



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:27 am BST

PDB ID : 5LVS  
Title : Self-assembled protein-aromatic foldamer complexes with 2:3 and 2:2:1 stoichiometries  
Authors : Jewginski, M.; LANGLOIS D'ESTAINOT, B.; Granier, T.; Huc, Y.  
Deposited on : 2016-09-14  
Resolution : 1.42 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

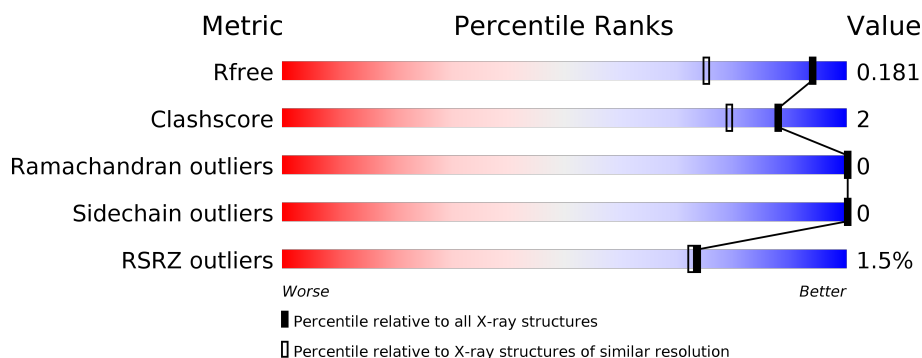
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.42 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	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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	259	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	B	259	<div> <div>2%</div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5064 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.

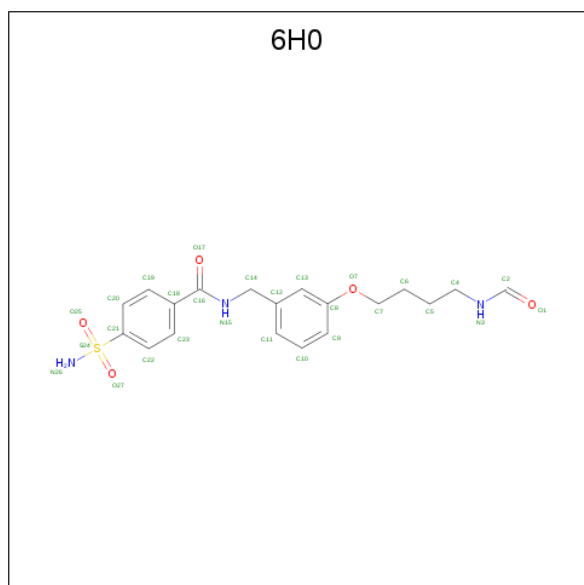
- Molecule 1 is a protein called Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	7	0
			2070	1334	354	380	2			
1	B	259	Total	C	N	O	S	0	9	0
			2083	1342	354	385	2			

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

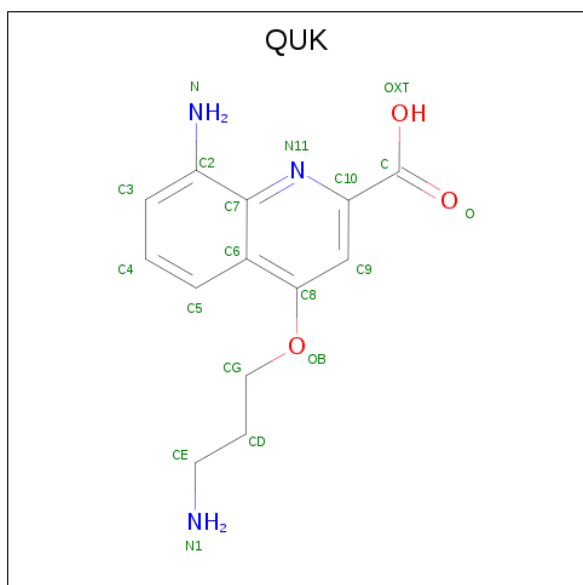
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- 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).



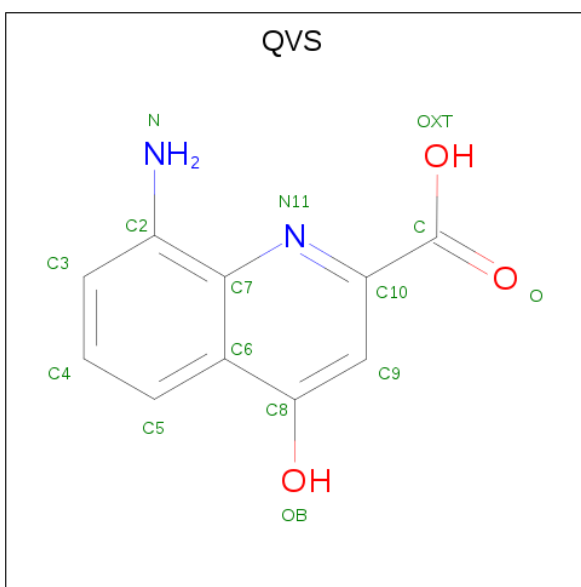
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
3	B	1	Total	C	N	O	S	0	0
			28	19	3	5	1		

- Molecule 4 is 8-azanyl-4-(3-azanylpropoxy)quinoline-2-carboxylic acid (three-letter code: QUK) (formula:  $C_{13}H_{15}N_3O_3$ ).



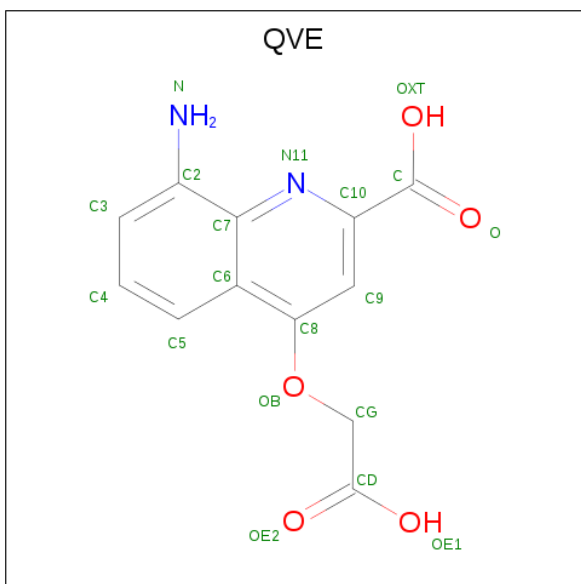
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	13	2	2		
4	A	1	Total	C	N	O	0	0
			14	10	2	2		
4	B	1	Total	C	N	O	0	0
			17	13	2	2		
4	B	1	Total	C	N	O	0	0
			14	10	2	2		

- Molecule 5 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
5	A	1	Total	C	N	O	0	0
			14	10	2	2		
5	B	1	Total	C	N	O	0	0
			14	10	2	2		

- 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
			19	12	2	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			19	12	2	5		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



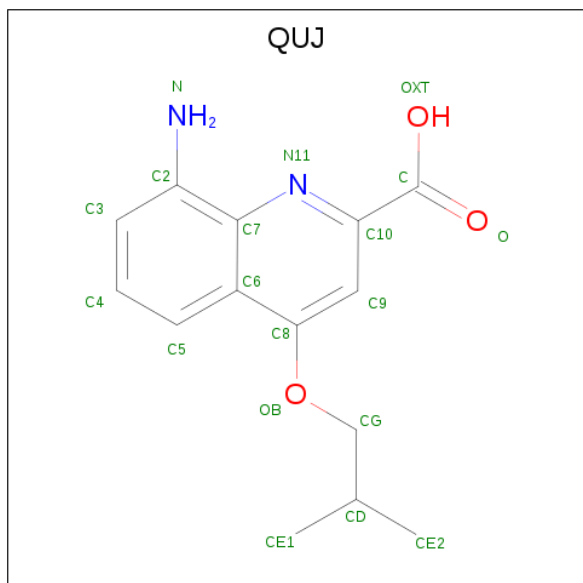
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	1
			12	6	6		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

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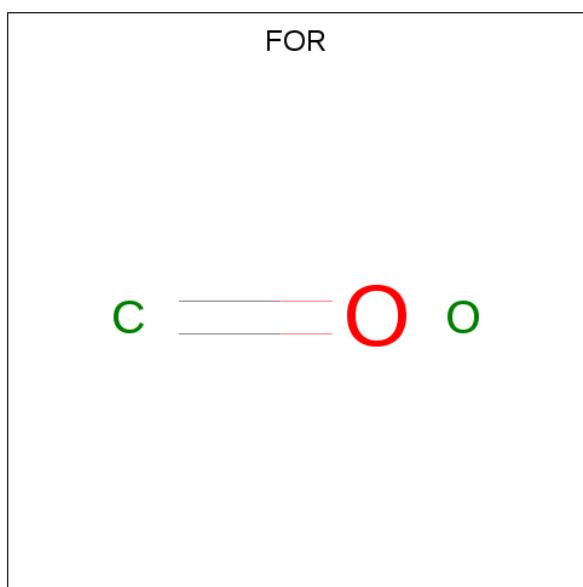
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 8-azanyl-4-(2-methylpropoxy)quinoline-2-carboxylic acid (three-letter code: QUJ) (formula:  $C_{14}H_{16}N_2O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			18	14	2	2		
8	A	1	Total	C	N	O	0	0
			19	14	2	3		
8	B	1	Total	C	N	O	0	0
			18	14	2	2		
8	B	1	Total	C	N	O	0	0
			15	10	2	3		

- Molecule 9 is FORMYL GROUP (three-letter code: FOR) (formula:  $CH_2O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			2	1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	289	Total	O	0	0
			289	289		
10	B	286	Total	O	0	0
			286	286		

### 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	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.73Å 54.81Å 84.70Å 90.00° 112.77° 90.00°	Depositor
Resolution (Å)	45.85 – 1.42 45.85 – 1.42	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.85-1.42) 99.0 (45.85-1.42)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.149 , 0.178 0.156 , 0.181	Depositor DCC
$R_{free}$ test set	6182 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	5064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, FOR, QVE, 6H0, QUK, QUJ, 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	0.69	0/2140	0.86	3/2911 (0.1%)
1	B	0.68	0/2159	0.87	2/2933 (0.1%)
All	All	0.68	0/4299	0.87	5/5844 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	PHE	CB-CG-CD2	-6.20	116.46	120.80
1	A	52	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	140	LEU	CB-CG-CD2	5.67	120.64	111.00
1	B	179	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	226	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	2070	0	1995	8	0
1	B	2083	0	2023	7	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	0	0	0
3	B	28	0	0	2	0
4	A	31	0	0	0	0
4	B	31	0	0	0	0
5	A	14	0	0	0	0
5	B	14	0	0	0	0
6	A	19	0	0	0	0
6	B	19	0	0	0	0
7	A	30	0	40	0	0
7	B	48	0	64	2	0
8	A	37	0	0	2	0
8	B	33	0	0	0	0
9	A	2	0	2	0	0
10	A	289	0	0	1	1
10	B	286	0	0	3	1
All	All	5064	0	4124	17	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (17) 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)
8:A:311:QUJ:N	3:B:303:6H0:C2	1.68	1.50
1:A:60[B]:LEU:O	1:A:60[B]:LEU:HD12	1.94	0.68
1:B:135:GLN:NE2	10:B:401:HOH:O	2.27	0.68
1:A:216[A]:SER:O	1:A:217[A]:VAL:HG13	2.01	0.61
1:A:135:GLN:NE2	10:A:402:HOH:O	2.36	0.56
1:A:60[B]:LEU:C	1:A:60[B]:LEU:HD12	2.25	0.56
1:A:60[B]:LEU:HD21	1:A:69:GLU:OE2	2.07	0.54
1:A:216[A]:SER:O	1:A:217[A]:VAL:CG1	2.59	0.50
8:A:311:QUJ:C2	3:B:303:6H0:C2	2.76	0.50
1:B:149[B]:VAL:HG12	10:B:497:HOH:O	2.11	0.49
1:B:54:ALA:HB3	7:B:312:GOL:H12	1.96	0.47
1:B:179:ASP:HA	7:B:312:GOL:H11	1.98	0.45
1:A:133:ALA:O	1:A:139:GLY:HA3	2.18	0.42
1:B:132:LYS:HG2	10:B:592:HOH:O	2.20	0.41
1:B:60[B]:LEU:C	1:B:60[B]:LEU:HD12	2.41	0.40
1:B:133:ALA:O	1:B:139:GLY:HA3	2.20	0.40
1:A:89:ARG:O	1:A:122:HIS:HA	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ASP:OD2	1:B:85:ASP:OD2[4_454]	2.17	0.03
10:A:547:HOH:O	10:B:449:HOH:O[3_445]	2.17	0.03

