



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:31 pm BST

PDB ID : 6Q9T
Title : Protein-aromatic foldamer complex crystal structure
Authors : Post, S.; Langlois d'Estaintot, B.; Fischer, L.; Granier, T.; Huc, I.
Deposited on : 2018-12-18
Resolution : 2.68 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

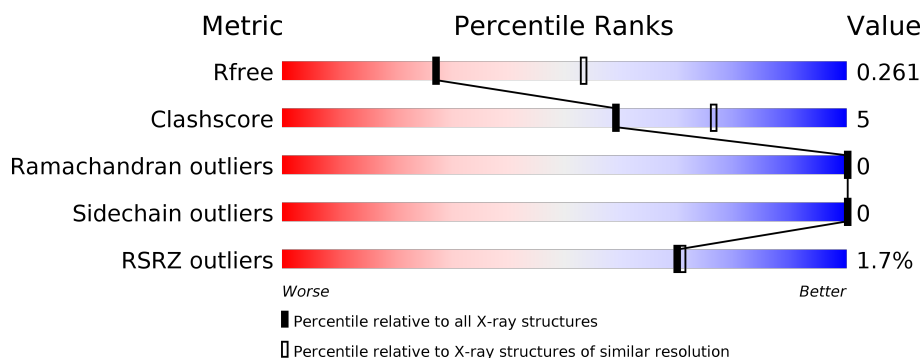
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	259	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>8%</div> </div> </div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 2009 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.

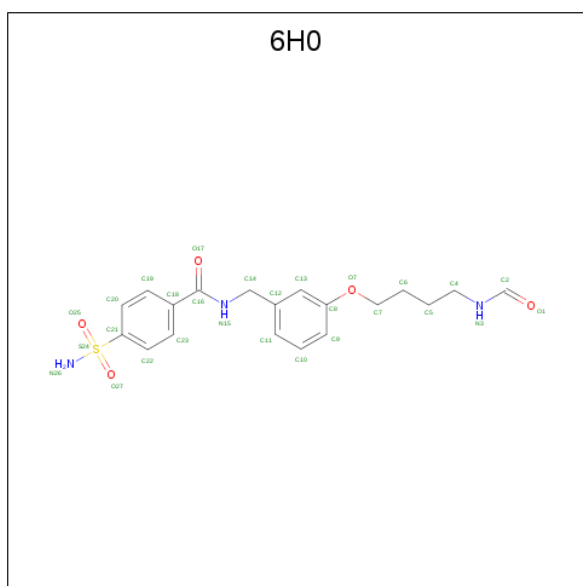
- Molecule 1 is a protein called Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	1	0
			1778	1142	306	328	2			

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

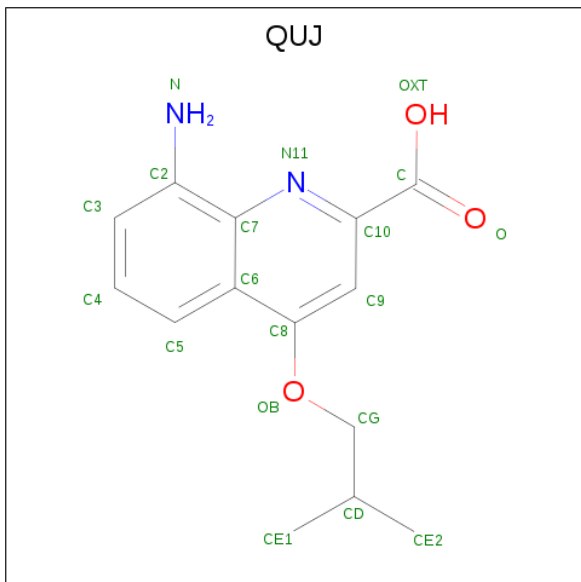
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

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



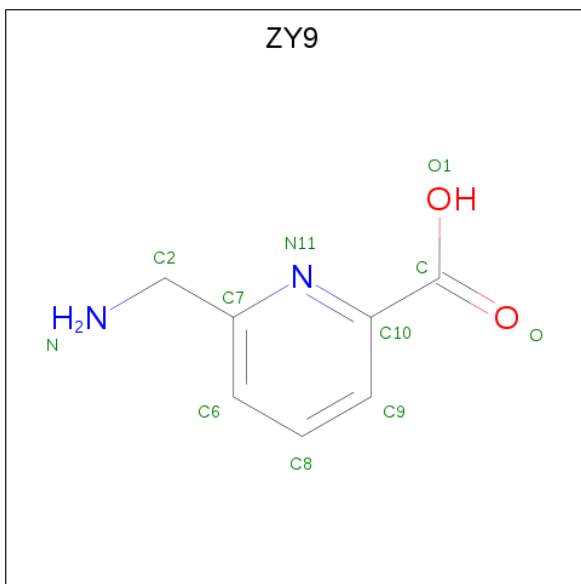
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			18	14	2	2		

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



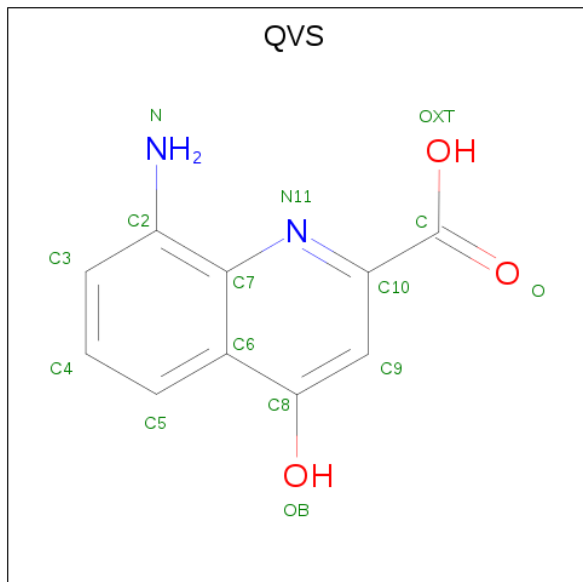
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	7	2	1		

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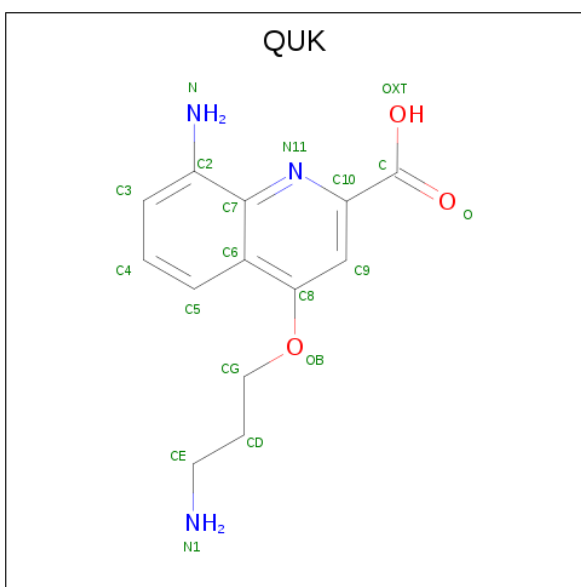
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	7	2	1		
5	A	1	Total	C	N	O	0	0
			10	7	2	1		
5	A	1	Total	C	N	O	0	0
			10	7	2	1		
5	A	1	Total	C	N	O	0	0
			10	7	2	1		

- Molecule 6 is 8-azanyl-4-oxidanyl-quinoline-2-carboxylic acid (three-letter code: QVS) (formula: $C_{10}H_8N_2O_3$).



