



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:55 am BST

PDB ID : 5L9E
Title : CRYSTAL STRUCTURE OF HUMAN CARBONIC ANHYDRASE II IN
COMPLEX WITH A QUINOLINE OLIGOAMIDE FOLDAMER
Authors : Vallade, M.; Langlois d'Estaintot, B.; Granier, T.; Huc, I.
Deposited on : 2016-06-10
Resolution : 2.90 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

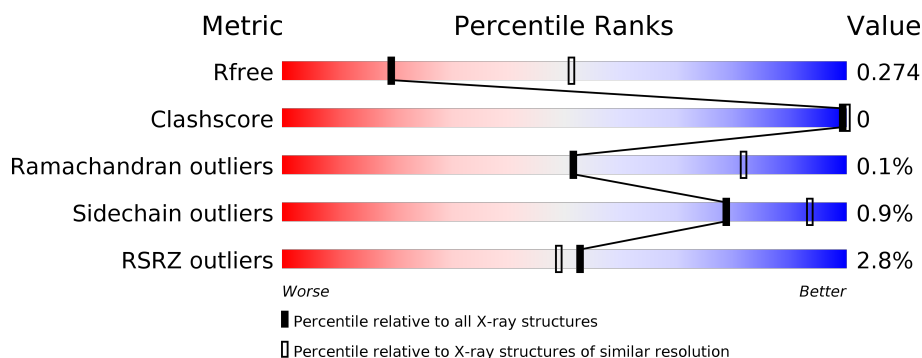
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 ≥ 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	260	<div> <div>2%</div> <div>98%</div> <div>.</div> </div>
1	B	260	<div> <div>2%</div> <div>98%</div> <div>.</div> </div>
1	C	260	<div> <div>3%</div> <div>98%</div> <div>..</div> </div>
1	D	260	<div> <div>4%</div> <div>97%</div> <div>..</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8501 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.

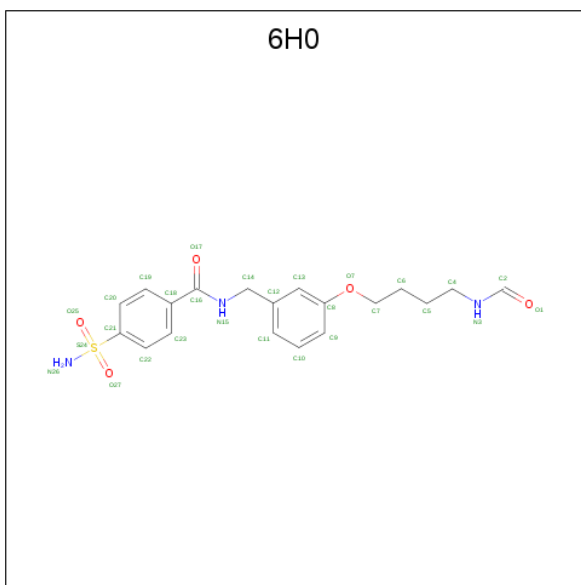
- Molecule 1 is a protein called Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2003	1287	340	374	2			
1	B	259	Total	C	N	O	S	0	0	0
			2005	1289	340	374	2			
1	C	257	Total	C	N	O	S	0	0	0
			1968	1273	330	363	2			
1	D	256	Total	C	N	O	S	0	0	0
			1933	1248	325	358	2			

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

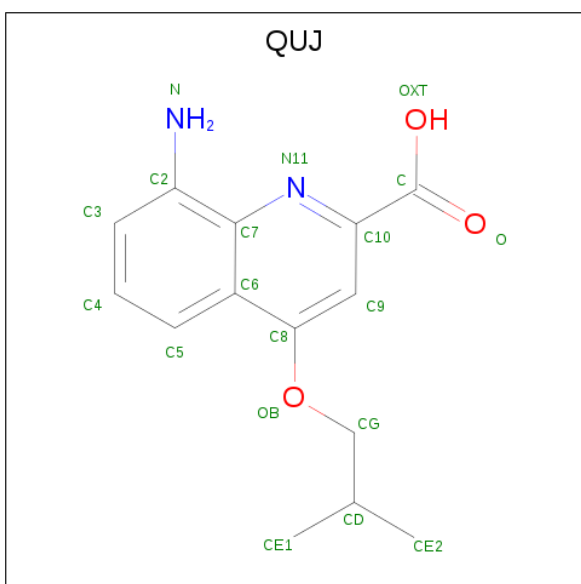
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Zn	0	0
			5	5		
2	A	10	Total	Zn	0	0
			10	10		
2	D	6	Total	Zn	0	0
			6	6		
2	C	6	Total	Zn	0	0
			6	6		

- Molecule 3 is {N}-[[3-(4-formamidobutoxy)phenyl]methyl]-4-sulfamoyl-benzamide (three-letter code: 6H0) (formula: C₁₉H₂₃N₃O₅S).



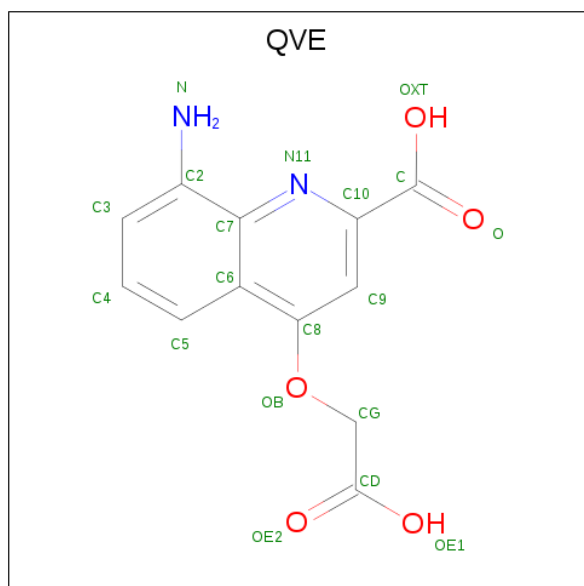
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
3	B	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
3	C	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
3	D	1	Total	C	N	O	S	0	0
			28	19	3	5	1		

- Molecule 4 is 8-azanyl-4-(2-methylpropoxy)quinoline-2-carboxylic acid (three-letter code: QUJ) (formula: C₁₄H₁₆N₂O₃).



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
			16	12	2	2		
4	B	1	Total	C	N	O	0	0
			14	10	2	2		
4	B	1	Total	C	N	O	0	0
			16	12	2	2		
4	B	1	Total	C	N	O	0	0
			16	12	2	2		
4	C	1	Total	C	N	O	0	0
			14	10	2	2		
4	C	1	Total	C	N	O	0	0
			17	13	2	2		
4	D	1	Total	C	N	O	0	0
			14	10	2	2		

- Molecule 5 is 8-azanyl-4-(2-hydroxy-2-oxoethoxy)quinoline-2-carboxylic acid (three-letter code: QVE) (formula: C₁₂H₁₀N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	12	2	4		
5	A	1	Total	C	N	O	0	0
			19	12	2	5		
5	B	1	Total	C	N	O	0	0
			18	12	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			19	12	2	5		
5	C	1	Total	C	N	O	0	0
			18	12	2	4		
5	C	1	Total	C	N	O	0	0
			19	12	2	5		
5	D	1	Total	C	N	O	0	0
			18	12	2	4		
5	D	1	Total	C	N	O	0	0
			19	12	2	5		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

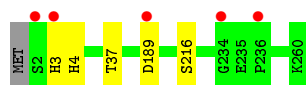
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	47	Total 47	O 47	0	0
7	B	33	Total 33	O 33	0	0
7	C	44	Total 44	O 44	0	0
7	D	36	Total 36	O 36	0	0

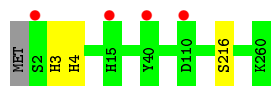
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

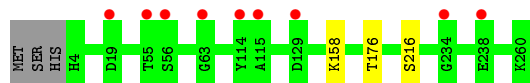
● Molecule 1: Carbonic anhydrase 2



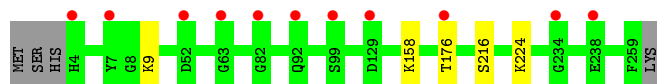
● Molecule 1: Carbonic anhydrase 2



● Molecule 1: Carbonic anhydrase 2



● Molecule 1: Carbonic anhydrase 2



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.97Å 75.14Å 141.10Å 90.00° 100.08° 90.00°	Depositor
Resolution (Å)	85.39 – 2.90 85.39 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (85.39-2.90) 98.1 (85.39-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.242 , 0.273 0.245 , 0.274	Depositor DCC
R_{free} test set	1397 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.771	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8501	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, QUJ, 6H0, QVE

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	0.44	0/2064	0.68	3/2815 (0.1%)
1	B	0.44	0/2067	0.68	1/2821 (0.0%)
1	C	0.43	0/2028	0.63	0/2767
1	D	0.43	0/1993	0.63	0/2725
All	All	0.44	0/8152	0.65	4/11128 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	HIS	N-CA-CB	8.03	125.05	110.60
1	A	4	HIS	N-CA-CB	5.85	121.13	110.60
1	A	3	HIS	N-CA-C	5.82	126.70	111.00
1	A	189	ASP	CB-CG-OD1	5.13	122.92	118.30

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	2003	0	1874	0	0
1	B	2005	0	1864	0	0
1	C	1968	0	1835	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1933	0	1763	1	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
3	C	28	0	0	0	0
3	D	28	0	0	0	0
4	A	30	0	0	0	0
4	B	46	0	0	0	0
4	C	31	0	0	0	0
4	D	14	0	0	0	0
5	A	37	0	0	0	0
5	B	37	0	0	0	0
5	C	37	0	0	0	0
5	D	37	0	0	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	D	6	0	8	0	0
7	A	47	0	0	0	0
7	B	33	0	0	0	0
7	C	44	0	0	0	0
7	D	36	0	0	0	0
All	All	8501	0	7368	2	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 0.

All (2) 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:D:158:LYS:NZ	1:D:176:THR:O	2.44	0.51
1:C:158:LYS:NZ	1:C:176:THR:O	2.45	0.50

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	257/260 (99%)	246 (96%)	11 (4%)	0	100	100
1	B	257/260 (99%)	245 (95%)	11 (4%)	1 (0%)	34	66
1	C	255/260 (98%)	245 (96%)	10 (4%)	0	100	100
1	D	254/260 (98%)	243 (96%)	11 (4%)	0	100	100
All	All	1023/1040 (98%)	979 (96%)	43 (4%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	HIS

5.3.2 Protein sidechains

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	205/225 (91%)	203 (99%)	2 (1%)	76	92
1	B	204/225 (91%)	203 (100%)	1 (0%)	88	96
1	C	196/225 (87%)	195 (100%)	1 (0%)	88	96
1	D	187/225 (83%)	184 (98%)	3 (2%)	62	86
All	All	792/900 (88%)	785 (99%)	7 (1%)	78	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	216	SER
1	B	216	SER
1	C	216	SER
1	D	9	LYS
1	D	216	SER
1	D	224	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	229	ASN
1	B	254	GLN
1	C	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 51 ligands modelled in this entry, 27 are monoatomic - leaving 24 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	QVE	A	306	2,4	14,20,20	0.94	1 (7%)	18,28,28	2.27	7 (38%)
4	QUJ	A	303	3,5	15,15,20	2.20	2 (13%)	19,21,28	2.92	5 (26%)
6	GOL	D	310	-	5,5,5	0.25	0	5,5,5	0.34	0
4	QUJ	D	303	3,5	15,15,20	2.14	1 (6%)	19,21,28	2.64	5 (26%)
4	QUJ	A	305	5	17,17,20	1.80	2 (11%)	20,23,28	2.79	8 (40%)
4	QUJ	B	303	3,5	15,15,20	2.08	2 (13%)	19,21,28	3.14	5 (26%)
5	QVE	C	306	2,4	14,20,20	0.88	1 (7%)	18,28,28	2.16	6 (33%)
3	6H0	A	302	2,4	29,29,29	2.02	6 (20%)	37,38,38	1.57	3 (8%)
5	QVE	B	306	2,4	14,20,20	0.87	1 (7%)	18,28,28	2.68	5 (27%)
6	GOL	C	311	-	5,5,5	0.28	0	5,5,5	0.07	0
5	QVE	C	304	4	16,19,20	1.82	2 (12%)	20,26,28	3.09	7 (35%)
5	QVE	B	304	4	16,19,20	2.15	2 (12%)	20,26,28	3.60	10 (50%)
5	QVE	D	304	4	16,19,20	1.98	2 (12%)	20,26,28	2.99	6 (30%)
4	QUJ	C	305	5	18,18,20	1.97	2 (11%)	21,24,28	2.97	7 (33%)
3	6H0	C	302	2,4	29,29,29	2.04	5 (17%)	37,38,38	1.51	3 (8%)
3	6H0	B	302	2,4	29,29,29	1.86	5 (17%)	37,38,38	1.71	3 (8%)
4	QUJ	B	305	5	17,17,20	1.86	2 (11%)	20,23,28	2.77	8 (40%)
4	QUJ	B	312	5	17,17,20	1.95	1 (5%)	20,23,28	3.31	8 (40%)
4	QUJ	C	303	3,5	15,15,20	2.18	2 (13%)	19,21,28	2.85	5 (26%)
6	GOL	A	314	-	5,5,5	0.30	0	5,5,5	0.32	0
5	QVE	D	305	2,4	14,20,20	0.84	1 (7%)	18,28,28	2.20	7 (38%)
5	QVE	A	304	4	16,19,20	2.06	2 (12%)	20,26,28	3.25	8 (40%)
6	GOL	B	311	-	5,5,5	0.33	0	5,5,5	0.33	0
3	6H0	D	302	2,4	29,29,29	1.91	6 (20%)	37,38,38	1.42	3 (8%)

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	QVE	A	306	2,4	-	2/3/9/9	0/2/2/2
4	QUJ	A	303	3,5	-	2/2/2/9	0/2/2/2
6	GOL	D	310	-	-	0/4/4/4	-
4	QUJ	D	303	3,5	-	2/2/2/9	0/2/2/2
4	QUJ	A	305	5	-	2/5/5/9	0/2/2/2
4	QUJ	B	303	3,5	-	2/2/2/9	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	QVE	C	306	2,4	-	2/3/9/9	0/2/2/2
3	6H0	A	302	2,4	-	4/23/23/23	0/2/2/2
5	QVE	B	306	2,4	-	1/3/9/9	0/2/2/2
6	GOL	C	311	-	-	2/4/4/4	-
5	QVE	C	304	4	-	4/5/7/9	0/2/2/2
5	QVE	B	304	4	-	4/5/7/9	0/2/2/2
5	QVE	D	304	4	-	5/5/7/9	0/2/2/2
4	QUJ	C	305	5	-	4/6/6/9	0/2/2/2
3	6H0	C	302	2,4	-	6/23/23/23	0/2/2/2
3	6H0	B	302	2,4	-	6/23/23/23	0/2/2/2
4	QUJ	B	305	5	-	3/5/5/9	0/2/2/2
4	QUJ	B	312	5	-	4/5/5/9	0/2/2/2
4	QUJ	C	303	3,5	-	2/2/2/9	0/2/2/2
6	GOL	A	314	-	-	2/4/4/4	-
5	QVE	D	305	2,4	-	2/3/9/9	0/2/2/2
5	QVE	A	304	4	-	3/5/7/9	0/2/2/2
6	GOL	B	311	-	-	2/4/4/4	-
3	6H0	D	302	2,4	-	7/23/23/23	0/2/2/2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	304	QVE	C10-C	-7.78	1.40	1.48
4	C	303	QUJ	C10-C	-7.59	1.40	1.48
4	A	303	QUJ	C10-C	-7.57	1.40	1.48
4	D	303	QUJ	C10-C	-7.37	1.40	1.48
4	C	305	QUJ	C10-C	-7.30	1.41	1.48
4	B	312	QUJ	C10-C	-7.17	1.41	1.48
4	B	303	QUJ	C10-C	-6.98	1.41	1.48
5	A	304	QVE	C10-C	-6.97	1.41	1.48
4	B	305	QUJ	C10-C	-6.40	1.41	1.48
5	D	304	QVE	C10-C	-6.34	1.42	1.48
4	A	305	QUJ	C10-C	-5.73	1.42	1.48
5	C	304	QVE	C10-C	-5.51	1.42	1.48
3	C	302	6H0	C14-C12	-5.39	1.39	1.51
3	B	302	6H0	C14-C12	-5.21	1.40	1.51
3	D	302	6H0	C14-C12	-5.00	1.40	1.51
3	A	302	6H0	C14-C12	-4.88	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	6H0	O25-S24	4.75	1.52	1.43
3	C	302	6H0	C21-S24	-4.64	1.69	1.77
3	C	302	6H0	O27-S24	4.60	1.52	1.43
3	B	302	6H0	O25-S24	4.57	1.52	1.43
3	D	302	6H0	O25-S24	4.51	1.52	1.43
3	B	302	6H0	O27-S24	4.49	1.52	1.43
3	D	302	6H0	O27-S24	4.40	1.51	1.43
3	A	302	6H0	C21-S24	-4.37	1.70	1.77
3	A	302	6H0	O25-S24	4.20	1.51	1.43
3	D	302	6H0	C18-C16	-4.03	1.41	1.50
3	A	302	6H0	O27-S24	4.01	1.51	1.43
3	A	302	6H0	C18-C16	-3.99	1.41	1.50
5	D	304	QVE	C10-N11	3.95	1.37	1.33
5	C	304	QVE	C10-N11	3.69	1.37	1.33
3	C	302	6H0	C18-C16	-3.54	1.42	1.50
4	A	305	QUJ	C10-N11	3.48	1.36	1.33
5	A	304	QVE	C10-N11	3.31	1.36	1.33
3	B	302	6H0	C18-C16	-3.29	1.43	1.50
3	D	302	6H0	C21-S24	-3.20	1.72	1.77
3	A	302	6H0	C2-N3	2.77	1.38	1.33
4	C	305	QUJ	C10-N11	2.70	1.36	1.33
4	B	305	QUJ	C10-N11	2.57	1.35	1.33
4	B	303	QUJ	C10-N11	2.53	1.35	1.33
5	A	306	QVE	C10-N11	2.45	1.36	1.33
5	B	304	QVE	C10-N11	2.35	1.35	1.33
5	D	305	QVE	C10-N11	2.29	1.36	1.33
4	A	303	QUJ	C10-N11	2.28	1.35	1.33
5	C	306	QVE	C10-N11	2.23	1.36	1.33
4	C	303	QUJ	C10-N11	2.21	1.35	1.33
3	B	302	6H0	C2-N3	2.19	1.37	1.33
5	B	306	QVE	C10-N11	2.14	1.36	1.33
3	D	302	6H0	C2-N3	2.05	1.37	1.33

