



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2020 – 04:07 PM EDT

PDB ID : 6VKV  
Title : Co-crystal structure of GS-6207 bound to HIV-1 capsid hexamer  
Authors : Bester, S.M.; Kvaratskhelia, M.  
Deposited on : 2020-01-22  
Resolution : 2.22 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

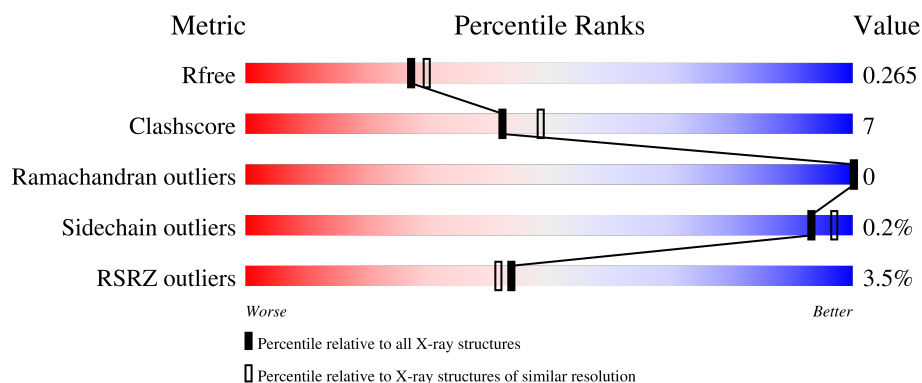
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	231	<div> <div>2%</div> <div>80% 16% 5%</div> </div>
1	B	231	<div> <div>5%</div> <div>77% 18% 5%</div> </div>
1	C	231	<div> <div>3%</div> <div>84% 11% 5%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5783 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.

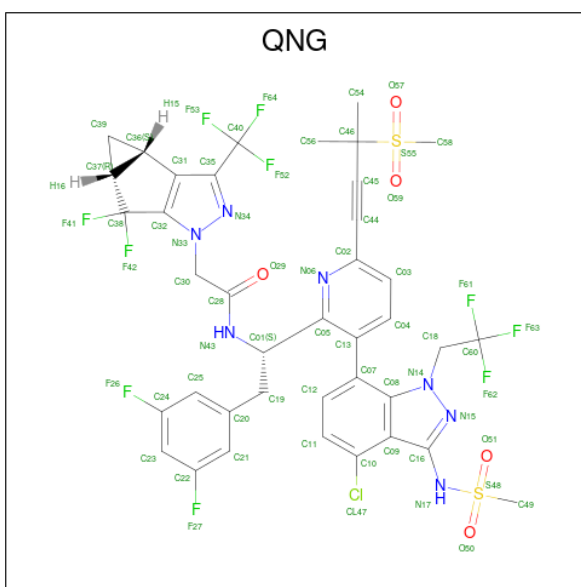
- Molecule 1 is a protein called Capsid protein p24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	1	0
			1715	1077	303	321	14			
1	B	220	Total	C	N	O	S	0	2	0
			1724	1082	304	324	14			
1	C	220	Total	C	N	O	S	0	0	0
			1704	1071	299	320	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	ALA	engineered mutation	UNP B6DRA0
A	45	CYS	GLU	engineered mutation	UNP B6DRA0
A	184	ALA	TRP	engineered mutation	UNP B6DRA0
A	185	ALA	MET	engineered mutation	UNP B6DRA0
B	14	CYS	ALA	engineered mutation	UNP B6DRA0
B	45	CYS	GLU	engineered mutation	UNP B6DRA0
B	184	ALA	TRP	engineered mutation	UNP B6DRA0
B	185	ALA	MET	engineered mutation	UNP B6DRA0
C	14	CYS	ALA	engineered mutation	UNP B6DRA0
C	45	CYS	GLU	engineered mutation	UNP B6DRA0
C	184	ALA	TRP	engineered mutation	UNP B6DRA0
C	185	ALA	MET	engineered mutation	UNP B6DRA0

- Molecule 2 is N-[(1S)-1-(3-{4-chloro-3-[(methylsulfonyl)amino]-1-(2,2,2-trifluoroethyl)-1H-indazol-7-yl}-6-[3-methyl-3-(methylsulfonyl)but-1-yn-1-yl]pyridin-2-yl)-2-(3,5-difluorophenyl)ethyl]-2-[(3bS,4aR)-5,5-difluoro-3-(trifluoromethyl)-3b,4,4a,5-tetrahydro-1H-cyclopropa[3,4]cyclopenta[1,2-c]pyrazol-1-yl]acetamide (three-letter code: QNG) (formula: C<sub>39</sub>H<sub>32</sub>ClF<sub>10</sub>N<sub>7</sub>O<sub>5</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	1
			128	78	2	20	14	10	4		
2	B	1	Total	C	Cl	F	N	O	S	0	1
			128	78	2	20	14	10	4		
2	C	1	Total	C	Cl	F	N	O	S	0	1
			128	78	2	20	14	10	4		

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

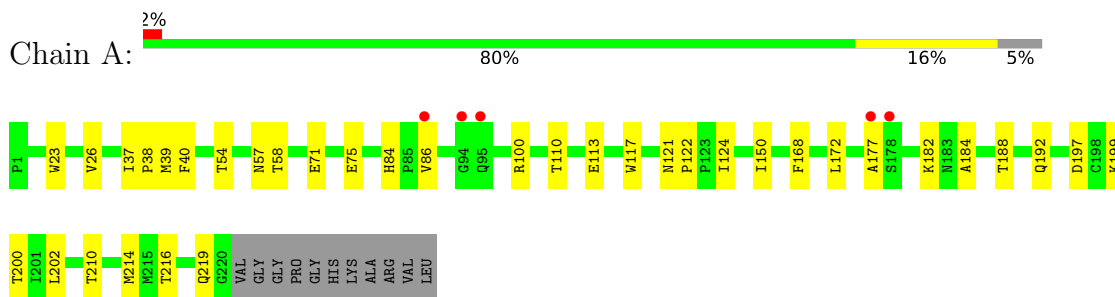
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	73	Total 73	O 73	0	0
5	B	76	Total 76	O 76	0	0
5	C	88	Total 88	O 88	0	0

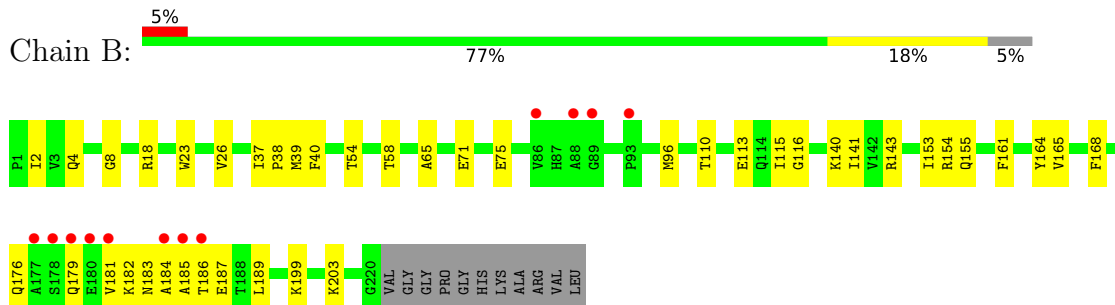
### 3 Residue-property plots [i](#)

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.

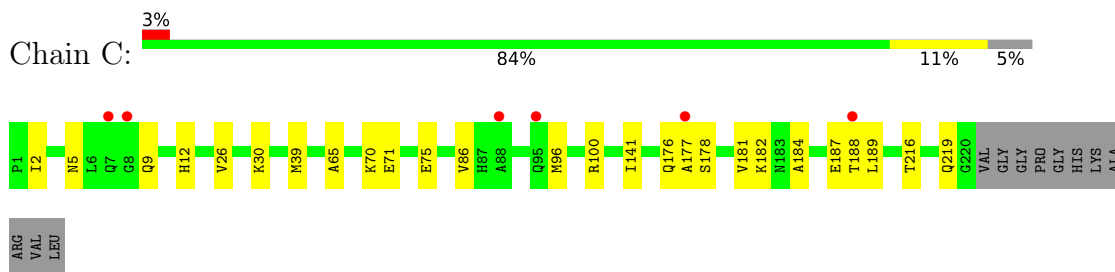
#### • Molecule 1: Capsid protein p24



#### • Molecule 1: Capsid protein p24



#### • Molecule 1: Capsid protein p24



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.05Å 160.05Å 57.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.26 – 2.22 46.71 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.26-2.22) 99.7 (46.71-2.22)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.231 , 0.269 0.231 , 0.265	Depositor DCC
$R_{free}$ test set	2051 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.8967e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: QNG, IOD, CL

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	0.37	0/1752	0.54	0/2380
1	B	0.36	0/1761	0.52	0/2392
1	C	0.34	0/1741	0.56	0/2366
All	All	0.36	0/5254	0.54	0/7138

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	1715	0	1718	26	0
1	B	1724	0	1723	28	0
1	C	1704	0	1706	19	0
2	A	128	0	0	2	0
2	B	128	0	0	0	0
2	C	128	0	0	1	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	0	1	0
4	C	6	0	0	0	0
5	A	73	0	0	3	0
5	B	76	0	0	4	0
5	C	88	0	0	1	0
All	All	5783	0	5147	74	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 7.

