



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 26, 2020 – 02:11 PM EST

PDB ID : 6VGC  
Title : Crystal Structures of FLAP bound to DG-031  
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N.E.; Chandrasekhar, S.; Sloan, A.V.; Gooding, K.; Harvey, A.; Yu, X.P.;  
Kahl, S.D.; Norman, B.H.  
Deposited on : 2020-01-07  
Resolution : 2.37 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
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) : 2.14.6

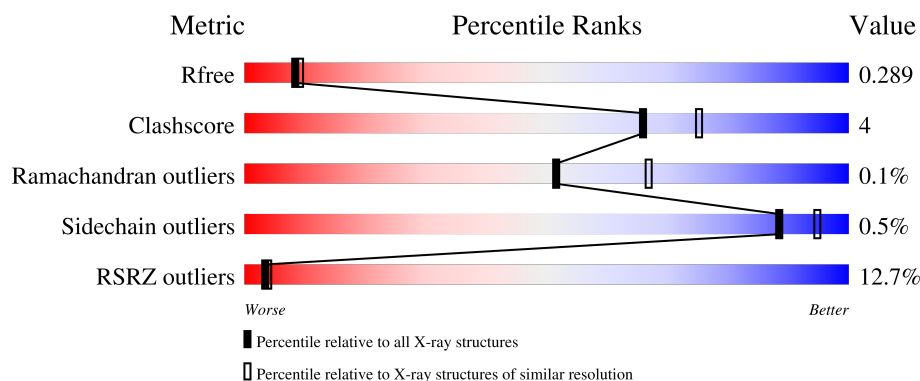
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	171	
1	B	171	
1	C	171	
1	D	171	
1	E	171	

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Mol	Chain	Length	Quality of chain
1	F	171	<div><div></div><div></div><div></div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7340 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 5-lipoxygenase-activating protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1134	757	175	198	4			
1	B	149	Total	C	N	O	S	0	0	0
			1174	782	184	204	4			
1	C	151	Total	C	N	O	S	0	0	0
			1191	796	183	208	4			
1	D	155	Total	C	N	O	S	0	0	0
			1221	815	187	215	4			
1	E	154	Total	C	N	O	S	0	0	0
			1225	815	194	212	4			
1	F	148	Total	C	N	O	S	0	0	0
			1152	772	174	202	4			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P20292
A	0	SER	-	expression tag	UNP P20292
A	1	LEU	-	expression tag	UNP P20292
A	148	ALA	LYS	conflict	UNP P20292
A	162	GLU	-	expression tag	UNP P20292
A	163	GLY	-	expression tag	UNP P20292
A	164	HIS	-	expression tag	UNP P20292
A	165	HIS	-	expression tag	UNP P20292
A	166	HIS	-	expression tag	UNP P20292
A	167	HIS	-	expression tag	UNP P20292
A	168	HIS	-	expression tag	UNP P20292
A	169	HIS	-	expression tag	UNP P20292
B	-1	MET	-	initiating methionine	UNP P20292
B	0	SER	-	expression tag	UNP P20292
B	1	LEU	-	expression tag	UNP P20292
B	148	ALA	LYS	conflict	UNP P20292
B	162	GLU	-	expression tag	UNP P20292

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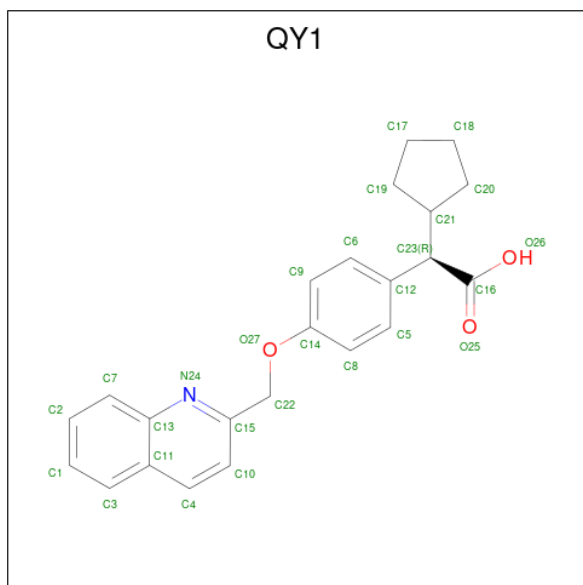
Chain	Residue	Modelled	Actual	Comment	Reference
B	163	GLY	-	expression tag	UNP P20292
B	164	HIS	-	expression tag	UNP P20292
B	165	HIS	-	expression tag	UNP P20292
B	166	HIS	-	expression tag	UNP P20292
B	167	HIS	-	expression tag	UNP P20292
B	168	HIS	-	expression tag	UNP P20292
B	169	HIS	-	expression tag	UNP P20292
C	-1	MET	-	initiating methionine	UNP P20292
C	0	SER	-	expression tag	UNP P20292
C	1	LEU	-	expression tag	UNP P20292
C	148	ALA	LYS	conflict	UNP P20292
C	162	GLU	-	expression tag	UNP P20292
C	163	GLY	-	expression tag	UNP P20292
C	164	HIS	-	expression tag	UNP P20292
C	165	HIS	-	expression tag	UNP P20292
C	166	HIS	-	expression tag	UNP P20292
C	167	HIS	-	expression tag	UNP P20292
C	168	HIS	-	expression tag	UNP P20292
C	169	HIS	-	expression tag	UNP P20292
D	-1	MET	-	initiating methionine	UNP P20292
D	0	SER	-	expression tag	UNP P20292
D	1	LEU	-	expression tag	UNP P20292
D	148	ALA	LYS	conflict	UNP P20292
D	162	GLU	-	expression tag	UNP P20292
D	163	GLY	-	expression tag	UNP P20292
D	164	HIS	-	expression tag	UNP P20292
D	165	HIS	-	expression tag	UNP P20292
D	166	HIS	-	expression tag	UNP P20292
D	167	HIS	-	expression tag	UNP P20292
D	168	HIS	-	expression tag	UNP P20292
D	169	HIS	-	expression tag	UNP P20292
E	-1	MET	-	initiating methionine	UNP P20292
E	0	SER	-	expression tag	UNP P20292
E	1	LEU	-	expression tag	UNP P20292
E	148	ALA	LYS	conflict	UNP P20292
E	162	GLU	-	expression tag	UNP P20292
E	163	GLY	-	expression tag	UNP P20292
E	164	HIS	-	expression tag	UNP P20292
E	165	HIS	-	expression tag	UNP P20292
E	166	HIS	-	expression tag	UNP P20292
E	167	HIS	-	expression tag	UNP P20292
E	168	HIS	-	expression tag	UNP P20292

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Chain	Residue	Modelled	Actual	Comment	Reference
E	169	HIS	-	expression tag	UNP P20292
F	-1	MET	-	initiating methionine	UNP P20292
F	0	SER	-	expression tag	UNP P20292
F	1	LEU	-	expression tag	UNP P20292
F	148	ALA	LYS	conflict	UNP P20292
F	162	GLU	-	expression tag	UNP P20292
F	163	GLY	-	expression tag	UNP P20292
F	164	HIS	-	expression tag	UNP P20292
F	165	HIS	-	expression tag	UNP P20292
F	166	HIS	-	expression tag	UNP P20292
F	167	HIS	-	expression tag	UNP P20292
F	168	HIS	-	expression tag	UNP P20292
F	169	HIS	-	expression tag	UNP P20292

- Molecule 2 is (2R)-cyclopentyl{4-[(quinolin-2-yl)methoxy]phenyl}acetic acid (three-letter code: QY1) (formula: C<sub>23</sub>H<sub>23</sub>NO<sub>3</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	23	1	3		
2	B	1	Total	C	N	O	0	0
			27	23	1	3		
2	C	1	Total	C	N	O	0	0
			27	23	1	3		
2	D	1	Total	C	N	O	0	0
			27	23	1	3		