## 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	264/259 (102%)	258 (98%)	6 (2%)	0	100	100
1	B	265/259 (102%)	259 (98%)	6 (2%)	0	100	100
All	All	529/518 (102%)	517 (98%)	12 (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	218/224 (97%)	218 (100%)	0	100	100
1	B	223/224 (100%)	223 (100%)	0	100	100
All	All	441/448 (98%)	441 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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	$\# Z  > 2$
3	6H0	A	302	8,2	29,29,29	2.22	8 (27%)	37,38,38	2.31	13 (35%)
3	6H0	B	303	2	29,29,29	1.83	9 (31%)	37,38,38	1.26	2 (5%)
5	QVS	A	304	4,6	15,15,16	1.75	2 (13%)	19,21,23	1.99	6 (31%)
7	GOL	A	307	-	5,5,5	0.52	0	5,5,5	0.60	0
7	GOL	B	313	-	5,5,5	0.28	0	5,5,5	0.44	0
7	GOL	B	307	-	5,5,5	0.52	0	5,5,5	0.41	0
8	QUJ	A	311	4	19,19,20	1.74	2 (10%)	23,26,28	2.18	4 (17%)
8	QUJ	B	314	4	13,16,20	1.28	2 (15%)	17,23,28	2.09	5 (29%)
6	QVE	B	306	5	14,20,20	0.75	0	18,28,28	2.55	6 (33%)
7	GOL	B	311	-	5,5,5	0.30	0	5,5,5	0.82	0
7	GOL	A	310	-	5,5,5	0.15	0	5,5,5	0.69	0
7	GOL	B	308[B]	-	5,5,5	0.39	0	5,5,5	0.62	0
7	GOL	A	308	-	5,5,5	0.44	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	QVS	B	305	4,6	15,15,16	1.89	2 (13%)	19,21,23	2.56	4 (21%)
7	GOL	B	308[A]	-	5,5,5	0.62	0	5,5,5	0.83	0
8	QUJ	A	314	4	17,20,20	1.13	2 (11%)	21,28,28	2.02	6 (28%)
4	QUK	A	303	8,5	18,18,20	1.64	2 (11%)	21,24,27	2.39	5 (23%)
4	QUK	A	313	9,8	15,15,20	1.71	2 (13%)	19,21,27	4.17	7 (36%)
4	QUK	B	315	9,8	15,15,20	1.51	1 (6%)	19,21,27	3.26	7 (36%)
6	QVE	A	305	5	14,20,20	0.99	1 (7%)	18,28,28	1.95	6 (33%)
7	GOL	B	309	-	5,5,5	0.37	0	5,5,5	0.40	0
7	GOL	A	306	-	5,5,5	0.42	0	5,5,5	0.88	0
7	GOL	B	312	-	5,5,5	0.38	0	5,5,5	0.48	0
7	GOL	A	309	-	5,5,5	0.22	0	5,5,5	0.65	0
7	GOL	B	310	-	5,5,5	0.64	0	5,5,5	0.53	0
8	QUJ	B	301	3,4	19,19,20	1.60	2 (10%)	23,26,28	2.45	5 (21%)
9	FOR	A	312	4	0,1,1	0.00	-	-	-	-
4	QUK	B	304	8,5	18,18,20	1.77	2 (11%)	21,24,27	2.58	6 (28%)

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	6H0	A	302	8,2	-	4/23/23/23	0/2/2/2
3	6H0	B	303	2	-	4/23/23/23	0/2/2/2
5	QVS	A	304	4,6	-	0/2/2/4	0/2/2/2
7	GOL	A	307	-	-	0/4/4/4	-
7	GOL	B	313	-	-	0/4/4/4	-
7	GOL	B	307	-	-	0/4/4/4	-
8	QUJ	A	311	4	-	0/7/7/9	0/2/2/2
8	QUJ	B	314	4	-	0/0/4/9	0/2/2/2
6	QVE	B	306	5	-	3/3/9/9	0/2/2/2
7	GOL	B	311	-	-	2/4/4/4	-
7	GOL	A	310	-	-	0/4/4/4	-
7	GOL	B	308[B]	-	-	1/4/4/4	-
7	GOL	A	308	-	-	0/4/4/4	-
5	QVS	B	305	4,6	-	0/2/2/4	0/2/2/2
7	GOL	B	308[A]	-	-	0/4/4/4	-
8	QUJ	A	314	4	-	3/5/9/9	0/2/2/2
4	QUK	A	303	8,5	-	0/6/6/9	0/2/2/2
4	QUK	A	313	9,8	-	0/2/2/9	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	QUK	B	315	9,8	-	0/2/2/9	0/2/2/2
6	QVE	A	305	5	-	0/3/9/9	0/2/2/2
7	GOL	B	309	-	-	0/4/4/4	-
7	GOL	A	306	-	-	0/4/4/4	-
7	GOL	B	312	-	-	4/4/4/4	-
7	GOL	A	309	-	-	0/4/4/4	-
7	GOL	B	310	-	-	0/4/4/4	-
8	QUJ	B	301	3,4	-	0/7/7/9	0/2/2/2
4	QUK	B	304	8,5	-	1/6/6/9	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	304	QUK	C10-C	-6.44	1.41	1.48
8	A	311	QUJ	C10-C	-6.31	1.42	1.48
3	A	302	6H0	O27-S24	6.09	1.55	1.43
8	B	301	QUJ	C10-C	-5.96	1.42	1.48
4	A	303	QUK	C10-C	-5.83	1.42	1.48
5	B	305	QVS	C10-C	-5.78	1.42	1.48
5	A	304	QVS	C10-C	-5.14	1.43	1.48
3	A	302	6H0	O25-S24	4.93	1.52	1.43
4	A	313	QUK	C10-C	-4.81	1.43	1.48
3	B	303	6H0	S24-N26	-4.42	1.51	1.60
4	B	315	QUK	C10-C	-4.42	1.44	1.48
3	A	302	6H0	C14-C12	-4.17	1.42	1.51
5	B	305	QVS	C10-N11	3.90	1.37	1.33
5	A	304	QVS	C10-N11	3.79	1.37	1.33
3	B	303	6H0	C14-C12	-3.56	1.43	1.51
3	A	302	6H0	C19-C18	3.43	1.45	1.39
3	A	302	6H0	C22-C21	3.22	1.43	1.38
3	B	303	6H0	O27-S24	3.19	1.49	1.43
3	B	303	6H0	C21-S24	-2.97	1.72	1.77
3	A	302	6H0	C18-C16	-2.93	1.44	1.50
3	B	303	6H0	C23-C18	2.87	1.44	1.39
3	A	302	6H0	S24-N26	-2.70	1.55	1.60
8	A	311	QUJ	C2-C7	-2.53	1.38	1.42
4	B	304	QUK	C10-N11	2.50	1.35	1.33
4	A	303	QUK	C10-N11	2.49	1.35	1.33
4	A	313	QUK	C4-C5	2.48	1.42	1.36
3	B	303	6H0	C19-C18	2.47	1.43	1.39
6	A	305	QVE	C10-N11	2.37	1.36	1.33
3	B	303	6H0	O25-S24	2.35	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	6H0	O17-C16	2.35	1.28	1.23
3	B	303	6H0	C13-C8	2.32	1.43	1.38
8	B	301	QUJ	C10-N11	2.27	1.35	1.33
8	A	314	QUJ	C2-C7	-2.17	1.38	1.42
8	B	314	QUJ	C3-C2	2.12	1.43	1.38
8	A	314	QUJ	C5-C6	-2.11	1.37	1.42
8	B	314	QUJ	C2-C7	-2.10	1.38	1.42
3	B	303	6H0	C16-N15	2.05	1.38	1.33

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	313	QUK	C-C10-N11	12.25	126.67	114.66
4	B	304	QUK	C10-N11-C7	8.68	124.69	118.11
3	A	302	6H0	C19-C20-C21	8.34	128.08	119.45
4	A	313	QUK	C10-N11-C7	8.32	124.42	118.11
4	B	315	QUK	C10-N11-C7	8.21	124.33	118.11
4	B	315	QUK	C-C10-N11	7.88	122.38	114.66
8	B	301	QUJ	C10-N11-C7	7.79	124.02	118.11
4	A	303	QUK	C10-N11-C7	7.47	123.78	118.11
5	B	305	QVS	C10-N11-C7	7.34	123.67	118.11
6	B	306	QVE	C10-N11-C7	7.31	123.87	118.26
8	A	311	QUJ	C10-N11-C7	6.73	123.22	118.11
8	B	301	QUJ	C-C10-N11	6.21	120.74	114.66
8	A	311	QUJ	C-C10-N11	5.49	120.04	114.66
4	A	313	QUK	C3-C2-N	5.49	131.33	120.36
6	A	305	QVE	C10-N11-C7	5.09	122.17	118.26
3	B	303	6H0	O1-C2-N3	5.07	130.01	124.89
4	A	313	QUK	C7-C2-N	-4.96	108.61	118.07
8	A	314	QUJ	C10-N11-C7	4.89	122.01	118.26
4	A	303	QUK	C-C10-N11	4.81	119.37	114.66
4	B	304	QUK	C-C10-N11	4.77	119.34	114.66
4	B	315	QUK	OB-C8-C6	4.77	122.27	116.31
5	A	304	QVS	C10-N11-C7	4.62	121.61	118.11
5	B	305	QVS	C-C10-N11	4.60	119.17	114.66
6	B	306	QVE	C9-C10-N11	-4.46	118.16	122.23
8	B	314	QUJ	C3-C2-N	4.46	129.28	120.36
8	B	314	QUJ	C10-N11-C7	4.40	121.63	118.26
4	A	313	QUK	OB-C8-C6	4.31	121.69	116.31
3	A	302	6H0	C21-S24-N26	-4.20	102.45	108.38
4	A	313	QUK	C9-C10-C	-4.19	117.60	121.23
5	B	305	QVS	O-C-C10	-4.02	120.42	124.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	QUK	O-C-C10	-3.99	120.44	124.22
8	A	314	QUJ	C3-C2-N	3.95	128.27	120.36
4	B	315	QUK	C3-C2-N	3.95	128.26	120.36
8	A	311	QUJ	O-C-C10	-3.91	120.52	124.22
3	A	302	6H0	C20-C19-C18	-3.89	116.25	120.78
6	B	306	QVE	CG-OB-C8	3.86	122.99	117.56
3	A	302	6H0	O25-S24-N26	3.76	112.93	107.36
3	A	302	6H0	C22-C23-C18	3.73	125.12	120.78
5	B	305	QVS	C3-C2-N	3.72	127.79	120.36
5	A	304	QVS	C-C10-N11	3.71	118.30	114.66
4	B	304	QUK	O-C-C10	-3.57	120.84	124.22
8	B	301	QUJ	O-C-C10	-3.54	120.87	124.22
5	A	304	QVS	C3-C2-N	3.48	127.31	120.36
6	A	305	QVE	CG-OB-C8	3.45	122.40	117.56
4	A	313	QUK	C8-C9-C10	3.37	122.32	119.05
8	B	314	QUJ	C7-C2-N	-3.17	112.03	118.07
8	B	301	QUJ	C3-C2-N	3.13	126.62	120.36
5	A	304	QVS	O-C-C10	-3.13	121.26	124.22
4	B	315	QUK	C8-C9-C10	3.11	122.07	119.05
8	A	314	QUJ	C7-C2-N	-3.07	112.22	118.07
4	B	315	QUK	C7-C2-N	-3.00	112.34	118.07
8	A	314	QUJ	C9-C10-N11	-3.00	119.50	122.23
3	A	302	6H0	O27-S24-N26	2.85	111.59	107.36
4	B	304	QUK	CG-OB-C8	2.82	126.16	117.74
3	A	302	6H0	O1-C2-N3	-2.80	122.06	124.89
3	A	302	6H0	C23-C22-C21	-2.77	116.58	119.45
8	A	314	QUJ	C2-C7-N11	2.72	121.33	118.64
4	B	315	QUK	O-C-C10	-2.68	121.68	124.22
6	B	306	QVE	C3-C2-N	2.67	125.70	120.36
4	A	303	QUK	C3-C2-N	2.58	125.52	120.36
4	B	304	QUK	C3-C2-N	2.57	125.49	120.36
3	A	302	6H0	O25-S24-C21	-2.53	104.52	107.35
6	A	305	QVE	C3-C2-N	2.52	125.41	120.36
6	A	305	QVE	C9-C10-N11	-2.44	120.00	122.23
5	A	304	QVS	OB-C8-C6	2.44	119.35	116.31
8	B	314	QUJ	OB-C8-C6	2.43	119.34	116.31
8	B	314	QUJ	C9-C10-N11	-2.39	120.05	122.23
8	A	314	QUJ	CG-OB-C8	2.38	126.02	118.25
4	A	303	QUK	CG-OB-C8	2.34	124.72	117.74
3	A	302	6H0	C18-C16-N15	2.32	122.06	117.09
8	A	311	QUJ	C9-C10-C	2.28	123.20	121.23
8	B	301	QUJ	CG-OB-C8	2.24	125.57	118.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	6H0	C22-C21-C20	-2.24	117.32	120.44
3	A	302	6H0	C14-N15-C16	2.20	127.02	121.81
3	A	302	6H0	C20-C21-S24	2.19	122.91	119.73
3	B	303	6H0	O27-S24-N26	2.18	110.59	107.36
6	B	306	QVE	C6-C7-N11	-2.11	118.42	122.78
6	B	306	QVE	OB-C8-C6	2.10	120.87	115.01
5	A	304	QVS	C7-C2-N	-2.05	114.15	118.07
4	B	304	QUK	C6-C7-N11	-2.04	118.57	122.78
6	A	305	QVE	C6-C7-N11	-2.03	118.60	122.78
6	A	305	QVE	OB-C8-C6	2.00	120.62	115.01

There are no chirality outliers.

