Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2023 – 10:55 am GMT

PDB ID	:	5L6K
Title	:	Crystal Structure of Human Carbonic Anhydrase II in Complex with a Quinoline Oligoamide Foldamer
Authors	:	Jewginski, M.; Langlois d'Estaintot, B.; Granier, T.; Huc, Y.
Deposited on	:	2016-05-30
Resolution	:	1.70 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:

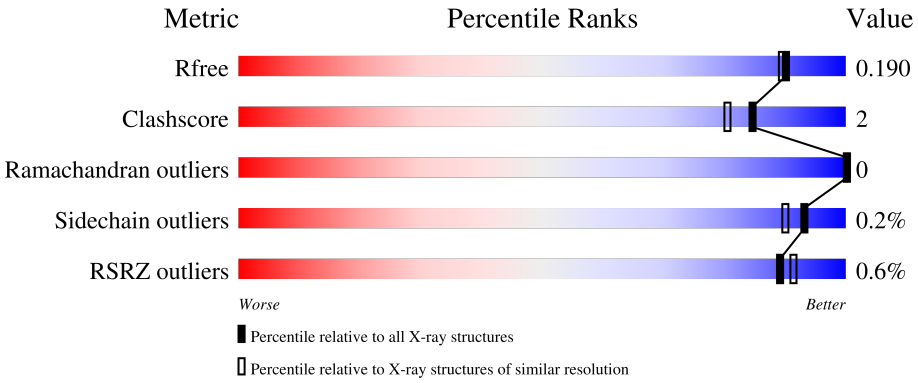
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	95% .
1	B	260	% 96% .

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 4929 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.

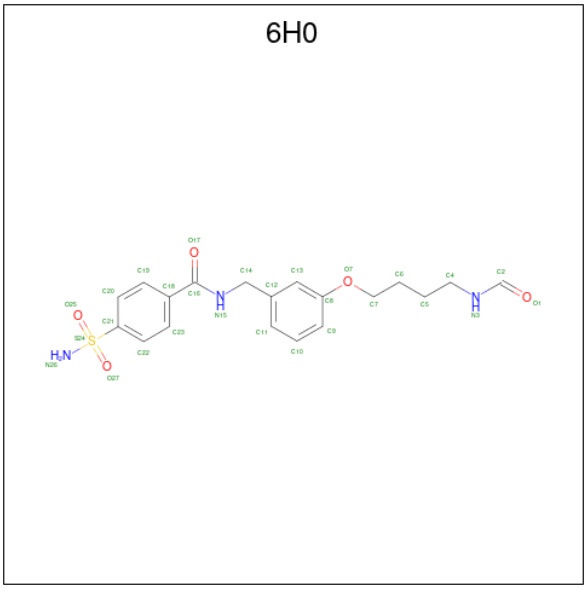
- Molecule 1 is a protein called Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	8	0
			2094	1351	358	383	2			
1	B	259	Total	C	N	O	S	0	6	0
			2081	1342	355	382	2			

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

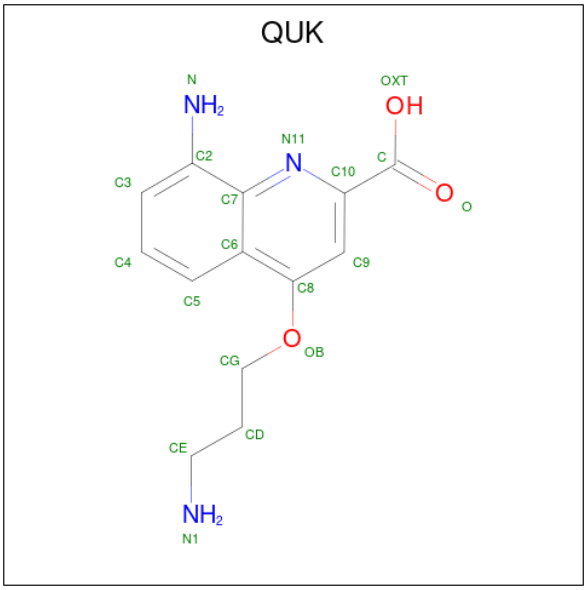
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is {N}-[[3-(4-formamidobutoxy)phenyl]methyl]-4-sulfamoyl-benzamide (three-letter code: 6H0) (formula: $C_{19}H_{23}N_3O_5S$).



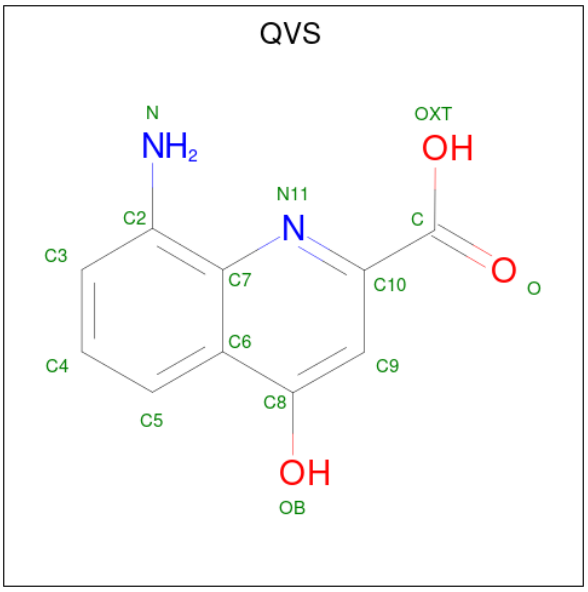
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	19	3	5	1		
3	B	1	Total	C	N	O	S	0	0
			28	19	3	5	1		

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



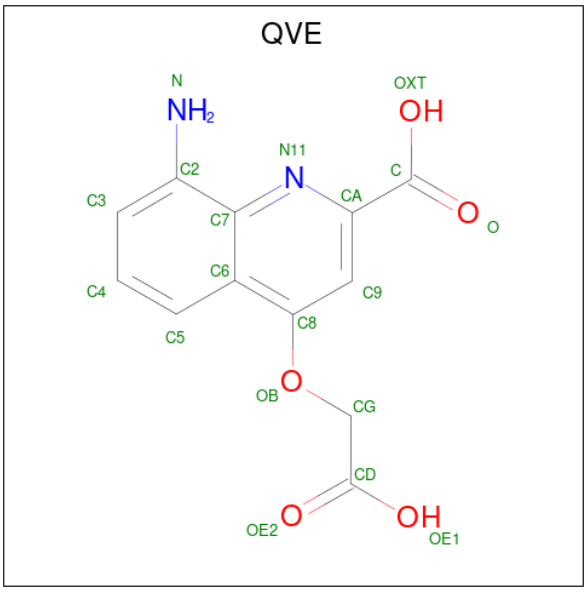
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	13	2	2		
4	A	1	Total	C	N	O	0	1
			14	10	2	2		
4	B	1	Total	C	N	O	0	0
			17	13	2	2		
4	B	1	Total	C	N	O	0	1
			14	10	2	2		

- Molecule 5 is 8-azanyl-4-oxidanyl-quinoline-2-carboxylic acid (three-letter code: QVS) (formula: $C_{10}H_8N_2O_3$).



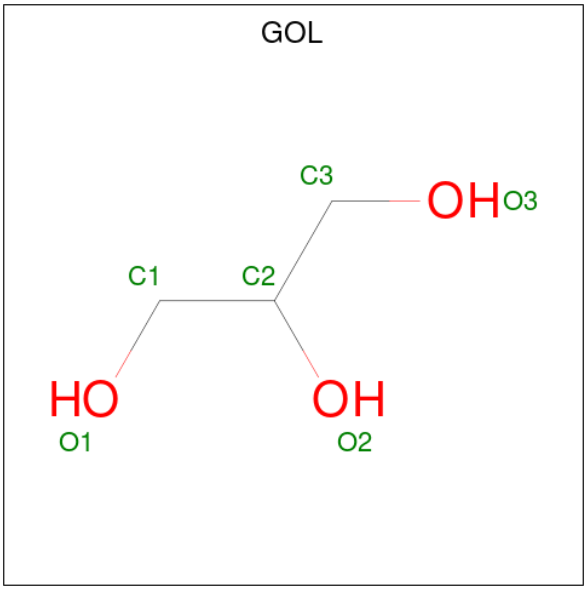
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 10 2 2	0	0
5	A	1	Total C N O 14 10 2 2	0	1
5	B	1	Total C N O 14 10 2 2	0	1
5	B	1	Total C N O 14 10 2 2	0	0

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



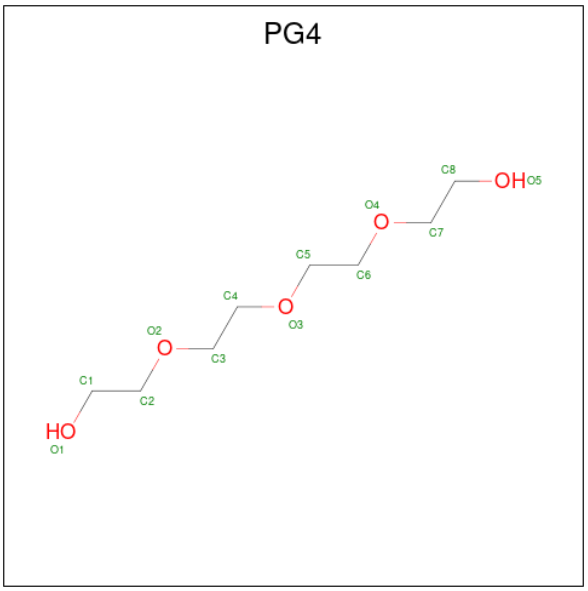
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 19 12 2 5	0	0
6	A	1	Total C N O 19 12 2 5	0	1
6	B	1	Total C N O 19 12 2 5	0	0
6	B	1	Total C N O 15 10 2 3	0	1

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



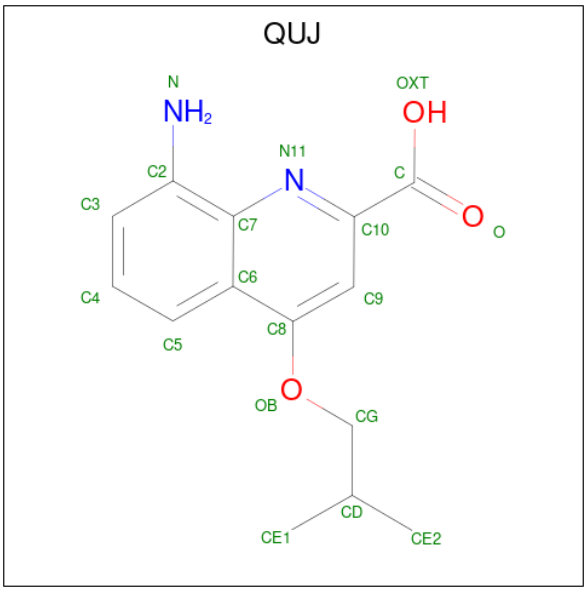
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 3 2 1	0	1
8	B	1	Total C O 7 4 3	0	1

- Molecule 9 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
9	A	1	Total C N O 18 14 2 2	0	1

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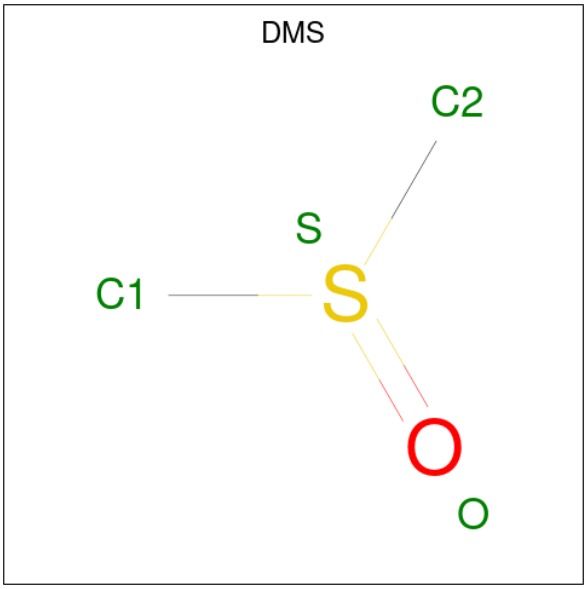
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O 17 13 2 2	0	0
9	B	1	Total C N O 17 13 2 2	0	0
9	B	1	Total C N O 18 14 2 2	0	1

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Na 1 1	0	0

- Molecule 11 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O S 4 2 1 1	0	0

- Molecule 12 is water.

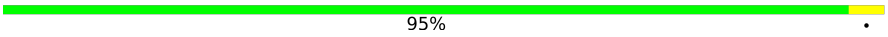
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	229	Total O 229 229	0	0
12	B	168	Total O 168 168	0	0

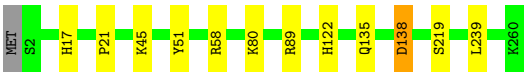
3 Residue-property plots (i)

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

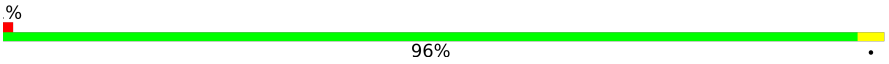
Chain A:

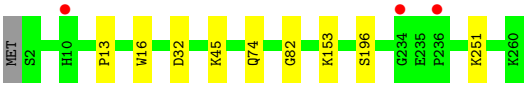




- Molecule 1: Carbonic anhydrase 2

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.07Å 84.87Å 77.22Å 90.00° 97.81° 90.00°	Depositor
Resolution (Å)	76.50 – 1.70 56.82 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (76.50-1.70) 99.7 (56.82-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.154 , 0.181 0.163 , 0.190	Depositor DCC
R_{free} test set	3137 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4929	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QUK, DMS, ZN, 6H0, GOL, PG4, NA, QVS, QVE, QUJ

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	0.89	2/2178 (0.1%)	0.96	3/2956 (0.1%)
1	B	0.82	1/2162 (0.0%)	0.91	0/2934
All	All	0.86	3/4340 (0.1%)	0.94	3/5890 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	196	SER	CA-CB	5.89	1.61	1.52
1	A	219	SER	CB-OG	-5.06	1.35	1.42
1	A	51	TYR	CG-CD1	5.00	1.45	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	58	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	51	TYR	CB-CG-CD1	5.19	124.11	121.00
1	A	138	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2094	0	2043	7	0
1	B	2081	0	2042	4	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
4	A	31	0	0	0	0
4	B	31	0	0	1	0
5	A	28	0	0	3	0
5	B	28	0	0	2	0
6	A	38	0	0	0	0
6	B	34	0	0	1	0
7	A	12	0	16	0	0
7	B	12	0	16	0	0
8	A	3	0	0	4	0
8	B	7	0	6	3	0
9	A	35	0	0	2	0
9	B	35	0	0	1	0
10	A	1	0	0	0	0
11	A	4	0	6	0	0
12	A	229	0	0	6	0
12	B	168	0	0	1	0
All	All	4929	0	4129	20	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:310[B]:PG4:C2	5:A:312[B]:QVS:C3	2.60	0.80
8:A:310[B]:PG4:C2	5:A:312[B]:QVS:C2	2.65	0.75
1:A:17[A]:HIS:HE1	12:A:408:HOH:O	1.74	0.71
1:A:45:LYS:NZ	12:A:403:HOH:O	2.29	0.66
1:A:135:GLN:NE2	12:A:404:HOH:O	2.32	0.62
8:B:302[A]:PG4:H21	5:B:304[A]:QVS:C3	2.31	0.59
8:A:310[B]:PG4:C2	12:A:465:HOH:O	2.50	0.57
1:B:251:LYS:NZ	12:B:401:HOH:O	2.42	0.53
8:B:302[A]:PG4:H21	5:B:304[A]:QVS:C2	2.42	0.49
8:A:310[B]:PG4:O1	9:A:311[B]:QUJ:C3	2.62	0.47
8:B:302[A]:PG4:O1	9:B:303[A]:QUJ:C3	2.58	0.46
1:A:89:ARG:O	1:A:122:HIS:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:311[B]:QUJ:O	4:B:310[B]:QUK:C3	2.64	0.44
5:A:312[B]:QVS:O	6:B:311[B]:QVE:C3	2.65	0.43
1:A:138:ASP:HA	12:A:468:HOH:O	2.19	0.42
1:A:80:LYS:HE2	12:A:456:HOH:O	2.20	0.41
1:B:13:PRO:HA	1:B:16:TRP:CD2	2.55	0.41
1:A:239:LEU:N	1:A:239:LEU:HD22	2.36	0.41
1:B:45:LYS:O	1:B:82:GLY:HA2	2.21	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ASP:OD2	1:B:74:GLN:NE2[1_655]	2.18	0.02