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	305	QUJ	C10-N11-C7	9.93	125.64	118.11
4	B	312	QUJ	C10-N11-C7	9.86	125.59	118.11
5	C	304	QVE	C10-N11-C7	9.38	125.22	118.11
5	D	304	QVE	C10-N11-C7	9.30	125.17	118.11
5	B	304	QVE	C10-N11-C7	9.21	125.10	118.11
5	A	304	QVE	C10-N11-C7	9.13	125.03	118.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	QUJ	C10-N11-C7	9.05	124.97	118.11
4	A	305	QUJ	C10-N11-C7	8.75	124.74	118.11
4	A	303	QUJ	C10-N11-C7	8.61	124.64	118.11
5	B	306	QVE	CG-OB-C8	8.31	129.23	117.56
5	B	304	QVE	CG-OB-C8	8.10	128.94	117.56
4	B	305	QUJ	C10-N11-C7	7.95	124.14	118.11
4	C	303	QUJ	C10-N11-C7	7.57	123.85	118.11
5	A	304	QVE	O-C-C10	-7.11	117.48	124.22
5	B	304	QVE	O-C-C10	-7.06	117.53	124.22
4	D	303	QUJ	C10-N11-C7	6.60	123.12	118.11
5	A	306	QVE	C10-N11-C7	6.45	123.21	118.26
4	B	303	QUJ	C-C10-N11	6.35	120.88	114.66
4	B	312	QUJ	C9-C10-C	6.24	126.62	121.23
3	B	302	6H0	O1-C2-N3	-6.16	118.67	124.89
5	C	306	QVE	C10-N11-C7	6.12	122.95	118.26
4	C	303	QUJ	C-C10-N11	5.96	120.50	114.66
5	D	305	QVE	C10-N11-C7	5.89	122.78	118.26
5	A	304	QVE	CG-OB-C8	5.76	125.65	117.56
4	C	303	QUJ	O-C-C10	-5.65	118.87	124.22
4	B	303	QUJ	O-C-C10	-5.64	118.88	124.22
3	A	302	6H0	O25-S24-O27	-5.63	109.50	118.76
4	C	305	QUJ	C9-C10-C	5.57	126.04	121.23
5	C	304	QVE	O-C-C10	-5.55	118.97	124.22
3	C	302	6H0	O25-S24-O27	-5.51	109.70	118.76
3	B	302	6H0	O25-S24-O27	-5.44	109.82	118.76
4	A	303	QUJ	O-C-C10	-5.43	119.08	124.22
4	D	303	QUJ	O-C-C10	-5.42	119.09	124.22
5	B	306	QVE	C10-N11-C7	5.33	122.35	118.26
4	D	303	QUJ	C-C10-N11	5.29	119.84	114.66
3	D	302	6H0	O25-S24-O27	-5.27	110.09	118.76
5	D	304	QVE	O-C-C10	-5.22	119.28	124.22
5	D	304	QVE	C-C10-N11	5.21	119.77	114.66
4	B	312	QUJ	CG-OB-C8	5.20	123.48	118.01
4	B	305	QUJ	O-C-C10	-5.19	119.31	124.22
4	B	312	QUJ	O-C-C10	-5.04	119.45	124.22
5	C	304	QVE	C-C10-N11	4.94	119.50	114.66
4	A	305	QUJ	O-C-C10	-4.91	119.57	124.22
4	C	305	QUJ	O-C-C10	-4.72	119.75	124.22
3	C	302	6H0	O1-C2-N3	-4.51	120.34	124.89
4	A	303	QUJ	C-C10-N11	4.33	118.91	114.66
4	A	305	QUJ	C9-C10-C	4.11	124.78	121.23
4	A	303	QUJ	C3-C2-N	4.09	128.55	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	304	QVE	CG-OB-C8	4.05	123.25	117.56
4	D	303	QUJ	C3-C2-N	3.90	128.16	120.36
4	B	303	QUJ	C3-C2-N	3.87	128.11	120.36
4	C	303	QUJ	C3-C2-N	3.77	127.90	120.36
4	B	305	QUJ	CG-OB-C8	3.73	121.94	118.01
3	D	302	6H0	O1-C2-N3	-3.55	121.31	124.89
5	B	304	QVE	C-C10-N11	3.54	118.13	114.66
4	B	305	QUJ	C-C10-N11	3.47	118.06	114.66
5	A	304	QVE	C-C10-N11	3.42	118.01	114.66
4	B	305	QUJ	C9-C10-C	3.40	124.17	121.23
4	A	303	QUJ	C7-C2-N	-3.34	111.71	118.07
5	A	306	QVE	C9-C10-N11	-3.30	119.22	122.23
4	A	305	QUJ	C-C10-N11	3.27	117.86	114.66
3	A	302	6H0	O1-C2-N3	-3.21	121.64	124.89
3	A	302	6H0	O25-S24-C21	3.13	110.85	107.35
5	B	304	QVE	OB-C8-C6	3.11	123.72	115.01
5	C	306	QVE	C9-C10-N11	-3.09	119.41	122.23
4	B	312	QUJ	C3-C2-N	3.07	126.49	120.36
5	D	305	QVE	CG-OB-C8	3.03	121.81	117.56
5	D	305	QVE	C2-C7-N11	3.02	121.62	118.64
4	C	305	QUJ	C3-C2-N	2.98	126.32	120.36
5	B	304	QVE	C3-C2-N	2.92	126.19	120.36
4	B	303	QUJ	C7-C2-N	-2.91	112.53	118.07
5	B	306	QVE	C2-C7-N11	2.89	121.50	118.64
5	A	306	QVE	OB-C8-C6	2.88	123.06	115.01
5	D	305	QVE	OB-C8-C6	2.84	122.94	115.01
5	C	304	QVE	C2-C7-N11	2.80	121.41	118.64
5	B	304	QVE	C9-C10-C	2.77	123.62	121.23
5	C	306	QVE	OB-C8-C6	2.74	122.66	115.01
4	A	305	QUJ	C3-C2-N	2.73	125.81	120.36
4	B	305	QUJ	C3-C2-N	2.71	125.78	120.36
5	A	304	QVE	C9-C10-C	2.70	123.56	121.23
5	D	304	QVE	C2-C7-N11	2.63	121.24	118.64
5	D	305	QVE	C9-C10-N11	-2.62	119.84	122.23
4	C	305	QUJ	C6-C7-N11	-2.56	117.50	122.78
5	A	304	QVE	C3-C2-N	2.56	125.47	120.36
4	C	303	QUJ	C7-C2-N	-2.55	113.20	118.07
5	A	306	QVE	CG-OB-C8	2.55	121.14	117.56
5	D	304	QVE	C6-C7-N11	-2.54	117.54	122.78
5	D	304	QVE	CG-OB-C8	2.51	121.09	117.56
4	C	305	QUJ	C3-C2-C7	-2.51	116.12	120.06
5	B	304	QVE	OB-C8-C9	-2.50	116.52	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	306	QVE	CG-OB-C8	2.49	121.05	117.56
5	A	304	QVE	C6-C7-N11	-2.46	117.70	122.78
5	B	304	QVE	C6-C7-N11	-2.44	117.74	122.78
5	A	306	QVE	C6-C7-N11	-2.39	117.85	122.78
4	B	312	QUJ	OB-C8-C6	2.37	121.65	115.01
5	A	306	QVE	C2-C7-N11	2.37	120.98	118.64
4	D	303	QUJ	C7-C2-N	-2.36	113.56	118.07
5	C	304	QVE	C6-C7-N11	-2.36	117.91	122.78
5	D	305	QVE	C6-C7-N11	-2.36	117.92	122.78
4	B	305	QUJ	OB-C8-C6	2.35	121.58	115.01
5	B	306	QVE	C9-C10-N11	-2.35	120.09	122.23
5	C	306	QVE	C3-C2-N	2.31	124.98	120.36
4	A	305	QUJ	C3-C2-C7	-2.31	116.44	120.06
5	C	304	QVE	C9-C10-C	2.30	123.21	121.23
5	B	304	QVE	C3-C2-C7	-2.26	116.50	120.06
5	B	306	QVE	C6-C7-N11	-2.26	118.11	122.78
4	C	305	QUJ	OB-C8-C6	2.16	121.04	115.01
3	D	302	6H0	O25-S24-C21	2.15	109.75	107.35
5	D	305	QVE	OB-C8-C9	-2.14	117.71	124.69
5	C	306	QVE	C6-C7-N11	-2.13	118.39	122.78
3	B	302	6H0	C14-C12-C13	-2.12	116.05	120.64
4	B	312	QUJ	C6-C7-N11	-2.12	118.41	122.78
5	A	306	QVE	OB-C8-C9	-2.08	117.90	124.69
4	B	305	QUJ	C3-C2-C7	-2.06	116.82	120.06
4	B	312	QUJ	C3-C2-C7	-2.04	116.86	120.06
3	C	302	6H0	O27-S24-C21	2.01	109.59	107.35
4	A	305	QUJ	C6-C7-N11	-2.01	118.64	122.78
4	A	305	QUJ	OB-C8-C6	2.01	120.62	115.01
5	A	304	QVE	C3-C2-C7	-2.00	116.92	120.06

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	QUJ	O-C-C10-C9
4	A	303	QUJ	O-C-C10-N11
4	D	303	QUJ	O-C-C10-C9
4	D	303	QUJ	O-C-C10-N11
4	B	303	QUJ	O-C-C10-C9
4	B	303	QUJ	O-C-C10-N11
6	C	311	GOL	C1-C2-C3-O3
5	B	304	QVE	O-C-C10-N11

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Mol	Chain	Res	Type	Atoms
5	B	304	QVE	O-C-C10-C9
4	C	305	QUJ	O-C-C10-C9
4	C	305	QUJ	O-C-C10-N11
5	D	304	QVE	O-C-C10-N11
5	D	304	QVE	O-C-C10-C9
4	C	303	QUJ	O-C-C10-C9
4	C	303	QUJ	O-C-C10-N11
4	B	312	QUJ	O-C-C10-C9
4	B	312	QUJ	O-C-C10-N11
6	A	314	GOL	O1-C1-C2-C3
5	A	304	QVE	O-C-C10-N11
6	B	311	GOL	O1-C1-C2-C3
5	C	304	QVE	C9-C8-OB-CG
5	D	305	QVE	C9-C8-OB-CG
5	C	304	QVE	C6-C8-OB-CG
5	D	305	QVE	C6-C8-OB-CG
4	C	305	QUJ	C9-C8-OB-CG
3	D	302	6H0	N3-C4-C5-C6
4	A	305	QUJ	C9-C8-OB-CG
5	D	304	QVE	C9-C8-OB-CG
5	B	304	QVE	C6-C8-OB-CG
4	A	305	QUJ	C6-C8-OB-CG
4	C	305	QUJ	C6-C8-OB-CG
5	D	304	QVE	C6-C8-OB-CG
4	B	305	QUJ	C6-C8-OB-CG
5	B	304	QVE	C9-C8-OB-CG
4	B	312	QUJ	C9-C8-OB-CG
4	B	312	QUJ	C6-C8-OB-CG
4	B	305	QUJ	C9-C8-OB-CG
3	C	302	6H0	C5-C6-C7-O7
3	D	302	6H0	C5-C6-C7-O7
3	D	302	6H0	C9-C8-O7-C7
3	D	302	6H0	C13-C8-O7-C7
6	C	311	GOL	O2-C2-C3-O3
6	A	314	GOL	O1-C1-C2-O2
6	B	311	GOL	O1-C1-C2-O2
5	B	306	QVE	CD-CG-OB-C8
3	B	302	6H0	C4-C5-C6-C7
3	A	302	6H0	C20-C21-S24-O27
3	D	302	6H0	C6-C7-O7-C8
3	B	302	6H0	C5-C4-N3-C2
4	B	305	QUJ	CD-CG-OB-C8

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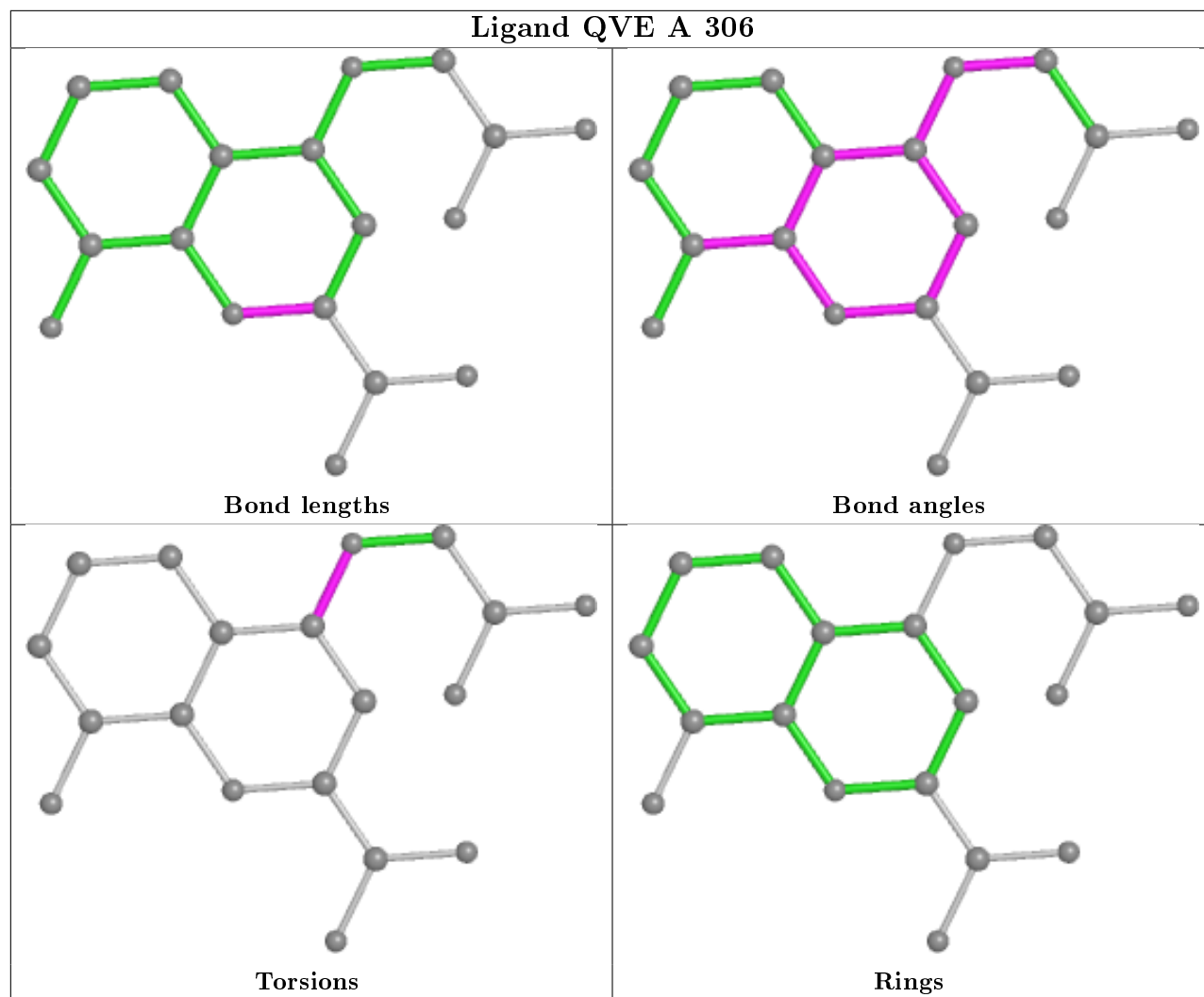
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Mol	Chain	Res	Type	Atoms
5	C	304	QVE	CD-CG-OB-C8
3	A	302	6H0	C22-C21-S24-O27
3	B	302	6H0	C20-C21-S24-O27
5	A	304	QVE	O-C-C10-C9
3	B	302	6H0	C22-C21-S24-O27
5	D	304	QVE	CD-CG-OB-C8
3	B	302	6H0	C5-C6-C7-O7
3	C	302	6H0	C9-C8-O7-C7
3	C	302	6H0	C13-C8-O7-C7
3	C	302	6H0	C5-C4-N3-C2
3	D	302	6H0	C22-C21-S24-O27
5	C	306	QVE	C6-C8-OB-CG
3	D	302	6H0	C20-C21-S24-O27
5	C	306	QVE	C9-C8-OB-CG
3	A	302	6H0	C20-C21-S24-N26
3	C	302	6H0	C22-C21-S24-O27
3	C	302	6H0	C20-C21-S24-O27
5	A	306	QVE	C9-C8-OB-CG
5	A	306	QVE	C6-C8-OB-CG
3	A	302	6H0	C22-C21-S24-N26
5	C	304	QVE	O-C-C10-N11
5	A	304	QVE	C9-C8-OB-CG
3	B	302	6H0	C20-C21-S24-N26

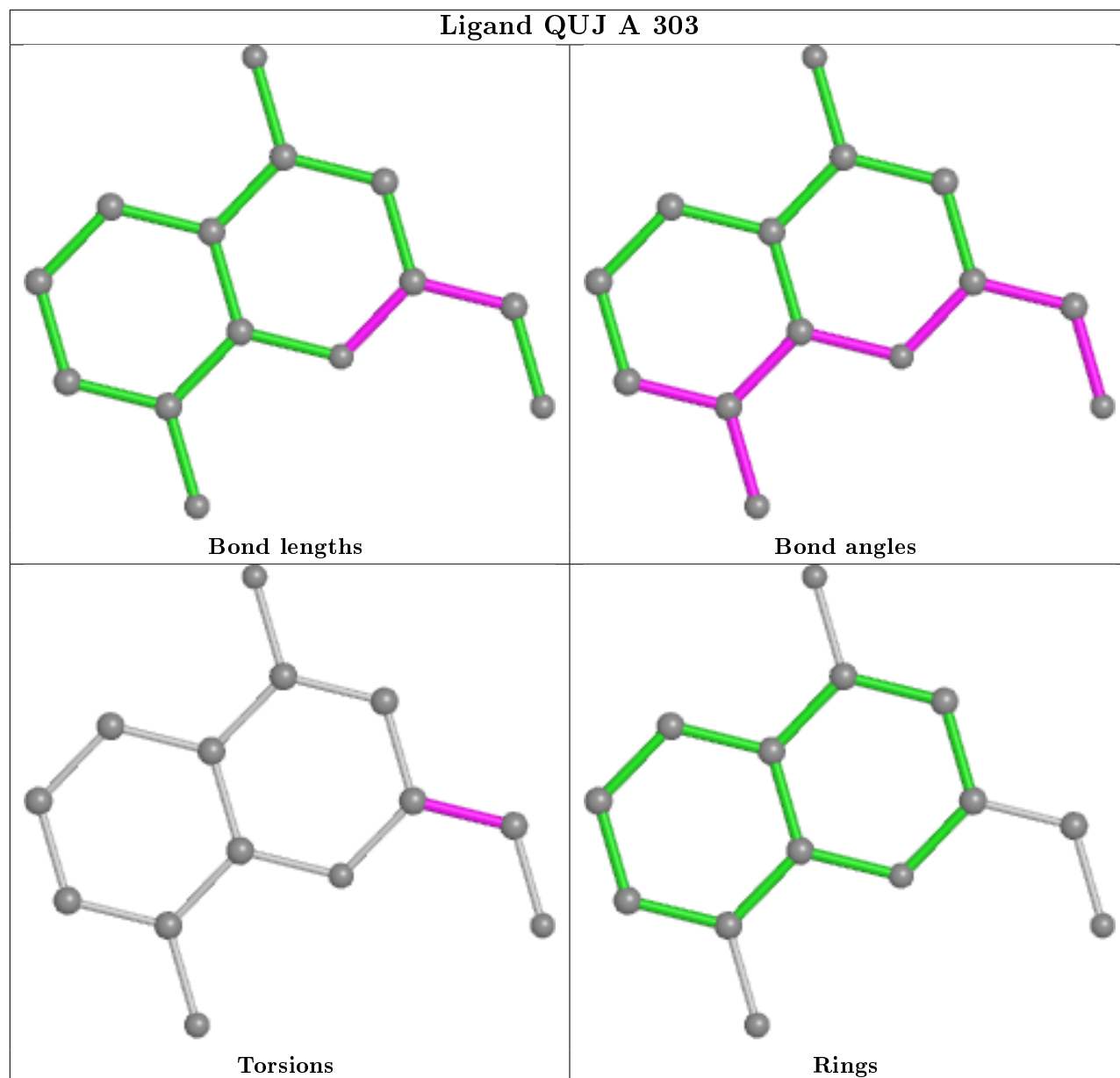
There are no ring outliers.