All (22) torsion outliers are listed below:

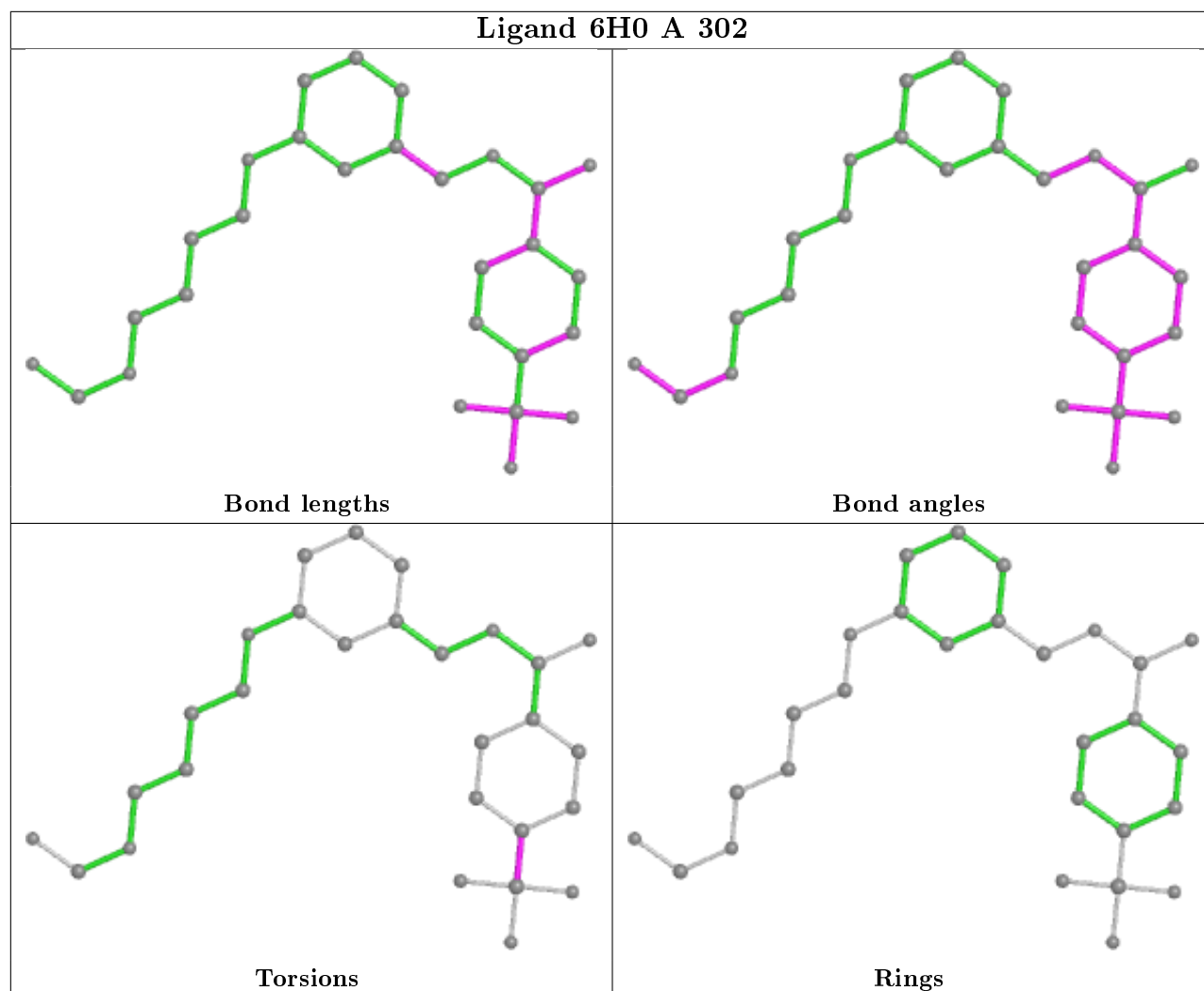
Mol	Chain	Res	Type	Atoms
7	B	312	GOL	O1-C1-C2-O2
7	B	312	GOL	O1-C1-C2-C3
4	B	304	QUK	O-C-C10-C9
6	B	306	QVE	C6-C8-OB-CG
6	B	306	QVE	C9-C8-OB-CG
7	B	311	GOL	O1-C1-C2-C3
7	B	312	GOL	C1-C2-C3-O3
7	B	312	GOL	O2-C2-C3-O3
3	A	302	6H0	C20-C21-S24-O25
8	A	314	QUJ	CE1-CD-CG-OB
7	B	311	GOL	O1-C1-C2-O2
3	A	302	6H0	C20-C21-S24-N26
3	A	302	6H0	C22-C21-S24-O25
3	B	303	6H0	C20-C21-S24-O25
3	B	303	6H0	C22-C21-S24-O25
8	A	314	QUJ	CD-CG-OB-C8
6	B	306	QVE	CD-CG-OB-C8
7	B	308[B]	GOL	O1-C1-C2-C3
8	A	314	QUJ	CE2-CD-CG-OB
3	A	302	6H0	C22-C21-S24-N26
3	B	303	6H0	C20-C21-S24-N26
3	B	303	6H0	C22-C21-S24-N26

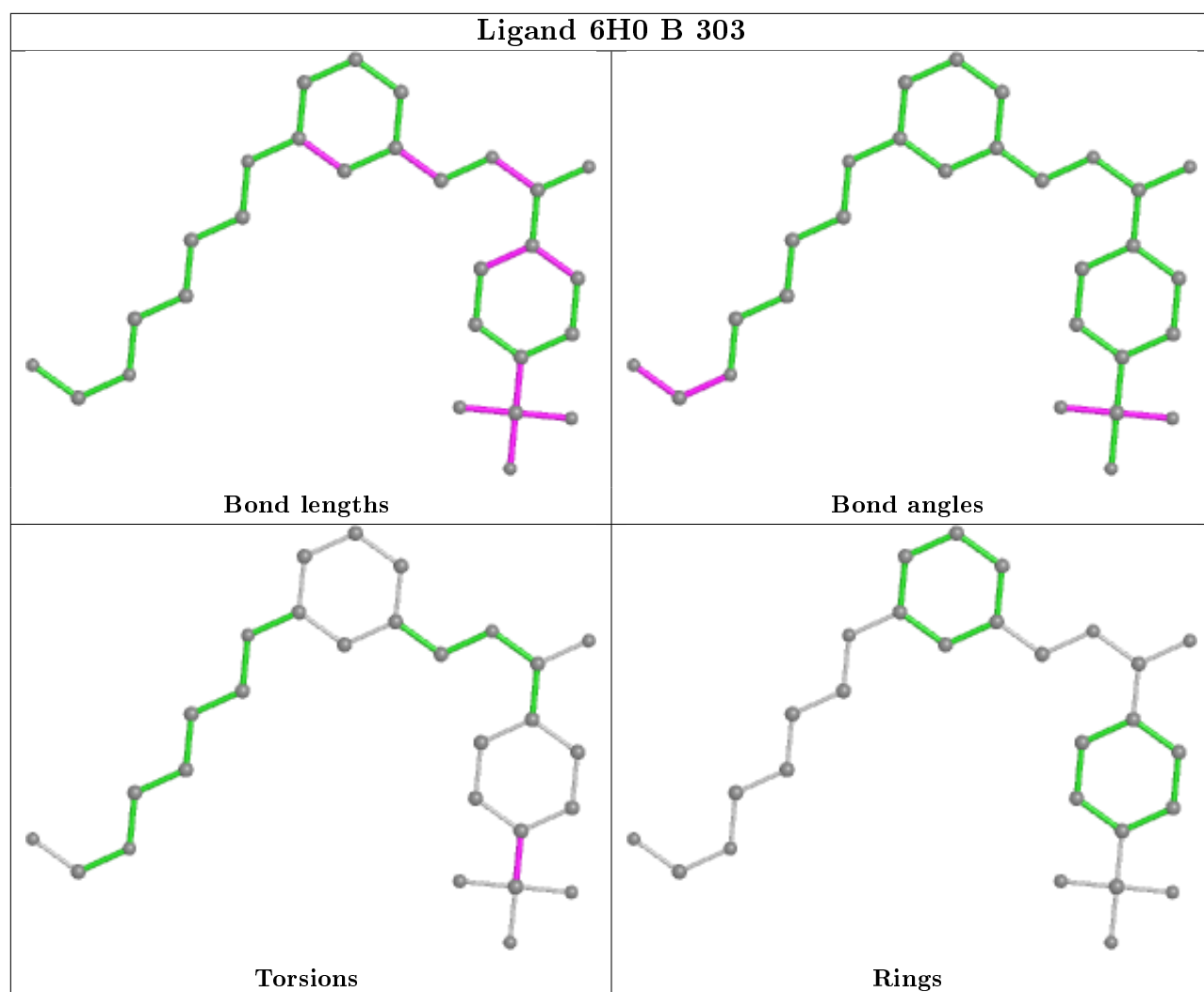
There are no ring outliers.