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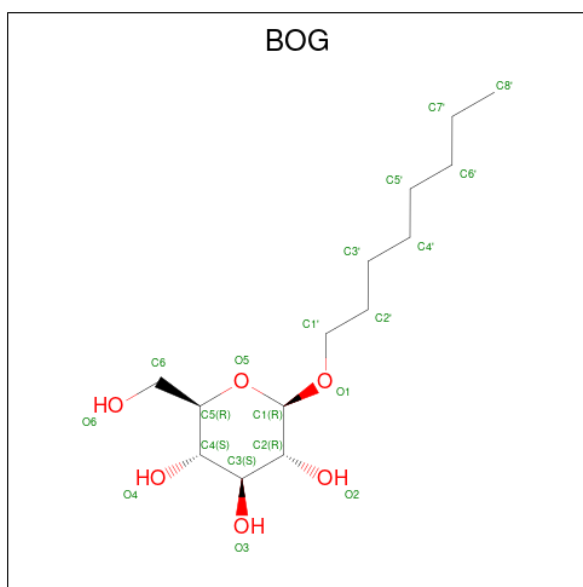
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			27	23	1	3		
2	F	1	Total	C	N	O	0	0
			27	23	1	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	14	Total	O	0	0
			14	14		

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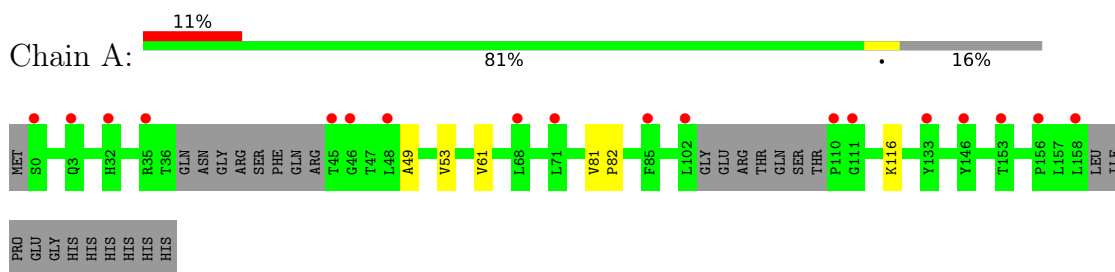
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	10	Total 10	O 10	0	0
5	D	8	Total 8	O 8	0	0
5	E	7	Total 7	O 7	0	0
5	F	9	Total 9	O 9	0	0



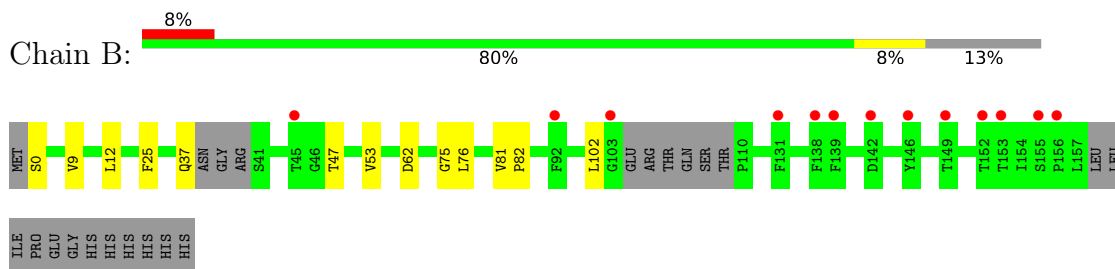
### 3 Residue-property plots [i](#)

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.

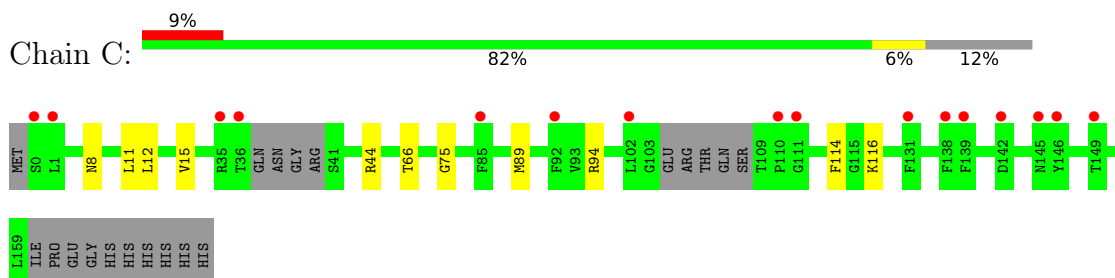
- Molecule 1: 5-lipoxygenase-activating protein



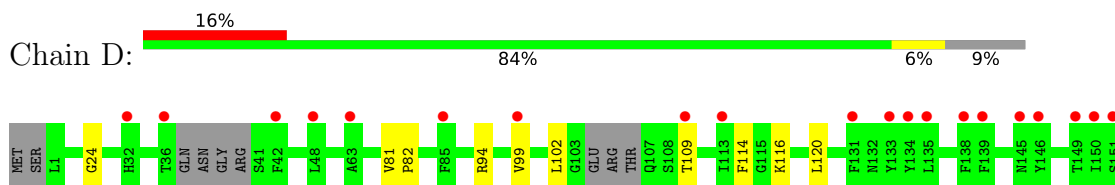
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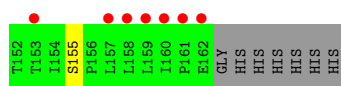


- Molecule 1: 5-lipoxygenase-activating protein

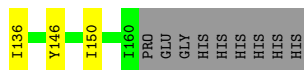
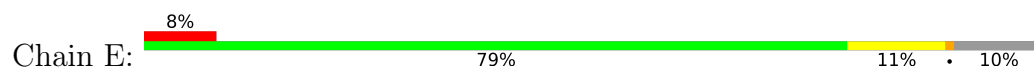


- Molecule 1: 5-lipoxygenase-activating protein

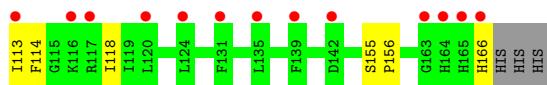
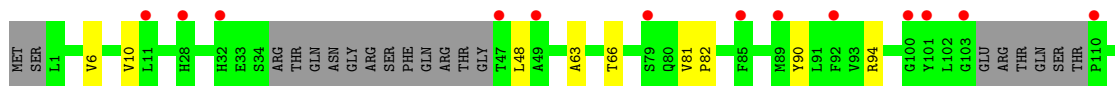
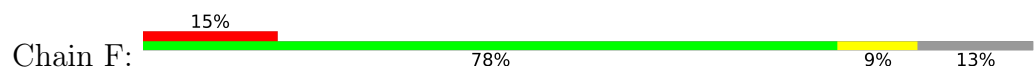




- Molecule 1: 5-lipoxygenase-activating protein



- Molecule 1: 5-lipoxygenase-activating protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.91Å 101.49Å 111.86Å 90.00° 99.83° 90.00°	Depositor
Resolution (Å)	30.00 – 2.37 52.07 – 2.37	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-2.37) 97.7 (52.07-2.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.254 , 0.285 0.256 , 0.289	Depositor DCC
$R_{free}$ test set	2896 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 65.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7340	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, QY1, BOG

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	0.38	0/1163	0.41	0/1580
1	B	0.38	0/1204	0.41	0/1634
1	C	0.37	0/1221	0.43	0/1660
1	D	0.37	0/1252	0.42	0/1703
1	E	0.37	0/1256	0.43	0/1705
1	F	0.37	0/1183	0.41	0/1611
All	All	0.37	0/7279	0.42	0/9893

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	1134	0	1122	8	0
1	B	1174	0	1157	8	0
1	C	1191	0	1186	9	0
1	D	1221	0	1215	7	0
1	E	1225	0	1231	11	0
1	F	1152	0	1124	11	0
2	A	27	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	0	2	0
2	C	27	0	0	5	0
2	D	27	0	0	1	0
2	E	27	0	0	7	0
2	F	27	0	0	3	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	F	20	0	28	0	0
5	A	11	0	0	1	0
5	B	14	0	0	0	0
5	C	10	0	0	0	0
5	D	8	0	0	0	0
5	E	7	0	0	0	0
5	F	9	0	0	0	0
All	All	7340	0	7063	57	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 4.