No monomer is involved in short contacts.

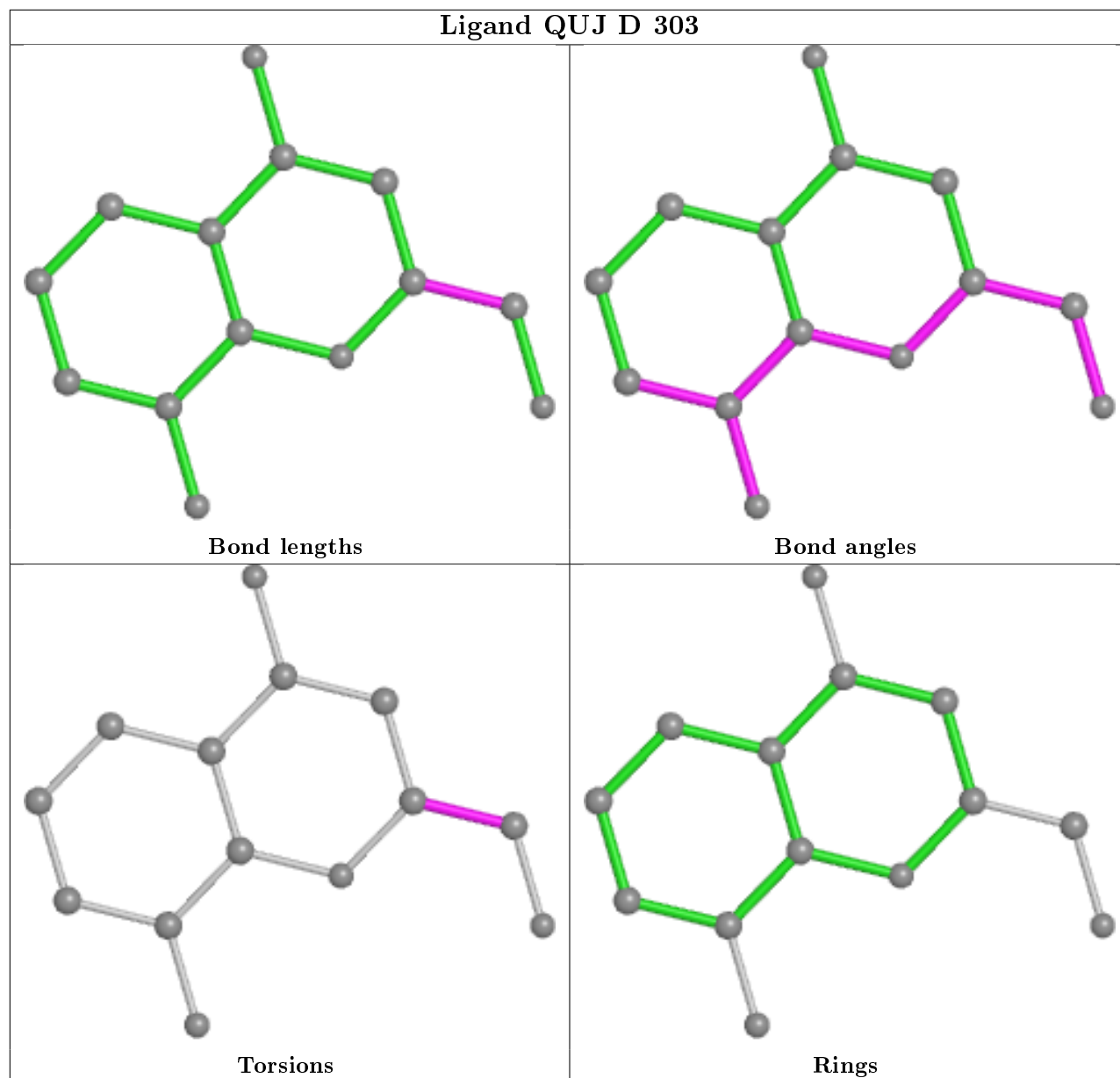
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