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	265/260 (102%)	260 (98%)	5 (2%)	0	100	100
1	B	263/260 (101%)	257 (98%)	6 (2%)	0	100	100
All	All	528/520 (102%)	517 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	225/225 (100%)	224 (100%)	1 (0%)	91 87
1	B	227/225 (101%)	227 (100%)	0	100 100
All	All	452/450 (100%)	451 (100%)	1 (0%)	93 90

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

Mol	Chain	Res	Type
1	A	21	PRO

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 3 are monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	6H0	B	306	9,2	29,29,29	1.45	5 (17%)	37,38,38	1.20	3 (8%)
11	DMS	A	314	-	3,3,3	0.48	0	3,3,3	0.88	0
8	PG4	A	310[B]	9	2,2,12	1.58	0	1,1,11	0.70	0
4	QUK	B	310[B]	9,5	15,15,20	2.50	1 (6%)	19,21,27	1.97	3 (15%)
9	QUJ	B	301	4,3	18,18,20	1.96	2 (11%)	21,24,28	2.35	4 (19%)
5	QVS	B	308	4,6	15,15,16	1.89	1 (6%)	19,21,23	2.33	6 (31%)
7	GOL	B	312	-	5,5,5	0.15	0	5,5,5	0.98	0
6	QVE	A	305	5	20,20,20	1.75	2 (10%)	27,28,28	1.87	5 (18%)
9	QUJ	B	303[A]	8,4	19,19,20	2.15	2 (10%)	23,26,28	1.72	3 (13%)
4	QUK	A	303	9,5	18,18,20	1.80	2 (11%)	21,24,27	2.39	5 (23%)
5	QVS	A	304	4,6	15,15,16	2.27	2 (13%)	19,21,23	2.42	5 (26%)
9	QUJ	A	311[B]	8,4	19,19,20	2.30	1 (5%)	23,26,28	1.76	6 (26%)
7	GOL	A	308	-	5,5,5	0.29	0	5,5,5	0.35	0
4	QUK	A	306[A]	9,5	15,15,20	2.14	2 (13%)	19,21,27	2.18	4 (21%)
7	GOL	A	309	-	5,5,5	0.57	0	5,5,5	0.86	0
5	QVS	A	312[B]	4,6	15,15,16	2.31	2 (13%)	19,21,23	1.87	4 (21%)
6	QVE	B	311[B]	5	16,16,20	2.21	2 (12%)	22,23,28	1.38	2 (9%)
9	QUJ	A	315	4,3	18,18,20	2.00	2 (11%)	21,24,28	2.77	6 (28%)
6	QVE	A	307[A]	5	20,20,20	1.93	3 (15%)	27,28,28	1.49	3 (11%)
5	QVS	B	304[A]	4,6	15,15,16	2.20	1 (6%)	19,21,23	2.10	6 (31%)
6	QVE	B	309	5	20,20,20	1.96	2 (10%)	27,28,28	1.60	5 (18%)
7	GOL	B	313	-	5,5,5	0.25	0	5,5,5	0.90	0
3	6H0	A	302	9,2	29,29,29	1.56	4 (13%)	37,38,38	1.92	6 (16%)
8	PG4	B	302[A]	9	6,6,12	1.50	1 (16%)	5,5,11	1.30	0
4	QUK	B	307	9,5	18,18,20	1.64	1 (5%)	21,24,27	2.61	6 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6H0	B	306	9,2	-	6/23/23/23	0/2/2/2
4	QUK	B	310[B]	9,5	-	0/2/2/9	0/2/2/2
9	QUJ	B	301	4,3	-	1/6/6/9	0/2/2/2
5	QVS	B	308	4,6	-	0/2/2/4	0/2/2/2
7	GOL	B	312	-	-	2/4/4/4	-
6	QVE	A	305	5	-	5/9/9/9	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	QUJ	B	303[A]	8,4	-	4/7/7/9	0/2/2/2
4	QUK	A	303	9,5	-	3/6/6/9	0/2/2/2
5	QVS	A	304	4,6	-	0/2/2/4	0/2/2/2
9	QUJ	A	311[B]	8,4	-	4/7/7/9	0/2/2/2
7	GOL	A	308	-	-	0/4/4/4	-
4	QUK	A	306[A]	9,5	-	2/2/2/9	0/2/2/2
7	GOL	A	309	-	-	0/4/4/4	-
5	QVS	A	312[B]	4,6	-	0/2/2/4	0/2/2/2
6	QVE	B	311[B]	5	-	0/4/4/9	0/2/2/2
9	QUJ	A	315	4,3	-	0/6/6/9	0/2/2/2
6	QVE	A	307[A]	5	-	0/9/9/9	0/2/2/2
5	QVS	B	304[A]	4,6	-	0/2/2/4	0/2/2/2
6	QVE	B	309	5	-	0/9/9/9	0/2/2/2
7	GOL	B	313	-	-	0/4/4/4	-
3	6H0	A	302	9,2	-	5/23/23/23	0/2/2/2
8	PG4	B	302[A]	9	-	3/4/4/10	-
4	QUK	B	307	9,5	-	2/6/6/9	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	311[B]	QUJ	C10-C	-8.96	1.39	1.48
4	B	310[B]	QUK	C10-C	-8.64	1.39	1.48
5	A	304	QVS	C10-C	-8.17	1.40	1.48
9	B	303[A]	QUJ	C10-C	-8.12	1.40	1.48
6	B	311[B]	QVE	CA-C	-7.73	1.40	1.50
5	A	312[B]	QVS	C10-C	-7.72	1.40	1.48
5	B	304[A]	QVS	C10-C	-7.60	1.40	1.48
6	B	309	QVE	CA-C	-7.46	1.40	1.50
9	A	315	QUJ	C10-C	-7.46	1.40	1.48
9	B	301	QUJ	C10-C	-7.36	1.40	1.48
4	A	306[A]	QUK	C10-C	-7.21	1.41	1.48
6	A	307[A]	QVE	CA-C	-7.01	1.41	1.50
5	B	308	QVS	C10-C	-6.55	1.41	1.48
6	A	305	QVE	CA-C	-6.54	1.41	1.50
4	A	303	QUK	C10-C	-6.52	1.41	1.48
4	B	307	QUK	C10-C	-5.75	1.42	1.48
3	A	302	6H0	O25-S24	4.46	1.52	1.43
3	A	302	6H0	C14-C12	-3.81	1.43	1.51
3	B	306	6H0	C14-C12	-3.62	1.43	1.51
8	B	302[A]	PG4	O1-C1	-3.59	1.23	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	306	6H0	O25-S24	3.35	1.50	1.43
3	B	306	6H0	C18-C16	-3.11	1.43	1.50
9	A	315	QUJ	C10-N11	2.88	1.36	1.33
4	A	303	QUK	C10-N11	2.53	1.35	1.33
3	A	302	6H0	S24-N26	-2.46	1.55	1.60
6	B	311[B]	QVE	OXT-C	-2.34	1.23	1.30
3	A	302	6H0	C18-C16	-2.32	1.45	1.50
6	B	309	QVE	OXT-C	-2.31	1.23	1.30
9	B	303[A]	QUJ	C10-N11	2.30	1.35	1.33
3	B	306	6H0	C23-C18	2.29	1.43	1.39
6	A	305	QVE	OXT-C	-2.28	1.23	1.30
3	B	306	6H0	C14-N15	2.28	1.50	1.46
6	A	307[A]	QVE	C2-C7	-2.26	1.38	1.42
9	B	301	QUJ	C10-N11	2.17	1.35	1.33
6	A	307[A]	QVE	OXT-C	-2.17	1.23	1.30
4	A	306[A]	QUK	C10-N11	2.16	1.35	1.33
5	A	304	QVS	C10-N11	2.03	1.35	1.33
5	A	312[B]	QVS	C2-C7	-2.03	1.39	1.42

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	315	QUJ	C10-N11-C7	9.21	125.10	118.11
4	B	307	QUK	C10-N11-C7	8.22	124.34	118.11
4	A	303	QUK	C10-N11-C7	7.14	123.52	118.11
9	B	301	QUJ	C10-N11-C7	6.45	123.00	118.11
6	A	305	QVE	CG-OB-C8	6.29	124.12	116.95
4	B	307	QUK	C-C10-N11	6.27	120.81	114.66
4	A	306[A]	QUK	C10-N11-C7	6.25	122.85	118.11
3	A	302	6H0	O27-S24-N26	6.06	116.35	107.36
5	A	304	QVS	C10-N11-C7	5.89	122.58	118.11
4	B	310[B]	QUK	C10-N11-C7	5.89	122.58	118.11
5	A	312[B]	QVS	C10-N11-C7	5.65	122.40	118.11
9	B	301	QUJ	C-C10-N11	5.63	120.18	114.66
9	B	303[A]	QUJ	C10-N11-C7	5.57	122.33	118.11
5	B	304[A]	QVS	C10-N11-C7	5.52	122.29	118.11
4	A	303	QUK	C-C10-N11	5.45	120.00	114.66
9	A	315	QUJ	O-C-C10	-5.32	119.18	124.22
5	B	308	QVS	C-C10-N11	4.95	119.52	114.66
5	B	304[A]	QVS	C-C10-N11	4.86	119.43	114.66
5	A	304	QVS	O-C-C10	-4.85	119.63	124.22
3	A	302	6H0	O25-S24-O27	-4.83	110.83	118.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	6H0	C23-C22-C21	-4.72	114.56	119.45
5	B	308	QVS	C10-N11-C7	4.51	121.53	118.11
4	B	310[B]	QUK	C9-C10-C	4.30	124.94	121.23
5	A	304	QVS	C-C10-N11	4.25	118.83	114.66
5	A	304	QVS	C3-C2-N	4.12	128.59	120.36
6	B	311[B]	QVE	OB-C8-C6	4.11	121.45	116.31
5	B	308	QVS	C3-C2-N	4.04	128.44	120.36
9	B	301	QUJ	O-C-C10	-4.00	120.43	124.22
9	B	303[A]	QUJ	C9-C10-C	3.99	124.68	121.23
6	A	307[A]	QVE	CG-OB-C8	3.99	121.50	116.95
5	B	308	QVS	O-C-C10	-3.97	120.46	124.22
4	A	306[A]	QUK	C9-C10-C	3.96	124.65	121.23
4	A	306[A]	QUK	OB-C8-C6	3.85	121.12	116.31
9	A	315	QUJ	C-C10-N11	3.79	118.37	114.66
6	B	309	QVE	C-CA-N11	3.79	122.32	116.28
3	B	306	6H0	O27-S24-N26	3.78	112.96	107.36
3	A	302	6H0	C22-C23-C18	3.77	125.17	120.78
9	A	311[B]	QUJ	OB-C8-C6	3.77	125.54	115.01
5	A	312[B]	QVS	C-C10-N11	3.64	118.23	114.66
6	B	309	QVE	CG-OB-C8	3.62	121.08	116.95
4	A	303	QUK	C3-C2-N	3.52	127.40	120.36
9	A	311[B]	QUJ	O-C-C10	-3.45	120.95	124.22
9	A	311[B]	QUJ	C10-N11-C7	3.39	120.68	118.11
6	B	309	QVE	C3-C2-N	3.29	126.94	120.36
4	B	307	QUK	O-C-C10	-3.26	121.13	124.22
4	B	307	QUK	C3-C2-N	3.24	126.83	120.36
3	A	302	6H0	C19-C20-C21	3.13	122.69	119.45
6	A	305	QVE	C-CA-N11	3.09	121.20	116.28
6	A	305	QVE	CA-N11-C7	3.06	123.68	117.24
4	B	310[B]	QUK	OB-C8-C6	3.03	120.10	116.31
9	B	301	QUJ	C3-C2-N	2.98	126.32	120.36
5	B	304[A]	QVS	C3-C2-N	2.94	126.23	120.36
3	B	306	6H0	O1-C2-N3	-2.87	121.99	124.89
9	A	315	QUJ	C3-C2-N	2.85	126.06	120.36
6	A	305	QVE	C3-C2-N	2.74	125.84	120.36
4	A	303	QUK	O-C-C10	-2.73	121.64	124.22
4	A	306[A]	QUK	O-C-C10	-2.66	121.70	124.22
6	B	309	QVE	C9-CA-N11	-2.58	118.21	124.50
6	A	305	QVE	C9-CA-N11	-2.57	118.24	124.50
4	A	303	QUK	CG-OB-C8	2.56	125.40	117.74
6	A	307[A]	QVE	C3-C2-N	2.55	125.47	120.36
9	B	303[A]	QUJ	O-C-C10	-2.53	121.82	124.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	315	QUJ	C6-C7-N11	-2.53	117.56	122.78
5	A	312[B]	QVS	C7-C2-N	-2.48	113.35	118.07
6	B	311[B]	QVE	C-CA-N11	2.46	120.21	116.28
5	A	312[B]	QVS	C3-C2-N	2.44	125.24	120.36
6	A	307[A]	QVE	OB-C8-C6	2.43	121.81	115.01
5	B	308	QVS	OB-C8-C6	2.40	119.31	116.31
5	B	304[A]	QVS	O-C-C10	-2.40	121.95	124.22
5	B	304[A]	QVS	OB-C8-C6	2.39	119.29	116.31
9	A	311[B]	QUJ	OB-CG-CD	2.38	119.06	108.70
6	B	309	QVE	CA-N11-C7	2.36	122.22	117.24
3	A	302	6H0	C20-C19-C18	-2.29	118.11	120.78
5	A	304	QVS	C7-C2-N	-2.28	113.72	118.07
5	B	308	QVS	C3-C2-C7	-2.26	116.51	120.06
9	A	315	QUJ	C2-C7-N11	2.18	120.79	118.64
4	B	307	QUK	C7-C2-N	-2.14	113.99	118.07
9	A	311[B]	QUJ	OB-C8-C9	-2.13	117.74	124.69
5	B	304[A]	QVS	C7-C2-N	-2.09	114.09	118.07
3	B	306	6H0	O27-S24-C21	-2.08	105.03	107.35
4	B	307	QUK	C9-C10-C	2.06	123.01	121.23
9	A	311[B]	QUJ	C2-C7-N11	-2.04	116.62	118.64

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	QUK	O-C-C10-C9
4	A	306[A]	QUK	O-C-C10-N11
4	A	306[A]	QUK	O-C-C10-C9
4	B	307	QUK	O-C-C10-N11
4	B	307	QUK	O-C-C10-C9
6	A	305	QVE	OE1-CD-CG-OB
7	B	312	GOL	O1-C1-C2-O2
7	B	312	GOL	O1-C1-C2-C3
9	A	311[B]	QUJ	O-C-C10-C9
9	A	311[B]	QUJ	O-C-C10-N11
9	B	303[A]	QUJ	O-C-C10-C9
9	B	303[A]	QUJ	O-C-C10-N11
6	A	305	QVE	OE2-CD-CG-OB
3	B	306	6H0	N3-C4-C5-C6
9	A	311[B]	QUJ	CE1-CD-CG-OB
8	B	302[A]	PG4	O1-C1-C2-O2
3	B	306	6H0	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
9	A	311[B]	QUJ	CE2-CD-CG-OB
9	B	301	QUJ	CD-CG-OB-C8
6	A	305	QVE	C6-C8-OB-CG
9	B	303[A]	QUJ	CE1-CD-CG-OB
3	A	302	6H0	C20-C21-S24-O25
6	A	305	QVE	C9-C8-OB-CG
9	B	303[A]	QUJ	CE2-CD-CG-OB
4	A	303	QUK	CE-CD-CG-OB
8	B	302[A]	PG4	C1-C2-O2-C3
3	A	302	6H0	C20-C21-S24-N26
3	A	302	6H0	C22-C21-S24-O25
3	B	306	6H0	C20-C21-S24-O25
8	B	302[A]	PG4	C4-C3-O2-C2
3	B	306	6H0	C22-C21-S24-O25
3	B	306	6H0	C20-C21-S24-N26
3	A	302	6H0	C4-C5-C6-C7
6	A	305	QVE	CD-CG-OB-C8
4	A	303	QUK	O-C-C10-N11
3	A	302	6H0	C22-C21-S24-N26
3	B	306	6H0	C22-C21-S24-N26

There are no ring outliers.