3 monomers are involved in 4 short contacts:

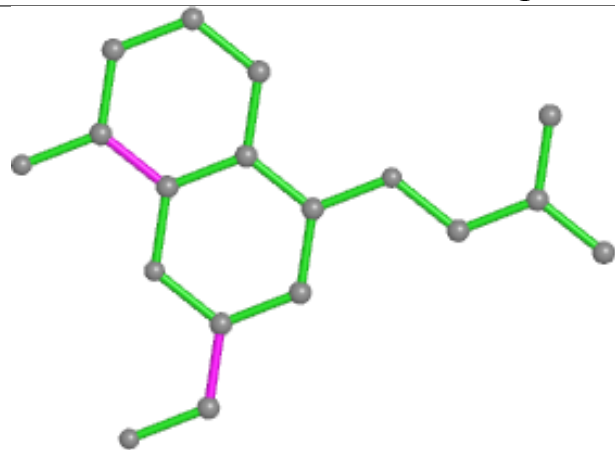
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	6H0	2	0
8	A	311	QUJ	2	0
7	B	312	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

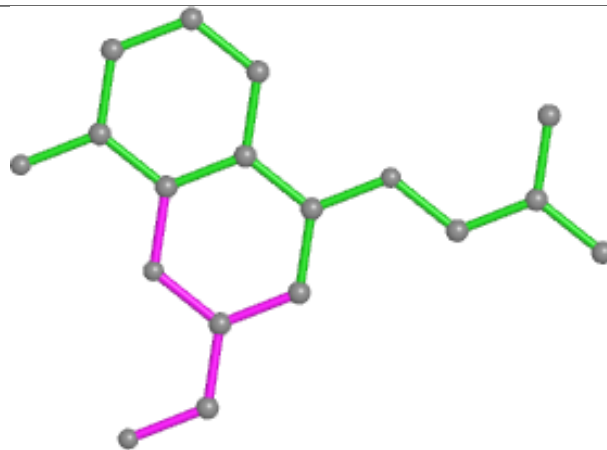




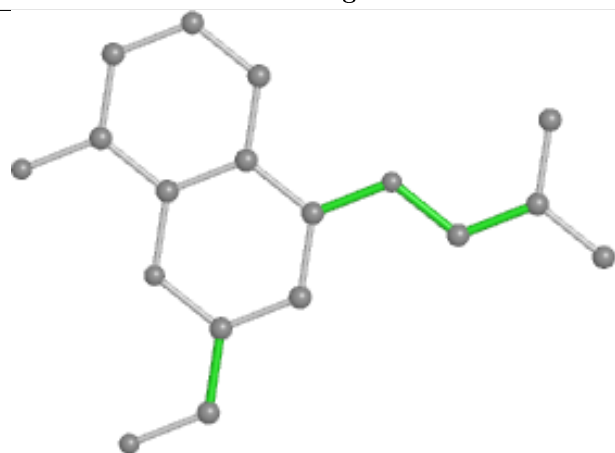
## Ligand QUJ A 311



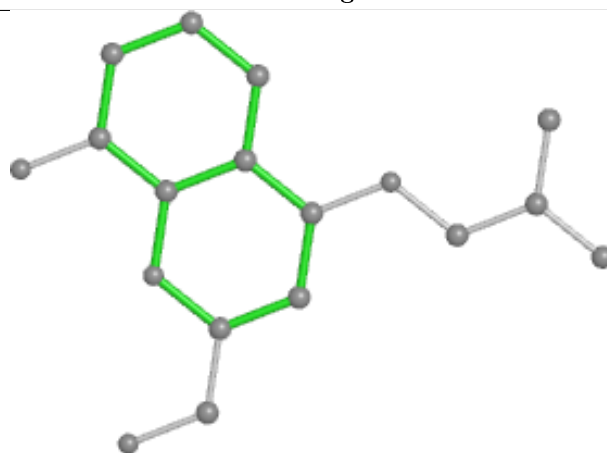
Bond lengths



Bond angles

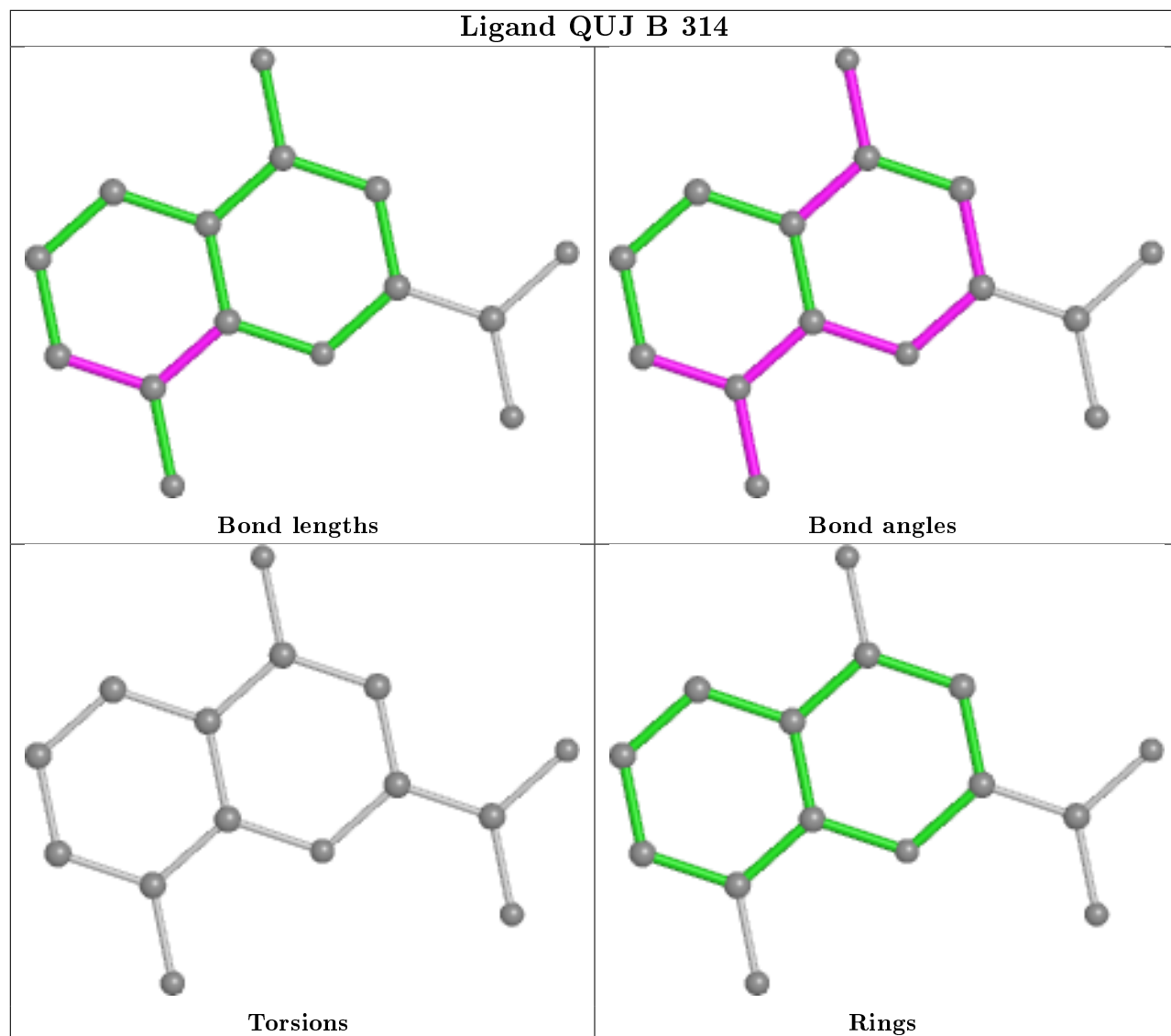


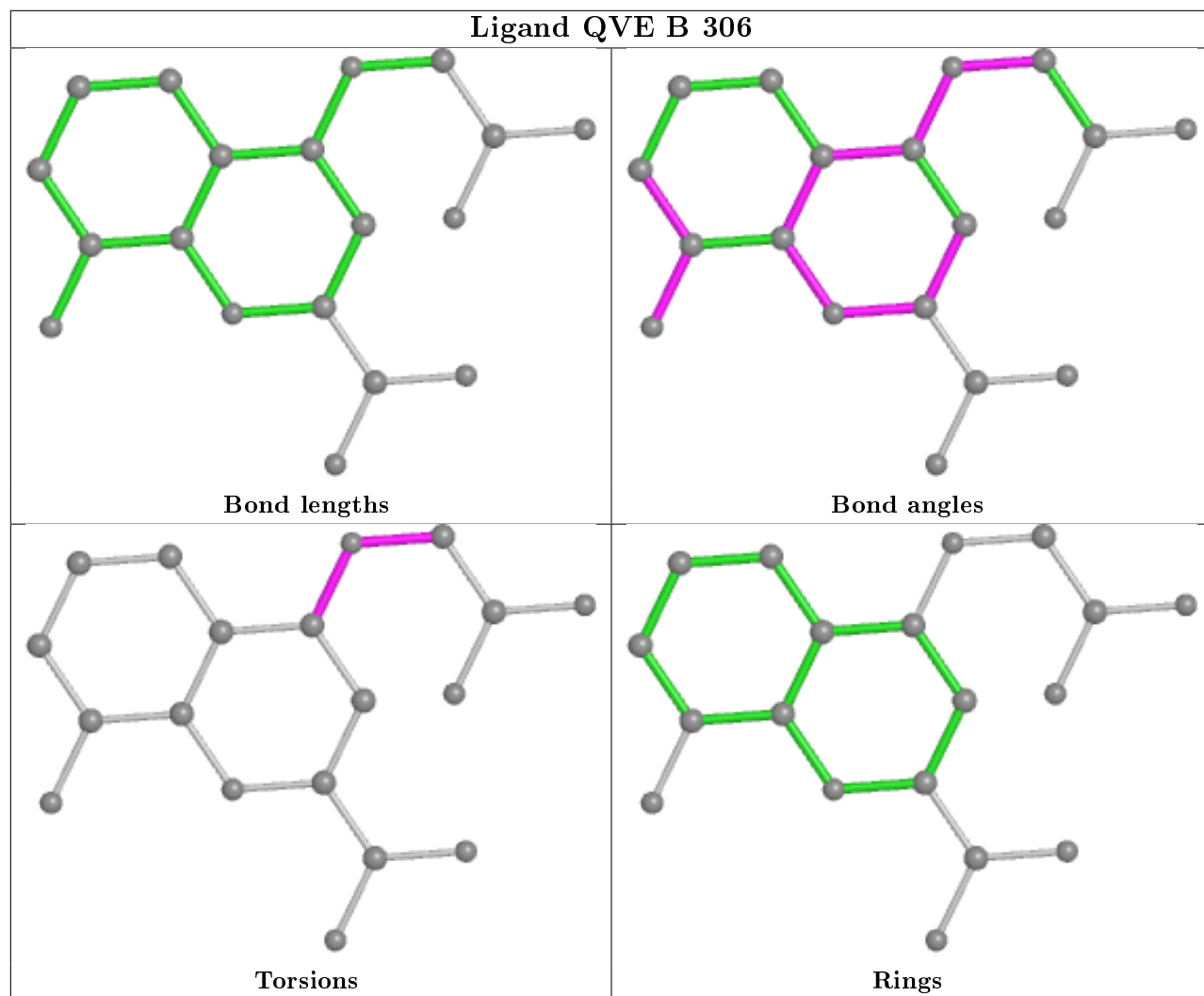
Torsions



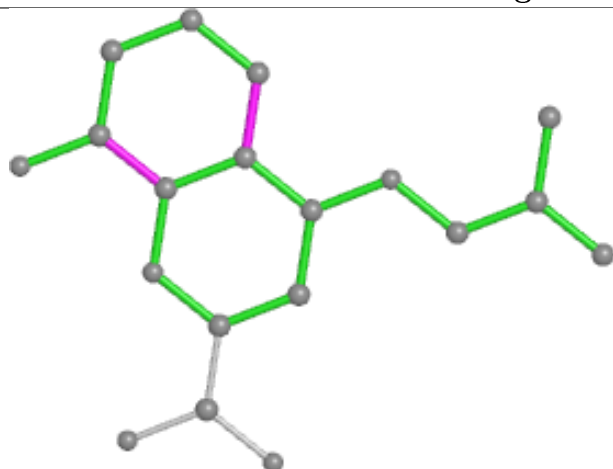