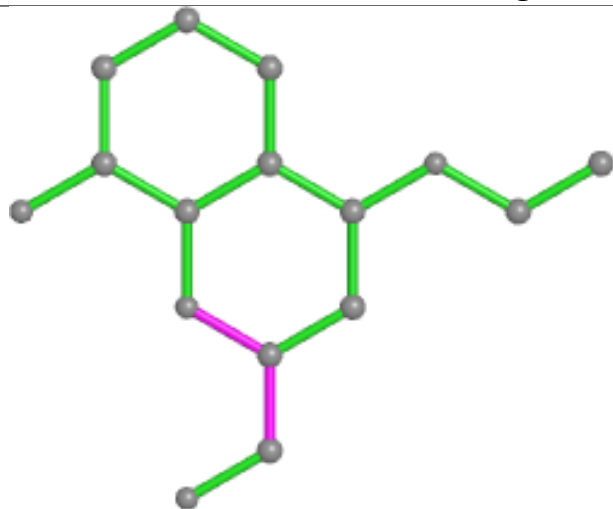
Ligand QUJ A 303



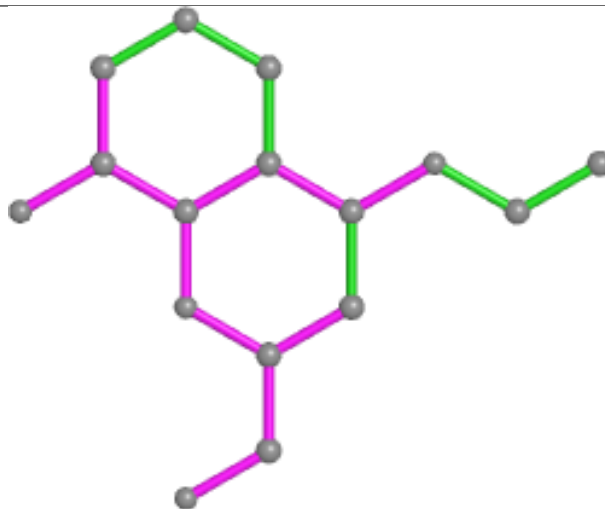
Ligand QUJ D 303



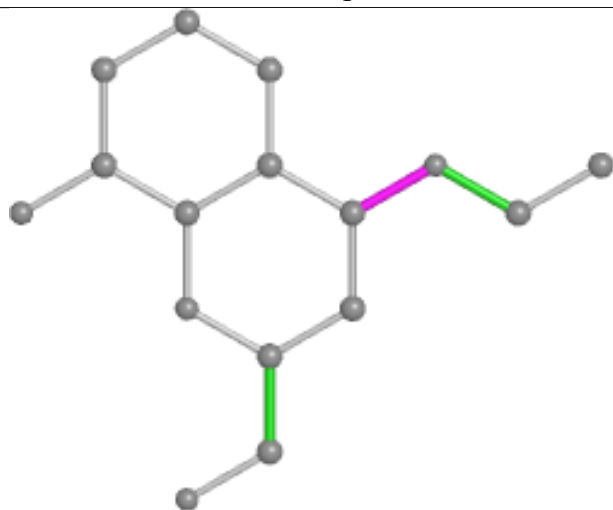
Ligand QUJ A 305



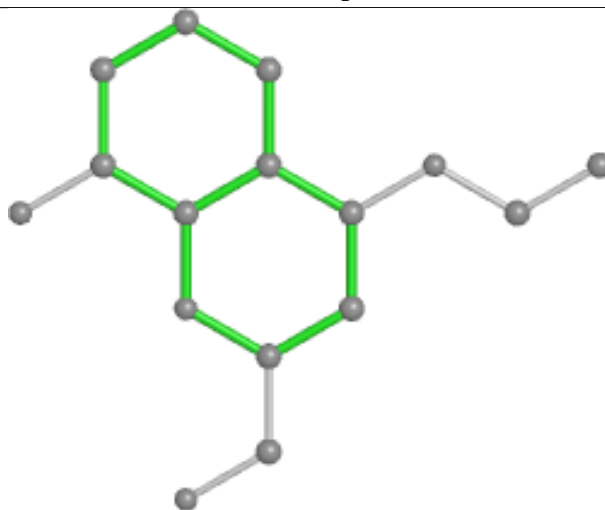
Bond lengths



Bond angles

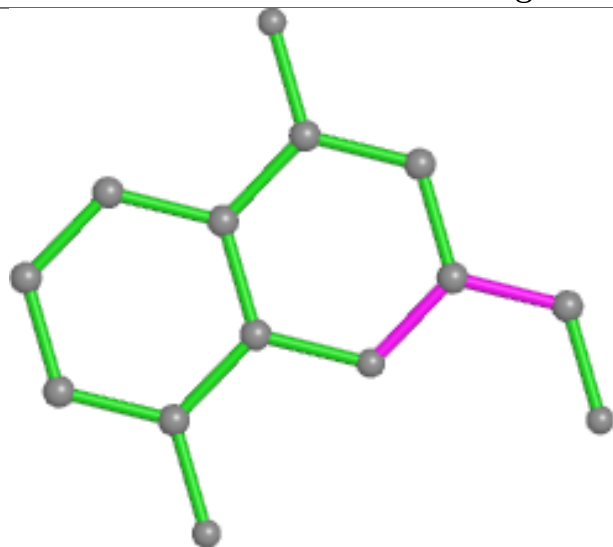


Torsions

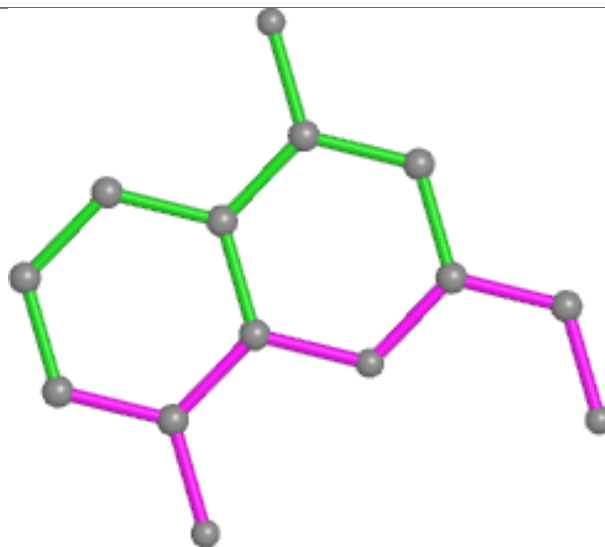


Rings

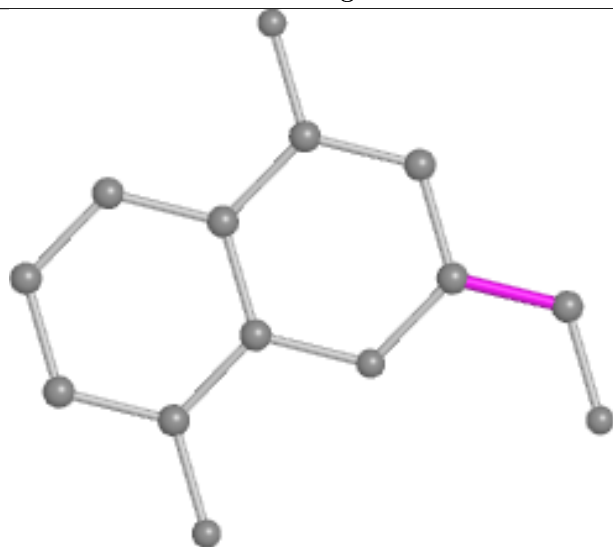
Ligand QUJ B 303



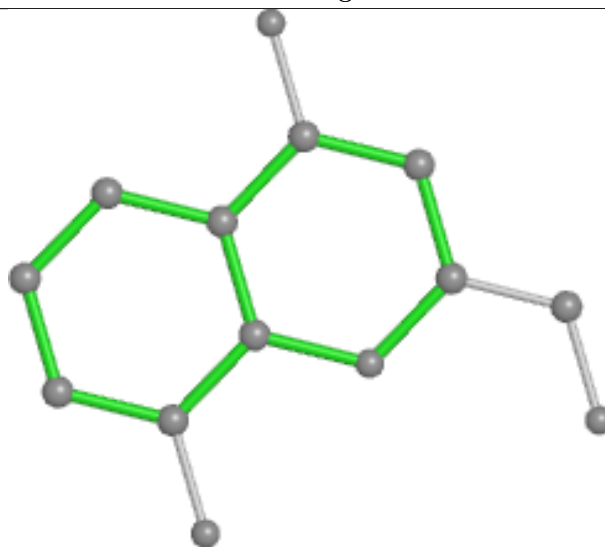
Bond lengths



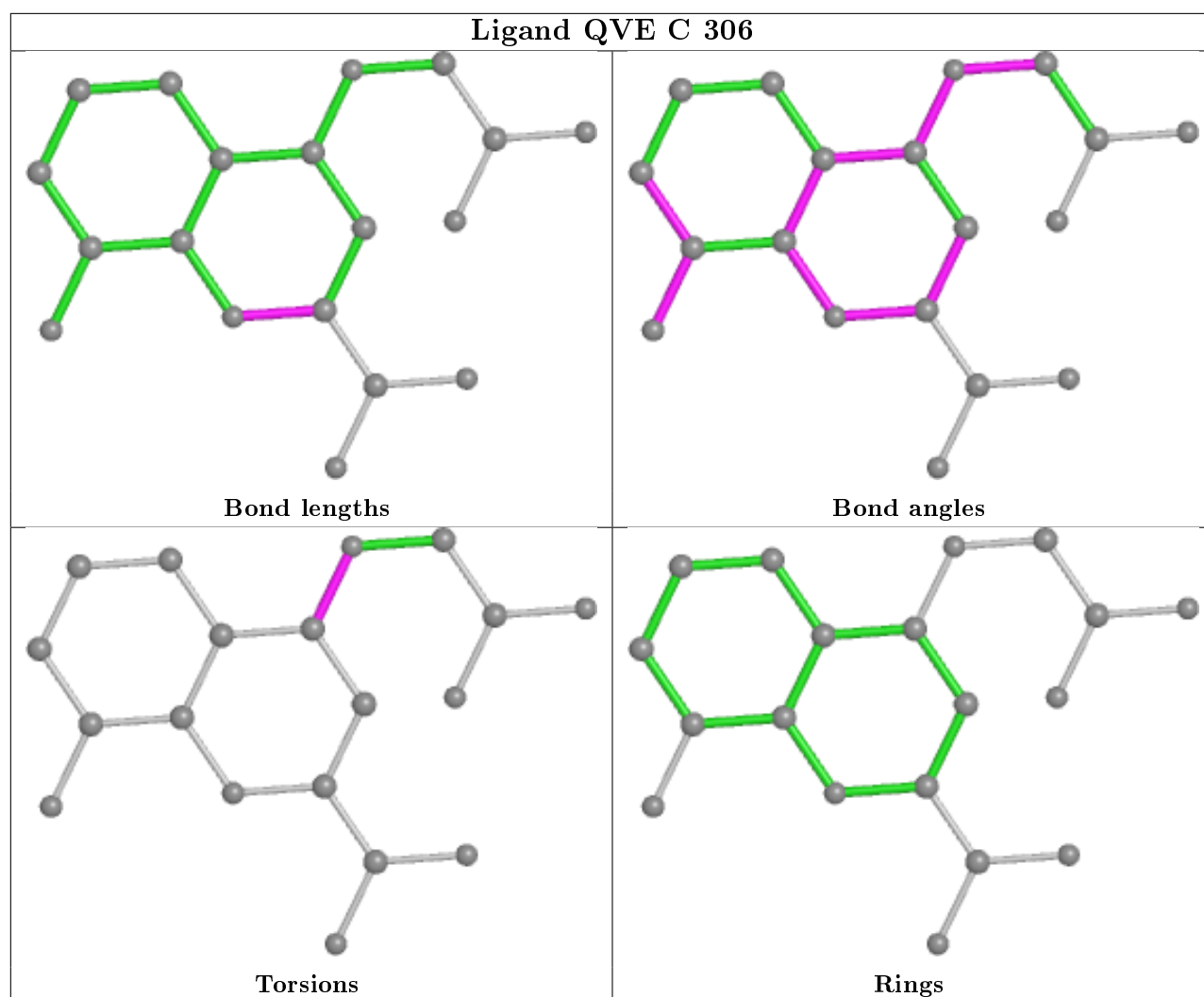
Bond angles



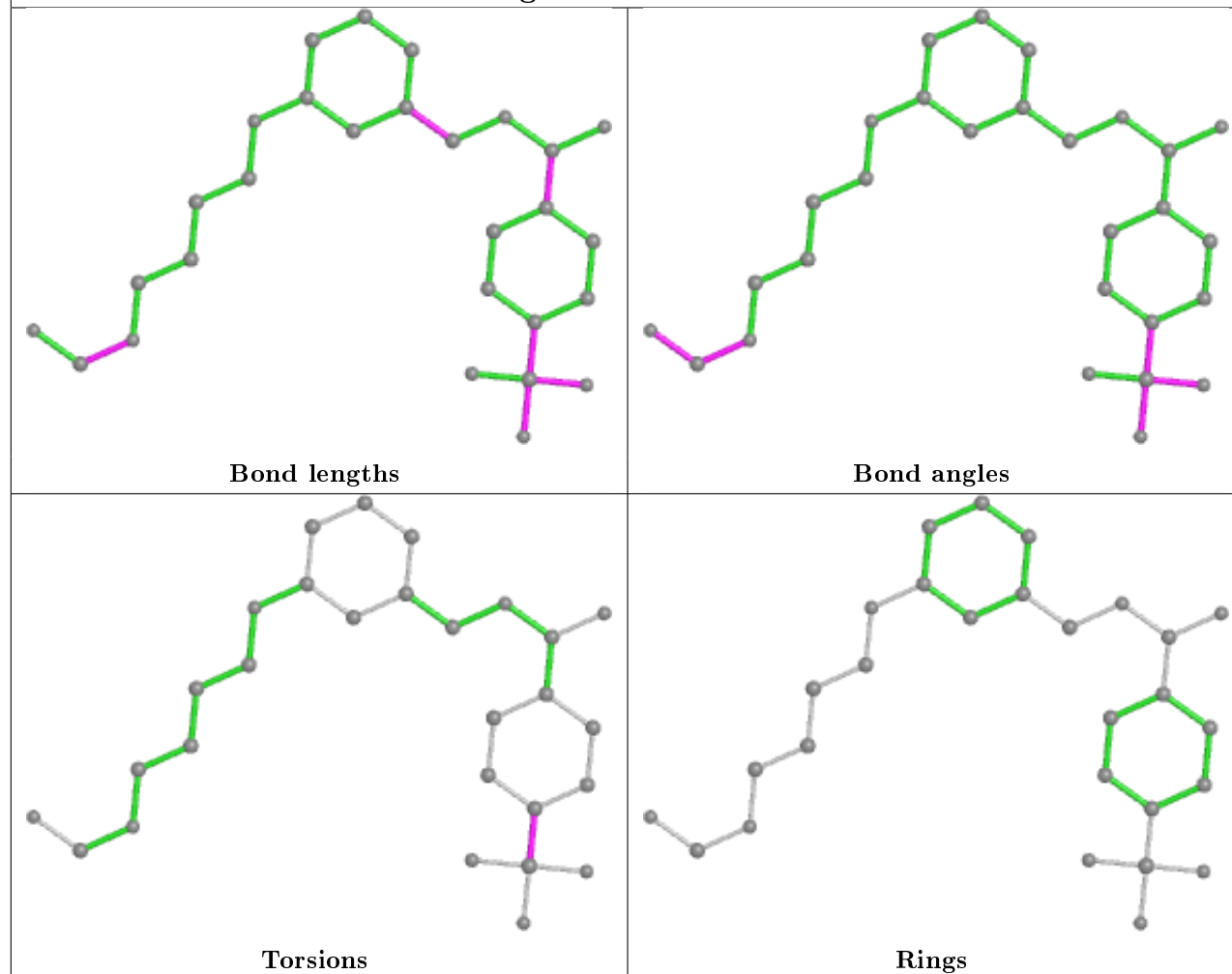
Torsions

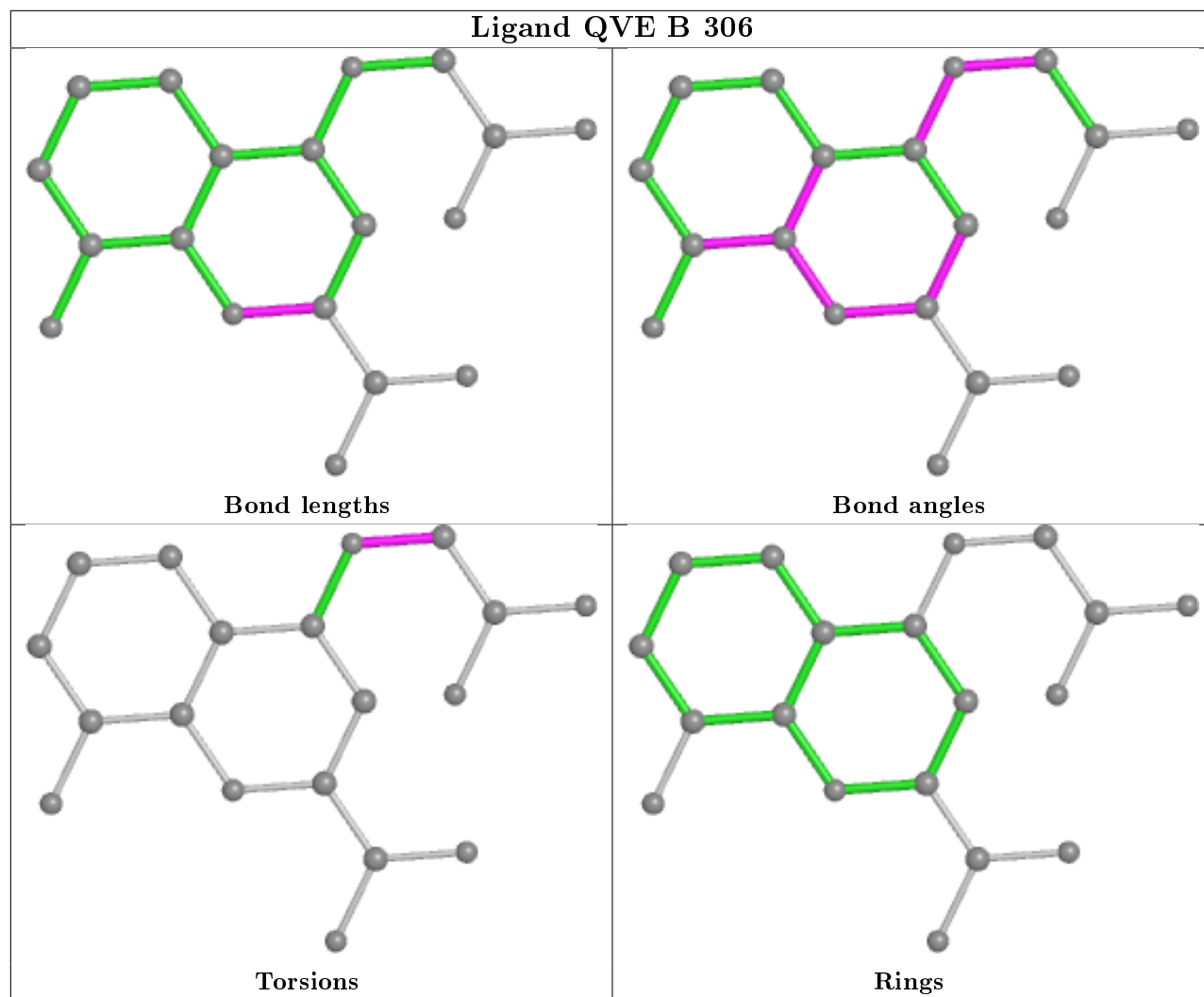


Rings

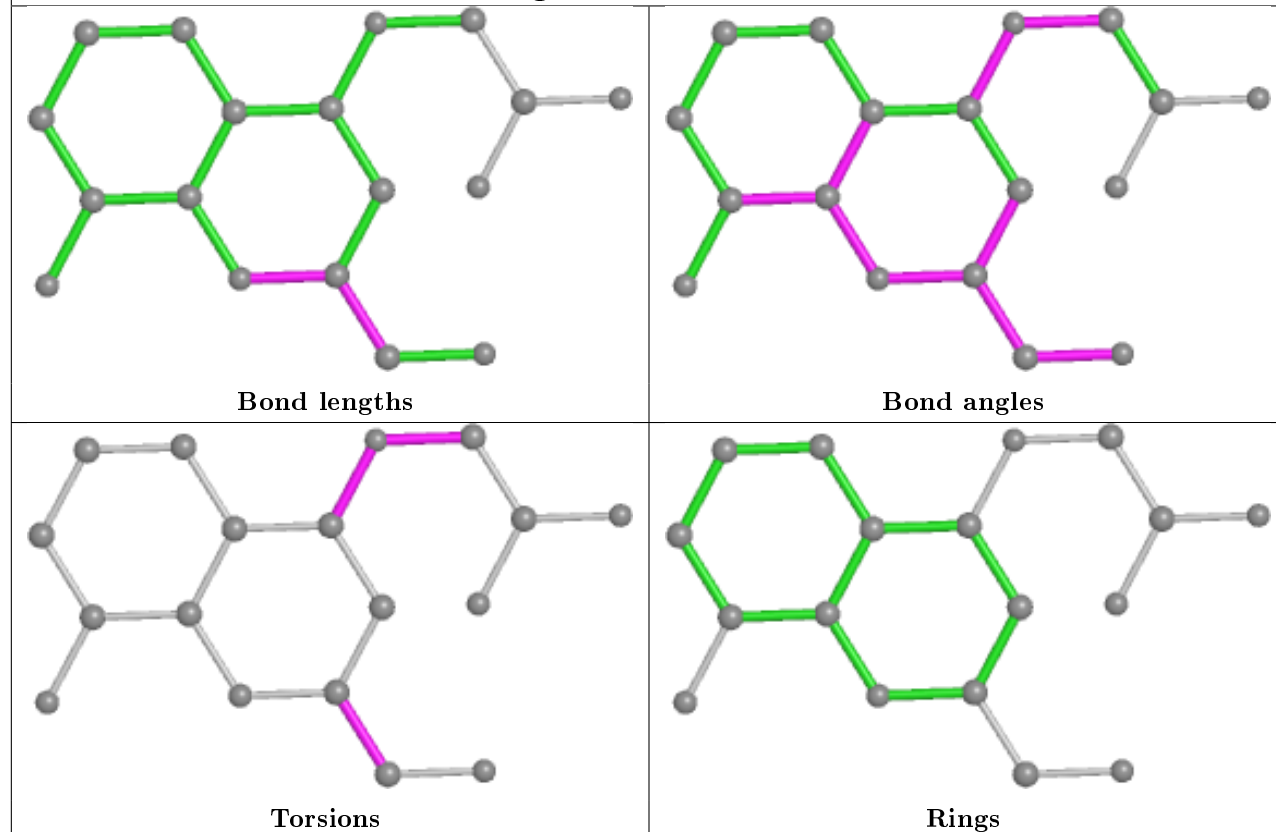


Ligand 6H0 A 302

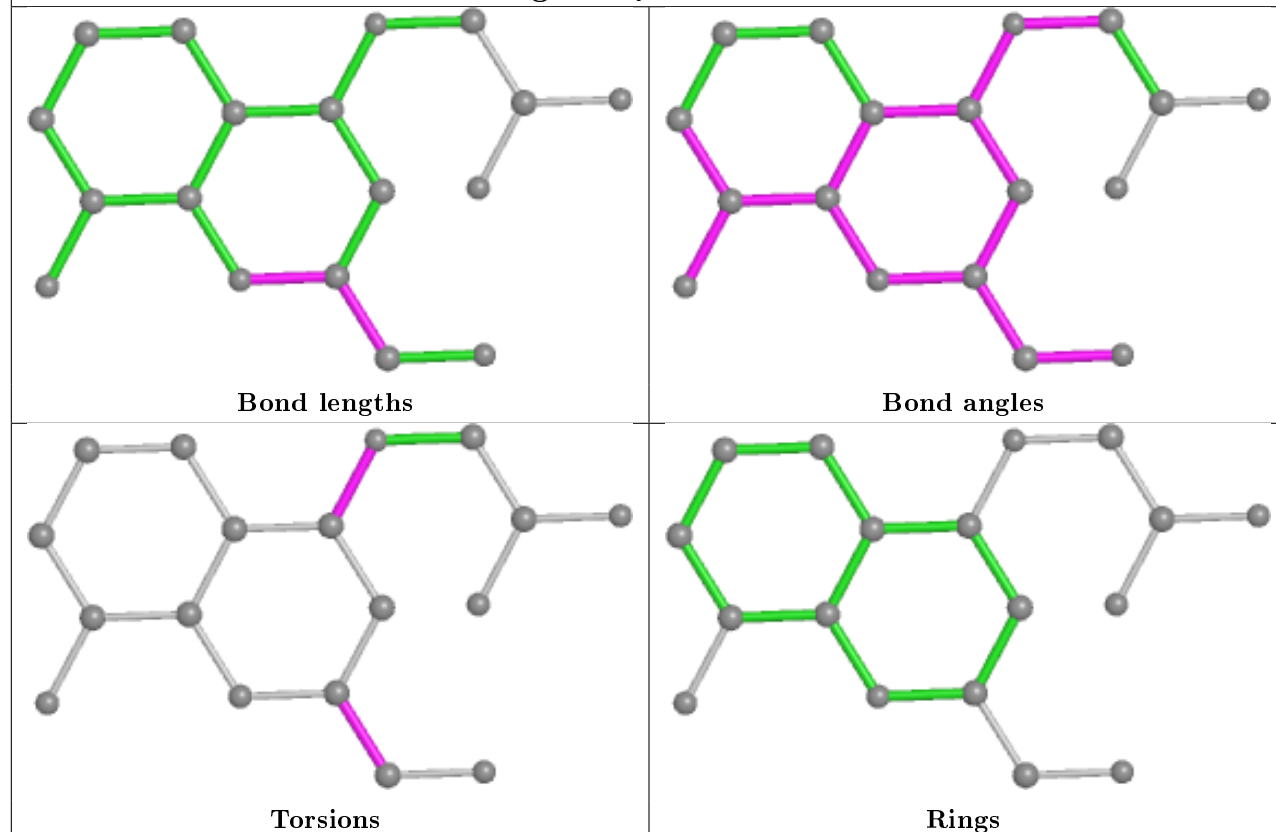


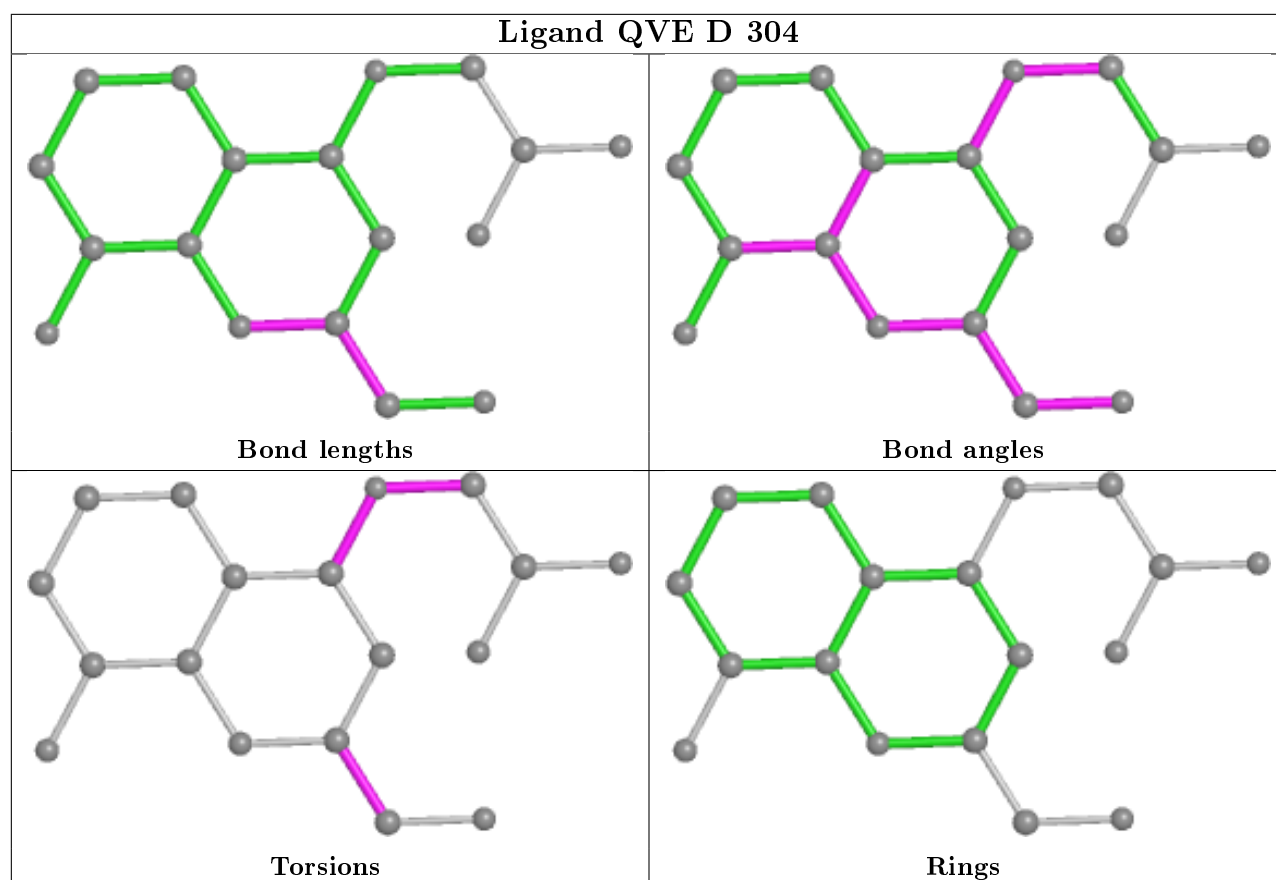


Ligand QVE C 304

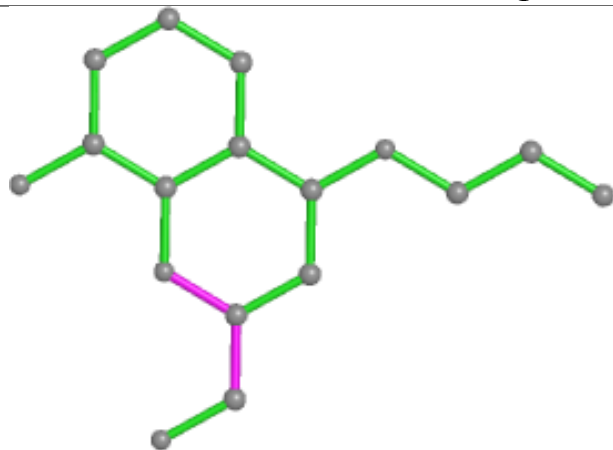


Ligand QVE B 304

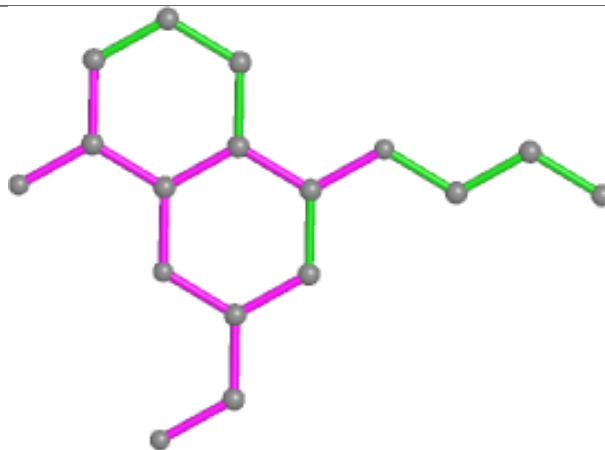




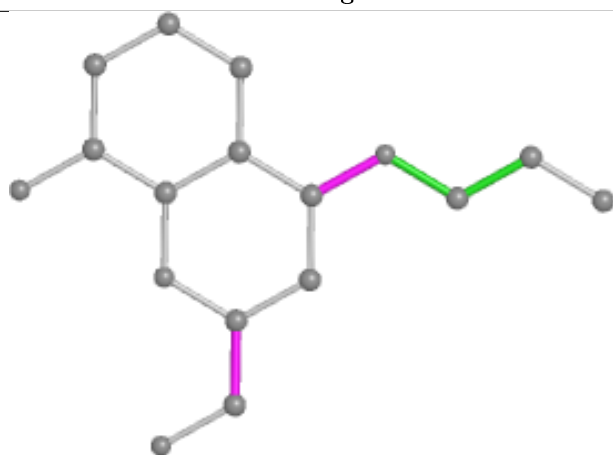
Ligand QUJ C 305



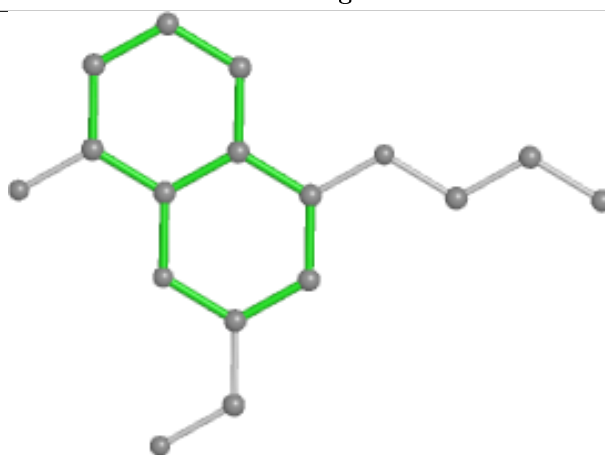
Bond lengths



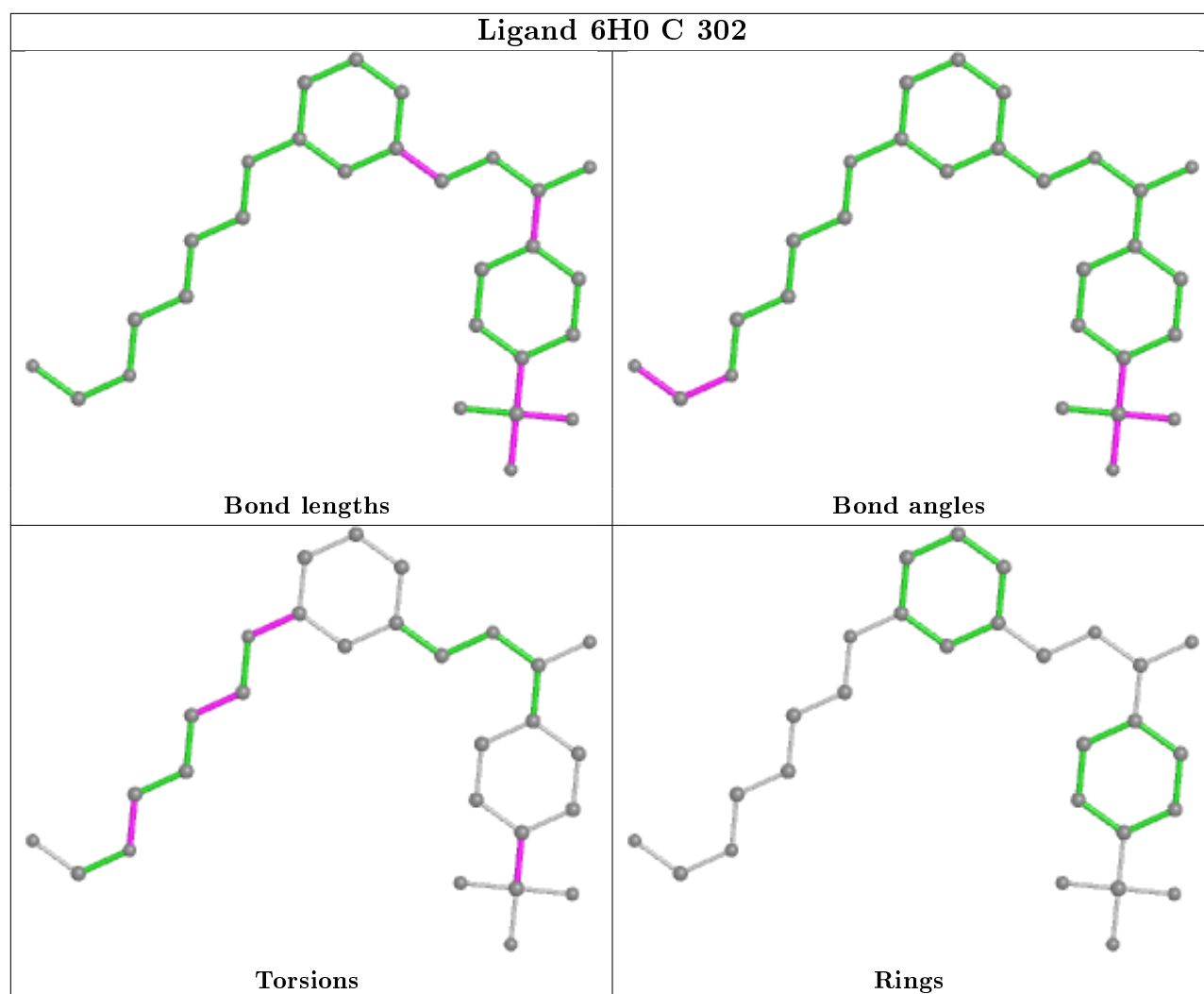
Bond angles



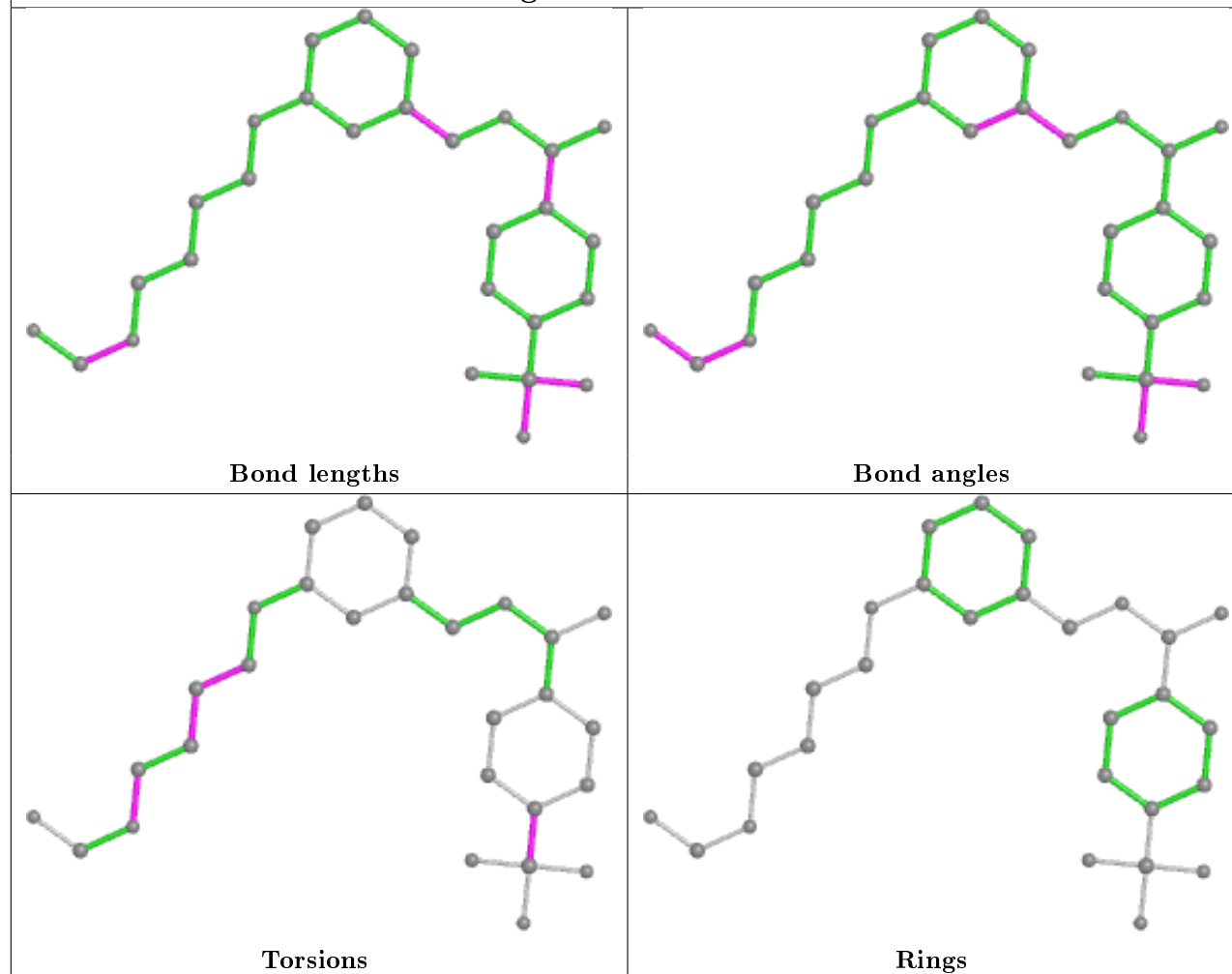
Torsions



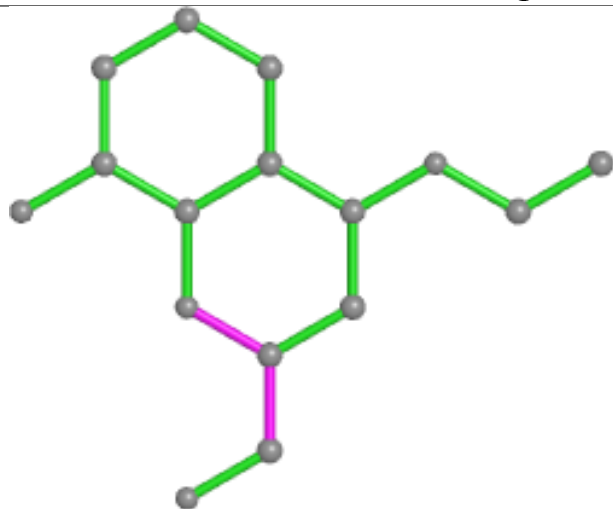
Rings



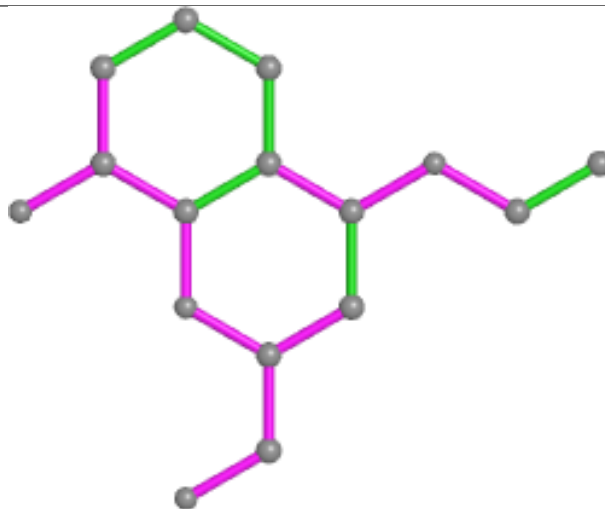
Ligand 6H0 B 302



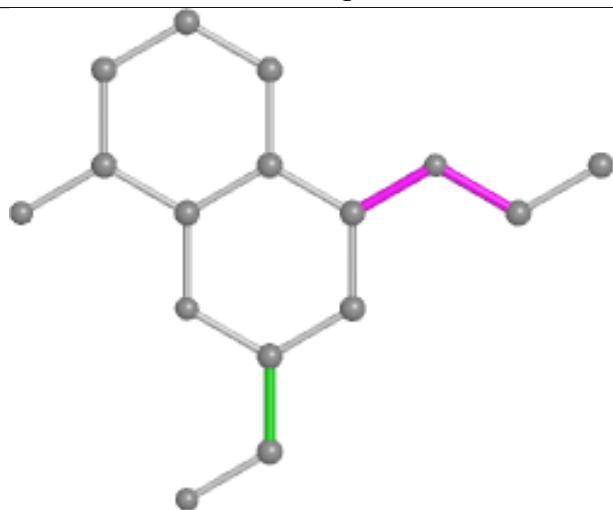
Ligand QUJ B 305



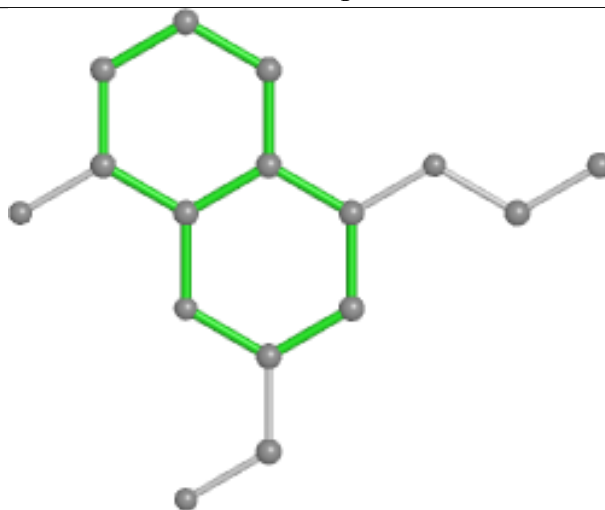
Bond lengths



Bond angles

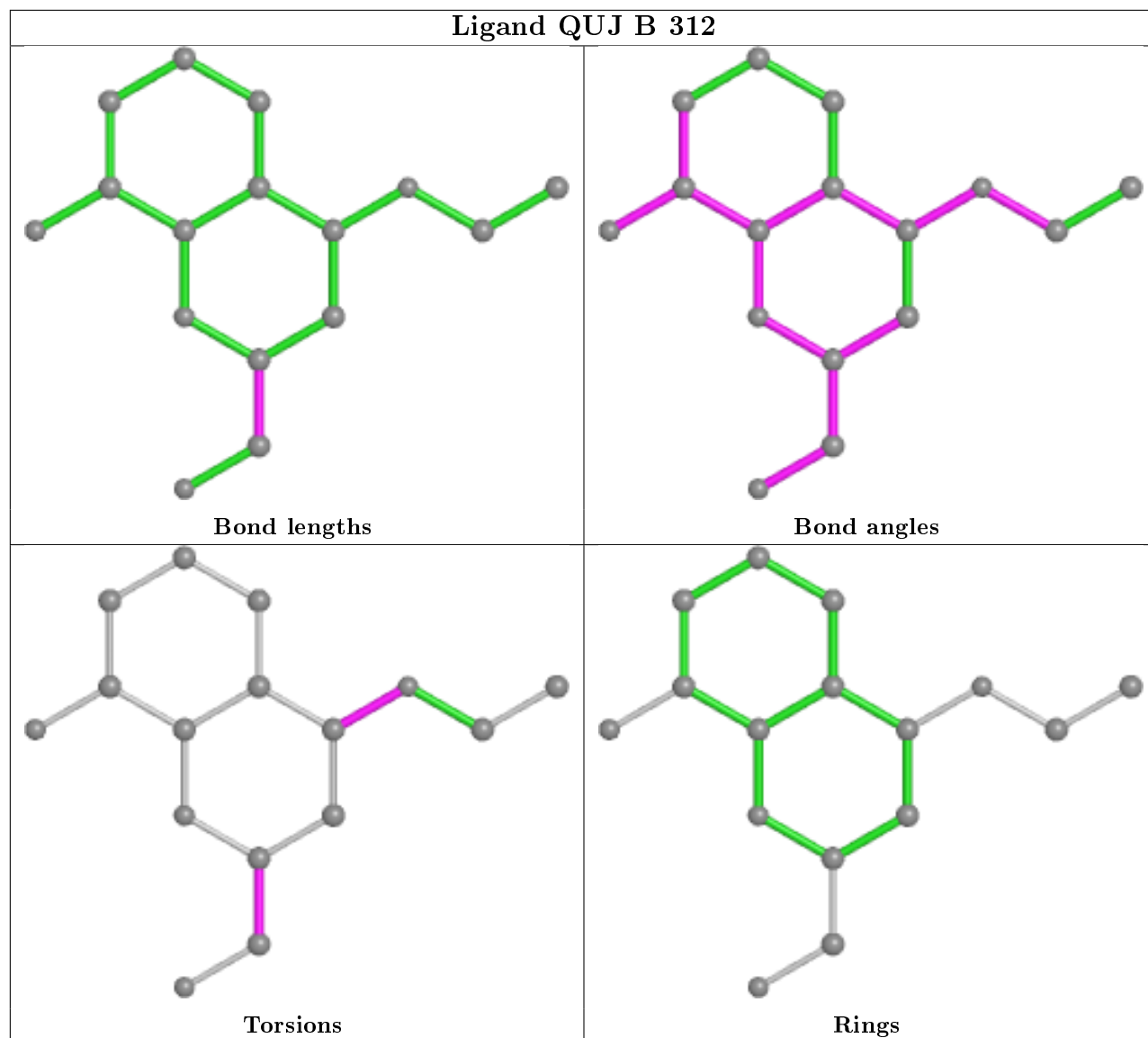


Torsions

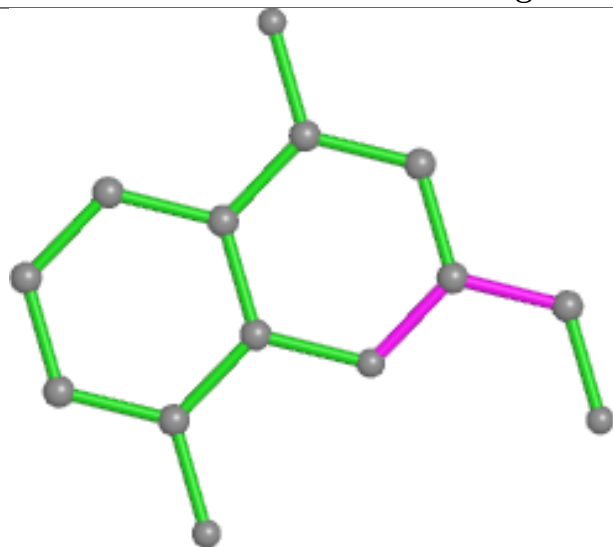


Rings

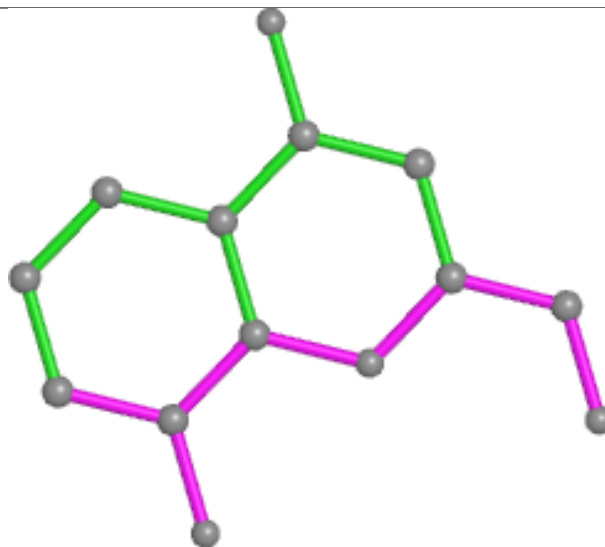
Ligand QUJ B 312



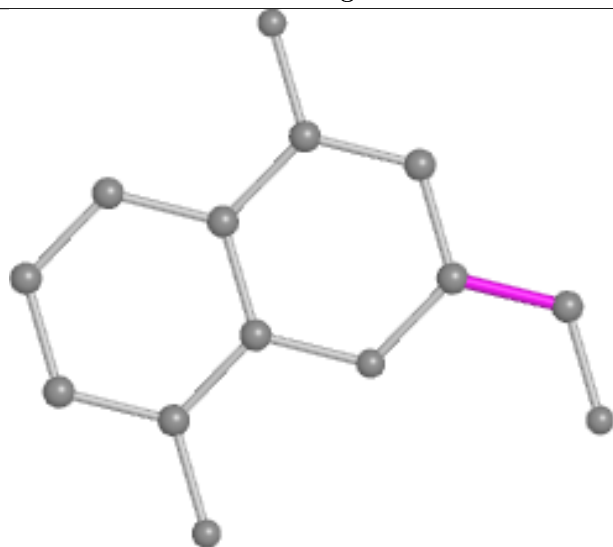
Ligand QUJ C 303



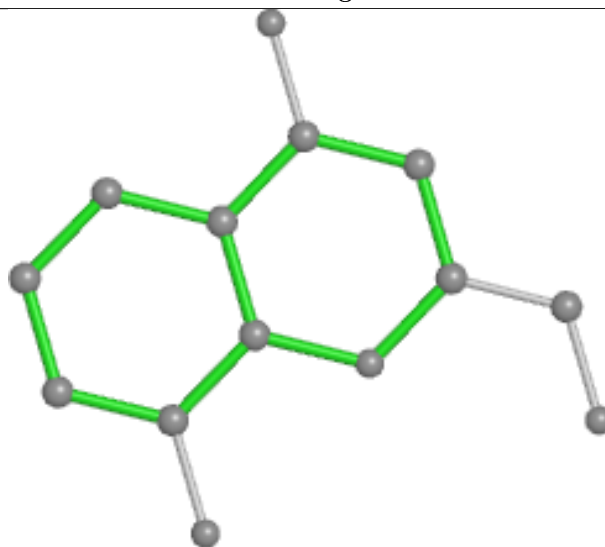
Bond lengths



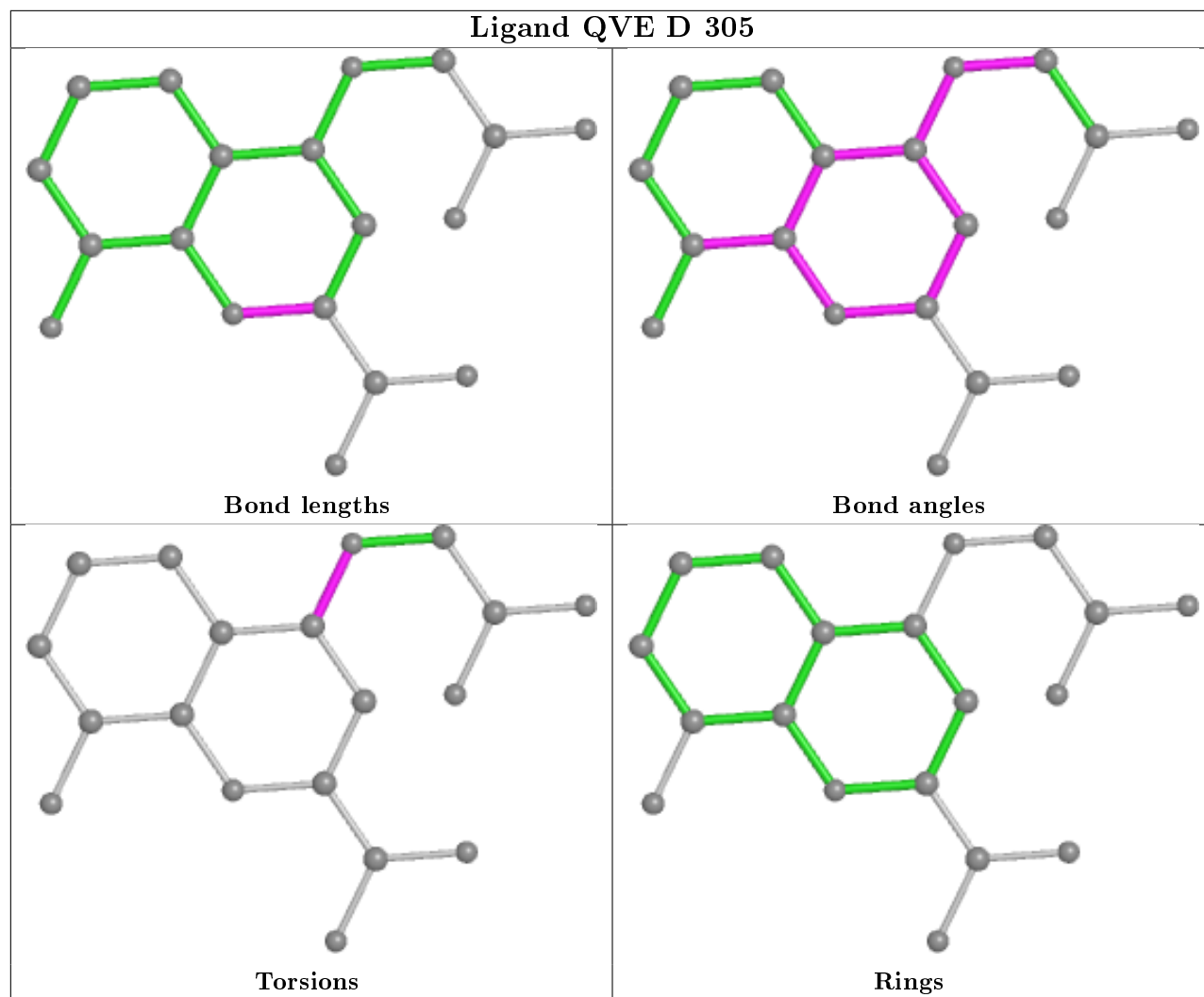
