



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2021 – 02:04 PM EST

PDB ID : 7KBL
Title : Biotin Carboxylase domain of Thermophilic 2-Oxoglutarate Carboxylase bound to Bicarbonate
Authors : Buhrman, G.K.; Rose, R.B.; Enriquez, P.; Truong, V.
Deposited on : 2020-10-02
Resolution : 2.30 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 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 : 2.16
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) : 2.16

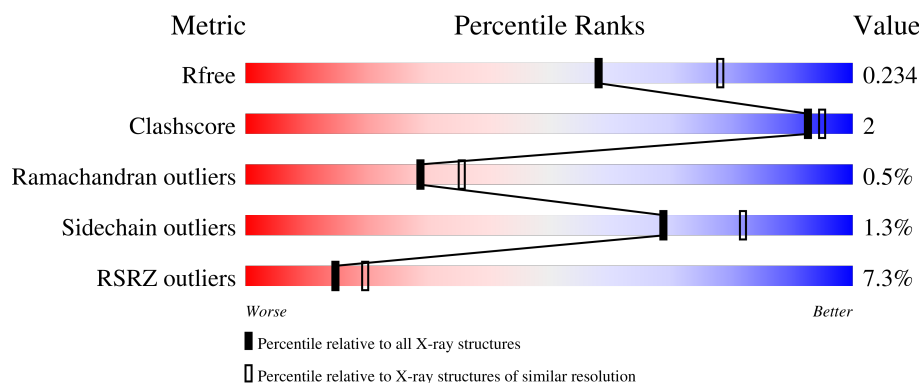
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	A	481	<div> <div>9%</div> <div>87%</div> <div>5%</div> <div>8%</div> </div>
1	B	481	<div> <div>5%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14087 atoms, of which 6782 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.

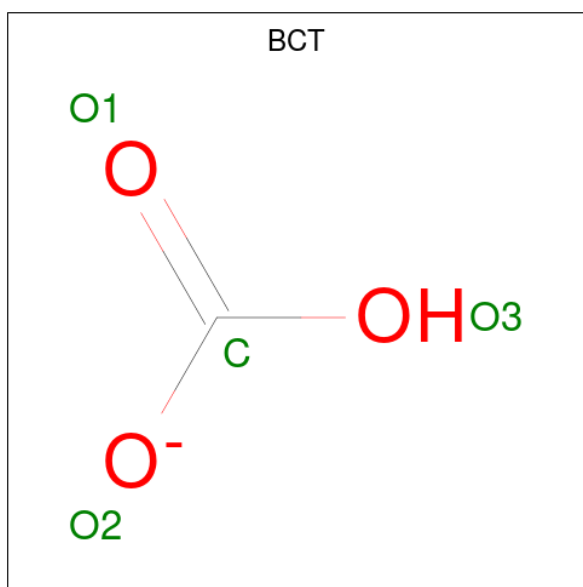
- Molecule 1 is a protein called 2-oxoglutarate carboxylase small subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	443	Total	C	H	N	O	S	0	0	0
			6559	2145	3195	576	628	15			
1	B	451	Total	C	H	N	O	S	0	0	0
			7162	2282	3585	614	665	16			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP D3DJ42
A	-7	LYS	-	expression tag	UNP D3DJ42
A	-6	HIS	-	expression tag	UNP D3DJ42
A	-5	HIS	-	expression tag	UNP D3DJ42
A	-4	HIS	-	expression tag	UNP D3DJ42
A	-3	HIS	-	expression tag	UNP D3DJ42
A	-2	HIS	-	expression tag	UNP D3DJ42
A	-1	HIS	-	expression tag	UNP D3DJ42
A	0	ALA	-	expression tag	UNP D3DJ42
B	-8	MET	-	initiating methionine	UNP D3DJ42
B	-7	LYS	-	expression tag	UNP D3DJ42
B	-6	HIS	-	expression tag	UNP D3DJ42
B	-5	HIS	-	expression tag	UNP D3DJ42
B	-4	HIS	-	expression tag	UNP D3DJ42
B	-3	HIS	-	expression tag	UNP D3DJ42
B	-2	HIS	-	expression tag	UNP D3DJ42
B	-1	HIS	-	expression tag	UNP D3DJ42
B	0	ALA	-	expression tag	UNP D3DJ42

