



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2024 – 01:41 pm GMT

PDB ID : 7O9N
Title : Crystal Structure of a Class D Carbapenemase Complexed with Bicarbonate
Authors : Zhou, Q.; He, Y.; Jin, Y.
Deposited on : 2021-04-16
Resolution : 1.97 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

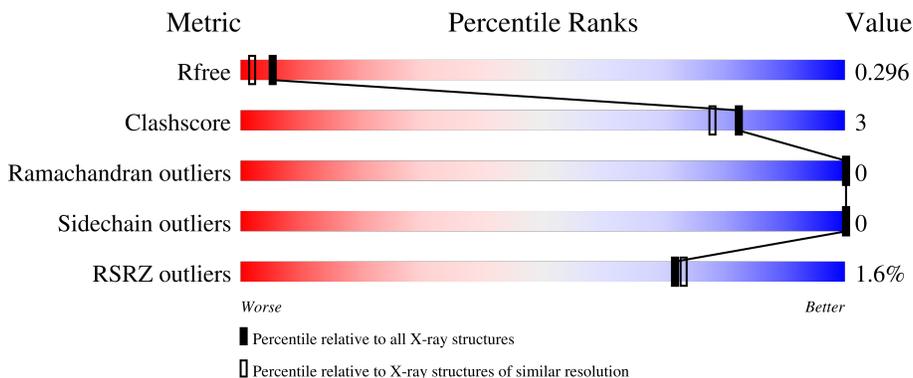
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	AAA	260	 89% 5% 6%
1	BBB	260	 88% 6% 6%
1	CCC	260	 88% 8% 5%
1	DDD	260	 87% 6% 7%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 16586 atoms, of which 7899 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 Beta-lactamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	244	3953	1270	1957	352	367	7	47	0	0
1	BBB	245	3987	1280	1974	355	370	8	47	1	0
1	CCC	248	4047	1304	2002	359	375	7	48	1	0
1	DDD	243	3960	1273	1961	353	366	7	49	1	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	6	MET	-	initiating methionine	UNP Q6XEC0
AAA	7	HIS	-	expression tag	UNP Q6XEC0
AAA	8	HIS	-	expression tag	UNP Q6XEC0
AAA	9	HIS	-	expression tag	UNP Q6XEC0
AAA	10	HIS	-	expression tag	UNP Q6XEC0
AAA	11	HIS	-	expression tag	UNP Q6XEC0
AAA	12	HIS	-	expression tag	UNP Q6XEC0
AAA	13	SER	-	expression tag	UNP Q6XEC0
AAA	14	ALA	-	expression tag	UNP Q6XEC0
AAA	15	GLY	-	expression tag	UNP Q6XEC0
AAA	16	GLU	-	expression tag	UNP Q6XEC0
AAA	17	ASN	-	expression tag	UNP Q6XEC0
AAA	18	LEU	-	expression tag	UNP Q6XEC0
AAA	19	TYR	-	expression tag	UNP Q6XEC0
AAA	20	PHE	-	expression tag	UNP Q6XEC0
AAA	21	GLN	-	expression tag	UNP Q6XEC0
AAA	22	GLY	-	expression tag	UNP Q6XEC0
BBB	6	MET	-	initiating methionine	UNP Q6XEC0
BBB	7	HIS	-	expression tag	UNP Q6XEC0
BBB	8	HIS	-	expression tag	UNP Q6XEC0
BBB	9	HIS	-	expression tag	UNP Q6XEC0

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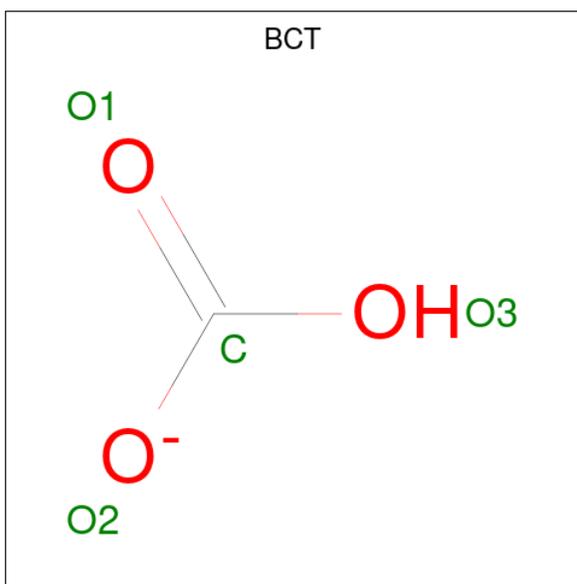
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	10	HIS	-	expression tag	UNP Q6XEC0
BBB	11	HIS	-	expression tag	UNP Q6XEC0
BBB	12	HIS	-	expression tag	UNP Q6XEC0
BBB	13	SER	-	expression tag	UNP Q6XEC0
BBB	14	ALA	-	expression tag	UNP Q6XEC0
BBB	15	GLY	-	expression tag	UNP Q6XEC0
BBB	16	GLU	-	expression tag	UNP Q6XEC0
BBB	17	ASN	-	expression tag	UNP Q6XEC0
BBB	18	LEU	-	expression tag	UNP Q6XEC0
BBB	19	TYR	-	expression tag	UNP Q6XEC0
BBB	20	PHE	-	expression tag	UNP Q6XEC0
BBB	21	GLN	-	expression tag	UNP Q6XEC0
BBB	22	GLY	-	expression tag	UNP Q6XEC0
CCC	6	MET	-	initiating methionine	UNP Q6XEC0
CCC	7	HIS	-	expression tag	UNP Q6XEC0
CCC	8	HIS	-	expression tag	UNP Q6XEC0
CCC	9	HIS	-	expression tag	UNP Q6XEC0
CCC	10	HIS	-	expression tag	UNP Q6XEC0
CCC	11	HIS	-	expression tag	UNP Q6XEC0
CCC	12	HIS	-	expression tag	UNP Q6XEC0
CCC	13	SER	-	expression tag	UNP Q6XEC0
CCC	14	ALA	-	expression tag	UNP Q6XEC0
CCC	15	GLY	-	expression tag	UNP Q6XEC0
CCC	16	GLU	-	expression tag	UNP Q6XEC0
CCC	17	ASN	-	expression tag	UNP Q6XEC0
CCC	18	LEU	-	expression tag	UNP Q6XEC0
CCC	19	TYR	-	expression tag	UNP Q6XEC0
CCC	20	PHE	-	expression tag	UNP Q6XEC0
CCC	21	GLN	-	expression tag	UNP Q6XEC0
CCC	22	GLY	-	expression tag	UNP Q6XEC0
DDD	6	MET	-	initiating methionine	UNP Q6XEC0
DDD	7	HIS	-	expression tag	UNP Q6XEC0
DDD	8	HIS	-	expression tag	UNP Q6XEC0
DDD	9	HIS	-	expression tag	UNP Q6XEC0
DDD	10	HIS	-	expression tag	UNP Q6XEC0
DDD	11	HIS	-	expression tag	UNP Q6XEC0
DDD	12	HIS	-	expression tag	UNP Q6XEC0
DDD	13	SER	-	expression tag	UNP Q6XEC0
DDD	14	ALA	-	expression tag	UNP Q6XEC0
DDD	15	GLY	-	expression tag	UNP Q6XEC0
DDD	16	GLU	-	expression tag	UNP Q6XEC0
DDD	17	ASN	-	expression tag	UNP Q6XEC0

