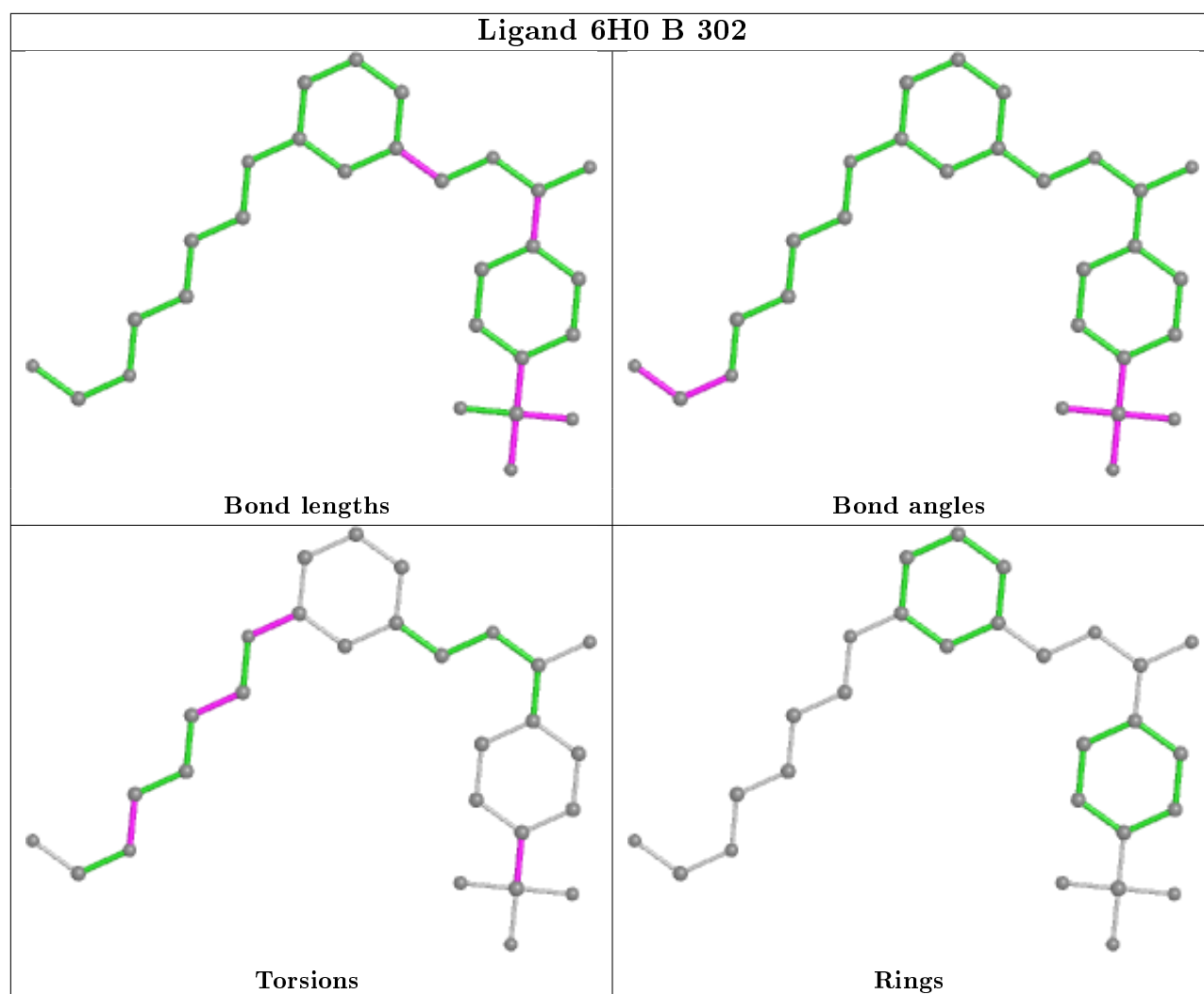


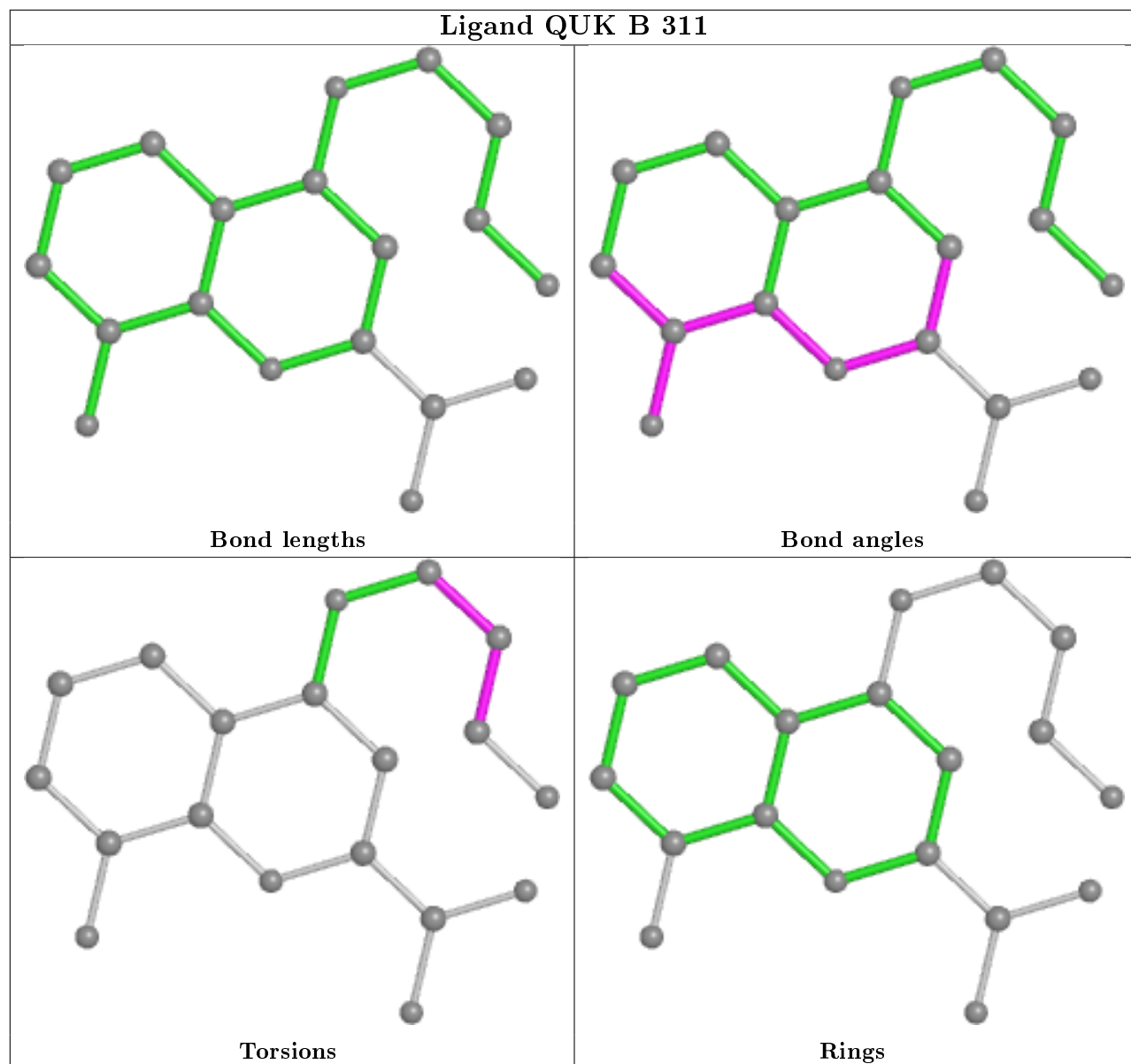


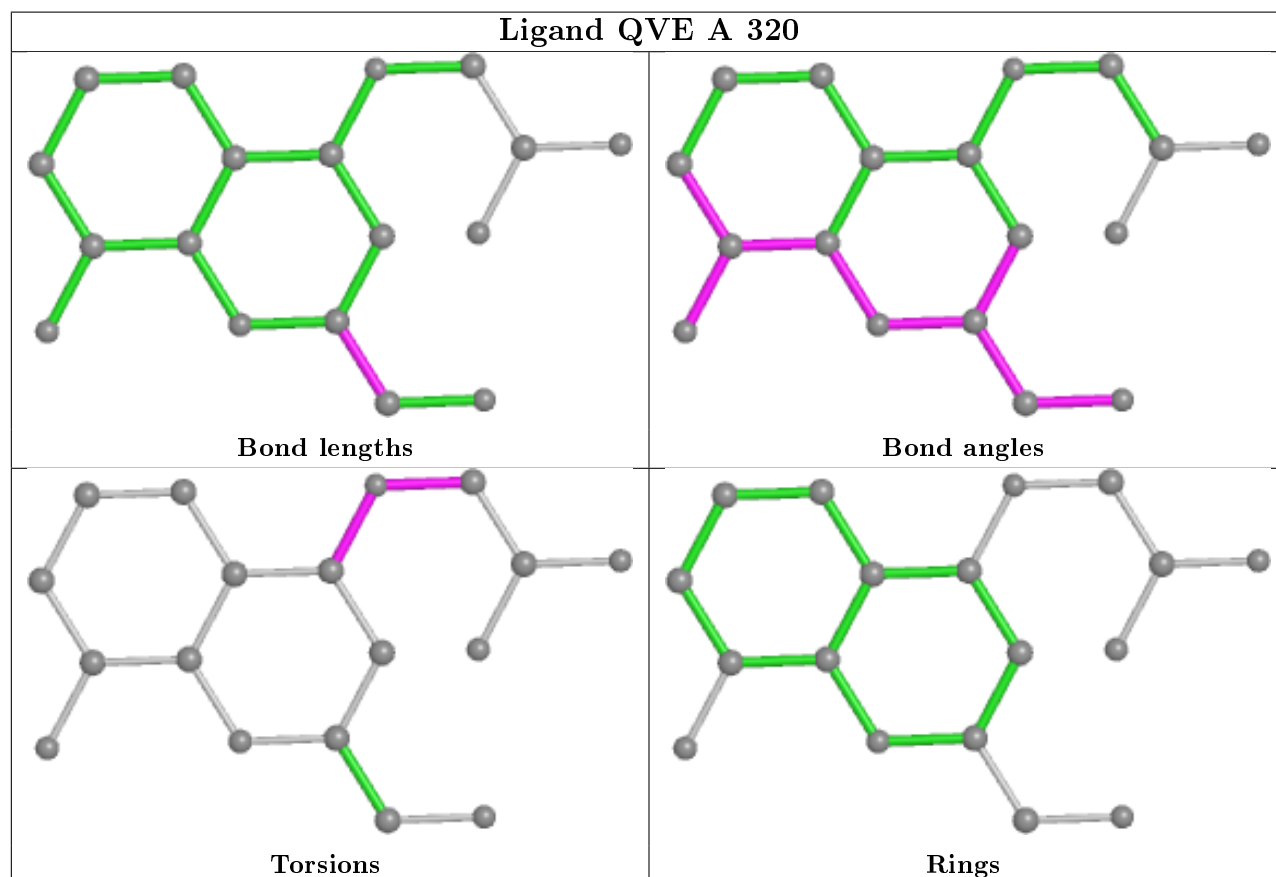
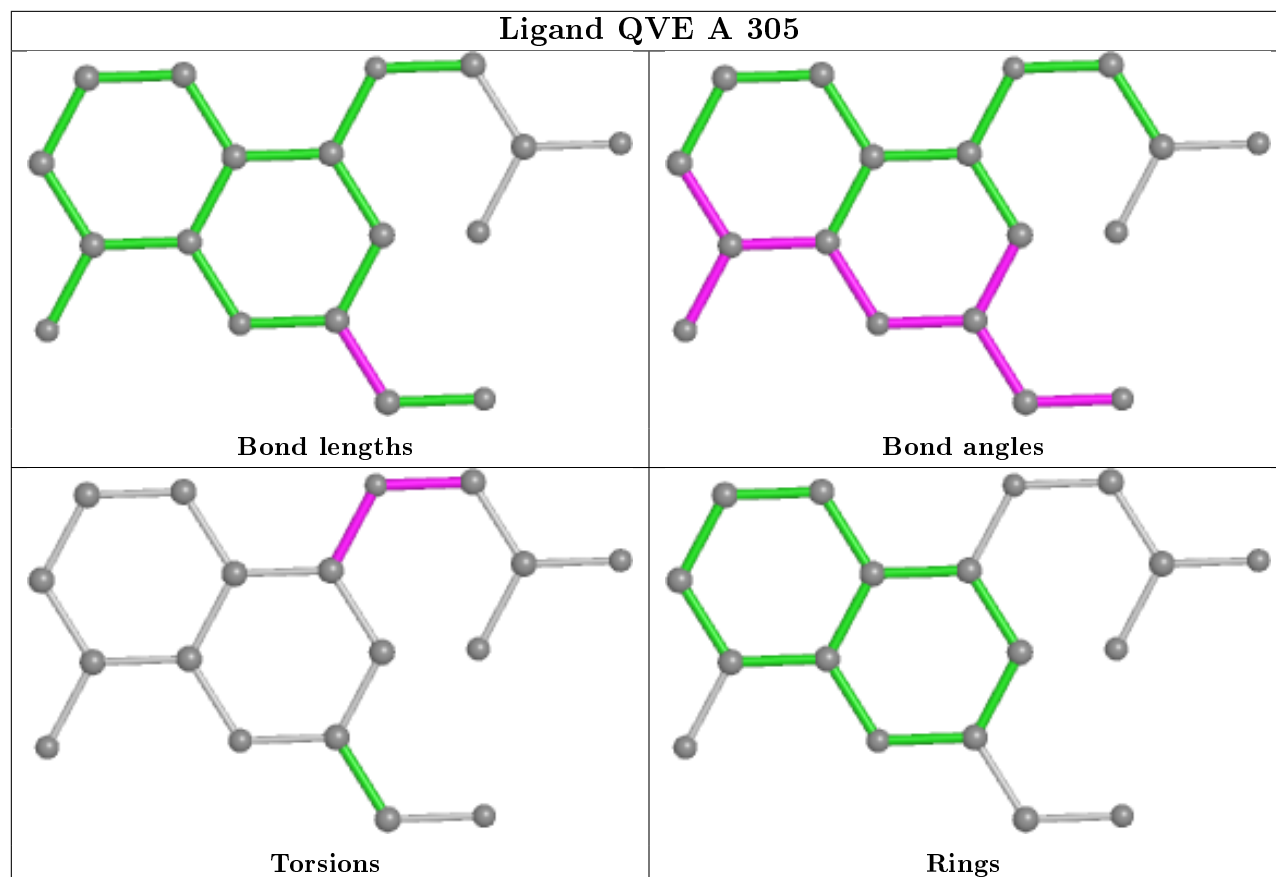