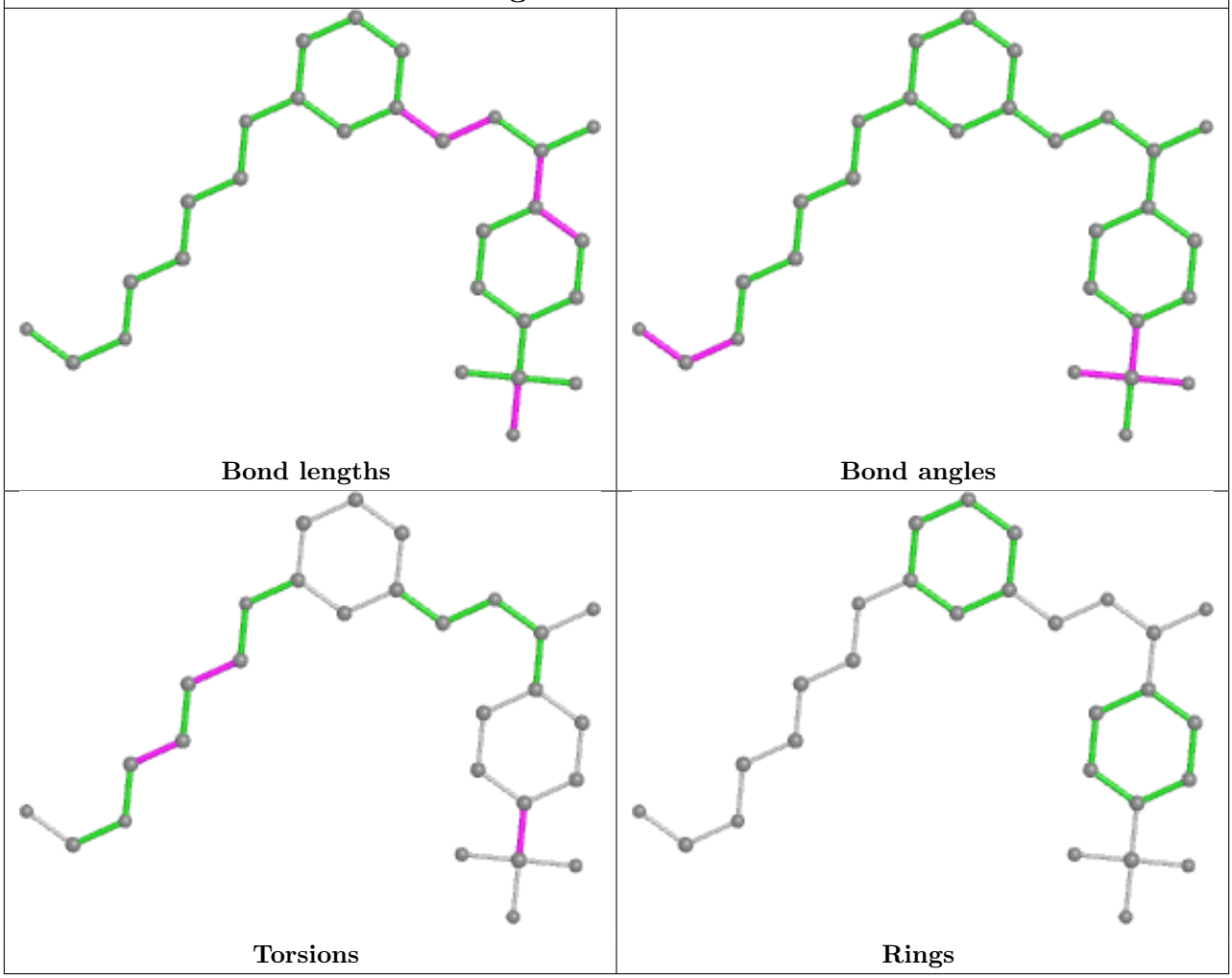
8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	310[B]	PG4	4	0
4	B	310[B]	QUK	1	0
9	B	303[A]	QUJ	1	0
9	A	311[B]	QUJ	2	0
5	A	312[B]	QVS	3	0
6	B	311[B]	QVE	1	0
5	B	304[A]	QVS	2	0
8	B	302[A]	PG4	3	0

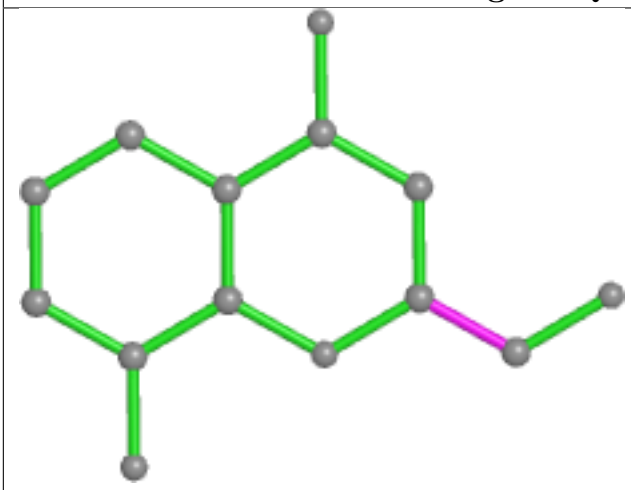
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

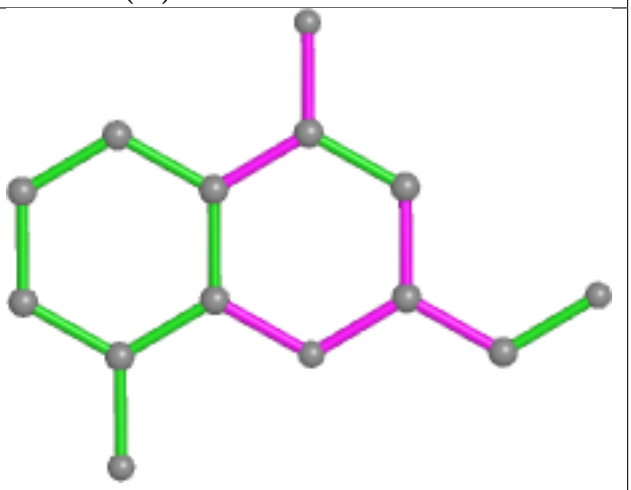
Ligand 6H0 B 306



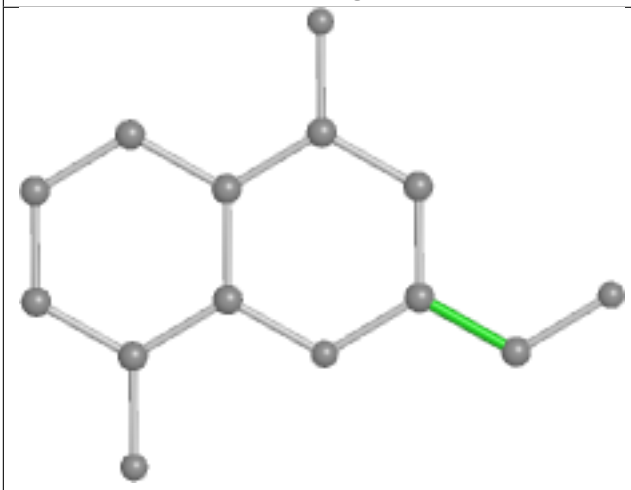
Ligand QUK B 310 (B)



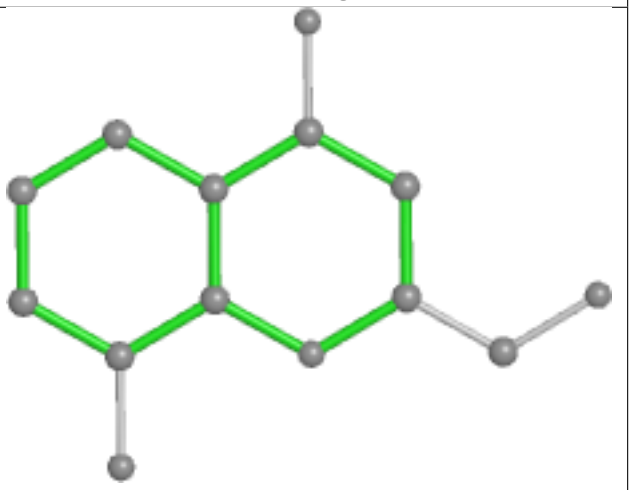
Bond lengths



Bond angles

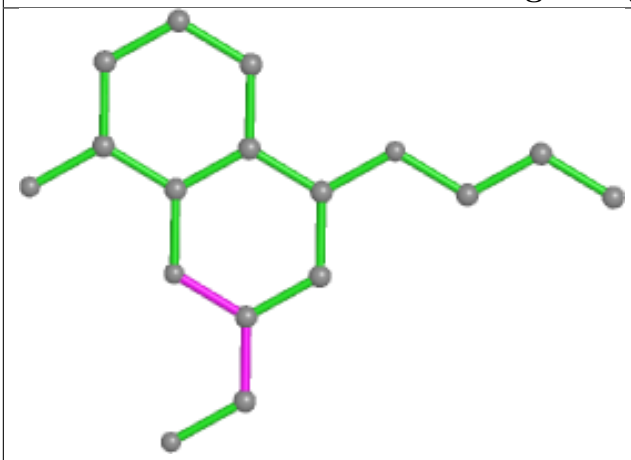


Torsions

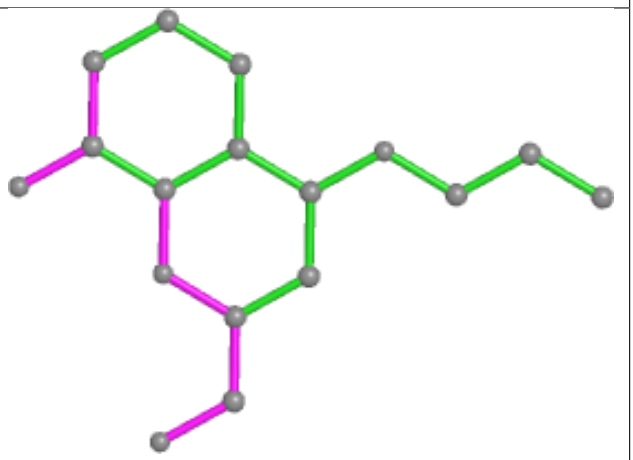


Rings

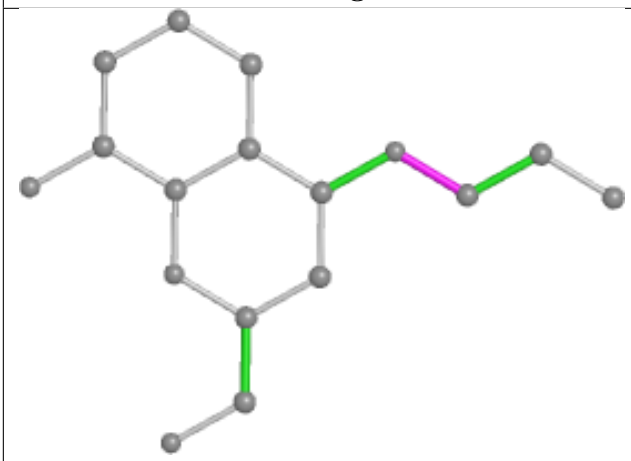
Ligand QUJ B 301



Bond lengths



Bond angles



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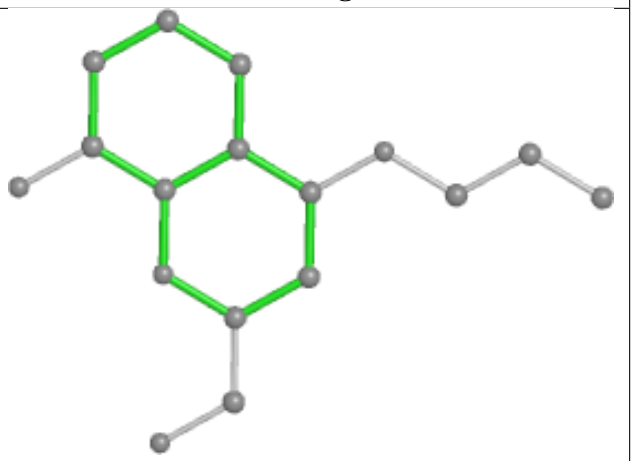
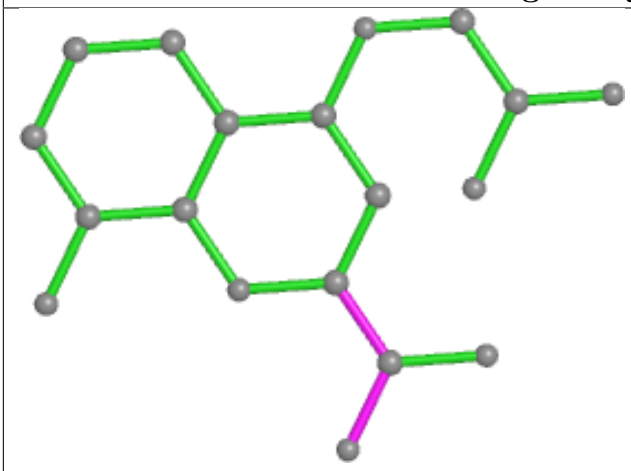
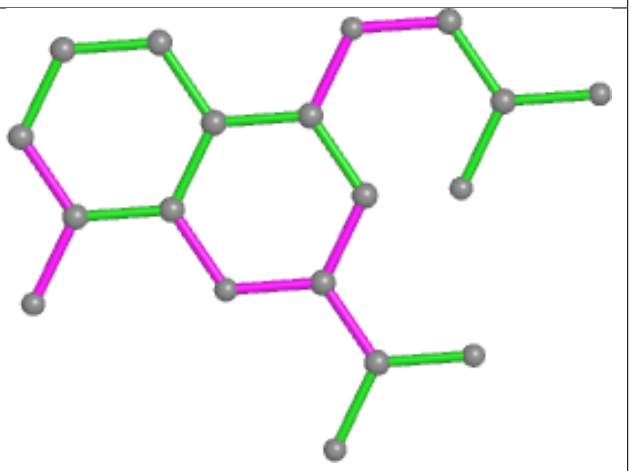