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	18	LEU	-	expression tag	UNP Q6XEC0
DDD	19	TYR	-	expression tag	UNP Q6XEC0
DDD	20	PHE	-	expression tag	UNP Q6XEC0
DDD	21	GLN	-	expression tag	UNP Q6XEC0
DDD	22	GLY	-	expression tag	UNP Q6XEC0

- Molecule 2 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	AAA	1	5	1	1	3	1	0
2	AAA	1	5	1	1	3	1	0
2	BBB	1	5	1	1	3	1	0
2	CCC	1	5	1	1	3	1	0
2	DDD	1	5	1	1	3	1	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	188	Total	O	0	0
			188	188		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	BBB	164	Total 165	O 165	0	1
3	CCC	112	Total 112	O 112	0	0
3	DDD	148	Total 149	O 149	0	1

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.

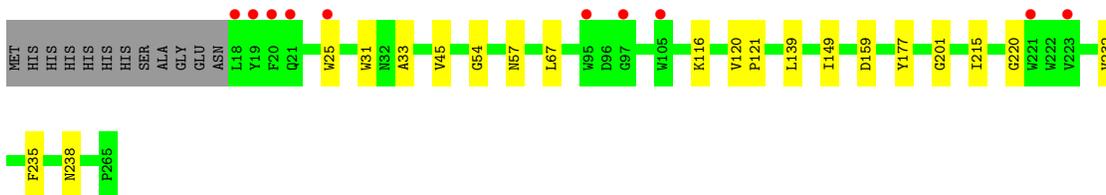
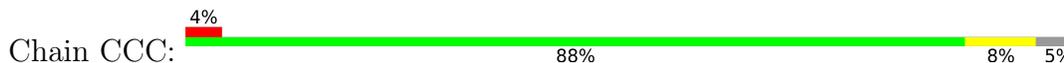
- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.81Å 106.40Å 124.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.50 – 1.97 68.40 – 1.97	Depositor EDS
% Data completeness (in resolution range)	100.0 (68.50-1.97) 99.9 (68.40-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.97Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.195 , 0.286 0.199 , 0.296	Depositor DCC
R_{free} test set	3747 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtrriage
Anisotropy	0.860	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16586	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 44.63 % 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 1.4842e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: KCX, BCT

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	AAA	0.77	0/2032	0.84	0/2746
1	BBB	0.75	0/2049	0.82	0/2768
1	CCC	0.75	0/2083	0.82	0/2815
1	DDD	0.76	0/2039	0.82	0/2756
All	All	0.76	0/8203	0.82	0/11085

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	AAA	1996	1957	1948	7	0
1	BBB	2013	1974	1964	10	0
1	CCC	2045	2002	1992	14	0
1	DDD	1999	1961	1952	12	0
2	AAA	8	2	0	0	0
2	BBB	4	1	0	0	0
2	CCC	4	1	0	0	0
2	DDD	4	1	0	0	0
3	AAA	188	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	165	0	0	2	0
3	CCC	112	0	0	1	0
3	DDD	149	0	0	3	0
All	All	8687	7899	7856	40	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 3.

