



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2021 – 02:11 pm GMT

PDB ID : 7B4C  
Title : Structural basis of reactivation of oncogenic p53 mutants by a small molecule: methylene quinuclidinone (MQ). Human p53DBD-R273C mutant bound to MQ: R273C-MQ (II)  
Authors : Degtjarik, O.; Rozenberg, H.; Shakked, Z.  
Deposited on : 2020-12-02  
Resolution : 1.71 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 : 1.8.4 (270009), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

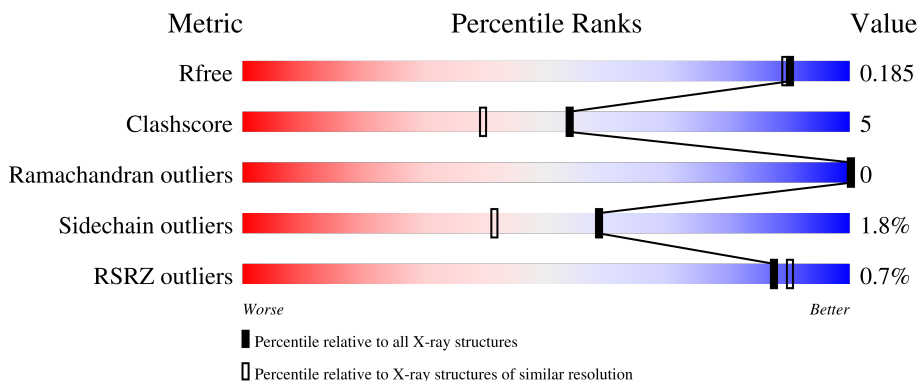
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.71 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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  $\geq 3$ , 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	200	
1	B	200	
1	C	200	
1	D	200	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6995 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 Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	191	1590	979	288	303	20	0	16	0
1	B	190	1560	960	282	294	24	0	14	0
1	C	191	1598	984	292	299	23	0	17	0
1	D	193	1595	983	293	297	22	0	16	0

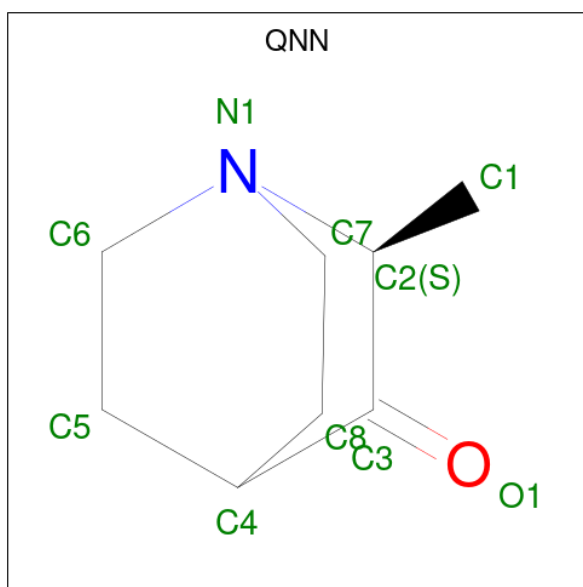
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	273	CYS	ARG	engineered mutation	UNP P04637
B	273	CYS	ARG	engineered mutation	UNP P04637
C	273	CYS	ARG	engineered mutation	UNP P04637
D	273	CYS	ARG	engineered mutation	UNP P04637

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

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

- Molecule 3 is (2 {S})-2-methyl-1-azabicyclo[2.2.2]octan-3-one (three-letter code: QNN) (formula: C<sub>8</sub>H<sub>13</sub>NO) (labeled as "Ligand of Interest" by depositor).



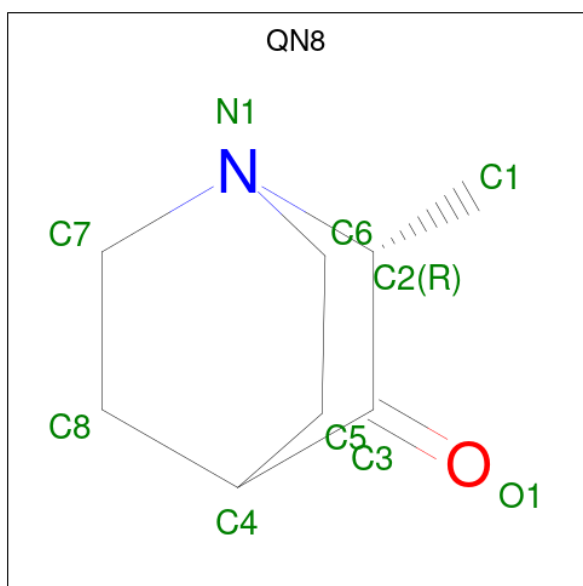
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	10	8	1	1	0	1
3	B	1	10	8	1	1	0	1
3	B	1	10	8	1	1	0	1
3	C	1	10	8	1	1	0	1
3	C	1	10	8	1	1	0	1
3	D	1	10	8	1	1	0	1

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			4	2 2		
4	B	1	Total	C O	0	0
			4	2 2		
4	C	1	Total	C O	0	0
			4	2 2		
4	D	1	Total	C O	0	0
			4	2 2		

- Molecule 5 is (2 {R})-2-methyl-1-azabicyclo[2.2.2]octan-3-one (three-letter code: QN8) (formula: C<sub>8</sub>H<sub>13</sub>NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	10	8	1	1	0	1

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	D	1	7	4	3	0	0
6	D	1	7	4	3	0	0

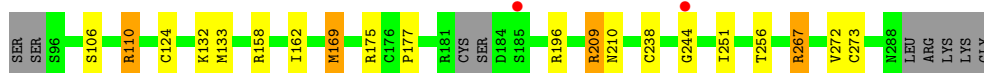
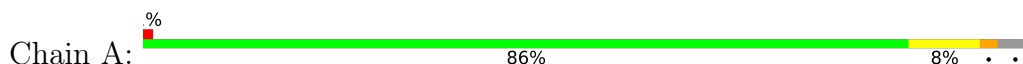
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	148	149	149	0	2
7	B	135	136	136	0	3
7	C	137	137	137	0	0
7	D	124	126	126	0	3

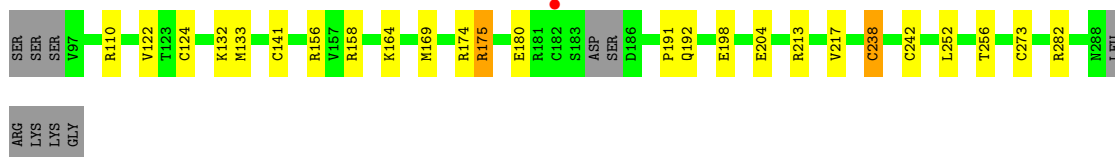
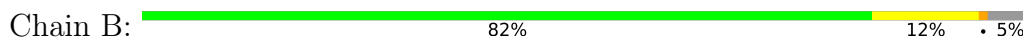
### 3 Residue-property plots [i](#)

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.

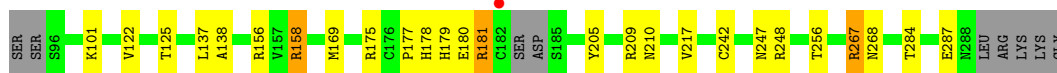
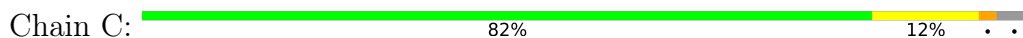
- Molecule 1: Cellular tumor antigen p53



- Molecule 1: Cellular tumor antigen p53



- Molecule 1: Cellular tumor antigen p53



- Molecule 1: Cellular tumor antigen p53



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.88Å 71.08Å 84.92Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	42.75 – 1.71 42.75 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.2 (42.75-1.71) 98.3 (42.75-1.71)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 1.71Å)	Xtrriage
Refinement program	REFMAC 5.8.0266	Depositor
R, $R_{free}$	0.149 , 0.182 0.154 , 0.185	Depositor DCC
$R_{free}$ test set	4333 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtrriage
Anisotropy	0.901	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.064 for -k,-h,-l 0.059 for k,h,-l 0.366 for h,-k,-l	Xtrriage
Reported twinning fraction	0.640 for H, K, L 0.360 for -h,-k,l	Depositor
Outliers	0 of 87211 reflections	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6995	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.30% 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: QN8, ZN, EDO, QNN, PEG