Rings

## Ligand QUJ B 314

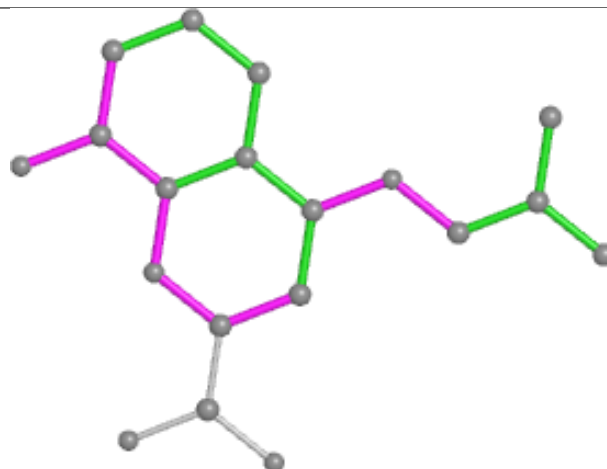




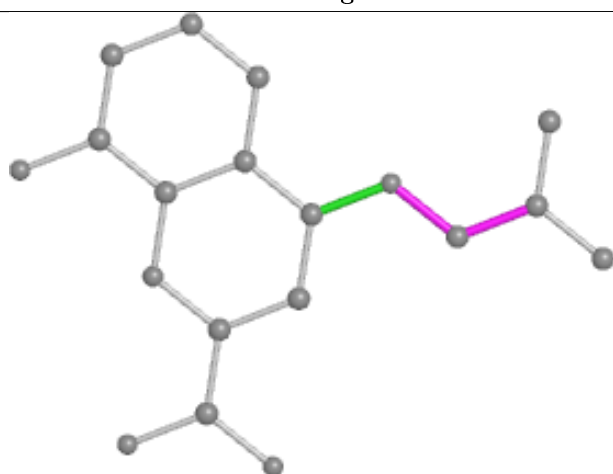
## Ligand QUJ A 314



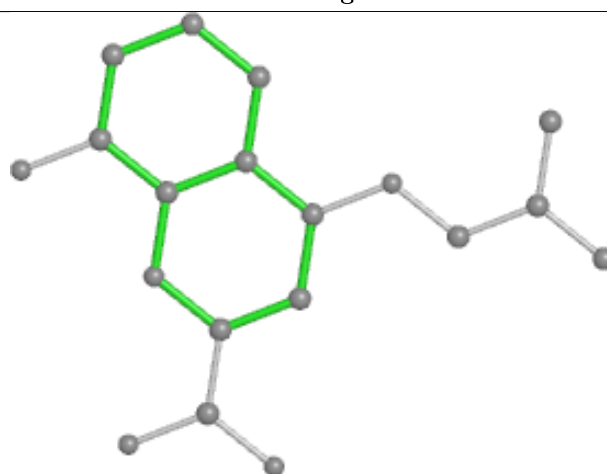
Bond lengths



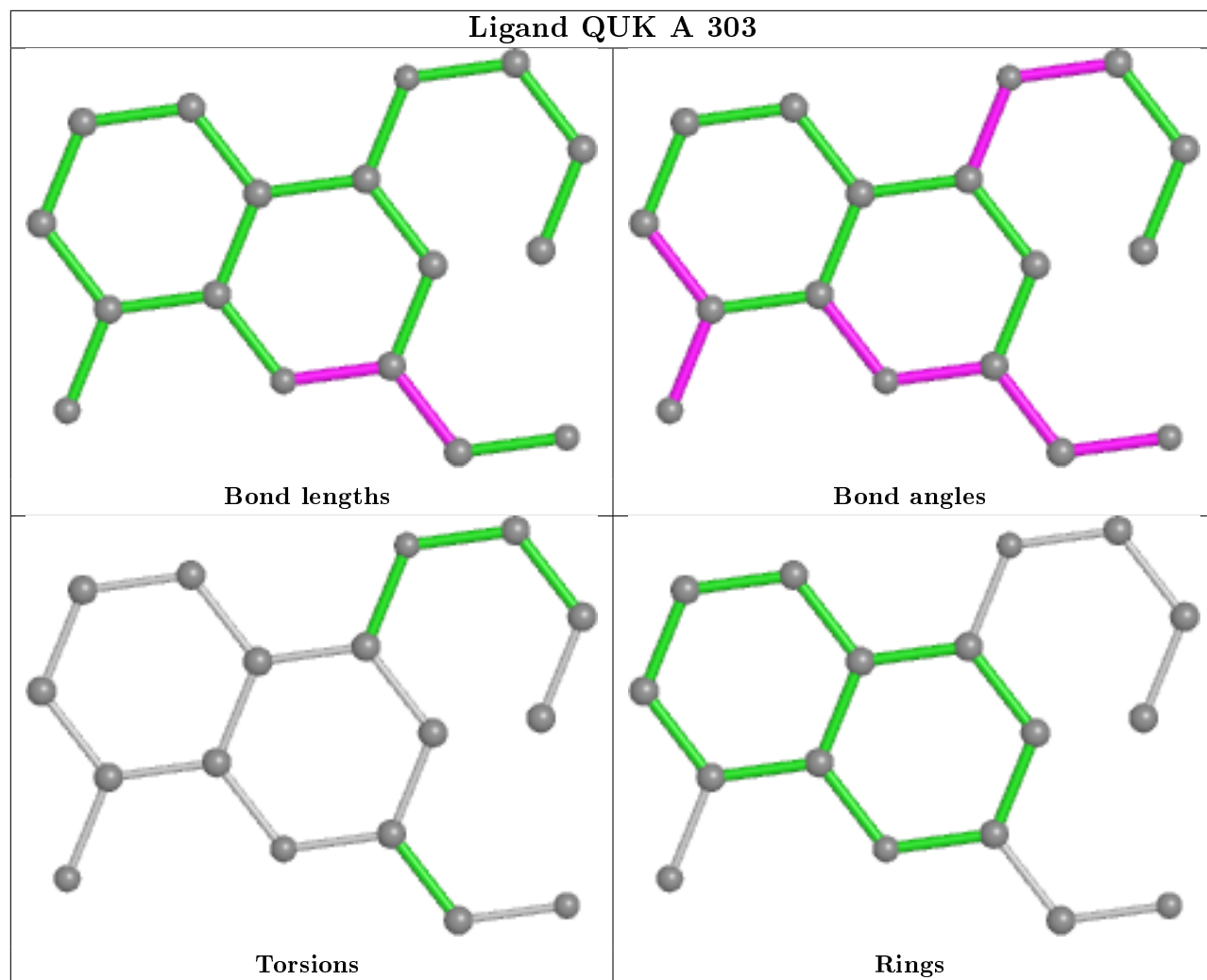
Bond angles

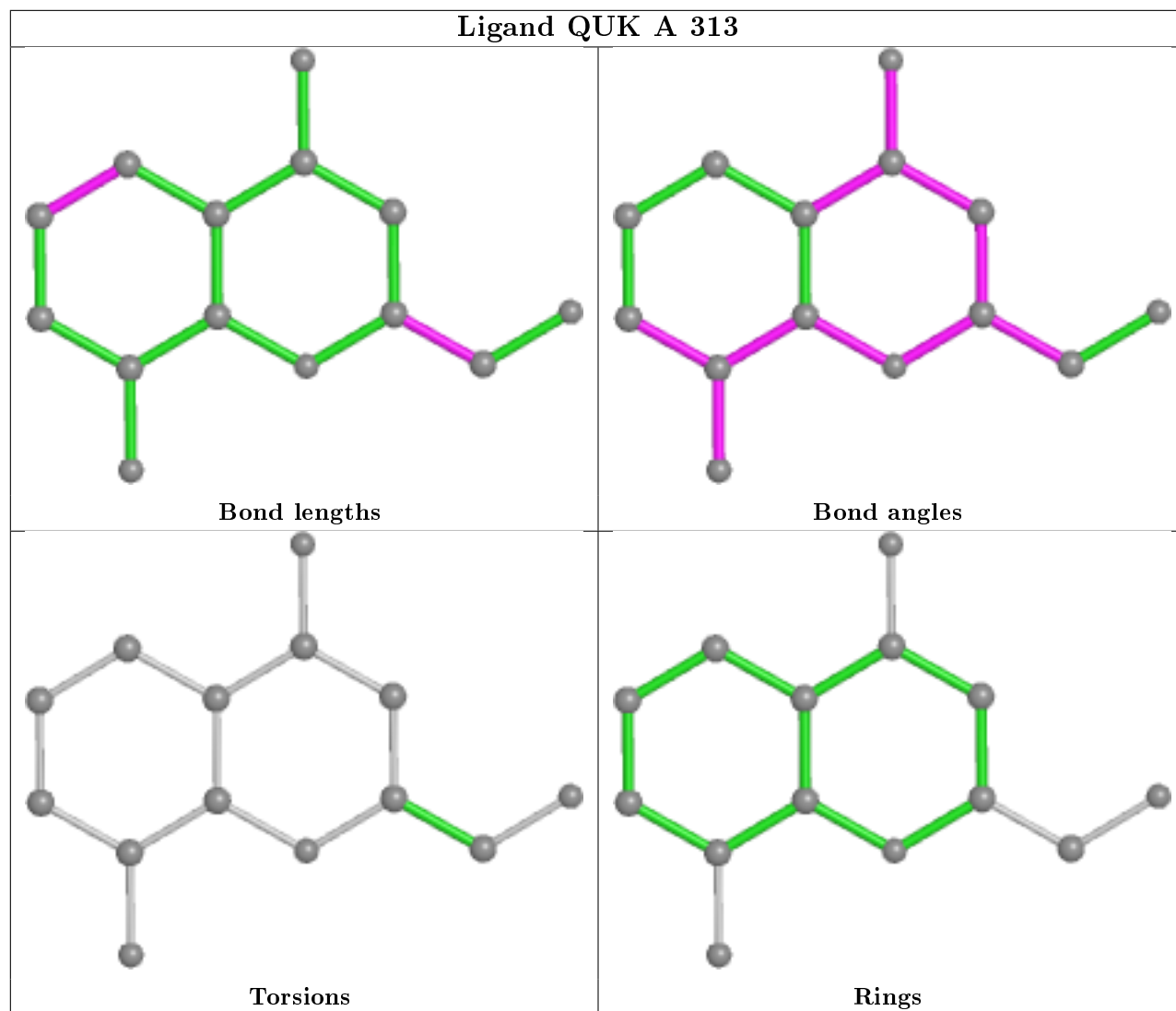


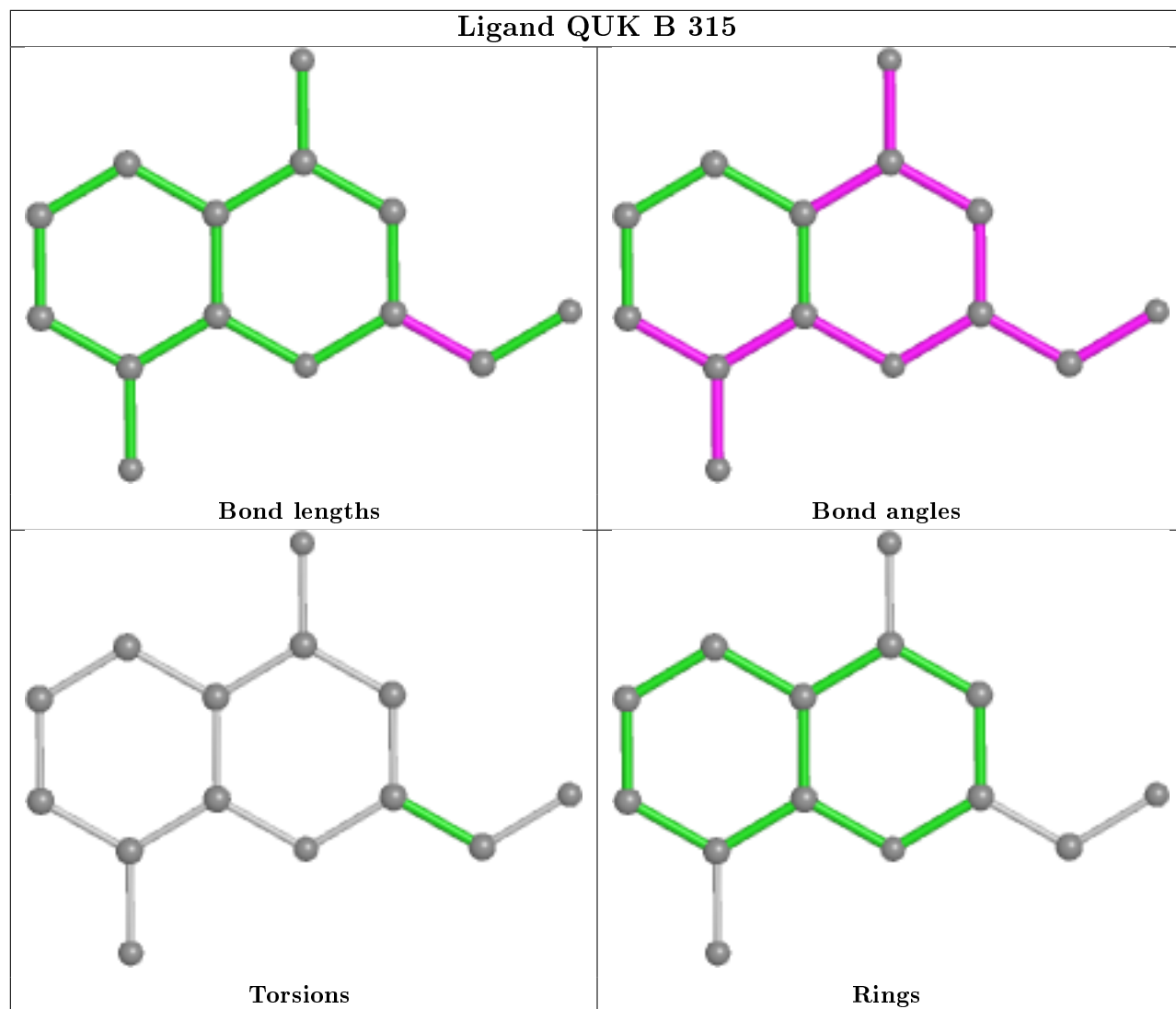
Torsions

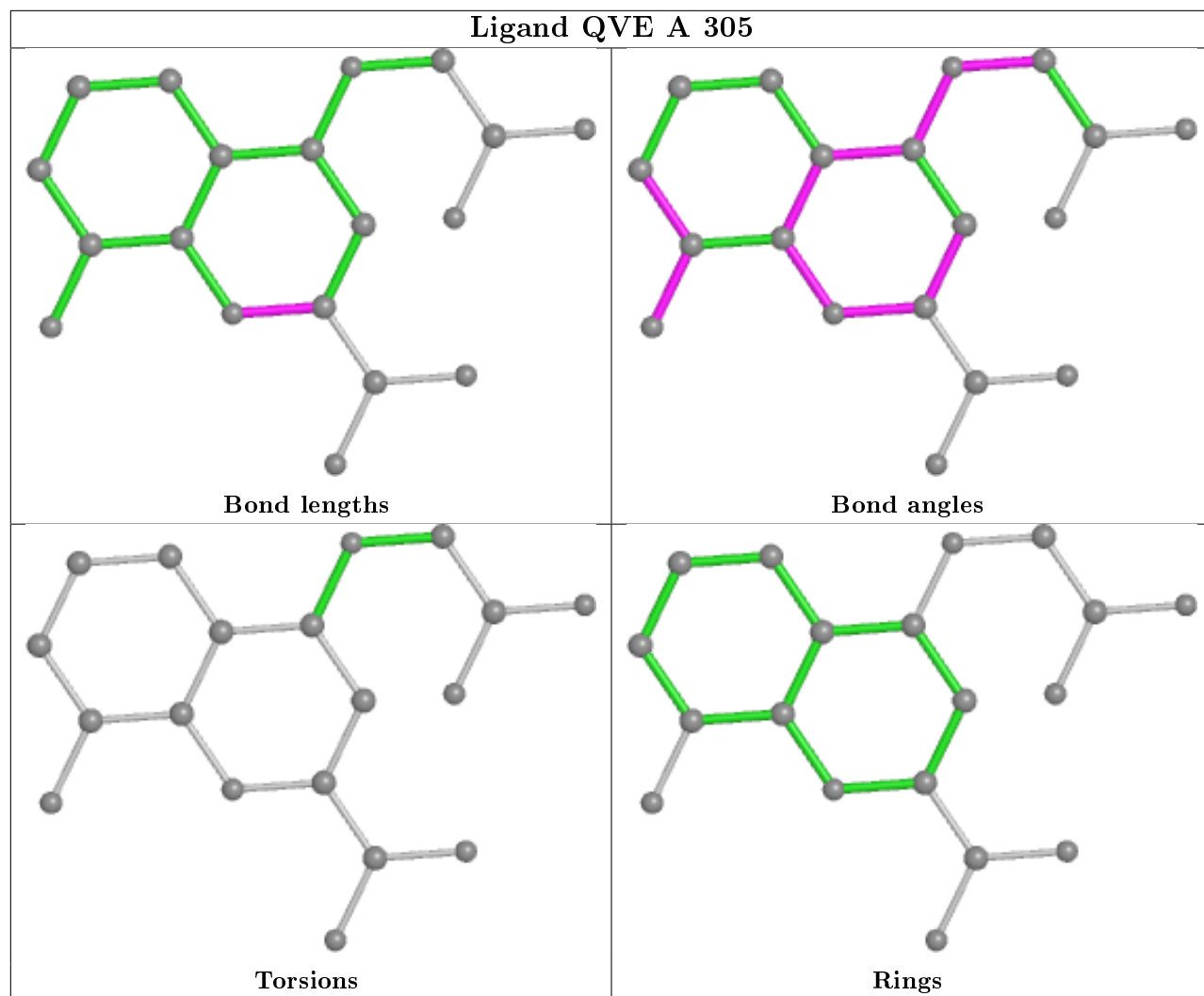


Rings

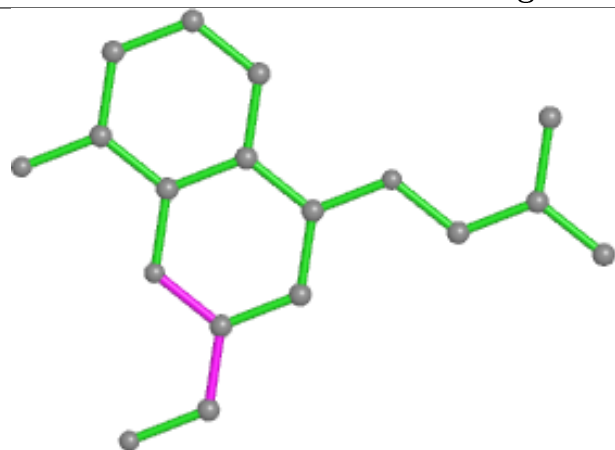




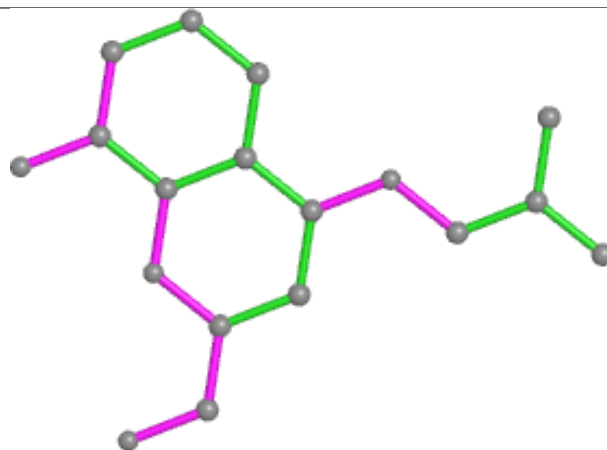




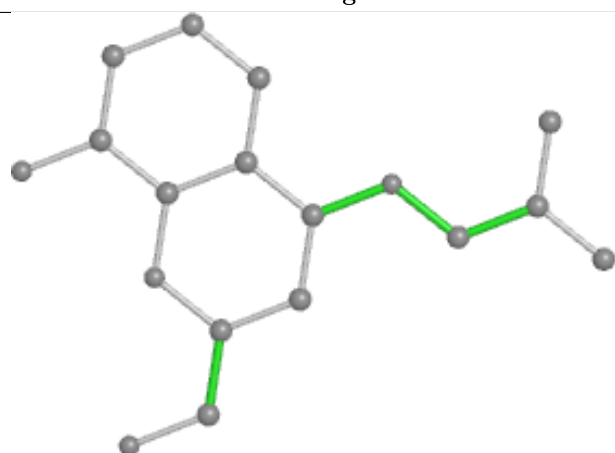