All (74) 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:192:GLN:HA	1:A:199:LYS:HE3	1.56	0.88
1:B:176:GLN:HA	5:B:413:HOH:O	1.74	0.86
1:C:184:ALA:HA	1:C:187:GLU:HG3	1.61	0.83
1:A:86:VAL:HG21	1:A:100:ARG:HD3	1.64	0.79
1:B:26:VAL:HG21	1:B:39:MET:HG2	1.65	0.78
4:A:307:CL:CL	5:A:430:HOH:O	2.42	0.74
1:B:182:LYS:HE2	5:B:413:HOH:O	1.90	0.71
1:A:86:VAL:CG2	1:A:100:ARG:HD3	2.22	0.69
1:A:86:VAL:HG23	1:A:100:ARG:HH11	1.63	0.64
1:C:86:VAL:HG21	1:C:100:ARG:CD	2.28	0.64
1:A:110:THR:OG1	1:A:113:GLU:HG3	1.98	0.64
1:A:71:GLU:O	1:A:75:GLU:HG3	1.98	0.64
1:C:86:VAL:HG23	1:C:100:ARG:NH1	2.13	0.63
1:C:188:THR:HG23	1:C:189:LEU:HG	1.81	0.62
1:A:26:VAL:HG21	1:A:39:MET:HG2	1.83	0.61
1:C:86:VAL:HG21	1:C:100:ARG:HD3	1.82	0.60
1:B:179:GLN:O	1:B:183:ASN:HB2	2.02	0.60
1:C:176:GLN:HA	1:C:182:LYS:NZ	2.17	0.59
1:A:117:TRP:HB3	1:A:124:ILE:HG23	1.84	0.57
1:B:143:ARG:HG2	1:B:176:GLN:H	1.67	0.57
1:B:71:GLU:O	1:B:75:GLU:HG3	2.05	0.57
1:C:184:ALA:O	1:C:187:GLU:HB2	2.04	0.57
1:C:216:THR:O	1:C:219:GLN:HG2	2.06	0.55
1:A:216:THR:HA	1:A:219:GLN:HG3	1.89	0.54
1:B:181:VAL:O	1:B:184:ALA:HB3	2.06	0.54
1:A:202:LEU:HD13	1:A:214:MET:HE3	1.90	0.53
1:B:18:ARG:HG3	4:B:306:CL:CL	2.46	0.53
1:B:2:ILE:HD11	1:B:115:ILE:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LYS:O	1:B:203:LYS:HD3	2.10	0.52
1:B:96:MET:SD	1:B:116:GLY:HA3	2.50	0.52
1:B:155:GLN:HB2	1:B:164:TYR:CG	2.45	0.51
1:C:177:ALA:H	1:C:182:LYS:HE2	1.76	0.51
1:C:30:LYS:NZ	5:C:403:HOH:O	2.43	0.51
1:A:177:ALA:HB2	5:A:427:HOH:O	2.10	0.51
1:C:70:LYS:HE2	2:C:301[B]:QNG:C16	2.41	0.51
1:B:110:THR:OG1	1:B:113:GLU:HG3	2.12	0.50
1:A:86:VAL:CG2	1:A:100:ARG:CD	2.89	0.49
1:B:4:GLN:OE1	1:B:8:GLY:HA2	2.13	0.49
1:B:153:ILE:HG21	1:B:168:PHE:HA	1.95	0.49
1:B:140:LYS:HG2	1:B:143:ARG:HH21	1.76	0.49
1:B:182:LYS:CB	1:B:182:LYS:NZ	2.77	0.48
1:A:84:HIS:O	1:A:100:ARG:NH1	2.44	0.48
1:A:23:TRP:CZ3	1:A:40:PHE:HB2	2.49	0.48
1:A:57:ASN:OD1	2:A:301[A]:QNG:N43	2.46	0.48
1:A:86:VAL:HG21	1:A:100:ARG:CD	2.40	0.47
1:A:184:ALA:O	1:A:188:THR:OG1	2.25	0.47
1:C:71:GLU:O	1:C:75:GLU:HG3	2.16	0.46
1:C:26:VAL:HG21	1:C:39:MET:HG3	1.96	0.46
1:A:100:ARG:HG3	5:A:456:HOH:O	2.15	0.46
1:B:161:PHE:O	1:B:165:VAL:HG23	2.16	0.46
1:B:54:THR:O	1:B:58:THR:HG23	2.15	0.46
1:C:86:VAL:HG21	1:C:100:ARG:HD2	1.98	0.46
1:B:199:LYS:HG2	1:B:203:LYS:HE2	1.98	0.46
1:A:37:ILE:HB	1:A:38:PRO:HD3	1.97	0.46
1:A:150:ILE:HD11	1:A:168:PHE:CE1	2.50	0.45
1:A:57:ASN:OD1	2:A:301[B]:QNG:N43	2.49	0.45
1:A:210:THR:O	1:A:214:MET:HG3	2.17	0.45
1:A:54:THR:O	1:A:58:THR:HG23	2.15	0.45
1:B:37:ILE:HB	1:B:38:PRO:HD3	1.99	0.44
1:A:197:ASP:O	1:A:200:THR:HG22	2.19	0.43
1:C:65:ALA:HB1	1:C:141:ILE:HD13	2.01	0.43
1:B:185:ALA:O	1:B:189:LEU:HB3	2.18	0.42
1:C:2:ILE:HD13	1:C:12:HIS:HA	2.01	0.42
1:C:178:SER:OG	1:C:181:VAL:HG23	2.19	0.42
1:A:172:LEU:HG	1:A:182:LYS:HG2	2.01	0.42
1:B:186:THR:OG1	1:B:187:GLU:HG3	2.21	0.41
1:B:65:ALA:HB1	1:B:141:ILE:HD13	2.02	0.41
1:B:154:ARG:NH1	5:B:405:HOH:O	2.53	0.41
1:A:121:ASN:HA	1:A:122:PRO:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LYS:CE	5:B:413:HOH:O	2.60	0.40
1:C:86:VAL:CG2	1:C:100:ARG:CD	2.97	0.40
1:B:181:VAL:HA	1:B:184:ALA:CB	2.52	0.40
1:C:5:ASN:HD21	1:C:9:GLN:CG	2.35	0.40
1:B:23:TRP:CZ3	1:B:40:PHE:HB2	2.56	0.40

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	219/231 (95%)	215 (98%)	4 (2%)	0	100	100
1	B	220/231 (95%)	215 (98%)	5 (2%)	0	100	100
1	C	218/231 (94%)	215 (99%)	3 (1%)	0	100	100
All	All	657/693 (95%)	645 (98%)	12 (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	187/193 (97%)	187 (100%)	0	100	100
1	B	188/193 (97%)	188 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	186/193 (96%)	185 (100%)	1 (0%)	88	94
All	All	561/579 (97%)	560 (100%)	1 (0%)	93	97

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

Mol	Chain	Res	Type
1	C	96	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	179	GLN
1	C	63	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 19 are monoatomic - leaving 6 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	QNG	C	301[B]	-	60,70,70	2.51	20 (33%)	80,114,114	3.18	29 (36%)
2	QNG	A	301[B]	-	60,70,70	2.66	19 (31%)	80,114,114	3.46	28 (35%)
2	QNG	A	301[A]	-	60,70,70	2.60	19 (31%)	80,114,114	3.37	23 (28%)
2	QNG	B	301[A]	-	60,70,70	2.56	20 (33%)	80,114,114	3.57	28 (35%)
2	QNG	C	301[A]	-	60,70,70	2.61	19 (31%)	80,114,114	3.44	25 (31%)
2	QNG	B	301[B]	-	60,70,70	2.54	21 (35%)	80,114,114	3.37	23 (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
2	QNG	C	301[B]	-	-	1/41/72/72	0/7/7/7
2	QNG	A	301[B]	-	-	2/41/72/72	0/7/7/7
2	QNG	A	301[A]	-	-	7/41/72/72	0/7/7/7
2	QNG	B	301[A]	-	-	13/41/72/72	0/7/7/7
2	QNG	C	301[A]	-	-	11/41/72/72	0/7/7/7
2	QNG	B	301[B]	-	-	5/41/72/72	0/7/7/7