All (40) 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:CCC:67:LEU:HD11	1:CCC:215:ILE:HD12	1.76	0.67
1:BBB:201:GLY:O	1:CCC:116:LYS:NZ	2.34	0.58
1:CCC:31:TRP:HB2	1:CCC:57:ASN:HB3	1.85	0.58
1:BBB:31:TRP:HB2	1:BBB:57:ASN:HB3	1.89	0.55
1:CCC:33:ALA:O	3:CCC:401:HOH:O	2.18	0.54
1:AAA:31:TRP:HB2	1:AAA:57:ASN:HB3	1.90	0.53
1:CCC:220:GLY:O	1:CCC:238:ASN:HA	2.09	0.52
1:DDD:220:GLY:O	1:DDD:238:ASN:HA	2.09	0.51
1:AAA:220:GLY:O	1:AAA:238:ASN:HA	2.11	0.51
1:BBB:220:GLY:O	1:BBB:238:ASN:HA	2.12	0.50
1:AAA:96:ASP:O	3:AAA:401:HOH:O	2.20	0.50
1:BBB:116:LYS:NZ	1:CCC:201:GLY:O	2.38	0.50
1:DDD:31:TRP:HB2	1:DDD:57:ASN:HB3	1.94	0.49
1:DDD:25:TRP:CE3	1:DDD:54:GLY:HA3	2.48	0.48
1:AAA:116:LYS:NZ	1:DDD:201:GLY:O	2.37	0.47
1:CCC:159:ASP:HA	1:CCC:215:ILE:CD1	2.45	0.47
1:AAA:177:TYR:CZ	1:AAA:232:VAL:HG21	2.49	0.47
1:DDD:177:TYR:CZ	1:DDD:232:VAL:HG21	2.50	0.46
1:DDD:104:THR:HG23	3:DDD:513:HOH:O	2.15	0.46
1:BBB:177:TYR:CZ	1:BBB:232:VAL:HG21	2.51	0.45
1:CCC:25:TRP:CE3	1:CCC:54:GLY:HA3	2.52	0.45
1:DDD:118:SER:HB3	3:DDD:475:HOH:O	2.17	0.44
1:BBB:120:VAL:N	1:BBB:121:PRO:CD	2.79	0.44
1:DDD:120:VAL:N	1:DDD:121:PRO:CD	2.80	0.44
1:AAA:120:VAL:N	1:AAA:121:PRO:CD	2.80	0.43
1:CCC:120:VAL:N	1:CCC:121:PRO:CD	2.80	0.43
1:DDD:25:TRP:CZ3	1:DDD:54:GLY:HA3	2.54	0.43
1:DDD:26:GLN:HG2	3:DDD:523:HOH:O	2.19	0.43
1:BBB:248:GLY:HA3	3:BBB:466:HOH:O	2.19	0.42
1:BBB:248:GLY:CA	3:BBB:466:HOH:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:177:TYR:CZ	1:CCC:232:VAL:HG21	2.54	0.42
1:BBB:115[A]:MET:HG2	1:BBB:123:TYR:OH	2.20	0.41
1:CCC:25:TRP:CZ3	1:CCC:54:GLY:HA3	2.55	0.41
1:CCC:45:VAL:O	1:CCC:235:PHE:HA	2.21	0.41
1:AAA:25:TRP:CE3	1:AAA:54:GLY:HA3	2.55	0.41
1:DDD:120:VAL:HB	1:DDD:121:PRO:HD3	2.02	0.41
1:CCC:159:ASP:HA	1:CCC:215:ILE:HD12	2.03	0.41
1:CCC:139:LEU:HD12	1:CCC:149:ILE:CG2	2.50	0.40
1:BBB:45:VAL:O	1:BBB:235:PHE:HA	2.21	0.40
1:DDD:139:LEU:HD12	1:DDD:149:ILE:CG2	2.51	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	AAA	241/260 (93%)	233 (97%)	8 (3%)	0	100	100
1	BBB	243/260 (94%)	238 (98%)	5 (2%)	0	100	100
1	CCC	246/260 (95%)	238 (97%)	8 (3%)	0	100	100
1	DDD	241/260 (93%)	235 (98%)	6 (2%)	0	100	100
All	All	971/1040 (93%)	944 (97%)	27 (3%)	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	AAA	211/225 (94%)	211 (100%)	0	100	100
1	BBB	213/225 (95%)	213 (100%)	0	100	100
1	CCC	216/225 (96%)	216 (100%)	0	100	100
1	DDD	212/225 (94%)	212 (100%)	0	100	100
All	All	852/900 (95%)	852 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	KCX	AAA	73	1	9,11,12	0.47	0	5,12,14	0.48	0
1	KCX	DDD	73	1	9,11,12	0.39	0	5,12,14	0.60	0
1	KCX	CCC	73	1	9,11,12	0.39	0	5,12,14	0.51	0
1	KCX	BBB	73	1	9,11,12	0.37	0	5,12,14	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	AAA	73	1	-	0/9/10/12	-
1	KCX	DDD	73	1	-	2/9/10/12	-
1	KCX	CCC	73	1	-	0/9/10/12	-
1	KCX	BBB	73	1	-	2/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	BBB	73	KCX	O-C-CA-CB
1	DDD	73	KCX	O-C-CA-CB
1	BBB	73	KCX	C-CA-CB-CG
1	DDD	73	KCX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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	BCT	BBB	301	-	2,3,3	0.52	0	2,3,3	2.21	1 (50%)
2	BCT	CCC	301	-	2,3,3	0.52	0	2,3,3	1.77	1 (50%)
2	BCT	DDD	301	-	2,3,3	1.02	0	2,3,3	1.70	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BCT	AAA	301	-	2,3,3	0.62	0	2,3,3	2.18	1 (50%)
2	BCT	AAA	302	-	2,3,3	0.78	0	2,3,3	2.04	1 (50%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	301	BCT	O2-C-O1	2.60	126.29	119.55
2	BBB	301	BCT	O2-C-O1	2.55	126.17	119.55
2	AAA	302	BCT	O2-C-O1	2.54	126.14	119.55
2	CCC	301	BCT	O2-C-O1	2.21	125.27	119.55
2	DDD	301	BCT	O2-C-O1	2.09	124.97	119.55

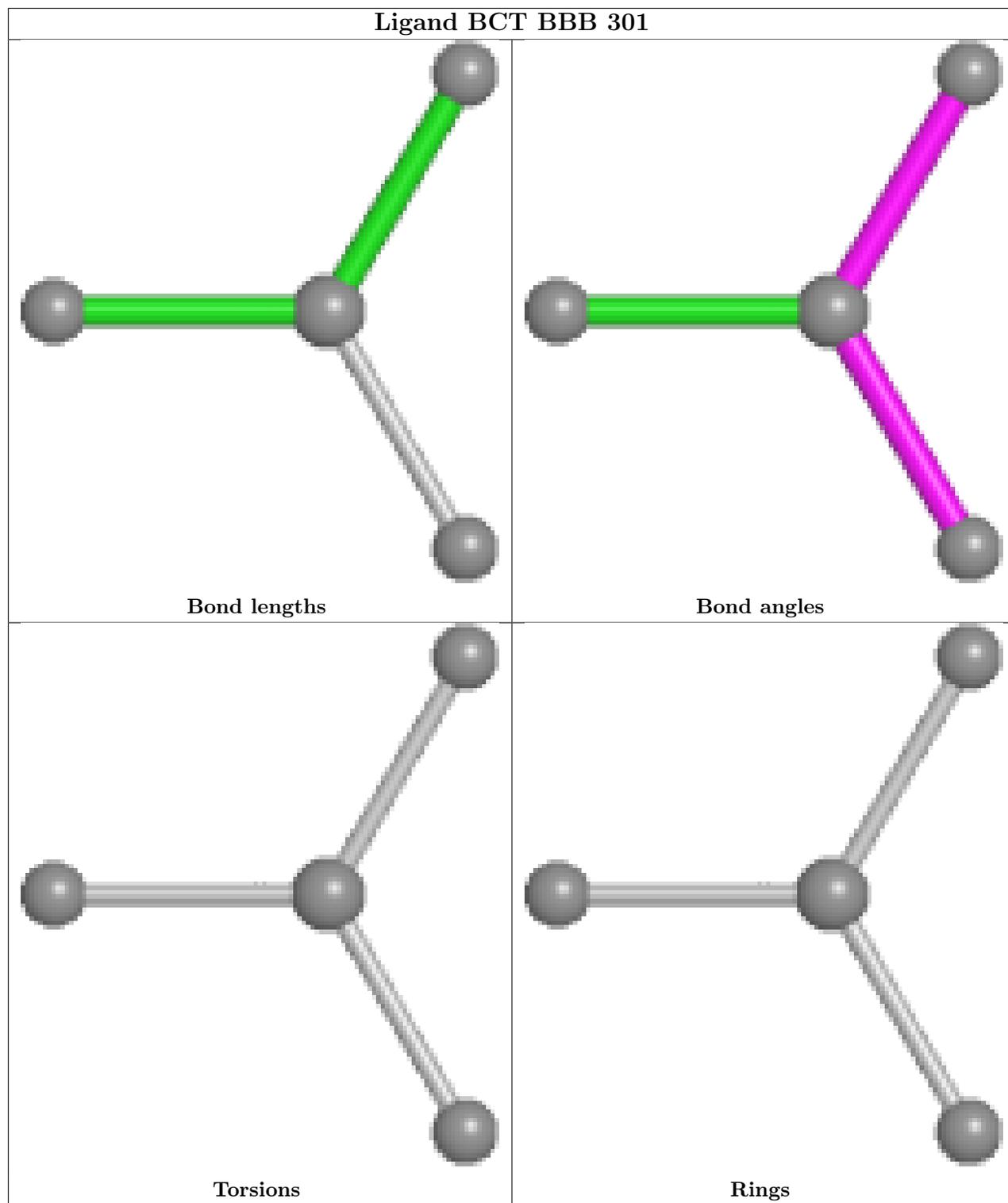
There are no chirality outliers.