All (57) 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:116:LYS:HZ1	2:A:201:QY1:C16	1.65	1.08
1:A:116:LYS:NZ	2:A:201:QY1:C16	2.27	0.98
2:E:201:QY1:O25	2:E:201:QY1:C19	2.25	0.83
2:B:201:QY1:C20	1:F:166:HIS:HD2	2.02	0.73
1:C:94:ARG:HG2	1:C:114:PHE:CE2	2.24	0.72
1:C:116:LYS:HG2	2:C:201:QY1:C8	2.21	0.69
1:A:116:LYS:NZ	2:A:201:QY1:O25	2.24	0.68
1:D:109:THR:HB	1:E:41:SER:HA	1.78	0.65
2:E:201:QY1:O25	2:E:201:QY1:C17	2.48	0.61
1:A:116:LYS:CE	2:A:201:QY1:O25	2.49	0.60
1:C:94:ARG:HG2	1:C:114:PHE:HE2	1.64	0.60
2:A:201:QY1:N24	5:A:301:HOH:O	2.30	0.60
1:F:6:VAL:O	1:F:10:VAL:HG23	2.01	0.60
2:E:201:QY1:C9	2:E:201:QY1:C10	2.81	0.58
1:B:53:VAL:HG22	1:B:102:LEU:HD22	1.84	0.58
1:F:63:ALA:HB2	2:F:201:QY1:C7	2.37	0.55
1:E:116:LYS:HD3	2:E:201:QY1:O26	2.08	0.54
1:D:94:ARG:HG2	1:D:114:PHE:CE1	2.44	0.53
1:C:66:THR:HG21	2:C:201:QY1:C10	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:THR:HG21	2:F:201:QY1:C10	2.39	0.52
1:E:90:TYR:HB2	1:E:118:ILE:HG21	1.92	0.52
2:C:201:QY1:C6	2:C:201:QY1:C19	2.89	0.51
1:F:94:ARG:HG2	1:F:114:PHE:CE2	2.46	0.51
2:E:201:QY1:C9	2:E:201:QY1:C15	2.89	0.48
1:E:146:TYR:CZ	1:E:150:ILE:HD11	2.48	0.48
1:A:61:VAL:HG11	1:B:62:ASP:HA	1.95	0.48
1:D:99:VAL:HA	1:D:102:LEU:HD12	1.96	0.48
1:C:116:LYS:HG2	2:C:201:QY1:C5	2.43	0.48
1:E:53:VAL:HG22	1:E:102:LEU:HD22	1.96	0.47
1:F:94:ARG:HG2	1:F:114:PHE:HE2	1.78	0.47
1:B:37:GLN:HE22	1:B:47:THR:H	1.63	0.47
1:B:12:LEU:HD11	1:B:75:GLY:HA3	1.96	0.46
2:E:201:QY1:C10	2:E:201:QY1:C14	2.93	0.46
1:B:0:SER:HB3	1:C:8:ASN:HB3	1.98	0.45
1:E:33:GLU:HG2	1:E:50:PHE:HA	1.98	0.45
1:A:81:VAL:HB	1:A:82:PRO:HD3	1.98	0.45
1:A:116:LYS:HZ2	2:A:201:QY1:C16	2.22	0.44
1:A:49:ALA:O	1:A:53:VAL:HG23	2.17	0.44
1:E:94:ARG:HG2	1:E:114:PHE:CE1	2.52	0.44
1:B:25:PHE:HA	2:C:201:QY1:C17	2.48	0.44
1:F:81:VAL:HB	1:F:82:PRO:HD3	1.99	0.44
1:E:81:VAL:HB	1:E:82:PRO:HD3	1.99	0.44
1:E:73:SER:O	1:E:77:LEU:HB2	2.18	0.43
1:D:81:VAL:HB	1:D:82:PRO:HD3	2.00	0.43
1:D:116:LYS:HD2	2:D:201:QY1:O25	2.19	0.43
1:F:113:ILE:HG13	1:F:113:ILE:H	1.72	0.43
2:B:201:QY1:C20	1:F:166:HIS:CD2	2.92	0.42
1:E:132:ASN:O	1:E:136:ILE:HG12	2.19	0.42
1:B:9:VAL:HG12	1:B:76:LEU:HD21	2.02	0.42
1:D:24:GLY:C	2:F:201:QY1:C20	2.89	0.41
1:F:90:TYR:HB2	1:F:118:ILE:HG21	2.02	0.41
1:C:11:LEU:O	1:C:15:VAL:HG12	2.21	0.41
1:C:89:MET:HE1	1:D:155:SER:O	2.20	0.41
1:C:12:LEU:HD11	1:C:75:GLY:HA3	2.04	0.40
1:B:81:VAL:HB	1:B:82:PRO:HD3	2.03	0.40
1:E:116:LYS:HZ2	2:E:201:QY1:C16	2.33	0.40
1:F:155:SER:HB3	1:F:156:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	138/171 (81%)	136 (99%)	2 (1%)	0	100	100
1	B	143/171 (84%)	140 (98%)	3 (2%)	0	100	100
1	C	145/171 (85%)	144 (99%)	1 (1%)	0	100	100
1	D	149/171 (87%)	147 (99%)	2 (1%)	0	100	100
1	E	150/171 (88%)	149 (99%)	1 (1%)	0	100	100
1	F	142/171 (83%)	139 (98%)	2 (1%)	1 (1%)	22	30
All	All	867/1026 (84%)	855 (99%)	11 (1%)	1 (0%)	51	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	48	LEU

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	119/146 (82%)	119 (100%)	0	100	100
1	B	122/146 (84%)	122 (100%)	0	100	100
1	C	126/146 (86%)	125 (99%)	1 (1%)	81	91
1	D	130/146 (89%)	129 (99%)	1 (1%)	81	91
1	E	130/146 (89%)	128 (98%)	2 (2%)	65	79
1	F	119/146 (82%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	746/876 (85%)	742 (100%)	4 (0%)	88	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	44	ARG
1	D	120	LEU
1	E	33	GLU
1	E	88	LEU

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

Mol	Chain	Res	Type
1	B	37	GLN
1	E	8	ASN
1	F	166	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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z  > 2$
2	QY1	A	201	-	27,30,30	0.82	0	35,41,41	0.69	0
2	QY1	E	201	-	27,30,30	0.81	0	35,41,41	0.71	0
2	QY1	B	201	-	27,30,30	0.82	0	35,41,41	0.68	0
2	QY1	C	201	-	27,30,30	0.81	0	35,41,41	0.71	0
2	QY1	F	201	-	27,30,30	0.81	0	35,41,41	0.76	0
2	QY1	D	201	-	27,30,30	0.81	0	35,41,41	0.67	0
4	BOG	F	202	-	20,20,20	0.51	0	25,25,25	0.60	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
2	QY1	A	201	-	-	0/13/24/24	0/4/4/4
2	QY1	E	201	-	-	4/13/24/24	0/4/4/4
2	QY1	B	201	-	-	0/13/24/24	0/4/4/4
2	QY1	C	201	-	-	5/13/24/24	0/4/4/4
2	QY1	F	201	-	-	7/13/24/24	0/4/4/4
2	QY1	D	201	-	-	0/13/24/24	0/4/4/4
4	BOG	F	202	-	-	7/11/31/31	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	201	QY1	C19-C21-C23-C12
2	E	201	QY1	C19-C21-C23-C16
2	E	201	QY1	C20-C21-C23-C12
2	E	201	QY1	C20-C21-C23-C16
2	C	201	QY1	C19-C21-C23-C16
2	F	201	QY1	C20-C21-C23-C12
2	F	201	QY1	C20-C21-C23-C16
4	F	202	BOG	O5-C5-C6-O6
4	F	202	BOG	C4-C5-C6-O6