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301[A]	QNG	C28-N43	7.06	1.49	1.34
2	B	301[B]	QNG	C28-N43	7.05	1.49	1.34
2	A	301[A]	QNG	S48-N17	6.92	1.72	1.63
2	C	301[A]	QNG	C28-N43	6.90	1.48	1.34
2	A	301[B]	QNG	C28-N43	6.84	1.48	1.34
2	A	301[B]	QNG	S48-N17	6.83	1.72	1.63
2	C	301[A]	QNG	S48-N17	6.76	1.72	1.63
2	A	301[A]	QNG	C28-N43	6.67	1.48	1.34
2	C	301[A]	QNG	C02-C44	6.43	1.55	1.44
2	A	301[B]	QNG	C02-C44	6.40	1.55	1.44
2	C	301[B]	QNG	S48-N17	6.25	1.71	1.63
2	C	301[B]	QNG	C28-N43	6.21	1.47	1.34
2	B	301[B]	QNG	S48-N17	6.20	1.71	1.63
2	A	301[A]	QNG	C02-C44	6.18	1.54	1.44
2	B	301[A]	QNG	C58-S55	6.14	1.83	1.76
2	C	301[B]	QNG	C02-C44	6.11	1.54	1.44
2	B	301[A]	QNG	S48-N17	6.11	1.71	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301[B]	QNG	C58-S55	6.10	1.83	1.76
2	C	301[A]	QNG	C46-C45	6.05	1.55	1.46
2	B	301[A]	QNG	C02-C44	5.96	1.54	1.44
2	B	301[B]	QNG	C58-S55	5.92	1.83	1.76
2	A	301[B]	QNG	C46-C45	5.72	1.55	1.46
2	B	301[B]	QNG	C02-C44	5.72	1.53	1.44
2	C	301[B]	QNG	C46-C45	5.69	1.55	1.46
2	A	301[A]	QNG	C58-S55	5.67	1.83	1.76
2	C	301[A]	QNG	C58-S55	5.65	1.83	1.76
2	B	301[A]	QNG	C46-C45	5.51	1.54	1.46
2	C	301[B]	QNG	C58-S55	5.46	1.83	1.76
2	A	301[A]	QNG	C46-C45	5.44	1.54	1.46
2	A	301[A]	QNG	C38-C32	5.15	1.55	1.49
2	B	301[B]	QNG	C46-C45	5.10	1.54	1.46
2	A	301[B]	QNG	C38-C32	5.02	1.55	1.49
2	C	301[A]	QNG	C38-C32	4.89	1.55	1.49
2	B	301[A]	QNG	C38-C32	4.88	1.55	1.49
2	A	301[B]	QNG	C07-C13	4.84	1.57	1.50
2	B	301[B]	QNG	C38-C32	4.82	1.55	1.49
2	C	301[B]	QNG	C38-C32	4.76	1.55	1.49
2	A	301[A]	QNG	C07-C13	4.75	1.56	1.50
2	C	301[A]	QNG	C07-C13	4.66	1.56	1.50
2	B	301[A]	QNG	O59-S55	4.52	1.47	1.44
2	C	301[B]	QNG	O59-S55	4.47	1.47	1.44
2	A	301[B]	QNG	O57-S55	4.47	1.47	1.44
2	A	301[B]	QNG	O59-S55	4.43	1.47	1.44
2	A	301[A]	QNG	O59-S55	4.36	1.47	1.44
2	C	301[B]	QNG	C07-C13	4.29	1.56	1.50
2	B	301[B]	QNG	C07-C13	4.26	1.56	1.50
2	C	301[A]	QNG	O59-S55	4.26	1.47	1.44
2	B	301[A]	QNG	O57-S55	4.22	1.47	1.44
2	B	301[B]	QNG	O59-S55	4.18	1.47	1.44
2	A	301[A]	QNG	O57-S55	4.08	1.47	1.44
2	B	301[B]	QNG	O57-S55	3.98	1.47	1.44
2	B	301[A]	QNG	C07-C13	3.94	1.55	1.50
2	C	301[A]	QNG	O57-S55	3.89	1.46	1.44
2	C	301[B]	QNG	O57-S55	3.85	1.46	1.44
2	C	301[B]	QNG	C09-C08	-3.61	1.38	1.42
2	A	301[A]	QNG	C16-N17	3.57	1.47	1.39
2	C	301[A]	QNG	C16-N17	3.54	1.47	1.39
2	A	301[B]	QNG	C16-N17	3.48	1.47	1.39
2	B	301[B]	QNG	C35-N34	3.48	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[A]	QNG	C35-N34	3.44	1.38	1.34
2	B	301[A]	QNG	C35-N34	3.42	1.38	1.34
2	C	301[A]	QNG	C49-S48	3.41	1.83	1.75
2	B	301[A]	QNG	C49-S48	3.40	1.83	1.75
2	A	301[B]	QNG	C49-S48	3.40	1.83	1.75
2	A	301[A]	QNG	C49-S48	3.39	1.83	1.75
2	C	301[B]	QNG	C49-S48	3.39	1.83	1.75
2	B	301[B]	QNG	C49-S48	3.37	1.83	1.75
2	A	301[B]	QNG	C18-C60	3.26	1.54	1.50
2	B	301[B]	QNG	C18-C60	3.25	1.54	1.50
2	B	301[A]	QNG	C18-C60	3.21	1.54	1.50
2	B	301[A]	QNG	C16-N17	3.20	1.46	1.39
2	A	301[A]	QNG	C18-C60	3.19	1.54	1.50
2	B	301[B]	QNG	C16-N17	3.18	1.46	1.39
2	B	301[B]	QNG	C09-C08	-3.17	1.38	1.42
2	C	301[B]	QNG	C16-N17	3.08	1.46	1.39
2	A	301[B]	QNG	C35-N34	3.01	1.38	1.34
2	C	301[B]	QNG	C35-N34	3.00	1.38	1.34
2	C	301[A]	QNG	C18-C60	3.00	1.54	1.50
2	A	301[A]	QNG	C31-C36	2.99	1.57	1.51
2	C	301[B]	QNG	C32-N33	-2.97	1.33	1.37
2	A	301[B]	QNG	C31-C36	2.95	1.57	1.51
2	C	301[A]	QNG	C31-C36	2.94	1.57	1.51
2	B	301[A]	QNG	C09-C08	-2.93	1.39	1.42
2	B	301[B]	QNG	C31-C36	2.92	1.57	1.51
2	A	301[A]	QNG	C09-C08	-2.91	1.39	1.42
2	C	301[B]	QNG	C31-C36	2.88	1.57	1.51
2	B	301[A]	QNG	C31-C36	2.85	1.57	1.51
2	C	301[A]	QNG	C09-C08	-2.75	1.39	1.42
2	B	301[B]	QNG	C32-N33	-2.74	1.33	1.37
2	A	301[B]	QNG	C09-C08	-2.72	1.39	1.42
2	A	301[A]	QNG	C35-N34	2.72	1.37	1.34
2	A	301[A]	QNG	C32-N33	-2.59	1.33	1.37
2	B	301[A]	QNG	C32-N33	-2.59	1.33	1.37
2	A	301[B]	QNG	C32-N33	-2.54	1.33	1.37
2	C	301[A]	QNG	C32-N33	-2.51	1.33	1.37
2	B	301[B]	QNG	O51-S48	2.26	1.47	1.43
2	B	301[A]	QNG	O51-S48	2.25	1.47	1.43
2	A	301[B]	QNG	O50-S48	2.25	1.47	1.43
2	C	301[B]	QNG	O50-S48	2.20	1.47	1.43
2	A	301[A]	QNG	O50-S48	2.20	1.47	1.43
2	C	301[B]	QNG	C18-C60	2.20	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301[B]	QNG	C11-C10	2.14	1.41	1.36
2	C	301[A]	QNG	O51-S48	2.14	1.47	1.43
2	B	301[B]	QNG	O50-S48	2.14	1.47	1.43
2	A	301[B]	QNG	O51-S48	2.12	1.47	1.43
2	C	301[B]	QNG	O51-S48	2.12	1.47	1.43
2	A	301[A]	QNG	O51-S48	2.11	1.47	1.43
2	C	301[B]	QNG	O29-C28	-2.11	1.19	1.23
2	B	301[B]	QNG	C11-C10	2.10	1.41	1.36
2	C	301[A]	QNG	O29-C28	-2.10	1.19	1.23
2	C	301[B]	QNG	C11-C10	2.10	1.41	1.36
2	B	301[A]	QNG	O50-S48	2.08	1.47	1.43
2	C	301[A]	QNG	C11-C10	2.06	1.41	1.36
2	B	301[B]	QNG	O29-C28	-2.05	1.19	1.23
2	A	301[A]	QNG	C11-C10	2.05	1.41	1.36
2	B	301[A]	QNG	O29-C28	-2.04	1.19	1.23
2	B	301[A]	QNG	C39-C37	2.01	1.53	1.50
2	B	301[B]	QNG	C39-C37	2.00	1.53	1.50

