



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2023 – 07:03 pm GMT

PDB ID : 5L70
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 : 2016-06-01
Resolution : 2.20 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 types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

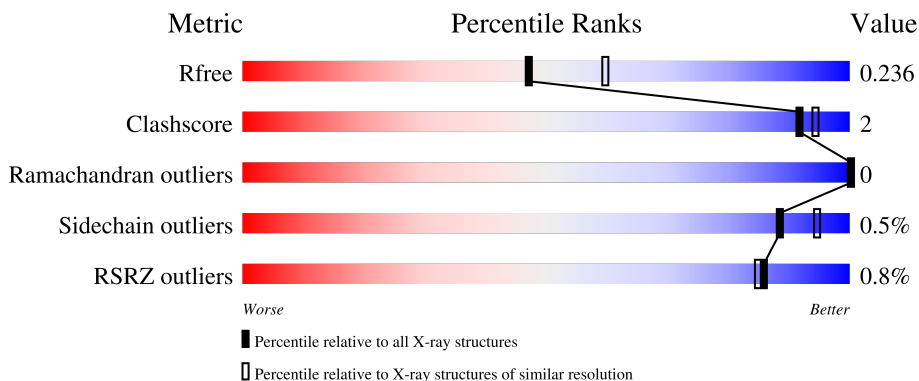
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

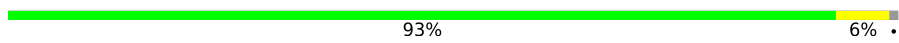
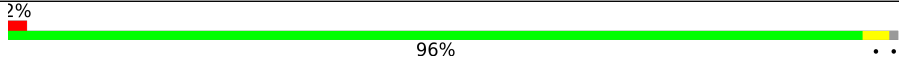
The reported resolution of this entry is 2.20 Å.

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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	 93% 6%
1	B	260	 2% 96%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4593 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.

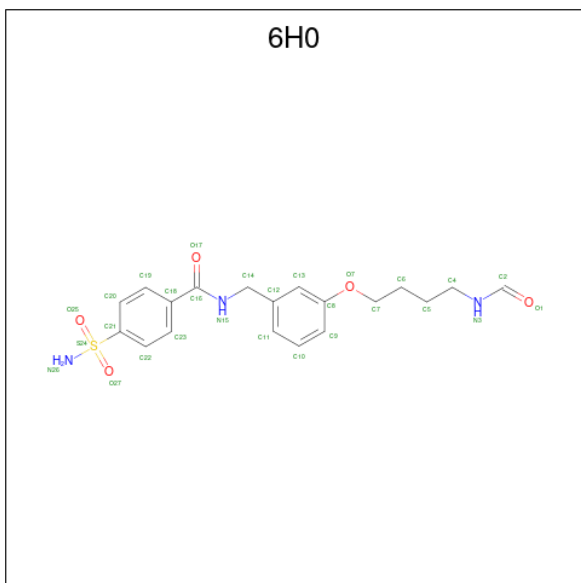
- Molecule 1 is a protein called Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	Total 2035	C 1308	N 343	O 382	S 2	0	3	0
1	B	258	Total 1989	C 1280	N 340	O 367	S 2	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total 9	Zn 9	0	0
2	B	4	Total 4	Zn 4	0	0

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



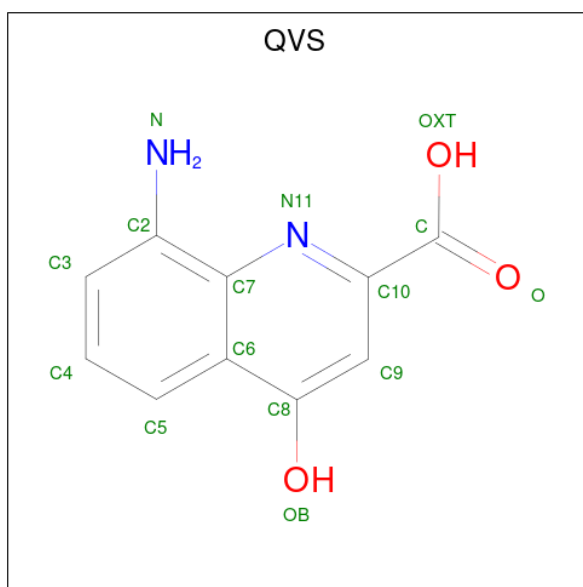
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
3	B	1	Total	C	N	O	S	0	0
			28	19	3	5	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



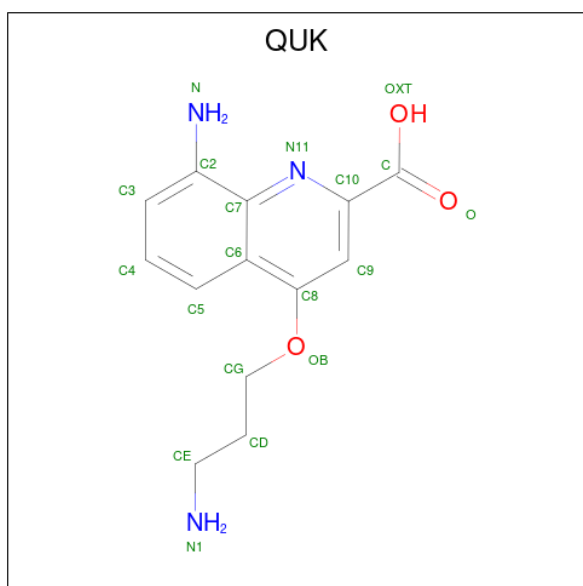
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 8-azanyl-4-oxidanyl-quinoline-2-carboxylic acid (three-letter code: QVS) (formula: C₁₀H₈N₂O₃).



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

- Molecule 6 is 8-azanyl-4-(3-azanylpropoxy)quinoline-2-carboxylic acid (three-letter code: QUK) (formula: $C_{13}H_{15}N_3O_3$).



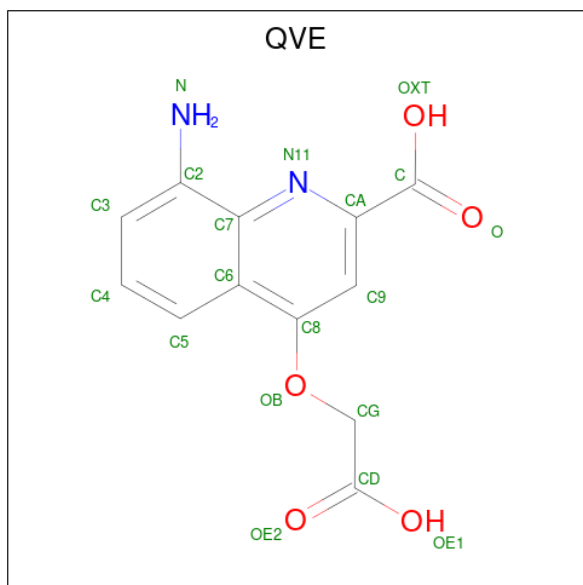
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	18	13	3	2	0	0

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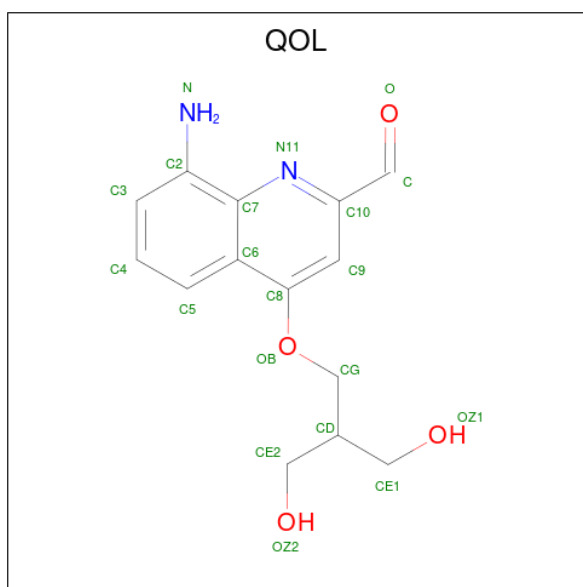
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	18	13	3	2	0	0

- Molecule 7 is 8-azanyl-4-(2-hydroxy-2-oxoethoxy)quinoline-2-carboxylic acid (three-letter code: QVE) (formula: C₁₂H₁₀N₂O₅).