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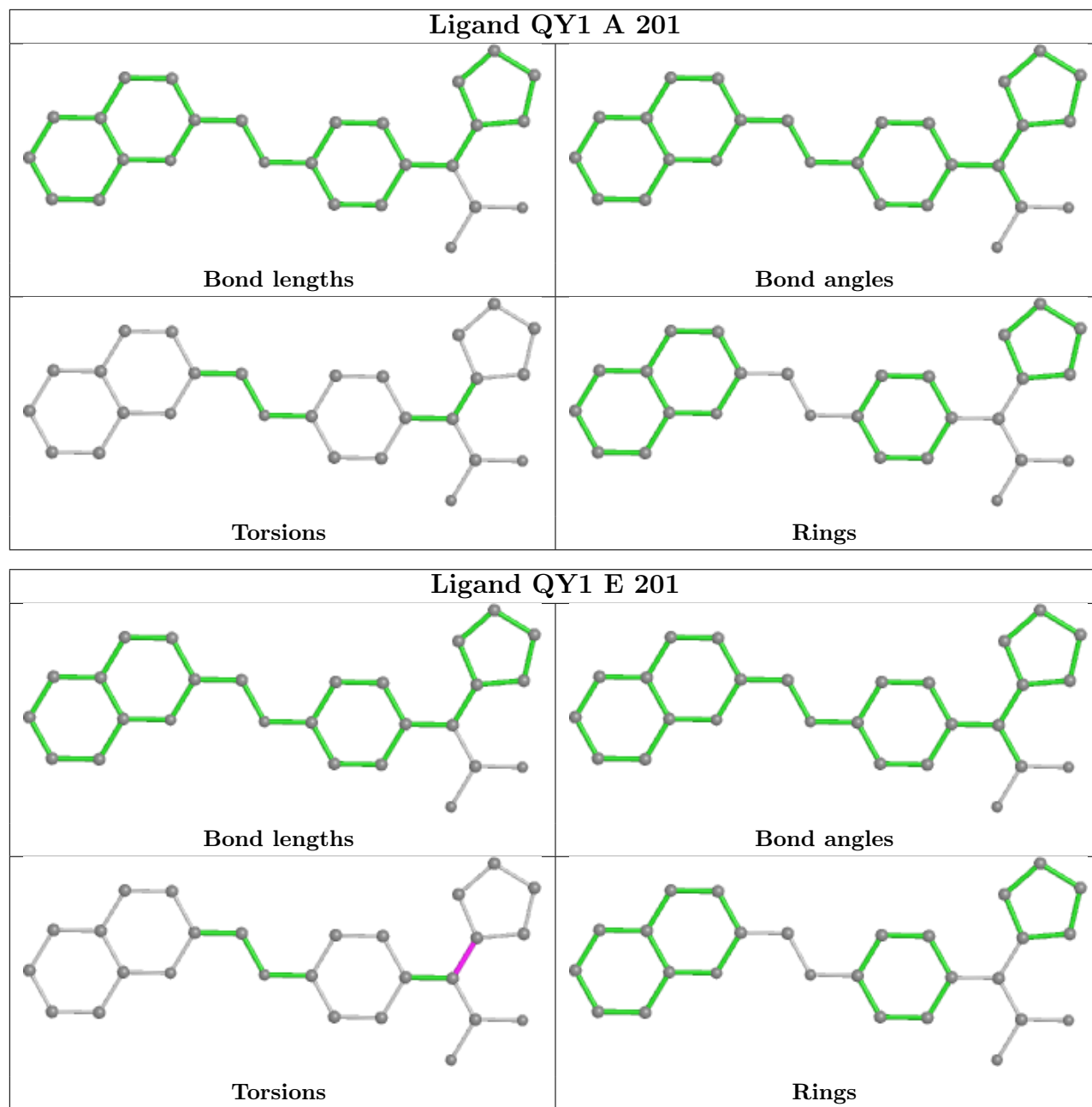
Mol	Chain	Res	Type	Atoms
2	C	201	QY1	C9-C14-O27-C22
2	C	201	QY1	C8-C14-O27-C22
2	F	201	QY1	C8-C14-O27-C22
2	F	201	QY1	C9-C14-O27-C22
4	F	202	BOG	C2'-C1'-O1-C1
4	F	202	BOG	C3'-C4'-C5'-C6'
4	F	202	BOG	O1-C1'-C2'-C3'
2	C	201	QY1	C20-C21-C23-C12
2	F	201	QY1	C19-C21-C23-C12
2	C	201	QY1	C20-C21-C23-C16
4	F	202	BOG	C2'-C3'-C4'-C5'
2	F	201	QY1	C6-C12-C23-C21
4	F	202	BOG	C5'-C6'-C7'-C8'
2	F	201	QY1	C5-C12-C23-C21

There are no ring outliers.

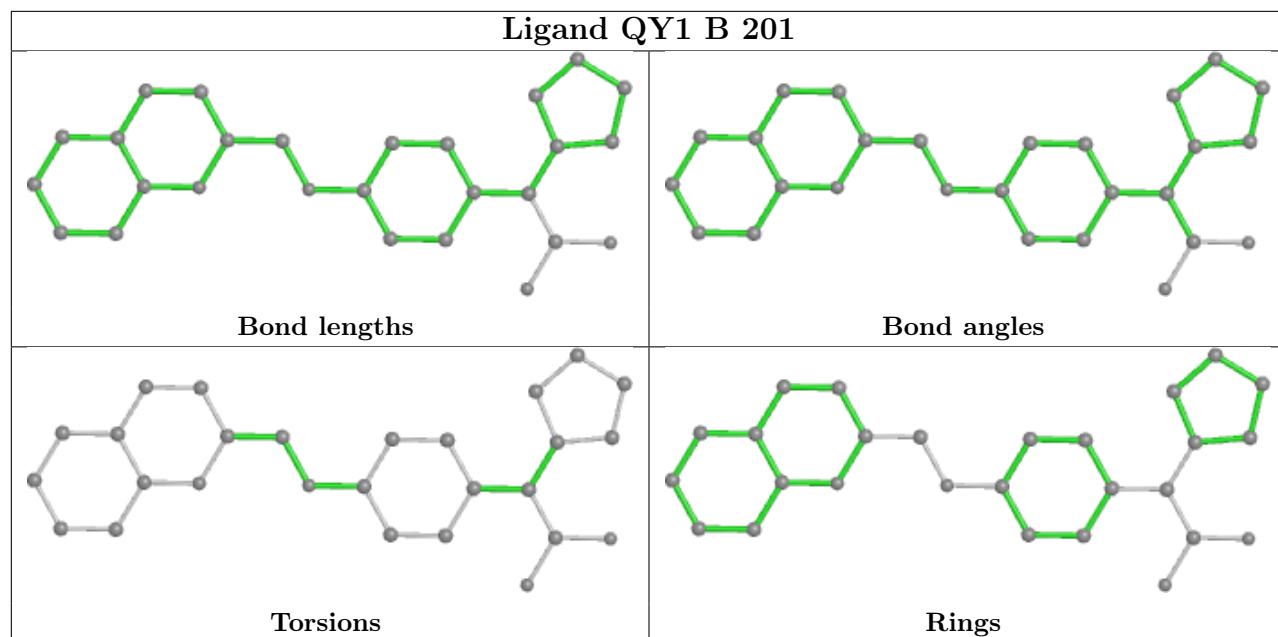
6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	QY1	6	0
2	E	201	QY1	7	0
2	B	201	QY1	2	0
2	C	201	QY1	5	0
2	F	201	QY1	3	0
2	D	201	QY1	1	0