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	0.97	0/1630	1.07	6/2215 (0.3%)
1	B	0.92	1/1597 (0.1%)	1.04	6/2170 (0.3%)
1	C	0.87	0/1634	1.00	6/2214 (0.3%)
1	D	0.89	1/1635 (0.1%)	0.97	0/2221
All	All	0.91	2/6496 (0.0%)	1.02	18/8820 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	204	GLU	CD-OE1	6.31	1.32	1.25
1	D	271	GLU	CD-OE1	5.49	1.31	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	B	175	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	B	174	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	C	181	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	A	267	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	110[A]	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	A	110[B]	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	A	175	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	C	267	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	175	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	C	158	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	205	TYR	CB-CG-CD2	5.74	124.45	121.00
1	B	282	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	110	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	B	213	ARG	NE-CZ-NH1	5.35	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	C	181	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	A	196	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	1590	0	1512	18	0
1	B	1560	0	1472	15	0
1	C	1598	0	1532	12	0
1	D	1595	0	1517	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	0	0	0
3	B	20	0	0	0	0
3	C	20	0	0	0	0
3	D	10	0	0	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
5	B	10	0	0	0	0
6	D	14	0	20	1	0
7	A	149	0	0	1	0
7	B	136	0	0	3	0
7	C	137	0	0	1	0
7	D	126	0	0	3	0
All	All	6995	0	6077	67	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (67) 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:251:ILE:HG13	1:A:272[B]:VAL:HG22	1.63	0.80
1:A:124[A]:CYS:SG	1:A:133[A]:MET:SD	2.82	0.76
1:D:162[A]:ILE:HD12	1:D:254:ILE:HD11	1.69	0.74
1:B:132:LYS:CE	1:B:273[B]:CYS:SG	2.76	0.74
1:B:124[A]:CYS:SG	1:B:133[A]:MET:SD	2.86	0.73
1:D:277[B]:CYS:HB2	1:D:280[B]:ARG:HH21	1.53	0.73
1:A:158:ARG:HB3	1:A:256[B]:THR:CG2	2.22	0.69
1:D:251:ILE:HG13	1:D:272[B]:VAL:HG22	1.74	0.69
1:D:251:ILE:HG13	1:D:272[B]:VAL:CG2	2.23	0.69
1:D:251:ILE:HD11	1:D:272[B]:VAL:CG2	2.26	0.65
1:D:251:ILE:HD11	1:D:272[B]:VAL:HG21	1.81	0.61
1:D:251:ILE:CD1	1:D:272[B]:VAL:CG2	2.79	0.61
1:B:132:LYS:NZ	1:B:273[B]:CYS:SG	2.74	0.60
1:A:251:ILE:HG13	1:A:272[B]:VAL:CG2	2.30	0.60
1:D:114:LEU:HD22	6:D:305:PEG:H21	1.84	0.59
1:D:256[B]:THR:HG21	7:D:498:HOH:O	2.02	0.58
1:D:277[B]:CYS:HB2	1:D:280[B]:ARG:NH2	2.18	0.58
1:A:132:LYS:HE2	1:A:273[B]:CYS:SG	2.43	0.58
1:D:122[B]:VAL:CG1	1:D:122[B]:VAL:O	2.52	0.58
1:C:177:PRO:HA	1:C:180:GLU:HG2	1.86	0.57
1:C:284:THR:O	1:C:287:GLU:HG2	2.05	0.57
1:D:122[B]:VAL:O	1:D:122[B]:VAL:HG13	2.05	0.56
1:A:251:ILE:HD11	1:A:272[B]:VAL:CG2	2.35	0.56
1:D:158:ARG:HB3	1:D:256[B]:THR:CG2	2.35	0.56
1:D:277[B]:CYS:CB	1:D:280[B]:ARG:HH21	2.17	0.56
1:D:251:ILE:CG1	1:D:272[B]:VAL:CG2	2.84	0.56
1:C:256:THR:HG22	1:C:267:ARG:HG3	1.89	0.55
1:A:158:ARG:HB3	1:A:256[B]:THR:HG23	1.87	0.55
1:A:251:ILE:HD11	1:A:272[B]:VAL:HG21	1.88	0.55
1:A:256[B]:THR:HG22	7:A:512:HOH:O	2.06	0.55
1:B:238[A]:CYS:SG	7:B:522[A]:HOH:O	2.58	0.54
1:D:209:ARG:HD2	7:D:503:HOH:O	2.08	0.53
1:B:256:THR:HG23	7:B:506:HOH:O	2.08	0.53
1:C:178:HIS:O	1:C:181:ARG:HD3	2.10	0.52
1:A:132:LYS:CE	1:A:273[B]:CYS:SG	2.98	0.52
1:C:158:ARG:CZ	1:C:217[B]:VAL:HG21	2.41	0.51
1:B:175:ARG:HD3	1:B:191:PRO:O	2.10	0.51
1:C:268[B]:ASN:ND2	7:C:402:HOH:O	2.43	0.50
1:C:137[B]:LEU:HD23	1:C:138:ALA:N	2.26	0.50
1:D:277[B]:CYS:CB	1:D:280[B]:ARG:NH2	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122[A]:VAL:HG11	1:C:125:THR:HB	1.93	0.49
1:A:251:ILE:CG1	1:A:272[B]:VAL:CG2	2.89	0.49
1:A:251:ILE:CD1	1:A:272[B]:VAL:CG2	2.91	0.49
1:B:133[B]:MET:SD	1:B:141[B]:CYS:HB3	2.52	0.49
1:C:101:LYS:O	1:C:267:ARG:HD2	2.13	0.48
1:D:137[A]:LEU:C	1:D:137[A]:LEU:HD23	2.34	0.48
1:A:177:PRO:HD3	1:A:244:GLY:O	2.14	0.47
1:A:162:ILE:HD12	1:A:169:MET:HE1	1.97	0.47
1:B:132:LYS:HE3	1:B:273[B]:CYS:SG	2.55	0.46
1:A:209:ARG:HG2	1:A:210:ASN:N	2.31	0.46
1:B:132:LYS:HE2	1:B:273[B]:CYS:SG	2.55	0.45
1:D:209:ARG:CD	7:D:503:HOH:O	2.63	0.45
1:A:158:ARG:HB3	1:A:256[B]:THR:HG22	1.97	0.45
1:B:158:ARG:CZ	1:B:217[B]:VAL:HG21	2.47	0.45
1:D:98:PRO:HG2	1:D:162[A]:ILE:HD11	1.99	0.44
1:C:179:HIS:HE1	1:C:242:CYS:SG	2.38	0.44
1:A:106:SER:HB2	1:B:242:CYS:SG	2.58	0.44
1:B:180:GLU:CD	1:B:192:GLN:HG2	2.38	0.43
1:B:164:LYS:HA	1:B:252:LEU:CD1	2.48	0.43
1:D:193:HIS:CE1	1:D:214:HIS:HB3	2.52	0.43
1:B:238[A]:CYS:CB	7:B:522[A]:HOH:O	2.66	0.43
1:D:251:ILE:CG1	1:D:272[B]:VAL:HG23	2.50	0.42
1:B:122[B]:VAL:HG13	1:B:122[B]:VAL:O	2.20	0.42
1:D:162[B]:ILE:HD11	1:D:169:MET:HG2	2.02	0.41
1:A:256[A]:THR:HG22	1:A:267:ARG:HG3	2.03	0.41
1:C:247:ASN:OD1	1:C:248[B]:ARG:NH2	2.54	0.41
1:C:156:ARG:HB3	1:C:217[A]:VAL:CG2	2.52	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	203/200 (102%)	201 (99%)	2 (1%)	0	100	100
1	B	199/200 (100%)	197 (99%)	2 (1%)	0	100	100
1	C	202/200 (101%)	200 (99%)	2 (1%)	0	100	100
1	D	205/200 (102%)	203 (99%)	2 (1%)	0	100	100
All	All	809/800 (101%)	801 (99%)	8 (1%)	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	182/179 (102%)	176 (97%)	6 (3%)	38	17
1	B	177/179 (99%)	173 (98%)	4 (2%)	50	31
1	C	184/179 (103%)	181 (98%)	3 (2%)	62	47
1	D	179/179 (100%)	176 (98%)	3 (2%)	60	44
All	All	722/716 (101%)	706 (98%)	16 (2%)	59	33

