



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2020 – 12:21 PM JST

PDB ID : 7COI  
Title : Crystal structure of the b-carbonic anhydrase CafA of the fungal pathogen *Aspergillus fumigatus*  
Authors : Jin, M.S.; Kim, S.; Yeon, J.; Sung, J.  
Deposited on : 2020-08-04  
Resolution : 1.80 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

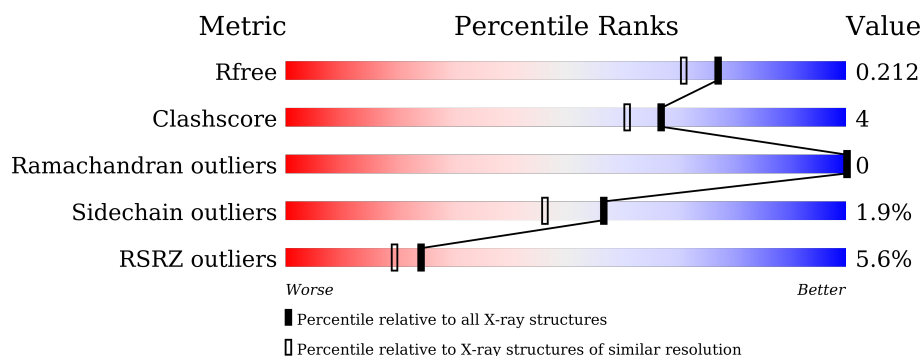
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	287	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>7%</div> <div>27%</div> </div> </div>
1	B	287	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>8%</div> <div>28%</div> </div> </div>
1	C	287	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>7%</div> <div>27%</div> </div> </div>
1	D	287	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>7%</div> <div>28%</div> </div> </div>

## 2 Entry composition [i](#)

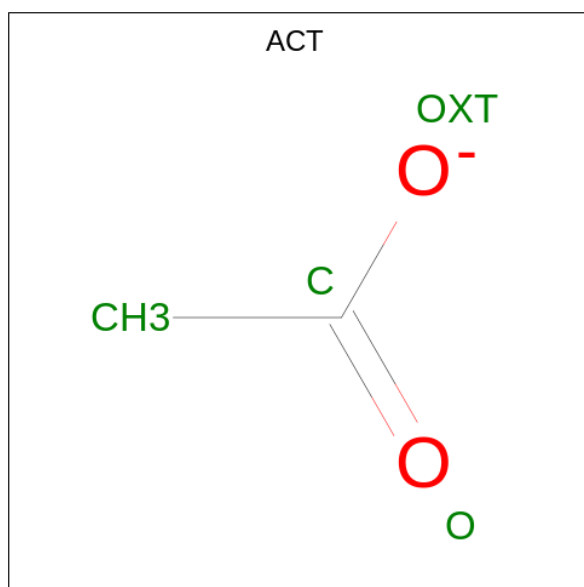
There are 4 unique types of molecules in this entry. The entry contains 7120 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Carbonic anhydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	1	0
			1603	1015	289	292	7			
1	B	208	Total	C	N	O	S	0	1	0
			1597	1010	288	292	7			
1	C	209	Total	C	N	O	S	0	1	0
			1603	1015	289	292	7			
1	D	208	Total	C	N	O	S	0	1	0
			1597	1010	288	292	7			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ) (labeled as "Ligand of Interest" by author).



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

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

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

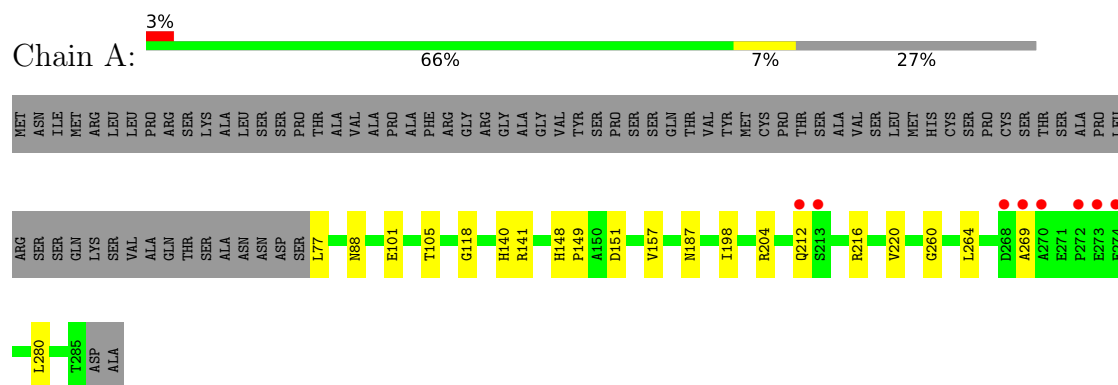
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	174	Total	O	0	0
			174	174		
4	B	235	Total	O	0	0
			235	235		
4	C	141	Total	O	0	0
			141	141		
4	D	150	Total	O	0	0
			150	150		

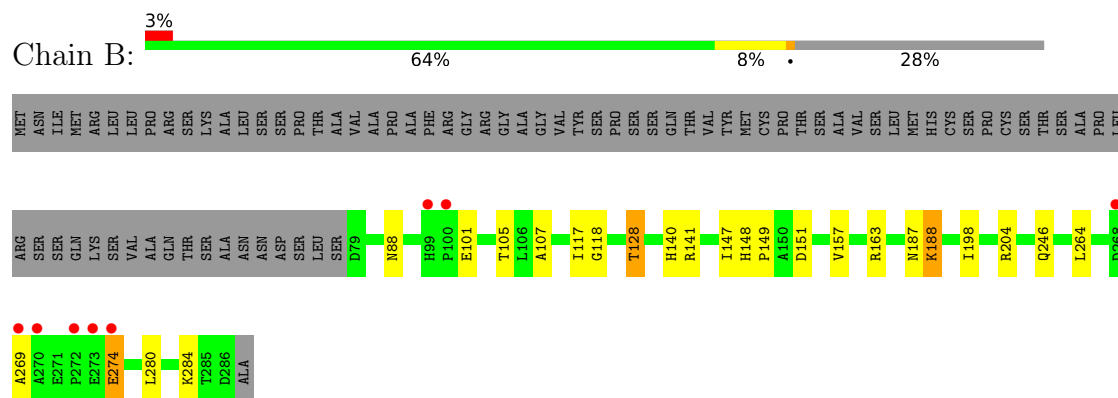
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

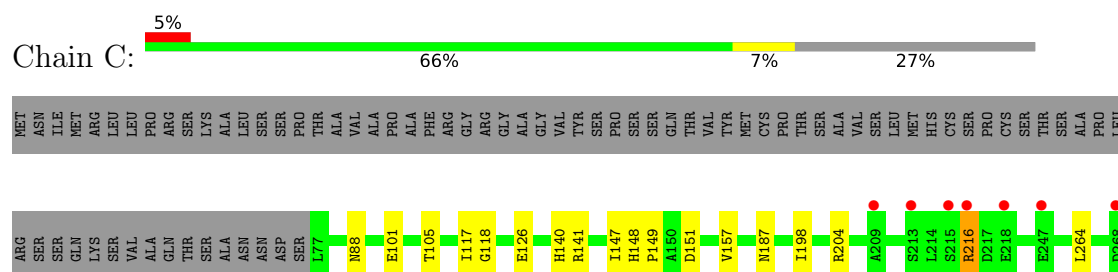
- Molecule 1: Carbonic anhydrase

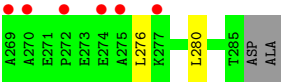


- Molecule 1: Carbonic anhydrase

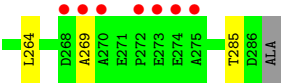
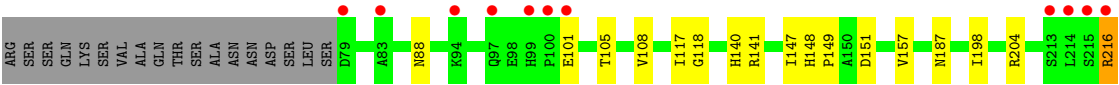
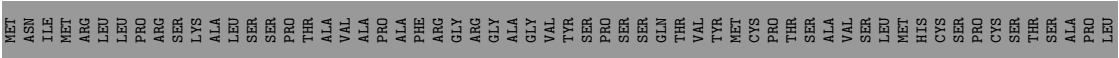