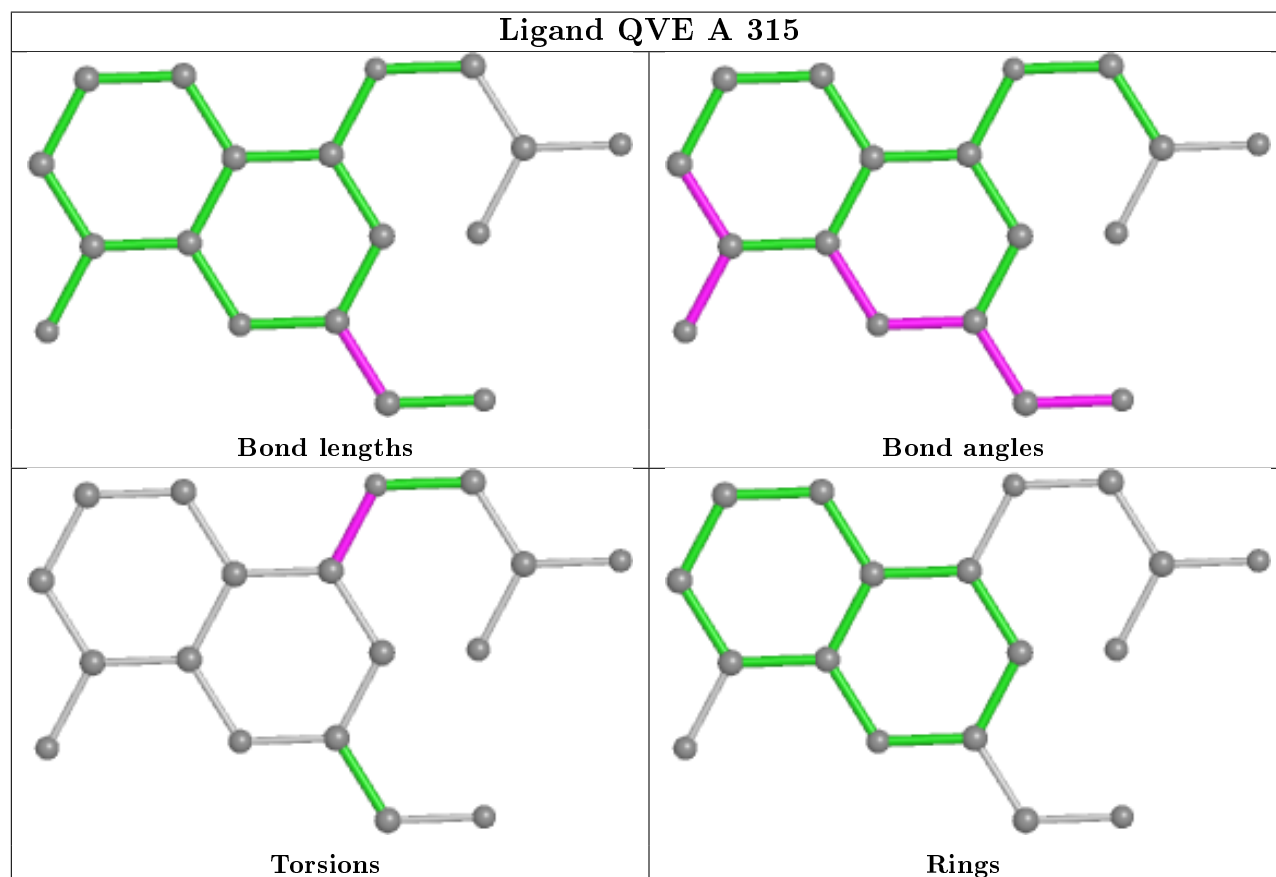
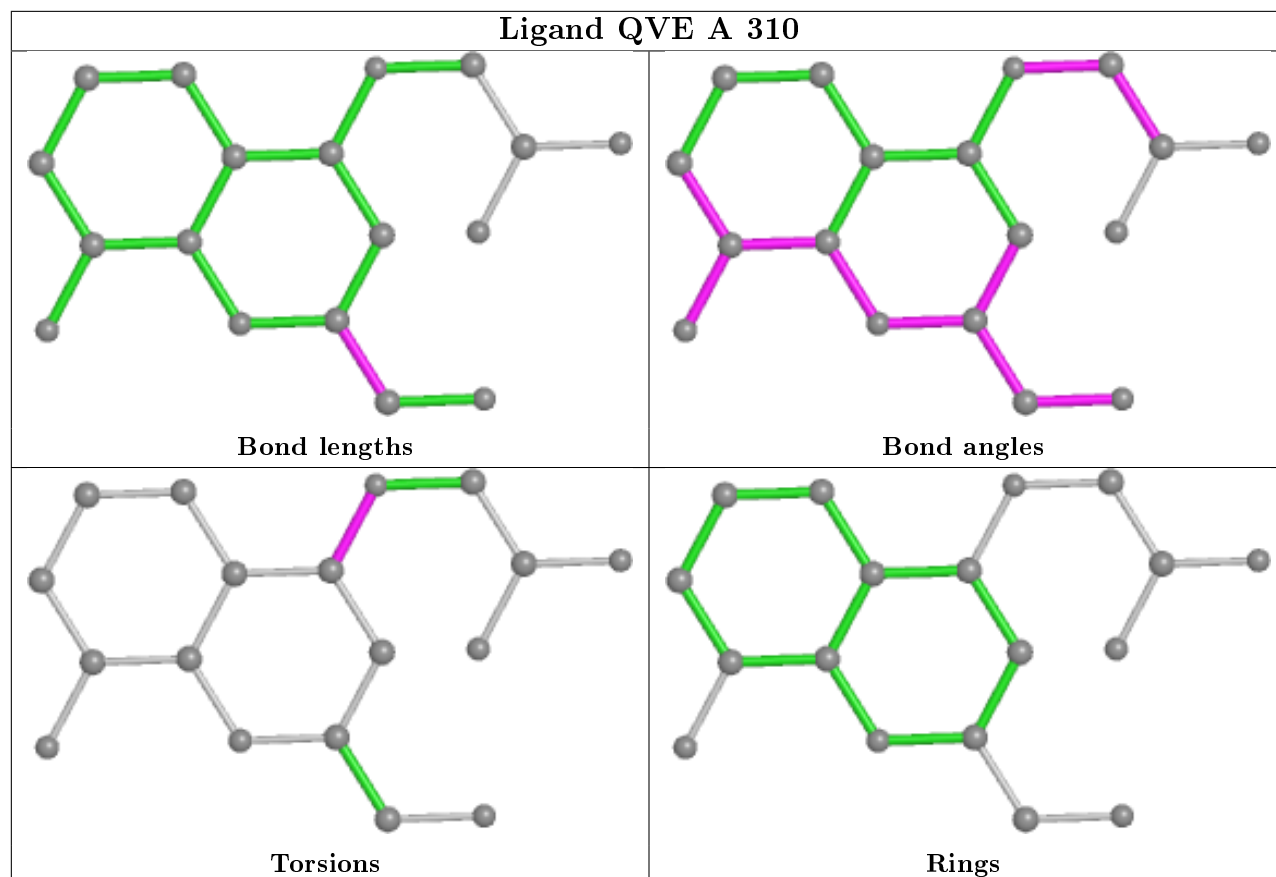