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110[A]	ARG
1	A	110[B]	ARG
1	A	169	MET
1	A	209	ARG
1	A	238[A]	CYS
1	A	238[B]	CYS
1	B	169	MET
1	B	198	GLU
1	B	238[A]	CYS
1	B	238[B]	CYS
1	C	169	MET
1	C	209	ARG
1	C	210	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
1	D	209	ARG
1	D	217[A]	VAL
1	D	217[B]	VAL

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

Mol	Chain	Res	Type
1	B	168	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 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

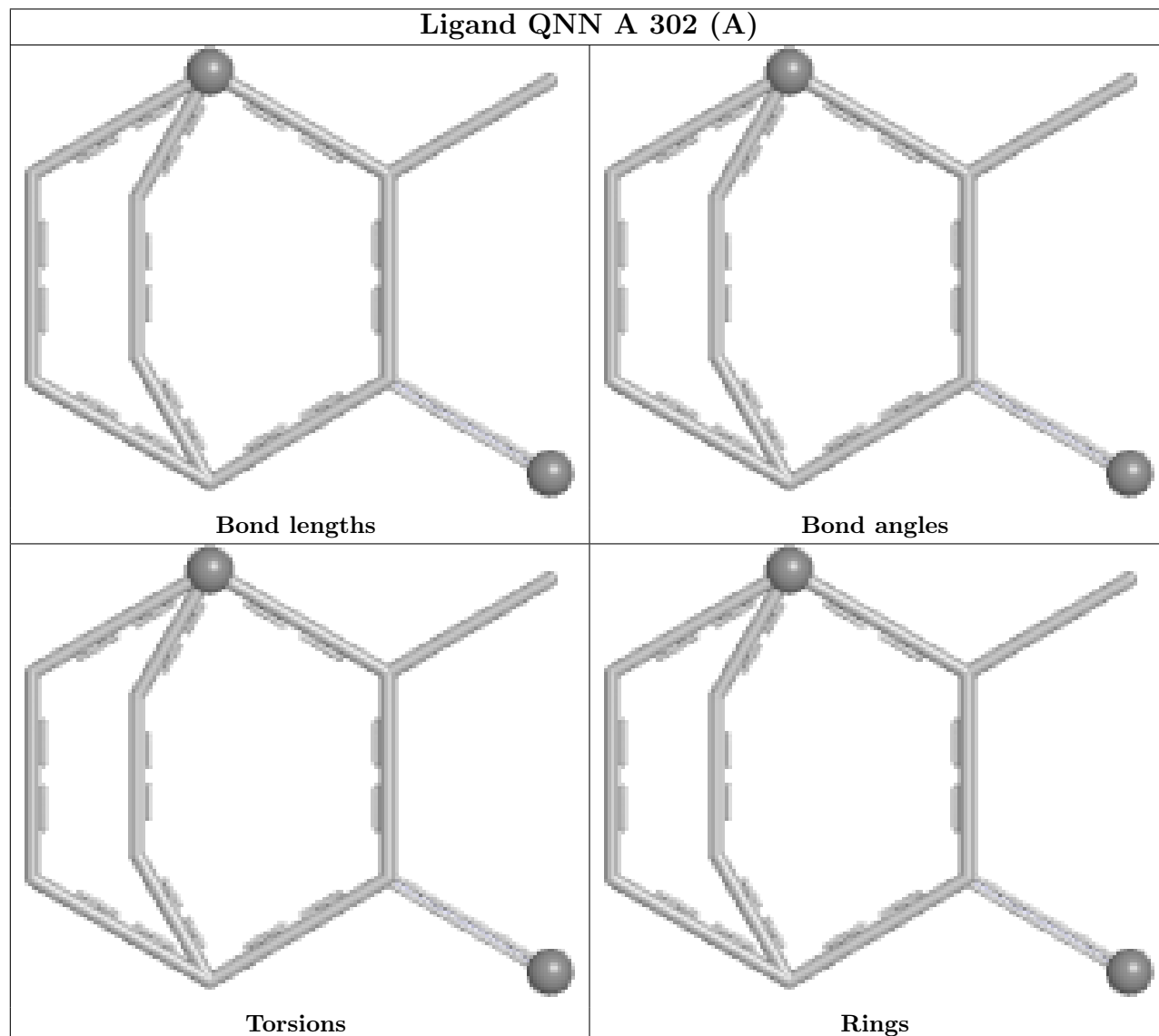
There are no torsion outliers.

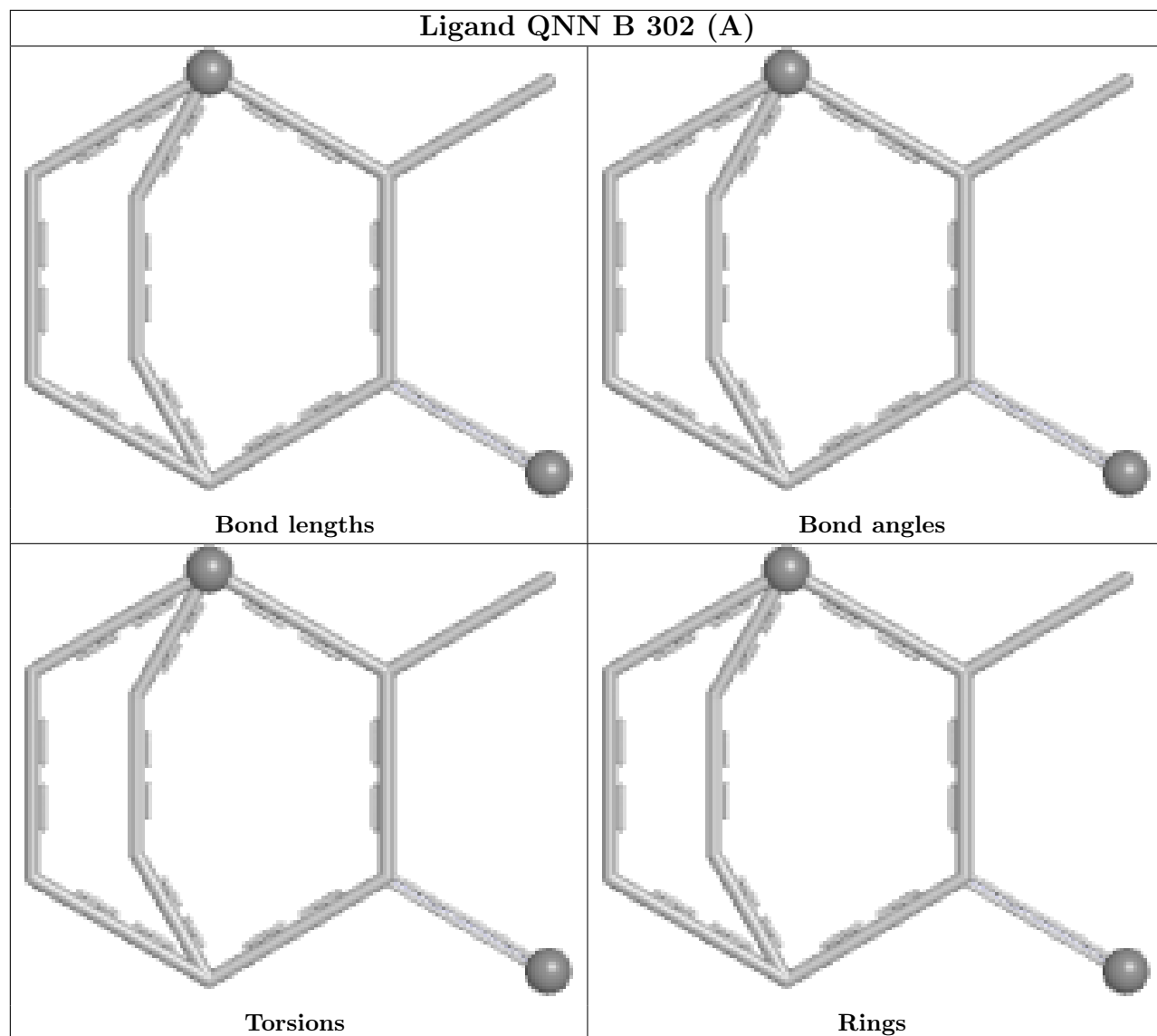
There are no ring outliers.