- Molecule 1: Carbonic anhydrase





● Molecule 1: Carbonic anhydrase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.66Å 88.71Å 144.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 1.80 29.86 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.88-1.80) 99.7 (29.86-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.54 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.172 , 0.204 0.183 , 0.212	Depositor DCC
$R_{free}$ test set	4069 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtrriage
Anisotropy	0.742	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7120	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.50 % 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 2.3400e-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: ZN, ACT

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	0.78	0/1635	0.78	0/2216
1	B	0.78	0/1629	0.84	1/2208 (0.0%)
1	C	0.74	0/1635	0.79	0/2216
1	D	0.74	0/1629	0.80	0/2208
All	All	0.76	0/6528	0.80	1/8848 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ARG	NE-CZ-NH2	-5.09	117.75	120.30

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	1603	0	1644	15	0
1	B	1597	0	1632	19	0
1	C	1603	0	1644	14	0
1	D	1597	0	1632	15	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	174	0	0	5	0
4	B	235	0	0	1	0
4	C	141	0	0	2	0
4	D	150	0	0	2	0
All	All	7120	0	6564	50	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 (50) 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:D:269:ALA:HB1	4:D:421:HOH:O	1.74	0.85
1:D:101:GLU:O	1:D:105:THR:HG23	1.83	0.79
1:B:101:GLU:O	1:B:105:THR:HG23	1.88	0.73
1:A:101:GLU:O	1:A:105:THR:HG23	1.89	0.72
1:C:101:GLU:O	1:C:105:THR:HG23	1.89	0.71
1:C:264:LEU:H	1:D:88:ASN:HD21	1.39	0.69
1:C:216:ARG:NH2	4:C:401:HOH:O	2.21	0.67
1:C:216:ARG:NH1	4:C:401:HOH:O	2.25	0.66
1:D:216:ARG:HD2	4:D:401:HOH:O	1.93	0.66
1:A:264:LEU:H	1:B:88:ASN:HD21	1.42	0.66
1:A:88:ASN:HD21	1:B:264:LEU:H	1.43	0.66
1:B:269:ALA:HB1	4:B:408:HOH:O	1.97	0.64
1:D:105:THR:O	1:D:108:VAL:HG22	1.99	0.62
1:C:88:ASN:HD21	1:D:264:LEU:H	1.48	0.61
1:A:187:ASN:HD21	1:A:204:ARG:HH22	1.48	0.60
1:D:187:ASN:HD21	1:D:204:ARG:HH22	1.48	0.59
1:A:269:ALA:HB1	4:A:406:HOH:O	2.02	0.58
1:C:187:ASN:HD21	1:C:204:ARG:HH22	1.49	0.58
1:B:187:ASN:HD21	1:B:204:ARG:HH22	1.53	0.55
1:A:198:ILE:HG21	1:C:149:PRO:HB3	1.90	0.54
1:C:264:LEU:H	1:D:88:ASN:ND2	2.04	0.54
4:A:464:HOH:O	1:B:128:THR:HG22	2.08	0.53
1:A:260:GLY:HA2	1:B:107:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASN:ND2	1:B:264:LEU:H	2.06	0.51
1:B:198:ILE:HG21	1:D:149:PRO:HB3	1.93	0.51
1:B:148:HIS:HB2	1:B:151:ASP:HB2	1.94	0.50
1:C:140:HIS:HB2	1:C:157:VAL:HG11	1.92	0.50
1:A:149:PRO:HB3	1:C:198:ILE:HG21	1.93	0.50
1:A:264:LEU:H	1:B:88:ASN:ND2	2.08	0.49
4:A:464:HOH:O	1:B:128:THR:CG2	2.60	0.49
1:C:117:ILE:HG21	1:C:147:ILE:HD11	1.95	0.49
1:C:88:ASN:ND2	1:D:264:LEU:H	2.10	0.49
1:A:220:VAL:HG12	4:A:452:HOH:O	2.12	0.48
1:A:140:HIS:HB2	1:A:157:VAL:HG11	1.94	0.48
1:A:148:HIS:HB2	1:A:151:ASP:HB2	1.96	0.48
1:D:117:ILE:HG21	1:D:147:ILE:HD11	1.96	0.48
1:C:148:HIS:HB2	1:C:151:ASP:HB2	1.96	0.47
1:B:246:GLN:HE22	1:B:284:LYS:NZ	2.12	0.47
1:B:274:GLU:N	1:B:274:GLU:OE1	2.47	0.47
1:A:212:GLN:NE2	4:A:405:HOH:O	2.48	0.47
1:B:117:ILE:HG21	1:B:147:ILE:HD11	1.97	0.47
1:B:140:HIS:HB2	1:B:157:VAL:HG11	1.98	0.46
1:A:118:GLY:O	1:A:141:ARG:HA	2.16	0.45
1:B:149:PRO:HB3	1:D:198:ILE:HG21	1.98	0.45
1:D:118:GLY:O	1:D:141:ARG:HA	2.17	0.44
1:D:140:HIS:HB2	1:D:157:VAL:HG11	1.99	0.44
1:B:118:GLY:O	1:B:141:ARG:HA	2.16	0.44
1:C:118:GLY:O	1:C:141:ARG:HA	2.18	0.43
1:D:148:HIS:HB2	1:D:151:ASP:HB2	2.00	0.42
1:B:188:LYS:HA	1:B:188:LYS:HD2	1.94	0.41

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	208/287 (72%)	205 (99%)	3 (1%)	0	100	100
1	B	207/287 (72%)	204 (99%)	3 (1%)	0	100	100
1	C	208/287 (72%)	205 (99%)	3 (1%)	0	100	100
1	D	207/287 (72%)	204 (99%)	3 (1%)	0	100	100
All	All	830/1148 (72%)	818 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	172/236 (73%)	169 (98%)	3 (2%)	60	51
1	B	171/236 (72%)	167 (98%)	4 (2%)	50	37
1	C	172/236 (73%)	168 (98%)	4 (2%)	50	37
1	D	171/236 (72%)	169 (99%)	2 (1%)	71	65
All	All	686/944 (73%)	673 (98%)	13 (2%)	57	46

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	216	ARG
1	A	280	LEU
1	B	128	THR
1	B	188	LYS
1	B	274	GLU
1	B	280	LEU
1	C	126	GLU
1	C	216	ARG
1	C	276	LEU
1	C	280	LEU
1	D	216	ARG
1	D	285	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	187	ASN
1	A	212	GLN
1	A	246	GLN
1	B	88	ASN
1	B	187	ASN
1	B	246	GLN
1	C	88	ASN
1	C	97	GLN
1	C	187	ASN
1	C	212	GLN
1	D	88	ASN
1	D	97	GLN
1	D	187	ASN
1	D	212	GLN

### 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	ACT	A	301	3	1,3,3	3.81	1 (100%)	0,3,3	0.00	-
2	ACT	B	301	3	1,3,3	1.74	0	0,3,3	0.00	-
2	ACT	C	301	3	1,3,3	2.50	1 (100%)	0,3,3	0.00	-
2	ACT	D	301	3	1,3,3	3.33	1 (100%)	0,3,3	0.00	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ACT	CH3-C	3.81	1.53	1.48
2	D	301	ACT	CH3-C	3.33	1.53	1.48
2	C	301	ACT	CH3-C	2.50	1.51	1.48

There are no bond angle outliers.