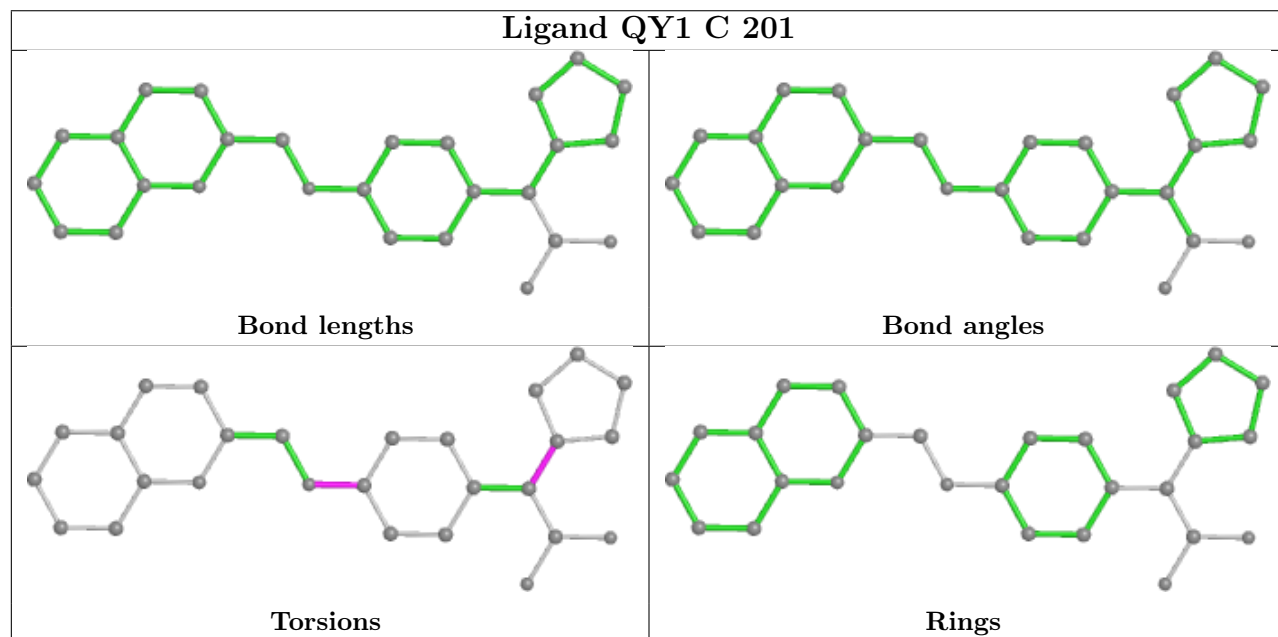
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