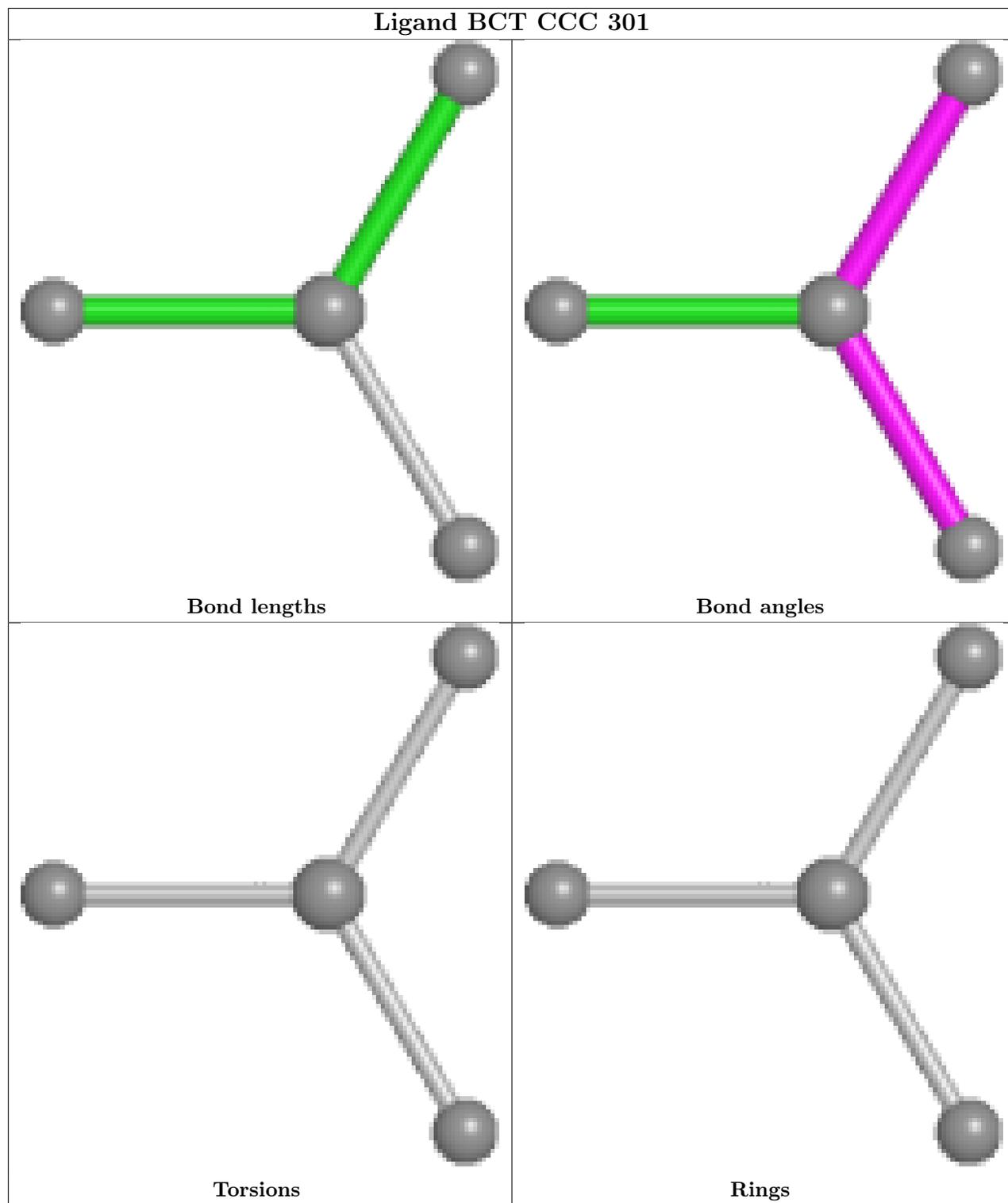
There are no torsion outliers.

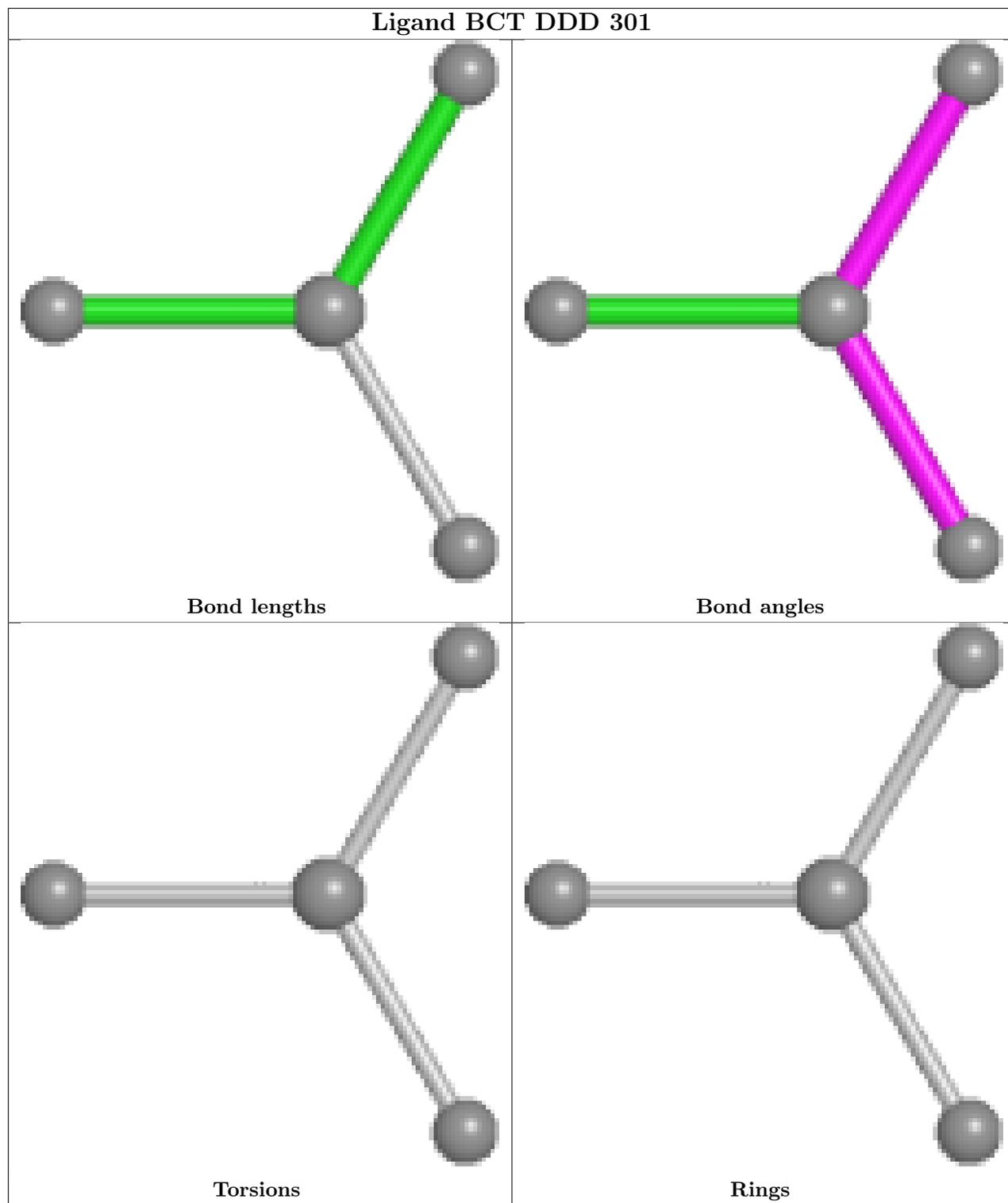
There are no ring outliers.