Bond angles

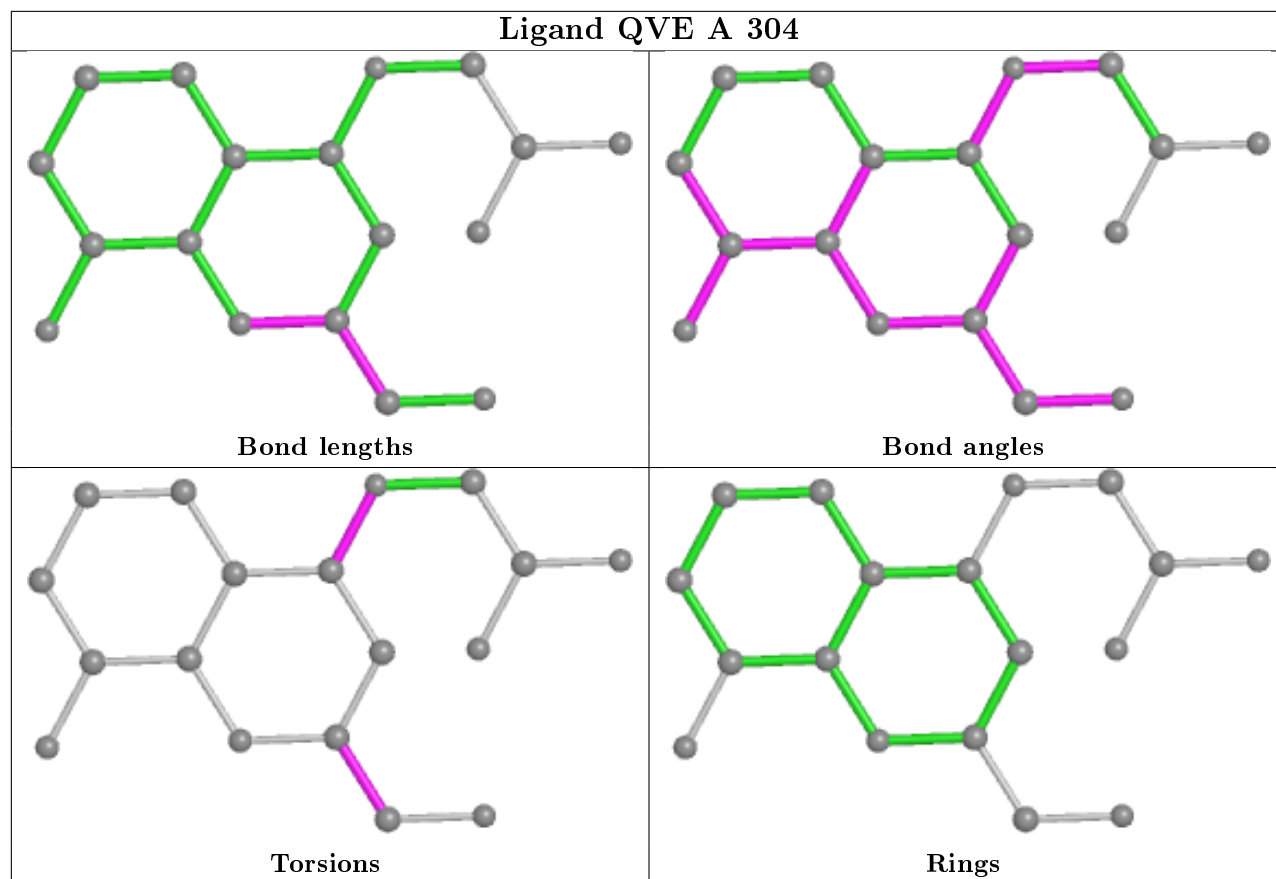


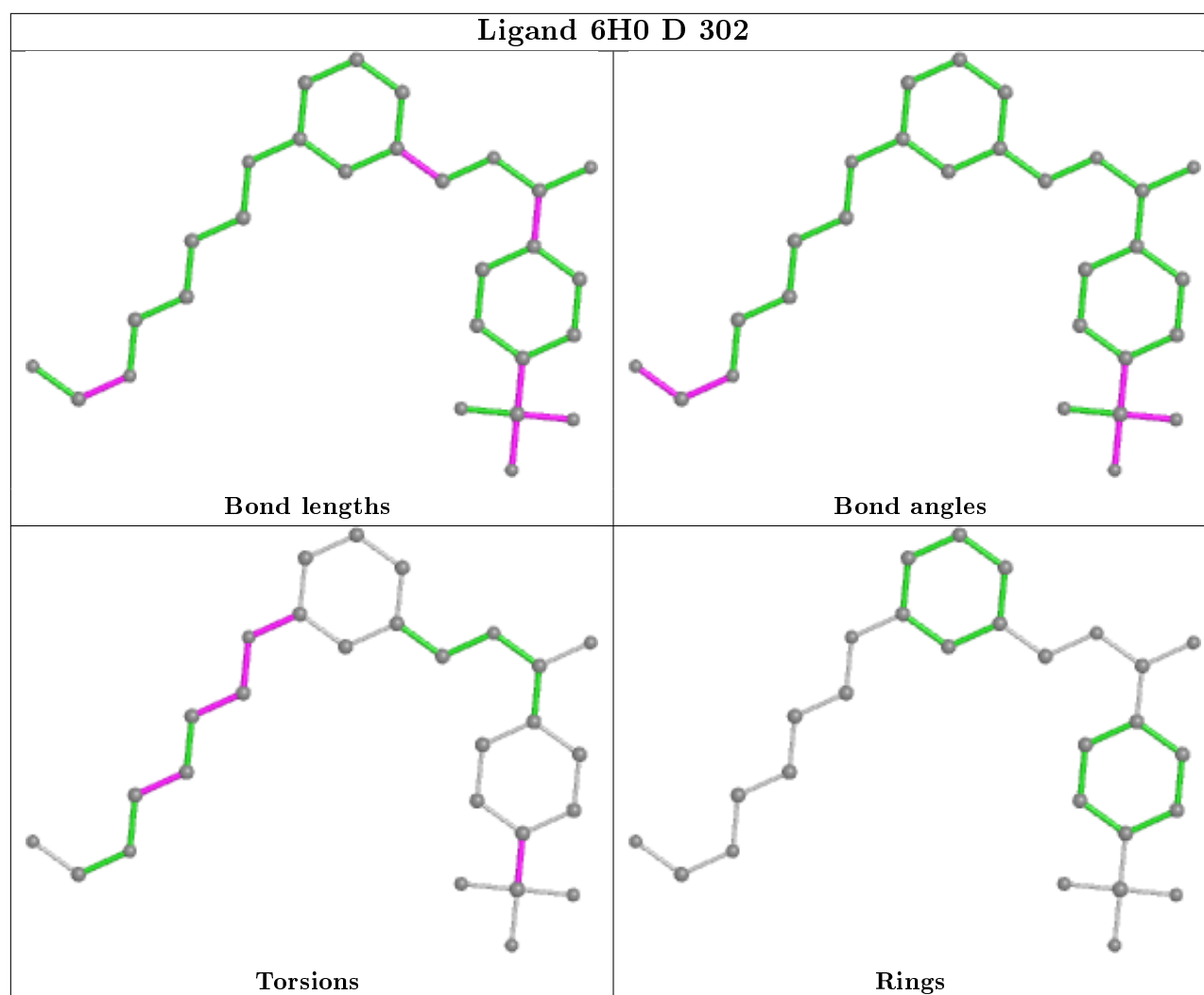
Torsions



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	259/260 (99%)	0.38	5 (1%) 66 65	46, 61, 75, 124	0
1	B	259/260 (99%)	0.38	4 (1%) 73 73	46, 62, 77, 124	0
1	C	257/260 (98%)	0.34	9 (3%) 44 38	48, 65, 79, 91	0
1	D	256/260 (98%)	0.45	11 (4%) 35 31	52, 71, 90, 107	0
All	All	1031/1040 (99%)	0.39	29 (2%) 53 49	46, 64, 84, 124	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	GLY	3.3
1	D	238	GLU	3.2
1	A	3	HIS	3.2
1	C	238	GLU	3.1
1	C	115	ALA	2.8
1	B	2	SER	2.8
1	D	176	THR	2.7
1	B	40	TYR	2.6
1	D	82	GLY	2.5
1	D	234	GLY	2.4
1	D	63	GLY	2.4
1	A	2	SER	2.4
1	C	234	GLY	2.3
1	D	7	TYR	2.3
1	A	189	ASP	2.2
1	C	129	ASP	2.2
1	D	4	HIS	2.2
1	C	63	GLY	2.2
1	D	129	ASP	2.2
1	D	92	GLN	2.1
1	D	52	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	99	SER	2.1
1	C	19	ASP	2.1
1	A	236	PRO	2.1
1	C	56	SER	2.1
1	C	114	TYR	2.1
1	B	15	HIS	2.1
1	C	55	THR	2.1
1	B	110	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
4	QUJ	D	303	14/19	0.77	0.31	78,83,89,91	0
4	QUJ	A	305	16/19	0.81	0.35	70,74,77,79	0
2	ZN	A	309	1/1	0.81	0.13	77,77,77,77	1
4	QUJ	B	312	16/19	0.82	0.27	81,89,96,99	0
2	ZN	C	312	1/1	0.83	0.43	124,124,124,124	1
6	GOL	B	311	6/6	0.83	0.44	124,124,124,124	0
4	QUJ	B	305	16/19	0.85	0.29	68,72,76,77	0
2	ZN	A	313	1/1	0.86	0.33	73,73,73,73	1
6	GOL	A	314	6/6	0.86	0.40	124,124,124,124	0
2	ZN	B	308	1/1	0.87	0.08	77,77,77,77	0
6	GOL	C	311	6/6	0.87	0.40	124,124,124,124	0
4	QUJ	C	305	17/19	0.88	0.22	76,82,90,91	0
2	ZN	A	315	1/1	0.88	0.14	77,77,77,77	0
6	GOL	D	310	6/6	0.88	0.43	124,124,124,124	0
4	QUJ	C	303	14/19	0.89	0.25	75,78,82,84	0