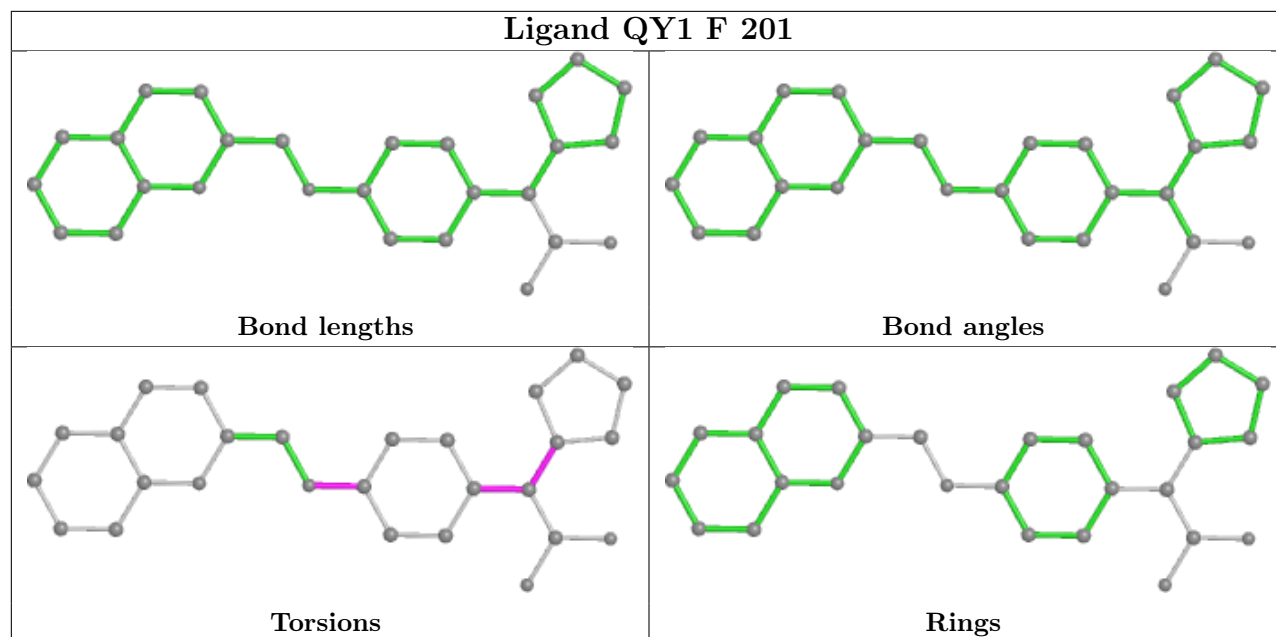
## Ligand QY1 B 201



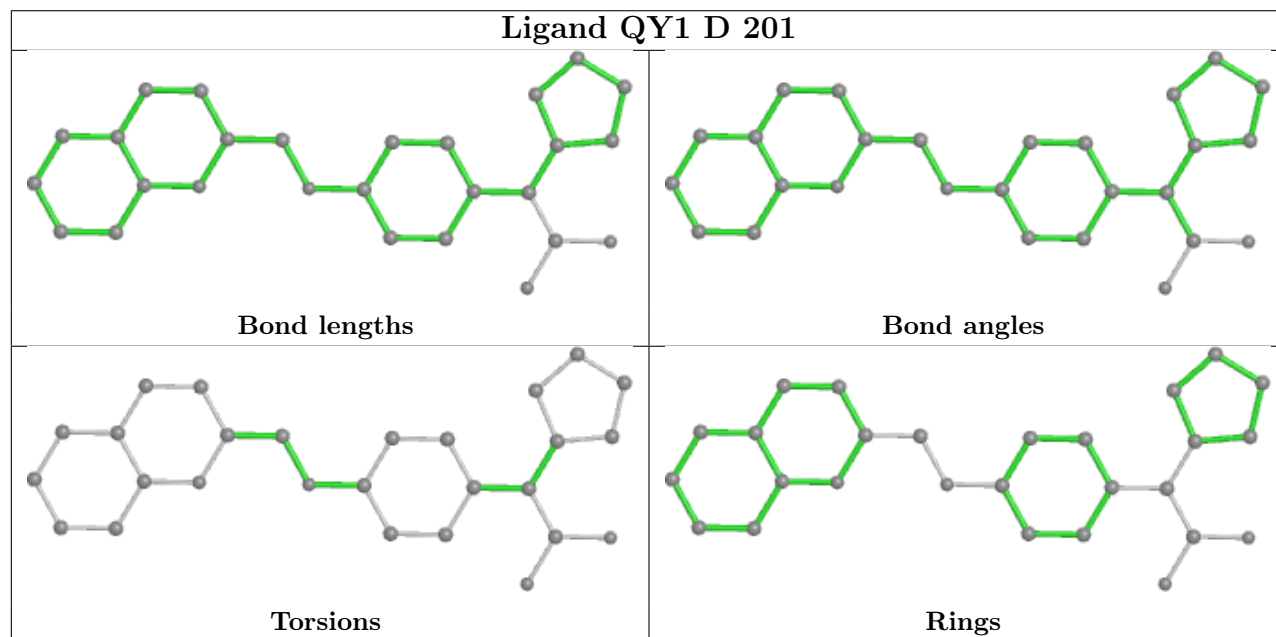
## Ligand QY1 C 201

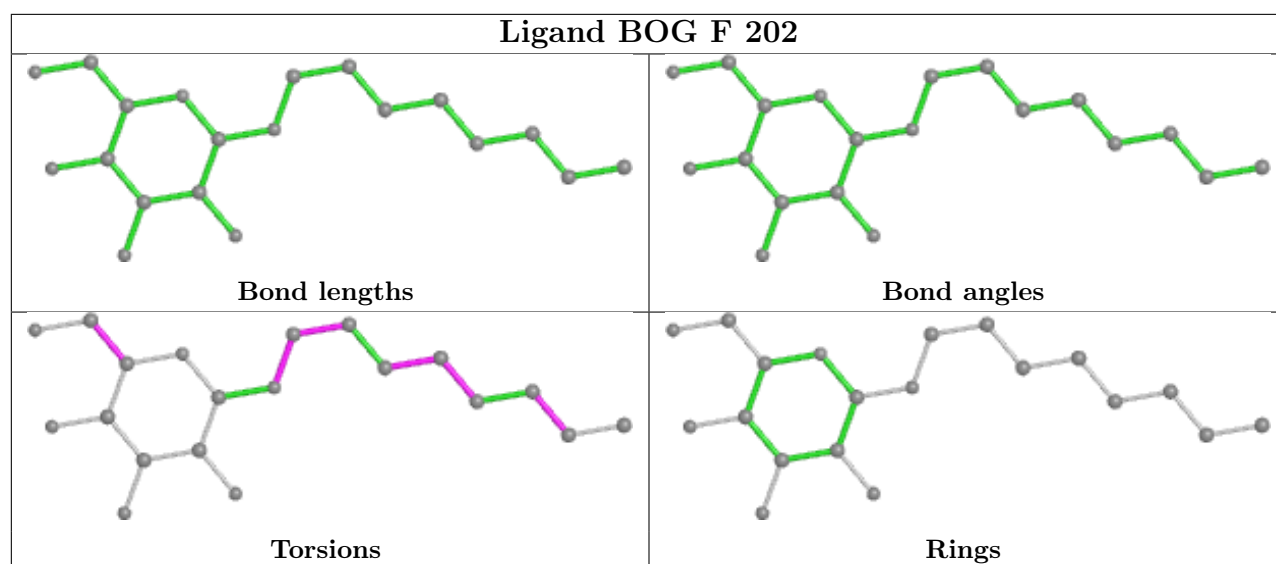


## Ligand QY1 F 201



## Ligand QY1 D 201





## 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	144/171 (84%)	1.01	18 (12%) <b>3</b> <b>4</b>	30, 46, 78, 81	0
1	B	149/171 (87%)	0.95	13 (8%) <b>10</b> <b>11</b>	20, 46, 86, 96	0
1	C	151/171 (88%)	0.82	16 (10%) <b>6</b> <b>7</b>	23, 50, 82, 87	0
1	D	155/171 (90%)	1.17	27 (17%) <b>1</b> <b>1</b>	41, 62, 88, 102	0
1	E	154/171 (90%)	0.94	14 (9%) <b>9</b> <b>10</b>	38, 59, 89, 98	0
1	F	148/171 (86%)	0.99	26 (17%) <b>1</b> <b>1</b>	42, 59, 85, 90	0
All	All	901/1026 (87%)	0.98	114 (12%) <b>3</b> <b>4</b>	20, 56, 85, 102	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	TYR	6.7
1	F	103	GLY	5.7
1	B	152	THR	5.4
1	B	156	PRO	4.6
1	F	49	ALA	4.6
1	A	45	THR	4.5
1	B	153	THR	4.5
1	E	85	PHE	4.5
1	B	138	PHE	4.5
1	F	32	HIS	4.4
1	D	131	PHE	4.3
1	C	36	THR	4.3
1	E	40	ARG	4.2
1	D	161	PRO	4.2
1	E	92	PHE	4.2
1	D	139	PHE	4.1
1	E	48	LEU	4.1
1	B	139	PHE	4.1
1	E	50	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	45	THR	4.0
1	B	142	ASP	3.8
1	E	110	PRO	3.8
1	D	146	TYR	3.7
1	A	35	ARG	3.6
1	D	85	PHE	3.6
1	A	146	TYR	3.6
1	A	133	TYR	3.6
1	D	133	TYR	3.6
1	F	110	PRO	3.6
1	F	100	GLY	3.6
1	C	92	PHE	3.4
1	D	36	THR	3.3
1	F	117	ARG	3.3
1	A	48	LEU	3.3
1	F	85	PHE	3.2
1	D	138	PHE	3.2
1	F	135	LEU	3.2
1	B	103	GLY	3.1
1	E	96	LYS	3.1
1	D	48	LEU	3.1
1	B	149	THR	3.0
1	C	85	PHE	3.0
1	C	1	LEU	3.0
1	D	159	LEU	3.0
1	C	110	PRO	3.0
1	F	131	PHE	2.9
1	D	160	ILE	2.8
1	B	92	PHE	2.8
1	D	153	THR	2.8
1	F	113	ILE	2.8
1	A	46	GLY	2.8
1	C	138	PHE	2.8
1	A	0	SER	2.8
1	D	99	VAL	2.7
1	A	110	PRO	2.7
1	D	113	ILE	2.7
1	D	150	ILE	2.7
1	F	11	LEU	2.7
1	D	145	ASN	2.6
1	B	131	PHE	2.6
1	F	92	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	35	ARG	2.6
1	D	32	HIS	2.6
1	F	142	ASP	2.6
1	A	3	GLN	2.6
1	E	3	GLN	2.6
1	E	135	LEU	2.6
1	D	162	GLU	2.6
1	F	163	GLY	2.6
1	F	79	SER	2.5
1	F	165	HIS	2.5
1	C	149	THR	2.5
1	F	120	LEU	2.5
1	A	32	HIS	2.5
1	A	111	GLY	2.5
1	B	155	SER	2.5
1	D	42	PHE	2.5
1	A	156	PRO	2.4
1	F	101	TYR	2.4
1	A	85	PHE	2.4
1	A	71	LEU	2.3
1	A	102	LEU	2.3
1	A	153	THR	2.3
1	D	158	LEU	2.3
1	E	35	ARG	2.3
1	E	38	ASN	2.3
1	D	157	LEU	2.3
1	F	116	LYS	2.3
1	C	102	LEU	2.3
1	D	134	TYR	2.3
1	E	89	MET	2.3
1	A	158	LEU	2.2
1	D	149	THR	2.2
1	C	145	ASN	2.2
1	C	0	SER	2.2
1	C	139	PHE	2.2
1	F	89	MET	2.2
1	D	151	SER	2.2
1	C	146	TYR	2.1
1	E	118	ILE	2.1
1	C	111	GLY	2.1
1	F	28	HIS	2.1
1	D	63	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	139	PHE	2.1
1	D	109	THR	2.1
1	E	36	THR	2.1
1	C	131	PHE	2.1
1	F	164	HIS	2.0
1	D	135	LEU	2.0
1	F	124	LEU	2.0
1	A	68	LEU	2.0
1	F	166	HIS	2.0
1	C	142	ASP	2.0
1	F	47	THR	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 monosaccharides in this entry.