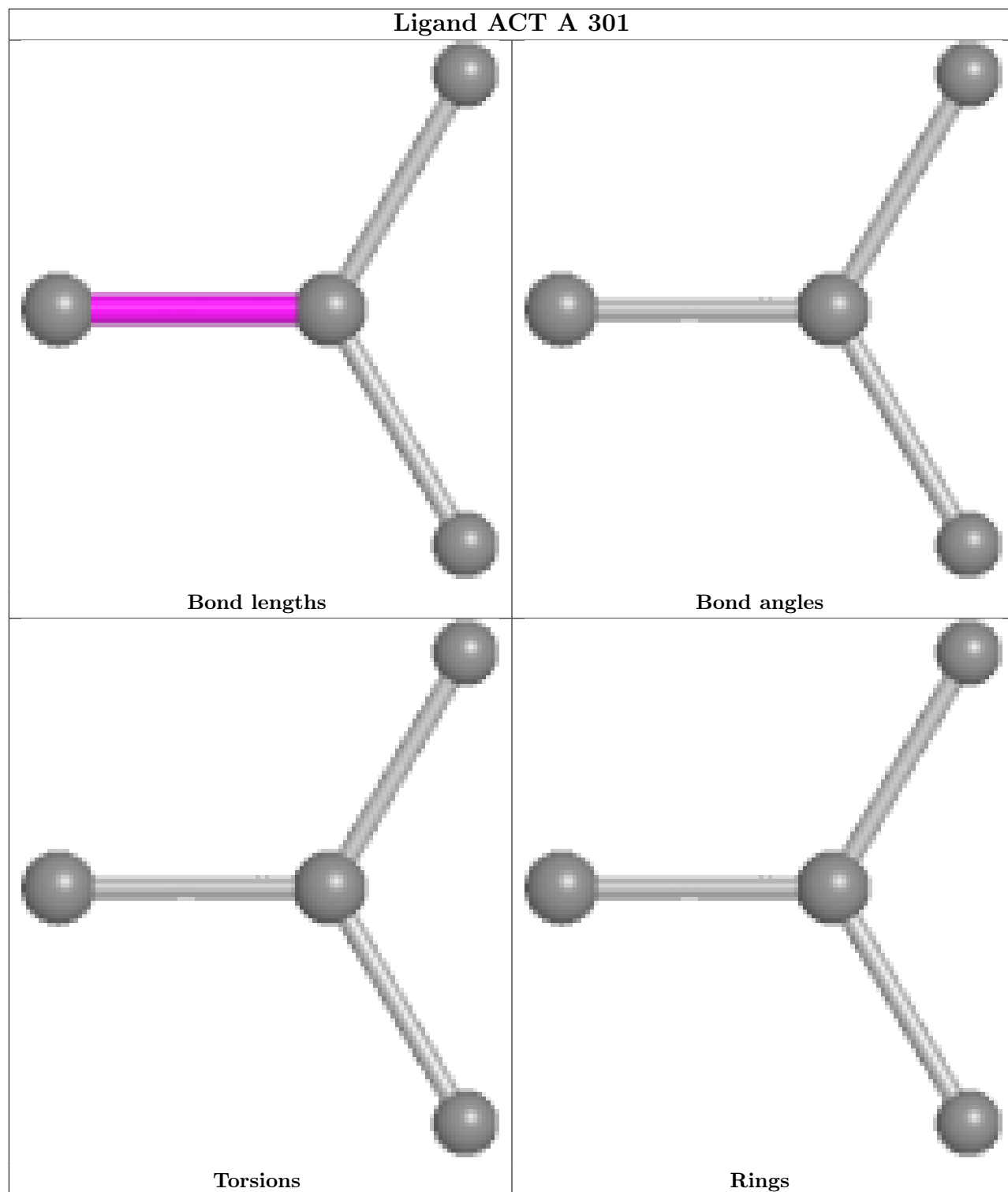
There are no chirality outliers.

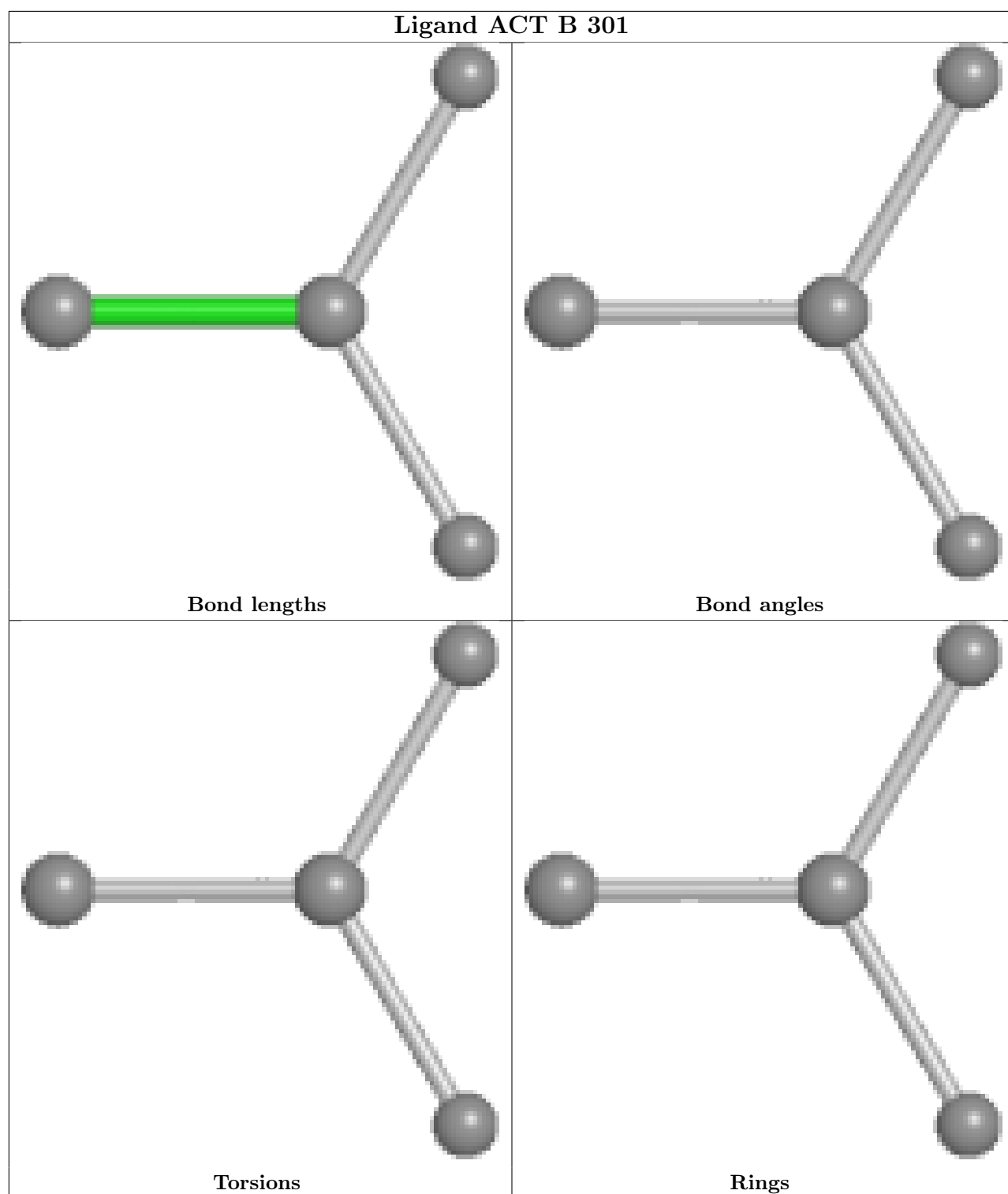
There are no torsion outliers.