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

- Molecule 8 is 8-azanyl-4-[2-(hydroxymethyl)-3-oxidanyl-propoxy]quinoline-2-carbaldehyde (three-letter code: QOL) (formula: C₁₄H₁₆N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	20	14	2	4	0	0
8	B	1	20	14	2	4	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	201	201	201	0	0
9	B	133	133	133	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: Carbonic anhydrase 2

Chain A:  93% 6%



- Molecule 1: Carbonic anhydrase 2

Chain B:  2% 96%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.21Å 83.37Å 79.41Å 90.00° 99.98° 90.00°	Depositor
Resolution (Å)	78.21 – 2.20 43.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.0 (78.21-2.20) 96.0 (43.54-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.174 , 0.238 0.181 , 0.236	Depositor DCC
R_{free} test set	1402 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtrriage
Anisotropy	0.012	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4593	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.06% 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: QVE, QVS, QUK, QOL, GOL, 6H0, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.63	0/2106	0.75	0/2869
1	B	0.57	0/2051	0.74	0/2800
All	All	0.60	0/4157	0.74	0/5669

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2035	0	1912	9	0
1	B	1989	0	1852	4	0
2	A	9	0	0	0	0
2	B	4	0	0	0	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
4	A	12	0	16	0	0
4	B	12	0	16	0	0
5	A	28	0	0	0	0
6	A	36	0	0	0	0
7	A	38	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	20	0	0	0	0
8	B	20	0	0	0	0
9	A	201	0	0	3	0
9	B	133	0	0	1	0
All	All	4593	0	3796	13	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 2.

All (13) 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:A:252[B]:ASN:O	1:A:252[B]:ASN:CG	2.32	0.68
1:A:10:HIS:CD2	9:A:565:HOH:O	2.53	0.60
1:B:157:GLN:NE2	9:B:401:HOH:O	2.34	0.59
1:A:189:ASP:HB2	1:A:212:LYS:HE3	1.86	0.58
1:B:133:ALA:O	1:B:139:GLY:HA3	2.06	0.56
1:A:133:ALA:O	1:A:139:GLY:HA3	2.06	0.55
1:A:167:LYS:NZ	9:A:402:HOH:O	2.42	0.53
1:A:3:HIS:CE1	9:A:480:HOH:O	2.70	0.44
1:B:89:ARG:O	1:B:122:HIS:HA	2.17	0.44
1:A:45:LYS:O	1:A:82:GLY:HA2	2.18	0.43
1:A:89:ARG:O	1:A:122:HIS:HA	2.18	0.43
1:A:116:ALA:HB3	1:A:147:LEU:HB2	2.01	0.42
1:B:45:LYS:O	1:B:82:GLY:HA2	2.19	0.42

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	259/260 (100%)	248 (96%)	11 (4%)	0	100	100
1	B	256/260 (98%)	248 (97%)	8 (3%)	0	100	100
All	All	515/520 (99%)	496 (96%)	19 (4%)	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	211/225 (94%)	210 (100%)	1 (0%)	88	94
1	B	201/225 (89%)	200 (100%)	1 (0%)	88	94
All	All	412/450 (92%)	410 (100%)	2 (0%)	88	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	SER
1	B	216	SER

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

Mol	Chain	Res	Type
1	A	3	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 13 are monoatomic - leaving 14 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
8	QOL	A	316	3,5	21,21,21	1.88	1 (4%)	23,28,28	2.82	5 (21%)
4	GOL	B	305	-	5,5,5	0.31	0	5,5,5	0.47	0
7	QVE	A	319	2,6	20,20,20	1.74	1 (5%)	27,28,28	1.66	8 (29%)
6	QUK	A	318	5,7	19,19,20	1.87	2 (10%)	22,25,27	2.71	7 (31%)
5	QVS	A	305	8,6	15,15,16	1.72	2 (13%)	19,21,23	3.00	5 (26%)
3	6H0	A	302	2,8	29,29,29	2.07	5 (17%)	37,38,38	1.53	3 (8%)
6	QUK	A	306	5,7	19,19,20	1.77	1 (5%)	22,25,27	2.81	7 (31%)
4	GOL	A	315	-	5,5,5	0.35	0	5,5,5	0.40	0
3	6H0	B	303	2,8	29,29,29	1.84	5 (17%)	37,38,38	1.59	5 (13%)
5	QVS	A	317	8,6	15,15,16	2.05	2 (13%)	19,21,23	2.87	6 (31%)
8	QOL	B	301	3,5	21,21,21	2.18	1 (4%)	23,28,28	2.44	6 (26%)
4	GOL	B	308	-	5,5,5	0.36	0	5,5,5	0.26	0
7	QVE	A	307	2,6	20,20,20	1.79	1 (5%)	27,28,28	2.03	8 (29%)
4	GOL	A	304	-	5,5,5	0.34	0	5,5,5	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	QOL	A	316	3,5	-	2/11/11/11	0/2/2/2
4	GOL	B	305	-	-	4/4/4/4	-
7	QVE	A	319	2,6	-	2/9/9/9	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	QUK	A	318	5,7	-	2/7/7/9	0/2/2/2
5	QVS	A	305	8,6	-	2/2/2/4	0/2/2/2
3	6H0	A	302	2,8	-	5/23/23/23	0/2/2/2
6	QUK	A	306	5,7	-	2/7/7/9	0/2/2/2
4	GOL	A	315	-	-	2/4/4/4	-
3	6H0	B	303	2,8	-	5/23/23/23	0/2/2/2
5	QVS	A	317	8,6	-	2/2/2/4	0/2/2/2
8	QOL	B	301	3,5	-	4/11/11/11	0/2/2/2
4	GOL	B	308	-	-	2/4/4/4	-
7	QVE	A	307	2,6	-	6/9/9/9	0/2/2/2
4	GOL	A	304	-	-	2/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	301	QOL	C10-C	-9.30	1.38	1.48
8	A	316	QOL	C10-C	-7.49	1.40	1.48
6	A	318	QUK	C10-C	-7.22	1.41	1.48
6	A	306	QUK	C10-C	-6.89	1.41	1.48
7	A	307	QVE	CA-C	-6.83	1.41	1.50
7	A	319	QVE	CA-C	-6.63	1.41	1.50
5	A	317	QVS	C10-C	-6.55	1.41	1.48
3	A	302	6H0	O27-S24	5.64	1.54	1.43
3	B	303	6H0	O27-S24	5.33	1.53	1.43
3	A	302	6H0	O25-S24	5.18	1.53	1.43
5	A	305	QVS	C10-C	-5.16	1.43	1.48
3	B	303	6H0	C14-C12	-4.75	1.41	1.51
3	A	302	6H0	C14-C12	-4.49	1.41	1.51
3	A	302	6H0	C18-C16	-4.45	1.40	1.50
3	A	302	6H0	C21-S24	-3.98	1.70	1.77
3	B	303	6H0	O25-S24	3.87	1.50	1.43
3	B	303	6H0	C21-S24	-3.15	1.72	1.77
5	A	317	QVS	C10-N11	3.03	1.36	1.33
3	B	303	6H0	C18-C16	-2.90	1.44	1.50
5	A	305	QVS	C10-N11	2.85	1.36	1.33
6	A	318	QUK	C10-N11	2.12	1.35	1.33

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	305	QVS	C10-N11-C7	9.77	125.52	118.11
6	A	306	QUK	C10-N11-C7	9.47	125.29	118.11
5	A	317	QVS	C10-N11-C7	9.46	125.28	118.11
6	A	318	QUK	C10-N11-C7	8.90	124.86	118.11
8	A	316	QOL	C-C10-N11	8.29	122.78	114.66
8	A	316	QOL	C10-N11-C7	7.90	124.10	118.11
8	B	301	QOL	C-C10-N11	6.64	121.16	114.66
8	B	301	QOL	C10-N11-C7	6.16	122.78	118.11
6	A	318	QUK	O-C-C10	-5.44	119.07	124.22
7	A	307	QVE	CG-OB-C8	5.43	123.13	116.95
3	A	302	6H0	O25-S24-O27	-5.38	109.91	118.76
3	B	303	6H0	O25-S24-O27	-5.35	109.96	118.76
3	A	302	6H0	O1-C2-N3	-5.32	119.52	124.89
6	A	306	QUK	C9-C10-C	4.88	125.44	121.23
5	A	305	QVS	O-C-C10	-4.83	119.64	124.22
5	A	317	QVS	O-C-C10	-4.83	119.65	124.22
8	B	301	QOL	C3-C2-N	4.64	129.64	120.36
3	B	303	6H0	O1-C2-N3	-4.61	120.24	124.89
6	A	306	QUK	O-C-C10	-4.54	119.92	124.22
8	A	316	QOL	C3-C2-N	4.50	129.35	120.36
7	A	307	QVE	C-CA-N11	4.49	123.45	116.28
6	A	318	QUK	C9-C10-C	4.17	124.83	121.23
5	A	305	QVS	C-C10-N11	4.16	118.74	114.66
8	A	316	QOL	C7-C2-N	-3.62	111.17	118.07
7	A	319	QVE	CA-N11-C7	3.60	124.82	117.24
5	A	305	QVS	C9-C10-C	3.52	124.27	121.23
8	B	301	QOL	C7-C2-N	-3.51	111.37	118.07
5	A	317	QVS	C-C10-N11	3.45	118.05	114.66
7	A	319	QVE	CG-OB-C8	3.45	120.88	116.95
6	A	306	QUK	C3-C2-N	3.41	127.18	120.36
7	A	307	QVE	C2-C7-N11	3.40	122.00	118.64
5	A	317	QVS	C9-C10-C	3.18	123.98	121.23
6	A	318	QUK	C3-C2-N	3.15	126.65	120.36
5	A	305	QVS	C3-C2-N	3.10	126.56	120.36
7	A	307	QVE	CA-N11-C7	3.08	123.72	117.24
5	A	317	QVS	C3-C2-N	3.04	126.45	120.36
7	A	319	QVE	C2-C7-N11	2.98	121.59	118.64
7	A	307	QVE	C9-CA-N11	-2.81	117.65	124.50
3	B	303	6H0	O25-S24-C21	2.81	110.49	107.35
7	A	319	QVE	C-CA-N11	2.79	120.73	116.28
7	A	319	QVE	C9-CA-N11	-2.74	117.82	124.50
6	A	306	QUK	C3-C2-C7	-2.65	115.89	120.06
7	A	307	QVE	OXT-C-O	-2.59	117.60	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	306	QUK	CG-OB-C8	2.57	125.42	117.74
8	A	316	QOL	OB-CG-CD	2.49	114.71	108.21
8	B	301	QOL	OB-CG-CD	2.47	114.66	108.21
8	B	301	QOL	O-C-C10	-2.45	121.90	124.22
3	B	303	6H0	O25-S24-N26	2.41	110.94	107.36
6	A	306	QUK	C6-C7-N11	-2.37	117.89	122.78
7	A	307	QVE	OXT-C-CA	2.33	120.00	114.69
6	A	318	QUK	CG-OB-C8	2.28	124.56	117.74
7	A	319	QVE	OXT-C-CA	2.27	119.85	114.69
7	A	319	QVE	OXT-C-O	-2.26	118.33	123.35
6	A	318	QUK	C6-C7-N11	-2.22	118.21	122.78
3	B	303	6H0	C23-C18-C19	-2.20	115.45	118.59
7	A	307	QVE	C3-C2-N	2.19	124.74	120.36
7	A	319	QVE	C6-C7-N11	-2.15	118.34	122.78
5	A	317	QVS	C6-C7-N11	-2.09	118.47	122.78
3	A	302	6H0	O27-S24-C21	2.07	109.66	107.35
6	A	318	QUK	C3-C2-C7	-2.03	116.87	120.06