No monomer is involved in short contacts.

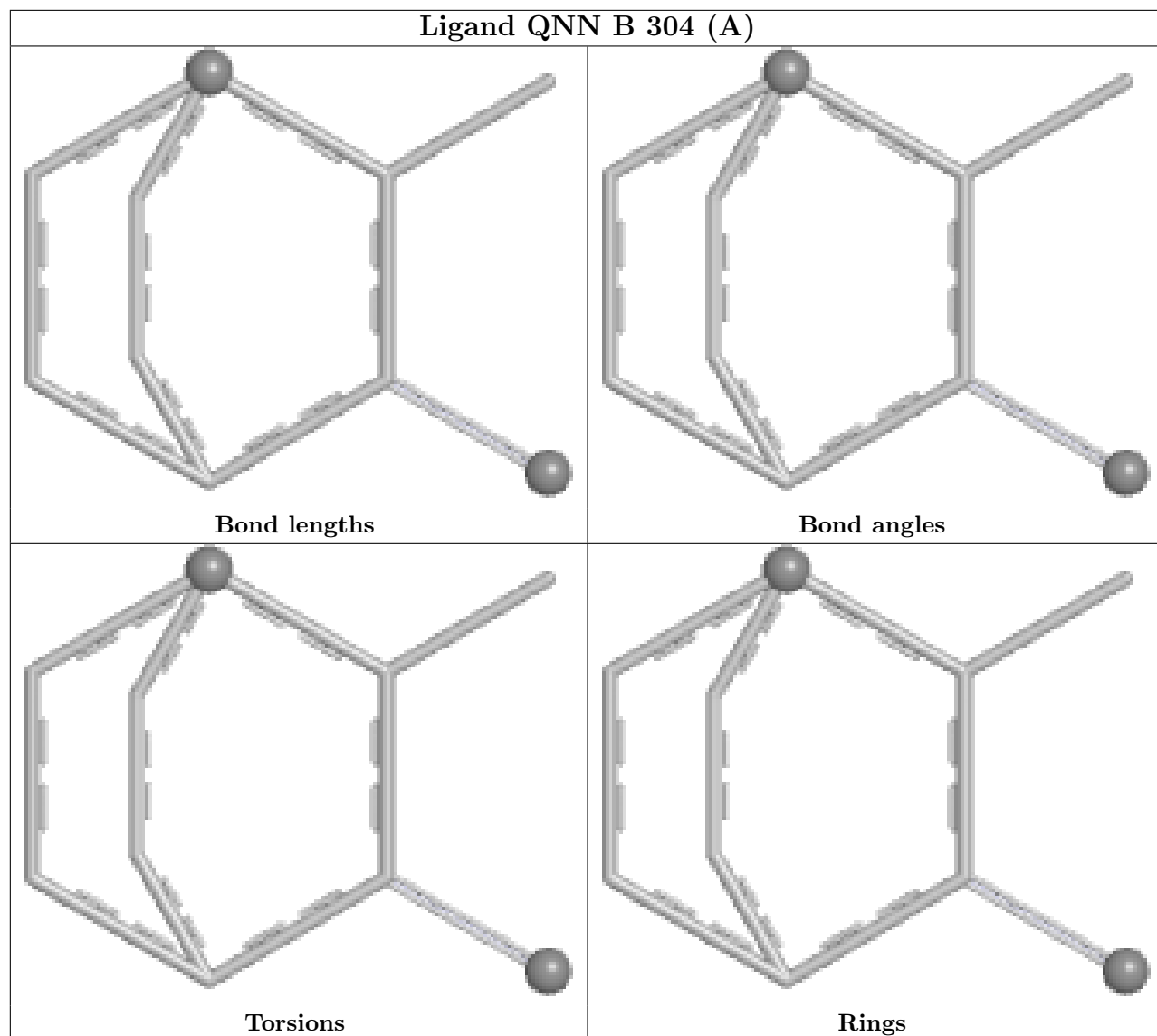
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

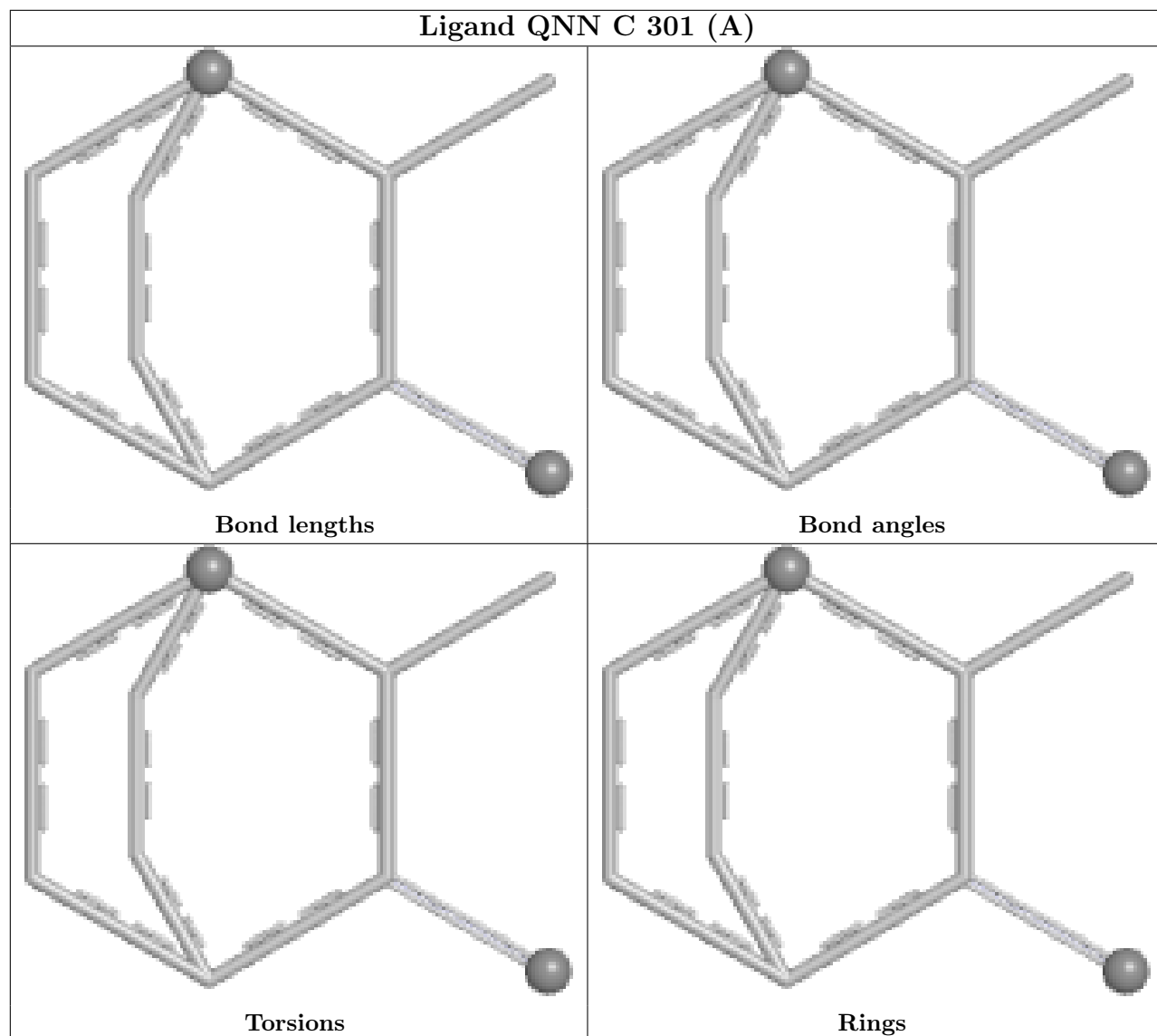
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