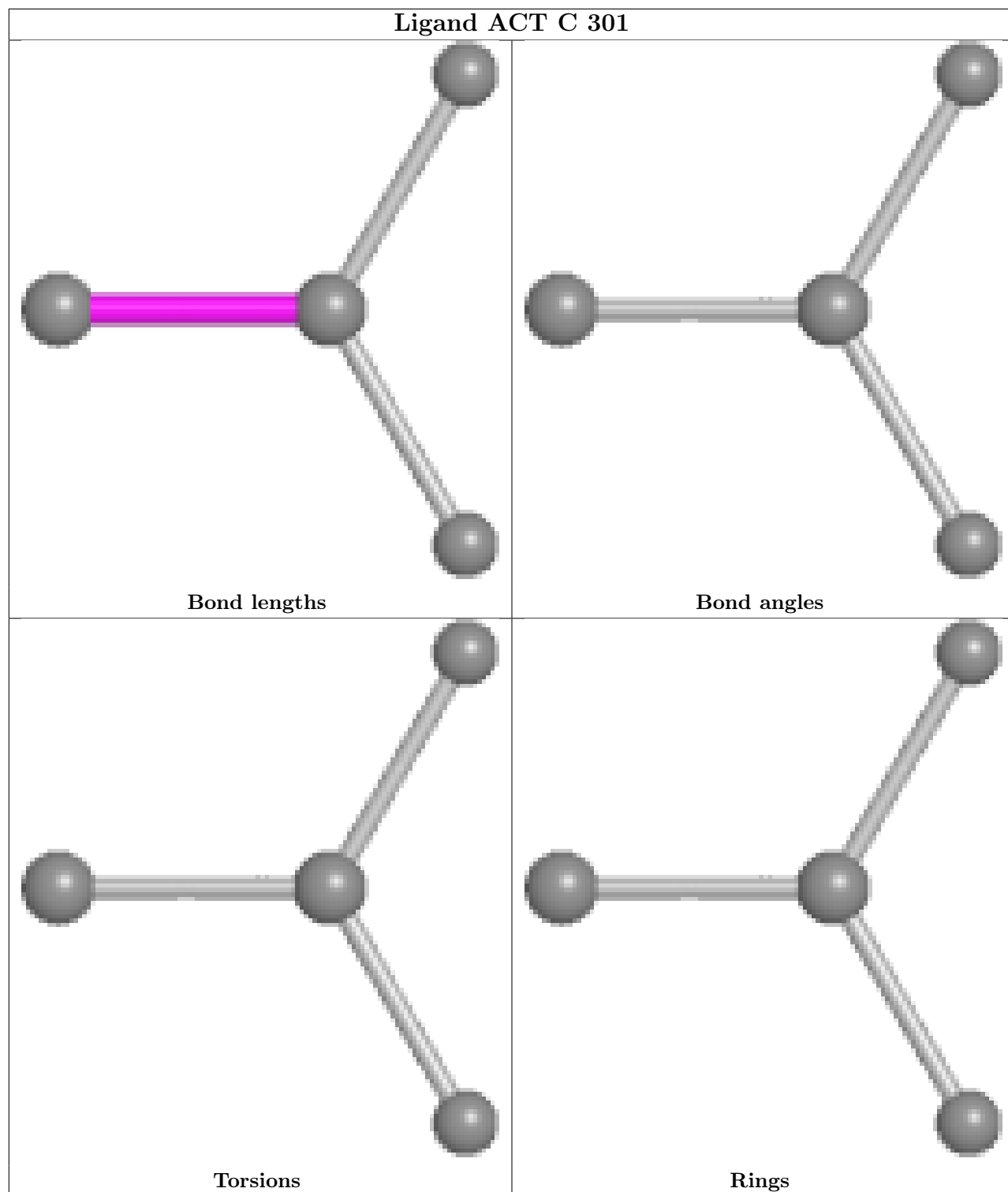
There are no ring outliers.

No monomer is involved in short contacts.