## Ligand QUJ B 301



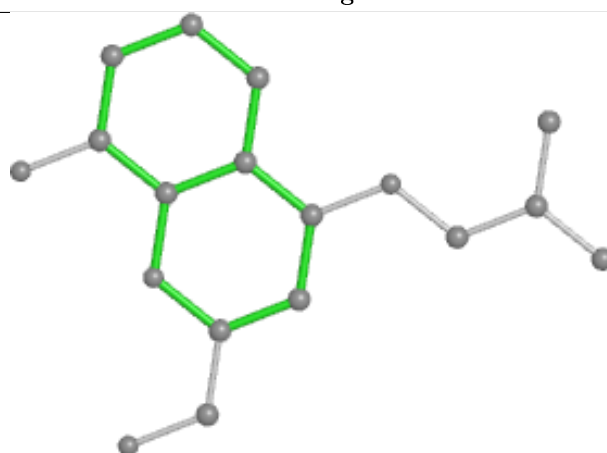
Bond lengths



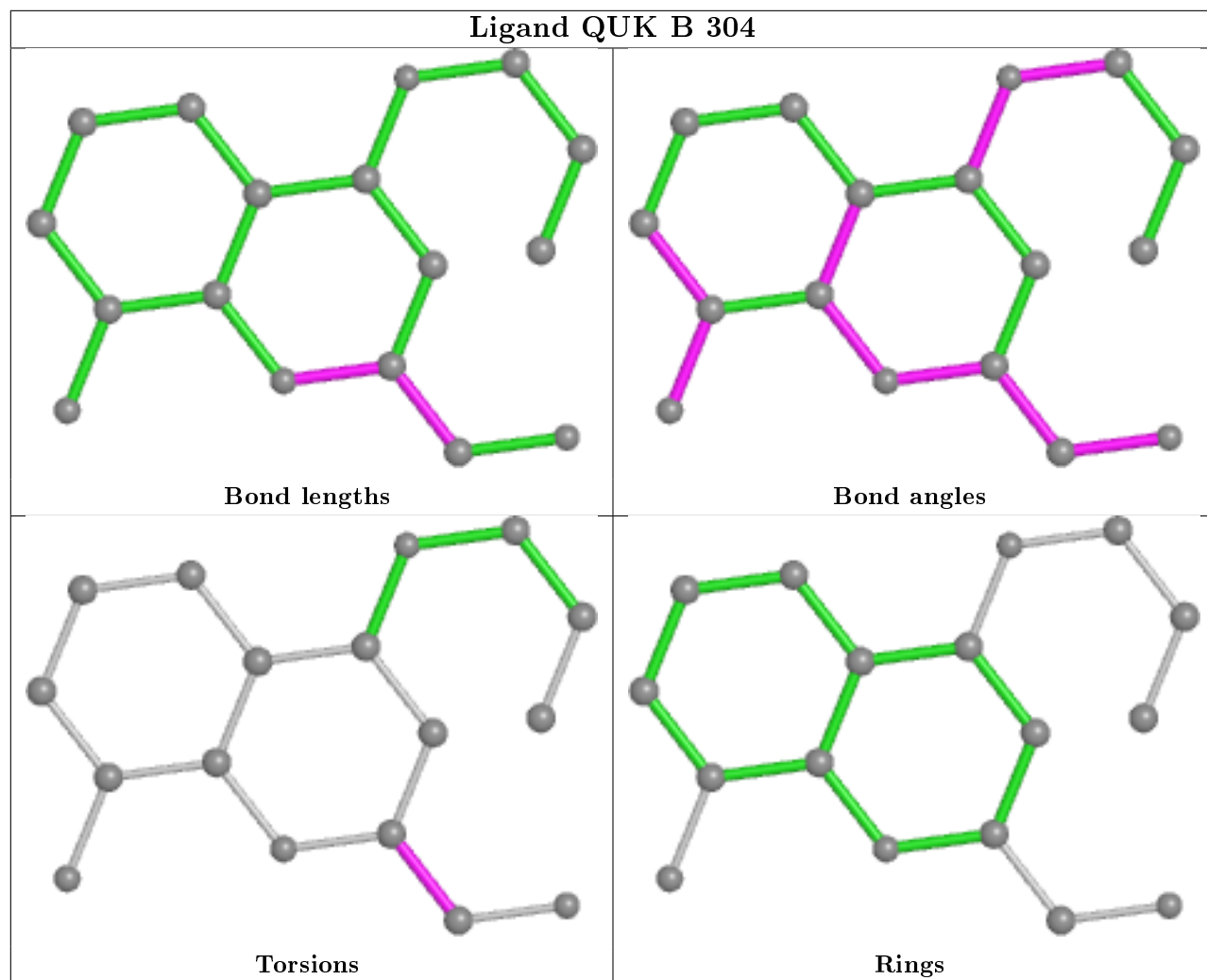
Bond angles



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	259/259 (100%)	0.34	4 (1%) 73 72	19, 26, 42, 55	0
1	B	259/259 (100%)	0.31	4 (1%) 73 72	18, 25, 40, 57	0
All	All	518/518 (100%)	0.33	8 (1%) 73 72	18, 25, 41, 57	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	HIS	4.1
1	B	40	TYR	3.7
1	A	234	GLY	3.7
1	B	252	ASN	2.8
1	B	42	PRO	2.6
1	A	36	HIS	2.6
1	A	40	TYR	2.3
1	A	236	PRO	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