- 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
2	A	1	Total	C	H	O	0	0
			5	1	1	3		
2	B	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	157	Total	O	0	0
			157	157		
3	B	199	Total	O	0	0
			199	199		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.50Å 125.15Å 125.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 2.30 29.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.75-2.30) 99.8 (29.75-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.181 , 0.234 0.182 , 0.234	Depositor DCC
R_{free} test set	1758 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.783	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14087	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 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	A	0.62	0/3433	0.71	3/4659 (0.1%)
1	B	0.65	0/3649	0.71	1/4927 (0.0%)
All	All	0.63	0/7082	0.71	4/9586 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	403	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	40	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	251	ARG	NE-CZ-NH2	-5.15	117.72	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	3364	3195	3197	11	0
1	B	3577	3585	3577	11	0
2	A	4	1	1	0	0
2	B	4	1	1	0	0
3	A	157	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	199	0	0	2	0
All	All	7305	6782	6776	21	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 2.

All (21) 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:B:437:THR:O	1:B:438:ARG:CB	2.44	0.64
1:A:40:ARG:HD3	1:B:358:TYR:CD1	2.40	0.56
1:B:438:ARG:HA	3:B:733:HOH:O	2.06	0.55
1:B:76:ALA:HA	1:B:100:THR:O	2.11	0.51
1:A:204:ASN:H	1:A:438:ARG:HH12	1.59	0.50
1:B:114:ASP:O	1:B:117:ARG:O	2.31	0.48
1:A:234:ASN:ND2	3:A:610:HOH:O	2.48	0.46
1:A:209:GLU:O	1:A:225:GLU:HA	2.18	0.44
1:A:339:ASN:O	1:A:416:THR:HA	2.17	0.44
1:B:71:GLU:OE1	3:B:601:HOH:O	2.21	0.43
1:B:121:VAL:HG11	1:B:265:ILE:HG21	2.01	0.42
1:B:202:ILE:HD12	1:B:284:TYR:CE2	2.54	0.42
1:A:296:HIS:CG	1:A:297:PRO:HD3	2.54	0.42
1:A:27:GLN:NE2	3:A:603:HOH:O	2.39	0.42
1:B:150:ILE:HD11	1:B:198:LEU:HD21	2.01	0.42
1:A:40:ARG:HD2	3:A:720:HOH:O	2.19	0.42
1:B:27:GLN:HA	1:B:46:ASP:OD2	2.20	0.41
1:A:297:PRO:O	1:A:301:MET:HG2	2.21	0.41
1:A:443:HIS:O	1:A:446:VAL:HG22	2.21	0.41
1:B:296:HIS:N	1:B:297:PRO:CD	2.84	0.41
1:A:155:LEU:O	1:A:198:LEU:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/481 (91%)	428 (98%)	10 (2%)	1 (0%)	47	58
1	B	449/481 (93%)	435 (97%)	11 (2%)	3 (1%)	22	26
All	All	888/962 (92%)	863 (97%)	21 (2%)	4 (0%)	29	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	118	SER
1	A	269	SER
1	B	163	GLY
1	B	269	SER

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	325/401 (81%)	321 (99%)	4 (1%)	71	84
1	B	373/401 (93%)	368 (99%)	5 (1%)	69	82
All	All	698/802 (87%)	689 (99%)	9 (1%)	69	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	355	GLU
1	A	369	HIS
1	A	409	TYR
1	B	173	GLU
1	B	369	HIS
1	B	372	SER
1	B	373	LYS
1	B	409	TYR

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	105	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](#)

2 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	B	501	-	0,3,3	0.00	-	0,3,3	0.00	-
2	BCT	A	501	-	0,3,3	0.00	-	0,3,3	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