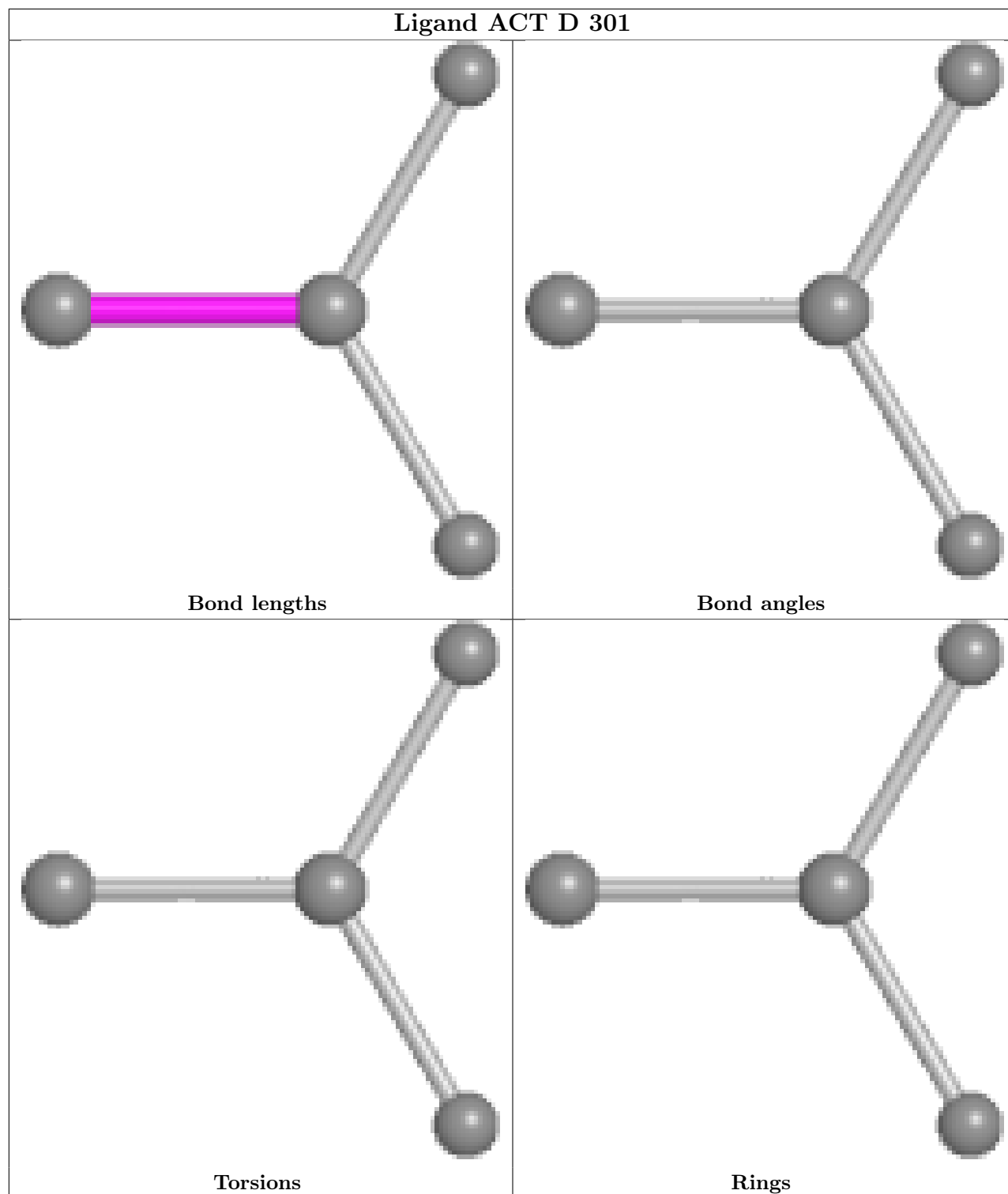
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	209/287 (72%)	0.07	8 (3%) 40 35	12, 21, 57, 90	0
1	B	208/287 (72%)	-0.14	8 (3%) 40 35	11, 17, 49, 79	0
1	C	209/287 (72%)	0.26	13 (6%) 20 16	14, 25, 50, 87	0
1	D	208/287 (72%)	0.18	18 (8%) 10 8	13, 21, 58, 78	0
All	All	834/1148 (72%)	0.09	47 (5%) 24 19	11, 22, 54, 90	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	ALA	7.8
1	A	270	ALA	6.3
1	A	272	PRO	6.3
1	C	272	PRO	6.2
1	B	269	ALA	5.6
1	C	274	GLU	4.8
1	D	270	ALA	4.6
1	D	273	GLU	4.2
1	B	270	ALA	4.1
1	A	273	GLU	4.0
1	D	272	PRO	3.9
1	B	273	GLU	3.9
1	D	269	ALA	3.9
1	D	100	PRO	3.8
1	C	270	ALA	3.7
1	D	274	GLU	3.7
1	C	213	SER	3.7
1	C	216	ARG	3.7
1	D	215	SER	3.5
1	A	268	ASP	3.5
1	D	101	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	275	ALA	3.4
1	B	272	PRO	3.4
1	A	213	SER	3.2
1	C	268	ASP	3.1
1	B	99	HIS	2.9
1	D	268	ASP	2.8
1	D	216	ARG	2.8
1	B	274	GLU	2.8
1	C	269	ALA	2.7
1	D	83	ALA	2.6
1	D	94	LYS	2.5
1	A	274	GLU	2.5
1	C	215	SER	2.4
1	A	212	GLN	2.4
1	D	213	SER	2.3
1	D	79	ASP	2.3
1	C	277	LYS	2.2
1	D	97	GLN	2.2
1	D	275	ALA	2.2
1	C	209	ALA	2.2
1	C	218	GLU	2.2
1	D	99	HIS	2.2
1	B	268	ASP	2.2
1	B	100	PRO	2.2
1	C	247	GLU	2.2
1	D	214	LEU	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](#)

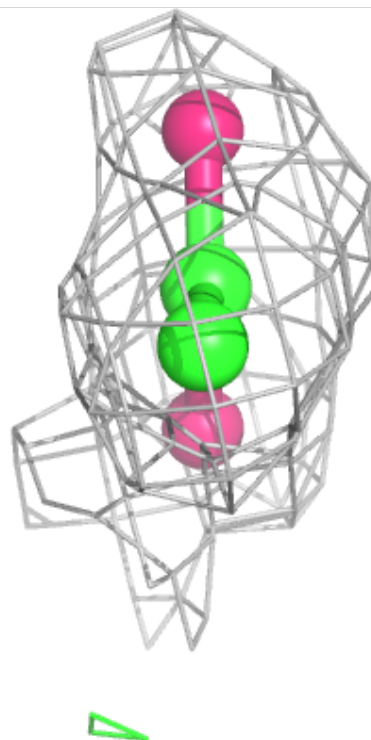
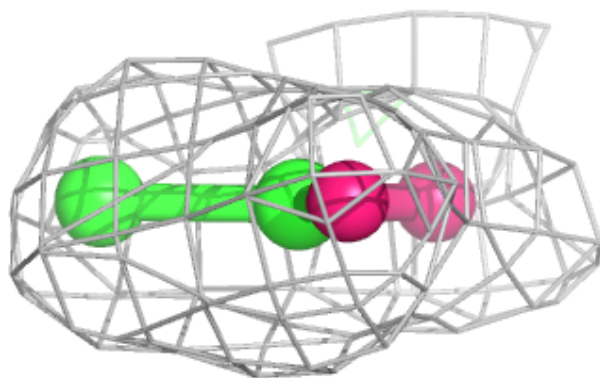
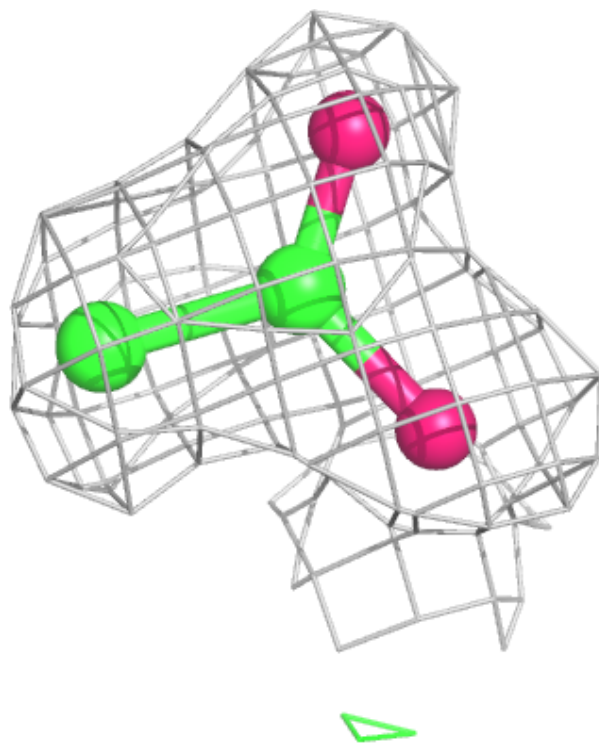
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	ACT	D	301	4/4	0.92	0.15	23,28,30,33	0
2	ACT	C	301	4/4	0.94	0.12	27,37,37,38	0
2	ACT	B	301	4/4	0.94	0.13	18,25,27,30	0
2	ACT	A	301	4/4	0.95	0.10	18,25,26,29	0
3	ZN	D	302	1/1	0.99	0.03	18,18,18,18	0
3	ZN	C	302	1/1	0.99	0.04	23,23,23,23	0
3	ZN	A	302	1/1	0.99	0.04	17,17,17,17	0
3	ZN	B	302	1/1	1.00	0.04	15,15,15,15	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.