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	315	GOL	O1-C1-C2-C3
4	B	305	GOL	O1-C1-C2-C3
4	B	305	GOL	C1-C2-C3-O3
4	B	308	GOL	O1-C1-C2-C3
5	A	305	QVS	O-C-C10-C9
5	A	305	QVS	O-C-C10-N11
5	A	317	QVS	O-C-C10-C9
5	A	317	QVS	O-C-C10-N11
8	A	316	QOL	CE2-CD-CG-OB
8	B	301	QOL	CE1-CD-CG-OB
8	B	301	QOL	CE2-CD-CG-OB
8	B	301	QOL	O-C-C10-C9
8	B	301	QOL	O-C-C10-N11
7	A	307	QVE	OE2-CD-CG-OB
4	A	304	GOL	O1-C1-C2-C3
3	B	303	6H0	C5-C6-C7-O7
4	A	315	GOL	O1-C1-C2-O2
4	B	305	GOL	O2-C2-C3-O3
4	B	308	GOL	O1-C1-C2-O2
7	A	307	QVE	OE1-CD-CG-OB

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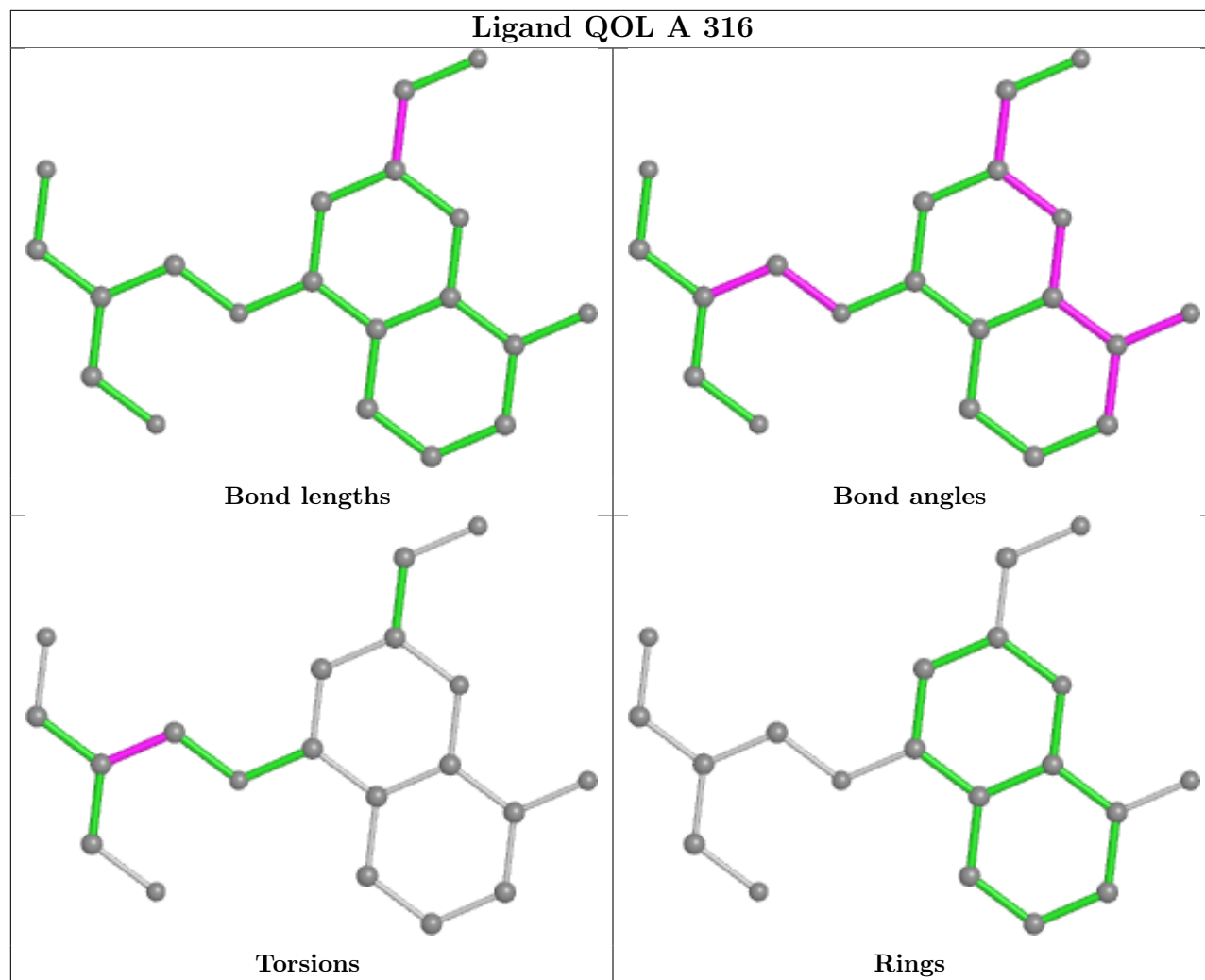
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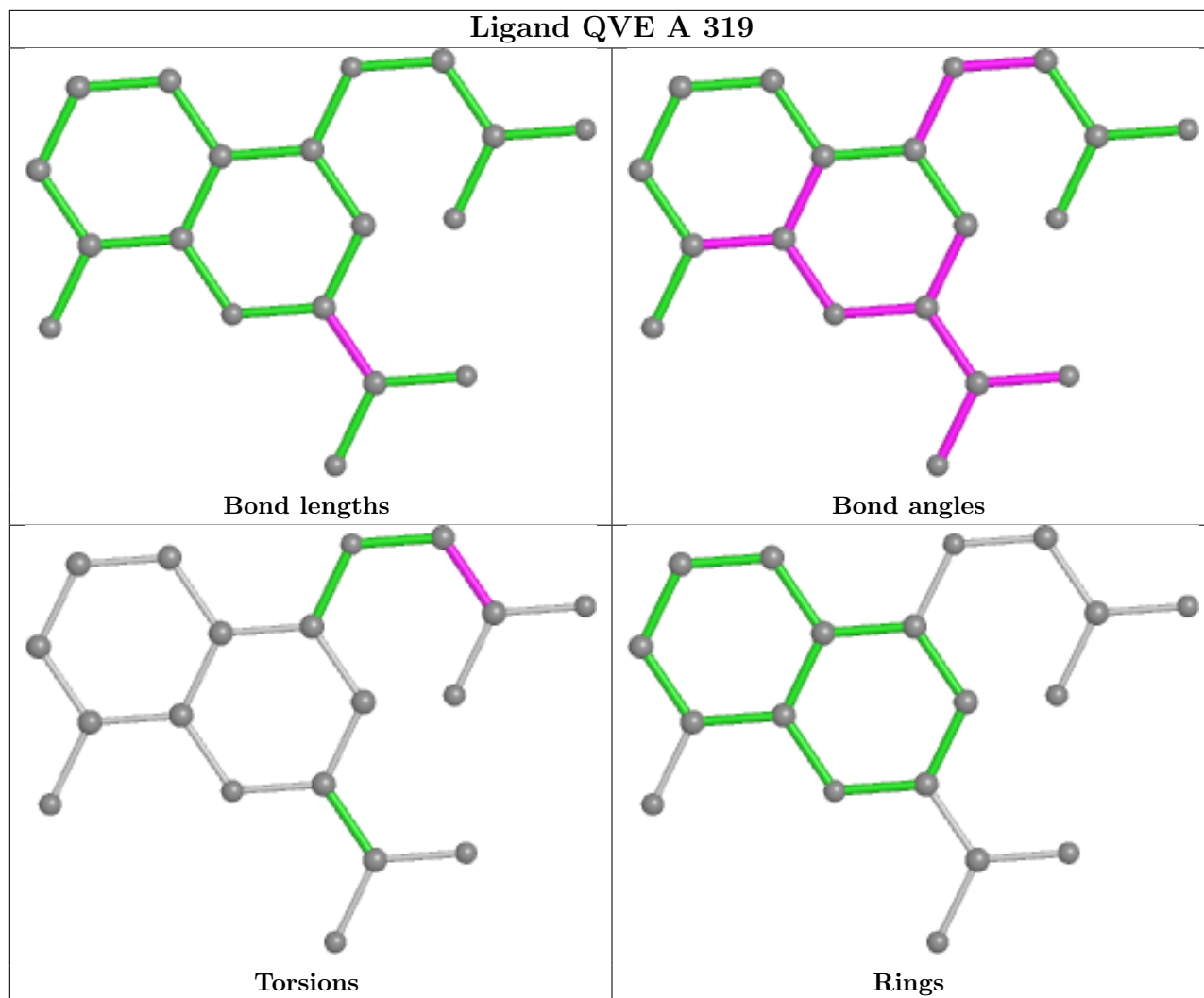
Mol	Chain	Res	Type	Atoms
6	A	318	QUK	CG-CD-CE-N1
3	A	302	6H0	C20-C21-S24-O27
3	A	302	6H0	C22-C21-S24-O27
3	B	303	6H0	C22-C21-S24-O27
3	A	302	6H0	C5-C6-C7-O7
3	B	303	6H0	C20-C21-S24-O27
4	A	304	GOL	O1-C1-C2-O2
8	A	316	QOL	CE1-CD-CG-OB
3	A	302	6H0	C20-C21-S24-N26
4	B	305	GOL	O1-C1-C2-O2
3	B	303	6H0	C22-C21-S24-N26
7	A	319	QVE	OE1-CD-CG-OB
3	B	303	6H0	C20-C21-S24-N26
7	A	307	QVE	C9-C8-OB-CG
7	A	319	QVE	OE2-CD-CG-OB
7	A	307	QVE	O-C-CA-C9
6	A	306	QUK	CG-CD-CE-N1
7	A	307	QVE	O-C-CA-N11
3	A	302	6H0	C22-C21-S24-N26
7	A	307	QVE	C6-C8-OB-CG
6	A	318	QUK	CE-CD-CG-OB
6	A	306	QUK	CD-CG-OB-C8