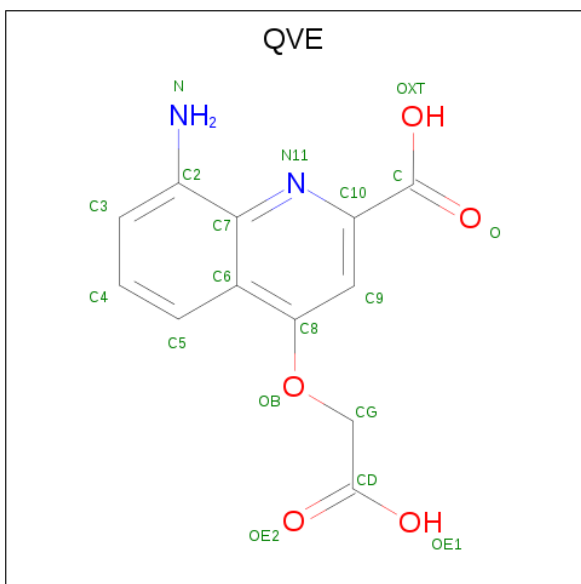
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	10	2	2		
6	A	1	Total	C	N	O	0	0
			14	10	2	2		

- Molecule 7 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
7	A	1	Total	C	N	O	0	0
			18	13	3	2		
7	A	1	Total	C	N	O	0	0
			19	13	3	3		

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



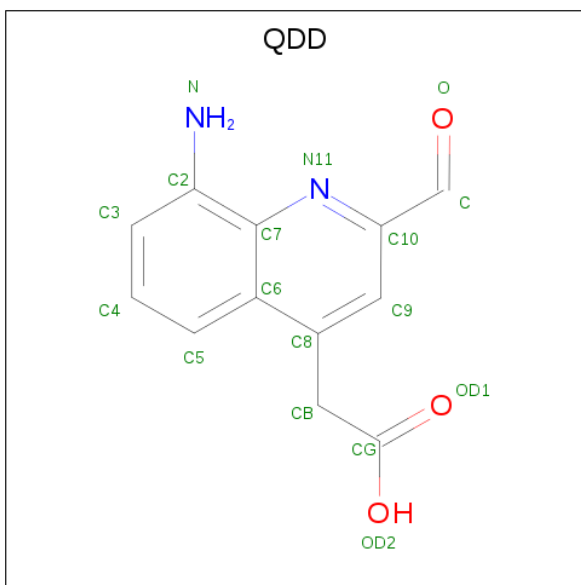
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			18	12	2	4		

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

- Molecule 9 is 2-(8-azanyl-2-methanoyl-quinolin-4-yl)ethanoic acid (three-letter code: QDD) (formula: C₁₂H₁₀N₂O₃).



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

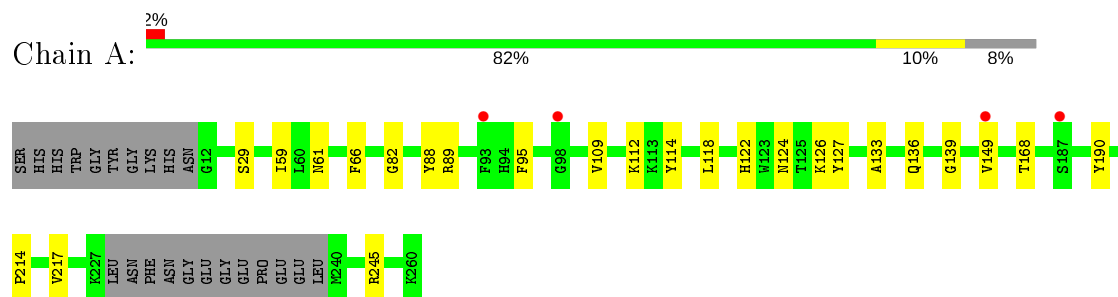
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	6	Total	O	0	0
			6	6		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	79.30Å 80.96Å 45.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.62 – 2.68 45.62 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.62-2.68) 98.5 (45.62-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.215 , 0.260 0.218 , 0.261	Depositor DCC
R_{free} test set	431 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2009	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.65% 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: QDD, QVE, ZN, 6H0, ZY9, QUK, QUJ, QVS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.77	0/1830	0.94	0/2503

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	1778	0	1631	16	0
2	A	1	0	0	0	0
3	A	28	0	0	0	0
4	A	18	0	0	0	0
5	A	60	0	0	0	0
6	A	28	0	0	0	0
7	A	37	0	0	1	0
8	A	36	0	0	0	0
9	A	17	0	0	0	0
10	A	6	0	0	0	0
All	All	2009	0	1631	17	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 5.

All (17) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PHE:CE2	1:A:118:LEU:HD13	2.42	0.54
1:A:88:TYR:CE2	1:A:124:ASN:HB2	2.44	0.53
1:A:66:PHE:CZ	1:A:95:PHE:CE1	2.97	0.52
1:A:82:GLY:HA2	1:A:190:TYR:OH	2.09	0.52
1:A:66:PHE:CZ	1:A:95:PHE:CD1	2.99	0.51
1:A:61:ASN:ND2	1:A:168:THR:C	2.66	0.49
1:A:89:ARG:O	1:A:122:HIS:HA	2.13	0.48
1:A:114:TYR:CE2	1:A:214:PRO:HG3	2.49	0.47
1:A:29:SER:O	1:A:245:ARG:NH1	2.46	0.47
1:A:109:VAL:O	1:A:112:LYS:HB3	2.15	0.47
1:A:59:ILE:HD11	1:A:66:PHE:CD1	2.49	0.46
1:A:133:ALA:O	1:A:139:GLY:HA3	2.16	0.45
1:A:149:VAL:HA	1:A:217:VAL:O	2.18	0.43
7:A:316:QUK:OB	7:A:316:QUK:N1	2.52	0.43
1:A:126:LYS:HD2	1:A:127:TYR:CZ	2.54	0.42
1:A:127:TYR:CZ	1:A:136:GLN:HG3	2.56	0.41
1:A:61:ASN:HD22	1:A:168:THR:C	2.24	0.41

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	233 / 259 (90%)	204 (88%)	29 (12%)	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	174/224 (78%)	174 (100%)	0	100	100

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

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

5.3.3 RNA [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 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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$
6	QVS	A	311	5	15,15,16	1.69	2 (13%)	19,21,23	3.51	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ZY9	A	309	8,5	10,10,11	3.52	2 (20%)	11,12,14	2.58	7 (63%)
4	QUJ	A	303	3,5	19,19,20	2.45	2 (10%)	23,26,28	2.24	7 (30%)
6	QVS	A	305	5,7	15,15,16	2.14	2 (13%)	19,21,23	2.50	6 (31%)
8	QVE	A	308	5	16,19,20	2.13	2 (12%)	20,26,28	2.42	6 (30%)
5	ZY9	A	312	9,6	10,10,11	3.58	2 (20%)	11,12,14	3.30	6 (54%)
9	QDD	A	313	5	15,18,18	1.91	3 (20%)	19,25,25	2.75	7 (36%)
5	ZY9	A	304	4,6	10,10,11	3.52	2 (20%)	11,12,14	2.81	6 (54%)
7	QUK	A	306	5,6	19,19,20	1.78	5 (26%)	22,25,27	2.66	5 (22%)
7	QUK	A	316	8	17,20,20	1.29	1 (5%)	20,27,27	2.47	4 (20%)
5	ZY9	A	307	8,7	10,10,11	4.19	4 (40%)	11,12,14	2.42	6 (54%)
8	QVE	A	315	5,7	16,19,20	2.76	3 (18%)	20,26,28	2.83	7 (35%)
5	ZY9	A	314	9,8	10,10,11	3.29	2 (20%)	11,12,14	2.63	5 (45%)
5	ZY9	A	310	5,6	10,10,11	5.45	5 (50%)	11,12,14	2.57	4 (36%)
3	6H0	A	302	2,4	29,29,29	2.47	8 (27%)	37,38,38	2.56	14 (37%)