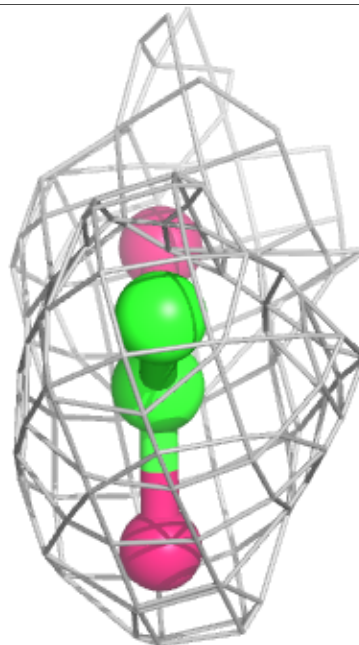
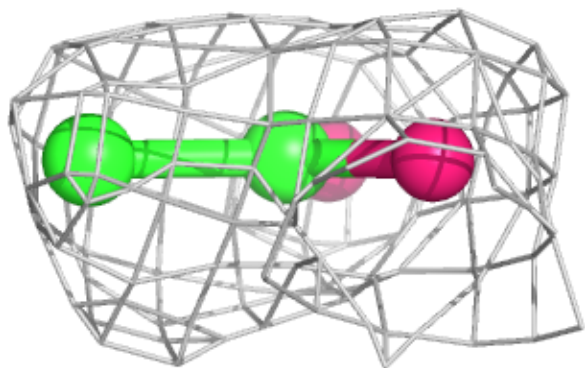
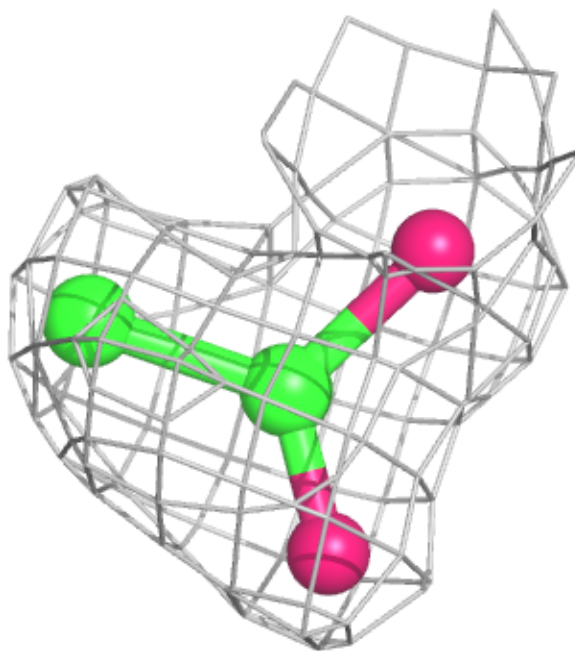
**Electron density around ACT D 301:**

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



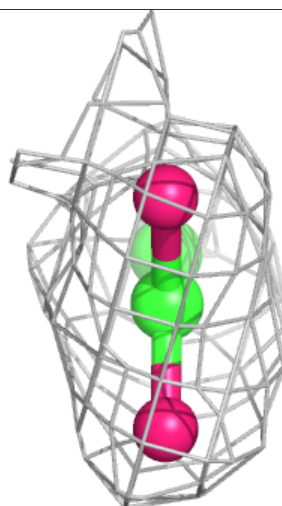
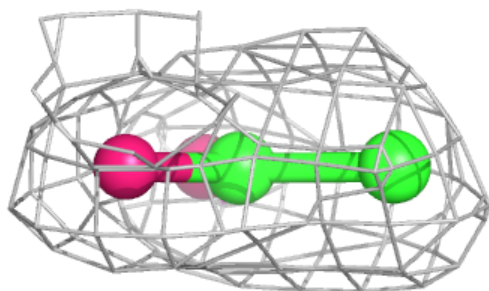
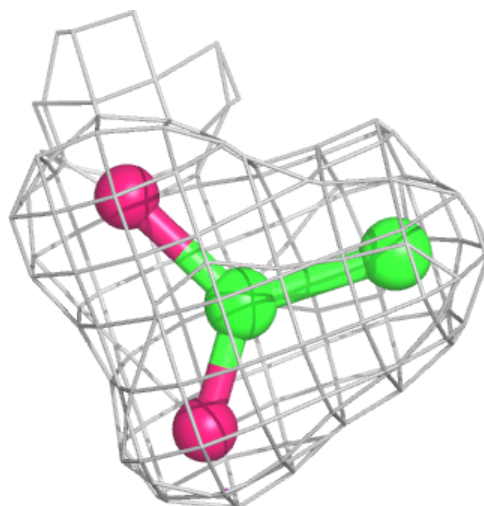
**Electron density around ACT C 301:**

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



**Electron density around ACT B 301:**

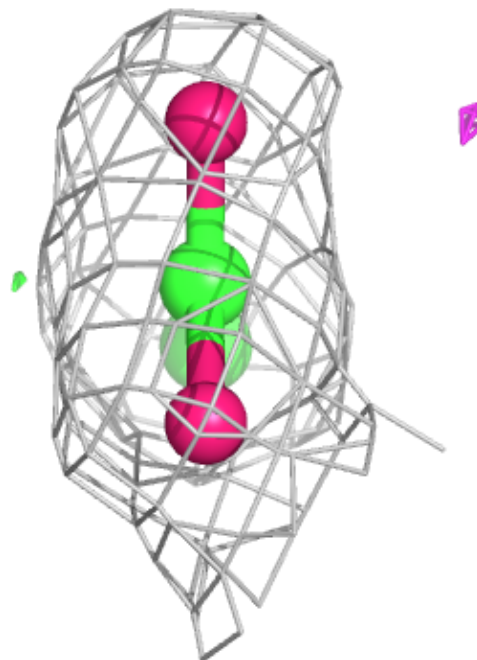
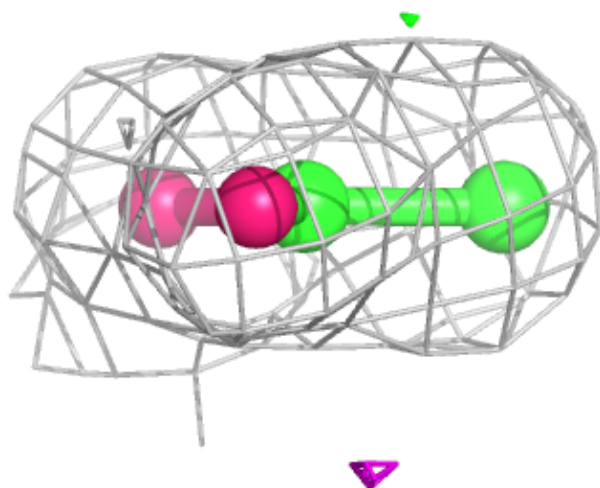
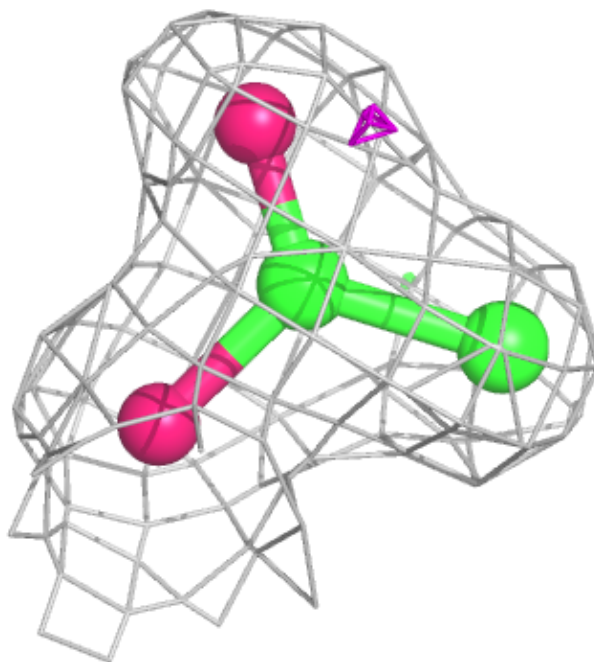
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