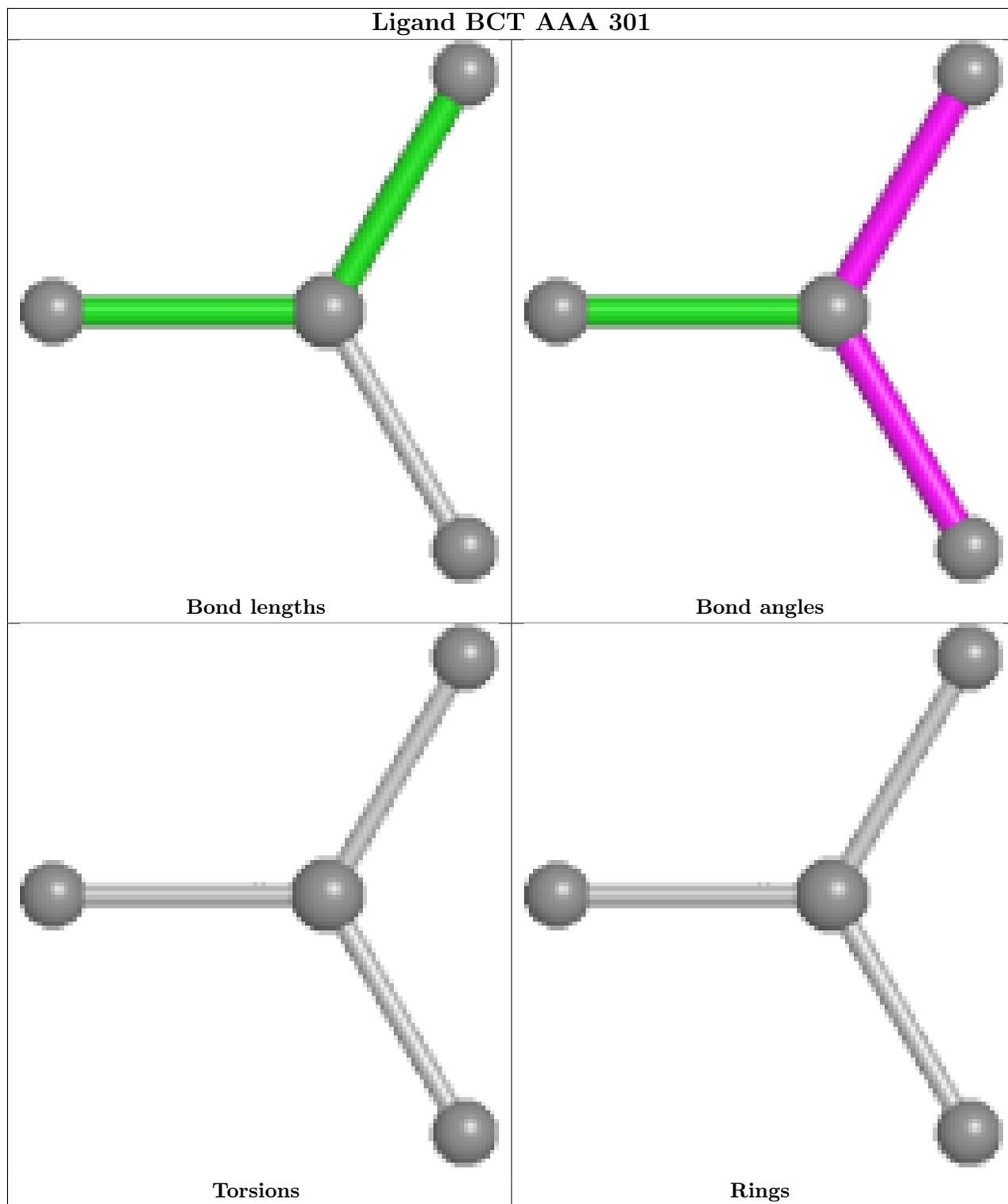
No monomer is involved in short contacts.