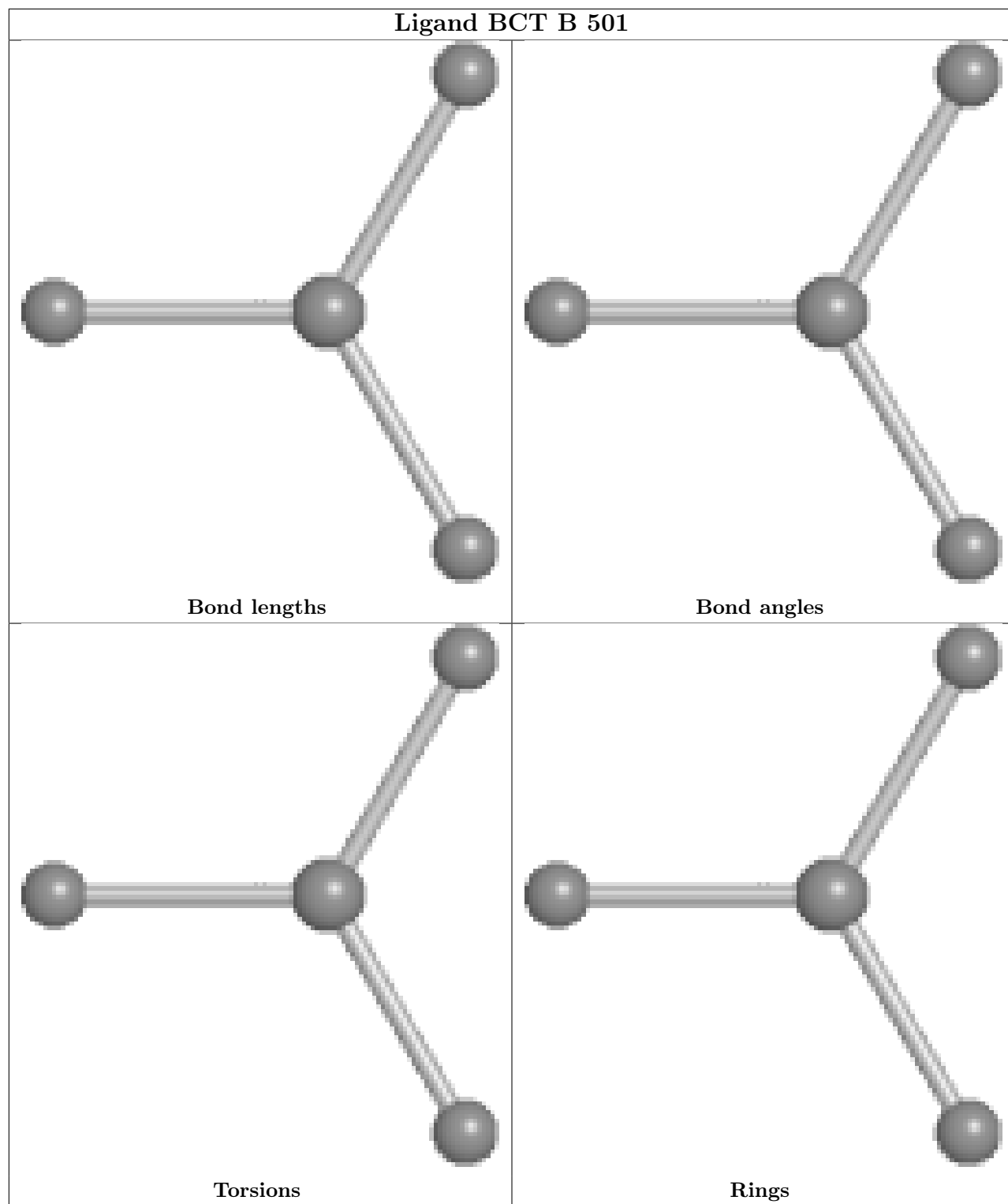
There are no chirality outliers.