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
6	QVS	A	311	5	-	0/2/2/4	0/2/2/2
5	ZY9	A	309	8,5	-	0/4/4/6	0/1/1/1
4	QUJ	A	303	3,5	-	2/7/7/9	0/2/2/2
6	QVS	A	305	5,7	-	0/2/2/4	0/2/2/2
8	QVE	A	308	5	-	3/5/7/9	0/2/2/2
5	ZY9	A	312	9,6	-	0/4/4/6	0/1/1/1
9	QDD	A	313	5	-	0/4/6/6	0/2/2/2
5	ZY9	A	304	4,6	-	0/4/4/6	0/1/1/1
7	QUK	A	306	5,6	-	2/7/7/9	0/2/2/2
7	QUK	A	316	8	-	1/5/9/9	0/2/2/2
5	ZY9	A	307	8,7	-	0/4/4/6	0/1/1/1
8	QVE	A	315	5,7	-	2/5/7/9	0/2/2/2
5	ZY9	A	314	9,8	-	2/4/4/6	0/1/1/1
5	ZY9	A	310	5,6	-	0/4/4/6	0/1/1/1
3	6H0	A	302	2,4	-	2/23/23/23	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	310	ZY9	C10-C	-12.86	1.35	1.48
5	A	307	ZY9	C2-C7	-11.95	1.37	1.51
5	A	312	ZY9	C2-C7	-10.66	1.39	1.51
5	A	310	ZY9	C2-C7	-9.84	1.40	1.51
8	A	315	QVE	C10-C	-9.74	1.38	1.48
5	A	309	ZY9	C2-C7	-9.39	1.40	1.51
5	A	314	ZY9	C2-C7	-9.36	1.40	1.51
4	A	303	QUJ	C10-C	-8.91	1.39	1.48
5	A	304	ZY9	C2-C7	-8.24	1.41	1.51
8	A	308	QVE	C10-C	-7.20	1.41	1.48
5	A	304	ZY9	C10-C	-7.14	1.41	1.48
3	A	302	6H0	C14-C12	-6.29	1.37	1.51
6	A	305	QVS	C10-C	-6.12	1.42	1.48
9	A	313	QDD	C10-C	-5.57	1.42	1.48
3	A	302	6H0	C21-S24	-5.38	1.68	1.77
3	A	302	6H0	O27-S24	5.30	1.53	1.43
5	A	309	ZY9	C10-C	-5.23	1.43	1.48
3	A	302	6H0	C18-C16	-4.95	1.39	1.50
3	A	302	6H0	O25-S24	4.72	1.52	1.43
6	A	311	QVS	C10-C	-4.71	1.43	1.48
7	A	306	QUK	C10-C	-4.30	1.44	1.48
5	A	314	ZY9	C10-C	-3.92	1.44	1.48
5	A	307	ZY9	C10-C	-3.75	1.44	1.48
4	A	303	QUJ	C10-N11	3.68	1.37	1.33
6	A	305	QVS	C10-N11	3.67	1.37	1.33
7	A	316	QUK	OB-CG	3.65	1.56	1.43
5	A	310	ZY9	C8-C6	3.55	1.46	1.38
5	A	310	ZY9	C7-N11	3.39	1.40	1.34
5	A	312	ZY9	C10-C	-2.99	1.45	1.48
7	A	306	QUK	C6-C7	-2.89	1.35	1.42
8	A	315	QVE	C10-N11	2.88	1.36	1.33
6	A	311	QVS	C6-C7	-2.69	1.35	1.42
7	A	306	QUK	C10-N11	2.60	1.35	1.33
9	A	313	QDD	CB-C8	-2.54	1.42	1.52
9	A	313	QDD	C7-N11	-2.51	1.32	1.37
8	A	308	QVE	C10-N11	2.44	1.35	1.33
3	A	302	6H0	S24-N26	2.38	1.65	1.60
5	A	307	ZY9	C9-C10	2.32	1.43	1.39
5	A	307	ZY9	C7-N11	2.26	1.38	1.34
7	A	306	QUK	C7-N11	-2.26	1.32	1.37
5	A	310	ZY9	C8-C9	2.25	1.43	1.38
7	A	306	QUK	C2-C7	-2.20	1.38	1.42
3	A	302	6H0	C13-C12	-2.15	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	315	QVE	C4-C5	2.15	1.41	1.36
3	A	302	6H0	C2-N3	2.08	1.37	1.33

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	311	QVS	C10-N11-C7	12.72	127.76	118.11
7	A	306	QUK	C10-N11-C7	8.97	124.91	118.11
7	A	316	QUK	C10-N11-C7	8.45	124.75	118.26
9	A	313	QDD	C10-N11-C7	8.28	124.39	118.11
6	A	305	QVS	C10-N11-C7	7.67	123.93	118.11
3	A	302	6H0	O25-S24-C21	7.35	115.55	107.35
8	A	315	QVE	C-C10-N11	7.34	121.85	114.66
5	A	310	ZY9	O-C-C10	-6.45	118.11	124.22
4	A	303	QUJ	C-C10-N11	6.25	120.78	114.66
8	A	315	QVE	C10-N11-C7	6.08	122.72	118.11
7	A	306	QUK	C-C10-N11	6.05	120.59	114.66
8	A	308	QVE	CG-OB-C8	-5.57	109.73	117.56
6	A	311	QVS	C9-C10-C	5.56	126.03	121.23
5	A	312	ZY9	O-C-C10	-5.53	118.98	124.22
8	A	308	QVE	C-C10-N11	5.46	120.01	114.66
5	A	312	ZY9	C10-N11-C7	5.35	126.10	118.41
5	A	304	ZY9	C2-C7-N11	5.17	124.68	115.89
5	A	312	ZY9	C9-C10-N11	-5.08	115.21	122.47
7	A	316	QUK	C9-C10-N11	-4.98	117.69	122.23
3	A	302	6H0	C8-C13-C12	4.93	125.16	119.73
5	A	314	ZY9	C2-C7-N11	4.83	124.10	115.89
4	A	303	QUJ	C10-N11-C7	4.75	121.71	118.11
8	A	308	QVE	C10-N11-C7	4.46	121.49	118.11
3	A	302	6H0	O25-S24-N26	-4.45	100.76	107.36
3	A	302	6H0	C14-C12-C11	4.36	129.96	120.91
4	A	303	QUJ	C7-C2-N	-4.13	110.20	118.07
5	A	312	ZY9	C2-C7-N11	4.10	122.87	115.89
5	A	314	ZY9	C6-C7-N11	-4.09	117.22	122.41
3	A	302	6H0	C14-C12-C13	-4.06	111.86	120.64
8	A	315	QVE	C7-C2-N	-3.97	110.49	118.07
5	A	304	ZY9	C6-C7-N11	-3.97	117.38	122.41
4	A	303	QUJ	C3-C2-N	3.95	128.25	120.36
8	A	315	QVE	C3-C2-N	3.89	128.14	120.36
8	A	315	QVE	O-C-C10	-3.89	120.54	124.22
5	A	304	ZY9	O-C-C10	-3.84	120.58	124.22
9	A	313	QDD	C9-C10-C	3.80	124.51	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	307	ZY9	C9-C10-N11	-3.66	117.24	122.47
3	A	302	6H0	O27-S24-N26	3.65	112.77	107.36
9	A	313	QDD	C3-C2-N	3.64	127.64	120.36
6	A	311	QVS	C2-C7-N11	3.58	122.18	118.64
5	A	309	ZY9	C6-C7-N11	-3.55	117.91	122.41
3	A	302	6H0	C21-S24-N26	-3.54	103.38	108.38
5	A	314	ZY9	C8-C6-C7	3.50	123.29	118.93
5	A	309	ZY9	C2-C7-N11	3.42	121.71	115.89
5	A	309	ZY9	O-C-C10	-3.35	121.05	124.22
9	A	313	QDD	O-C-C10	-3.29	121.10	124.22
3	A	302	6H0	O25-S24-O27	-3.29	113.36	118.76
5	A	307	ZY9	C2-C7-N11	3.27	121.45	115.89
7	A	316	QUK	C3-C2-N	3.24	126.85	120.36
5	A	309	ZY9	C8-C6-C7	3.23	122.96	118.93
5	A	310	ZY9	C6-C7-N11	-3.20	118.35	122.41
8	A	308	QVE	OB-CG-CD	-3.16	100.08	108.59
5	A	307	ZY9	C10-N11-C7	3.16	122.95	118.41
8	A	308	QVE	C3-C2-N	3.13	126.62	120.36
6	A	311	QVS	C6-C7-N11	-3.08	116.42	122.78
5	A	310	ZY9	C10-N11-C7	3.04	122.78	118.41
7	A	306	QUK	O-C-C10	-3.00	121.38	124.22
5	A	314	ZY9	C10-N11-C7	3.00	122.72	118.41
6	A	305	QVS	C9-C10-C	2.98	123.80	121.23
3	A	302	6H0	C7-O7-C8	2.97	125.68	117.93
5	A	307	ZY9	O-C-C10	-2.96	121.42	124.22
6	A	305	QVS	C4-C5-C6	-2.96	116.79	120.89
7	A	316	QUK	C7-C2-N	-2.93	112.49	118.07
5	A	309	ZY9	C10-N11-C7	2.77	122.40	118.41
5	A	304	ZY9	C10-N11-C7	2.74	122.35	118.41
5	A	307	ZY9	C9-C10-C	2.71	123.61	121.19
6	A	305	QVS	C-C10-N11	2.71	117.31	114.66
5	A	304	ZY9	C9-C10-C	-2.67	118.82	121.19
9	A	313	QDD	C2-C7-N11	-2.66	116.01	118.64
3	A	302	6H0	O1-C2-N3	-2.65	122.21	124.89
5	A	309	ZY9	C9-C10-N11	-2.64	118.69	122.47
5	A	312	ZY9	C9-C10-C	2.62	123.52	121.19
3	A	302	6H0	O27-S24-C21	2.61	110.26	107.35
9	A	313	QDD	CG-CB-C8	-2.60	108.66	114.71
8	A	308	QVE	C7-C2-N	-2.60	113.12	118.07
4	A	303	QUJ	C9-C10-C	-2.58	119.00	121.23
6	A	305	QVS	C3-C2-N	2.54	125.44	120.36
3	A	302	6H0	C10-C11-C12	-2.47	116.85	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	312	ZY9	C6-C7-N11	-2.46	119.28	122.41
6	A	311	QVS	C-C10-N11	2.43	117.04	114.66
5	A	314	ZY9	O-C-C10	-2.42	121.93	124.22
3	A	302	6H0	C11-C10-C9	2.30	123.51	120.25
8	A	315	QVE	CG-OB-C8	-2.27	114.36	117.56
5	A	304	ZY9	C8-C6-C7	2.23	121.71	118.93
4	A	303	QUJ	C4-C3-C2	-2.22	116.92	121.19
5	A	310	ZY9	C2-C7-N11	2.21	119.64	115.89
7	A	306	QUK	C3-C2-N	2.20	124.75	120.36
5	A	309	ZY9	C6-C8-C9	-2.18	117.15	120.25
3	A	302	6H0	C20-C21-S24	2.18	122.89	119.73
7	A	306	QUK	C6-C7-N11	-2.17	118.29	122.78
9	A	313	QDD	C-C10-N11	2.14	116.76	114.66
8	A	315	QVE	C2-C7-N11	2.12	120.74	118.64
4	A	303	QUJ	O-C-C10	-2.09	122.25	124.22
6	A	305	QVS	C6-C7-N11	-2.08	118.49	122.78
6	A	311	QVS	C3-C2-N	2.06	124.47	120.36
5	A	307	ZY9	C6-C7-N11	-2.03	119.83	122.41