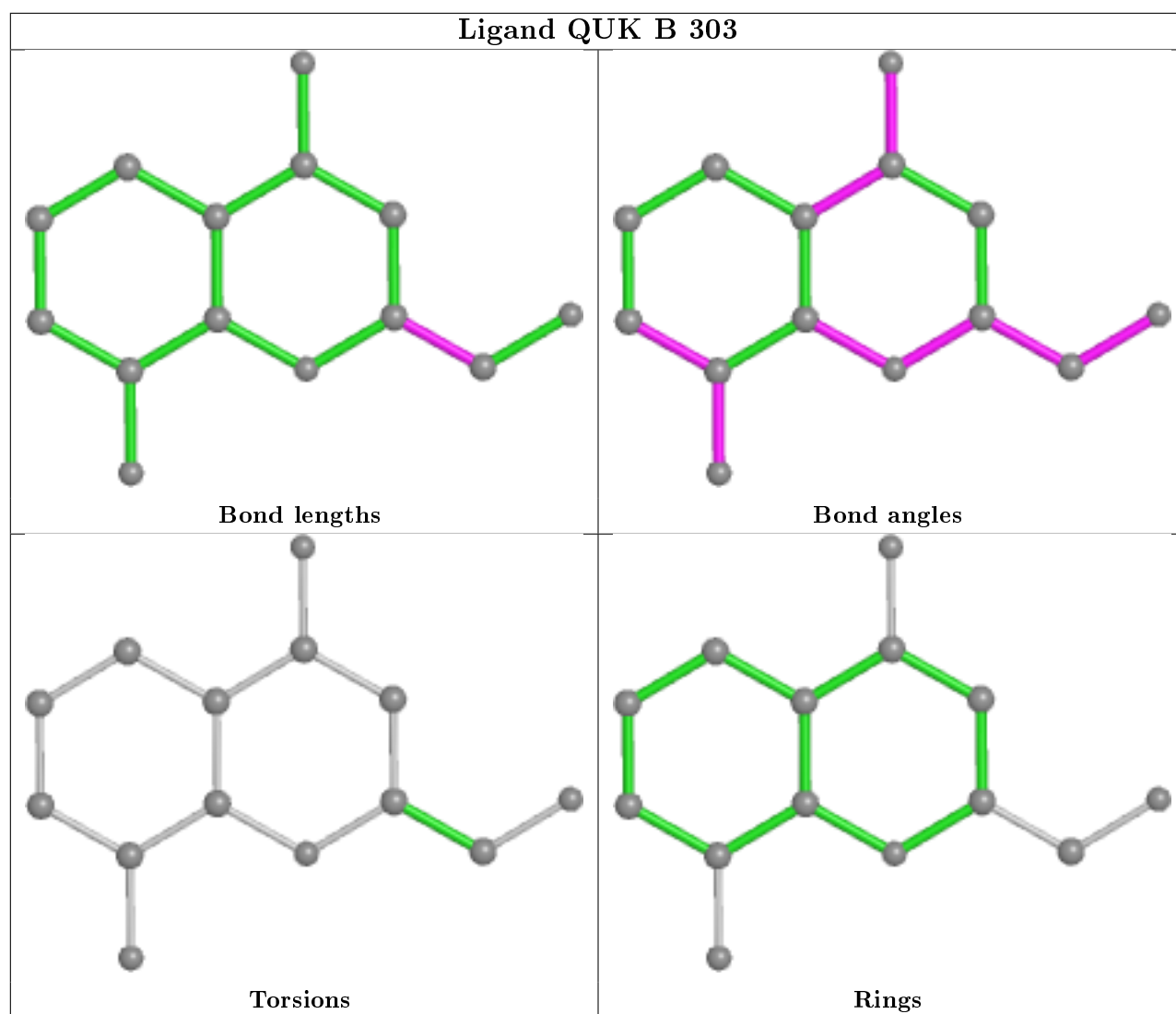


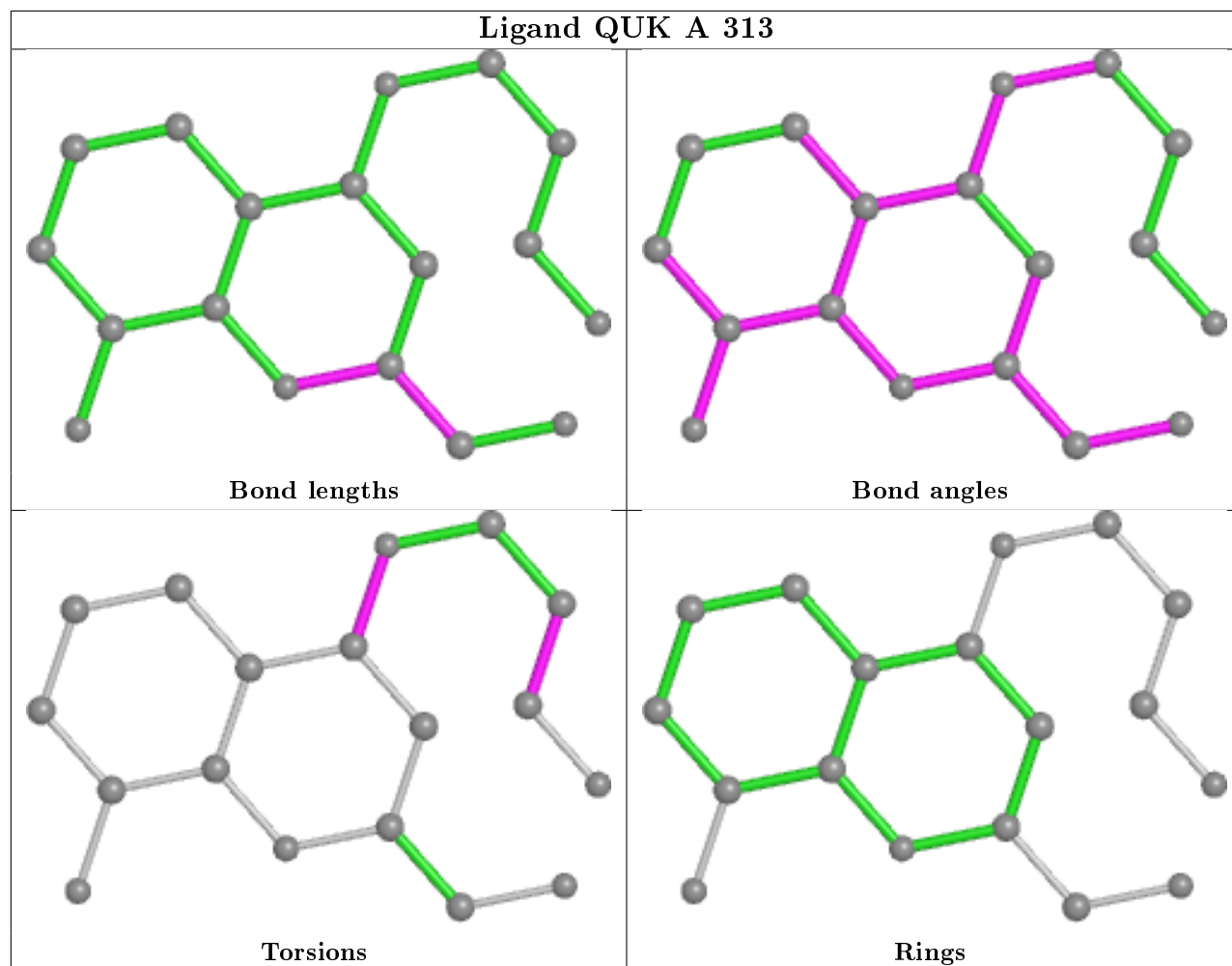


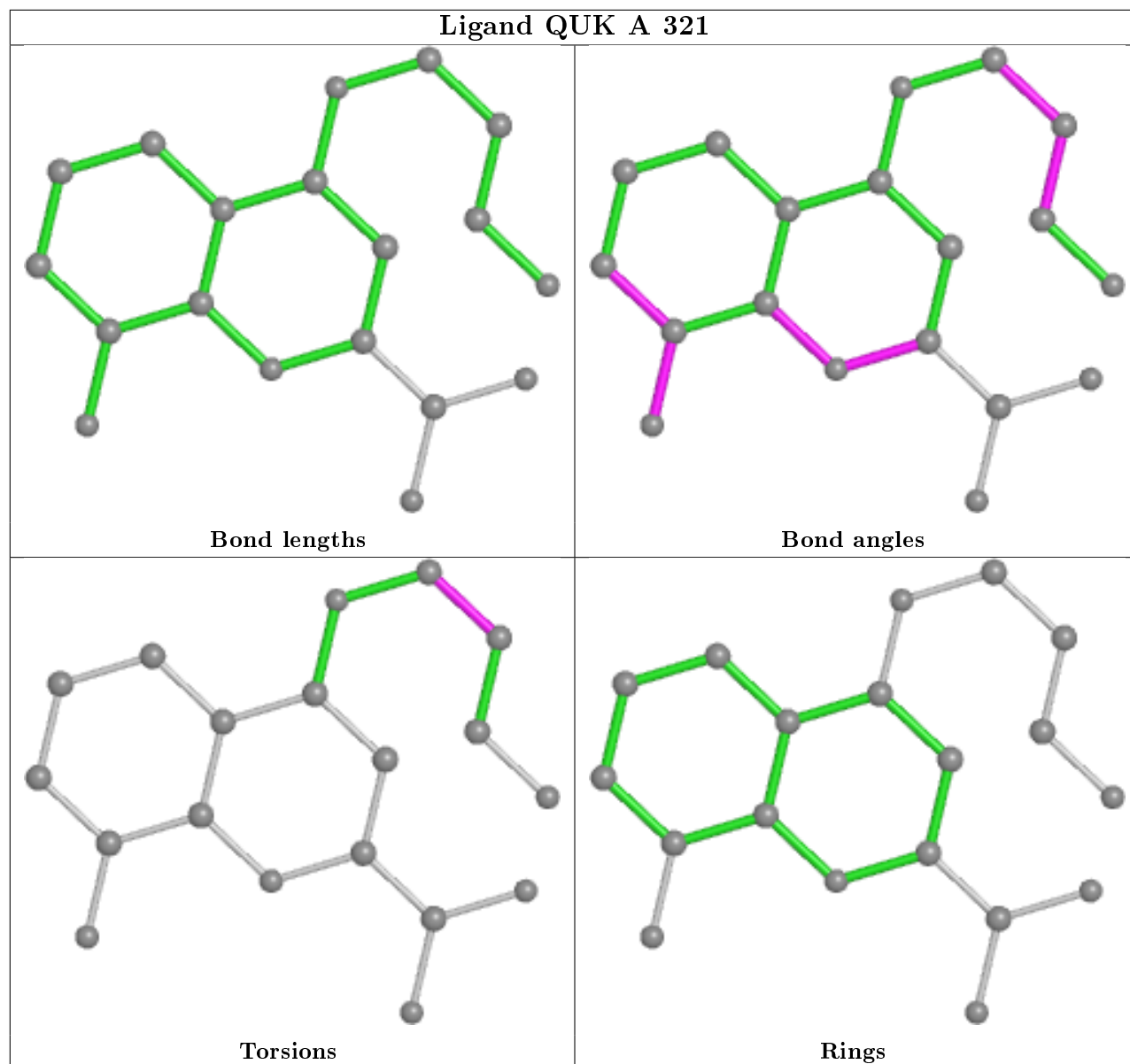