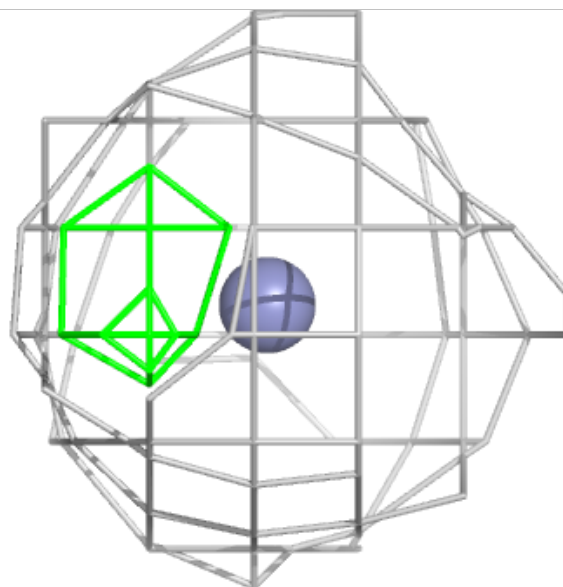
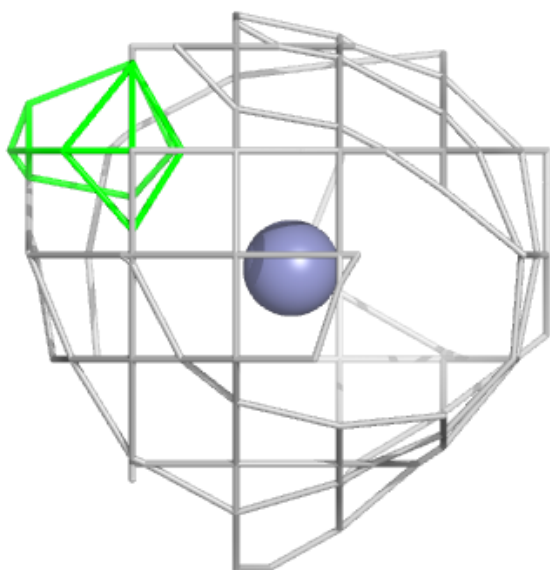
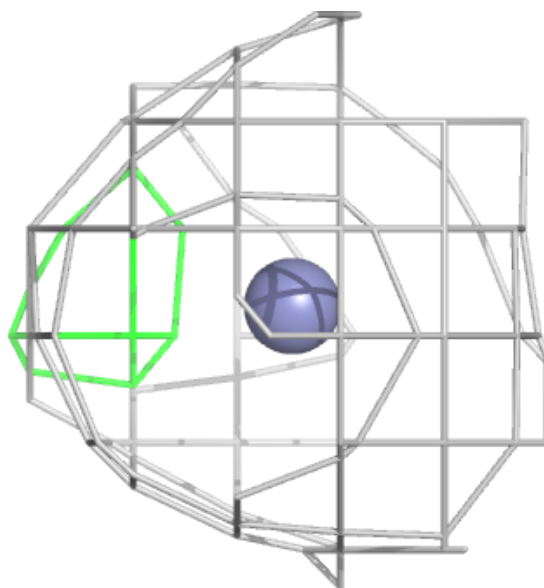
**Electron density around ACT A 301:**

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



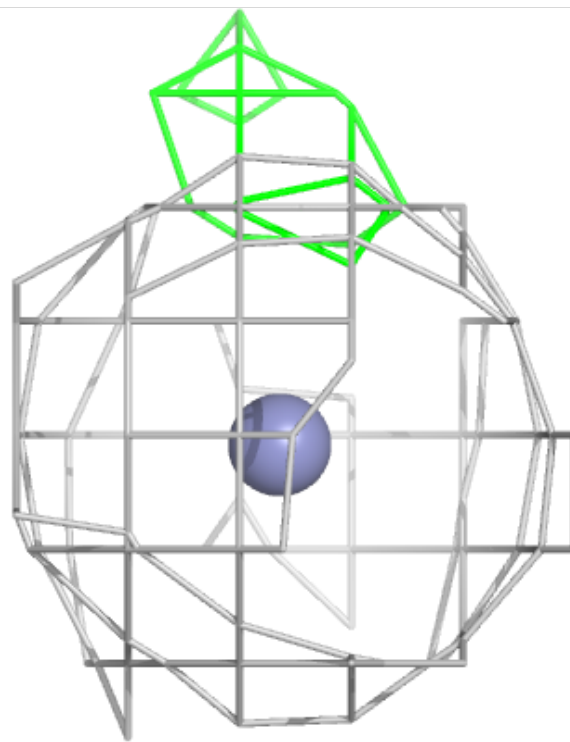
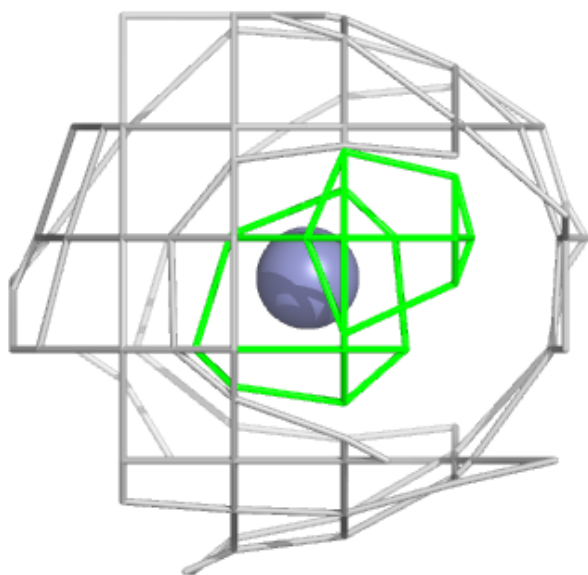
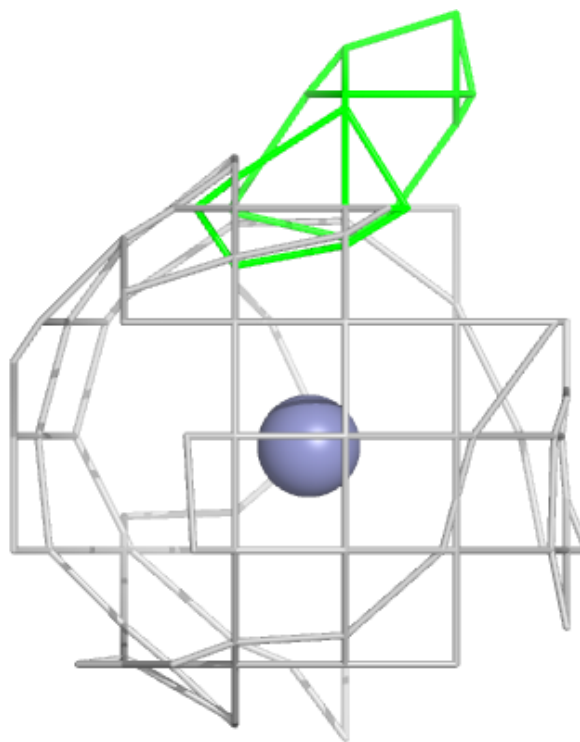
**Electron density around ZN D 302:**