There are no chirality outliers.

All (14) torsion outliers are listed below:

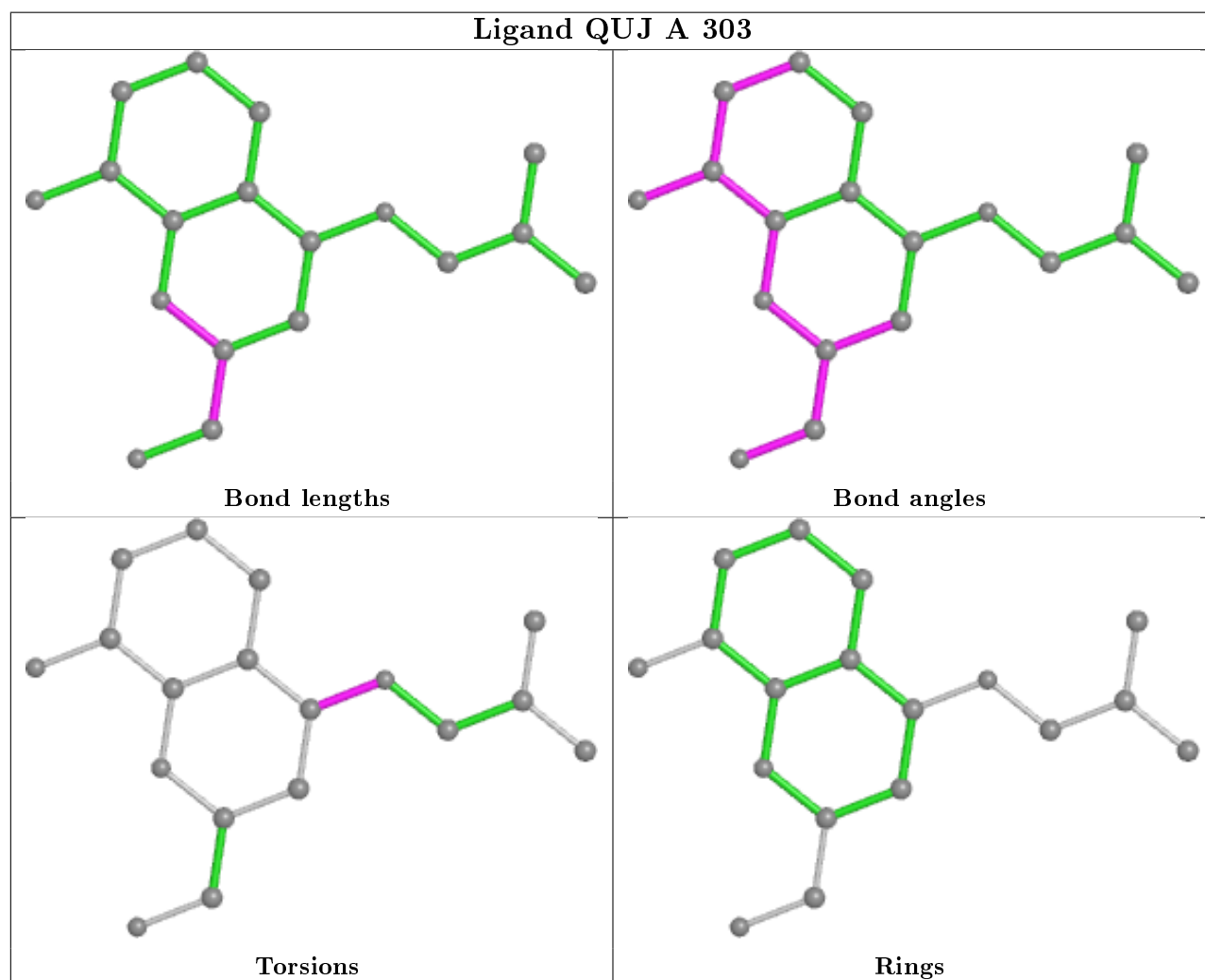
Mol	Chain	Res	Type	Atoms
5	A	314	ZY9	O-C-C10-N11
5	A	314	ZY9	O-C-C10-C9
8	A	308	QVE	C9-C8-OB-CG
7	A	306	QUK	CE-CD-CG-OB
7	A	316	QUK	CE-CD-CG-OB
4	A	303	QUJ	C6-C8-OB-CG
8	A	308	QVE	C6-C8-OB-CG
4	A	303	QUJ	C9-C8-OB-CG
8	A	315	QVE	C9-C8-OB-CG
8	A	315	QVE	C6-C8-OB-CG
3	A	302	6H0	C5-C6-C7-O7
8	A	308	QVE	CD-CG-OB-C8
7	A	306	QUK	CG-CD-CE-N1
3	A	302	6H0	C5-C4-N3-C2