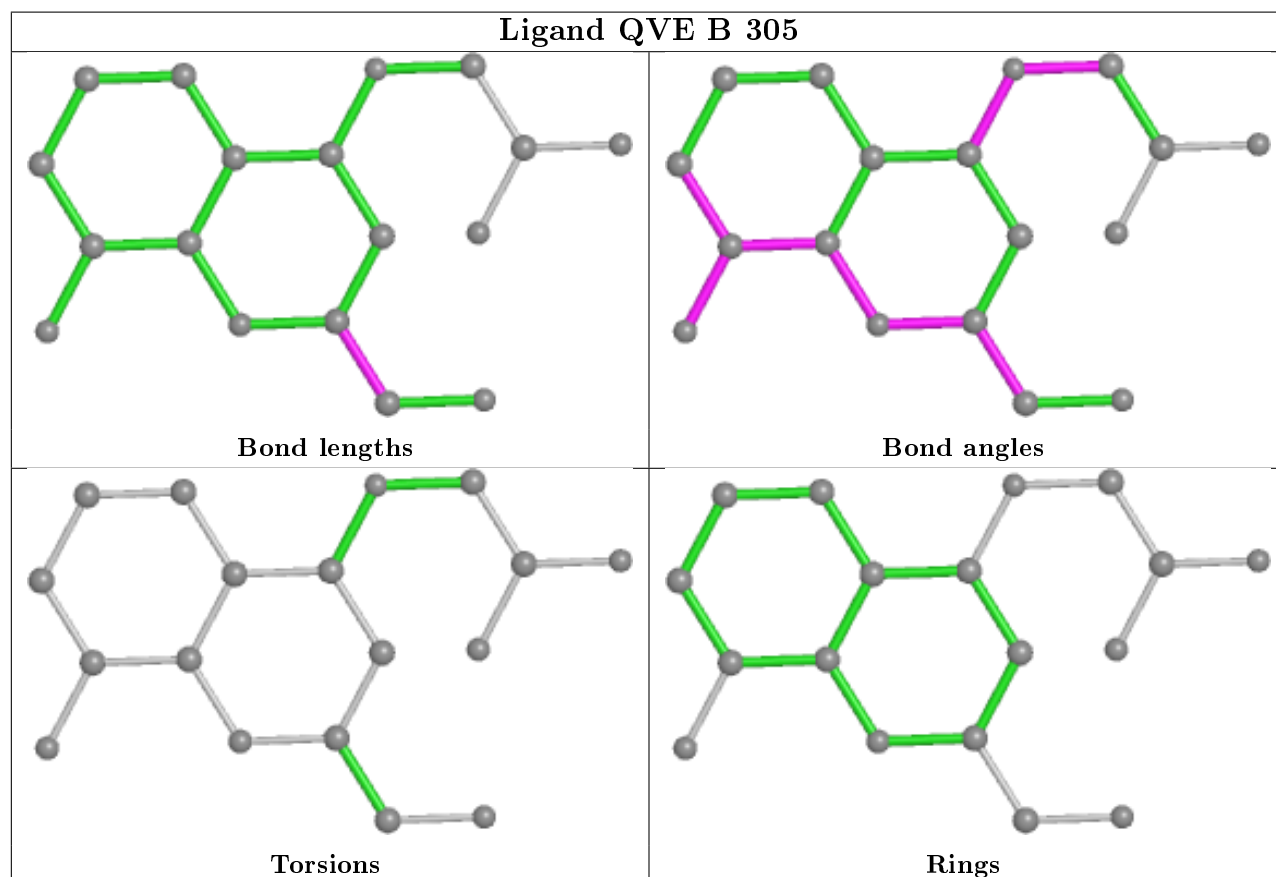
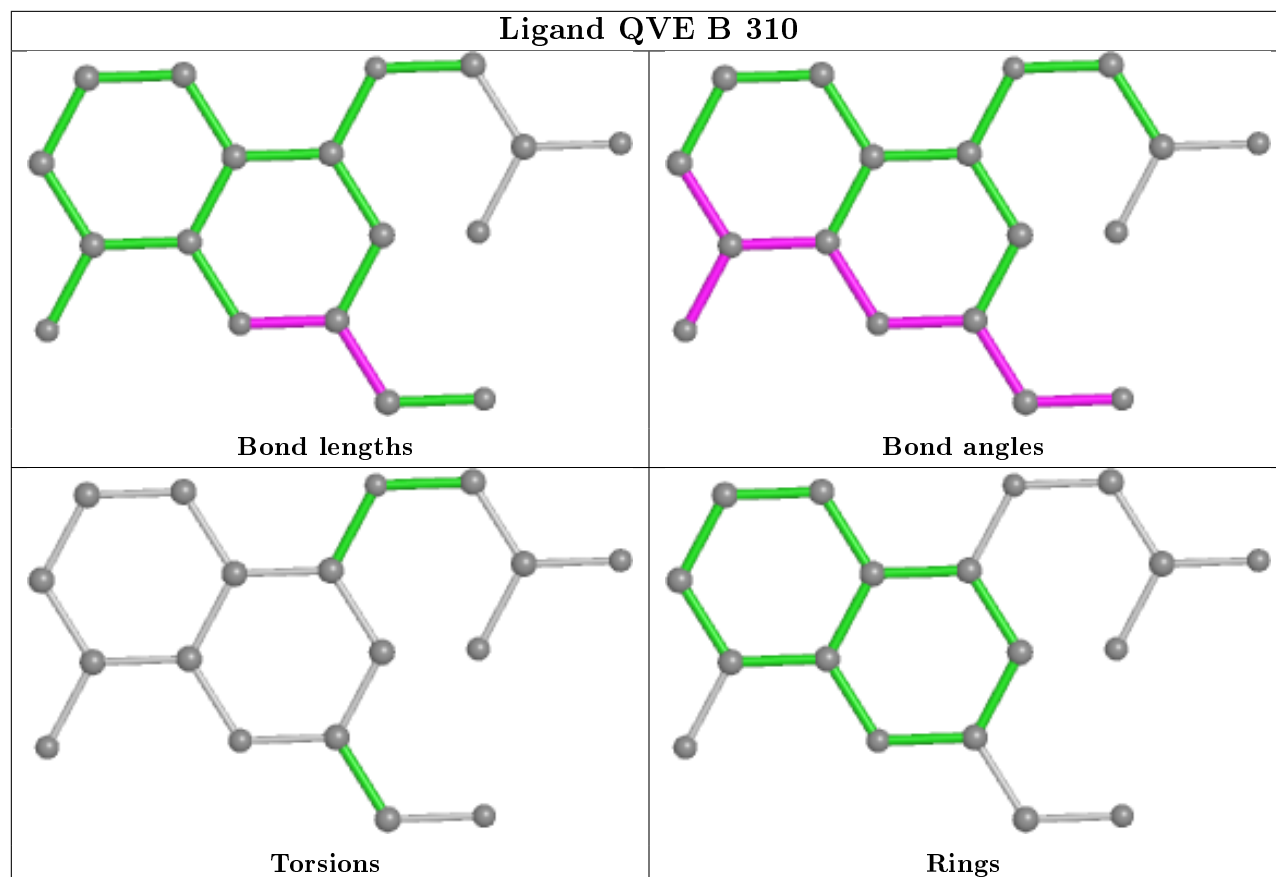