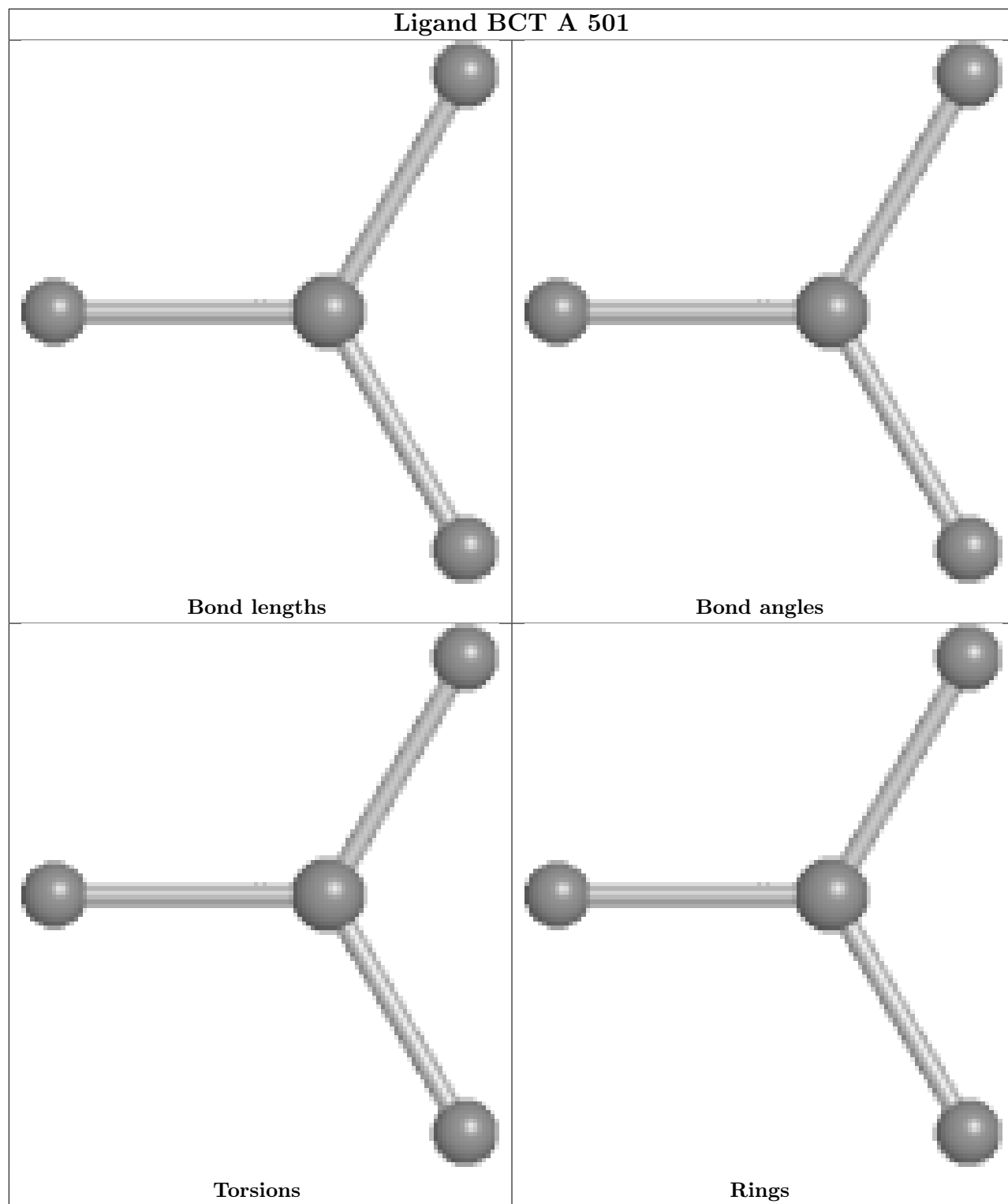
There are no torsion outliers.