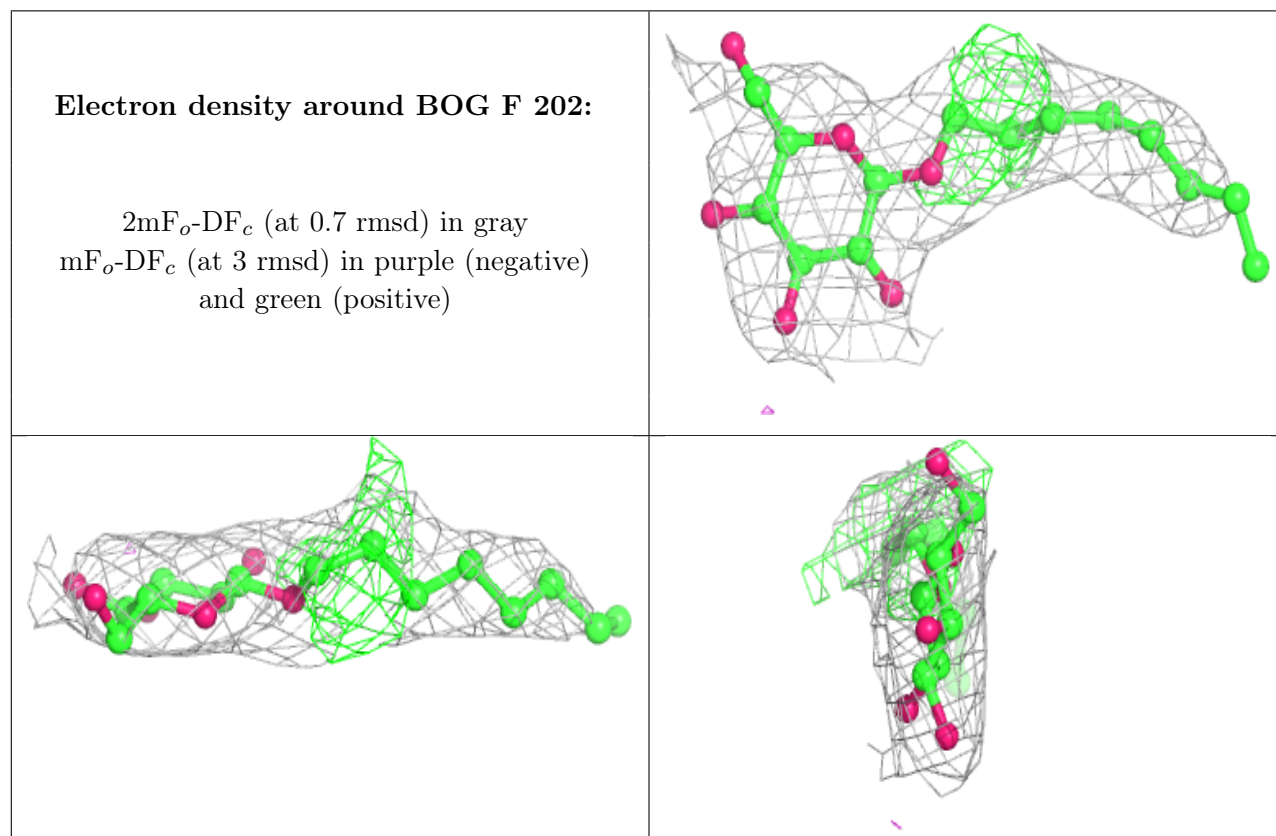
## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BOG	F	202	20/20	0.83	0.26	79,84,89,90	0
2	QY1	E	201	27/27	0.86	0.20	65,77,82,87	0
2	QY1	F	201	27/27	0.88	0.28	55,71,81,84	0
2	QY1	D	201	27/27	0.91	0.20	58,62,72,75	0
2	QY1	B	201	27/27	0.91	0.19	33,44,58,60	0
2	QY1	A	201	27/27	0.92	0.17	31,52,56,59	0
2	QY1	C	201	27/27	0.94	0.16	38,57,70,75	0
3	CA	B	202	1/1	0.96	0.23	81,81,81,81	0
3	CA	D	202	1/1	0.96	0.30	80,80,80,80	0

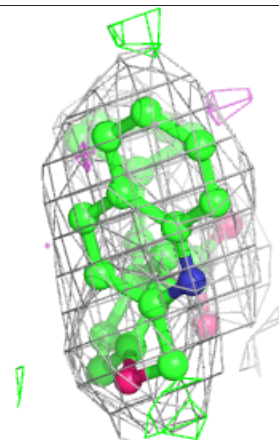
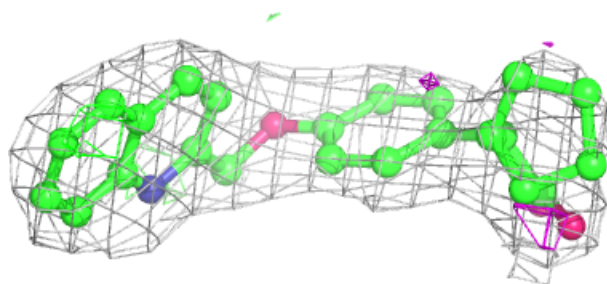
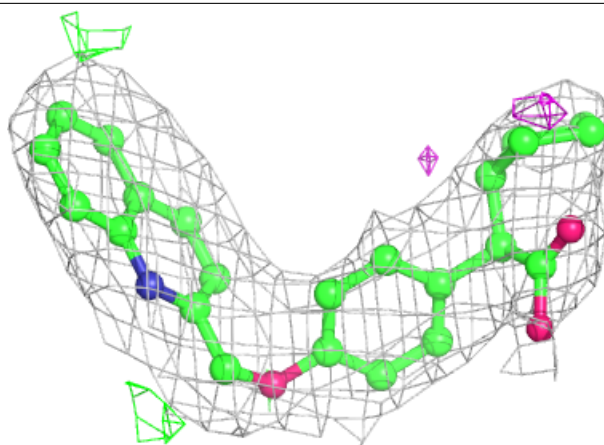
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

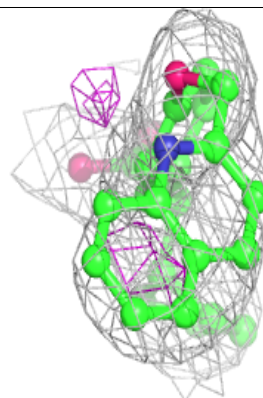
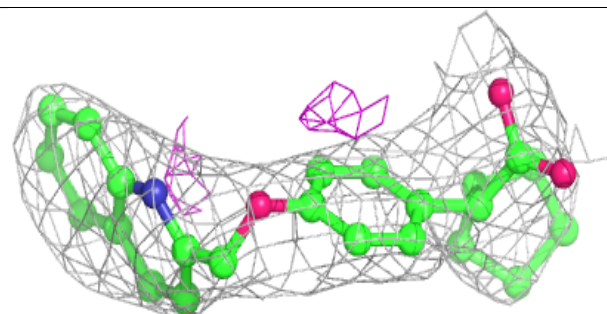
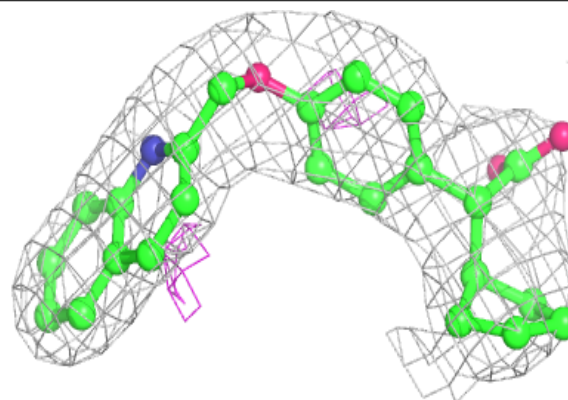