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301[B]	QNG	O59-S55-O57	-20.56	101.01	118.10
2	C	301[A]	QNG	O59-S55-O57	-19.81	101.63	118.10
2	B	301[A]	QNG	O59-S55-O57	-19.73	101.69	118.10
2	A	301[A]	QNG	O59-S55-O57	-19.48	101.91	118.10
2	B	301[B]	QNG	O59-S55-O57	-19.10	102.22	118.10
2	C	301[B]	QNG	O59-S55-O57	-18.37	102.82	118.10
2	C	301[A]	QNG	O51-S48-O50	-12.59	100.75	118.85
2	A	301[A]	QNG	O51-S48-O50	-12.25	101.24	118.85
2	B	301[A]	QNG	O51-S48-O50	-12.22	101.28	118.85
2	A	301[B]	QNG	O51-S48-O50	-12.14	101.40	118.85
2	B	301[B]	QNG	O51-S48-O50	-12.03	101.55	118.85
2	C	301[B]	QNG	O51-S48-O50	-10.43	103.86	118.85
2	A	301[A]	QNG	C39-C36-C31	9.64	128.58	115.70
2	B	301[A]	QNG	C39-C36-C31	9.58	128.50	115.70
2	B	301[B]	QNG	C39-C36-C31	9.41	128.28	115.70
2	A	301[B]	QNG	C39-C36-C31	9.33	128.18	115.70
2	C	301[A]	QNG	C39-C36-C31	9.30	128.14	115.70
2	B	301[A]	QNG	C40-C35-C31	-8.62	124.12	129.48
2	C	301[B]	QNG	C39-C36-C31	8.30	126.80	115.70
2	B	301[A]	QNG	C40-C35-N34	7.29	128.40	119.69
2	A	301[B]	QNG	C02-N06-C05	7.14	122.22	117.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301[B]	QNG	C40-C35-C31	-6.45	125.47	129.48
2	A	301[A]	QNG	C02-N06-C05	6.39	121.69	117.22
2	C	301[A]	QNG	C40-C35-C31	-6.21	125.62	129.48
2	C	301[A]	QNG	C02-N06-C05	6.16	121.53	117.22
2	B	301[B]	QNG	C40-C35-N34	6.10	126.98	119.69
2	B	301[A]	QNG	C02-N06-C05	6.00	121.42	117.22
2	C	301[A]	QNG	C40-C35-N34	5.97	126.83	119.69
2	B	301[B]	QNG	C02-N06-C05	5.10	120.79	117.22
2	A	301[A]	QNG	C40-C35-N34	5.00	125.67	119.69
2	A	301[B]	QNG	C40-C35-N34	4.88	125.52	119.69
2	C	301[B]	QNG	C40-C35-C31	-4.81	126.49	129.48
2	C	301[B]	QNG	C40-C35-N34	4.79	125.41	119.69
2	C	301[B]	QNG	C02-N06-C05	4.62	120.45	117.22
2	A	301[A]	QNG	C40-C35-C31	-4.34	126.78	129.48
2	C	301[B]	QNG	C49-S48-N17	4.02	111.21	106.63
2	A	301[B]	QNG	C40-C35-C31	-4.01	126.99	129.48
2	A	301[A]	QNG	C49-S48-N17	3.79	110.96	106.63
2	B	301[A]	QNG	F41-C38-C32	-3.75	107.30	112.81
2	A	301[B]	QNG	C54-C46-C45	-3.65	106.59	109.96
2	B	301[B]	QNG	C16-N17-S48	-3.62	117.70	124.17
2	B	301[A]	QNG	C18-N14-N15	3.49	123.63	117.08
2	B	301[B]	QNG	F41-C38-C32	-3.49	107.69	112.81
2	C	301[B]	QNG	C18-N14-N15	3.45	123.56	117.08
2	C	301[B]	QNG	C13-C05-C01	-3.39	118.36	122.91
2	C	301[A]	QNG	C18-N14-N15	3.33	123.33	117.08
2	A	301[A]	QNG	C18-N14-N15	3.30	123.26	117.08
2	B	301[B]	QNG	C18-N14-N15	3.28	123.22	117.08
2	B	301[B]	QNG	C49-S48-N17	3.25	110.33	106.63
2	B	301[A]	QNG	C16-N17-S48	-3.21	118.44	124.17
2	C	301[B]	QNG	C16-N17-S48	-3.12	118.60	124.17
2	C	301[B]	QNG	F61-C60-C18	-3.11	107.03	112.12
2	A	301[A]	QNG	F41-C38-C32	-3.11	108.24	112.81
2	A	301[B]	QNG	C18-N14-N15	3.10	122.89	117.08
2	B	301[A]	QNG	C32-C31-C35	3.06	107.73	104.23
2	C	301[B]	QNG	C01-N43-C28	-3.05	118.47	123.33
2	A	301[A]	QNG	F52-C40-C35	-2.99	107.64	112.32
2	B	301[B]	QNG	C19-C01-C05	-2.99	105.72	110.64
2	C	301[A]	QNG	F41-C38-C32	-2.98	108.44	112.81
2	A	301[A]	QNG	C13-C05-C01	-2.94	118.97	122.91
2	C	301[B]	QNG	F41-C38-C32	-2.90	108.55	112.81
2	B	301[B]	QNG	C32-C31-C35	2.89	107.54	104.23
2	A	301[A]	QNG	O57-S55-C58	2.89	112.22	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301[A]	QNG	C32-C31-C35	2.87	107.52	104.23
2	B	301[B]	QNG	C23-C22-C21	-2.85	119.92	123.52
2	B	301[A]	QNG	C23-C22-C21	-2.85	119.92	123.52
2	B	301[A]	QNG	C49-S48-N17	2.84	109.87	106.63
2	B	301[B]	QNG	O59-S55-C58	2.83	112.15	108.44
2	B	301[B]	QNG	C30-N33-N34	2.81	125.66	117.77
2	A	301[A]	QNG	C32-C31-C35	2.78	107.41	104.23
2	A	301[B]	QNG	C32-C31-C35	2.75	107.37	104.23
2	A	301[B]	QNG	C23-C22-C21	-2.74	120.05	123.52
2	A	301[B]	QNG	C49-S48-N17	2.74	109.76	106.63
2	B	301[A]	QNG	F53-C40-C35	-2.74	108.03	112.32
2	B	301[A]	QNG	C25-C24-C23	-2.73	120.07	123.52
2	B	301[B]	QNG	C25-C24-C23	-2.70	120.11	123.52
2	A	301[A]	QNG	C23-C22-C21	-2.69	120.11	123.52
2	B	301[A]	QNG	C13-C05-C01	-2.68	119.31	122.91
2	A	301[B]	QNG	C25-C24-C23	-2.66	120.15	123.52
2	B	301[A]	QNG	C19-C01-C05	-2.65	106.27	110.64
2	B	301[A]	QNG	C30-N33-N34	2.65	125.22	117.77
2	A	301[B]	QNG	F41-C38-C32	-2.63	108.95	112.81
2	B	301[A]	QNG	C24-C23-C22	2.62	120.20	116.13
2	C	301[A]	QNG	C25-C24-C23	-2.60	120.23	123.52
2	C	301[A]	QNG	C03-C02-N06	-2.60	120.28	123.27
2	C	301[A]	QNG	C23-C22-C21	-2.60	120.23	123.52
2	B	301[B]	QNG	C24-C23-C22	2.58	120.14	116.13
2	C	301[B]	QNG	C09-C10-CL47	-2.58	116.64	122.81
2	A	301[A]	QNG	C25-C24-C23	-2.57	120.27	123.52
2	B	301[B]	QNG	O51-S48-C49	2.57	112.40	108.28
2	C	301[A]	QNG	C30-N33-N34	2.55	124.95	117.77
2	C	301[B]	QNG	C30-N33-N34	2.54	124.91	117.77
2	A	301[A]	QNG	F61-C60-C18	-2.54	107.98	112.12
2	B	301[A]	QNG	O51-S48-C49	2.53	112.34	108.28
2	B	301[A]	QNG	C13-C07-C08	2.53	123.99	121.14
2	B	301[A]	QNG	C12-C07-C08	2.53	121.09	117.47
2	A	301[B]	QNG	C07-C13-C05	-2.52	117.96	122.73
2	C	301[B]	QNG	F53-C40-C35	-2.52	108.38	112.32
2	C	301[A]	QNG	C13-C05-C01	-2.51	119.54	122.91
2	A	301[B]	QNG	C04-C13-C07	2.51	123.34	119.27
2	A	301[A]	QNG	C24-C23-C22	2.50	120.02	116.13
2	A	301[B]	QNG	C24-C23-C22	2.49	120.01	116.13
2	A	301[B]	QNG	O57-S55-C58	2.49	111.70	108.44
2	C	301[B]	QNG	C23-C22-C21	-2.49	120.38	123.52
2	B	301[B]	QNG	C13-C05-C01	-2.45	119.63	122.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301[B]	QNG	O59-S55-C58	2.44	111.64	108.44
2	A	301[A]	QNG	C07-C13-C05	-2.44	118.12	122.73
2	C	301[B]	QNG	C32-C31-C35	2.43	107.01	104.23
2	A	301[B]	QNG	C03-C02-N06	-2.43	120.49	123.27
2	C	301[B]	QNG	F42-C38-C32	-2.41	109.27	112.81
2	C	301[A]	QNG	C19-C01-C05	-2.40	106.68	110.64
2	A	301[B]	QNG	C13-C05-C01	-2.40	119.69	122.91
2	C	301[B]	QNG	C19-C01-C05	-2.40	106.69	110.64
2	C	301[A]	QNG	C49-S48-N17	2.39	109.36	106.63
2	A	301[B]	QNG	C03-C02-C44	2.39	123.99	120.34
2	C	301[B]	QNG	C25-C24-C23	-2.37	120.52	123.52
2	C	301[B]	QNG	C12-C11-C10	-2.37	118.02	120.89
2	C	301[A]	QNG	C24-C23-C22	2.37	119.82	116.13
2	C	301[A]	QNG	O50-S48-C49	2.36	112.07	108.28
2	C	301[B]	QNG	O50-S48-C49	2.36	112.06	108.28
2	B	301[B]	QNG	C12-C07-C08	2.34	120.82	117.47
2	A	301[B]	QNG	F64-C40-C35	-2.33	108.68	112.32
2	C	301[A]	QNG	C30-C28-N43	2.33	120.66	115.26
2	B	301[A]	QNG	C54-C46-C45	-2.32	107.82	109.96
2	B	301[B]	QNG	C30-C28-N43	2.31	120.62	115.26
2	C	301[A]	QNG	O57-S55-C58	2.31	111.47	108.44
2	B	301[A]	QNG	O59-S55-C58	2.31	111.46	108.44
2	C	301[A]	QNG	O50-S48-N17	2.30	111.79	107.10
2	C	301[A]	QNG	O59-S55-C58	2.30	111.45	108.44
2	B	301[A]	QNG	O57-S55-C58	2.29	111.44	108.44
2	A	301[A]	QNG	C04-C13-C07	2.28	122.97	119.27
2	B	301[A]	QNG	C12-C07-C13	-2.26	114.92	119.12
2	A	301[B]	QNG	C16-N17-S48	-2.26	120.14	124.17
2	B	301[A]	QNG	C30-C28-N43	2.23	120.44	115.26
2	A	301[A]	QNG	O50-S48-N17	2.23	111.64	107.10
2	A	301[B]	QNG	O50-S48-C49	2.22	111.84	108.28
2	B	301[A]	QNG	O50-S48-C49	2.21	111.83	108.28
2	C	301[B]	QNG	C24-C23-C22	2.20	119.56	116.13
2	A	301[A]	QNG	C01-N43-C28	-2.19	119.84	123.33
2	C	301[A]	QNG	O29-C28-N43	-2.19	119.26	122.95
2	C	301[A]	QNG	C01-N43-C28	-2.16	119.88	123.33
2	C	301[B]	QNG	C07-C13-C05	-2.15	118.66	122.73
2	A	301[A]	QNG	C09-C10-CL47	-2.15	117.66	122.81
2	A	301[B]	QNG	C30-N33-N34	2.13	123.77	117.77
2	B	301[B]	QNG	F53-C40-C35	-2.12	109.01	112.32
2	C	301[A]	QNG	O51-S48-C49	2.10	111.65	108.28
2	A	301[B]	QNG	F63-C60-C18	-2.08	108.72	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301[B]	QNG	C01-N43-C28	-2.08	120.01	123.33
2	C	301[B]	QNG	C12-C07-C08	2.07	120.44	117.47
2	C	301[B]	QNG	O29-C28-N43	-2.06	119.47	122.95
2	A	301[B]	QNG	O50-S48-N17	2.06	111.30	107.10
2	A	301[A]	QNG	C03-C02-N06	-2.05	120.92	123.27
2	B	301[B]	QNG	F27-C22-C23	2.04	121.17	118.25
2	C	301[B]	QNG	C03-C02-N06	-2.02	120.95	123.27
2	B	301[A]	QNG	F27-C22-C23	2.02	121.14	118.25
2	C	301[B]	QNG	F64-C40-C35	-2.01	109.18	112.32

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301[A]	QNG	C02-C44-C45-C46
2	C	301[A]	QNG	C45-C46-S55-O57
2	C	301[A]	QNG	C45-C46-S55-O59
2	C	301[A]	QNG	C54-C46-S55-O59
2	C	301[A]	QNG	C56-C46-S55-O57
2	C	301[A]	QNG	C56-C46-S55-O59
2	B	301[A]	QNG	C02-C44-C45-C46
2	B	301[A]	QNG	C45-C46-S55-O57
2	B	301[A]	QNG	C45-C46-S55-O59
2	B	301[A]	QNG	C54-C46-S55-O57
2	B	301[A]	QNG	C54-C46-S55-O59
2	B	301[A]	QNG	C56-C46-S55-O57
2	B	301[A]	QNG	C56-C46-S55-O59
2	B	301[B]	QNG	N14-C18-C60-F61
2	B	301[B]	QNG	N14-C18-C60-F62
2	B	301[B]	QNG	N14-C18-C60-F63
2	A	301[B]	QNG	C45-C46-S55-O59
2	A	301[A]	QNG	C16-N17-S48-O51
2	C	301[B]	QNG	C02-C44-C45-C46
2	B	301[B]	QNG	C02-C44-C45-C46
2	A	301[A]	QNG	C02-C44-C45-C46
2	C	301[A]	QNG	C54-C46-S55-O57
2	A	301[A]	QNG	C16-N17-S48-O50
2	C	301[A]	QNG	C16-N17-S48-O51
2	B	301[A]	QNG	N34-C35-C40-F53
2	A	301[A]	QNG	N34-C35-C40-F52
2	A	301[B]	QNG	C16-N17-S48-O51
2	B	301[A]	QNG	C16-N17-S48-O51