Rings

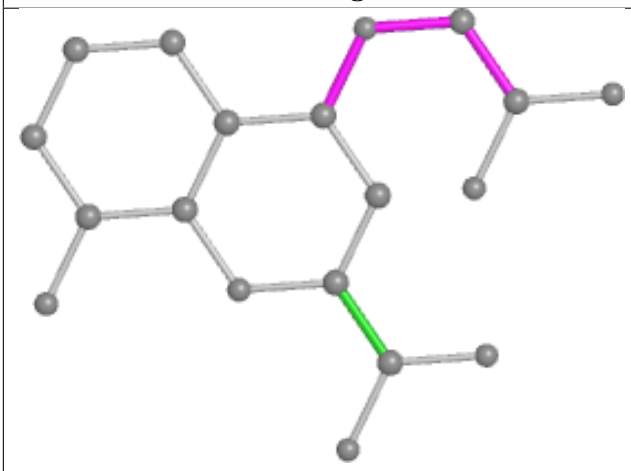
Ligand QVE A 305



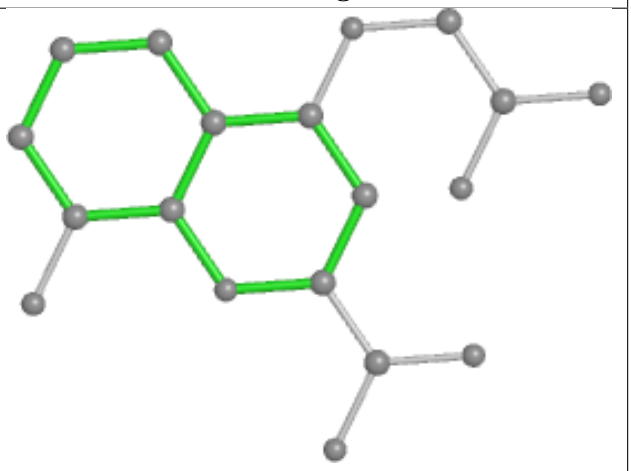
Bond lengths



Bond angles

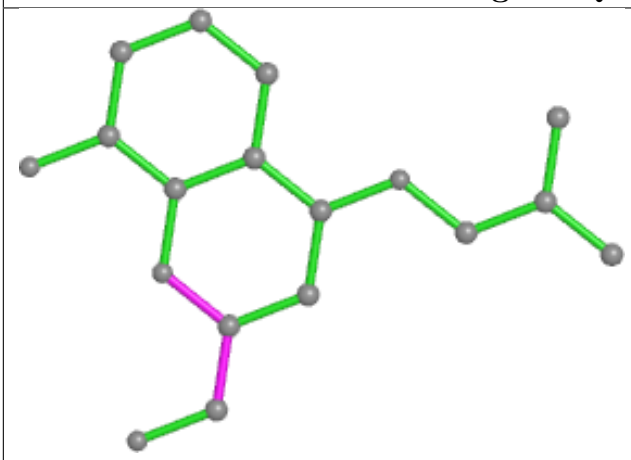


Torsions

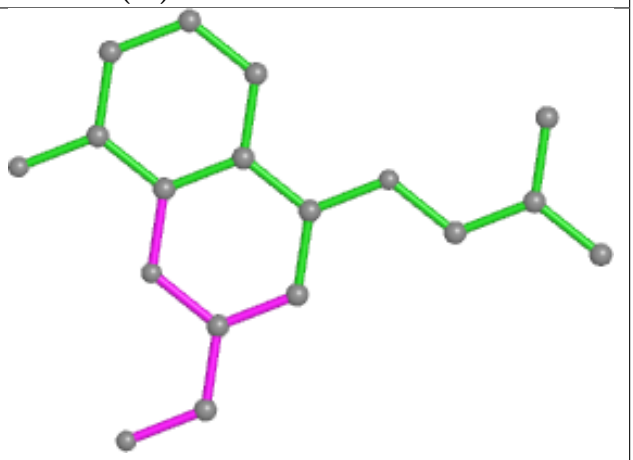


Rings

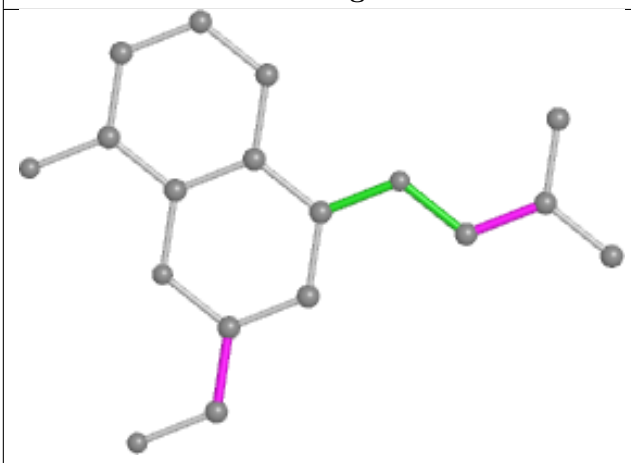
Ligand QUJ B 303 (A)



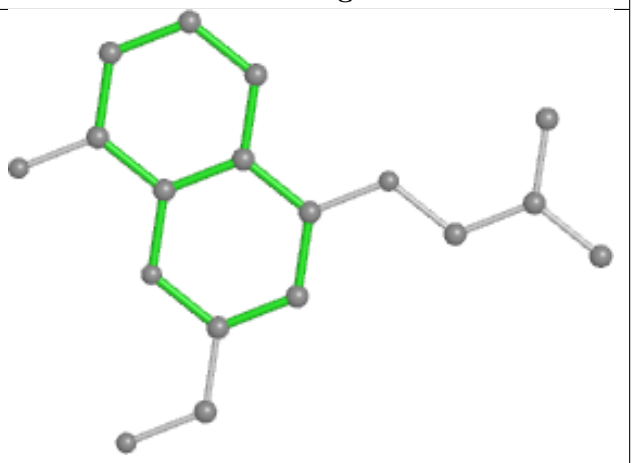
Bond lengths



Bond angles

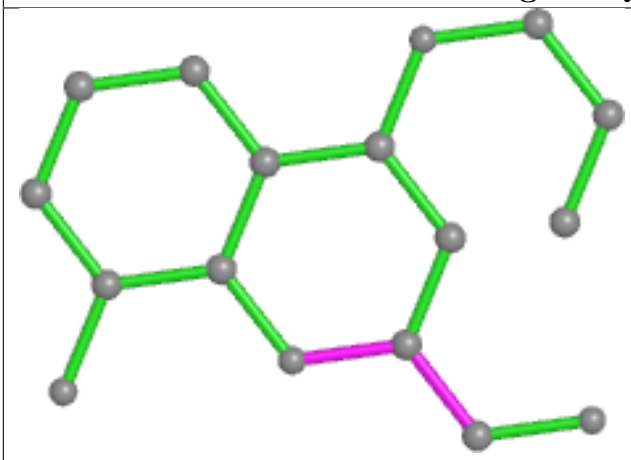


Torsions

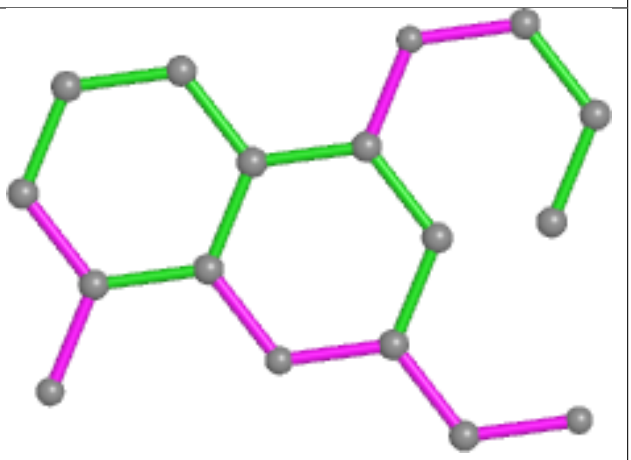


Rings

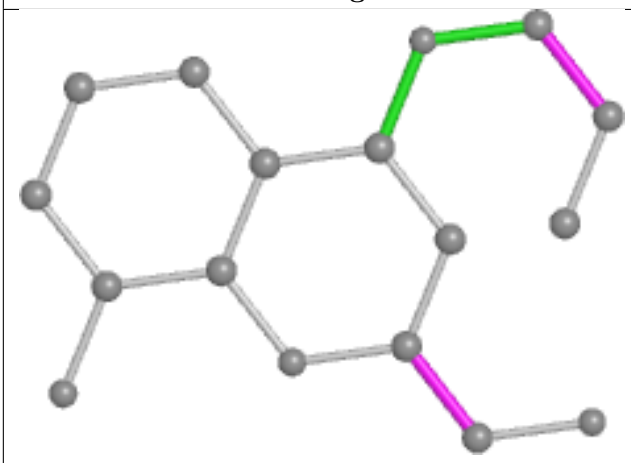
Ligand QUK A 303



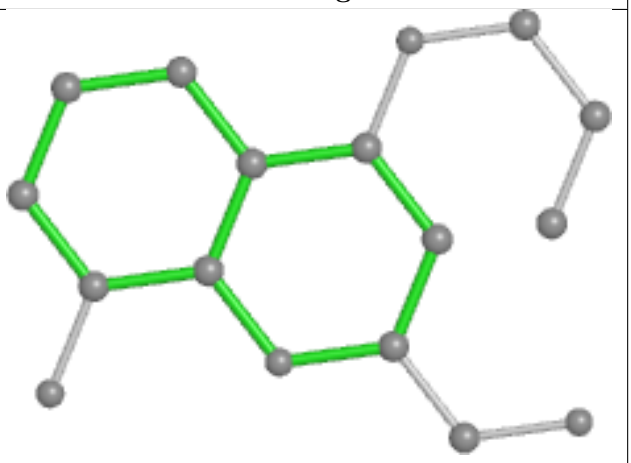
Bond lengths



Bond angles

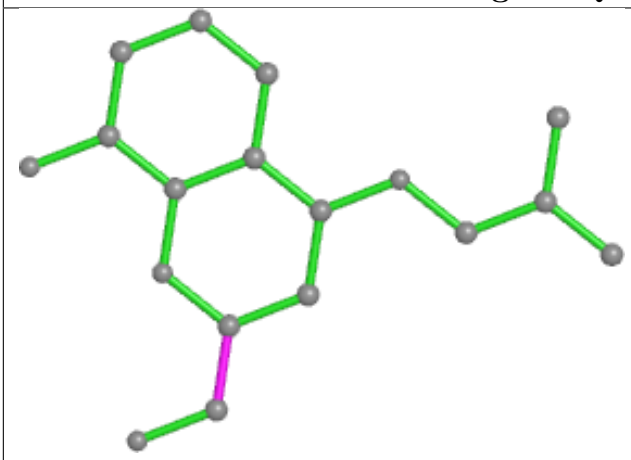


Torsions

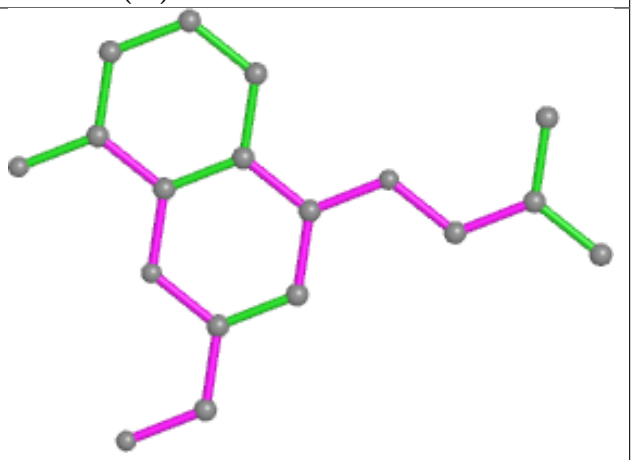


Rings

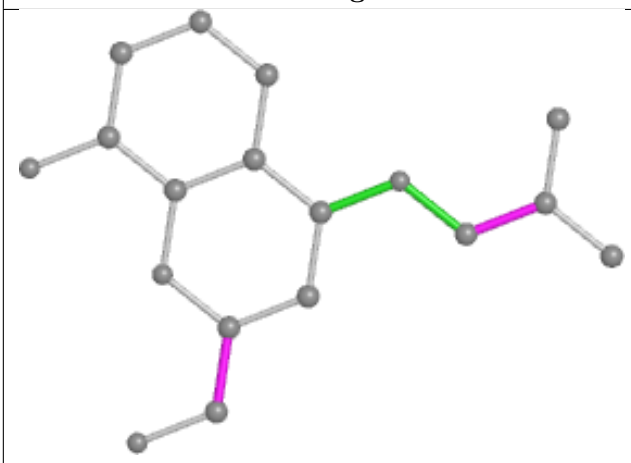
Ligand QUJ A 311 (B)



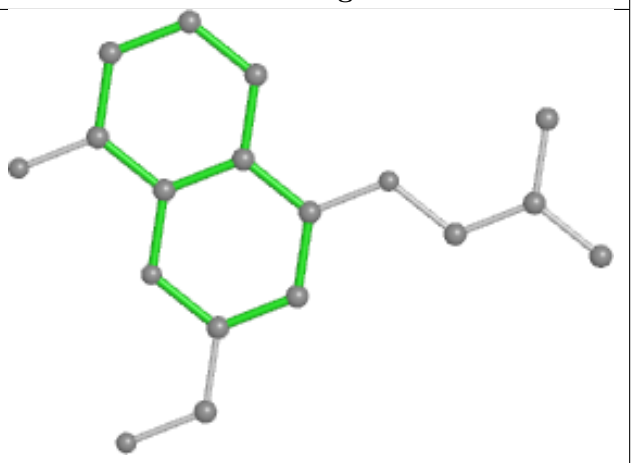
Bond lengths



Bond angles

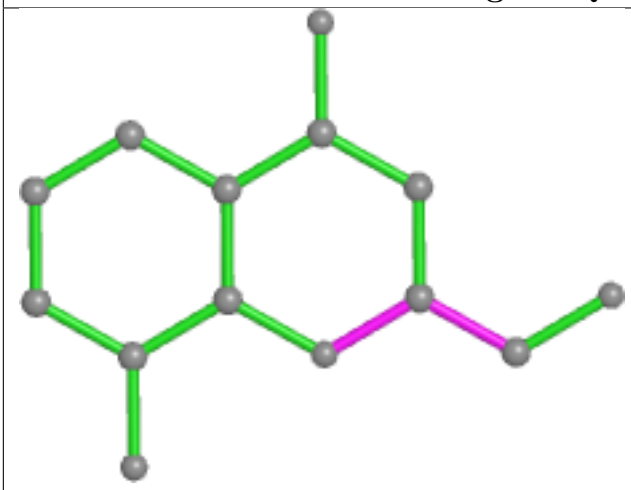


Torsions

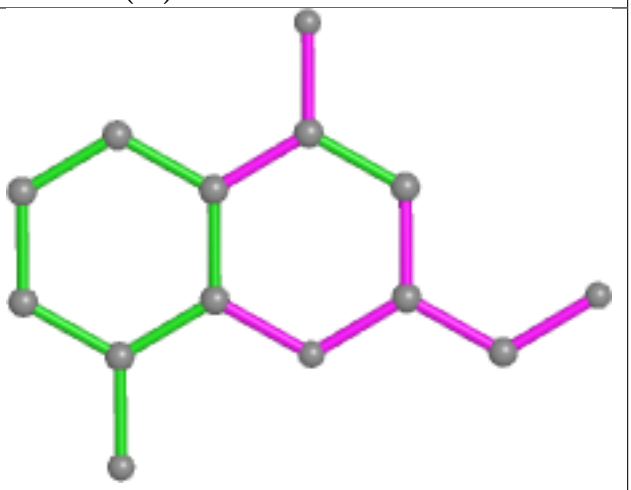


Rings

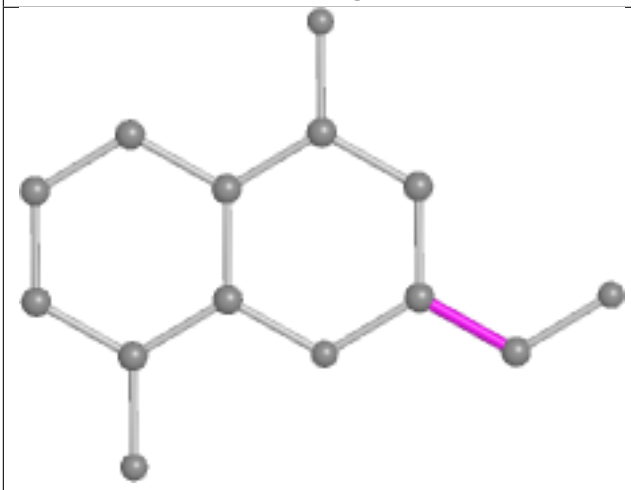
Ligand QUK A 306 (A)