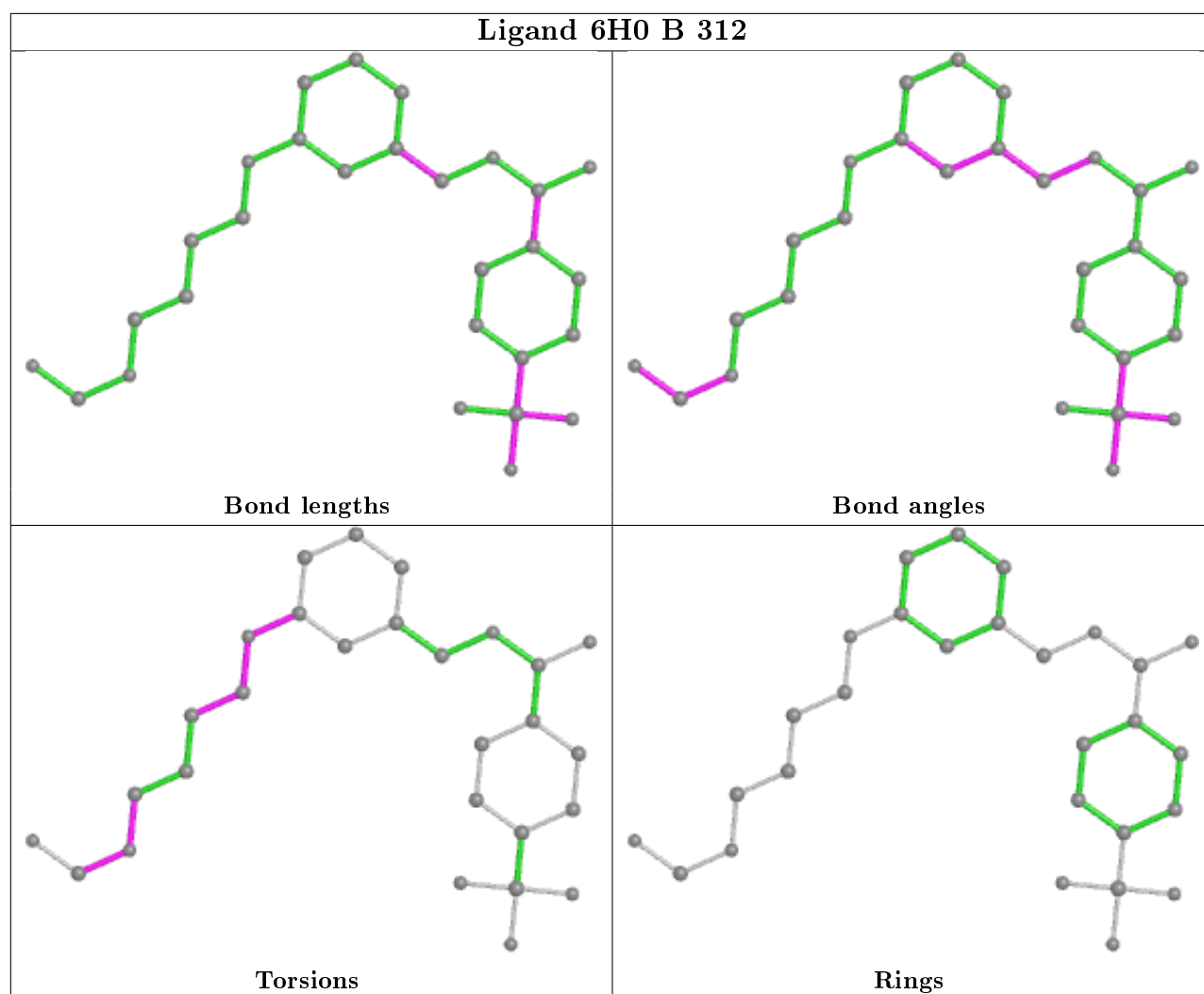


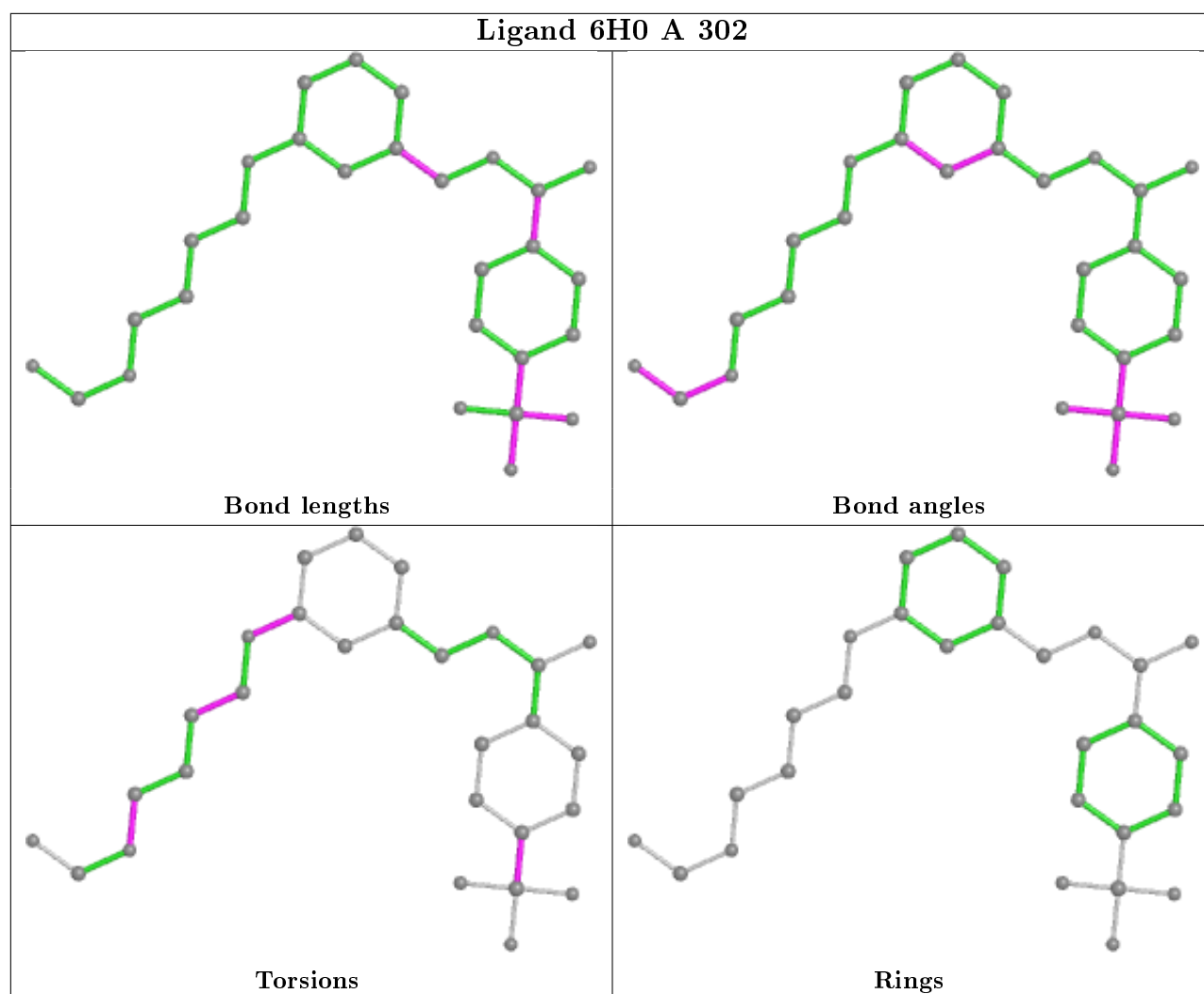


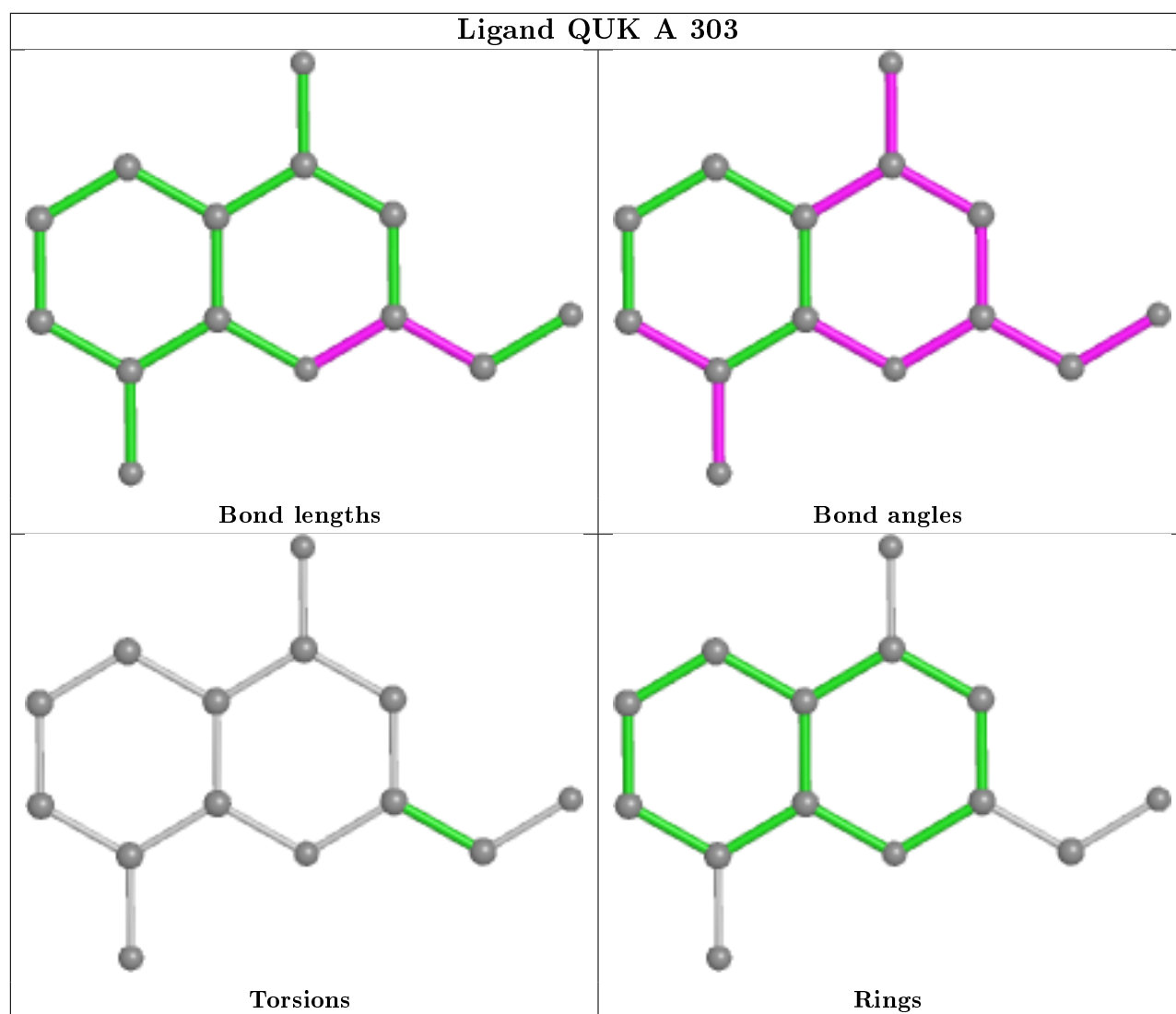












## 5.7 Other polymers [i](#)

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	257/257 (100%)	0.30	9 (3%) 44 40	63, 89, 120, 145	0
1	B	257/257 (100%)	0.22	7 (2%) 54 51	66, 90, 113, 119	0
All	All	514/514 (100%)	0.26	16 (3%) 49 45	63, 89, 115, 145	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	ILE	3.0
1	B	162	VAL	2.9
1	B	70	PHE	2.9
1	A	191	TRP	2.8
1	B	183	LEU	2.7
1	A	259	PHE	2.7
1	B	215	ILE	2.5
1	A	114	TYR	2.4
1	A	26	GLU	2.3
1	A	36	HIS	2.3
1	A	212	LYS	2.3
1	B	225	PHE	2.2
1	A	257	ALA	2.1
1	B	159	VAL	2.1
1	B	15	HIS	2.0
1	A	44	LEU	2.0

### 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 ⓘ

There are no carbohydrates 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
9	GOL	B	323	6/6	0.83	0.36	99,101,103,104	0
3	6H0	A	312	28/28	0.91	0.20	72,80,97,99	0
8	QDD	A	308	17/17	0.91	0.22	79,84,102,103	0
6	QVE	A	320	18/19	0.91	0.22	73,80,99,102	0
9	GOL	A	323	6/6	0.91	0.27	85,87,88,89	0
6	QVE	B	305	18/19	0.91	0.18	69,73,91,94	0
7	QVS	A	306	14/15	0.92	0.17	75,79,81,81	0
3	6H0	B	312	28/28	0.92	0.24	76,85,96,99	0
4	QUK	A	313	18/19	0.93	0.24	75,79,99,99	0
6	QVE	A	305	18/19	0.93	0.23	73,78,99,99	0
8	QDD	B	308	17/17	0.93	0.21	73,77,90,90	0
6	QVE	A	310	18/19	0.94	0.17	78,84,94,96	0
8	QDD	A	318	17/17	0.94	0.20	71,75,86,86	0
4	QUK	B	313	18/19	0.94	0.22	76,80,97,98	0
4	QUK	B	311	19/19	0.94	0.18	80,82,96,97	0
5	ZY9	A	319	10/11	0.94	0.19	71,73,75,75	0
4	QUK	A	303	14/19	0.94	0.18	74,78,81,83	0
9	GOL	B	322	6/6	0.95	0.38	80,82,83,83	0
6	QVE	B	310	18/19	0.95	0.15	71,77,86,88	0
6	QVE	A	315	18/19	0.95	0.20	68,73,87,87	0
4	QUK	A	311	19/19	0.95	0.16	84,86,99,100	0
6	QVE	B	320	18/19	0.95	0.18	76,81,90,92	0
4	QUK	B	303	14/19	0.96	0.15	70,72,75,75	0
7	QVS	B	306	14/15	0.96	0.17	68,70,73,73	0
5	ZY9	A	309	10/11	0.96	0.18	77,79,79,79	0
4	QUK	A	321	19/19	0.96	0.20	76,81,95,99	0
5	ZY9	B	317	10/11	0.96	0.21	73,74,74,75	0
8	QDD	B	318	17/17	0.96	0.19	74,75,83,84	0
5	ZY9	A	314	10/11	0.96	0.23	67,71,75,76	0
7	QVS	A	316	14/15	0.96	0.17	73,75,80,80	0
6	QVE	B	315	18/19	0.96	0.21	70,74,86,86	0
4	QUK	B	321	19/19	0.96	0.21	80,83,91,94	0

*Continued on next page...*

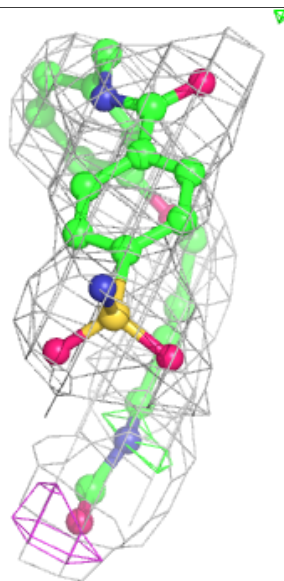
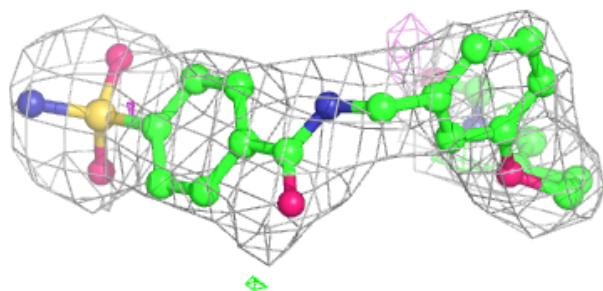
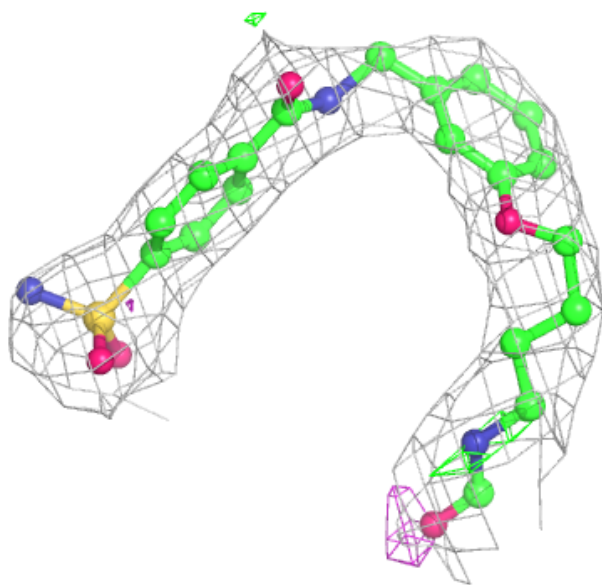
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ZY9	B	304	10/11	0.97	0.21	69,70,72,72	0
7	QVS	B	316	14/15	0.97	0.14	74,75,77,78	0
5	ZY9	B	319	10/11	0.97	0.21	76,78,78,79	0
5	ZY9	B	309	10/11	0.97	0.18	70,71,72,73	0
3	6H0	A	302	28/28	0.97	0.22	66,68,71,72	0
5	ZY9	A	304	10/11	0.97	0.18	75,77,77,78	0
5	ZY9	A	307	10/11	0.98	0.19	73,74,77,78	0
5	ZY9	B	307	10/11	0.98	0.18	68,70,70,71	0
9	GOL	A	322	6/6	0.98	0.20	69,70,72,73	0
3	6H0	B	302	28/28	0.98	0.23	70,73,76,77	0
5	ZY9	A	317	10/11	0.98	0.16	65,67,69,70	0
5	ZY9	B	314	10/11	0.99	0.19	71,73,75,75	0
2	ZN	B	301	1/1	1.00	0.20	69,69,69,69	0
2	ZN	A	301	1/1	1.00	0.19	65,65,65,65	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.