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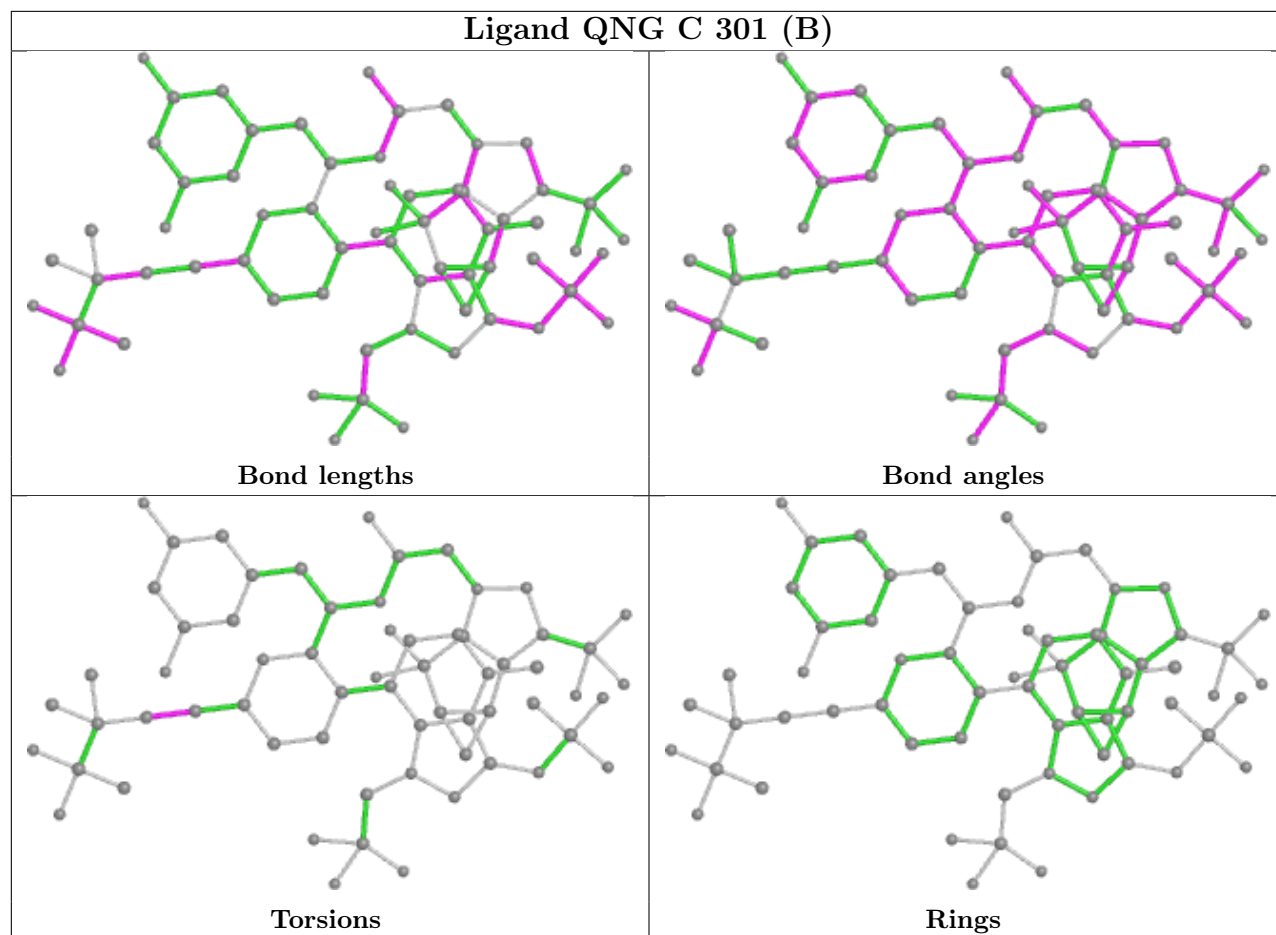
Mol	Chain	Res	Type	Atoms
2	B	301[A]	QNG	N34-C35-C40-F64
2	A	301[A]	QNG	N34-C35-C40-F53
2	A	301[A]	QNG	N34-C35-C40-F64
2	C	301[A]	QNG	C28-C30-N33-C32
2	B	301[A]	QNG	C28-C30-N33-C32
2	B	301[B]	QNG	C28-C30-N33-C32
2	B	301[A]	QNG	N34-C35-C40-F52
2	C	301[A]	QNG	C16-N17-S48-C49
2	A	301[A]	QNG	C16-N17-S48-C49
2	B	301[A]	QNG	N06-C02-C44-C45
2	C	301[A]	QNG	C28-C30-N33-N34

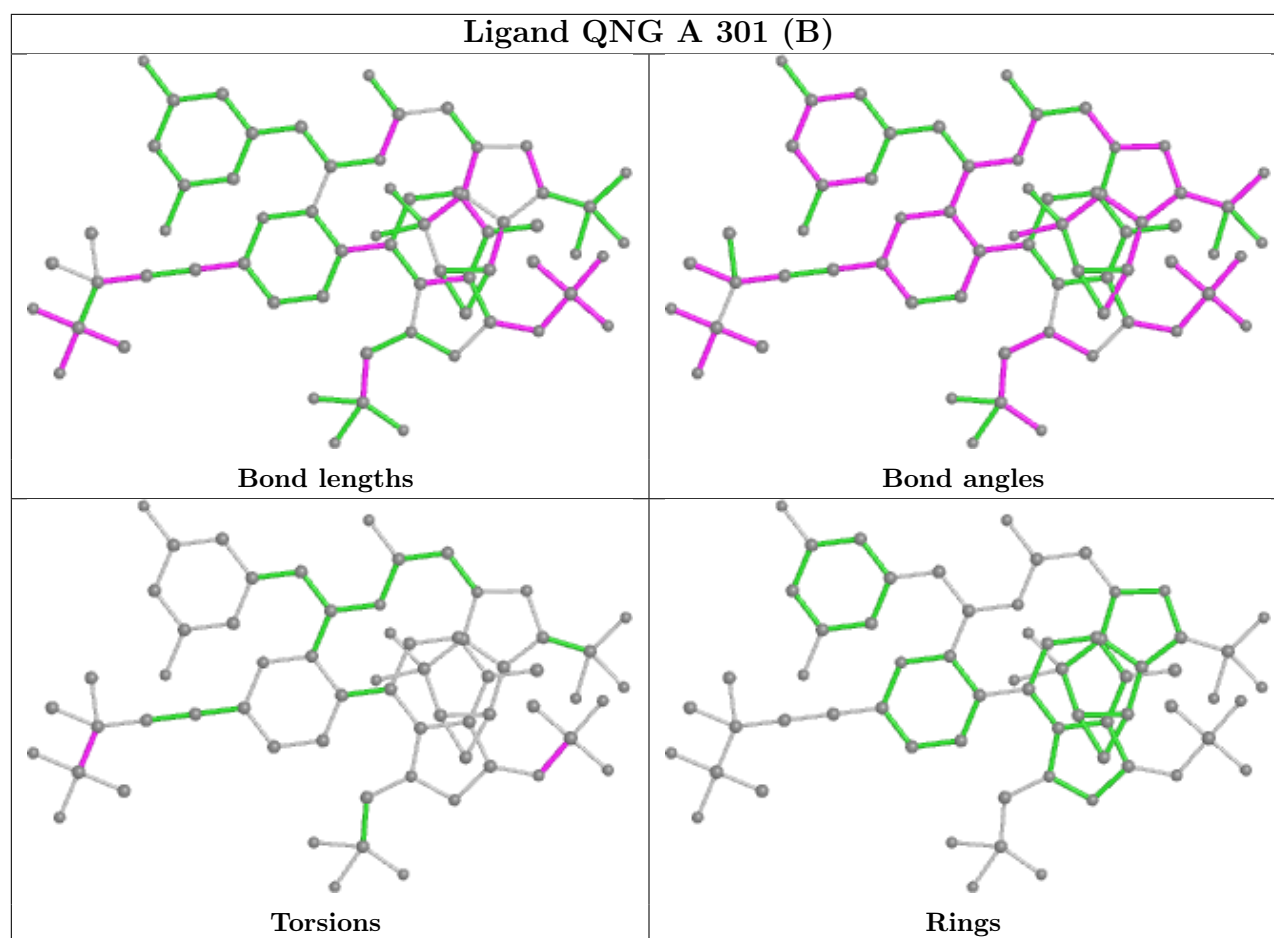
There are no ring outliers.

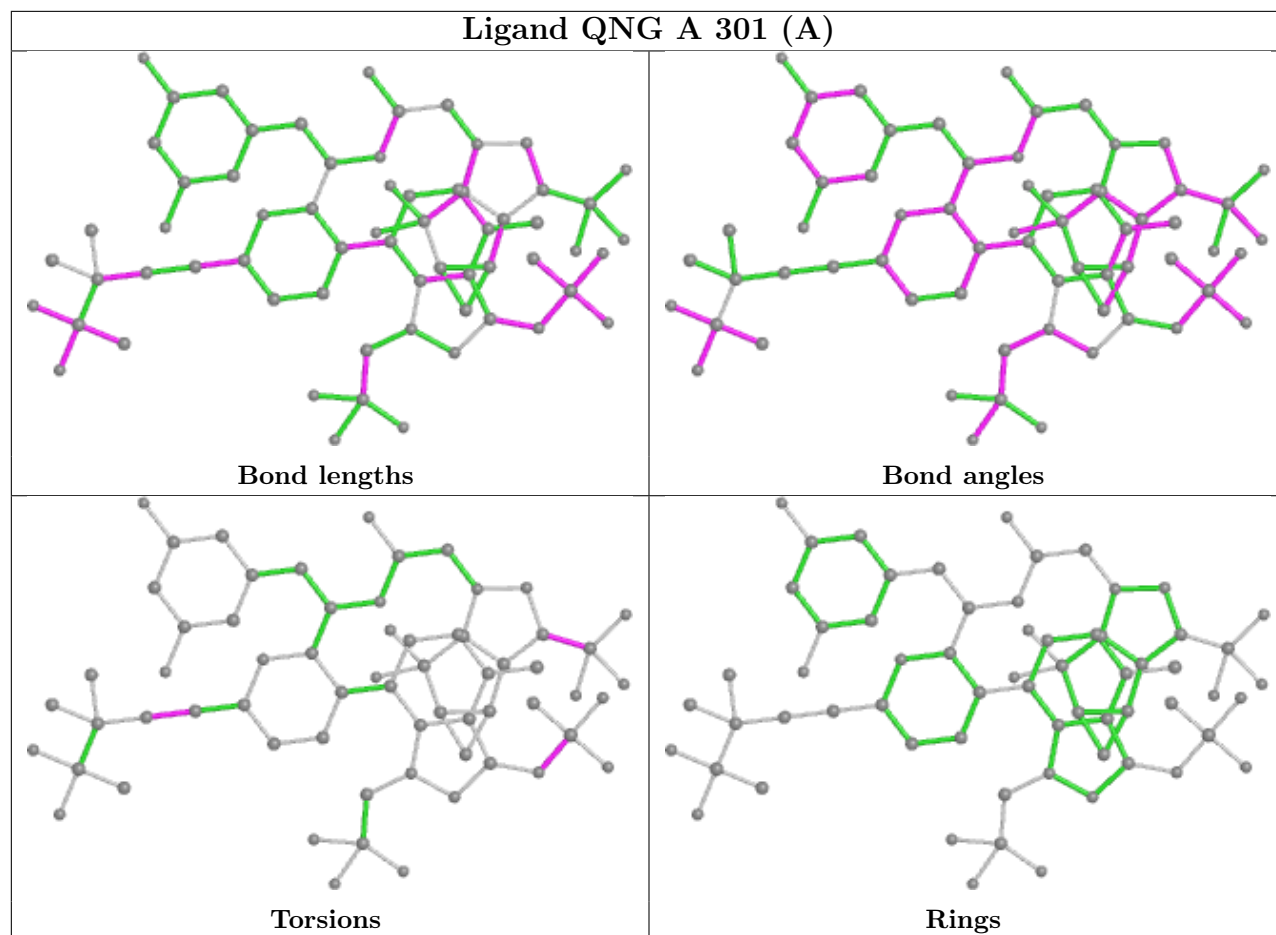
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301[B]	QNG	1	0
2	A	301[B]	QNG	1	0
2	A	301[A]	QNG	1	0