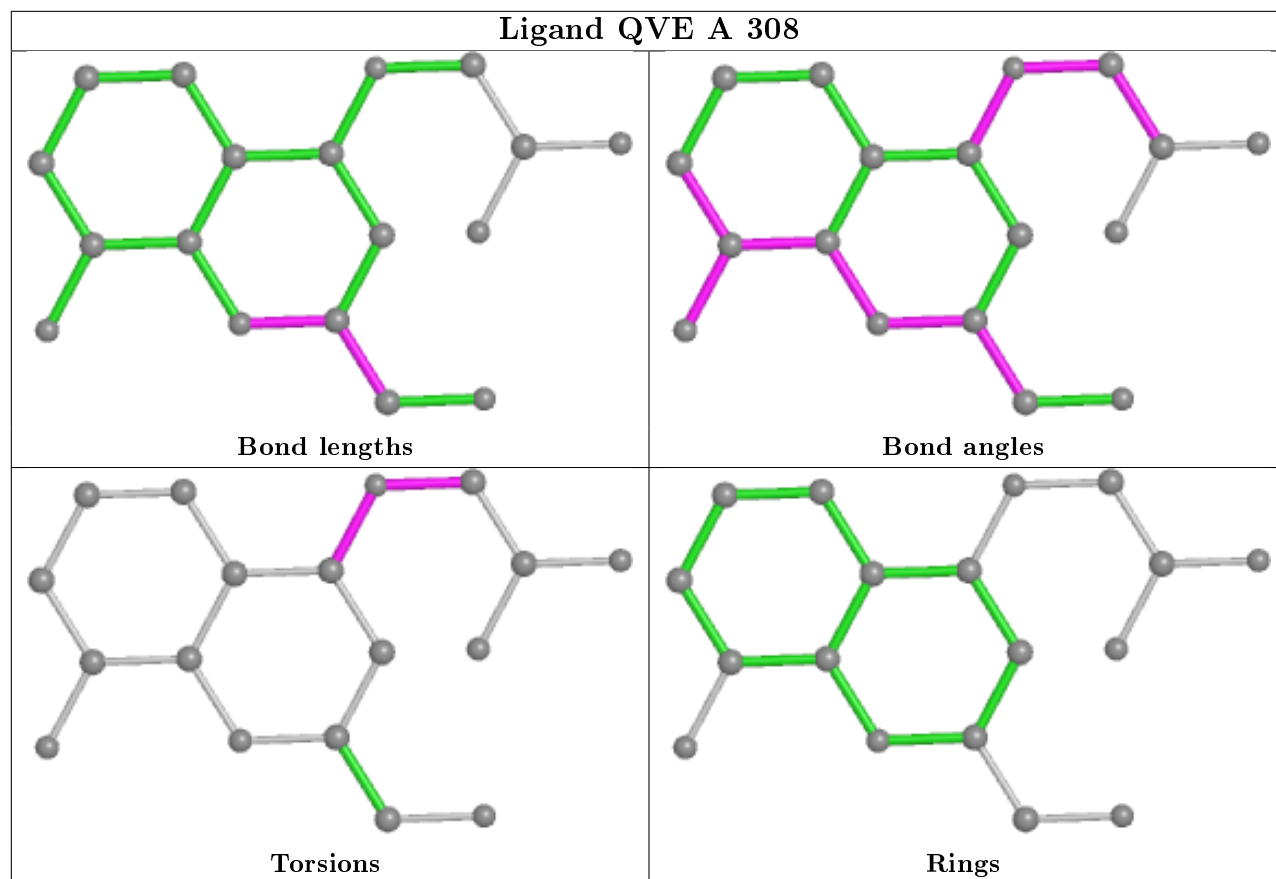
There are no ring outliers.

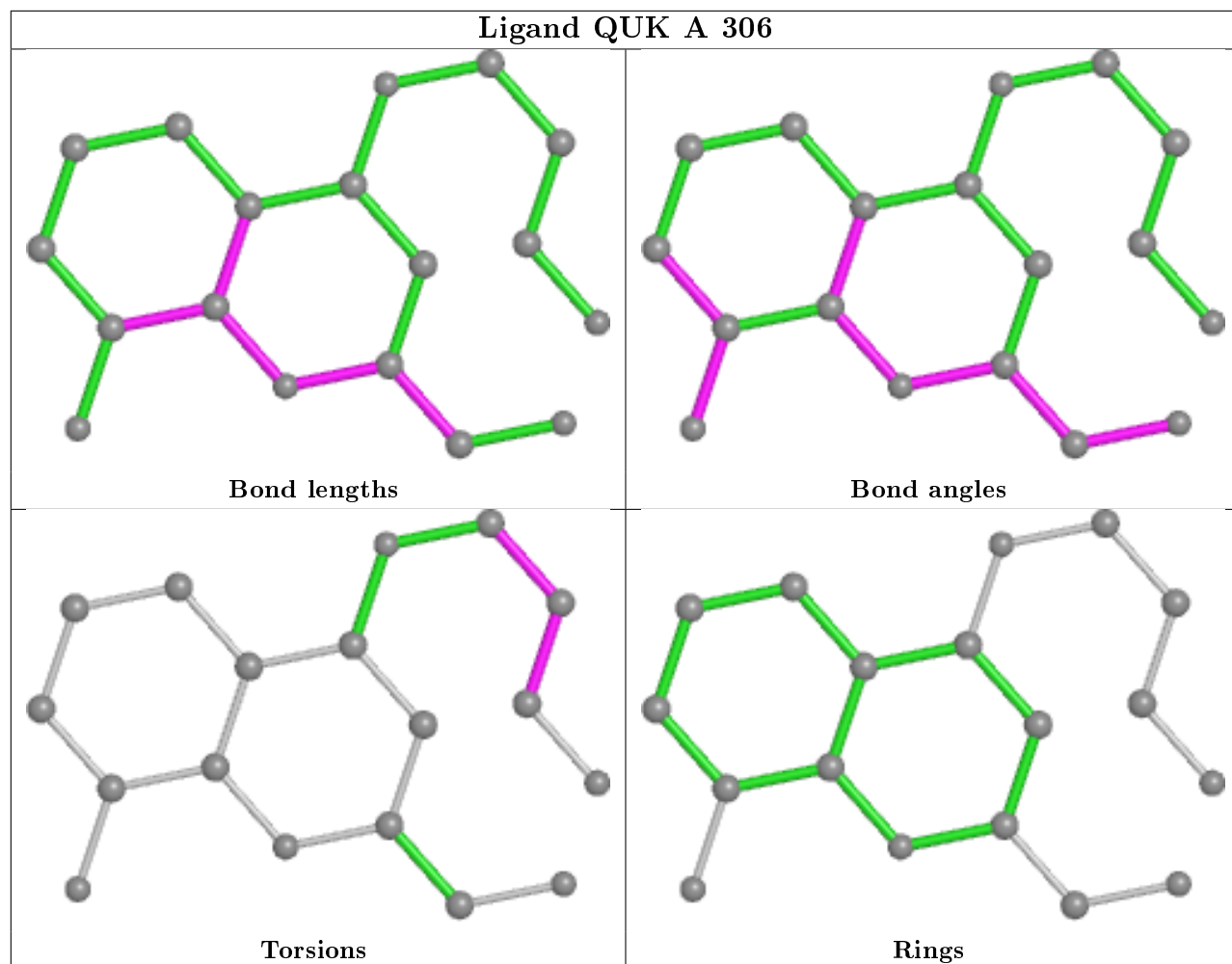
1 monomer is involved in 1 short contact:

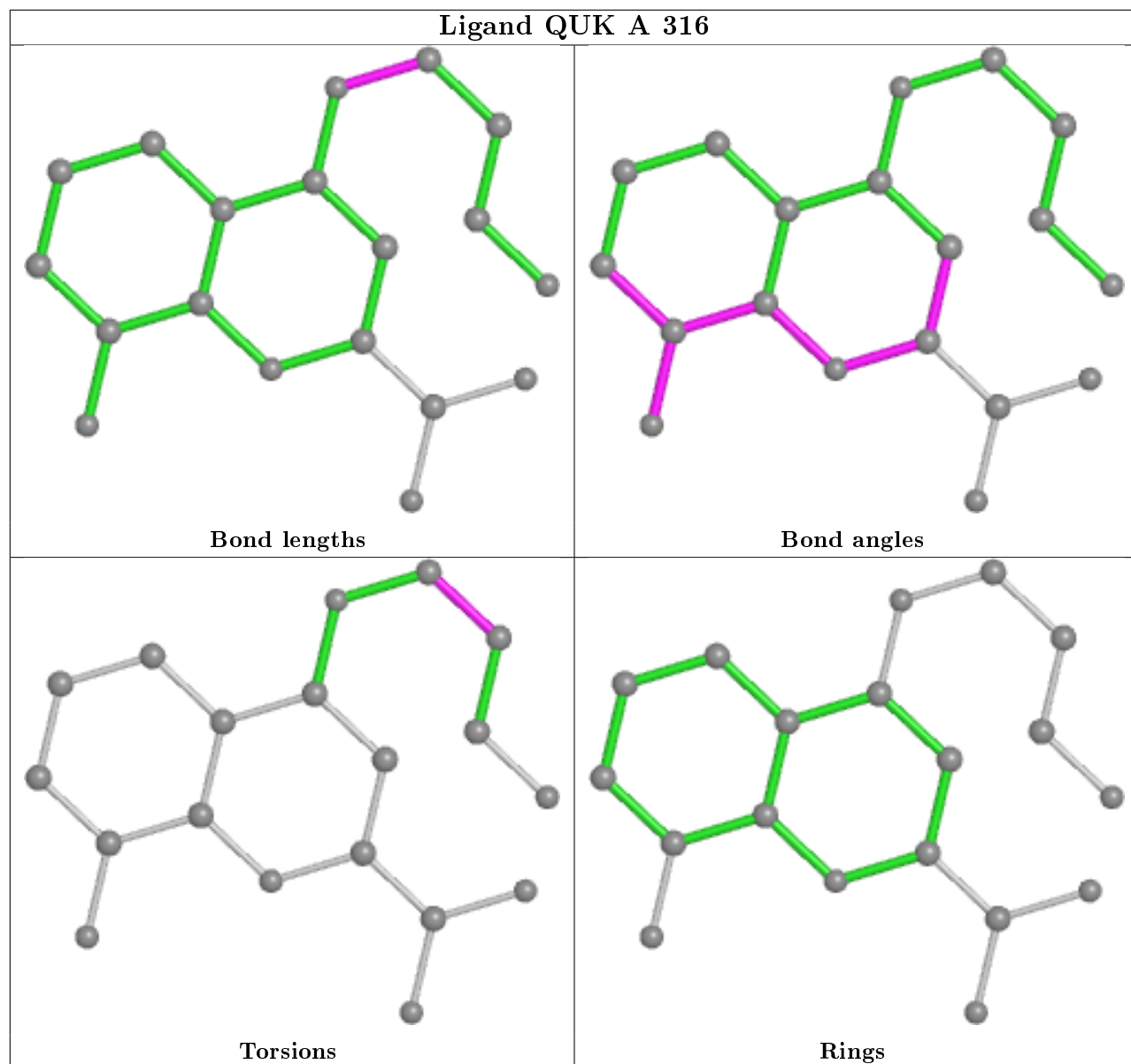
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	316	QUK	1	0

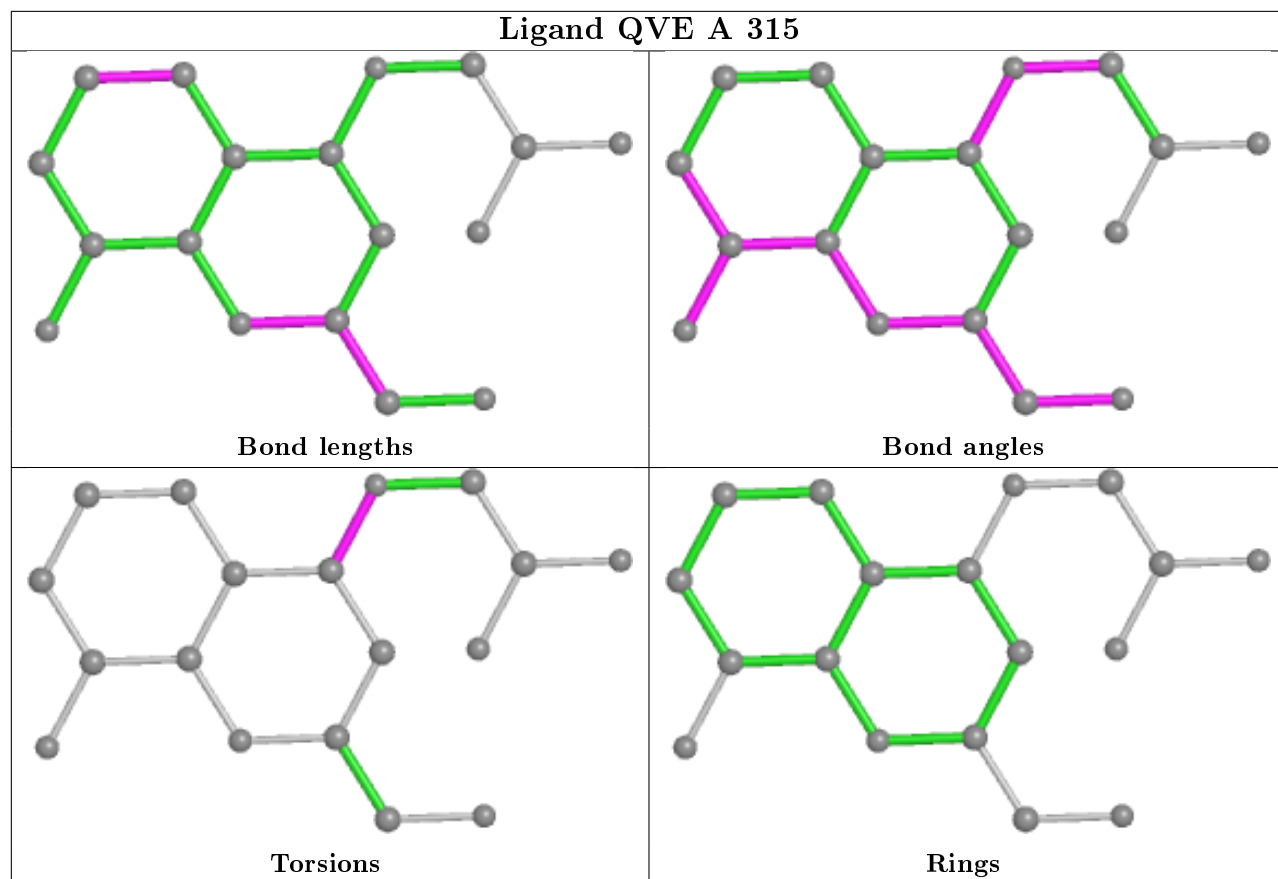
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