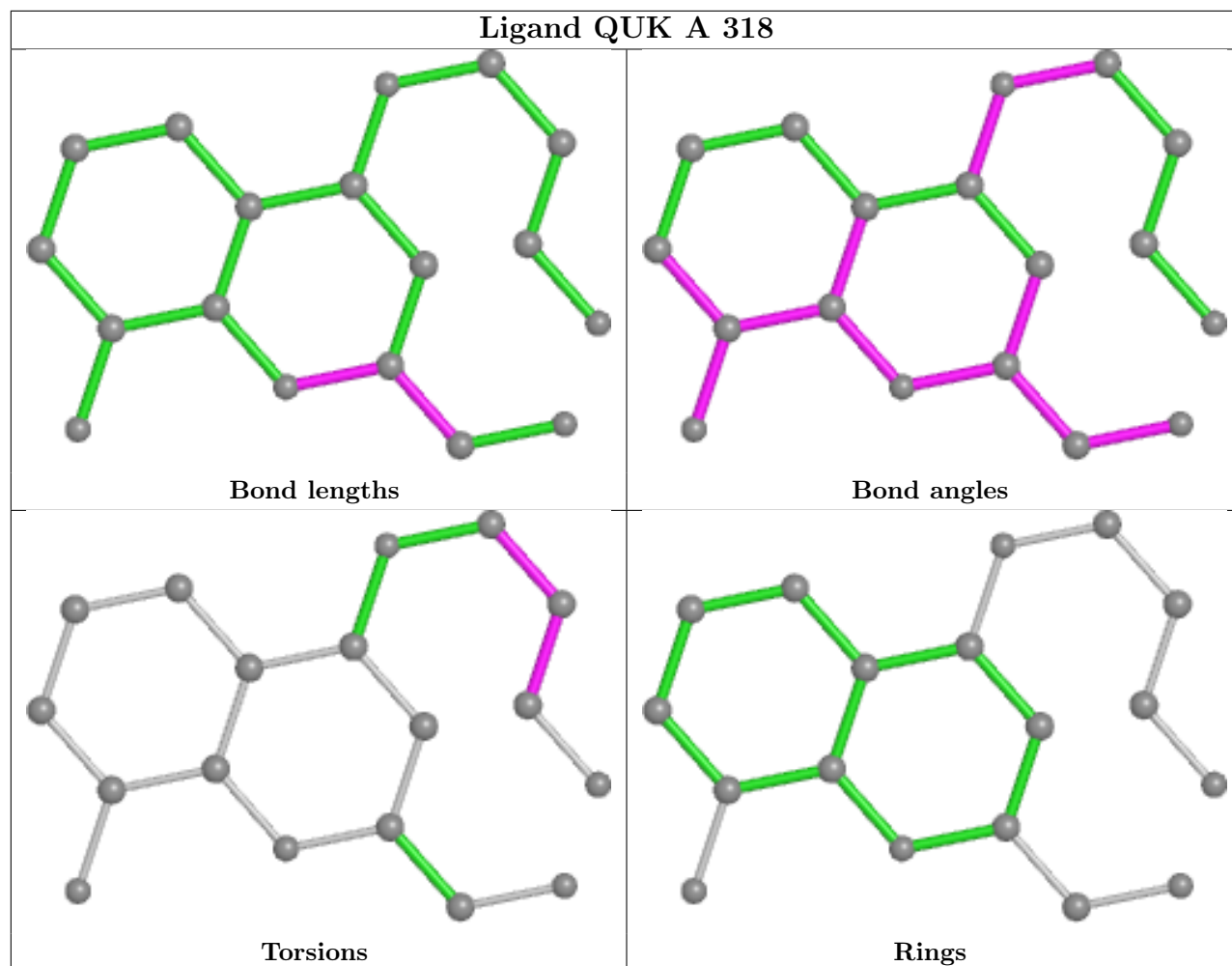
There are no ring outliers.

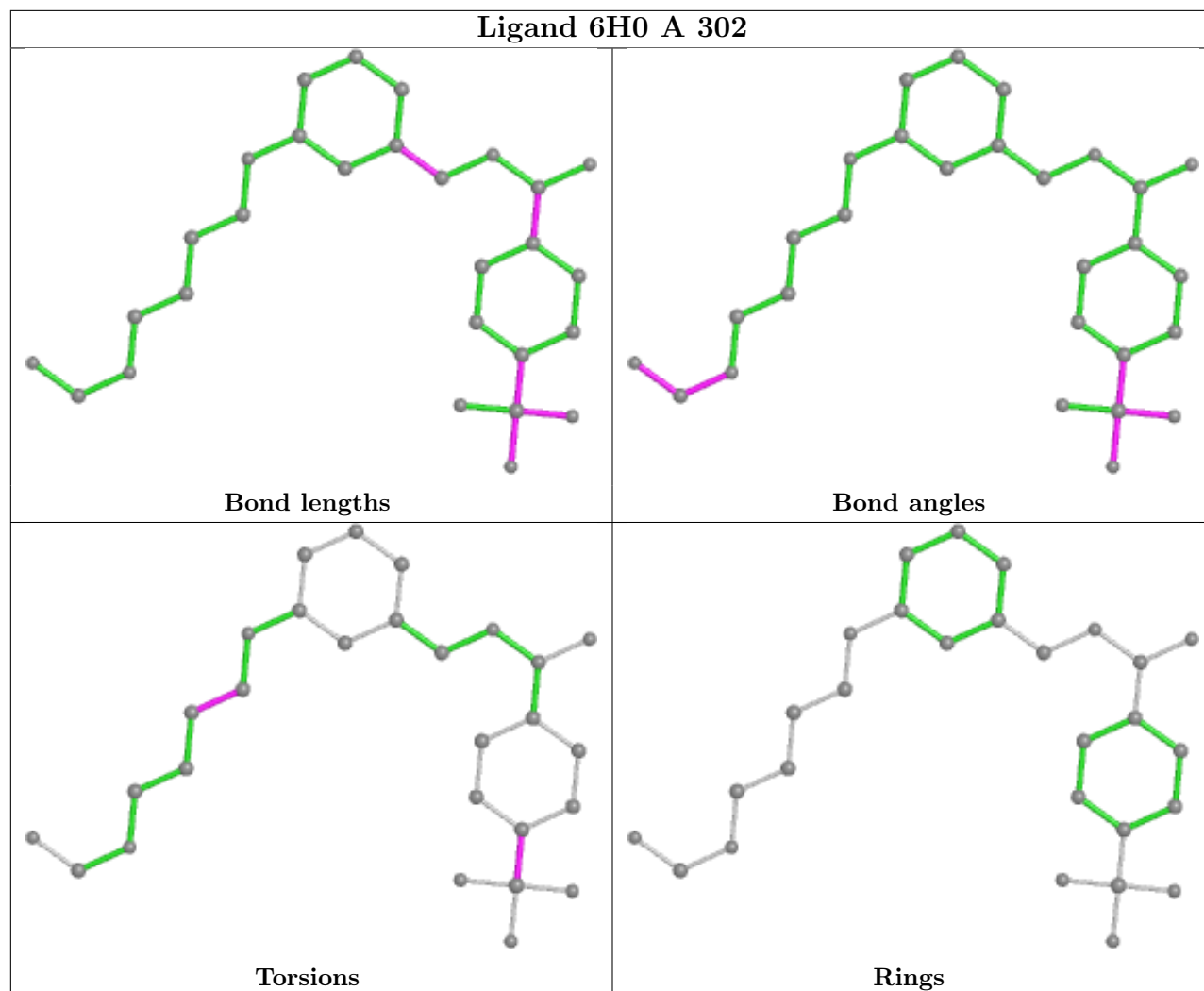
No monomer is involved in short contacts.