**Electron density around QY1 E 201:**

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

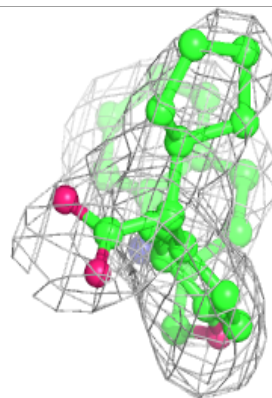
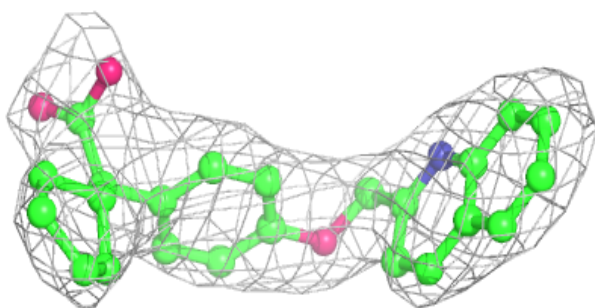
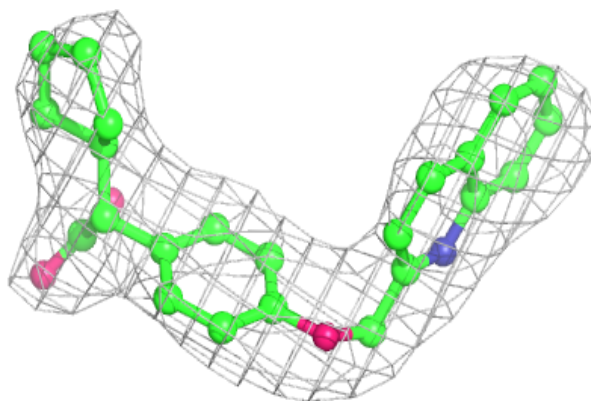
**Electron density around QY1 F 201:**

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

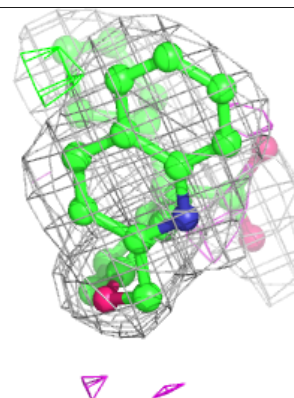
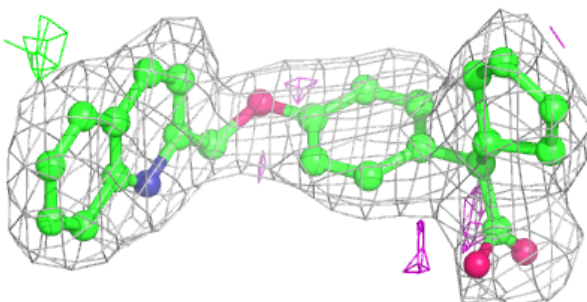
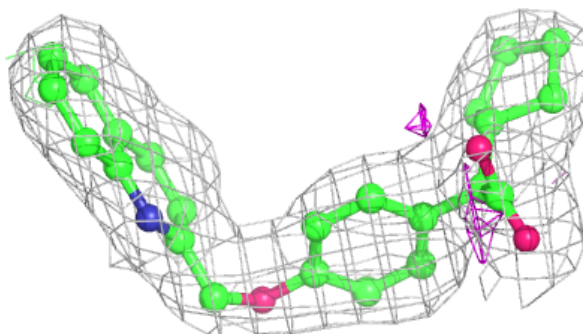


**Electron density around QY1 D 201:**

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

**Electron density around QY1 B 201:**

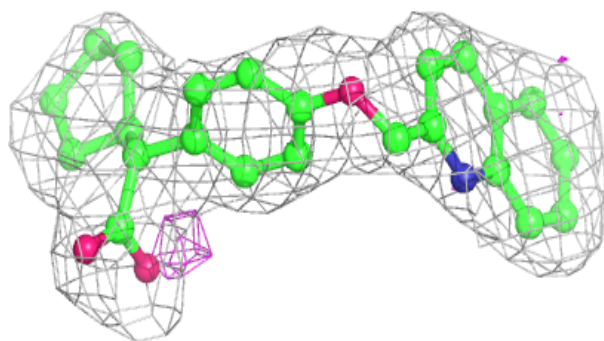
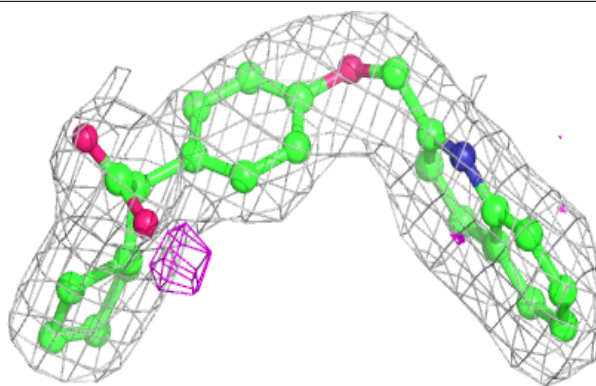
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



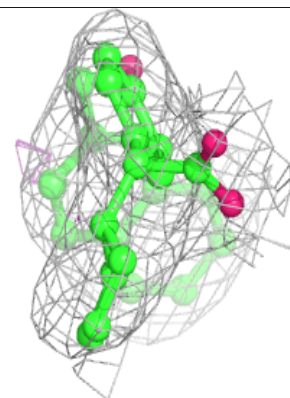
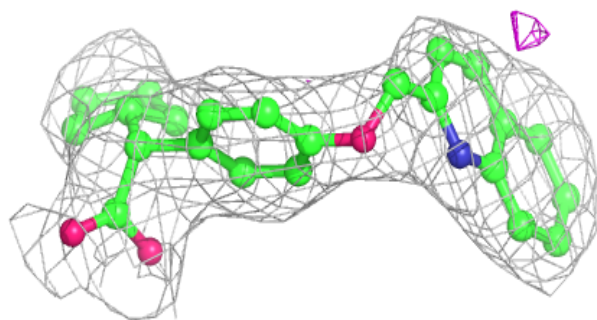
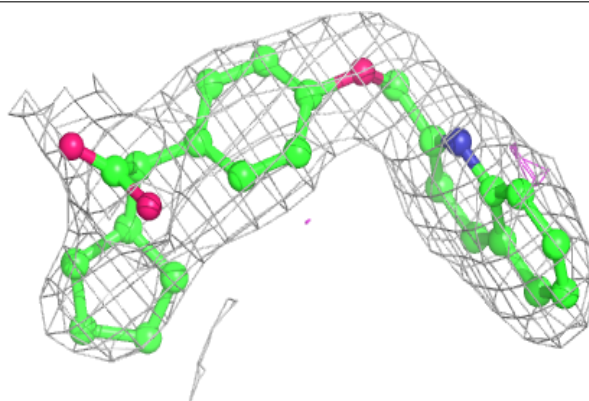


**Electron density around QY1 A 201:**

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

**Electron density around QY1 C 201:**

$2mF_o-DF_c$  (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.