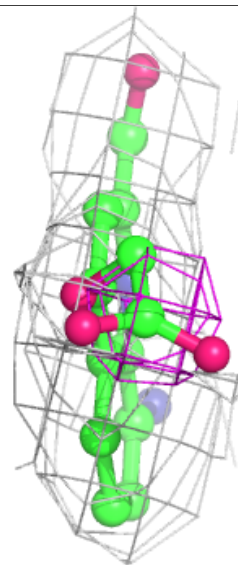
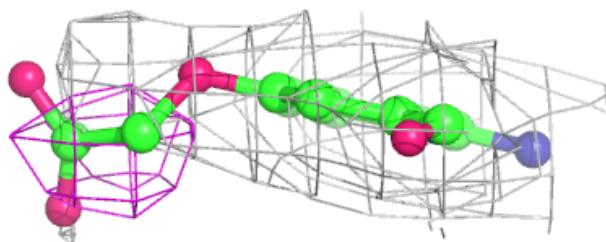
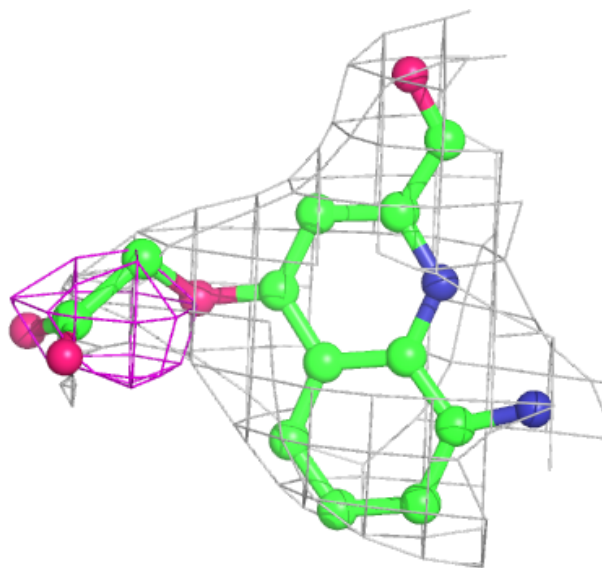
**Electron density around 6H0 A 312:**

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



**Electron density around QVE A 320:**

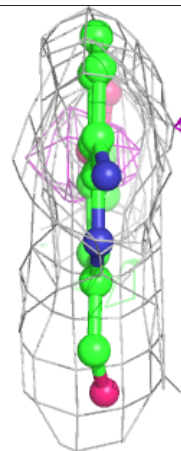
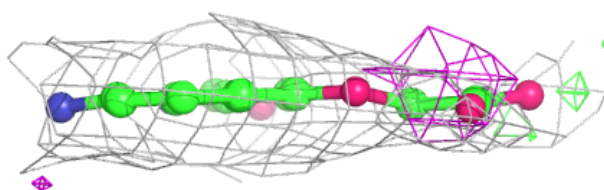
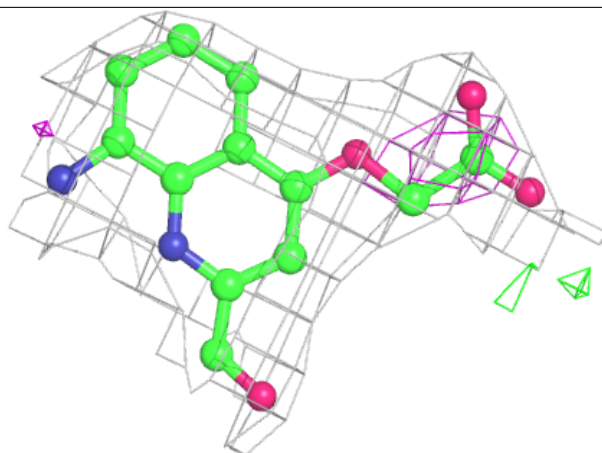
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





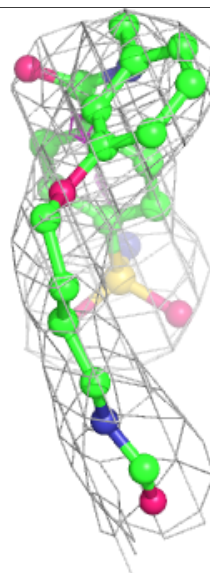
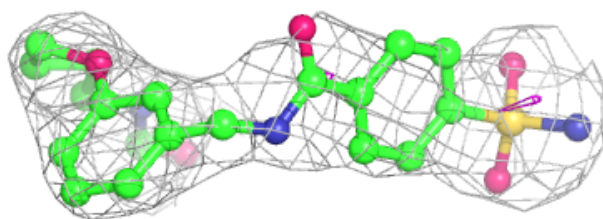
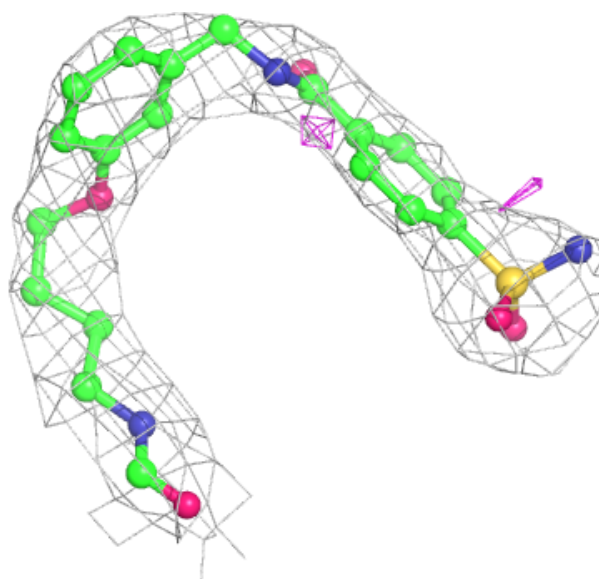
**Electron density around QVE B 305:**

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



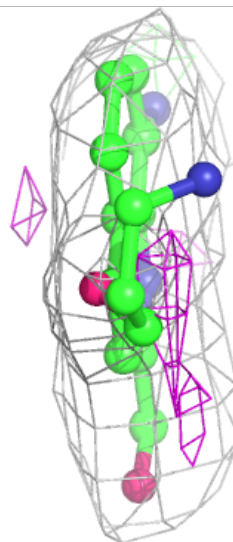
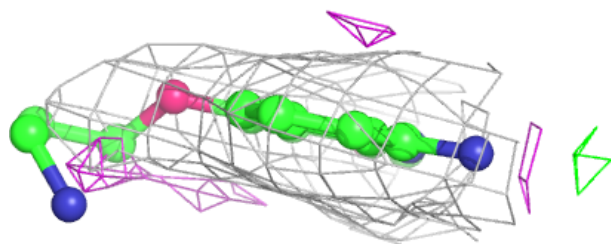
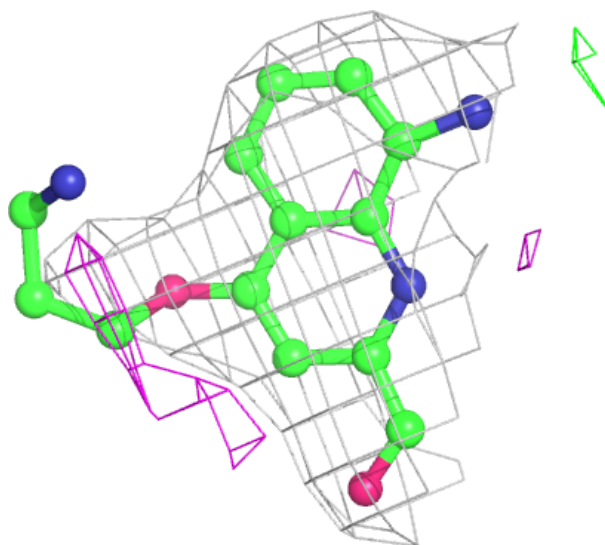
**Electron density around 6H0 B 312:**

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



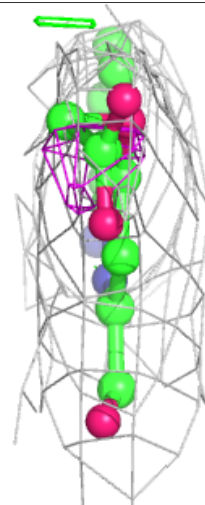
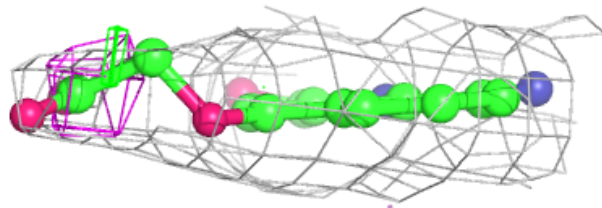
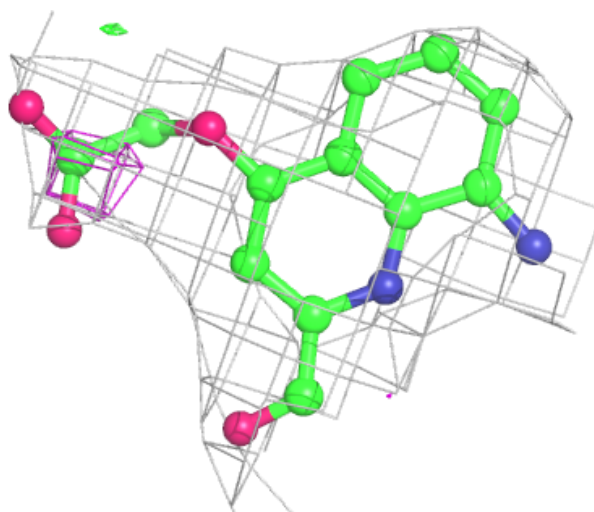
**Electron density around QUK A 313:**

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



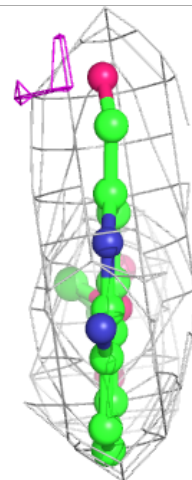
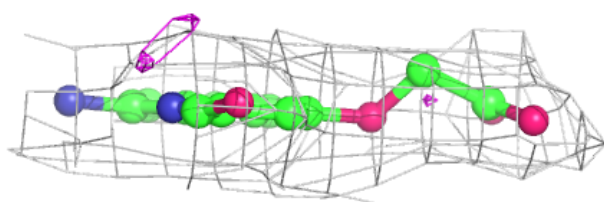
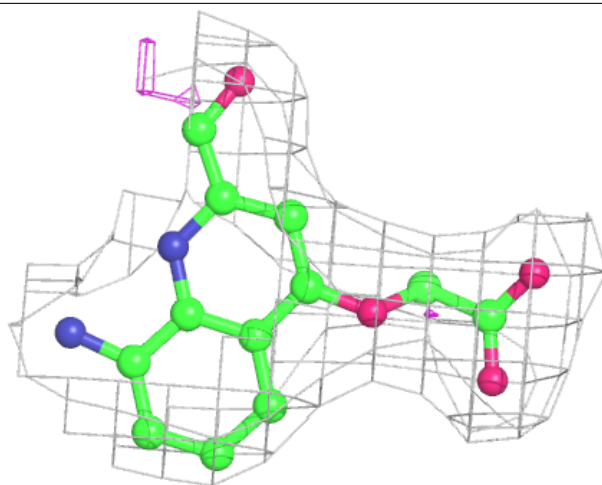
**Electron density around QVE A 305:**