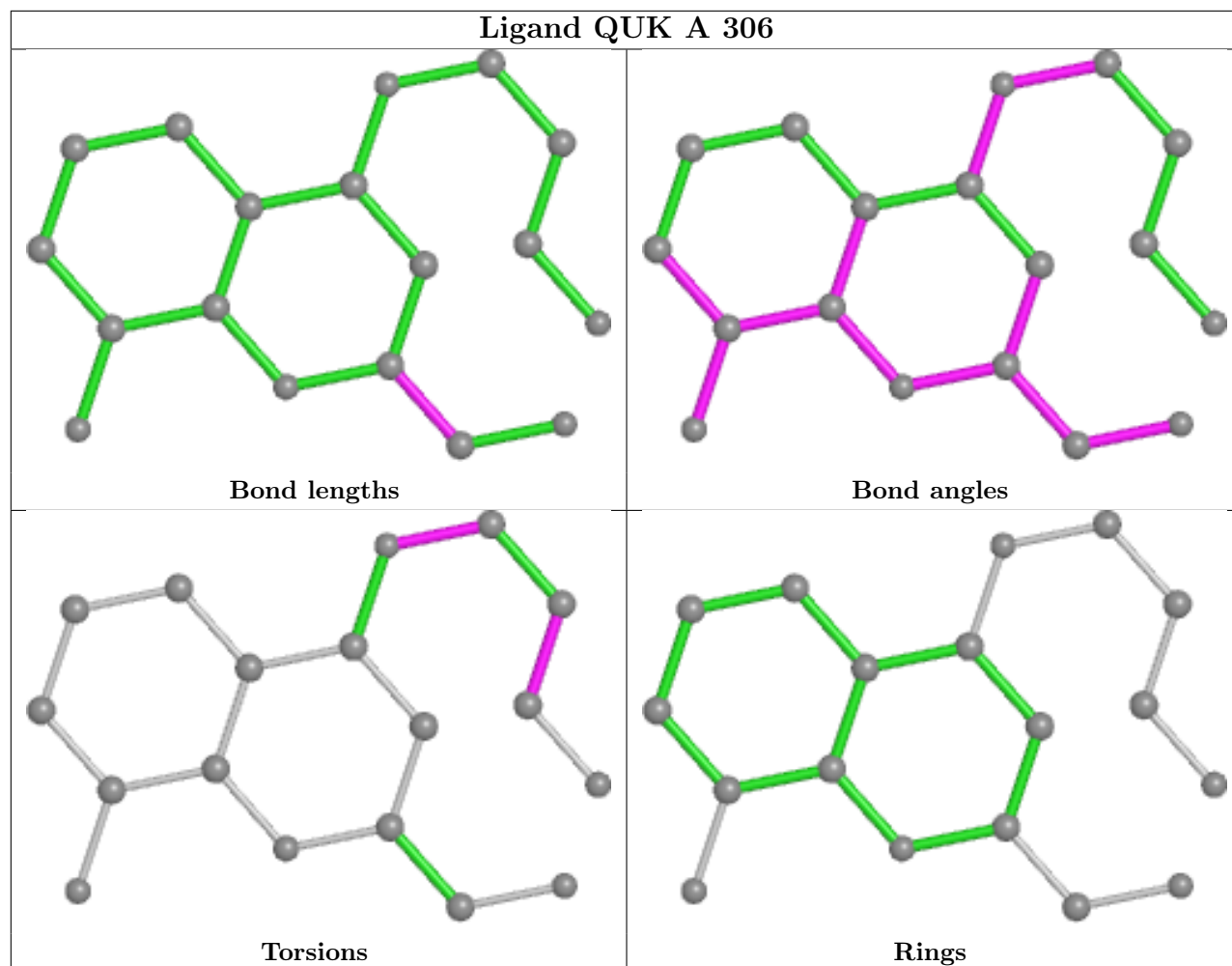
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