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 ⓘ

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, 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	A	443/481 (92%)	0.46	41 (9%) 8 11	24, 37, 84, 96	0
1	B	451/481 (93%)	0.14	24 (5%) 26 33	24, 35, 58, 91	0
All	All	894/962 (92%)	0.30	65 (7%) 15 20	24, 36, 78, 96	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	CYS	10.2
1	B	162	GLY	6.4
1	A	146	ILE	6.2
1	A	183	ALA	5.7
1	A	171	ARG	5.7
1	B	163	GLY	5.3
1	A	135	GLY	5.2
1	A	147	ALA	5.0
1	A	201	TYR	5.0
1	A	140	VAL	4.8
1	A	187	ALA	4.7
1	A	194	GLY	4.5
1	B	124	ARG	4.5
1	A	158	ALA	4.2
1	A	151	GLY	4.2
1	A	180	TYR	4.0
1	A	195	ASP	3.9
1	A	139	ASP	3.8
1	A	138	LYS	3.6
1	B	308	VAL	3.6
1	A	202	ILE	3.6
1	A	196	LEU	3.5
1	A	136	ILE	3.4
1	A	188	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	143	ALA	3.4
1	A	184	TYR	3.3
1	B	13	ILE	3.0
1	A	156	LEU	2.9
1	B	294	VAL	2.9
1	A	137	LEU	2.8
1	B	116	ALA	2.8
1	A	141	GLU	2.8
1	A	172	ASN	2.7
1	B	93	LEU	2.7
1	A	361	GLY	2.7
1	A	179	ASN	2.6
1	A	169	ILE	2.6
1	B	271	GLY	2.5
1	A	362	GLY	2.5
1	A	190	ALA	2.4
1	A	149	GLU	2.4
1	A	185	ASN	2.4
1	B	167	ILE	2.4
1	B	307	ILE	2.3
1	B	367	VAL	2.3
1	B	226	ARG	2.3
1	A	142	GLU	2.3
1	B	272	THR	2.3
1	B	296	HIS	2.3
1	A	152	TYR	2.3
1	B	18	ILE	2.2
1	A	203	GLU	2.2
1	B	297	PRO	2.2
1	A	15	CYS	2.2
1	B	292	ILE	2.2
1	B	293	GLN	2.2
1	A	145	ARG	2.2
1	B	14	ALA	2.2
1	A	132	GLY	2.2
1	A	150	ILE	2.1
1	B	15	CYS	2.1
1	B	17	VAL	2.1
1	B	117	ARG	2.1
1	B	321	ARG	2.1
1	A	148	LYS	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](#)

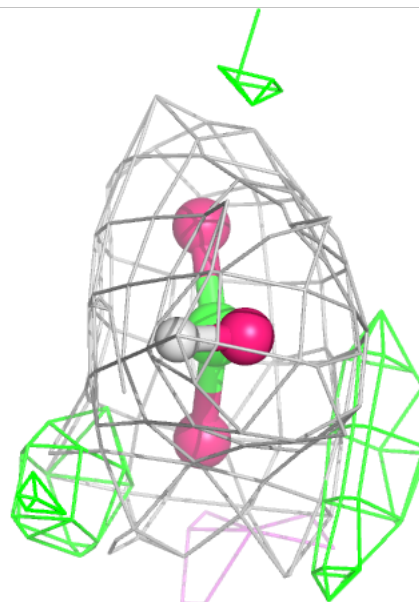
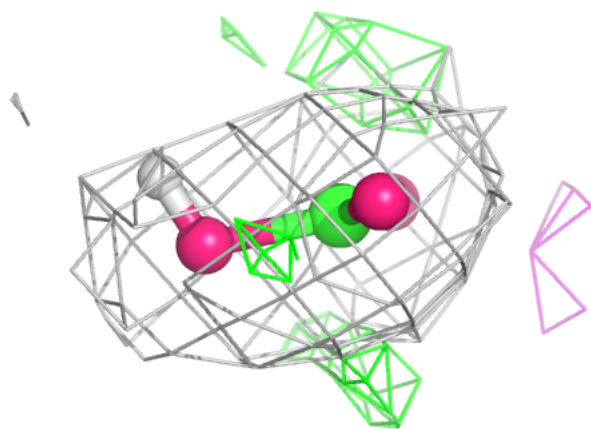
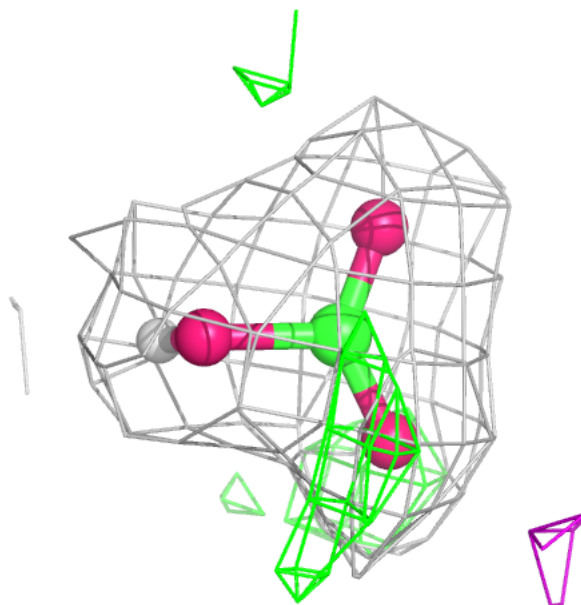
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