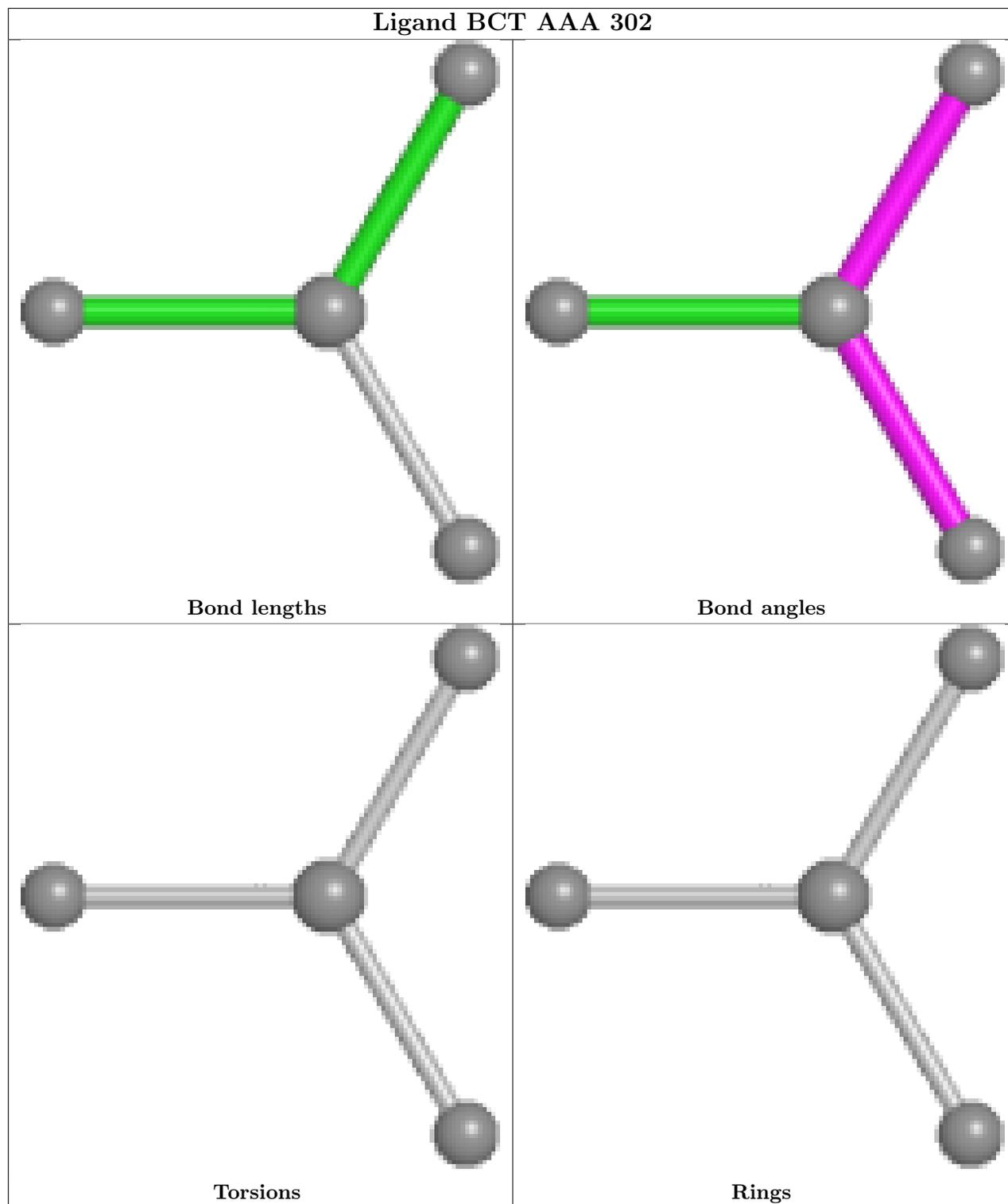
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	243/260 (93%)	-0.03	3 (1%) 79 80	11, 21, 39, 69	1 (0%)
1	BBB	244/260 (93%)	-0.04	1 (0%) 92 93	14, 24, 38, 81	3 (1%)
1	CCC	247/260 (95%)	0.10	10 (4%) 38 40	17, 26, 47, 73	4 (1%)
1	DDD	242/260 (93%)	0.11	2 (0%) 86 87	15, 28, 48, 70	1 (0%)
All	All	976/1040 (93%)	0.03	16 (1%) 72 73	11, 25, 44, 81	9 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	22	GLY	4.2
1	DDD	25	TRP	4.1
1	CCC	21	GLN	3.4
1	CCC	19	TYR	3.1
1	CCC	18	LEU	2.8
1	AAA	59	LEU	2.5
1	DDD	23	LYS	2.5
1	CCC	105	TRP	2.5
1	CCC	20	PHE	2.5
1	CCC	25	TRP	2.4
1	AAA	23	LYS	2.2
1	CCC	223	VAL	2.2
1	CCC	97	GLY	2.1
1	CCC	95	TRP	2.1
1	CCC	221	TRP	2.1
1	BBB	25	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	DDD	73	12/13	0.96	0.11	18,23,29,31	1
1	KCX	BBB	73	12/13	0.97	0.10	15,17,19,20	1
1	KCX	CCC	73	12/13	0.97	0.14	19,26,31,35	1
1	KCX	AAA	73	12/13	0.97	0.14	12,17,19,21	1

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

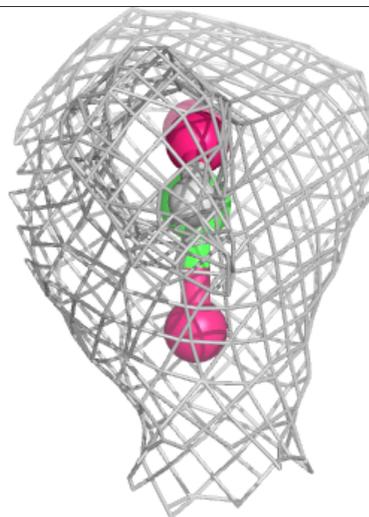
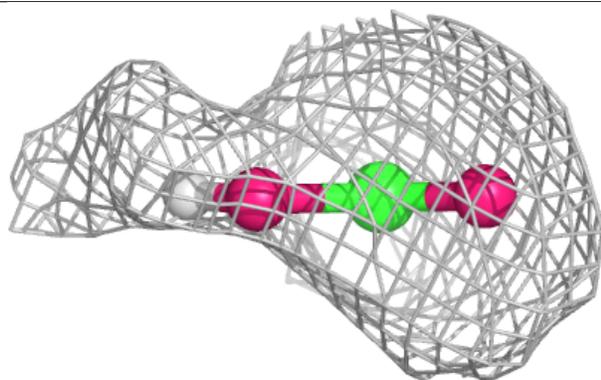
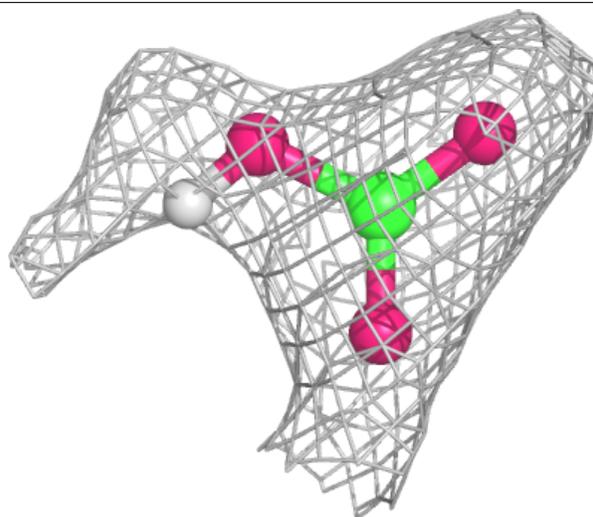
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BCT	DDD	301	4/4	0.95	0.13	40,42,43,49	1
2	BCT	BBB	301	4/4	0.96	0.11	35,40,41,43	1
2	BCT	AAA	302	4/4	0.98	0.07	30,31,37,37	1
2	BCT	CCC	301	4/4	0.99	0.09	14,17,21,22	1
2	BCT	AAA	301	4/4	0.99	0.07	14,18,18,18	1

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.