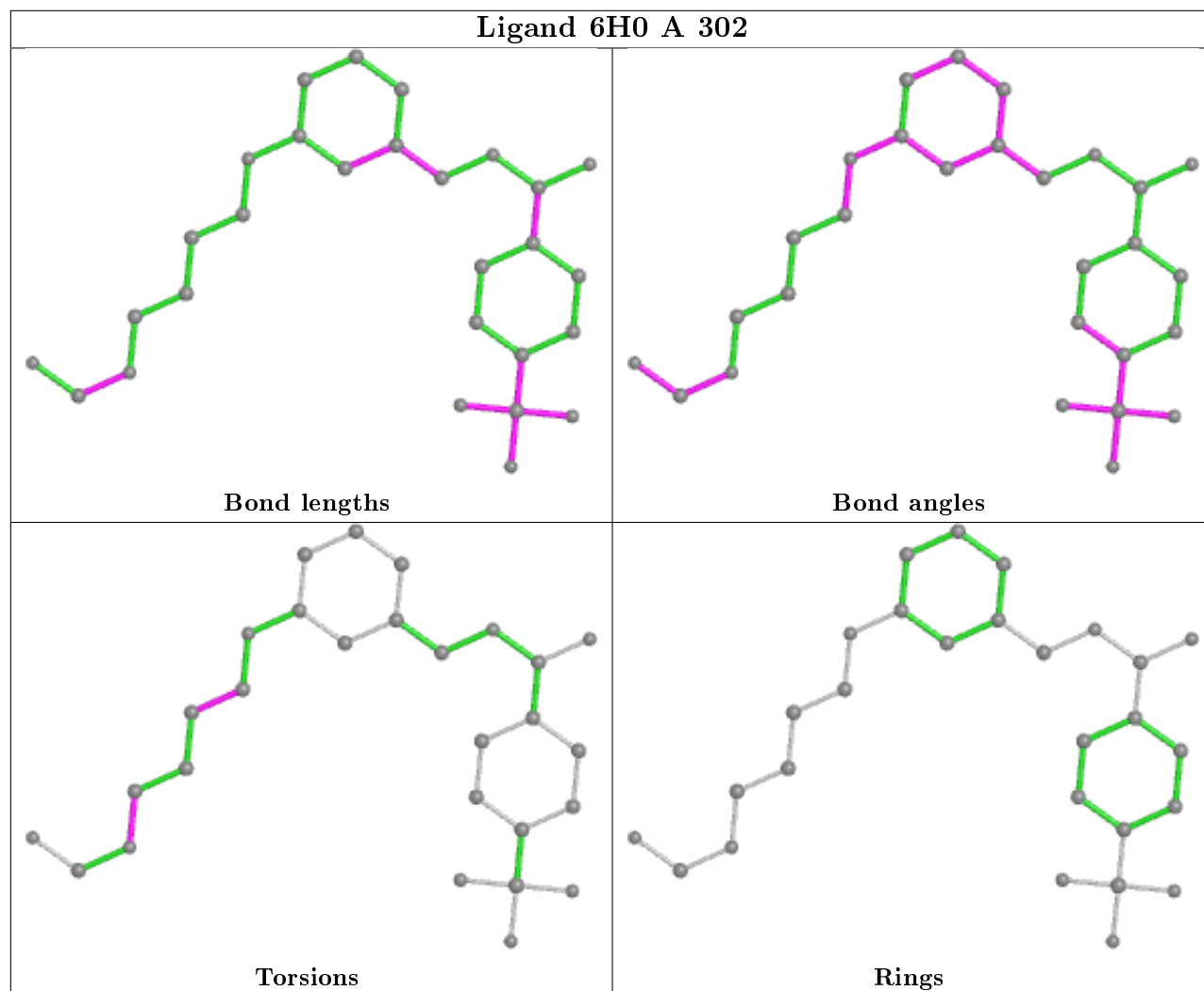












5.7 Other polymers [i](#)

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	237/259 (91%)	0.02	4 (1%) 70 71	45, 78, 124, 142	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	VAL	3.3
1	A	98	GLY	2.3
1	A	93	PHE	2.2
1	A	187	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
7	QUK	A	316	19/19	0.89	0.21	66,70,86,86	0
9	QDD	A	313	17/17	0.93	0.16	59,61,69,72	0
7	QUK	A	306	18/19	0.94	0.21	57,60,70,71	0

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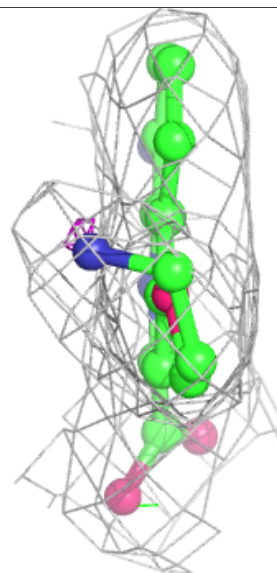
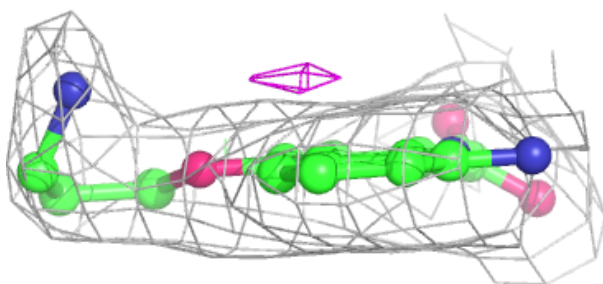
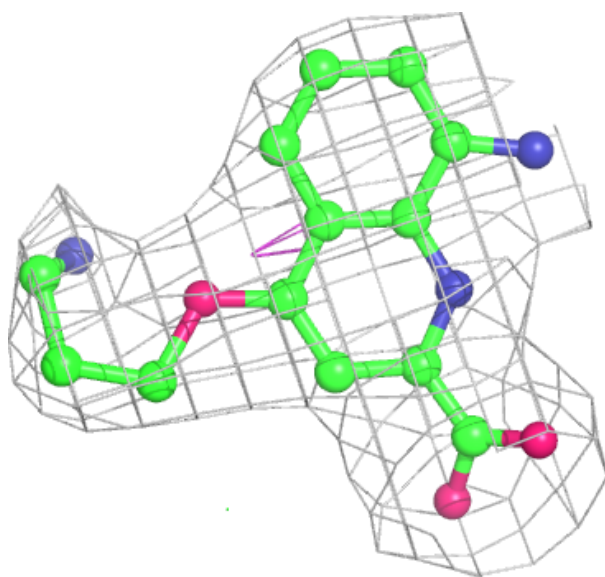
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	QVE	A	308	18/19	0.94	0.19	57,60,81,86	0
8	QVE	A	315	18/19	0.94	0.14	60,62,73,75	0
5	ZY9	A	314	10/11	0.94	0.15	62,64,65,65	0
6	QVS	A	311	14/15	0.95	0.17	57,61,64,64	0
4	QUJ	A	303	18/19	0.95	0.18	55,59,77,78	0
5	ZY9	A	310	10/11	0.95	0.14	62,64,65,65	0
6	QVS	A	305	14/15	0.96	0.14	54,55,57,58	0
5	ZY9	A	304	10/11	0.97	0.14	52,53,55,55	0
5	ZY9	A	312	10/11	0.97	0.14	55,57,60,60	0
3	6H0	A	302	28/28	0.97	0.17	46,55,60,63	0
2	ZN	A	301	1/1	0.98	0.06	87,87,87,87	0
5	ZY9	A	309	10/11	0.98	0.21	57,58,60,60	0
5	ZY9	A	307	10/11	0.98	0.20	53,56,58,58	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.