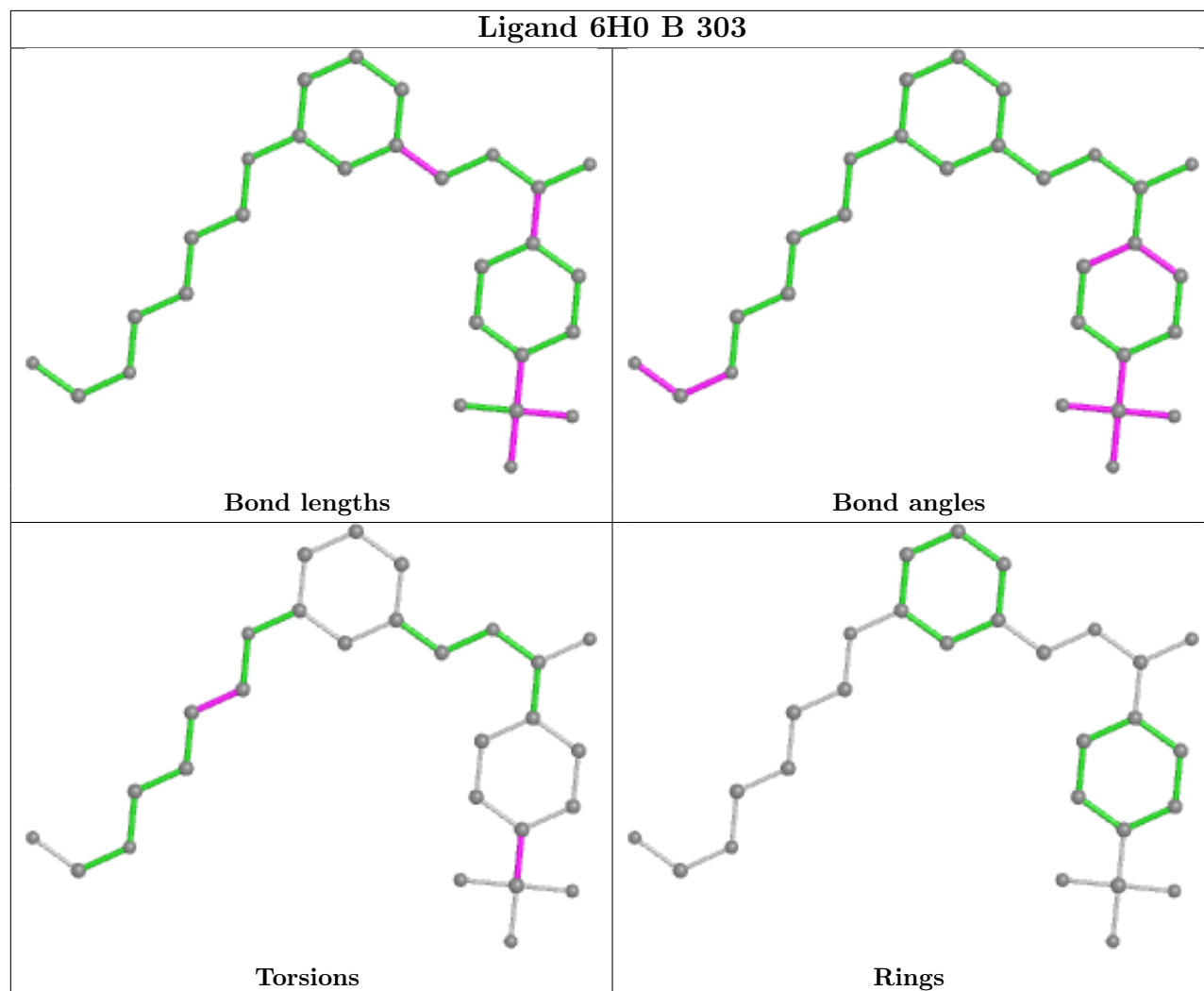


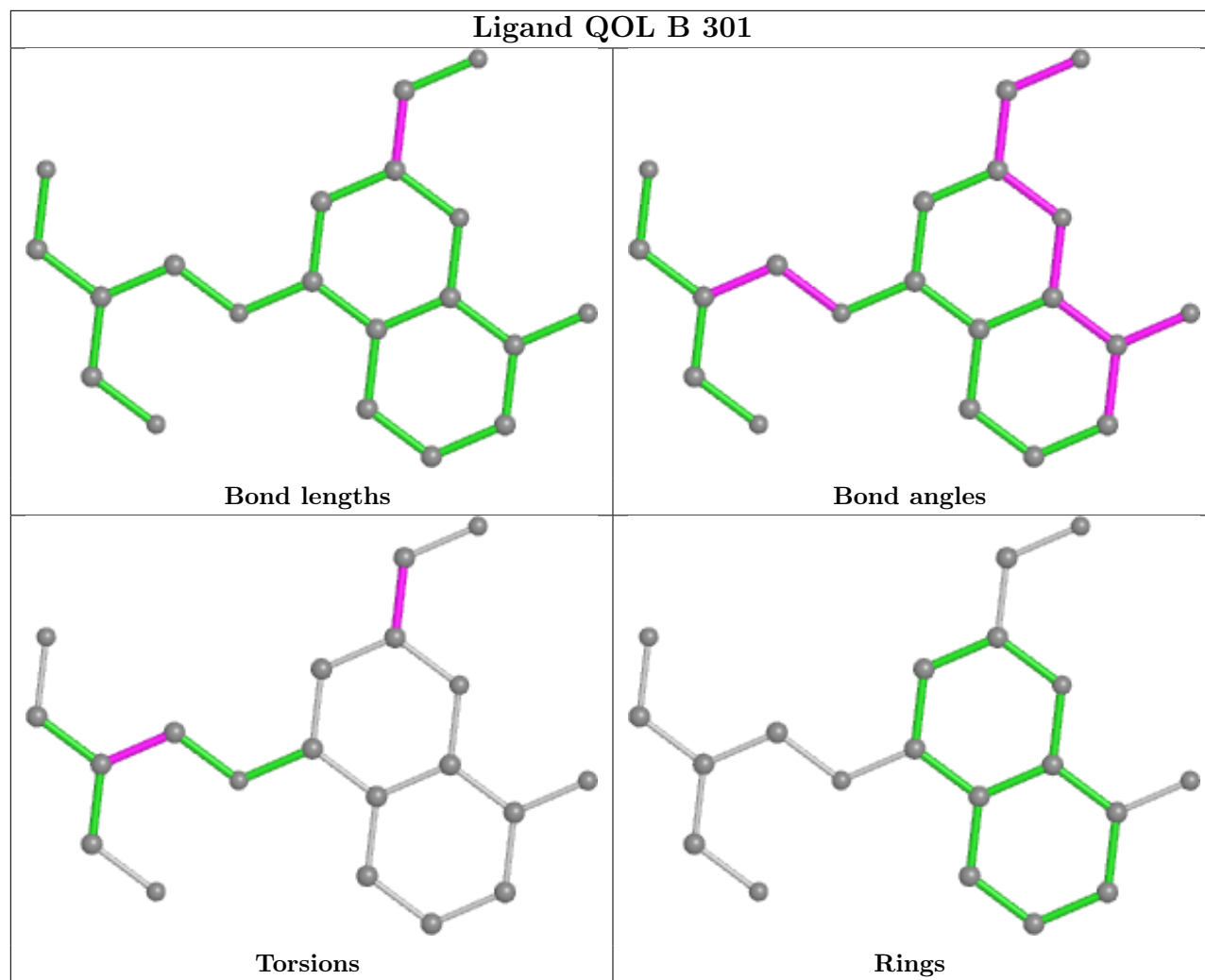


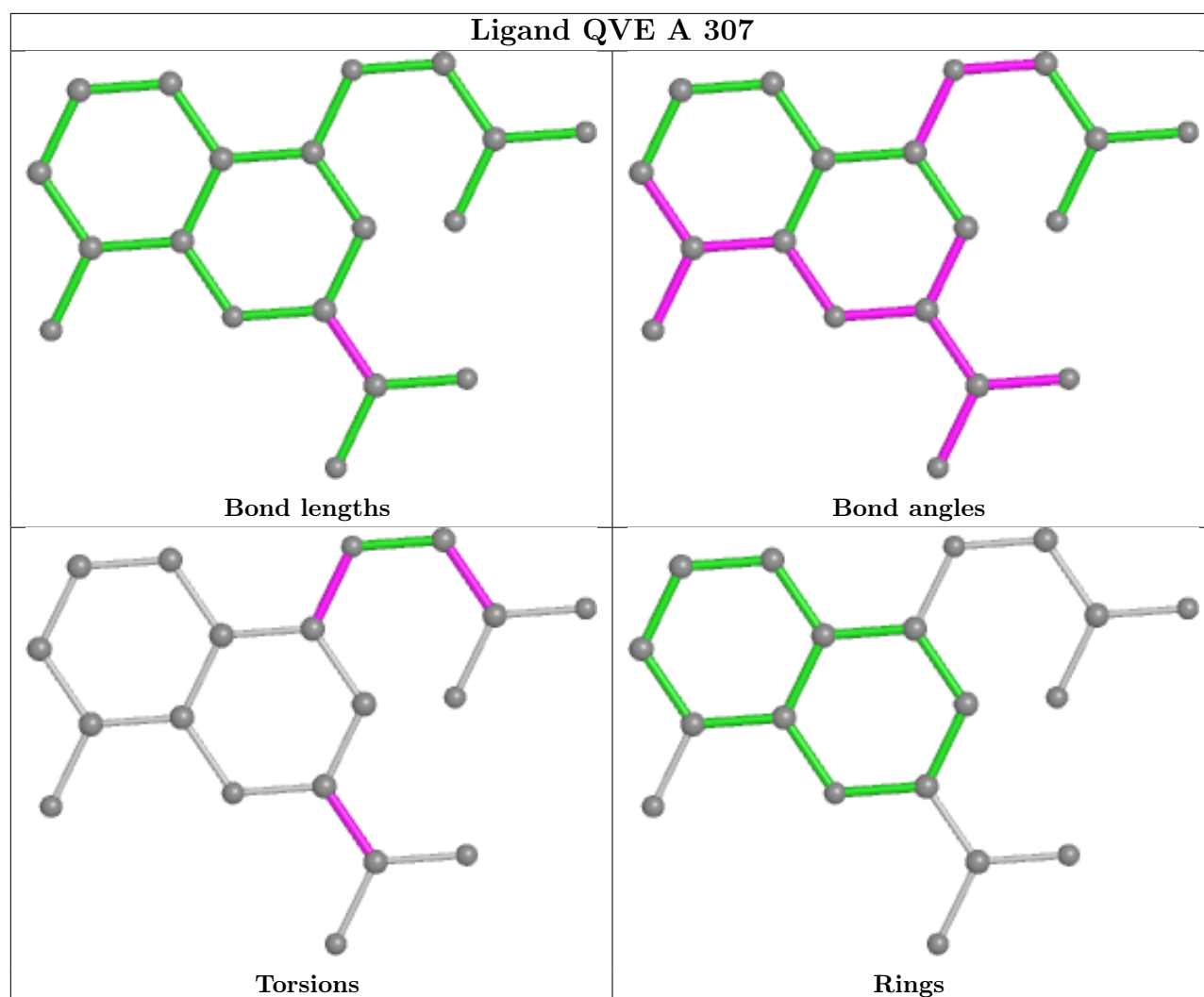












5.7 Other polymers [i](#)

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, 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	258/260 (99%)	-0.39	0 100 100	12, 26, 44, 60	0
1	B	258/260 (99%)	-0.06	4 (1%) 72 70	16, 37, 64, 90	0
All	All	516/520 (99%)	-0.23	4 (0%) 86 85	12, 31, 59, 90	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	236	PRO	2.9
1	B	225	PHE	2.4
1	B	234	GLY	2.3
1	B	42	PRO	2.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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, 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
2	ZN	A	314	1/1	0.87	0.13	34,34,34,34	1