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



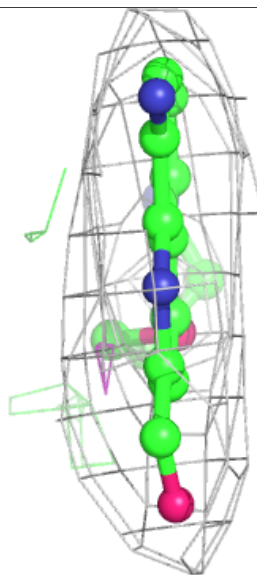
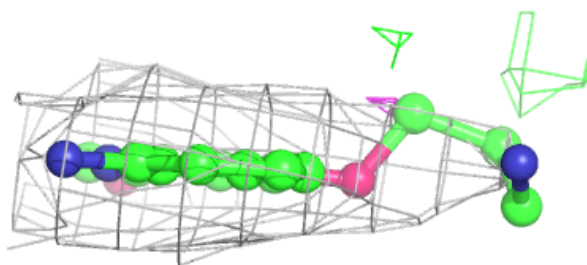
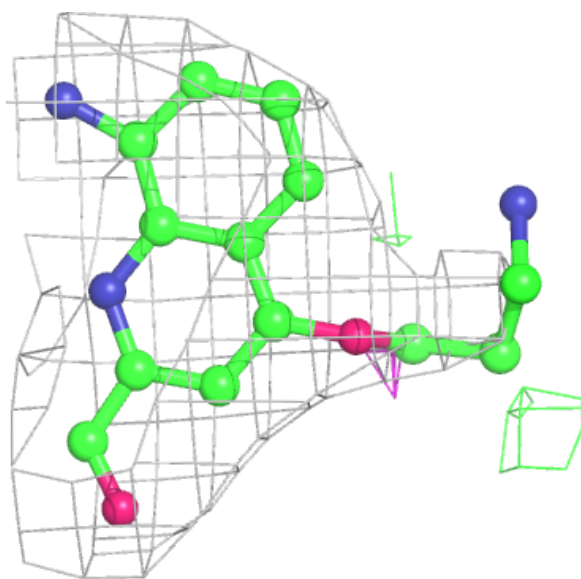
**Electron density around QVE A 310:**

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



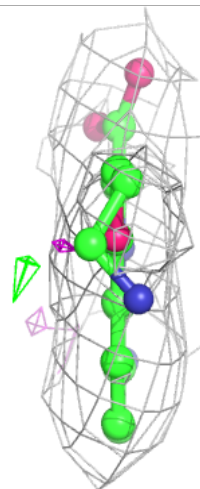
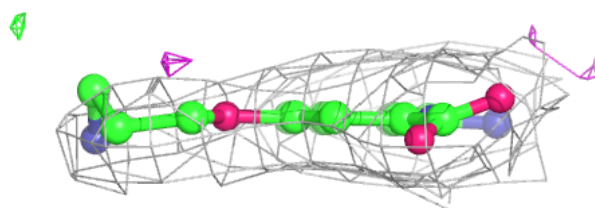
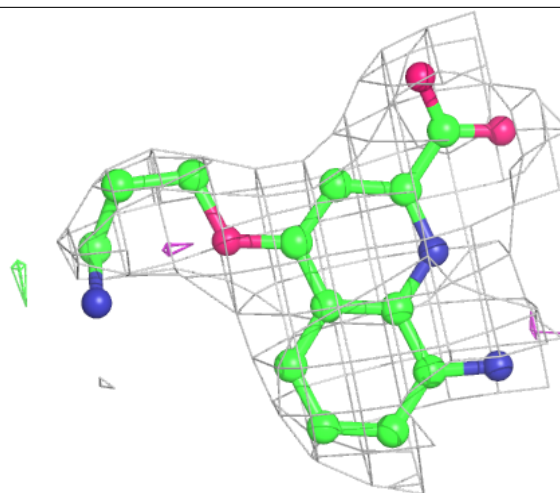
**Electron density around QUK B 313:**

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



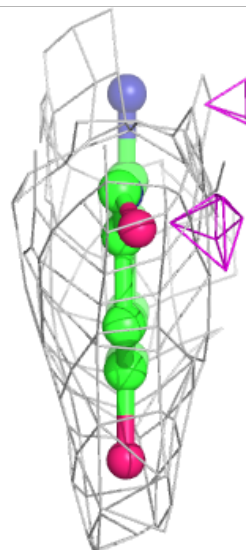
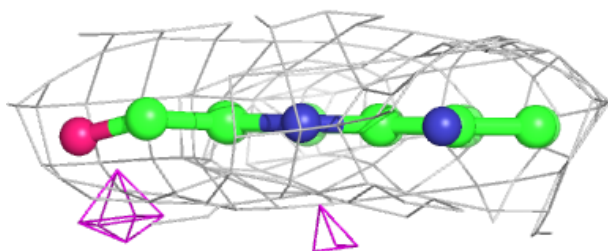
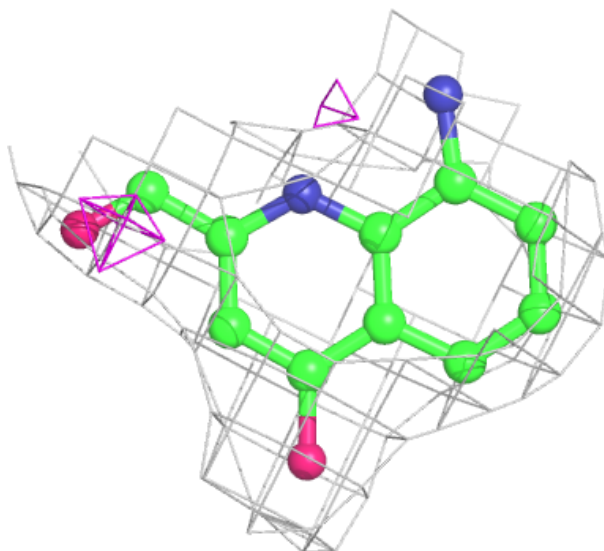
**Electron density around QUK B 311:**

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



**Electron density around QUK A 303:**

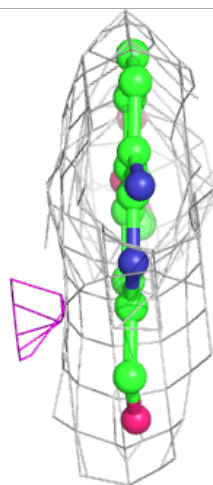
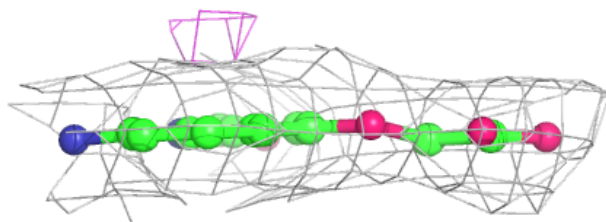
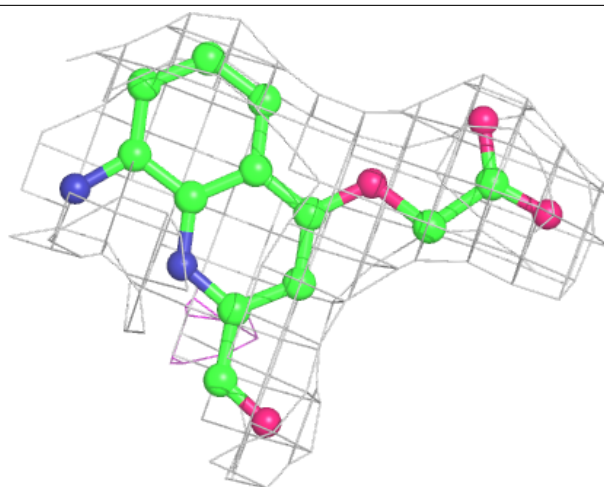
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





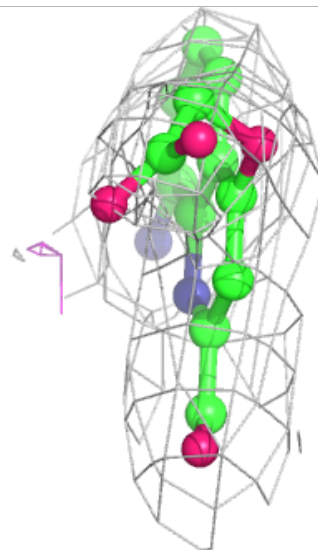
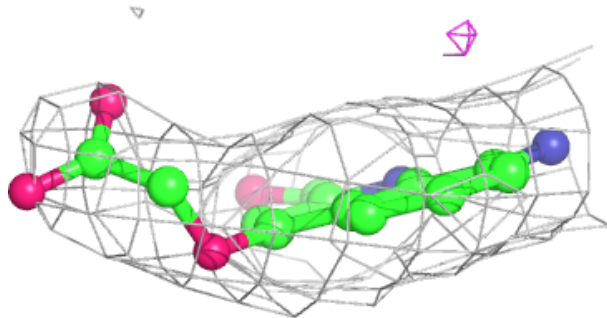
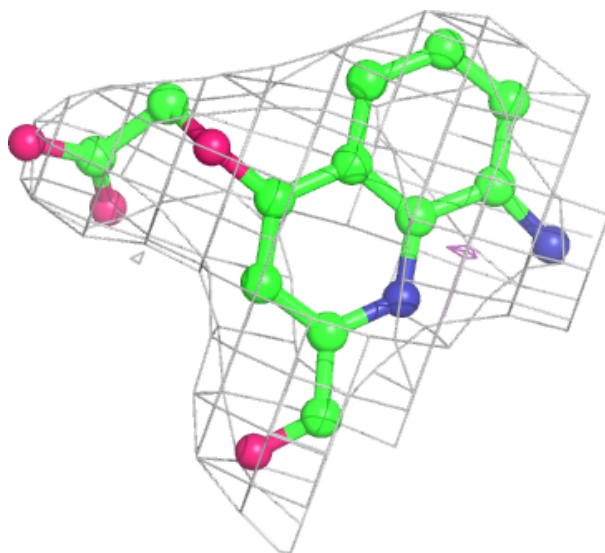
**Electron density around QVE B 310:**

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



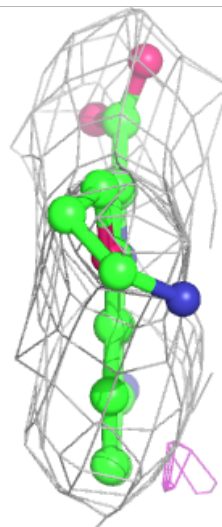
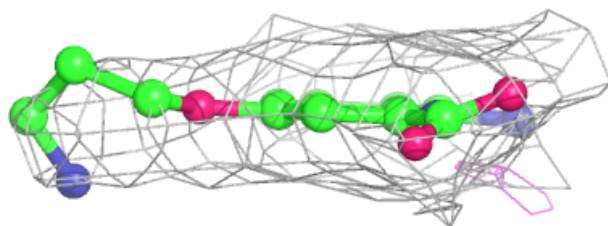
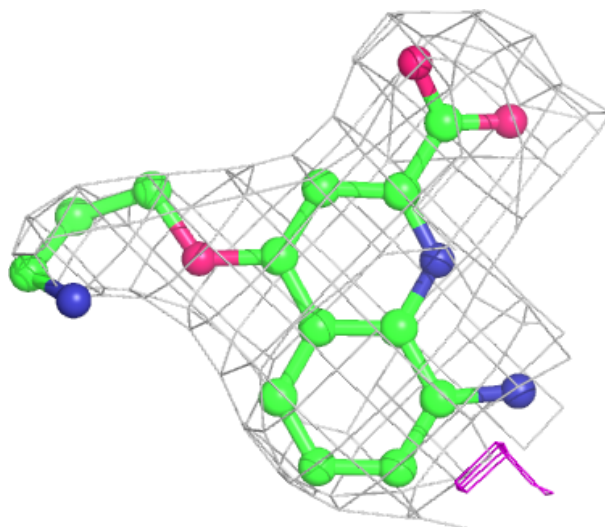
**Electron density around QVE A 315:**