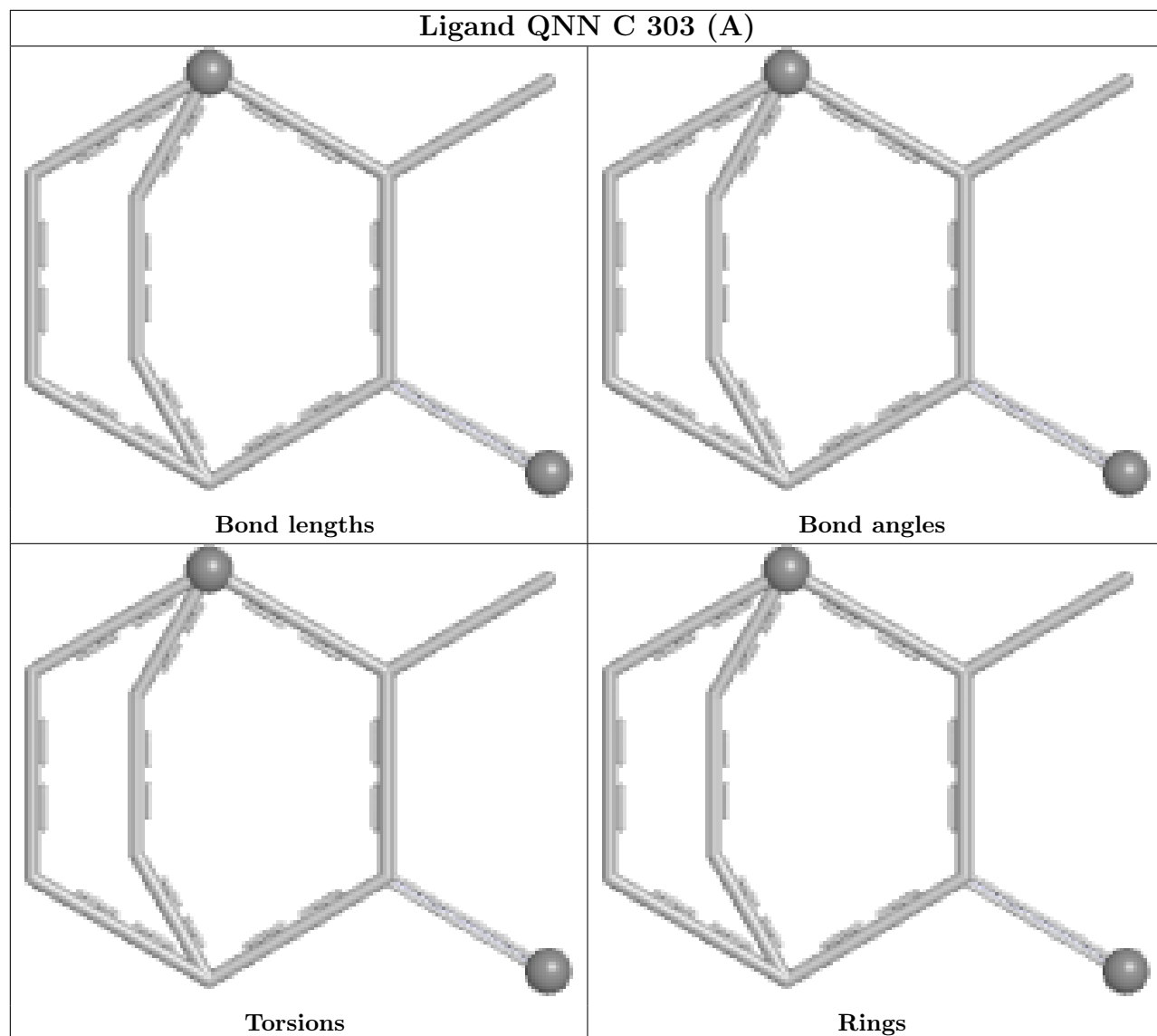


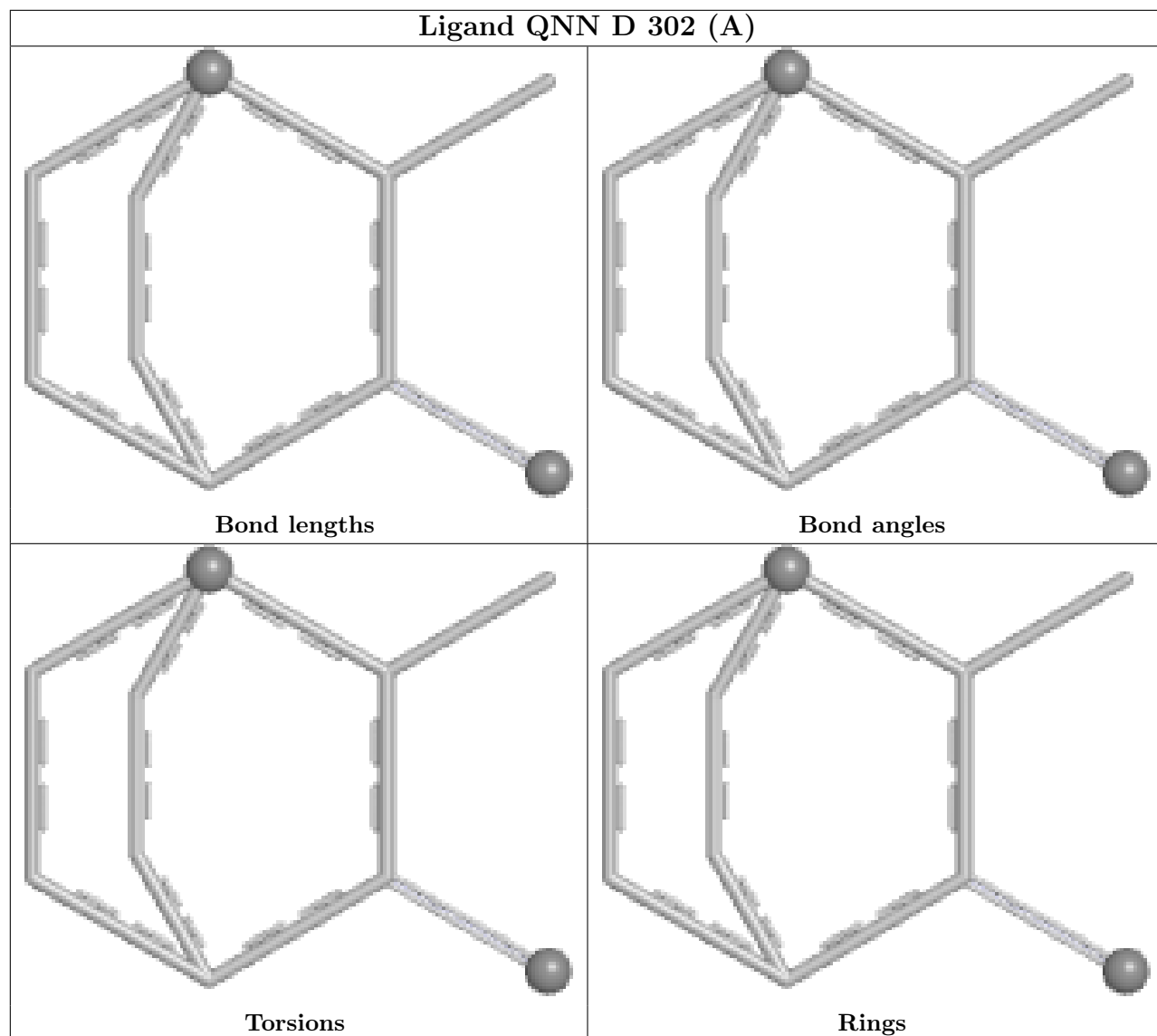


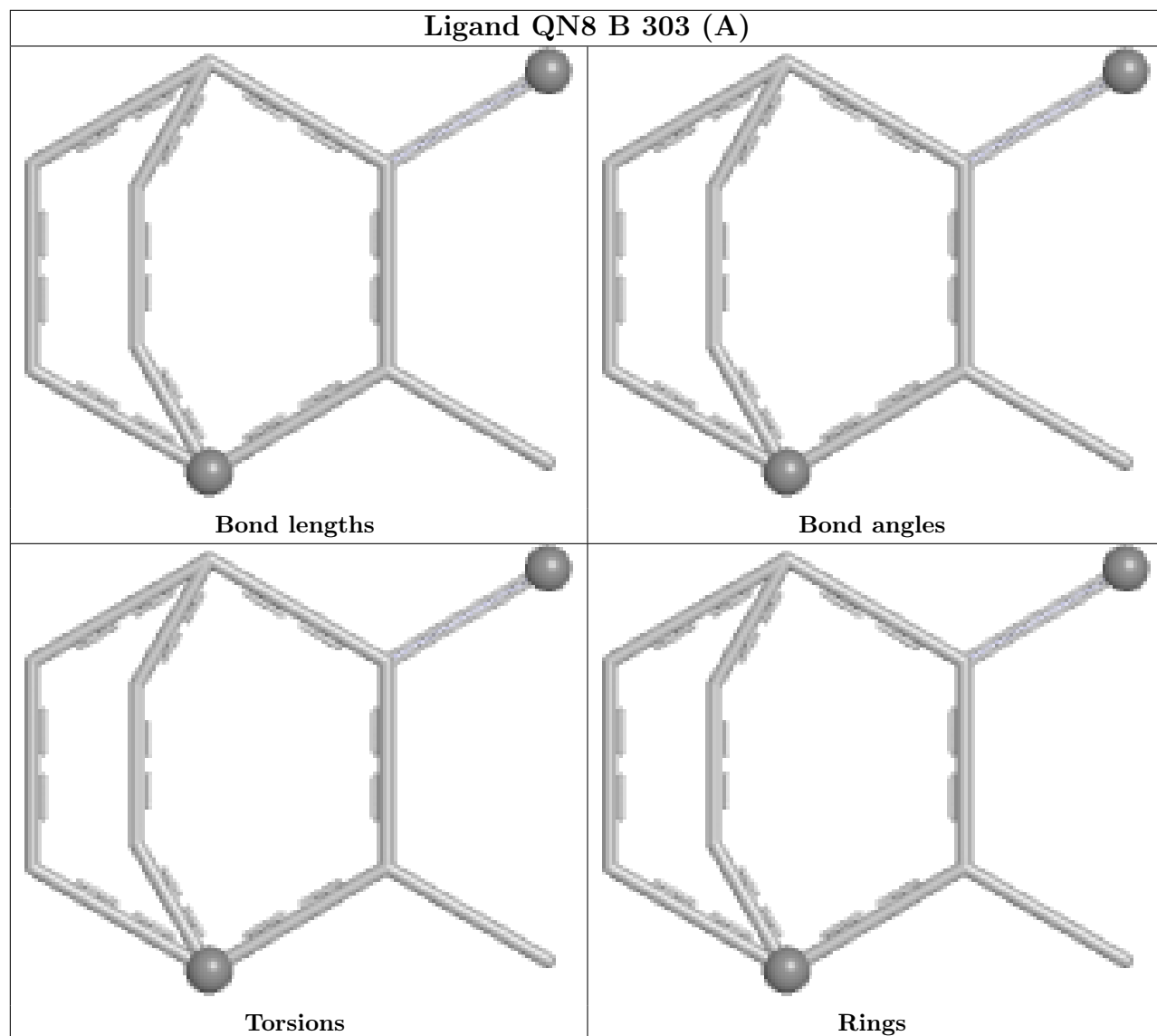












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	191/200 (95%)	-0.29	2 (1%) 82 85	14, 26, 48, 73	1 (0%)
1	B	190/200 (95%)	-0.19	1 (0%) 91 92	15, 32, 53, 66	1 (0%)
1	C	191/200 (95%)	-0.16	1 (0%) 91 92	19, 33, 55, 80	0
1	D	193/200 (96%)	-0.15	1 (0%) 91 92	17, 33, 59, 72	1 (0%)
All	All	765/800 (95%)	-0.20	5 (0%) 87 90	14, 31, 56, 80	3 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	182[A]	CYS	6.6
1	B	182[A]	CYS	4.5
1	D	95	SER	3.1
1	A	185	SER	2.2
1	A	244	GLY	2.1

### 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,

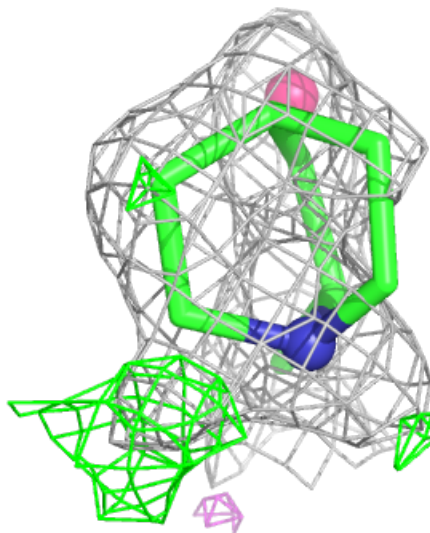
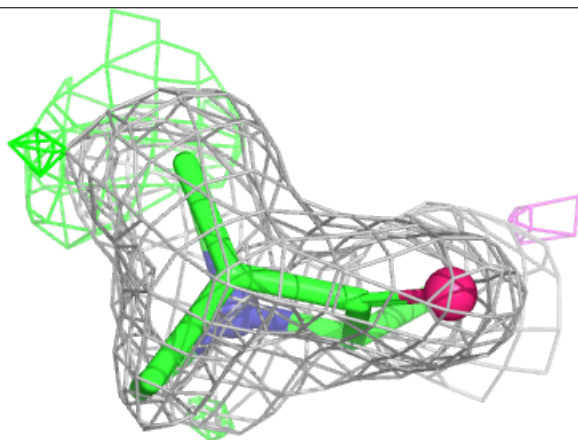
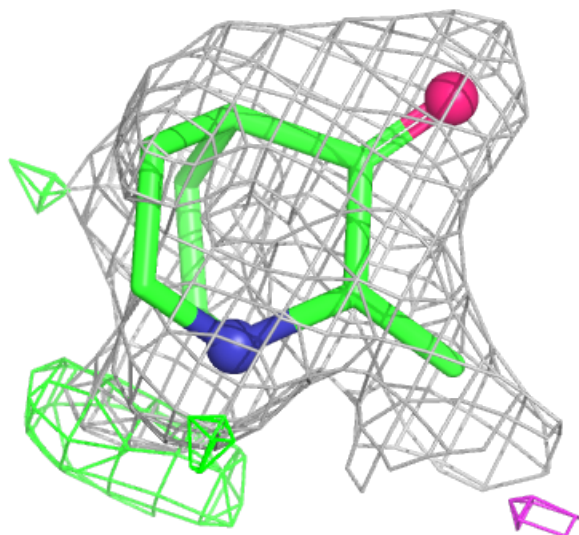