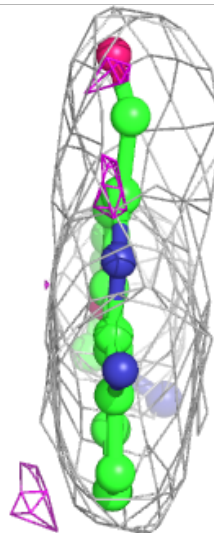
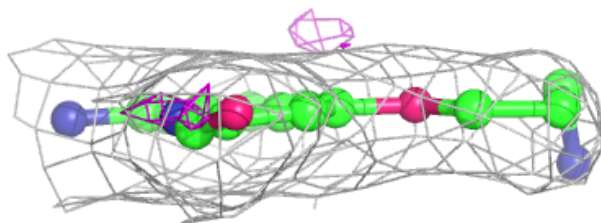
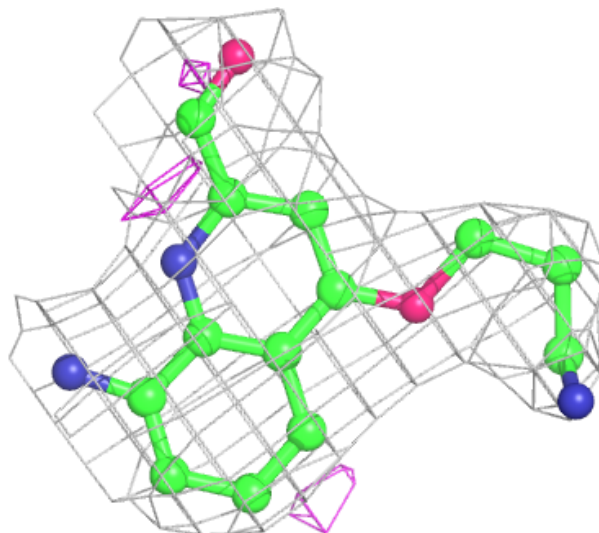
Electron density around QUK A 316:

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



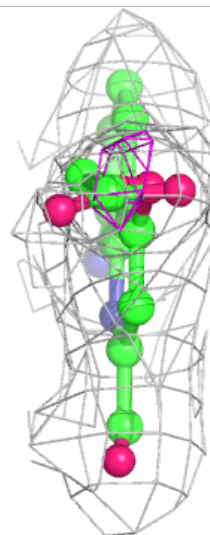
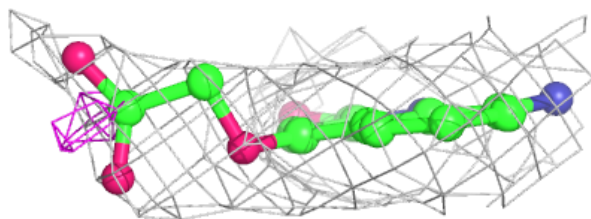
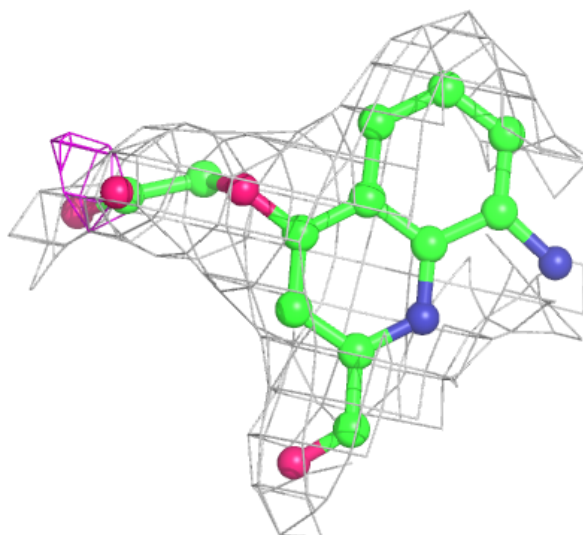
Electron density around QUK A 306:

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



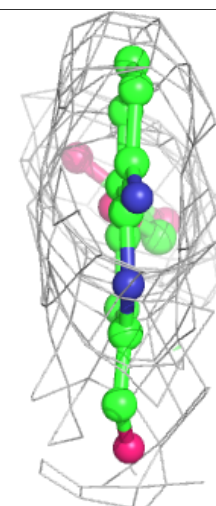
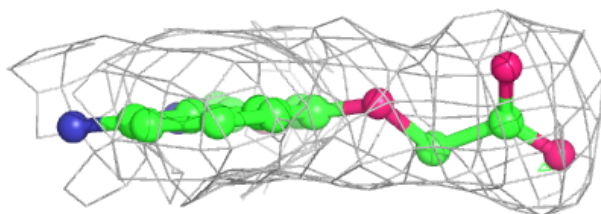
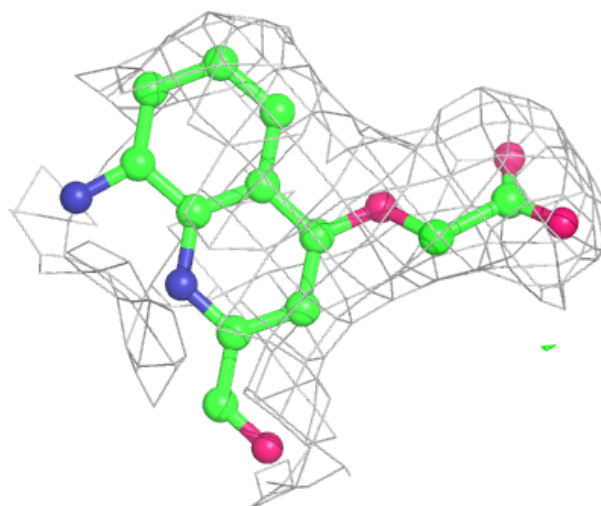
Electron density around QVE A 308:

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



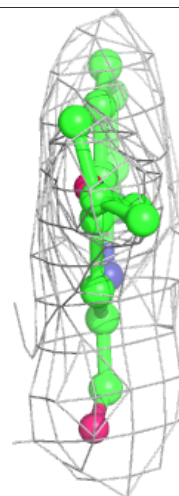
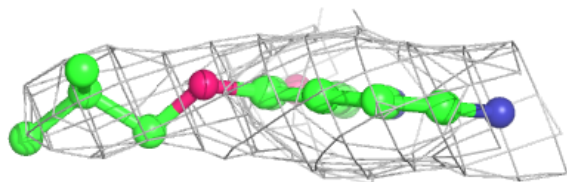
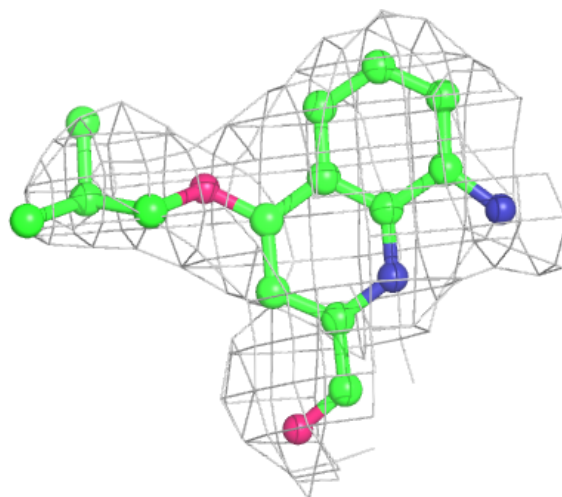
Electron density around QVE A 315:

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



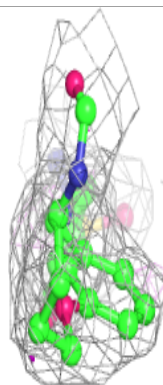
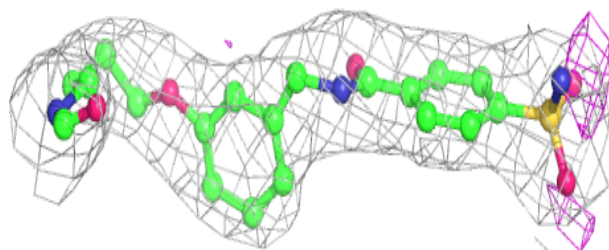
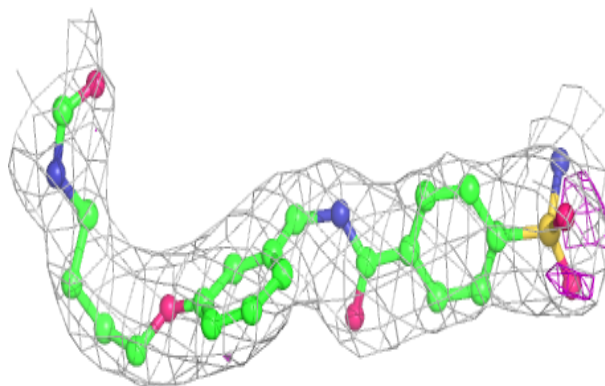
Electron density around Q U J A 303:

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



Electron density around 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.