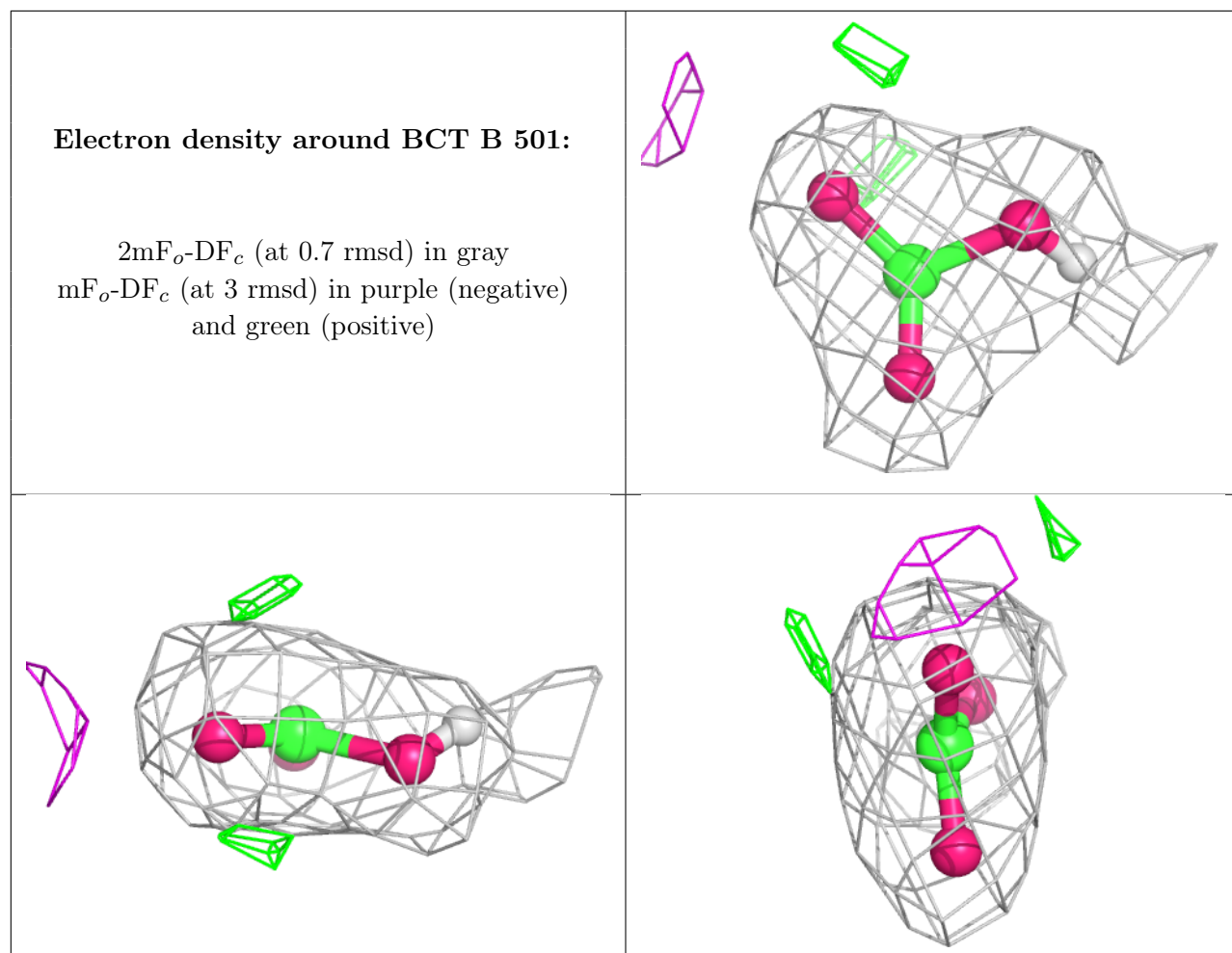
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BCT	A	501	4/4	0.97	0.23	27,31,34,45	0
2	BCT	B	501	4/4	0.98	0.23	26,31,34,34	0

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 BCT A 501:

$2mF_o-DF_c$ (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.