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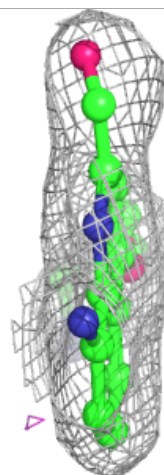
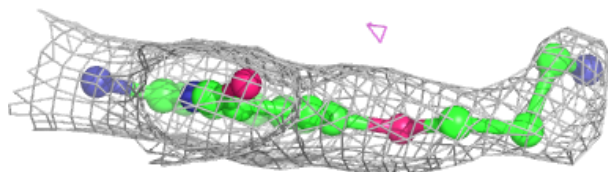
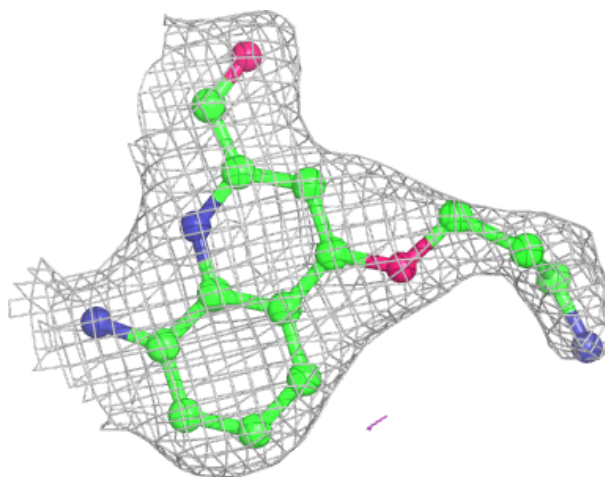
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	311	1/1	0.88	0.07	69,69,69,69	0
4	GOL	B	305	6/6	0.91	0.22	21,33,36,44	0
2	ZN	A	312	1/1	0.92	0.07	58,58,58,58	0
4	GOL	A	304	6/6	0.94	0.15	19,30,37,51	0
2	ZN	B	306	1/1	0.94	0.07	63,63,63,63	0
5	QVS	A	317	14/15	0.94	0.10	22,25,28,32	0
6	QUK	A	318	18/19	0.94	0.14	23,30,49,51	0
8	QOL	A	316	20/20	0.95	0.13	17,24,49,55	0
8	QOL	B	301	20/20	0.95	0.15	16,22,40,43	0
6	QUK	A	306	18/19	0.96	0.13	19,24,44,44	0
2	ZN	B	307	1/1	0.96	0.16	31,31,31,31	1
7	QVE	A	319	19/19	0.96	0.11	20,26,43,60	0
4	GOL	B	308	6/6	0.96	0.21	37,47,52,52	0
4	GOL	A	315	6/6	0.96	0.12	25,26,35,38	0
7	QVE	A	307	19/19	0.97	0.12	18,23,41,48	0
2	ZN	A	313	1/1	0.97	0.04	47,47,47,47	0
3	6H0	B	303	28/28	0.97	0.11	9,19,32,34	0
5	QVS	A	305	14/15	0.97	0.09	12,20,28,28	0
2	ZN	A	309	1/1	0.98	0.05	30,30,30,30	0
3	6H0	A	302	28/28	0.98	0.11	8,19,40,41	0
2	ZN	A	308	1/1	0.98	0.04	56,56,56,56	0
2	ZN	A	310	1/1	0.99	0.04	26,26,26,26	0
2	ZN	B	304	1/1	0.99	0.05	27,27,27,27	0
2	ZN	A	303	1/1	0.99	0.05	20,20,20,20	0
2	ZN	B	302	1/1	1.00	0.07	18,18,18,18	0
2	ZN	A	301	1/1	1.00	0.07	12,12,12,12	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.

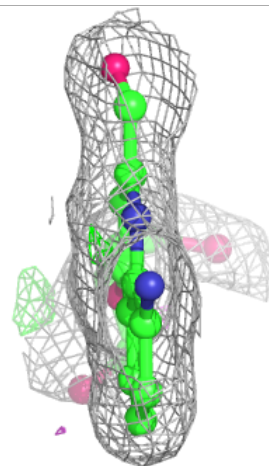
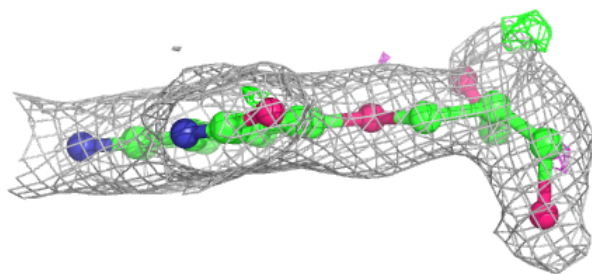
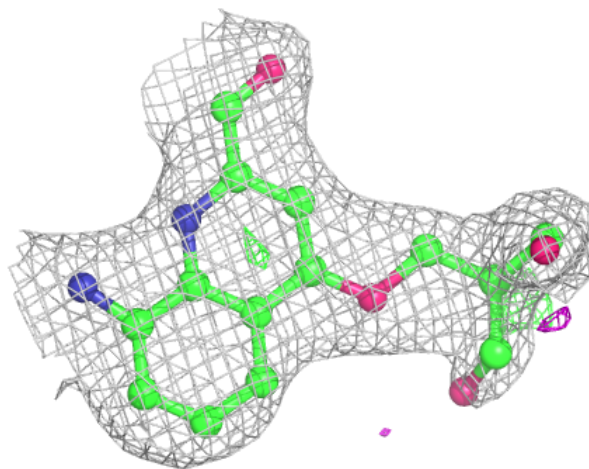
Electron density around QUK A 318:

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



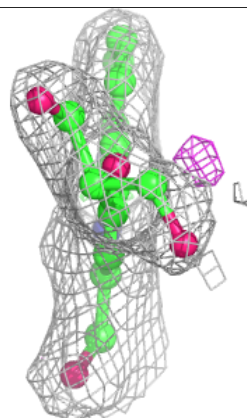
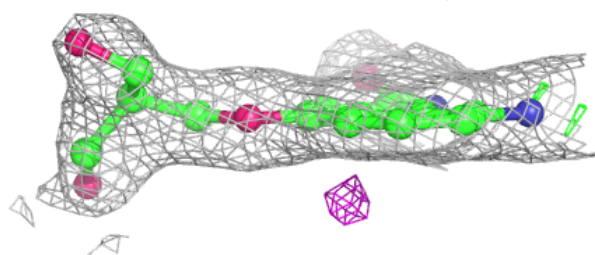
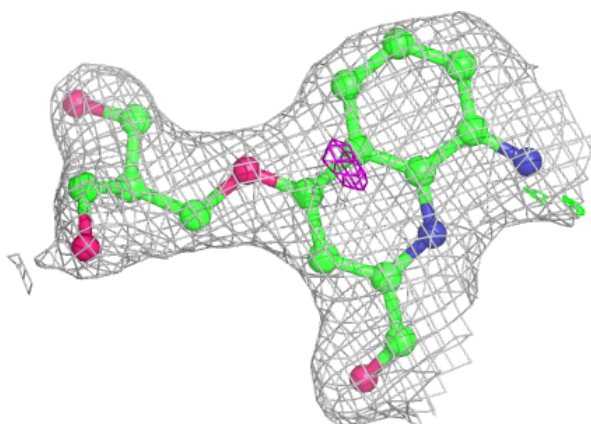
Electron density around QOL A 316:

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

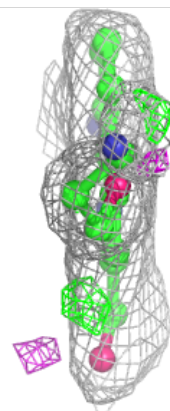
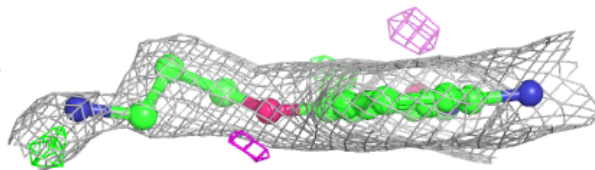
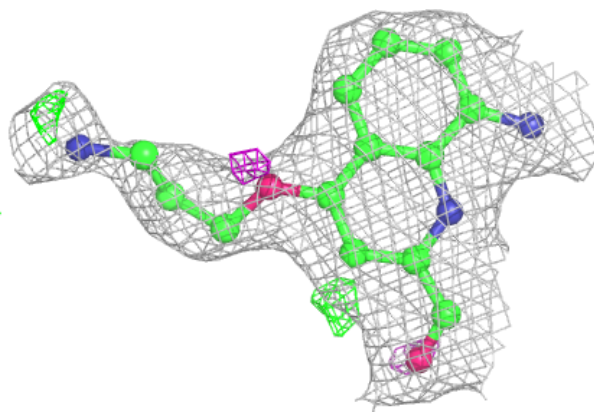


Electron density around QOL B 301:

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

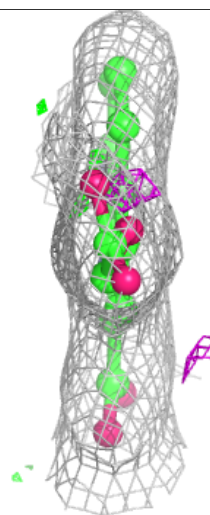
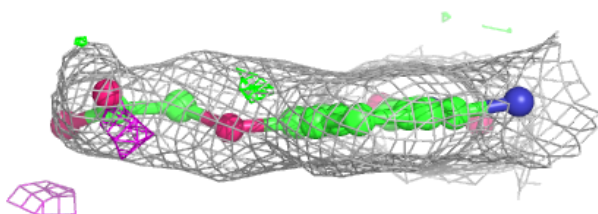
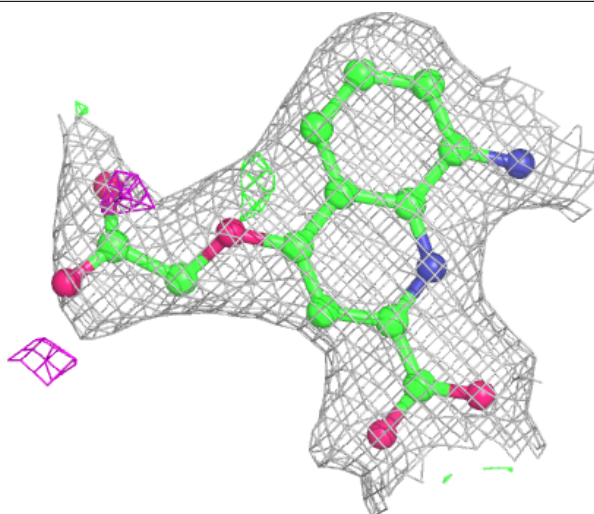
**Electron density around QUK A 306:**

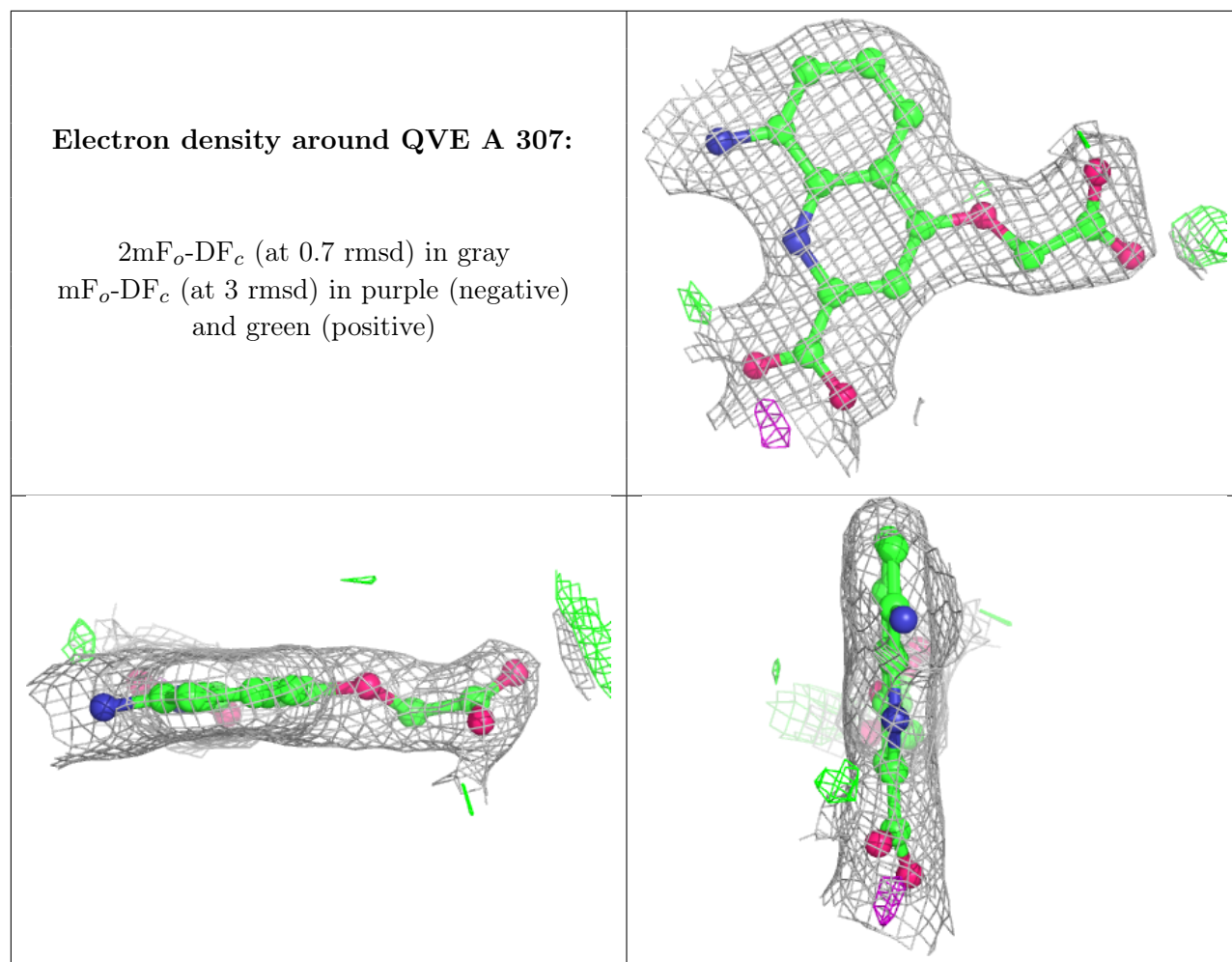
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around QVE A 319:

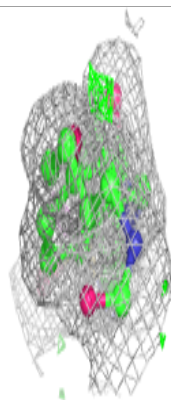
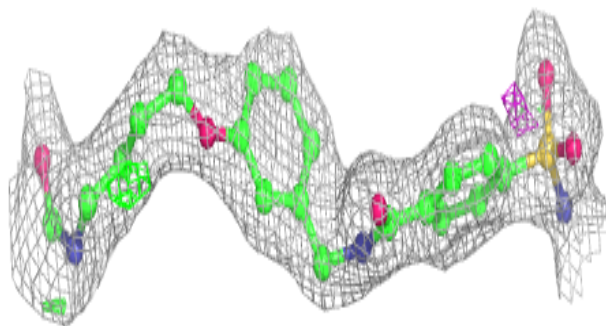
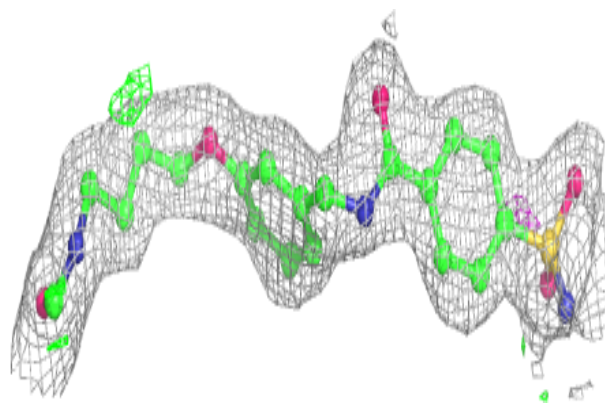
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



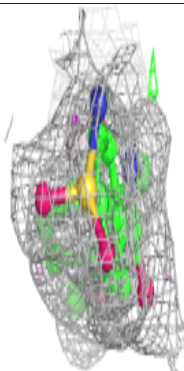
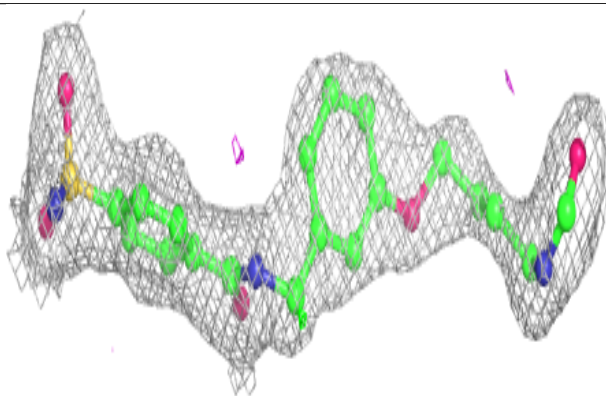
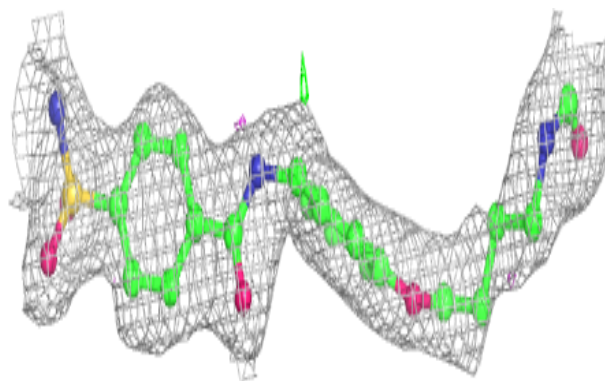


Electron density around 6H0 B 303:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.