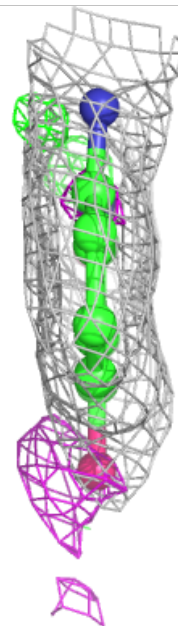
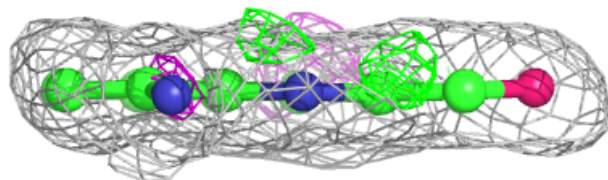
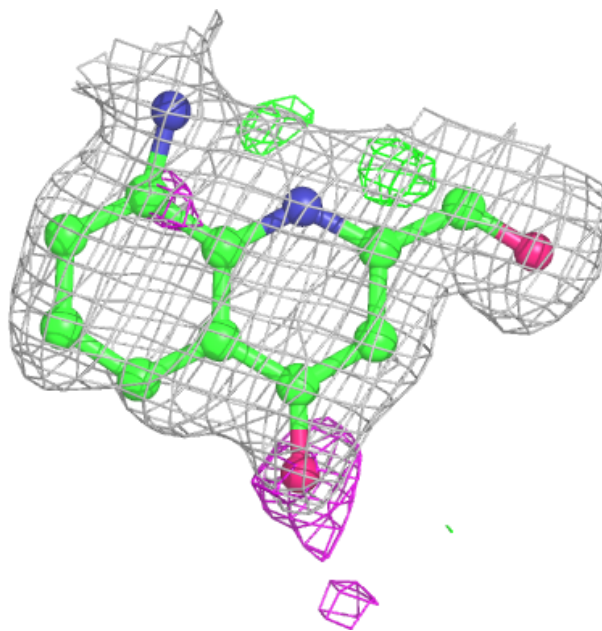
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	A	310	6/6	0.82	0.22	31,33,40,44	0
7	GOL	B	310	6/6	0.83	0.23	36,40,45,48	0
7	GOL	B	313	6/6	0.84	0.26	31,34,39,47	0
7	GOL	A	306	6/6	0.86	0.25	31,33,37,41	0
7	GOL	B	312	6/6	0.86	0.18	38,39,41,45	0
7	GOL	B	307	6/6	0.86	0.26	37,38,43,46	0
7	GOL	B	308[A]	6/6	0.89	0.17	17,19,20,25	6
7	GOL	B	308[B]	6/6	0.89	0.17	11,12,17,19	6
7	GOL	A	309	6/6	0.90	0.16	27,35,42,48	0
7	GOL	B	311	6/6	0.91	0.15	25,29,31,41	1
4	QUK	A	313	14/19	0.91	0.16	24,33,39,42	0
7	GOL	A	308	6/6	0.91	0.17	28,29,30,35	0
7	GOL	B	309	6/6	0.93	0.12	27,29,31,36	0
6	QVE	A	305	19/19	0.94	0.10	26,32,56,62	0
8	QUJ	A	314	19/19	0.94	0.11	21,30,38,43	0
4	QUK	B	315	14/19	0.94	0.11	24,31,39,39	0
7	GOL	A	307	6/6	0.95	0.11	18,20,22,25	0
8	QUJ	B	314	15/19	0.95	0.09	24,29,41,42	0
6	QVE	B	306	19/19	0.96	0.13	27,31,63,65	0
4	QUK	A	303	17/19	0.96	0.10	24,29,39,47	0
9	FOR	A	312	2/2	0.96	0.15	44,44,44,45	0
4	QUK	B	304	17/19	0.96	0.08	27,31,41,42	0
3	6H0	A	302	28/28	0.97	0.10	18,22,26,26	0
8	QUJ	A	311	18/19	0.97	0.08	25,28,36,39	0
5	QVS	B	305	14/15	0.97	0.09	23,24,27,32	0
5	QVS	A	304	14/15	0.97	0.08	22,23,26,30	0
3	6H0	B	303	28/28	0.98	0.09	19,24,28,30	0
8	QUJ	B	301	18/19	0.98	0.08	24,25,40,40	0
2	ZN	A	301	1/1	0.99	0.15	18,18,18,18	0
2	ZN	B	302	1/1	0.99	0.14	19,19,19,19	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.

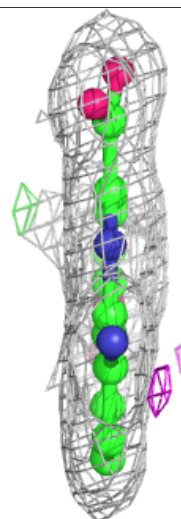
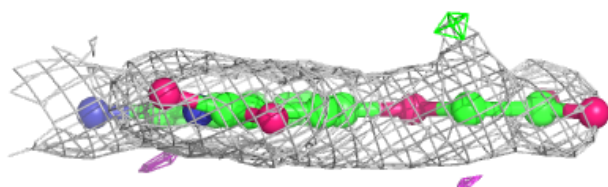
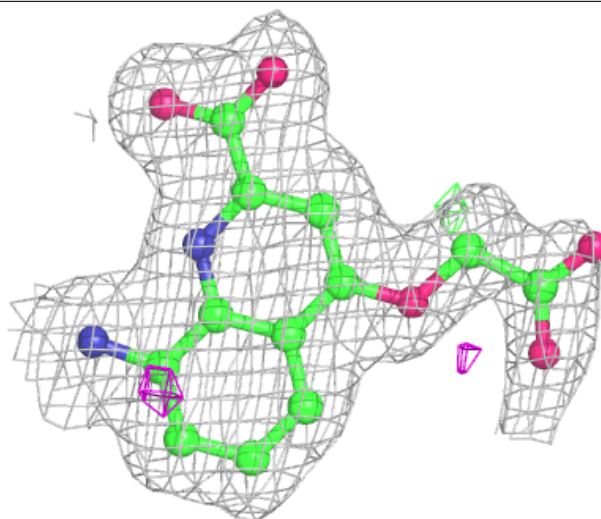
**Electron density around QUK A 313:**

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



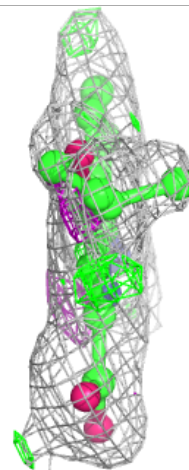
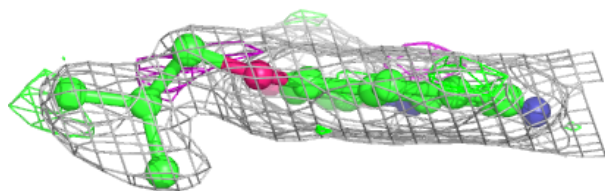
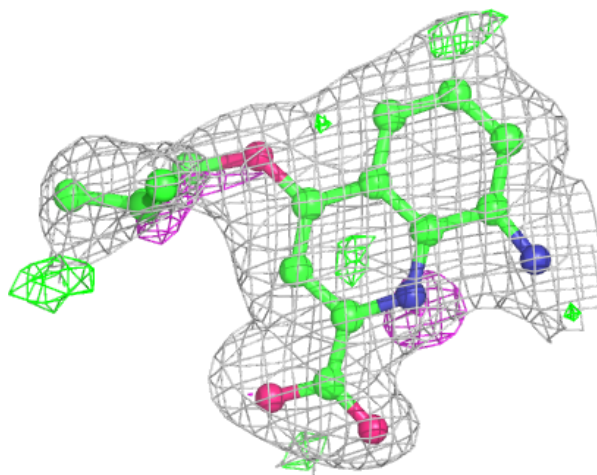
**Electron density around QVE A 305:**

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



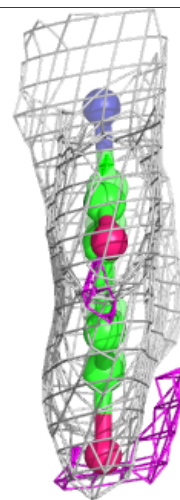
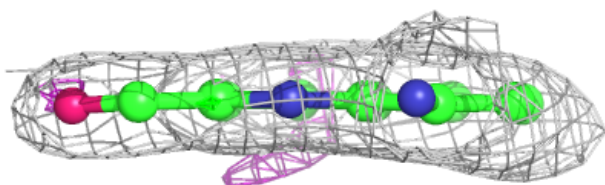
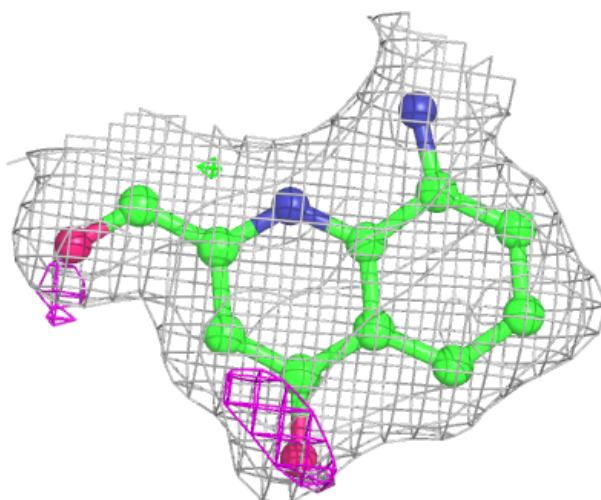
**Electron density around QUJ A 314:**

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



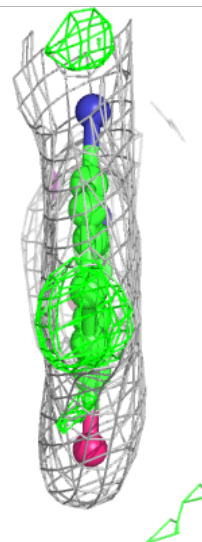
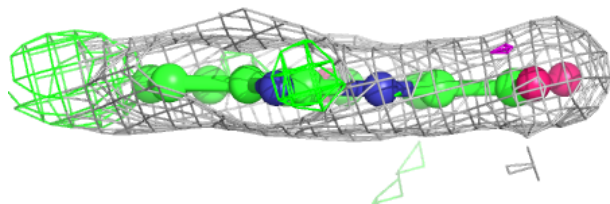
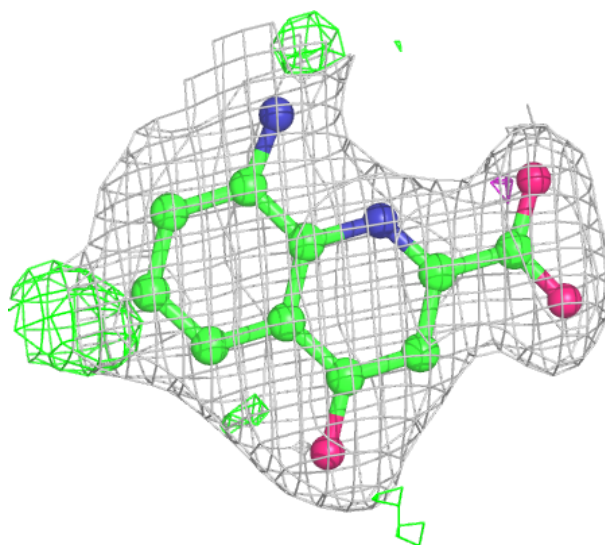
**Electron density around QUK B 315:**

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



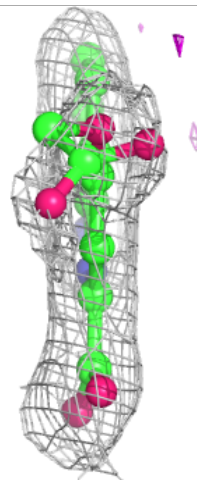
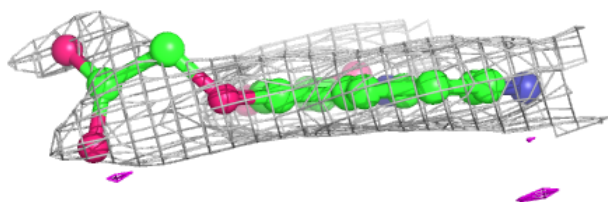
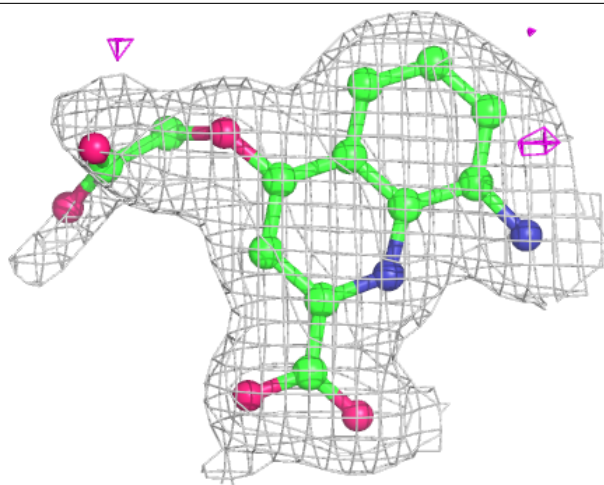
**Electron density around QUJ B 314:**