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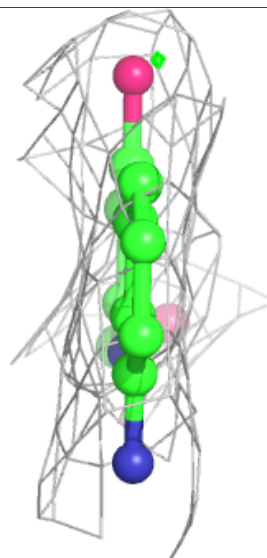
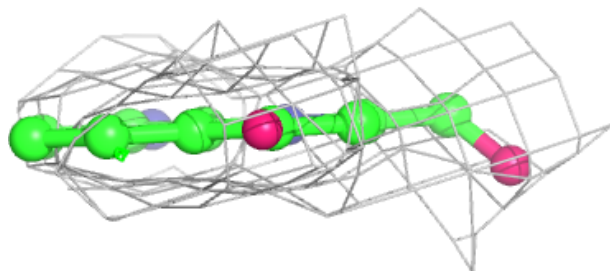
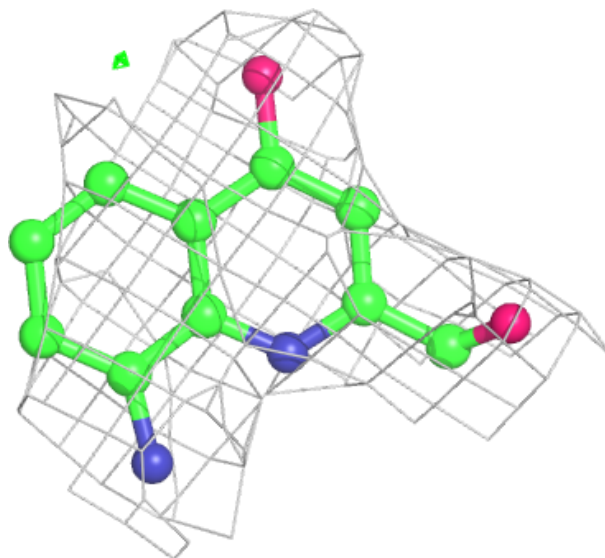
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	A	312	1/1	0.89	0.08	66,66,66,66	0
2	ZN	A	311	1/1	0.89	0.10	78,78,78,78	0
2	ZN	B	309	1/1	0.90	0.14	77,77,77,77	1
4	QUJ	B	303	14/19	0.90	0.26	66,69,72,74	0
5	QVE	D	304	18/19	0.90	0.27	72,76,78,79	0
4	QUJ	A	303	14/19	0.91	0.21	67,70,73,75	0
2	ZN	D	309	1/1	0.91	0.09	99,99,99,99	0
5	QVE	B	304	18/19	0.91	0.26	64,66,67,67	0
2	ZN	D	308	1/1	0.92	0.09	85,85,85,85	1
5	QVE	C	304	18/19	0.92	0.27	69,73,75,75	0
2	ZN	C	309	1/1	0.93	0.06	80,80,80,80	1
5	QVE	A	304	18/19	0.93	0.25	68,69,70,73	0
2	ZN	A	310	1/1	0.93	0.06	80,80,80,80	0
2	ZN	C	308	1/1	0.93	0.05	82,82,82,82	0
2	ZN	A	308	1/1	0.94	0.05	76,76,76,76	0
5	QVE	C	306	19/19	0.94	0.23	80,84,87,87	0
2	ZN	D	307	1/1	0.94	0.05	89,89,89,89	0
2	ZN	A	316	1/1	0.94	0.20	124,124,124,124	1
5	QVE	D	305	19/19	0.95	0.23	83,88,91,92	0
5	QVE	A	306	19/19	0.96	0.25	75,78,80,83	0
2	ZN	B	310	1/1	0.96	0.06	81,81,81,81	0
5	QVE	B	306	19/19	0.96	0.26	72,75,77,78	0
3	6H0	A	302	28/28	0.97	0.25	45,50,64,67	0
3	6H0	C	302	28/28	0.97	0.18	47,54,71,76	0
2	ZN	D	311	1/1	0.97	0.20	124,124,124,124	1
2	ZN	C	310	1/1	0.97	0.11	84,84,84,84	0
3	6H0	B	302	28/28	0.97	0.25	45,50,63,67	0
3	6H0	D	302	28/28	0.97	0.20	51,57,77,82	0
2	ZN	C	307	1/1	0.98	0.06	58,58,58,58	0
2	ZN	B	307	1/1	0.99	0.05	55,55,55,55	0
2	ZN	D	301	1/1	0.99	0.11	51,51,51,51	0
2	ZN	A	307	1/1	0.99	0.08	57,57,57,57	0
2	ZN	D	306	1/1	0.99	0.09	60,60,60,60	0
2	ZN	C	301	1/1	0.99	0.10	47,47,47,47	0
2	ZN	A	301	1/1	1.00	0.11	45,45,45,45	0
2	ZN	B	301	1/1	1.00	0.11	45,45,45,45	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.