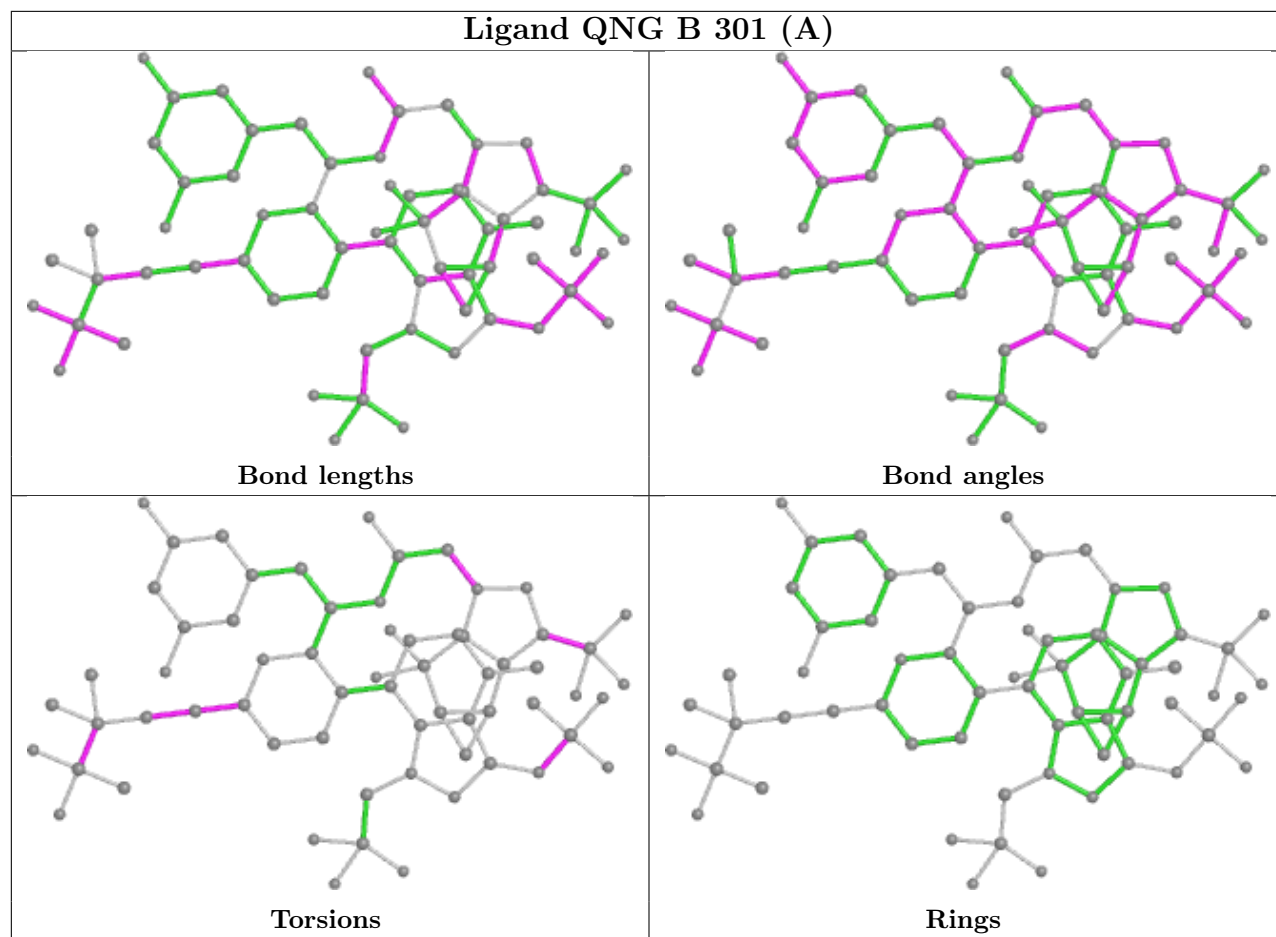
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