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



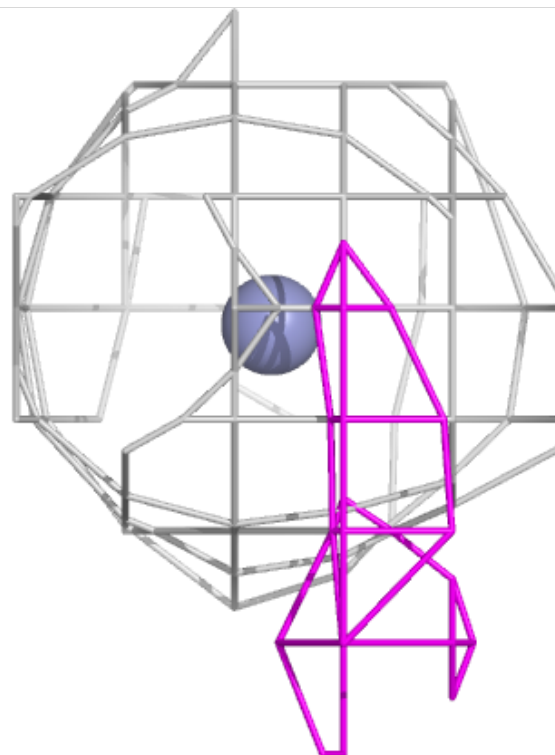
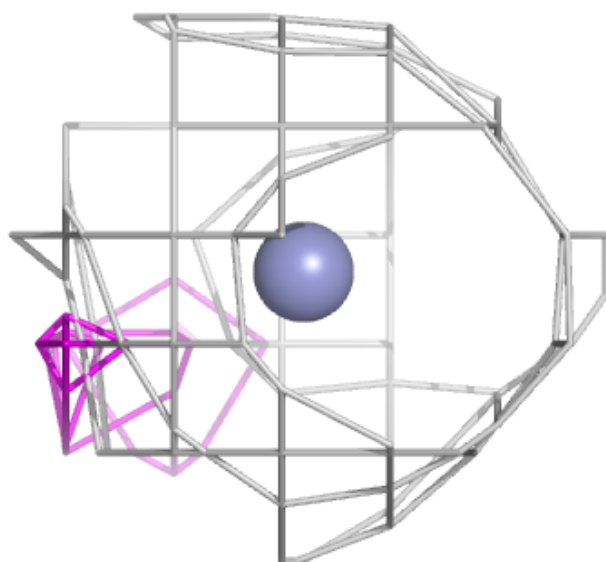
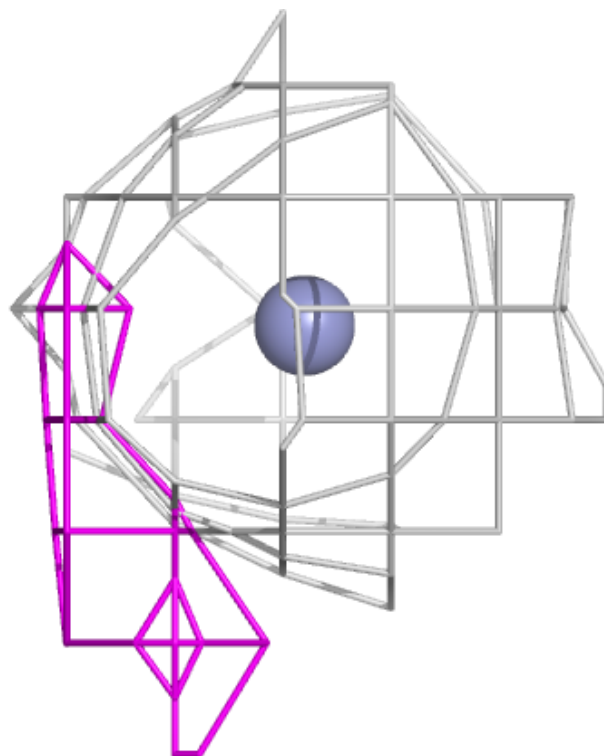
**Electron density around ZN C 302:**

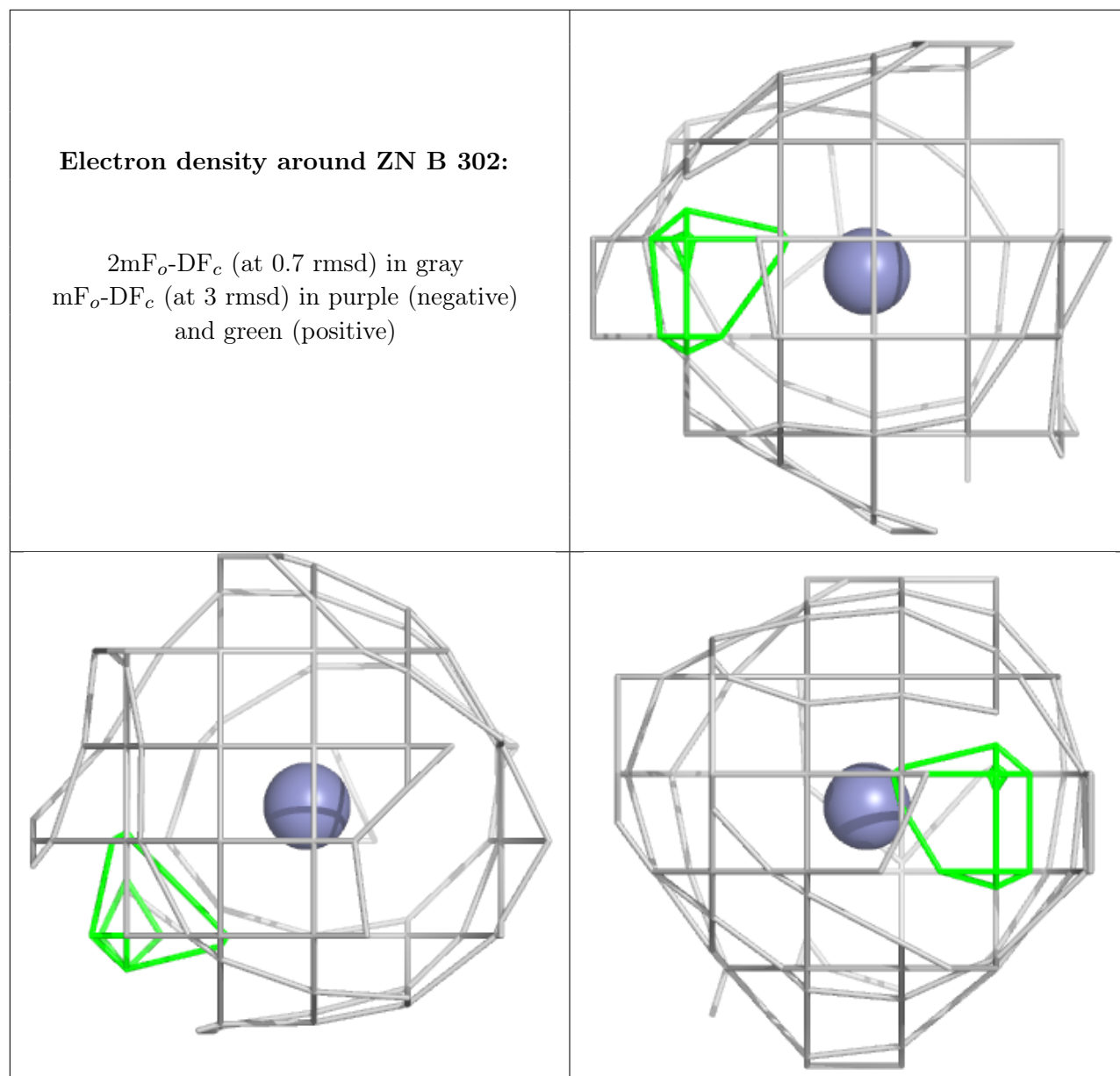
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN A 302:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.