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



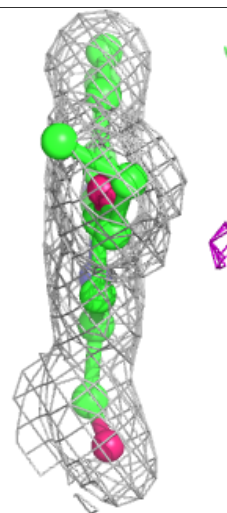
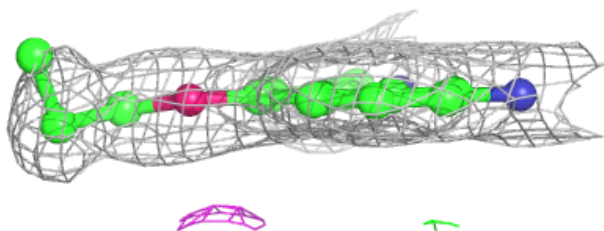
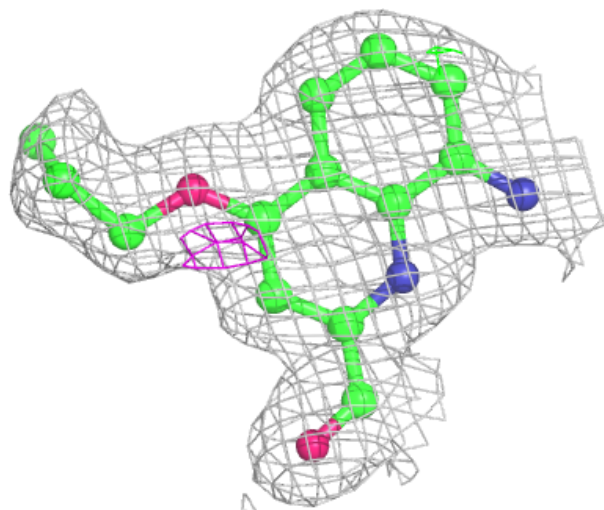
**Electron density around QVE B 306:**

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



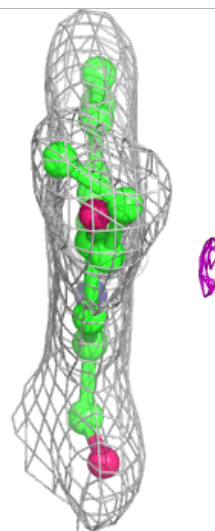
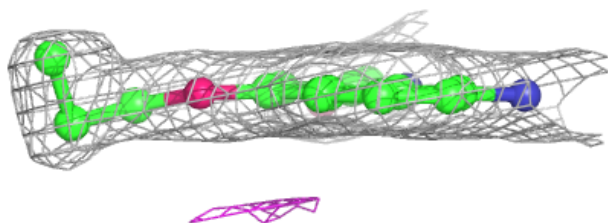
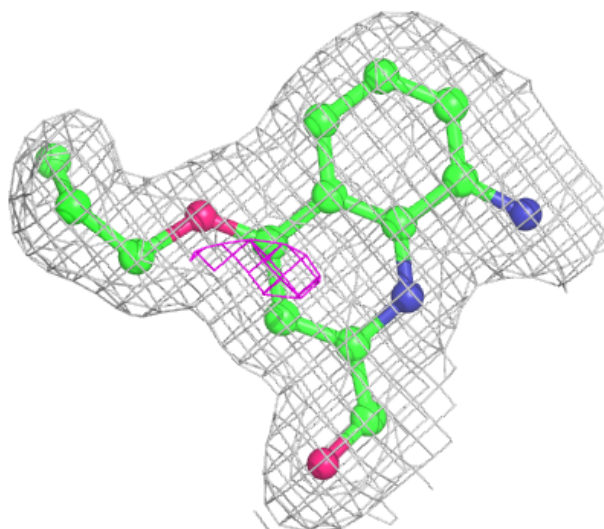
**Electron density around QUK A 303:**

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



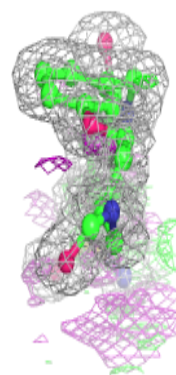
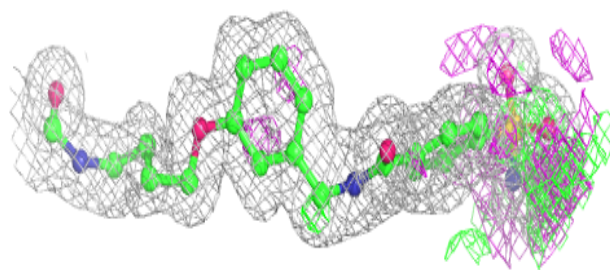
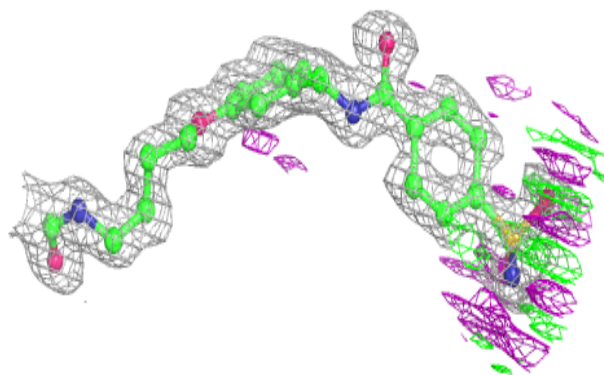
**Electron density around QUK B 304:**

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



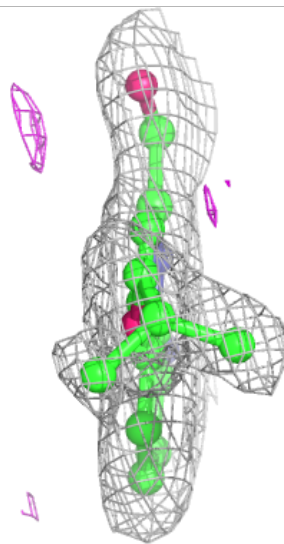
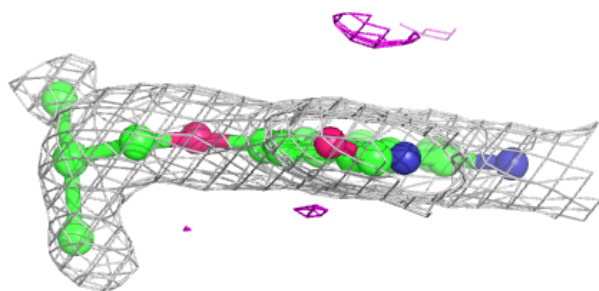
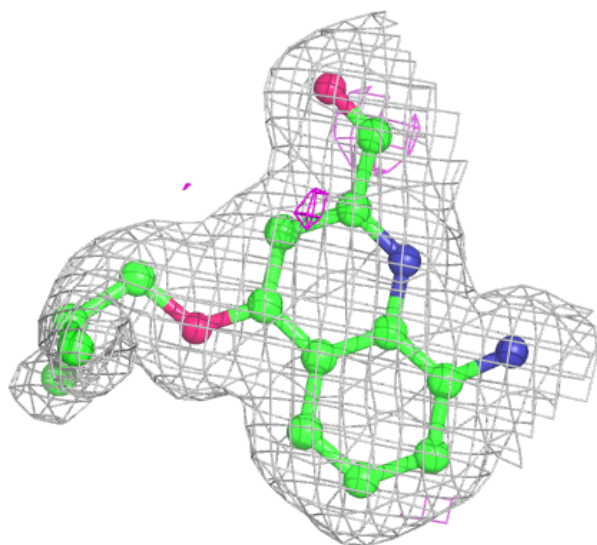
**Electron density around 6H0 A 302:**

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



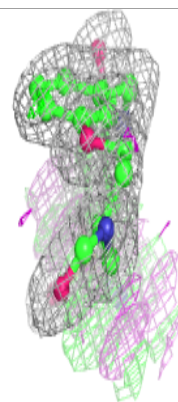
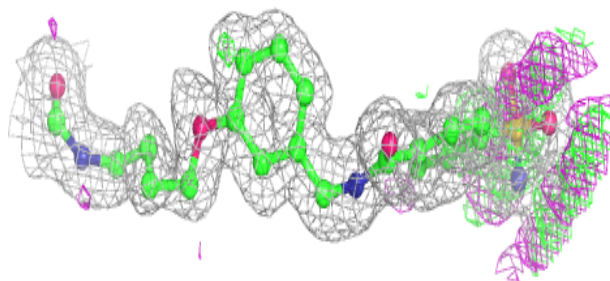
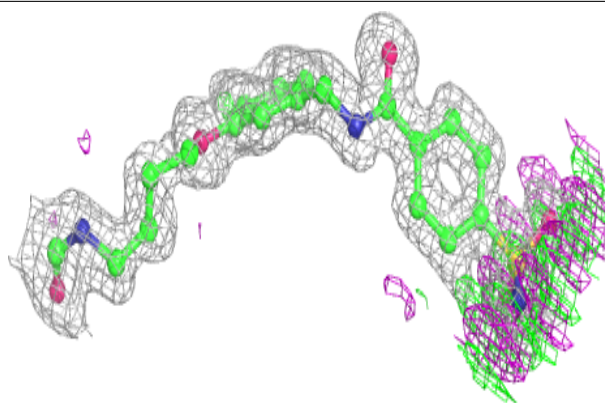
**Electron density around QUJ A 311:**

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



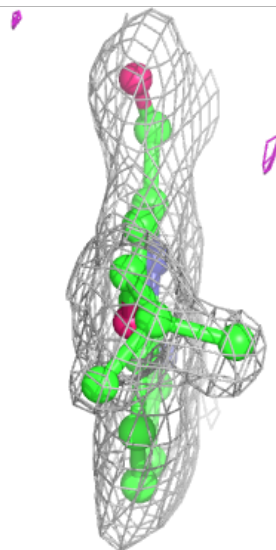
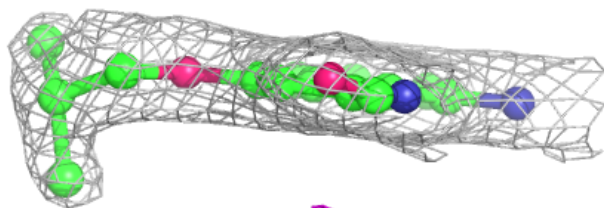
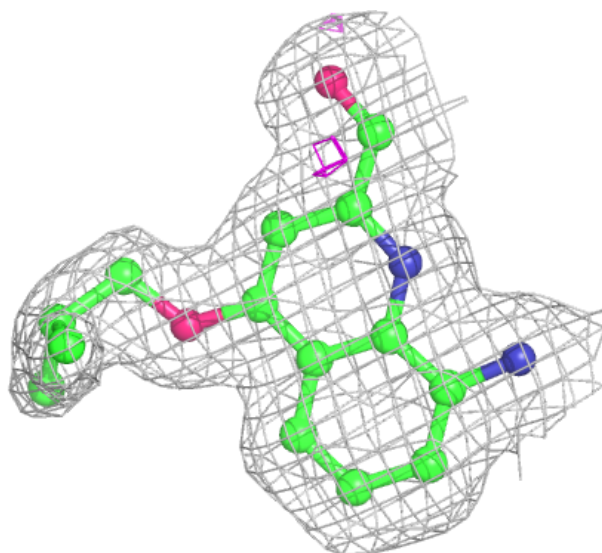
**Electron density around 6H0 B 303:**

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



**Electron density around QUJ B 301:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.