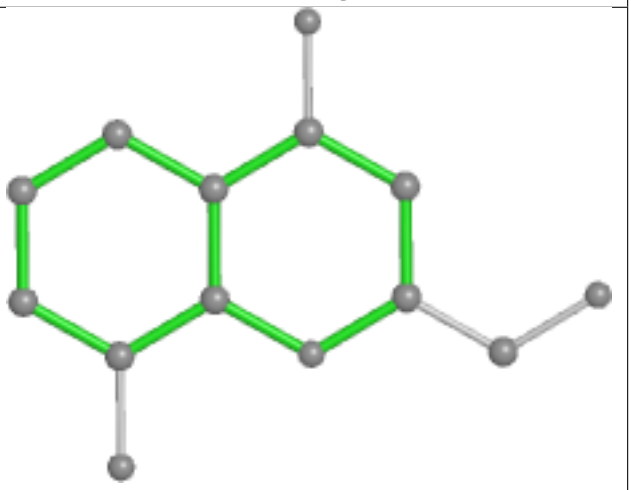
Bond lengths



Bond angles

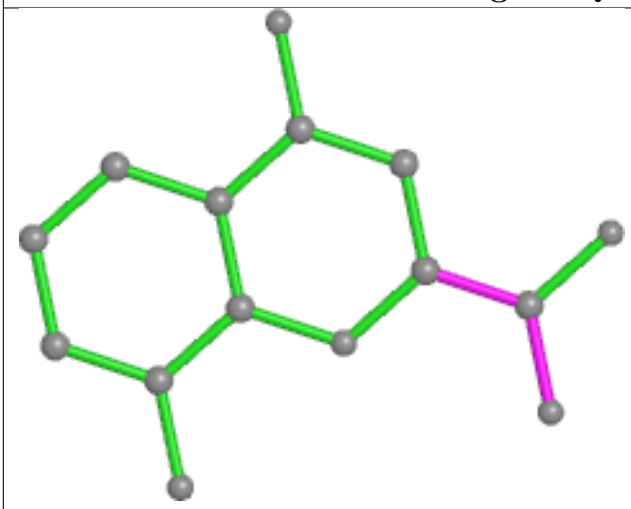


Torsions

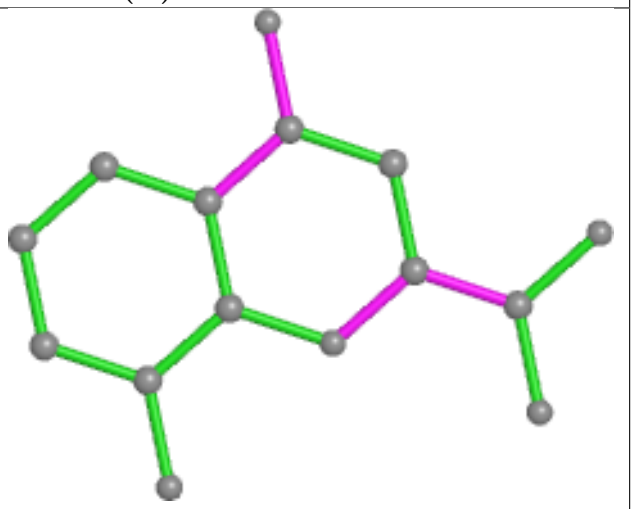


Rings

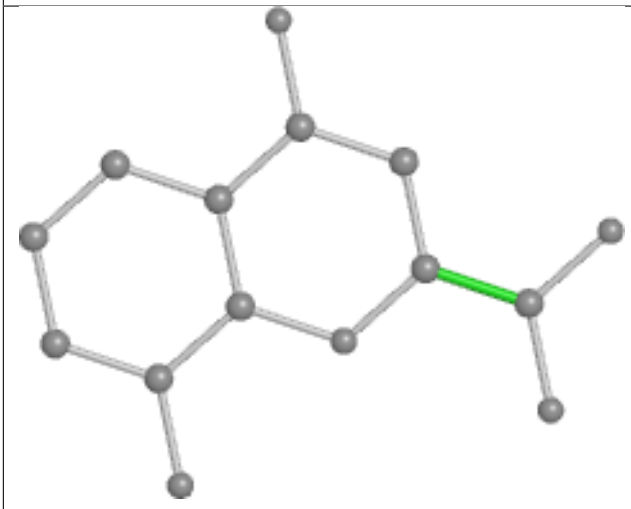
Ligand QVE B 311 (B)



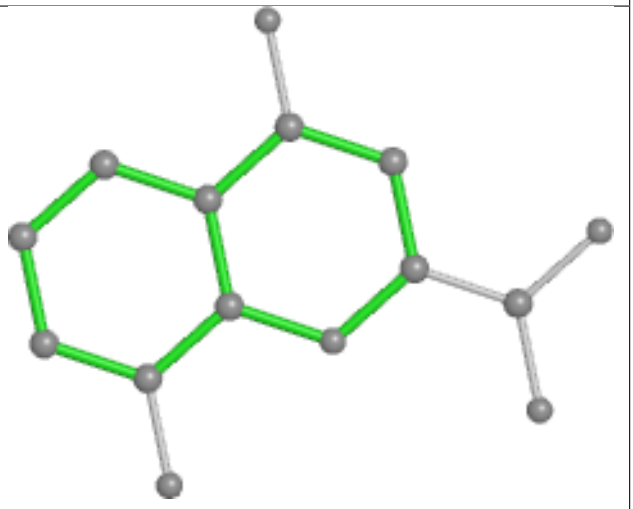
Bond lengths



Bond angles

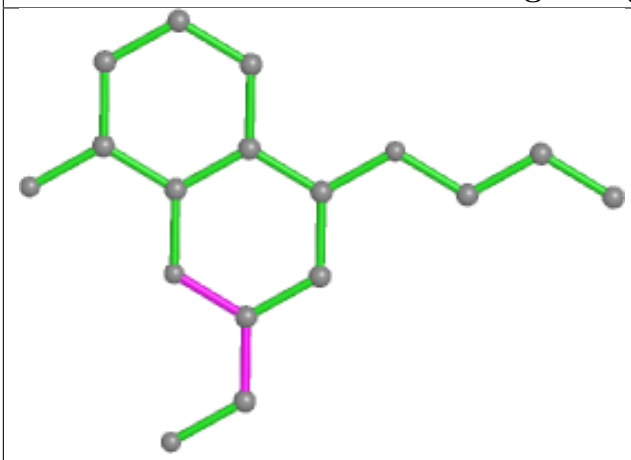


Torsions

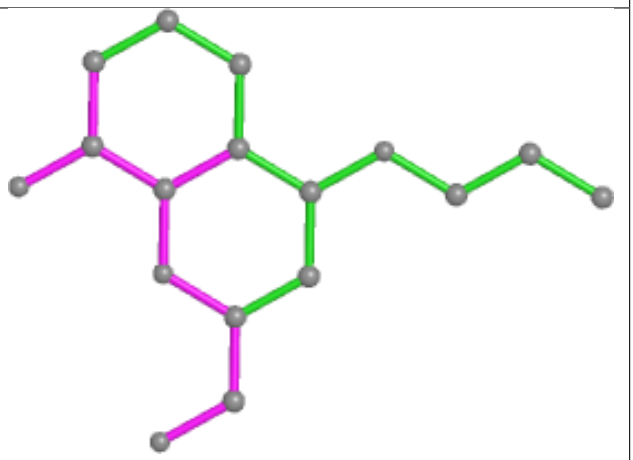


Rings

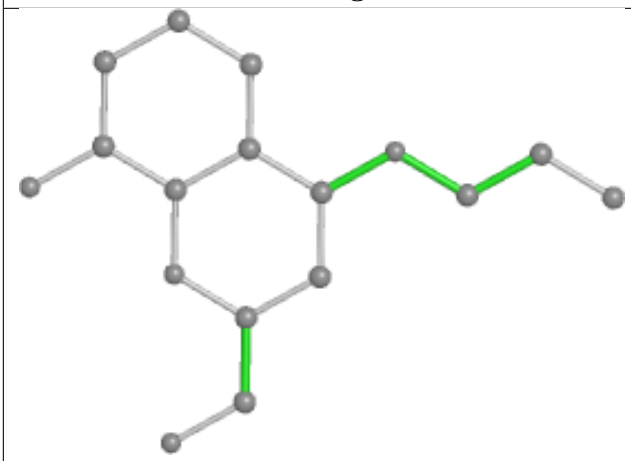
Ligand QUJ A 315



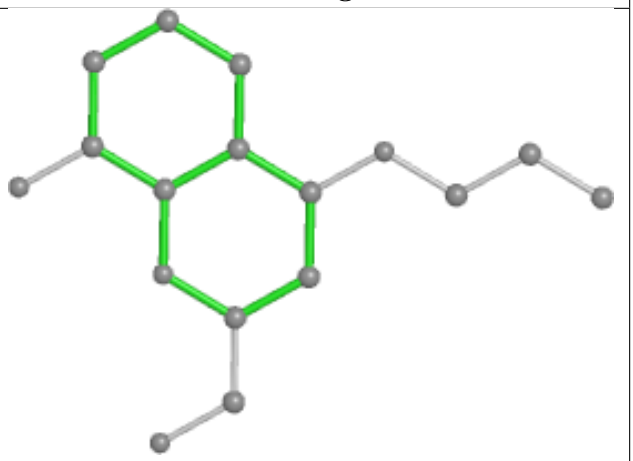
Bond lengths



Bond angles

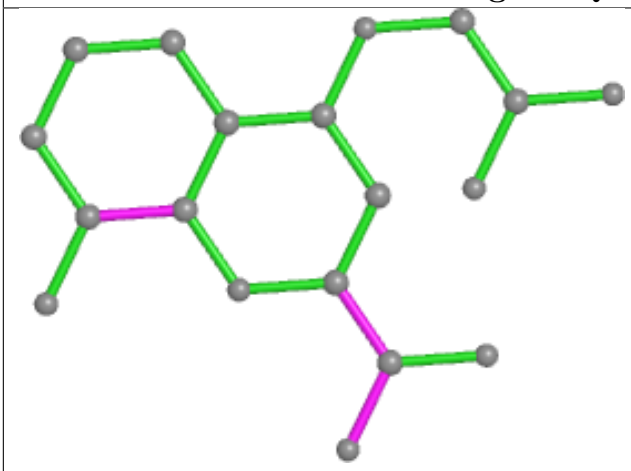


Torsions

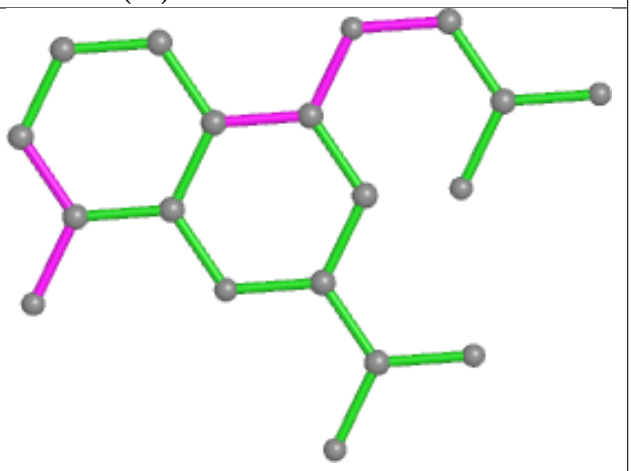


Rings

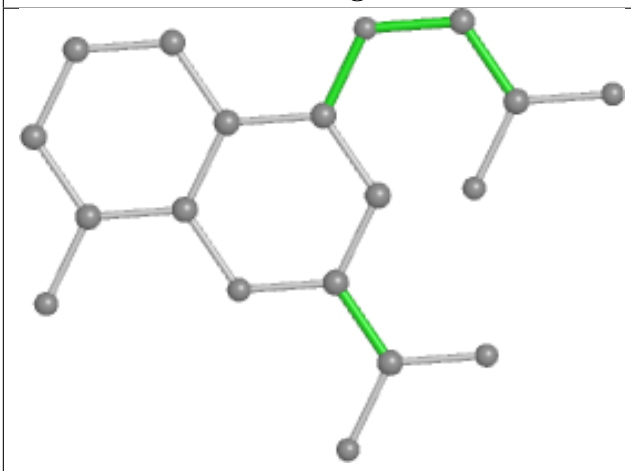
Ligand QVE A 307 (A)