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	D	303	4/4	0.69	0.14	36,36,36,37	4
3	QNN	C	303[A]	10/10	0.77	0.21	38,47,50,51	10
4	EDO	A	303	4/4	0.80	0.21	36,42,43,49	4
3	QNN	C	301[A]	10/10	0.81	0.19	39,42,43,44	10
3	QNN	D	302[A]	10/10	0.81	0.19	37,45,46,47	10
4	EDO	B	305	4/4	0.82	0.19	38,39,42,43	4
3	QNN	B	302[A]	10/10	0.82	0.17	34,43,45,47	10
5	QN8	B	303[A]	10/10	0.82	0.29	45,52,54,54	10
3	QNN	B	304[A]	10/10	0.84	0.22	38,44,45,45	10
6	PEG	D	304	7/7	0.86	0.23	26,29,31,31	7
3	QNN	A	302[A]	10/10	0.89	0.14	31,38,38,43	10
6	PEG	D	305	7/7	0.89	0.20	26,32,37,37	7
4	EDO	C	304	4/4	0.92	0.12	26,26,27,27	4
2	ZN	B	301	1/1	0.99	0.04	24,24,24,24	0
2	ZN	C	302	1/1	0.99	0.04	26,26,26,26	0
2	ZN	D	301	1/1	0.99	0.05	30,30,30,30	0
2	ZN	A	301	1/1	0.99	0.06	28,28,28,28	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 QNN C 303 (A):**