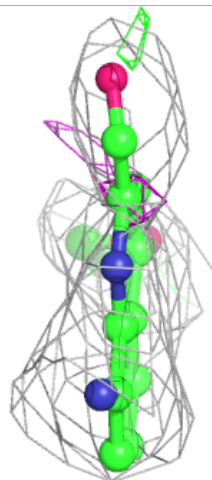
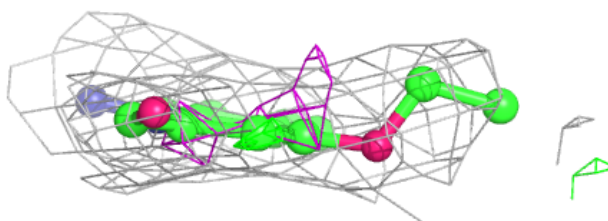
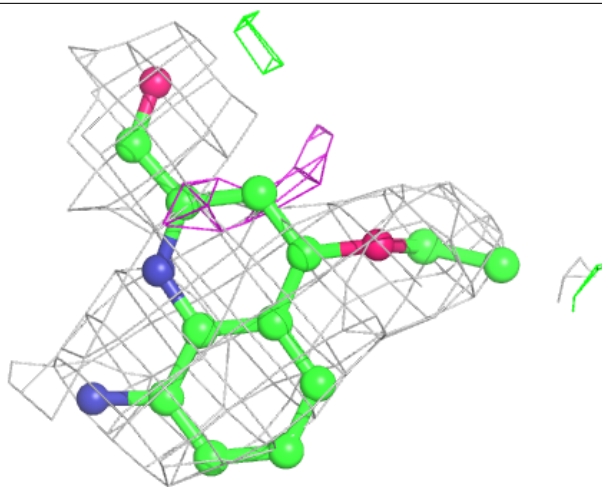
Electron density around QUJ D 303:

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



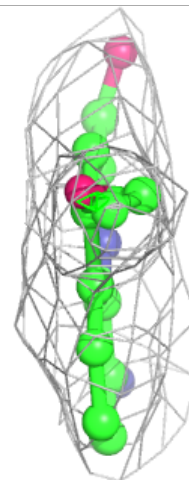
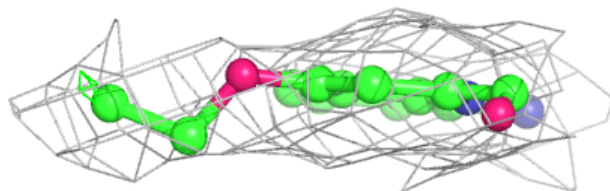
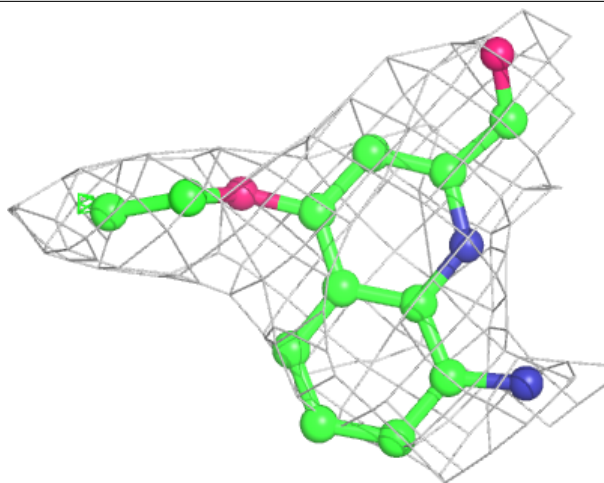
Electron density around QUJ A 305:

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



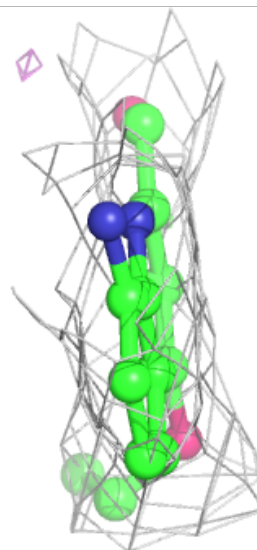
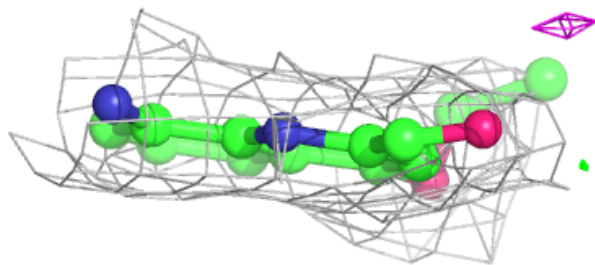
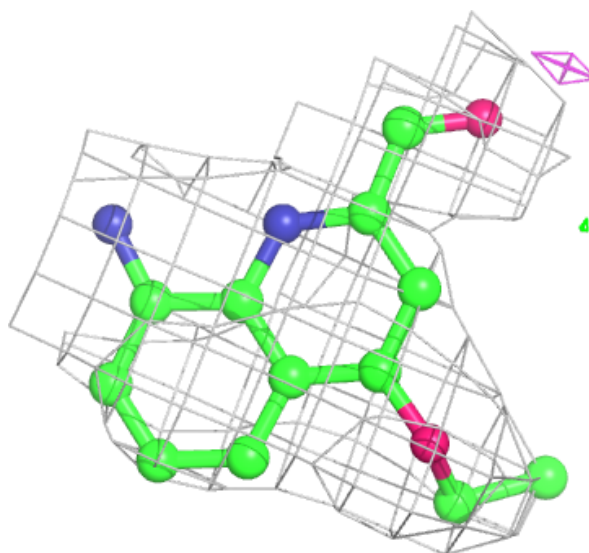
Electron density around QUJ B 312:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



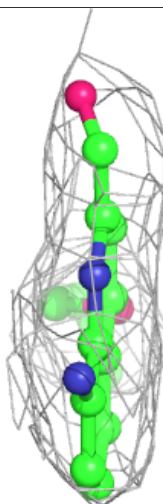
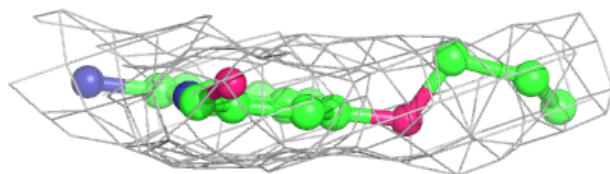
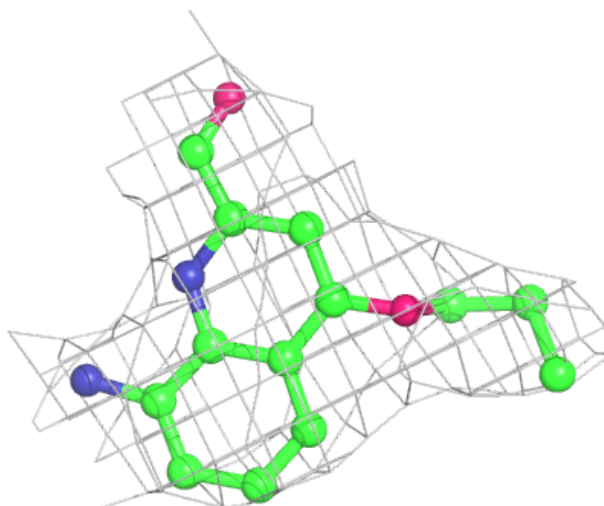
Electron density around QUJ B 305:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



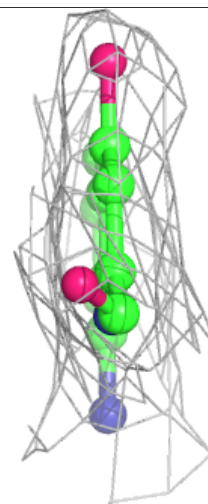
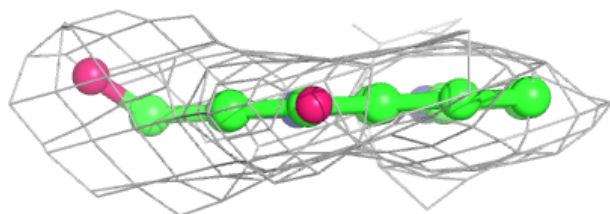
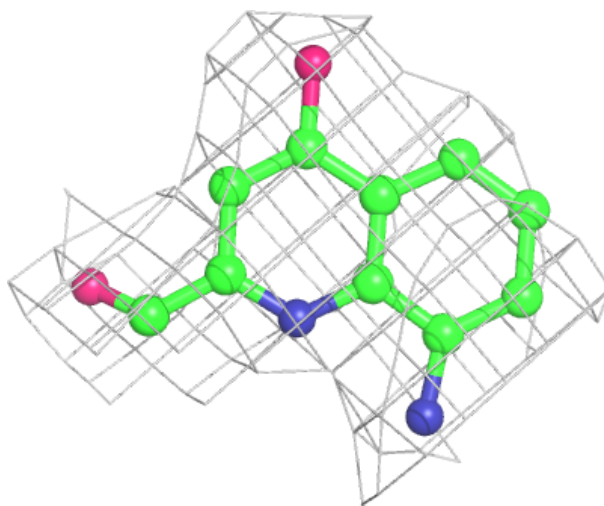
Electron density around QUJ C 305:

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and green (positive)



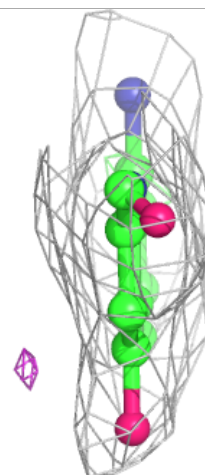
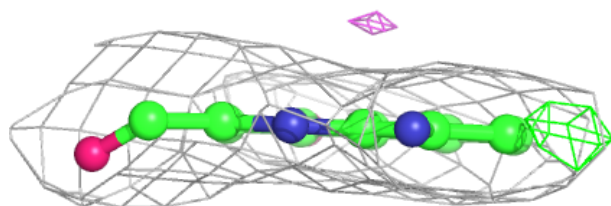
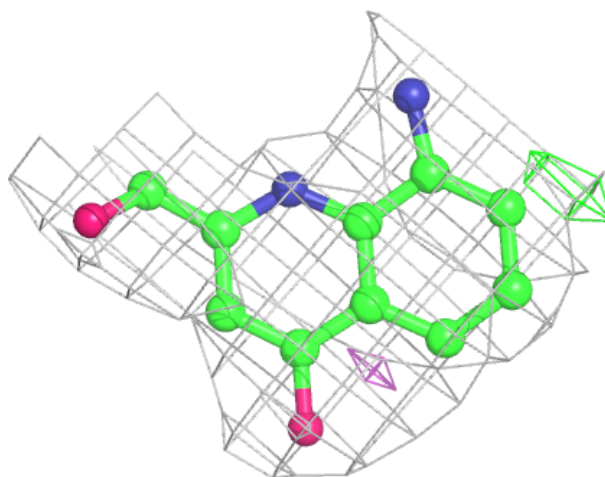
Electron density around QUJ C 303:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



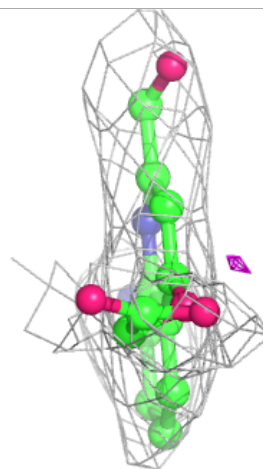
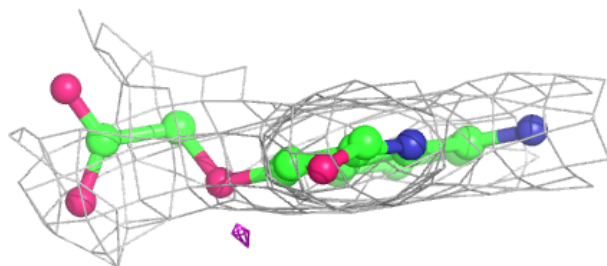
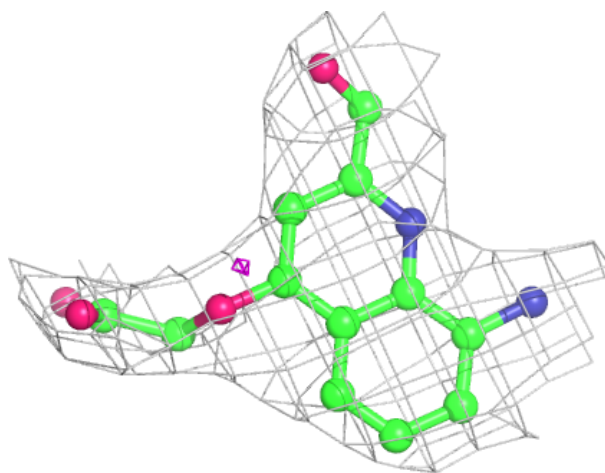
Electron density around QUJ B 303:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



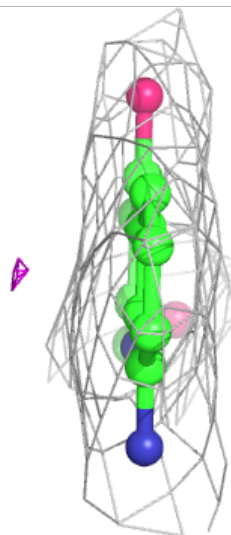
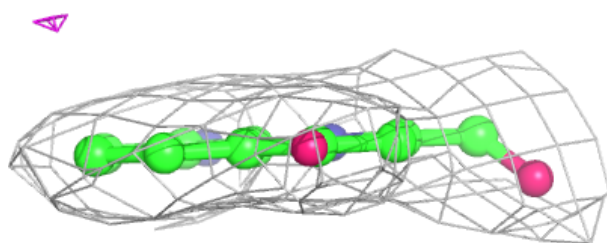
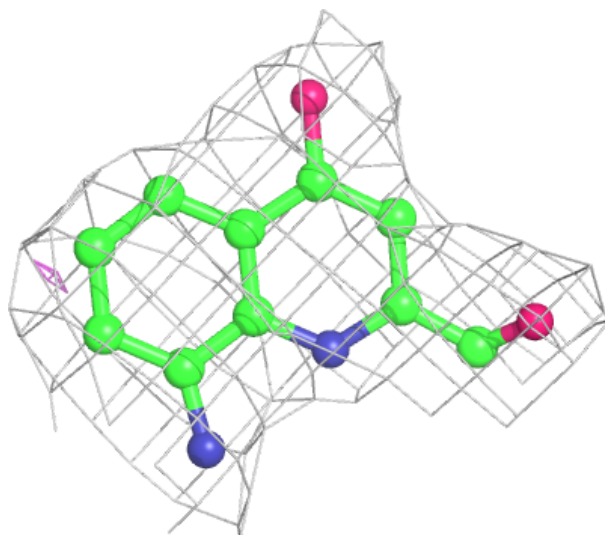
Electron density around QVE D 304:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



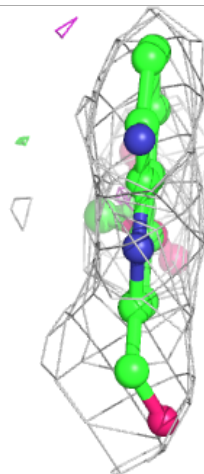
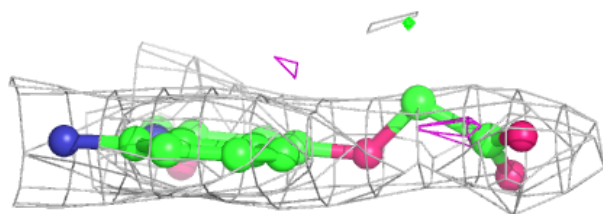
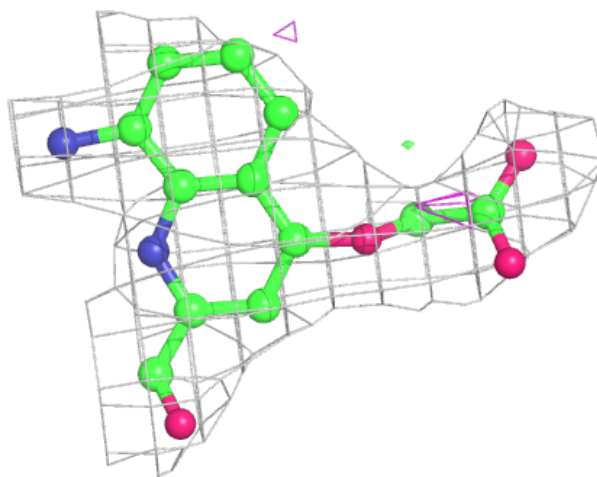
Electron density around QUJ A 303:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