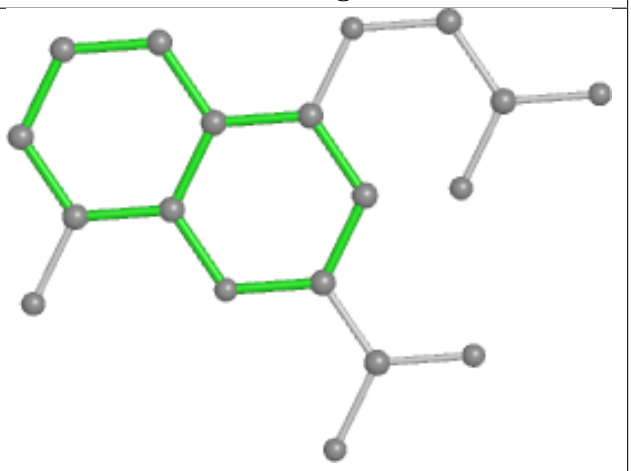
Bond lengths



Bond angles

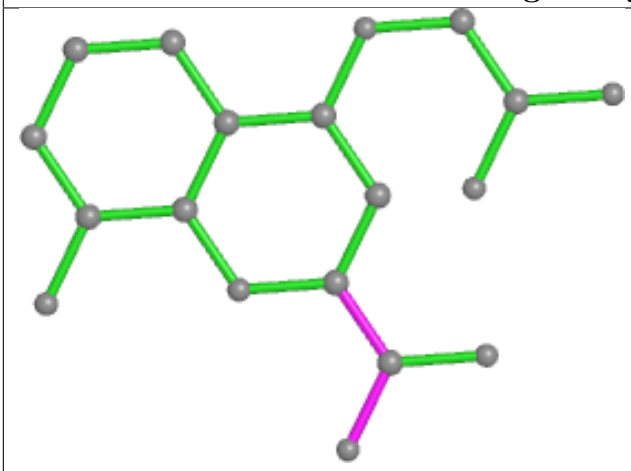


Torsions

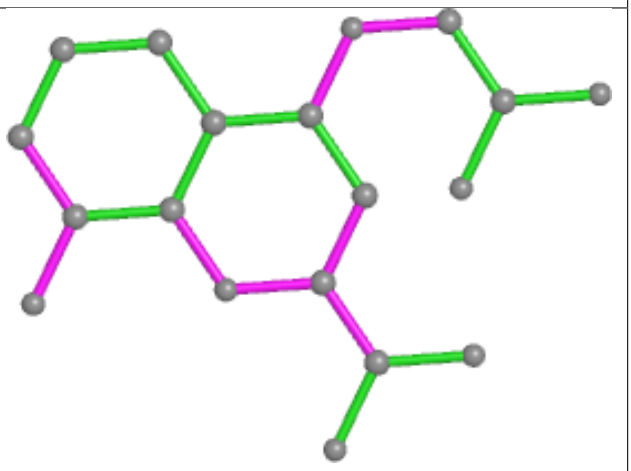


Rings

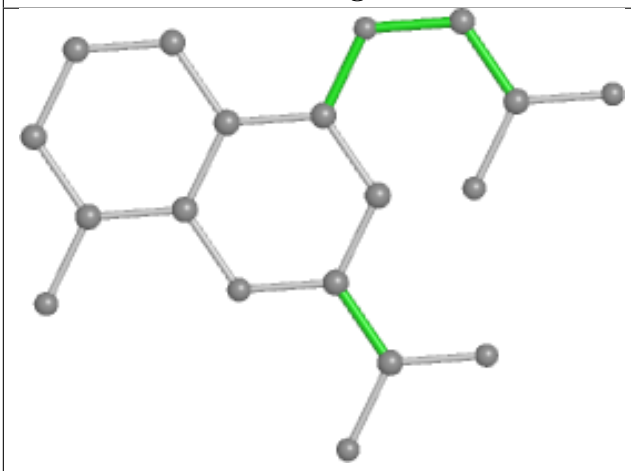
Ligand QVE B 309



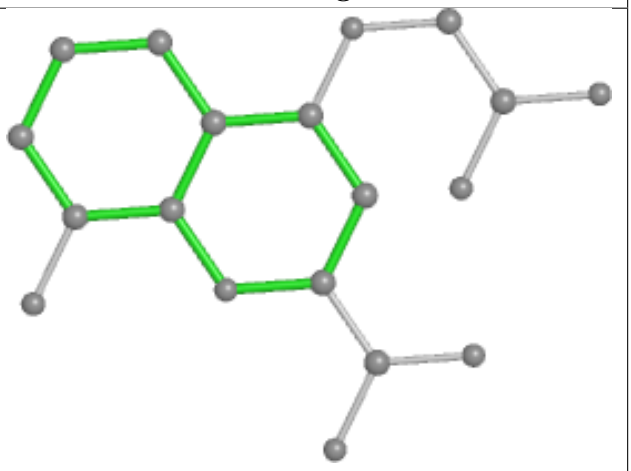
Bond lengths



Bond angles

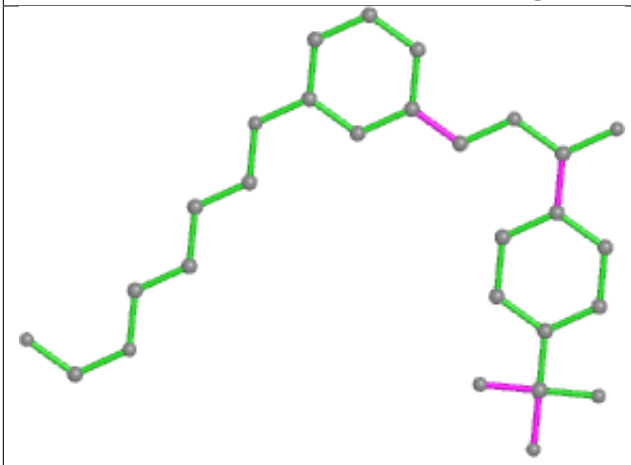


Torsions

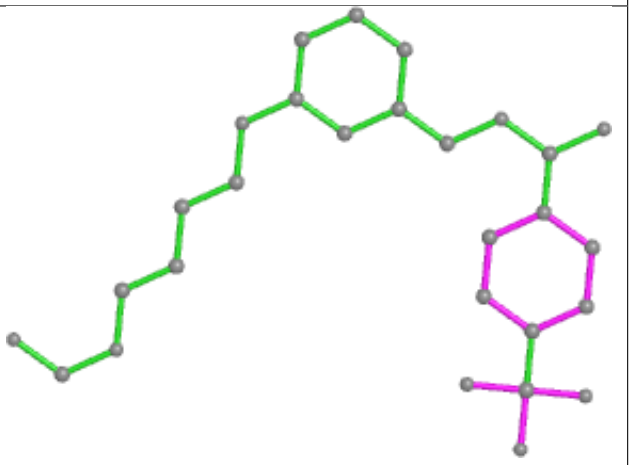


Rings

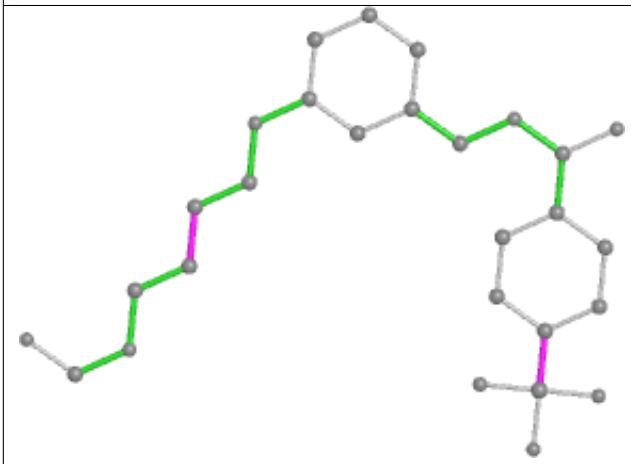
Ligand 6H0 A 302



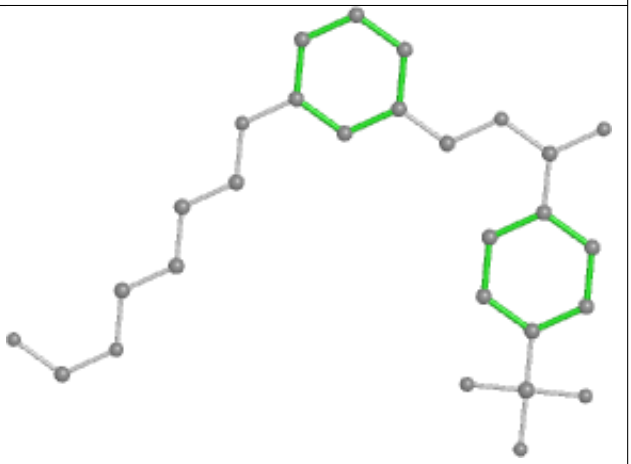
Bond lengths



Bond angles

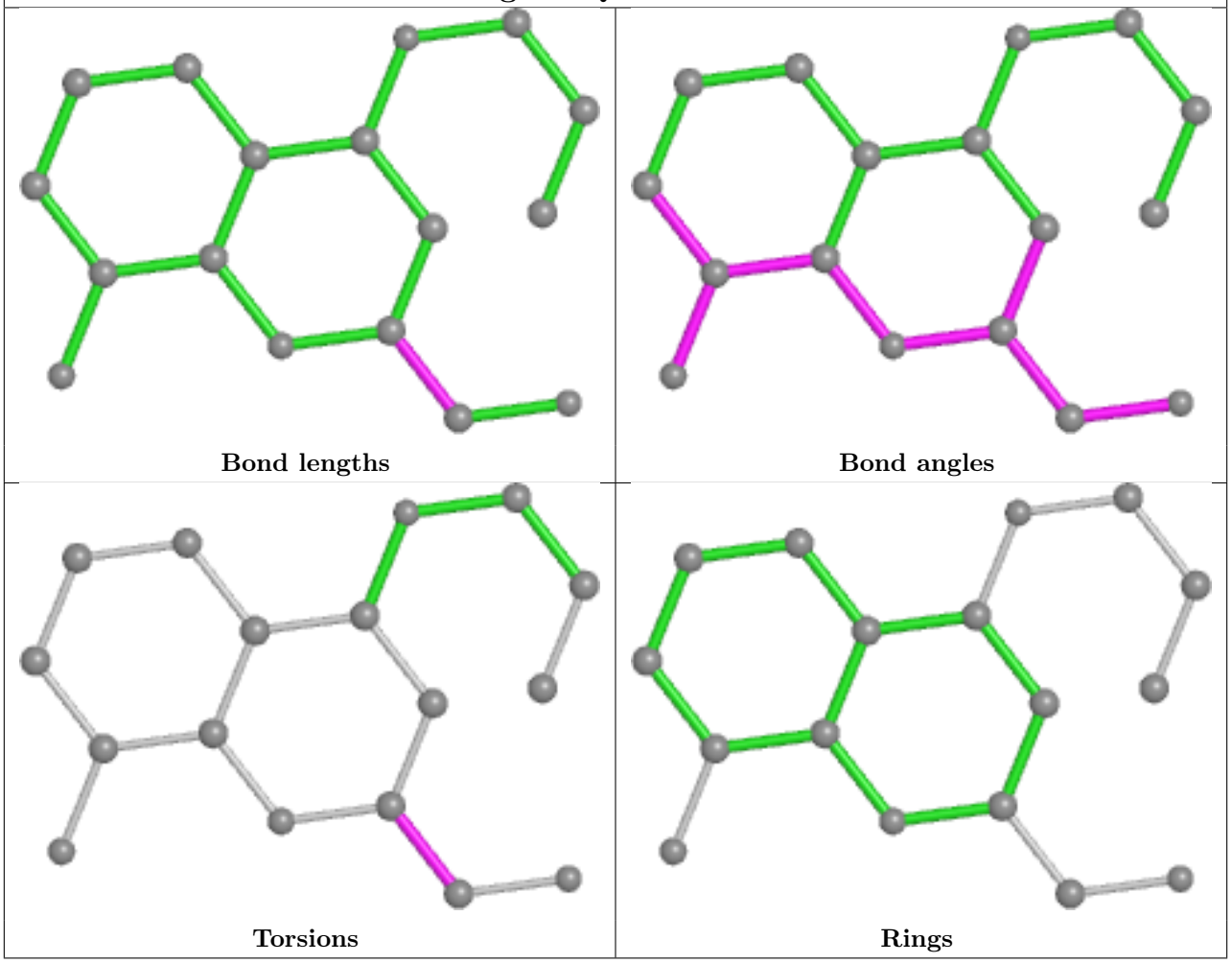


Torsions



Rings

Ligand QUK B 307



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, 95^{th} 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%)	-0.33	0 100 100	12, 20, 39, 64	0
1	B	259/260 (99%)	-0.25	3 (1%) 79 82	14, 24, 43, 76	0
All	All	518/520 (99%)	-0.29	3 (0%) 89 91	12, 22, 42, 76	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	HIS	3.4
1	B	234	GLY	3.0
1	B	236	PRO	2.1

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 monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
11	DMS	A	314	4/4	0.85	0.14	30,33,54,92	0
7	GOL	B	313	6/6	0.87	0.15	30,37,54,54	0

Continued on next page...

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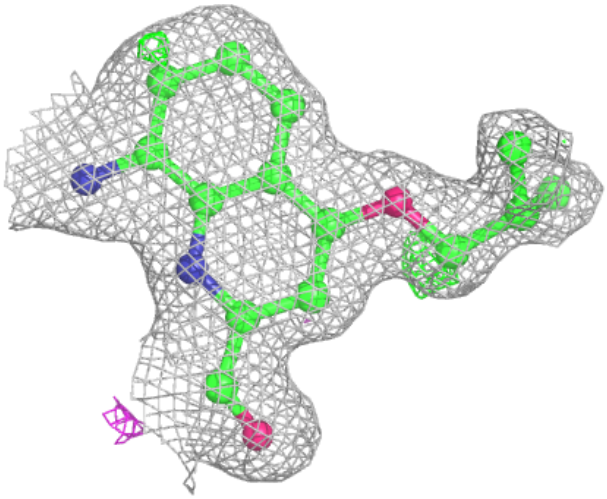
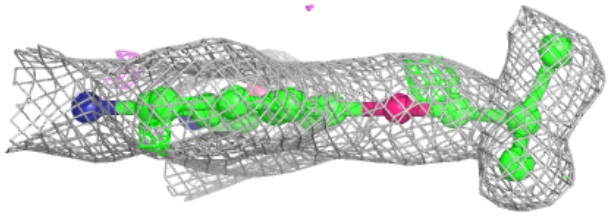
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PG4	B	302[A]	7/13	0.89	0.17	24,30,45,49	7
7	GOL	A	309	6/6	0.90	0.12	24,30,37,50	0
9	QUJ	B	303[A]	18/19	0.91	0.12	13,16,23,23	18
6	QVE	A	307[A]	19/19	0.92	0.10	10,17,30,31	19
4	QUK	A	306[A]	14/19	0.92	0.09	12,18,22,24	14
9	QUJ	A	311[B]	18/19	0.93	0.12	17,29,38,45	18
9	QUJ	A	315	17/19	0.93	0.10	19,23,40,41	0
6	QVE	A	305	19/19	0.93	0.09	22,28,62,79	0
7	GOL	B	312	6/6	0.93	0.12	25,30,31,42	0
10	NA	A	313	1/1	0.94	0.10	44,44,44,44	0
6	QVE	B	309	19/19	0.94	0.10	18,23,39,44	0
4	QUK	A	303	17/19	0.95	0.08	20,25,42,45	0
4	QUK	B	310[B]	14/19	0.95	0.10	22,34,43,51	14
8	PG4	A	310[B]	3/13	0.95	0.10	37,37,39,45	3
5	QVS	B	304[A]	14/15	0.96	0.07	12,18,23,26	14
4	QUK	B	307	17/19	0.96	0.07	20,23,36,40	0
9	QUJ	B	301	17/19	0.96	0.08	16,21,37,42	0
5	QVS	A	304	14/15	0.96	0.07	17,19,25,25	0
5	QVS	A	312[B]	14/15	0.96	0.14	20,36,46,48	14
6	QVE	B	311[B]	15/19	0.96	0.10	22,30,40,46	15
7	GOL	A	308	6/6	0.97	0.09	16,17,19,21	0
3	6H0	A	302	28/28	0.97	0.09	10,17,24,28	0
5	QVS	B	308	14/15	0.97	0.07	11,16,22,23	0
3	6H0	B	306	28/28	0.97	0.09	15,20,33,40	0
2	ZN	A	301	1/1	0.99	0.11	12,12,12,12	0
2	ZN	B	305	1/1	0.99	0.09	16,16,16,16	0

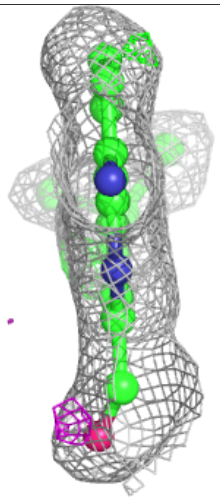
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around QUJ B 303 (A):

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

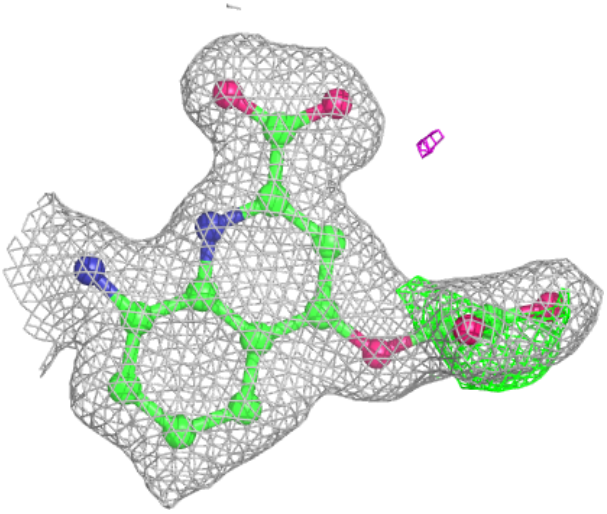


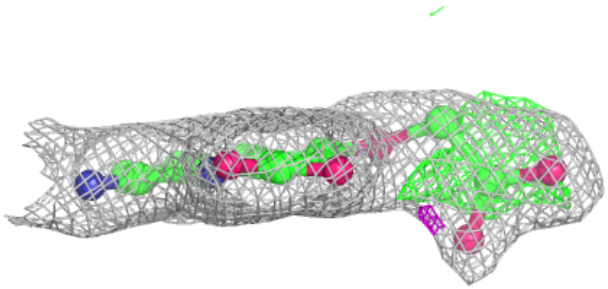


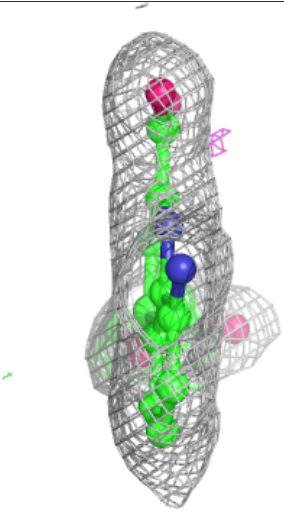


Electron density around QVE A 307 (A):