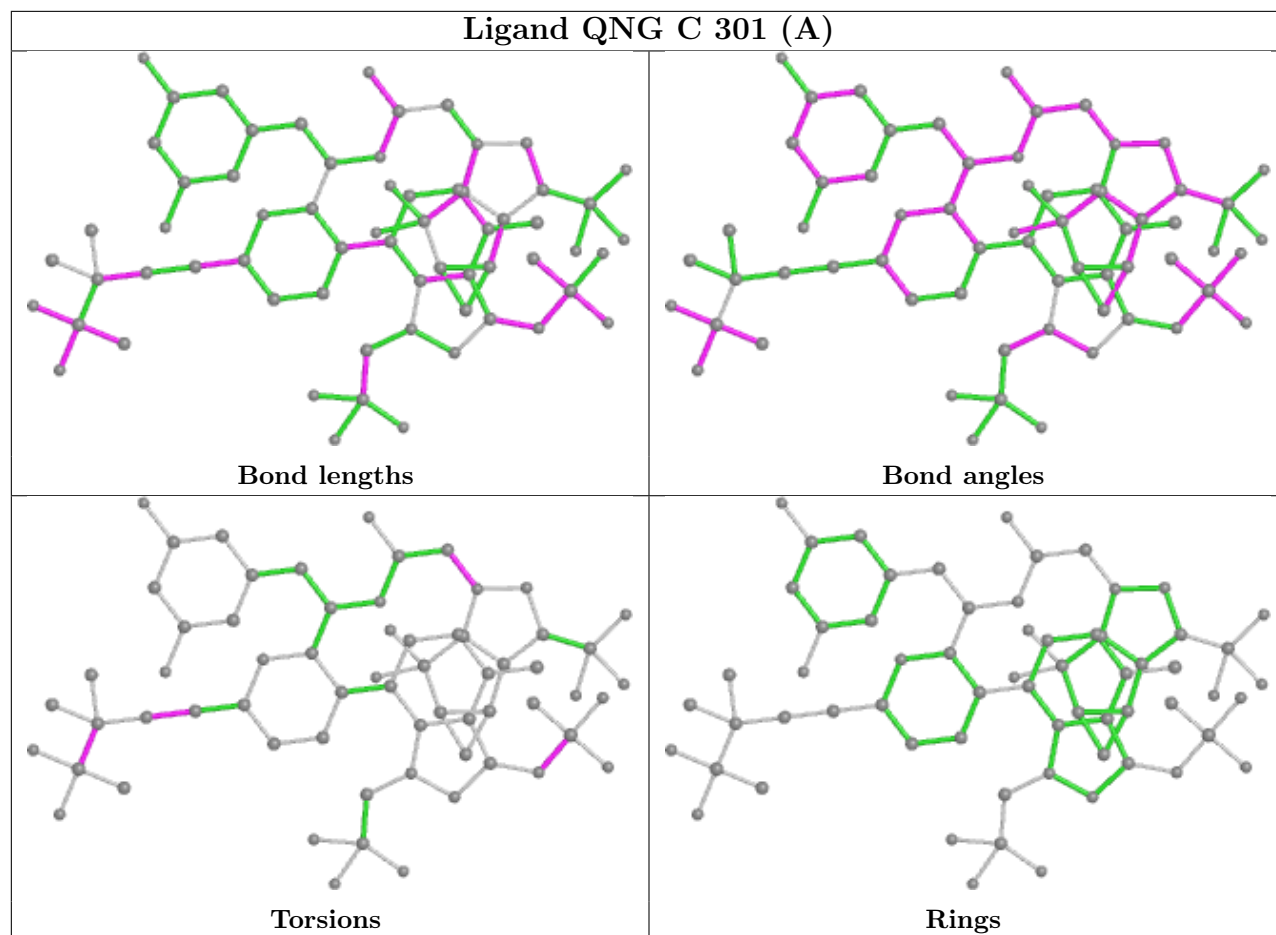


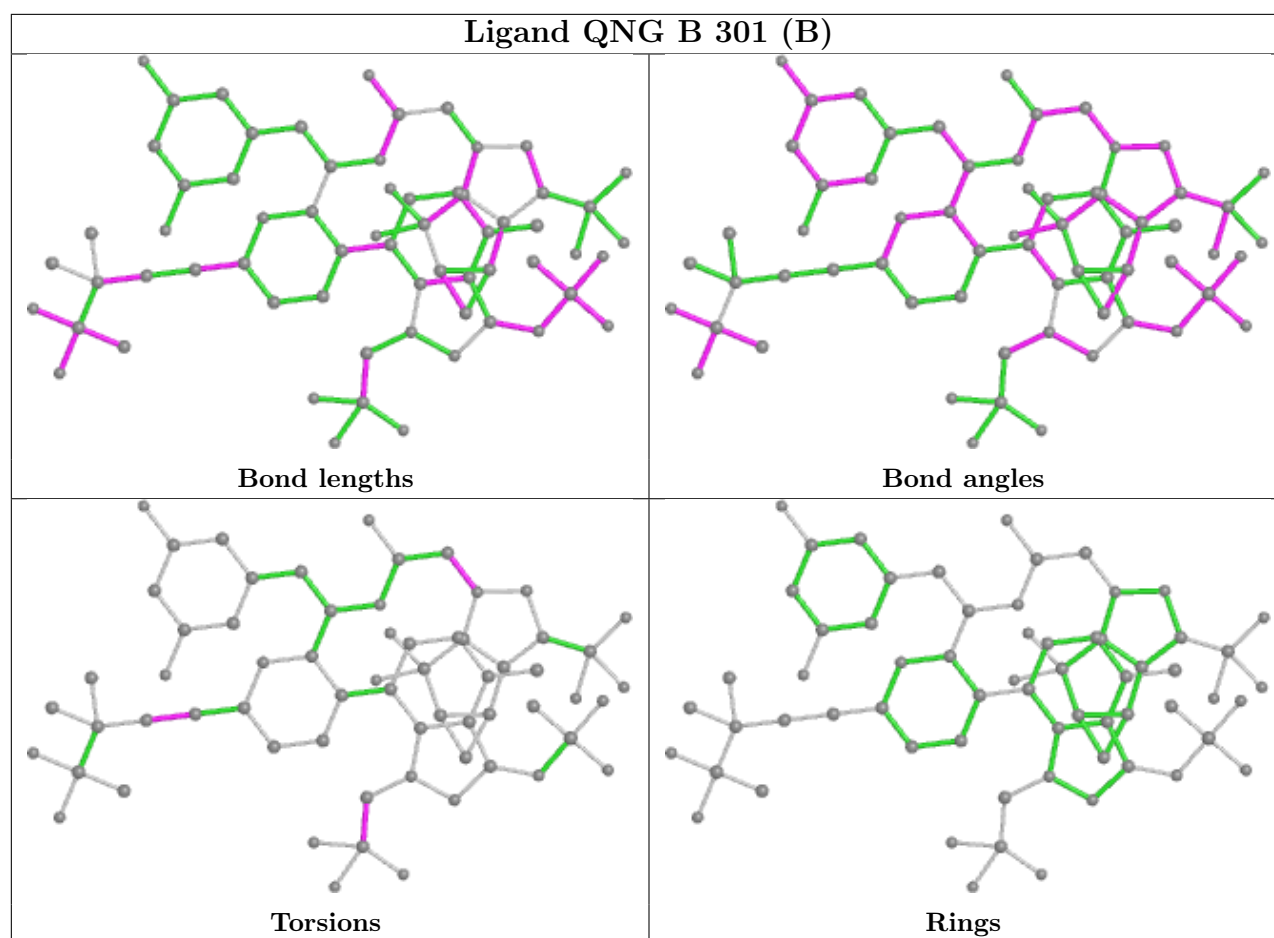












## 5.7 Other polymers [i](#)

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, 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	220/231 (95%)	-0.05	5 (2%) 60 58	21, 37, 67, 81	0
1	B	220/231 (95%)	0.20	12 (5%) 25 23	21, 39, 97, 154	0
1	C	220/231 (95%)	0.00	6 (2%) 54 52	19, 33, 72, 113	0
All	All	660/693 (95%)	0.05	23 (3%) 44 41	19, 36, 76, 154	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	GLU	9.0
1	B	181	VAL	7.2
1	B	177	ALA	6.3
1	B	184	ALA	4.8
1	B	185	ALA	4.7
1	B	86	VAL	4.1
1	C	188	THR	3.9
1	B	186	THR	3.5
1	C	7	GLN	3.4
1	B	179	GLN	3.0
1	C	95	GLN	2.8
1	C	88	ALA	2.7
1	B	93	PRO	2.7
1	B	178	SER	2.5
1	A	95	GLN	2.5
1	B	88	ALA	2.4
1	A	86	VAL	2.3
1	C	8	GLY	2.2
1	A	177	ALA	2.1
1	A	178	SER	2.1
1	B	89	GLY	2.1
1	A	94	GLY	2.1
1	C	177	ALA	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.

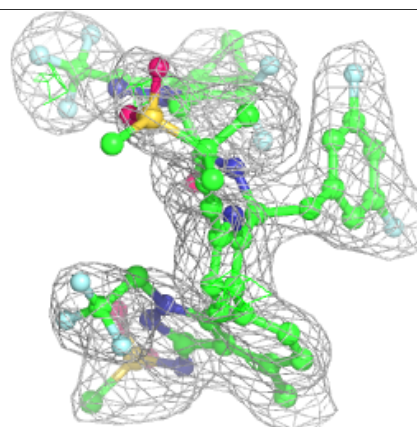
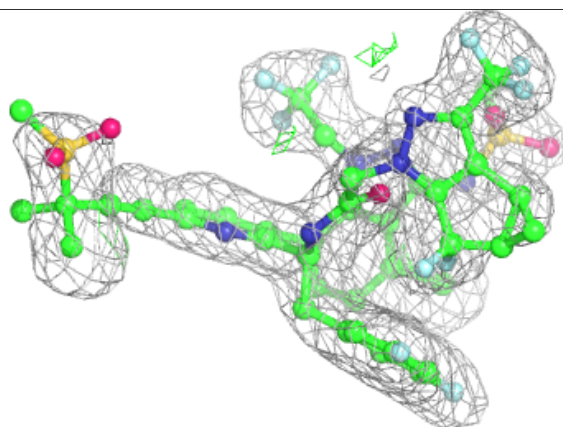
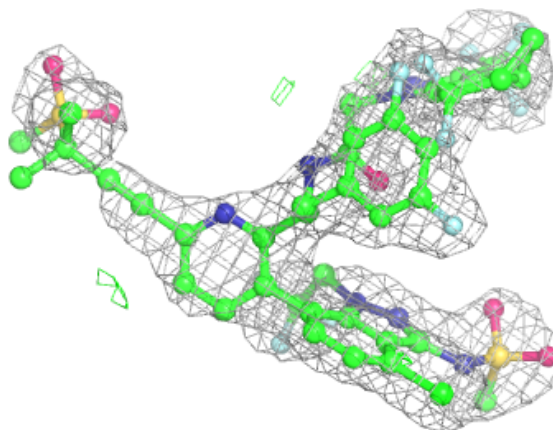
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	B	303	1/1	0.76	0.19	38,38,38,38	0
3	IOD	A	303	1/1	0.81	0.10	91,91,91,91	0
3	IOD	A	304	1/1	0.89	0.27	30,30,30,30	0
2	QNG	B	301[A]	64/64	0.90	0.22	18,30,38,44	64
2	QNG	B	301[B]	64/64	0.90	0.22	18,30,38,41	64
2	QNG	A	301[B]	64/64	0.93	0.19	26,32,39,41	64
2	QNG	C	301[A]	64/64	0.93	0.18	20,31,39,41	64
2	QNG	A	301[A]	64/64	0.93	0.19	25,32,40,42	64
2	QNG	C	301[B]	64/64	0.93	0.18	19,31,39,44	64
4	CL	C	305	1/1	0.94	0.27	26,26,26,26	0
4	CL	B	306	1/1	0.96	0.31	37,37,37,37	0
4	CL	C	308	1/1	0.96	0.23	42,42,42,42	0
4	CL	A	305	1/1	0.97	0.26	32,32,32,32	0
4	CL	A	306	1/1	0.97	0.22	27,27,27,27	0
4	CL	A	307	1/1	0.97	0.25	24,24,24,24	0
4	CL	A	308	1/1	0.97	0.27	37,37,37,37	0
4	CL	C	303	1/1	0.98	0.17	29,29,29,29	0
4	CL	C	307	1/1	0.98	0.22	18,18,18,18	0
4	CL	C	306	1/1	0.98	0.30	38,38,38,38	0
3	IOD	B	302	1/1	0.99	0.09	38,38,38,38	0
4	CL	C	304	1/1	0.99	0.13	27,27,27,27	0
3	IOD	A	302	1/1	0.99	0.10	42,42,42,42	0
4	CL	B	304	1/1	0.99	0.11	19,19,19,19	0
4	CL	B	305	1/1	1.00	0.26	3,3,3,3	0
3	IOD	C	302	1/1	1.00	0.13	35,35,35,35	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.

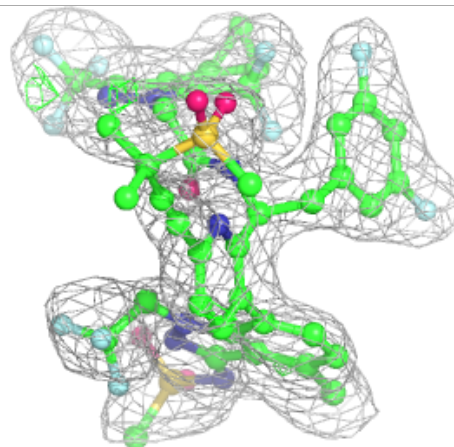
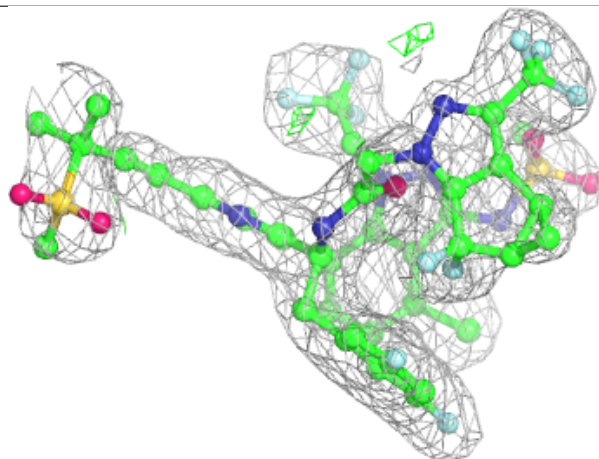
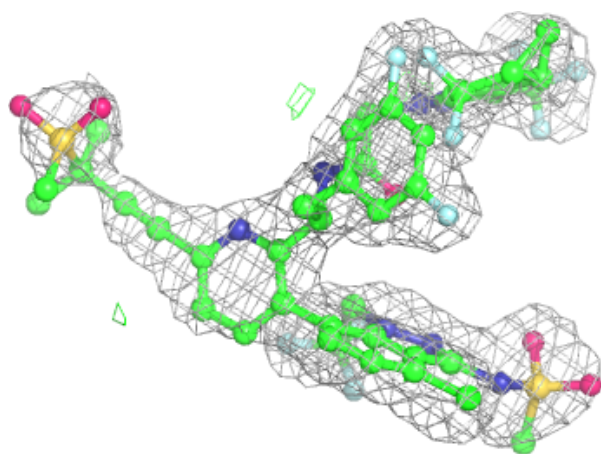
**Electron density around QNG B 301 (A):**