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



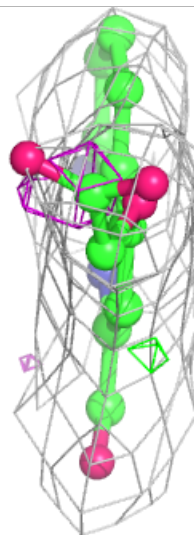
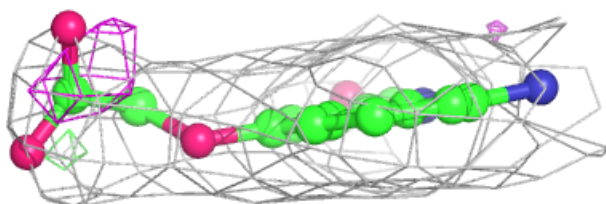
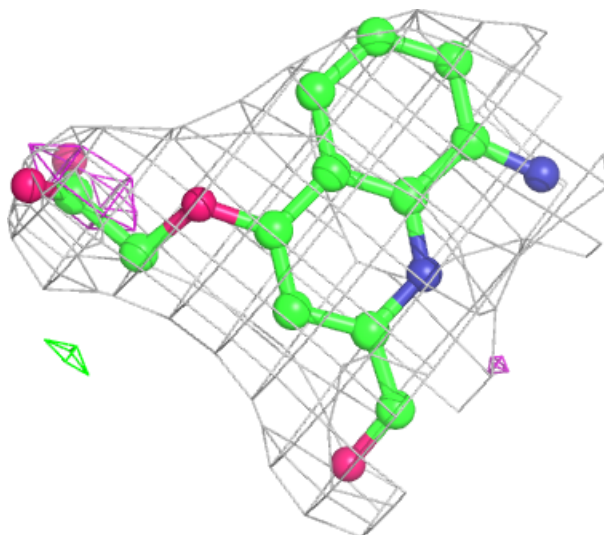
**Electron density around QUK A 311:**

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



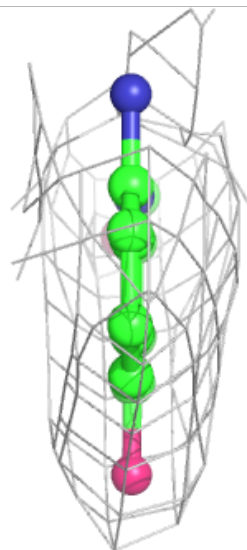
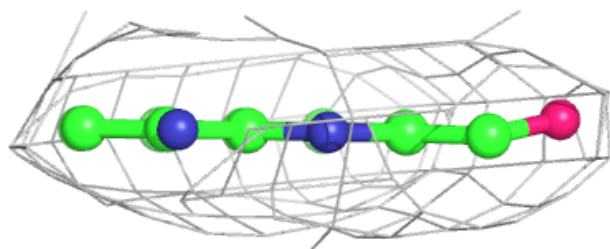
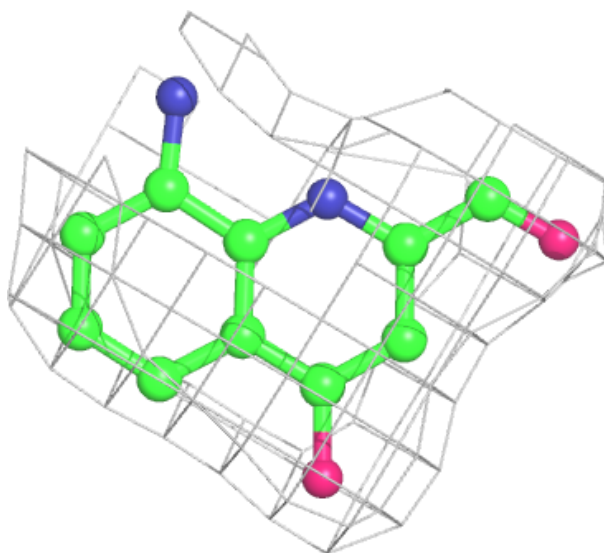
**Electron density around QVE B 320:**

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



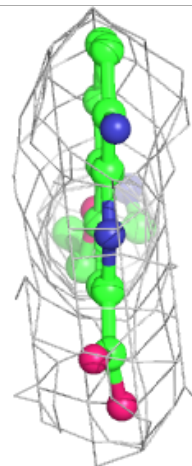
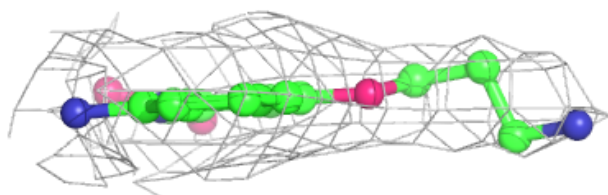
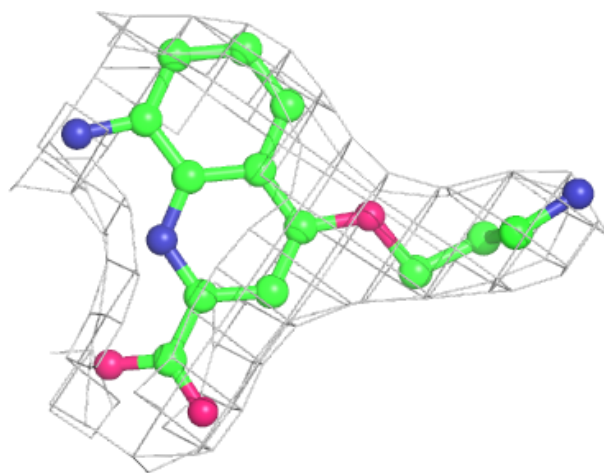
**Electron density around QUK B 303:**

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



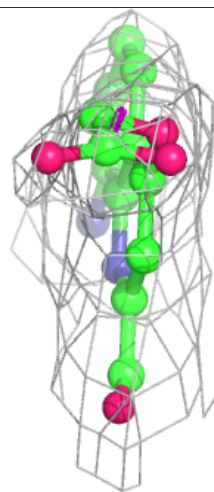
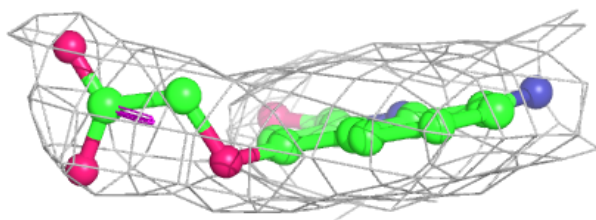
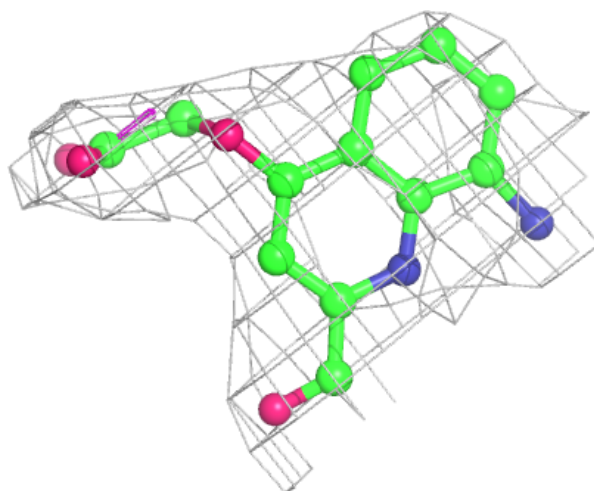
**Electron density around QUK A 321:**

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



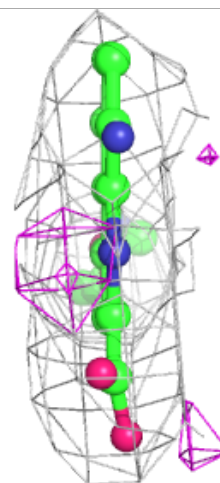
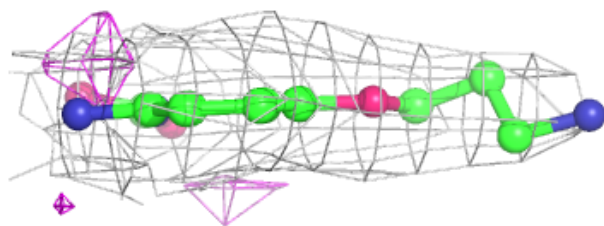
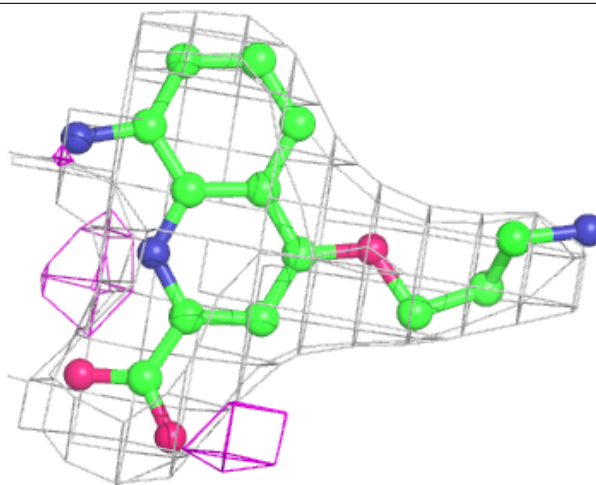
**Electron density around QVE B 315:**

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



**Electron density around QUK B 321:**

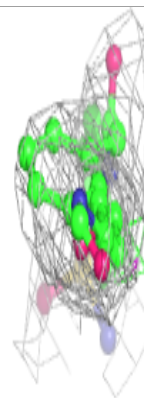
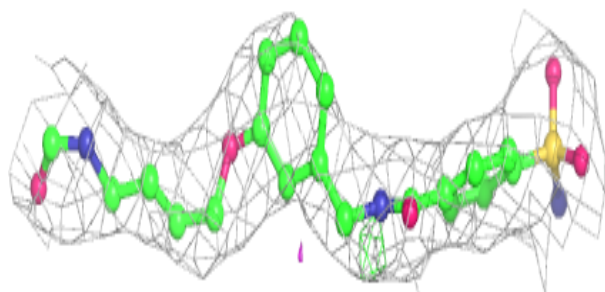
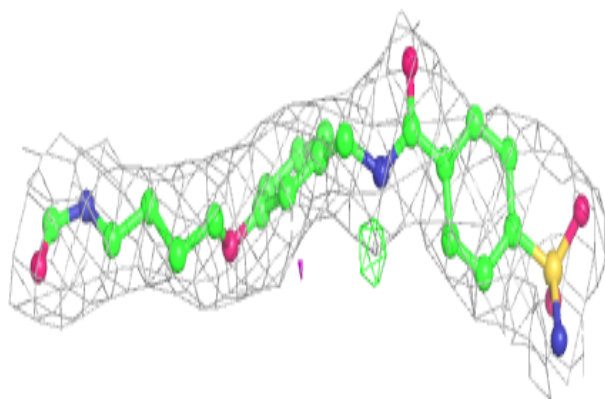
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



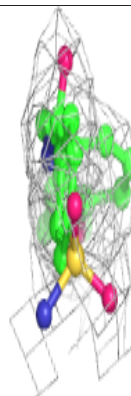
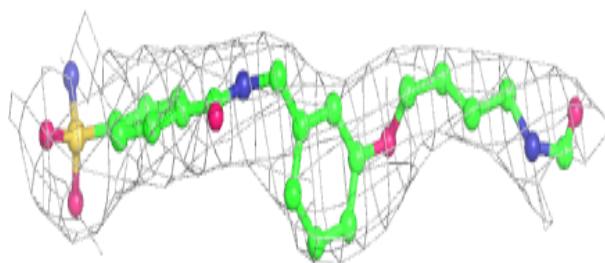
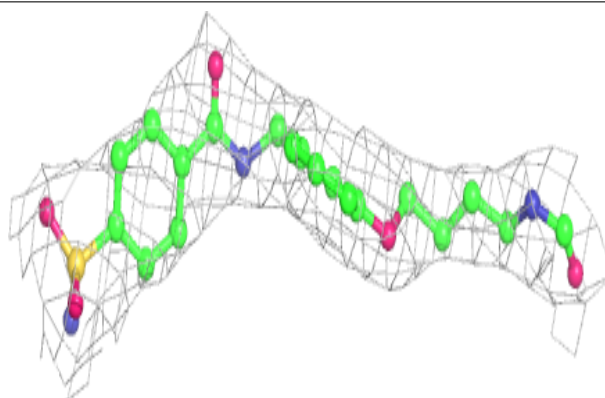


**Electron density around 6H0 A 302:**

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

**Electron density around 6H0 B 302:**

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



## 6.5 Other polymers

There are no such residues in this entry.