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

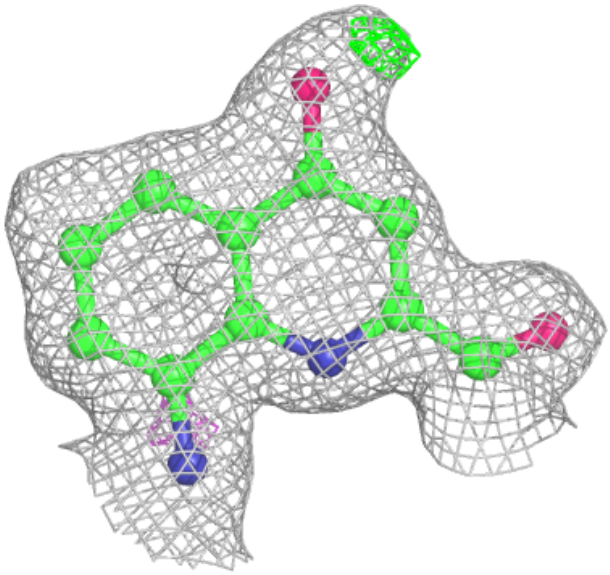


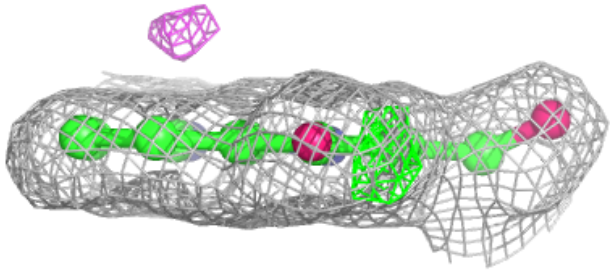


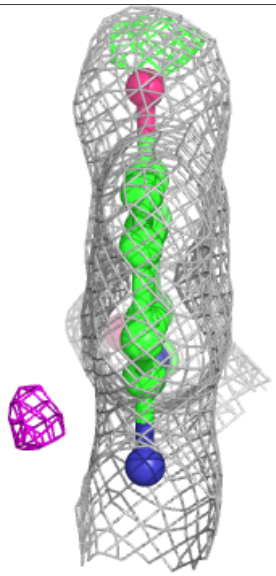


Electron density around QUK A 306 (A):

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

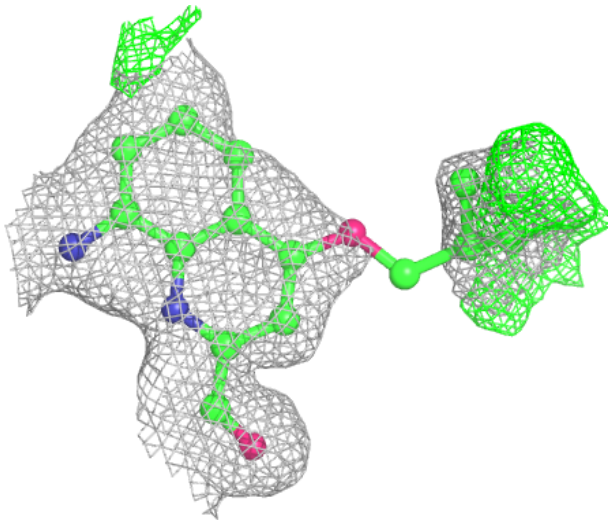


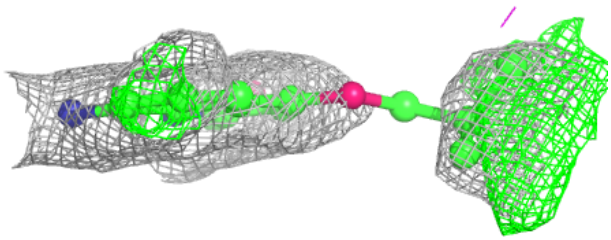


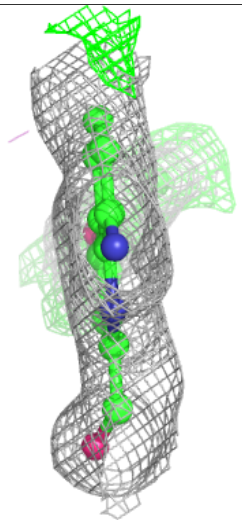


Electron density around QUJ A 311 (B):

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

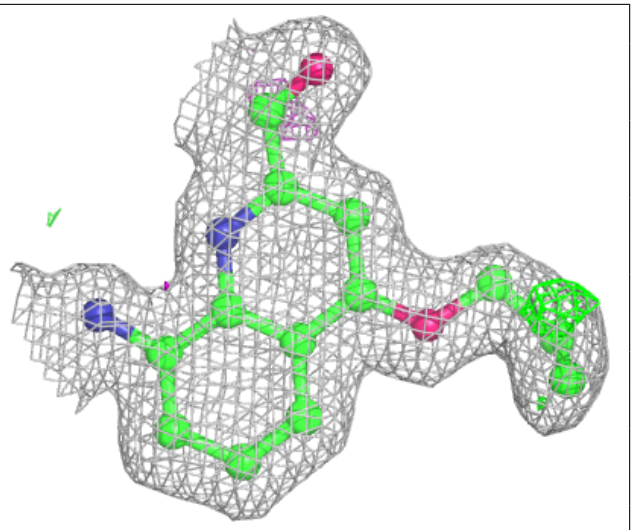


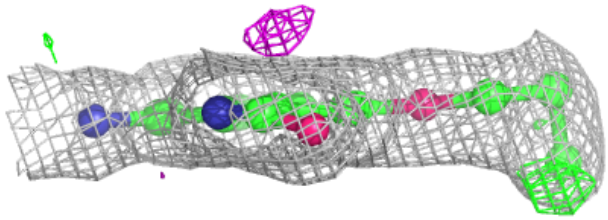


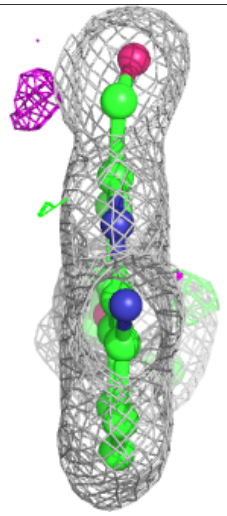


Electron density around QUJ A 315:

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

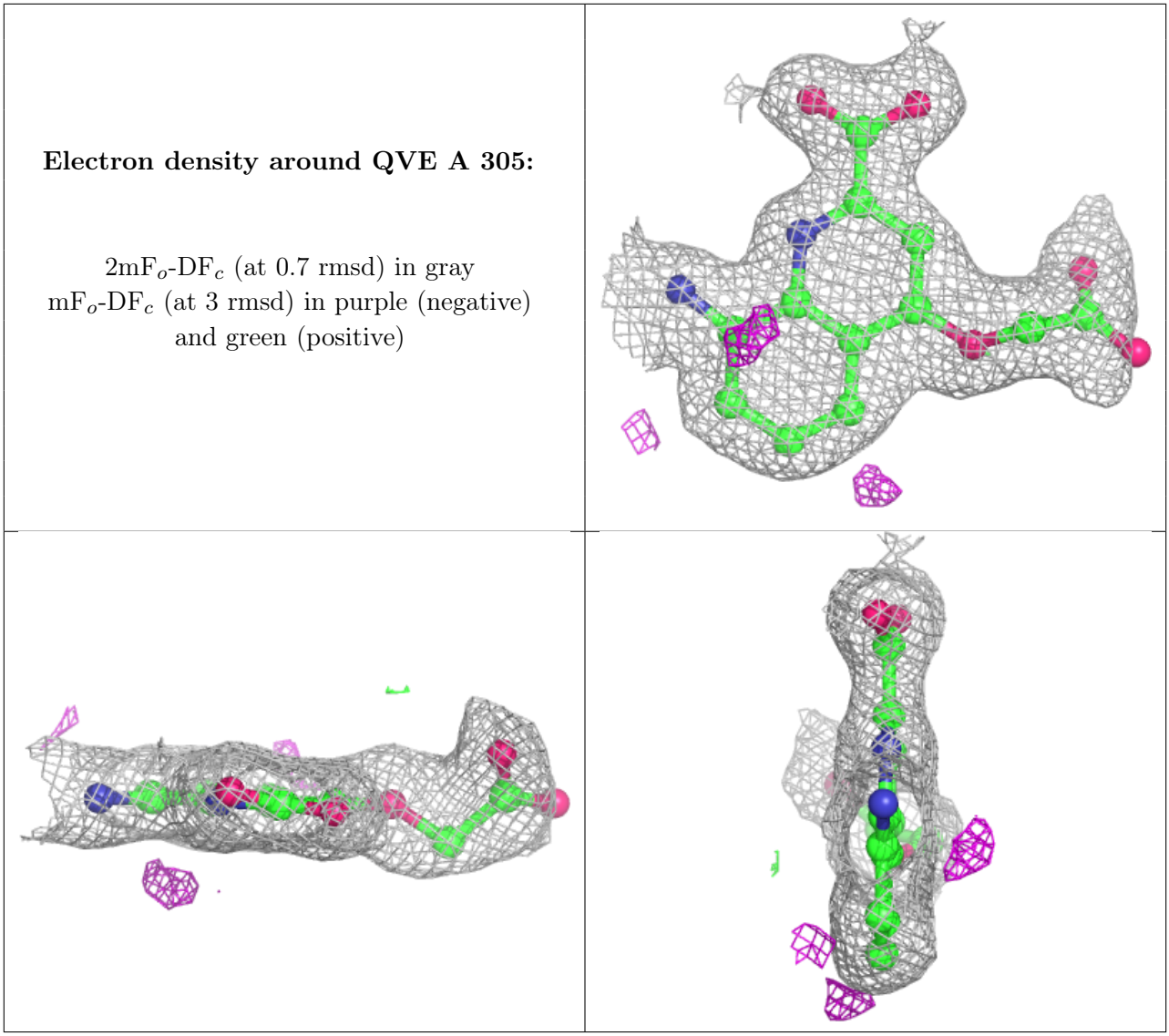






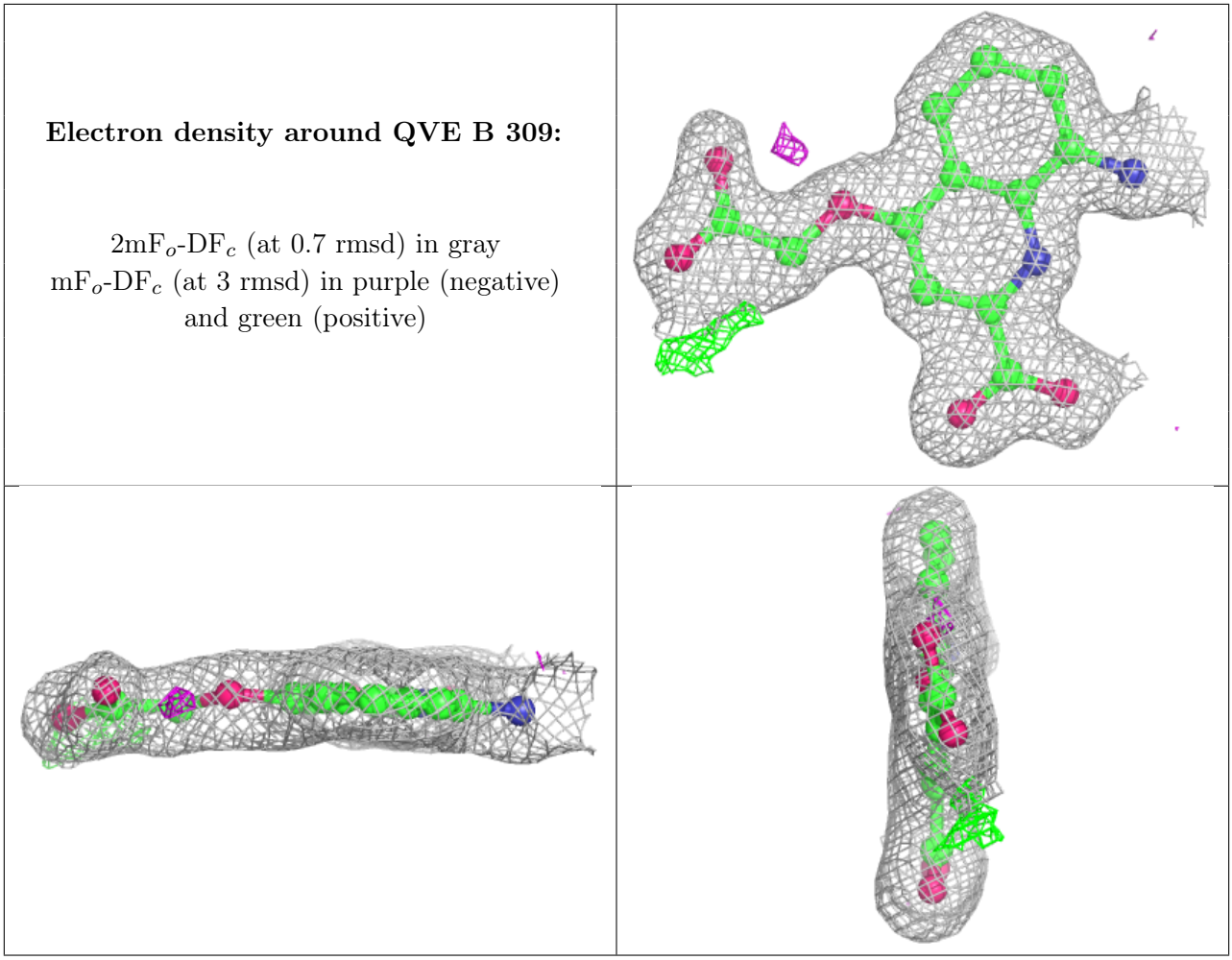
Electron density around QVE A 305:

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



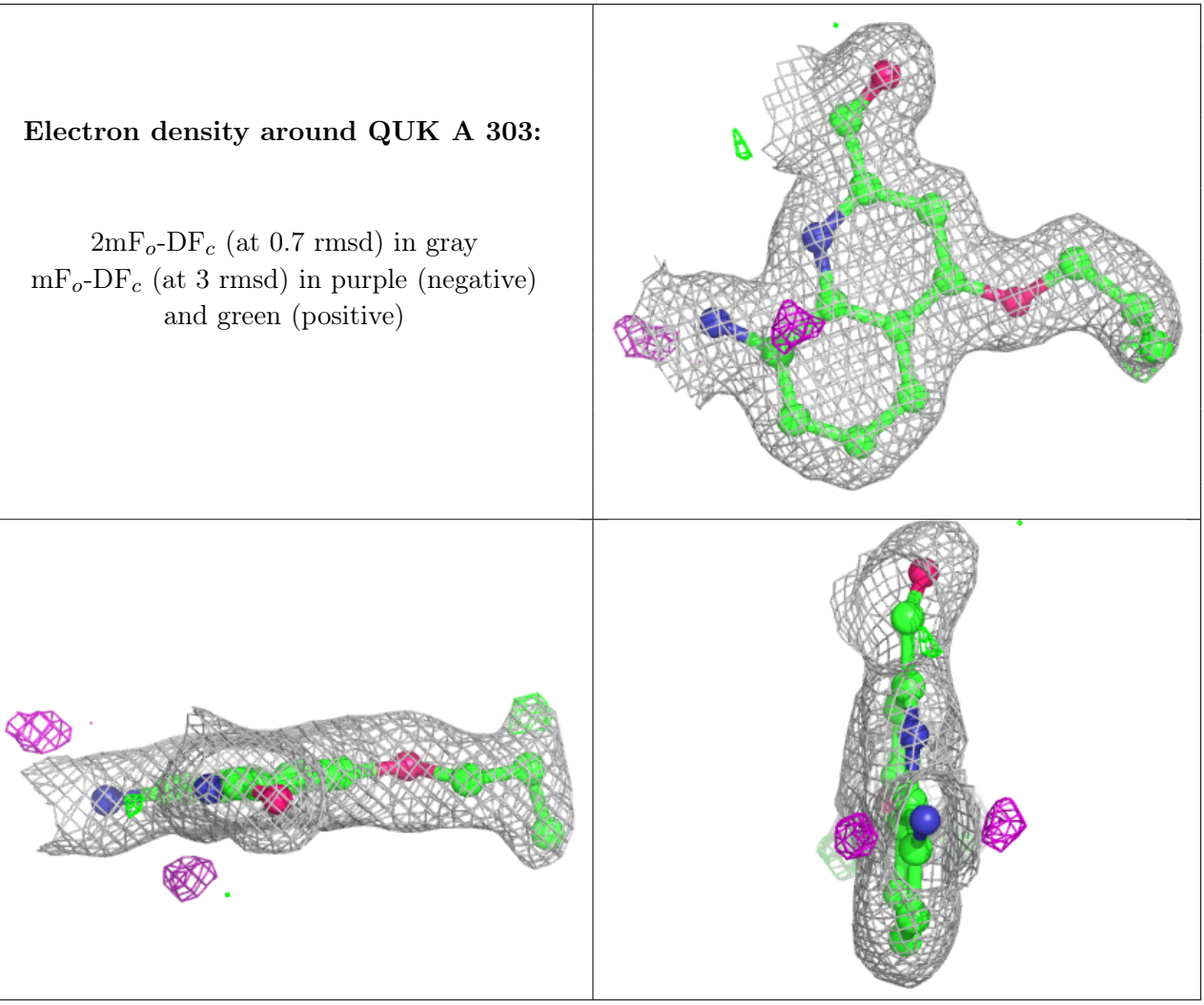
Electron density around QVE B 309:

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



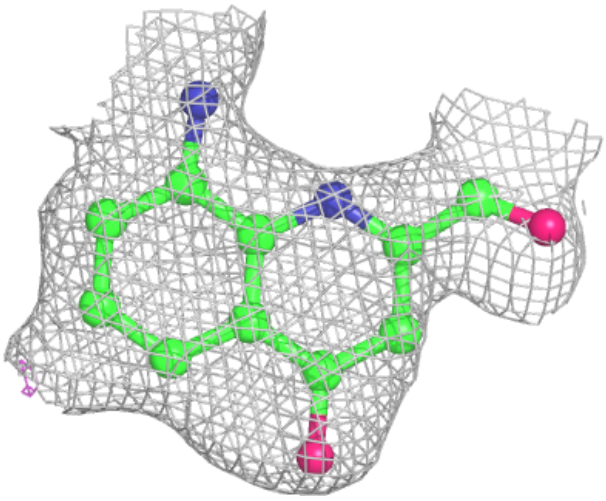
Electron density around QUK A 303:

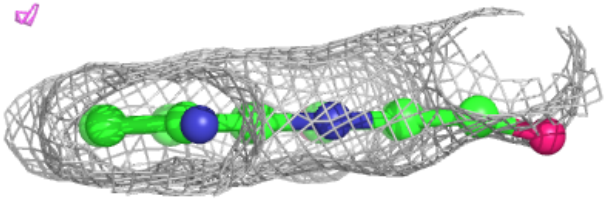
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

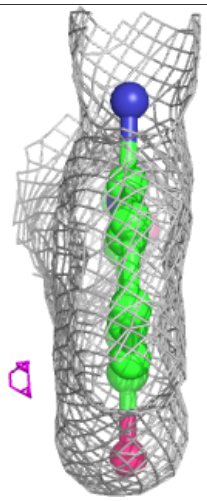


Electron density around QUK B 310 (B):

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

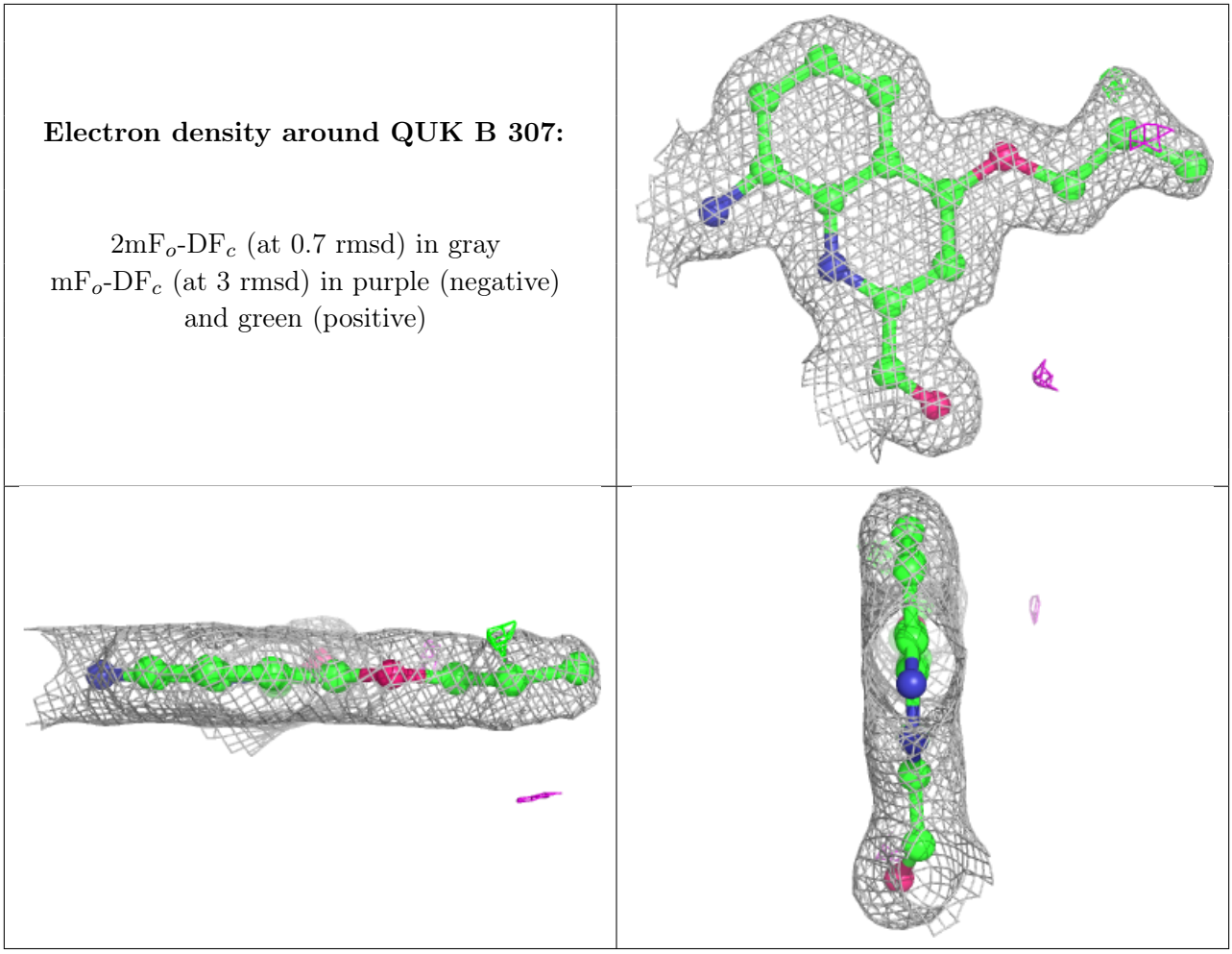






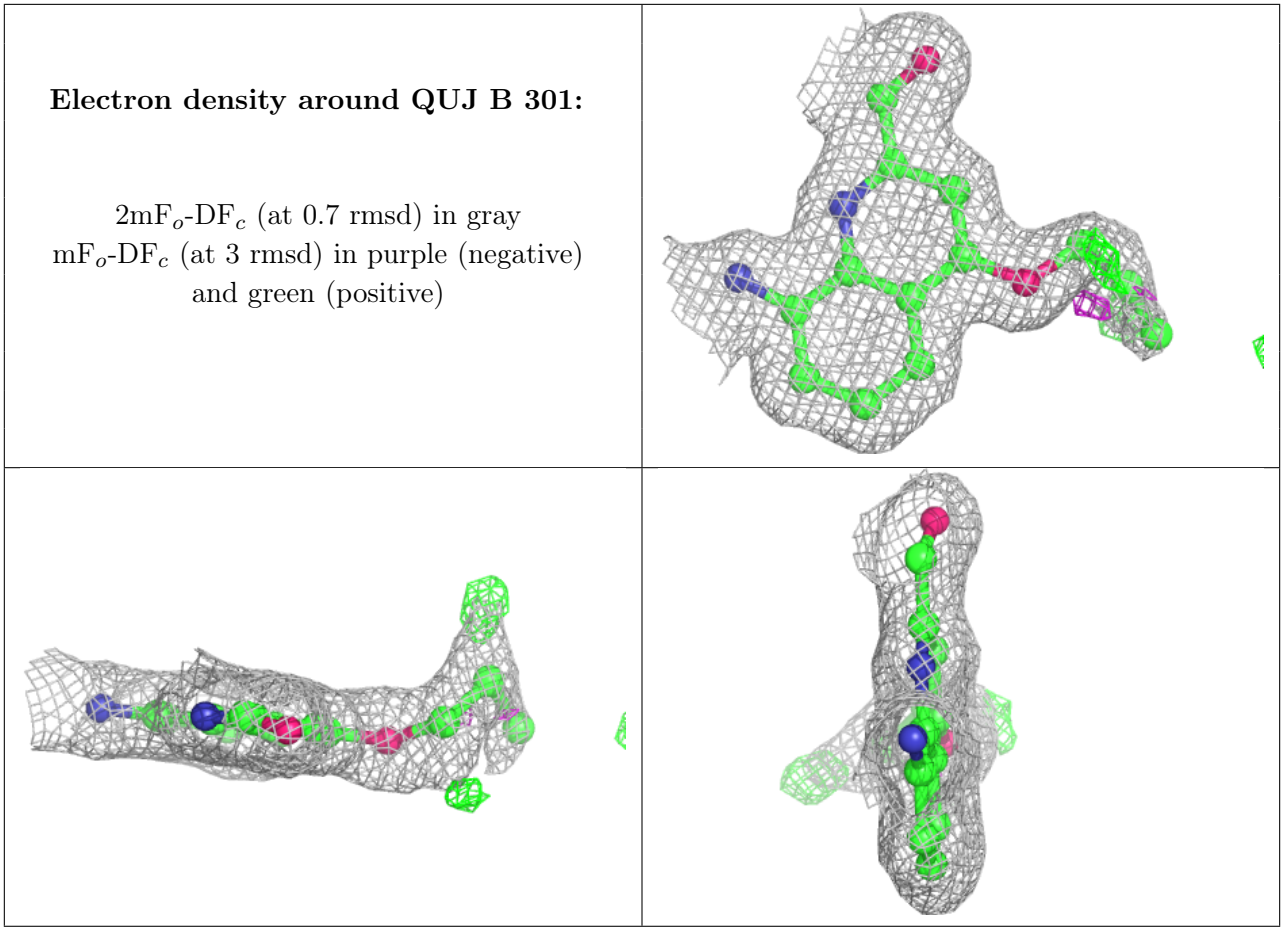
Electron density around QUK B 307:

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



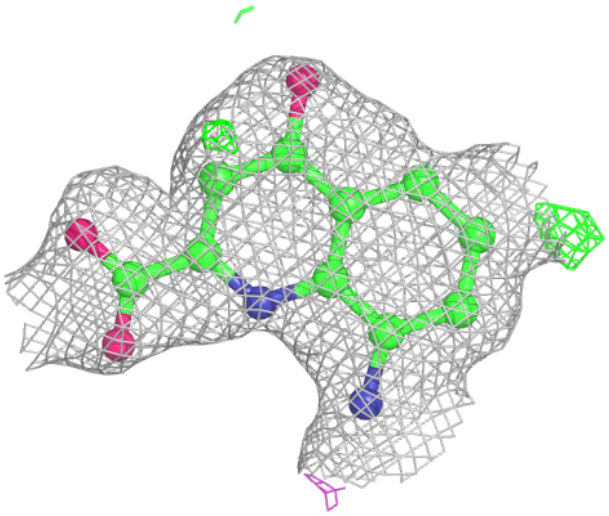
Electron density around QUJ B 301:

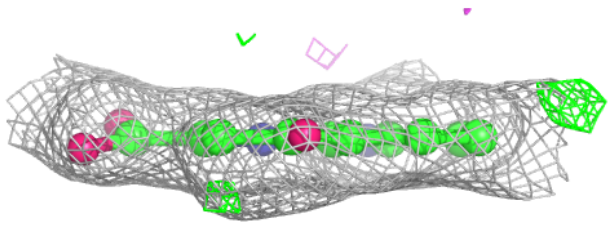
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

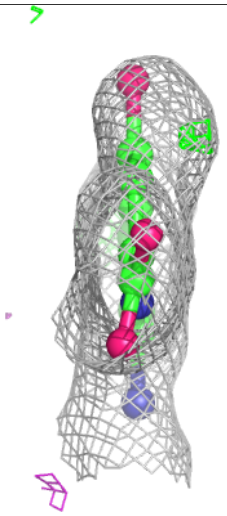


Electron density around QVE B 311 (B):

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

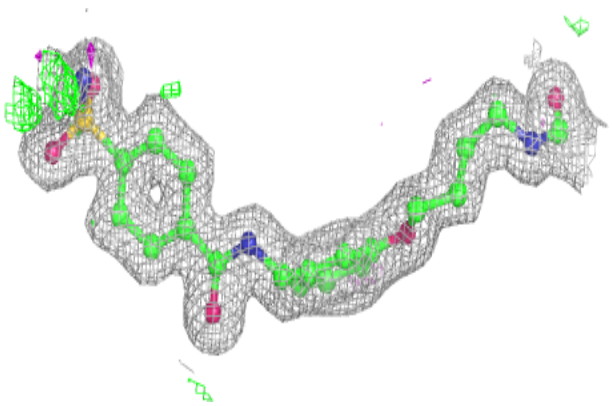


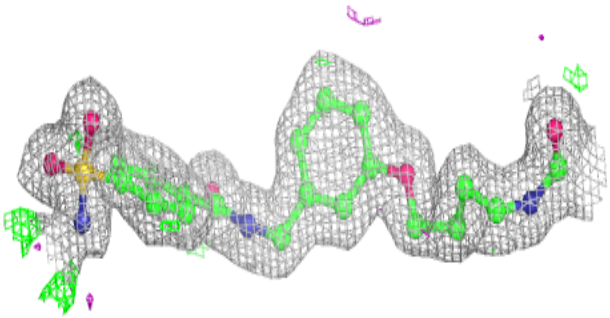




Electron density around 6H0 A 302:

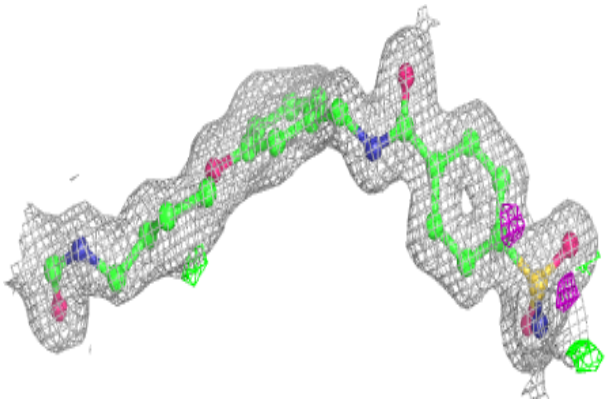
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

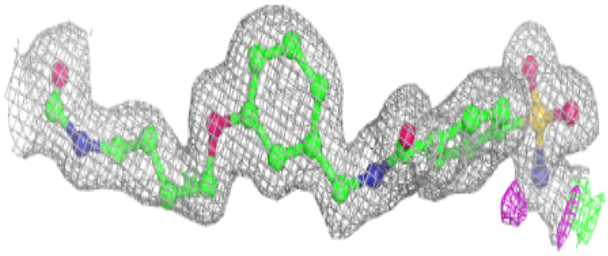


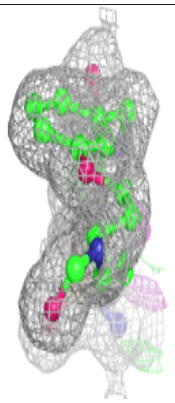


Electron density around 6H0 B 306:

$2mF_o$-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.