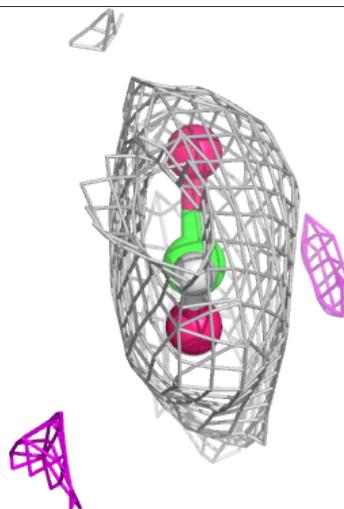
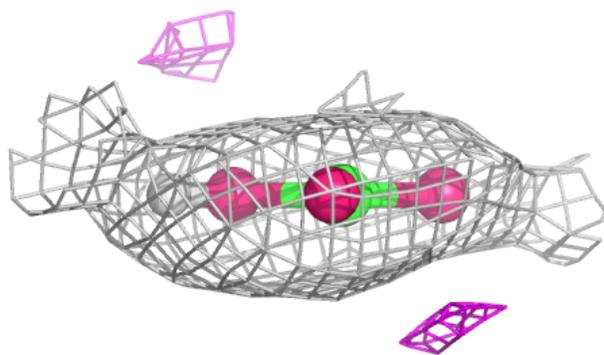
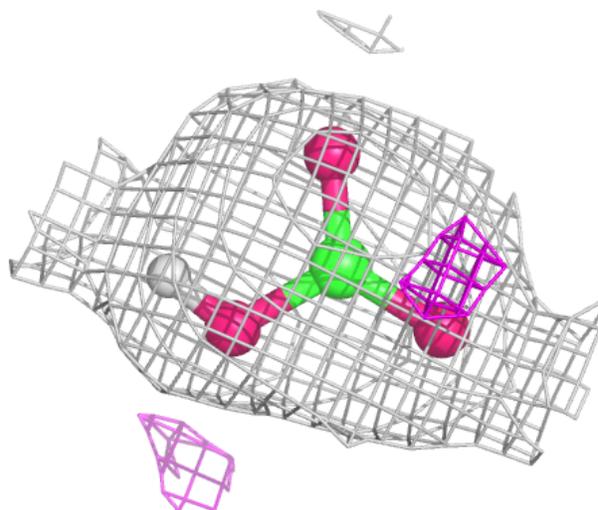
Electron density around BCT DDD 301:

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



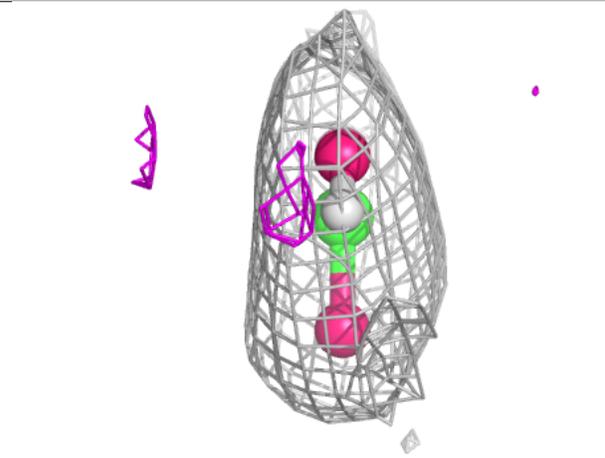
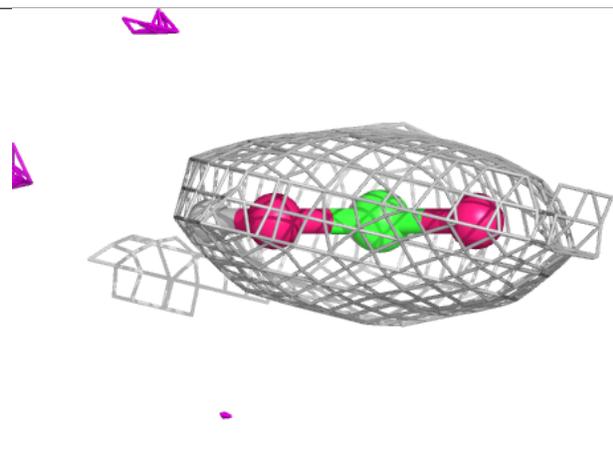
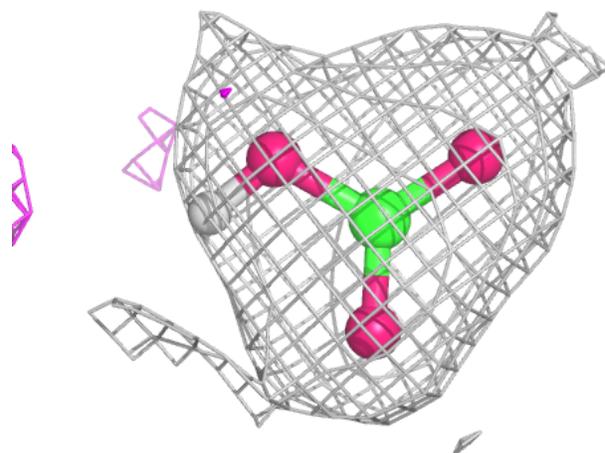
Electron density around BCT BBB 301:

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



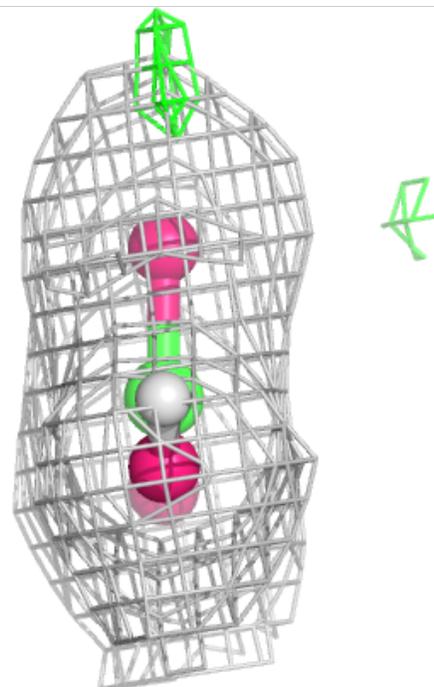
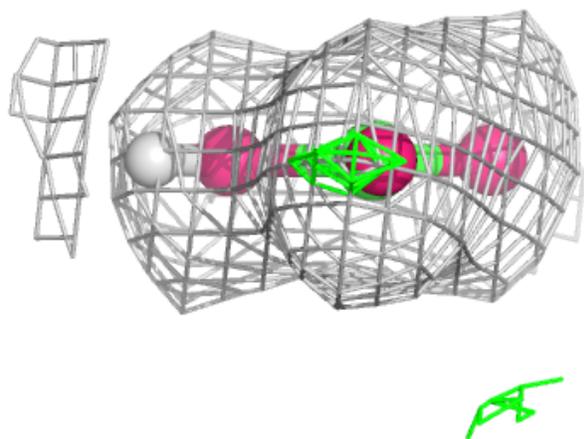
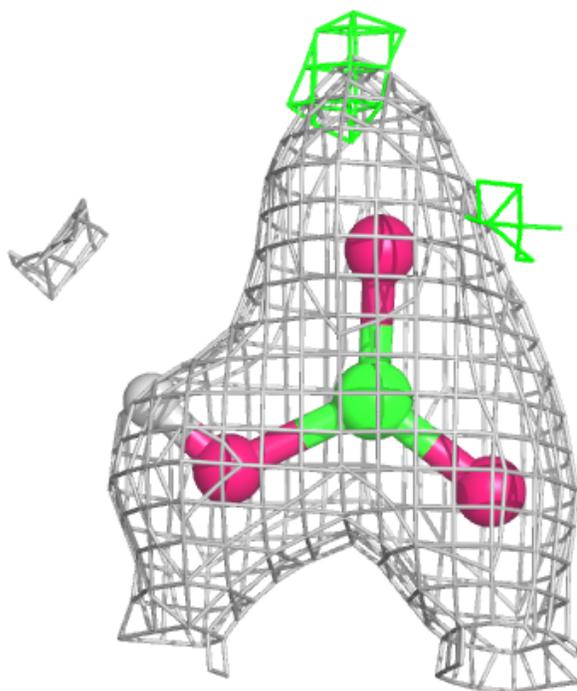
Electron density around BCT AAA 302:

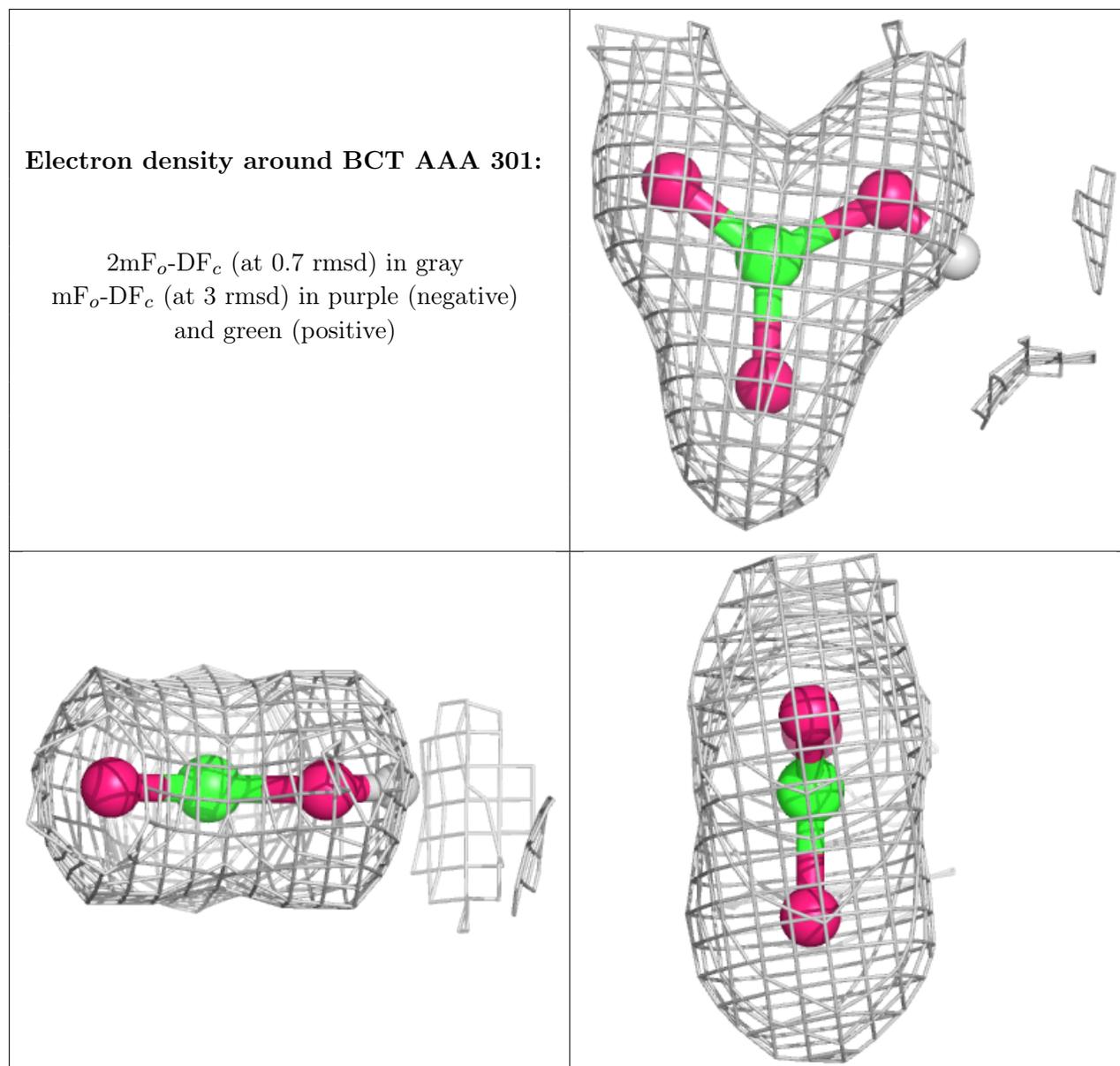
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCT CCC 301:

$2mF_o-DF_c$ (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.