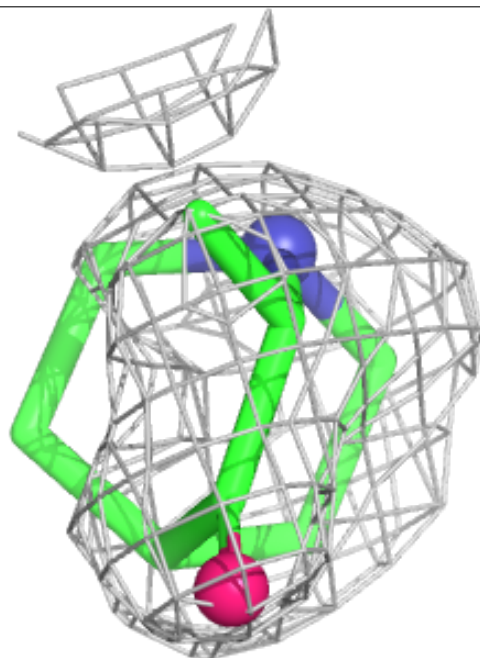
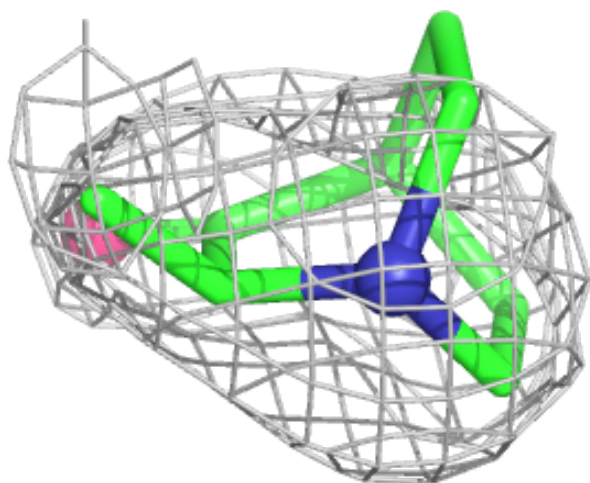
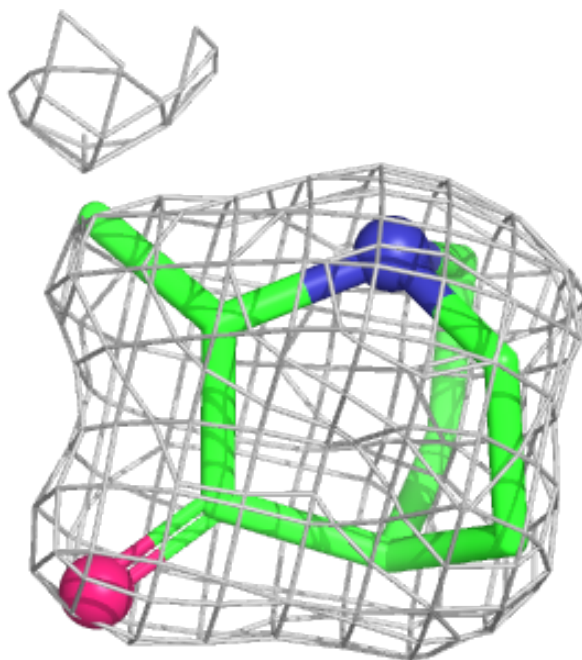
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





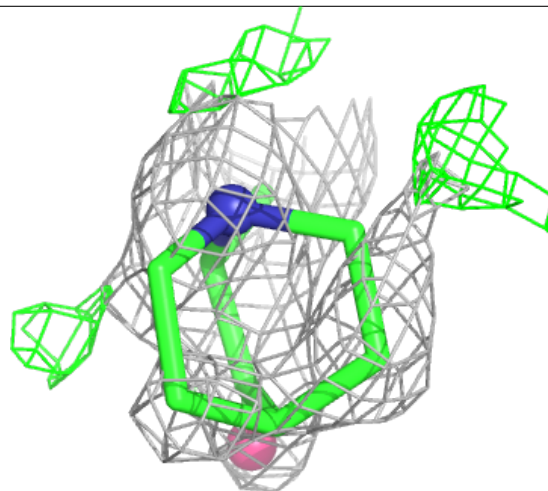
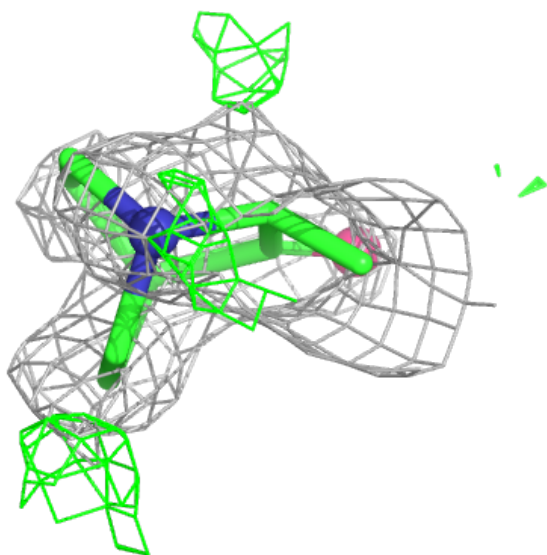
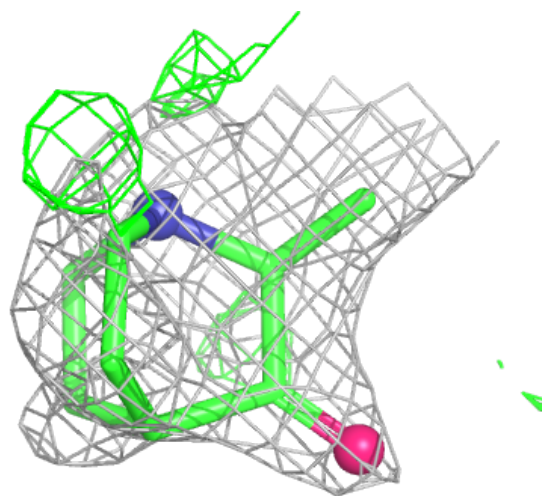
**Electron density around QNN C 301 (A):**

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



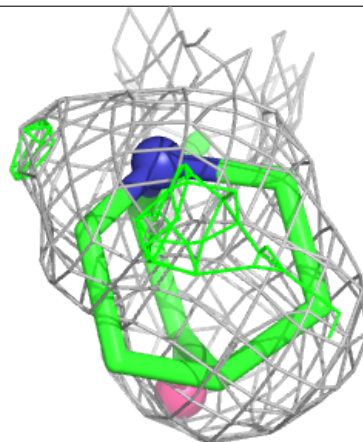
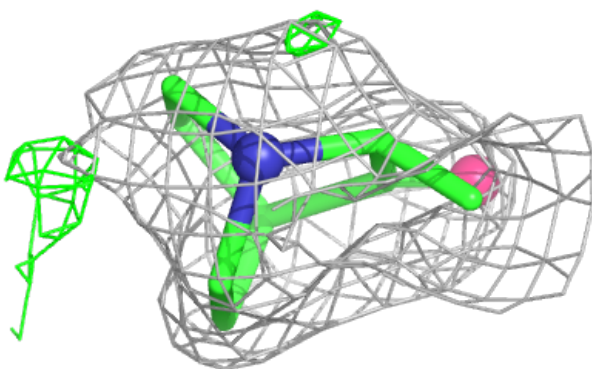
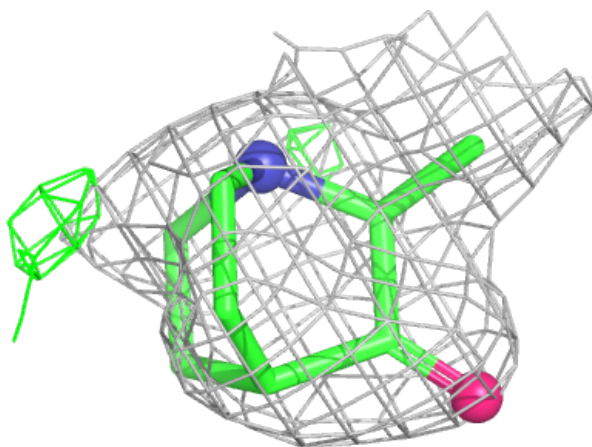
**Electron density around QNN D 302 (A):**