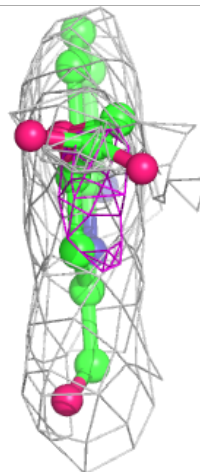
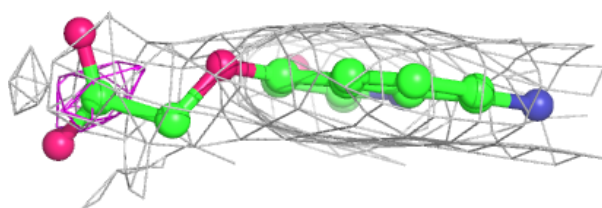
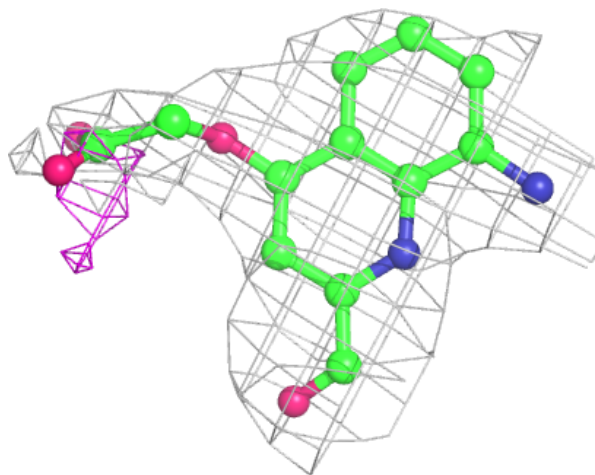
Electron density around QVE B 304:

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



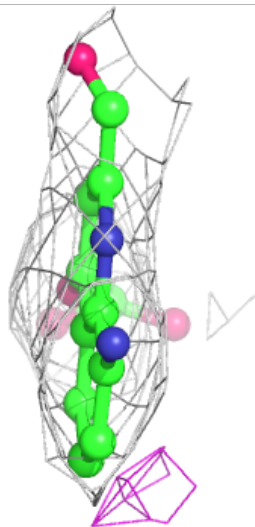
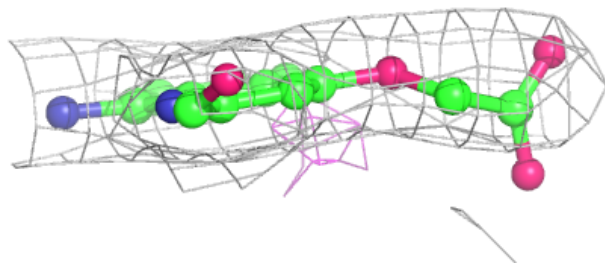
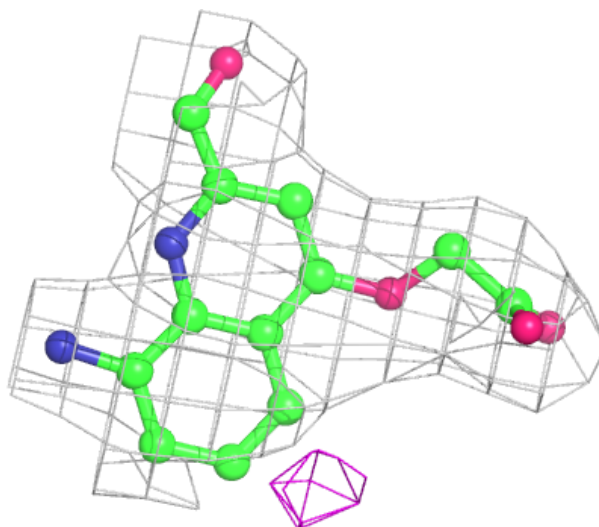
Electron density around QVE C 304:

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



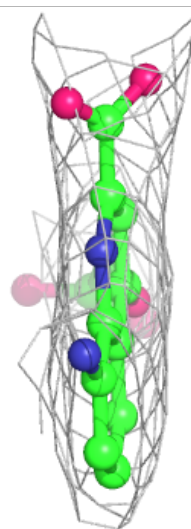
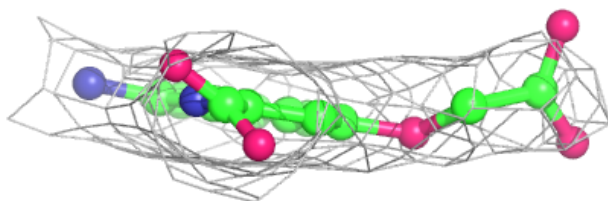
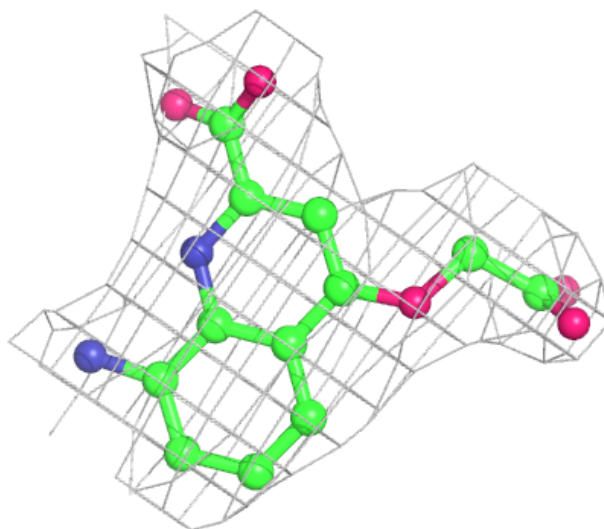
Electron density around QVE A 304:

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



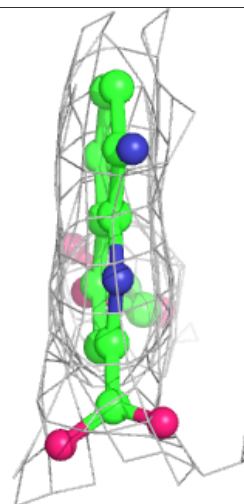
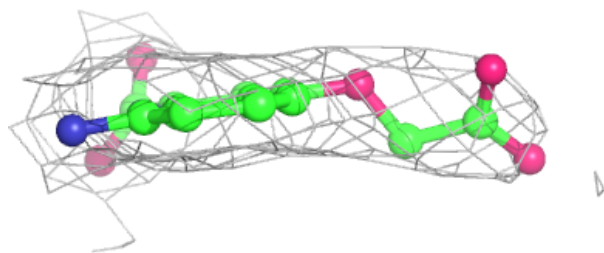
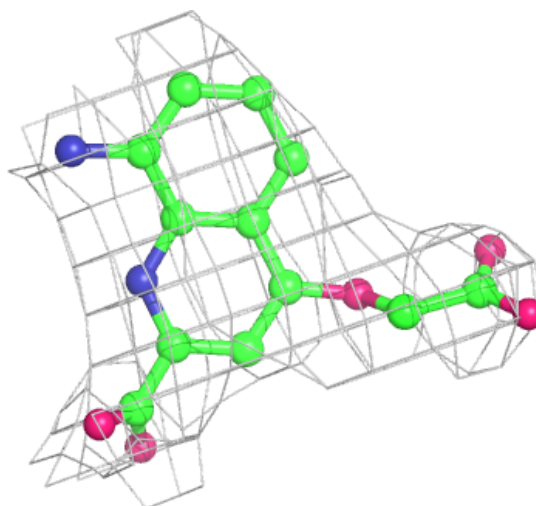
Electron density around QVE C 306:

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



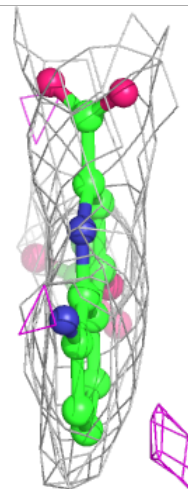
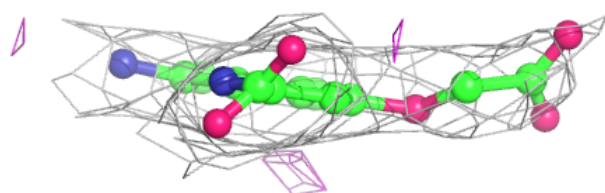
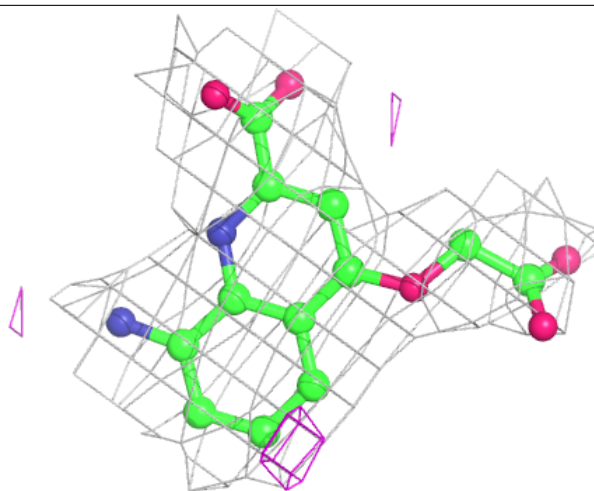
Electron density around QVE D 305:

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



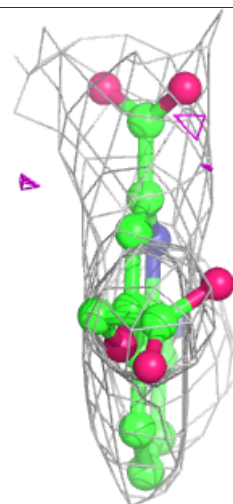
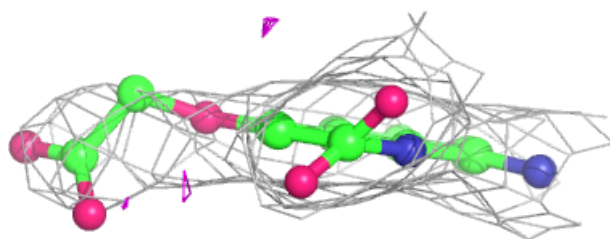
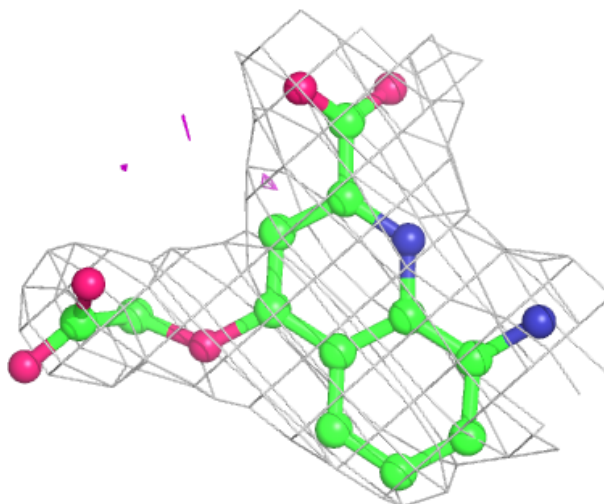
Electron density around QVE A 306:

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



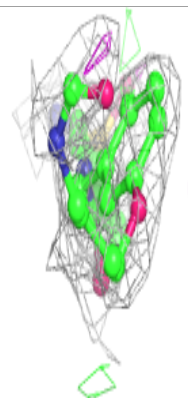
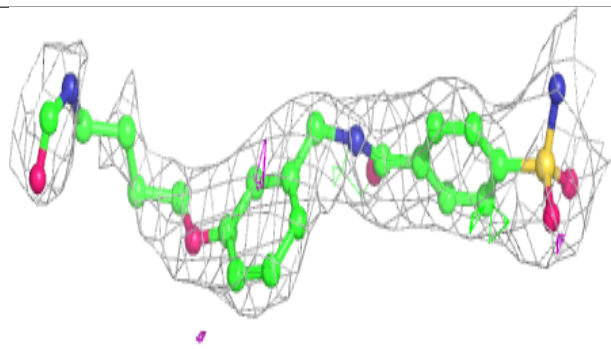
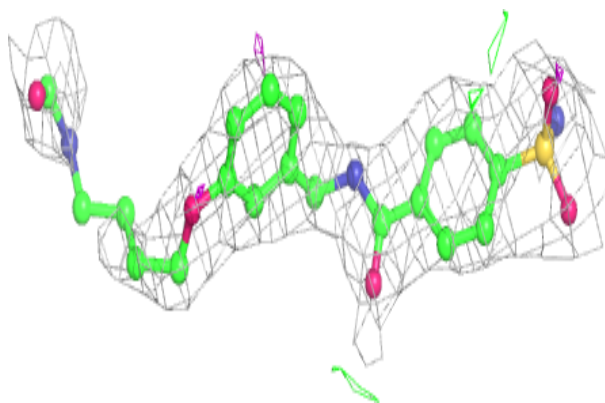
Electron density around QVE B 306:

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

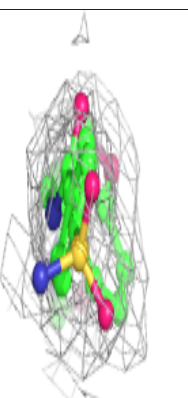
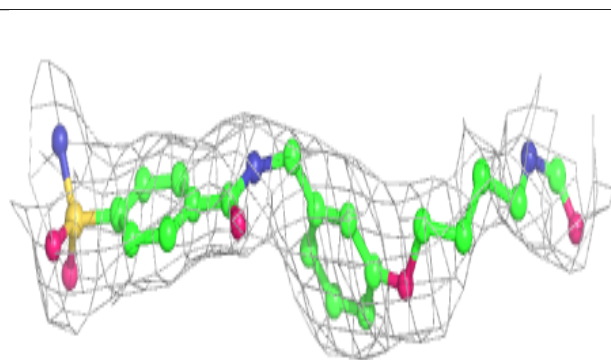
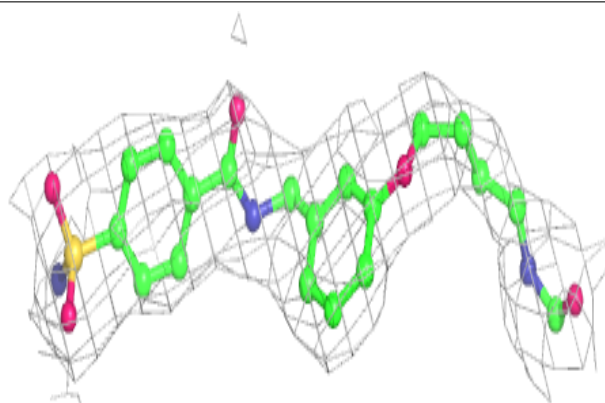


Electron density around 6H0 A 302:

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

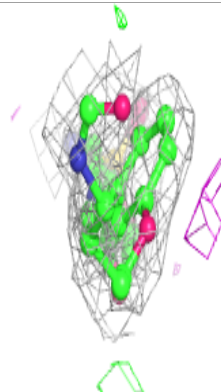
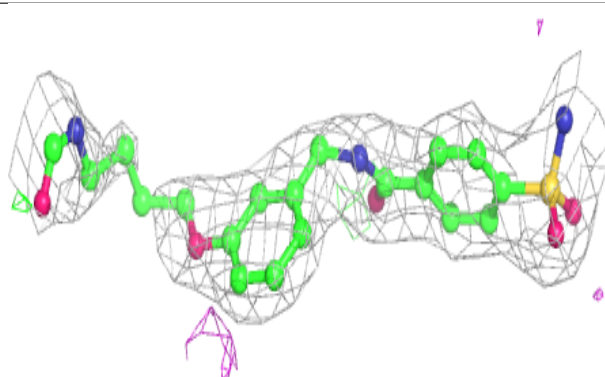
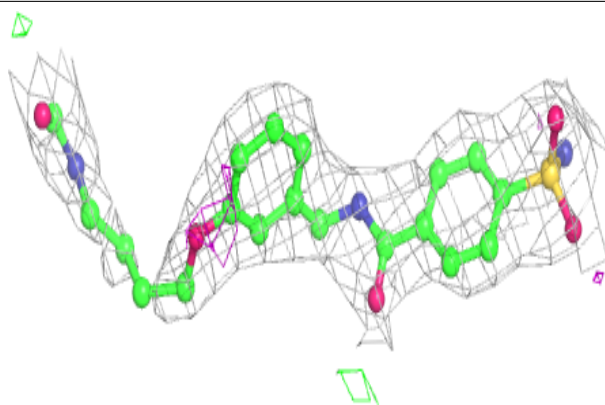
**Electron density around 6H0 C 302:**

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

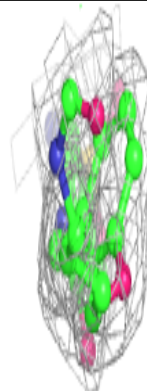
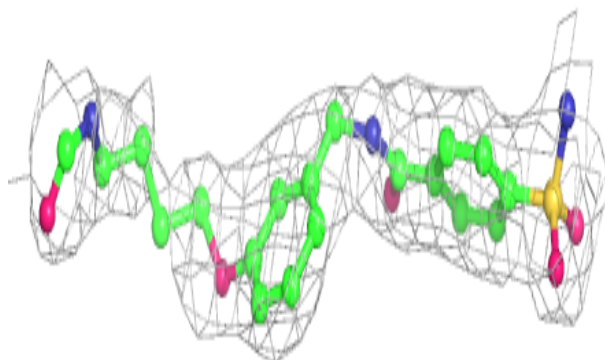
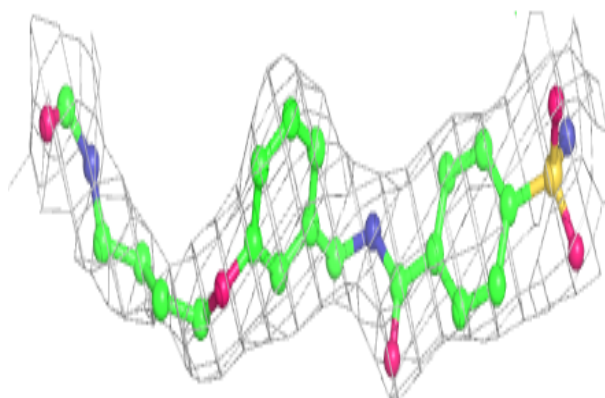


Electron density around 6H0 B 302:

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

**Electron density around 6H0 D 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 [i](#)

There are no such residues in this entry.