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



**Electron density around QNG B 301 (B):**

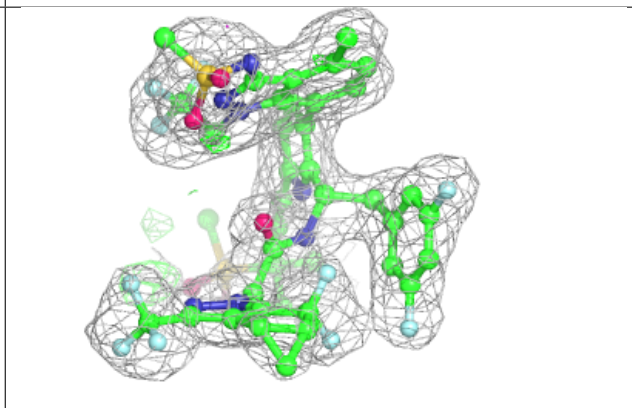
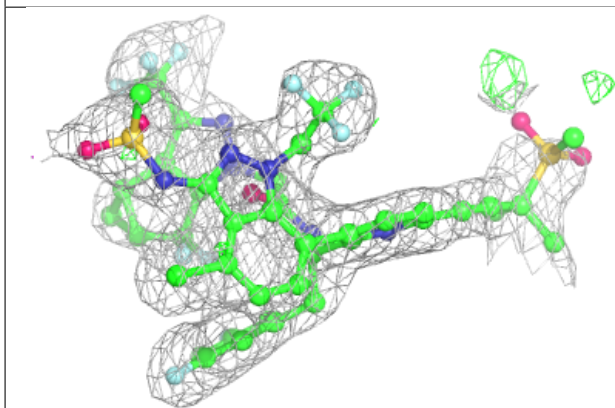
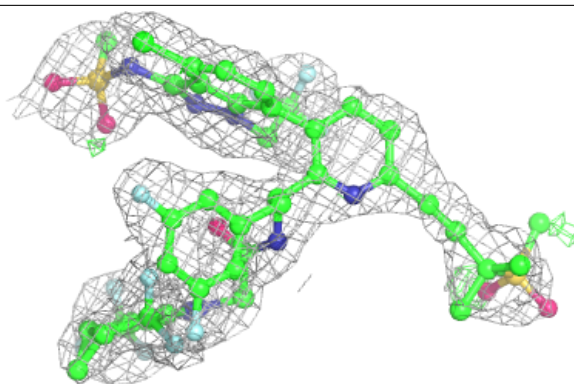
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



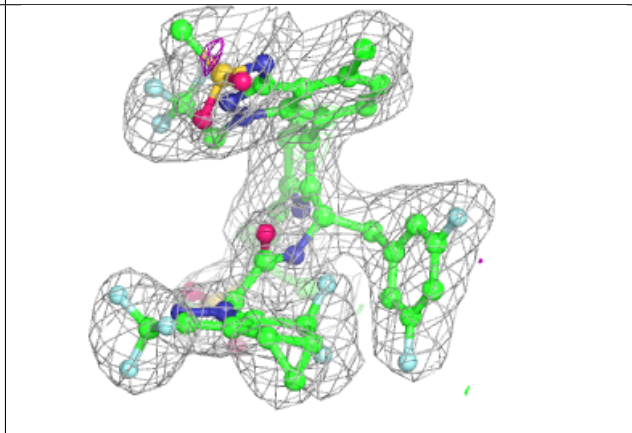
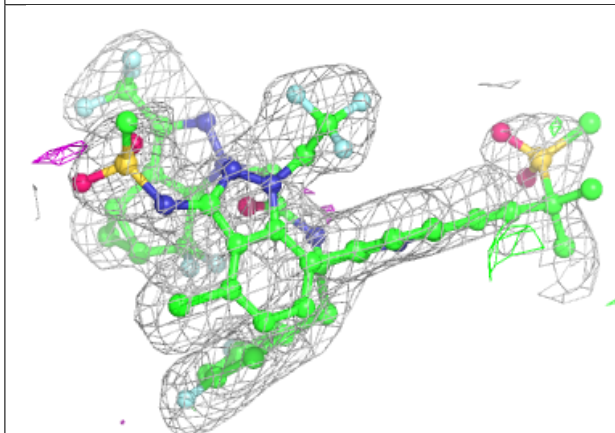
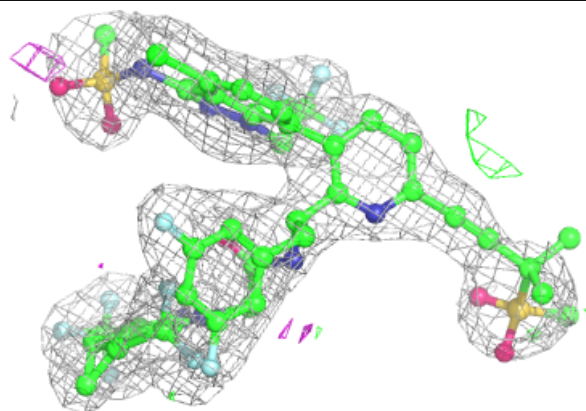


**Electron density around QNG A 301 (B):**

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

**Electron density around QNG C 301 (A):**

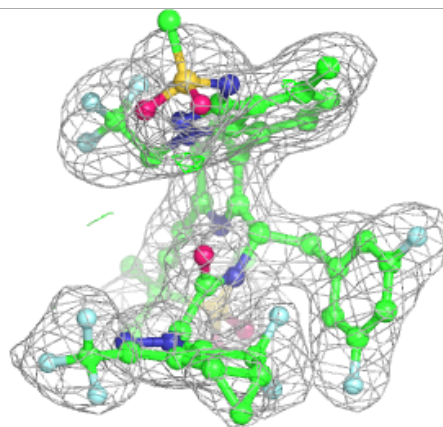
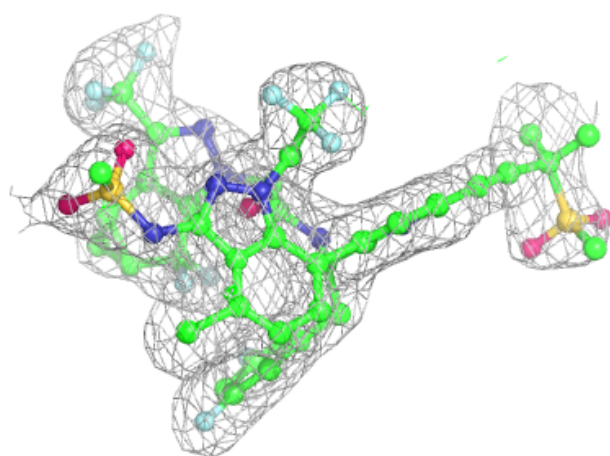
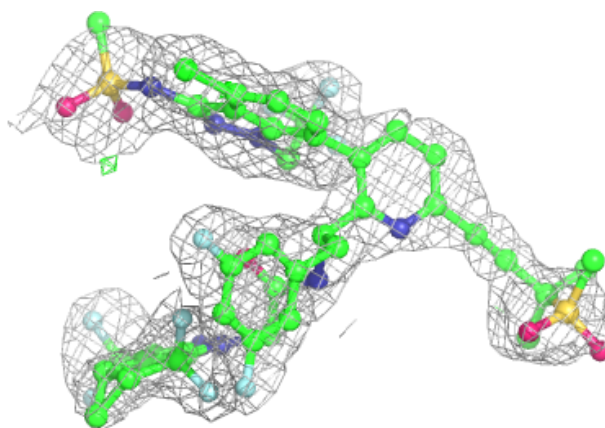
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





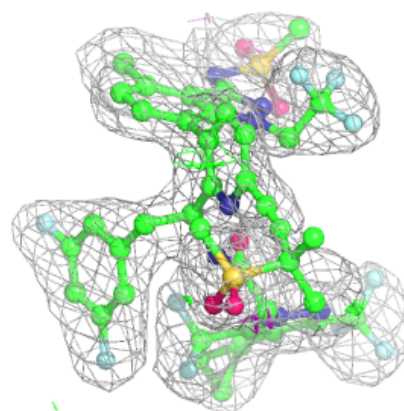
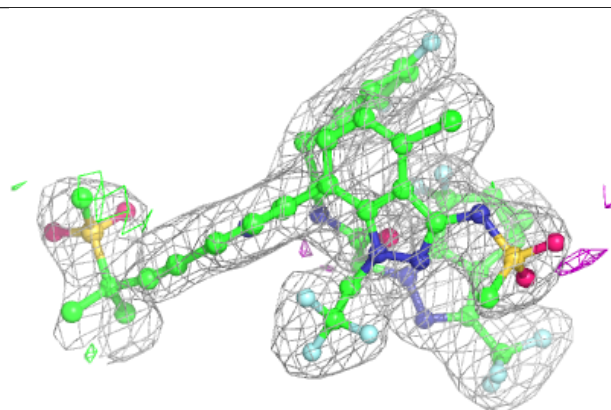
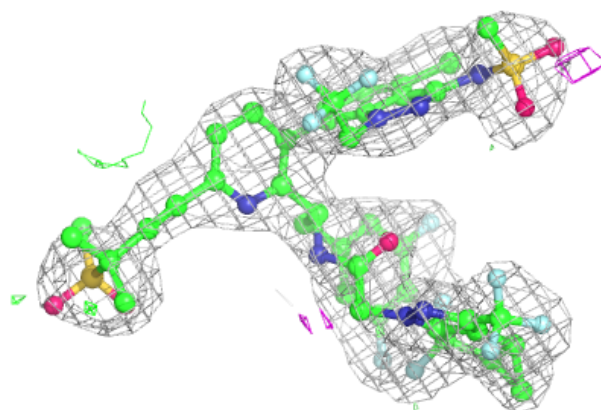
**Electron density around QNG A 301 (A):**

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



**Electron density around QNG C 301 (B):**

$2mF_o-DF_c$  (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.