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



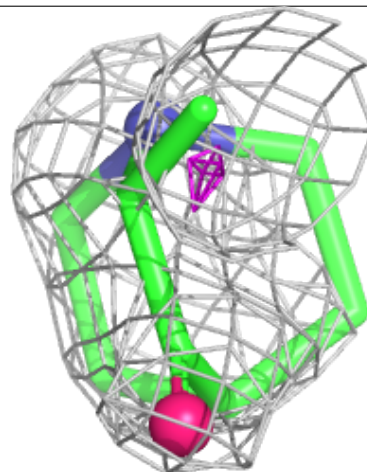
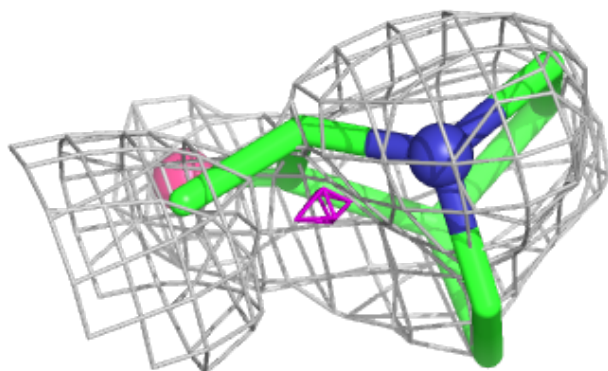
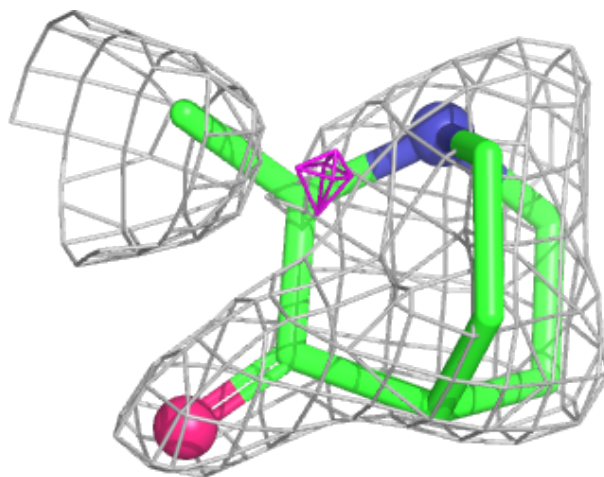
**Electron density around QNN B 302 (A):**

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



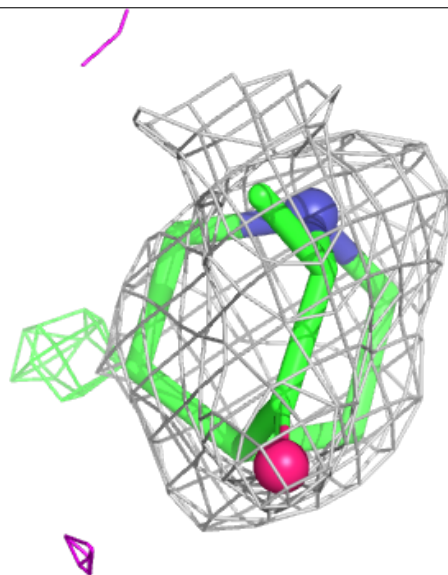
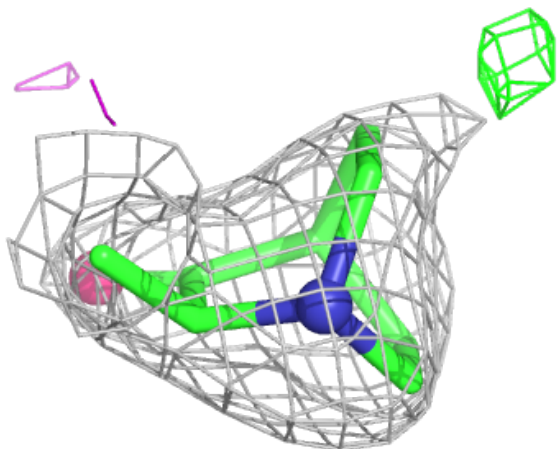
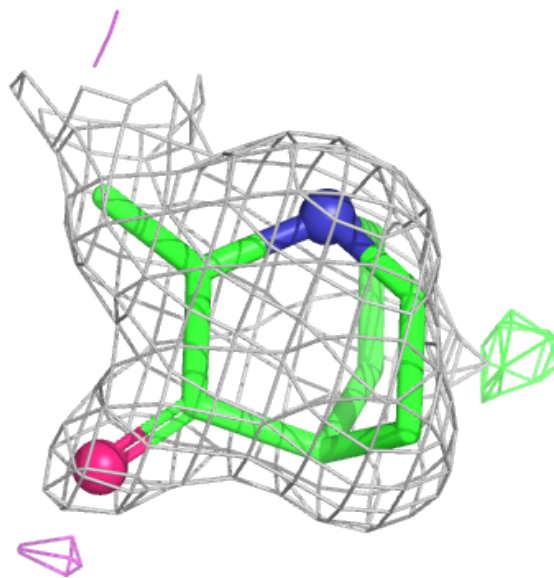
**Electron density around QN8 B 303 (A):**

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

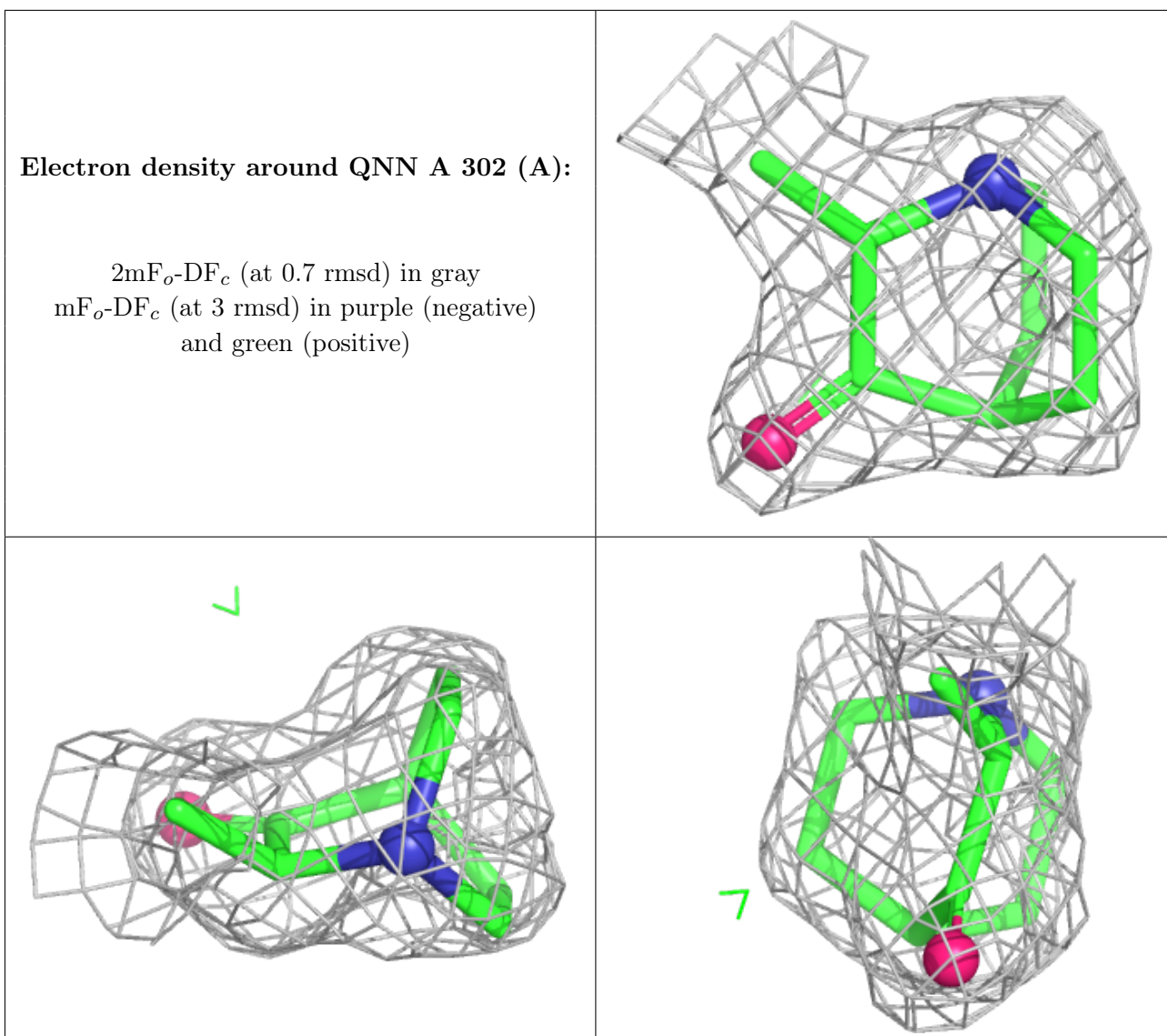


**Electron density around QNN B 304 (A):**

$2mF_o-DF_c$  (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.