



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 21, 2021 – 02:04 PM EST

PDB ID : 7KCT  
Title : Crystal Structure of the Hydrogenobacter thermophilus 2-Oxoglutarate Carboxylase (OGC) Biotin Carboxylase (BC) Domain Dimer in Complex with Adenosine 5'-Diphosphate Magnesium Salt (MgADP), Adenosine 5'-Diphosphate (ADP, and Bicarbonate Anion (Hydrogen Carbonate/HCO<sub>3</sub><sup>-</sup>)  
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Deposited on : 2020-10-07  
Resolution : 2.02 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 : 2.16  
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

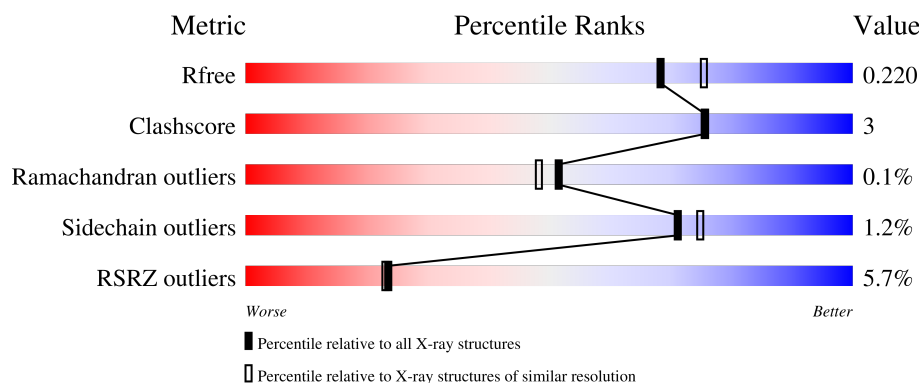
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	481	<div> <div>3%</div> <div>87%</div> <div>7%</div> <div>6%</div> </div>
1	B	481	<div> <div>8%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14245 atoms, of which 6856 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	453	Total	C	H	N	O	S	0	0	0
			6962	2250	3448	609	639	16			
1	B	453	Total	C	H	N	O	S	0	1	0
			6810	2214	3359	588	633	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	GLN	-	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	GLN	-	expression tag	UNP D3DJ42

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

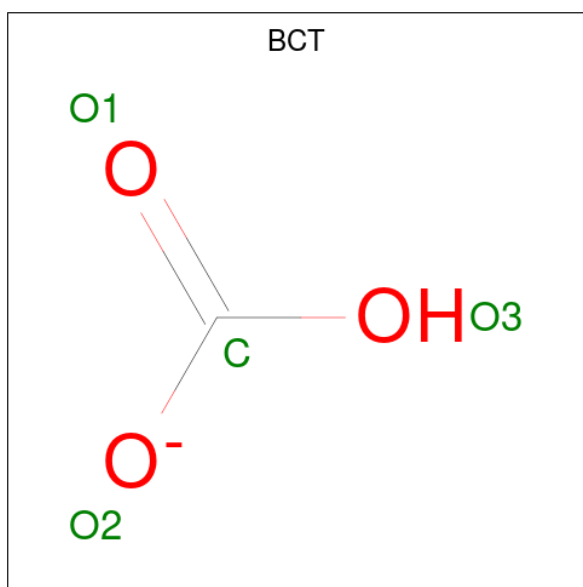


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	A	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	B	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	B	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			5	1	1	3		

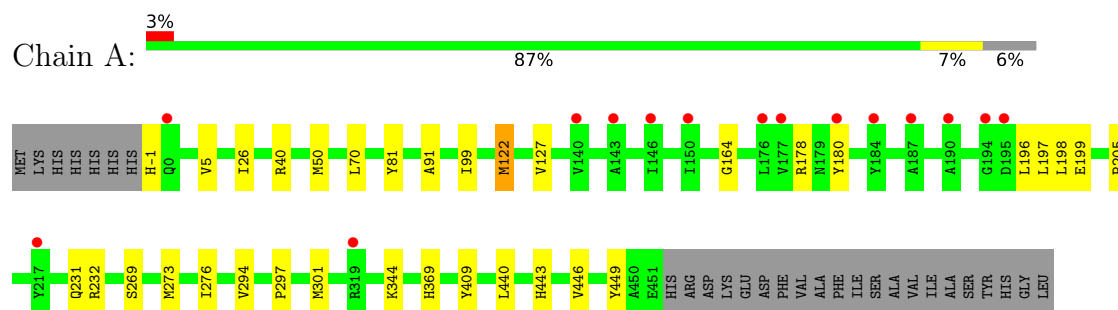
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	161	Total	O	0	0
			161	161		
5	B	149	Total	O	0	0
			149	149		

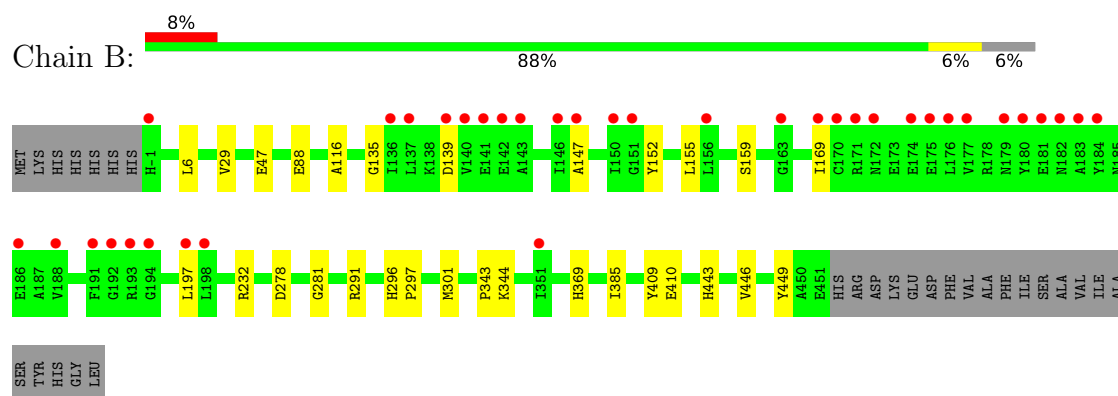
### 3 Residue-property plots

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: 2-oxoglutarate carboxylase small subunit



- Molecule 1: 2-oxoglutarate carboxylase small subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.28Å 86.88Å 86.11Å 90.00° 113.65° 90.00°	Depositor
Resolution (Å)	42.10 – 2.02 42.11 – 2.02	Depositor EDS
% Data completeness (in resolution range)	94.6 (42.10-2.02) 94.5 (42.11-2.02)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.11 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.174 , 0.219 0.174 , 0.220	Depositor DCC
$R_{free}$ test set	2014 reflections (3.32%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14245	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, MG, ADP

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	0.65	0/3586	0.76	2/4852 (0.0%)
1	B	0.64	0/3525	0.77	1/4777 (0.0%)
All	All	0.64	0/7111	0.76	3/9629 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	122	MET	CG-SD-CE	5.33	108.73	100.20
1	A	50	MET	CG-SD-CE	5.24	108.59	100.20

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	3514	3448	3474	22	0
1	B	3451	3359	3358	18	0
2	A	54	24	22	6	0
2	B	54	24	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	1	1	0	0
5	A	161	0	0	2	0
5	B	149	0	0	1	0
All	All	7389	6856	6876	43	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 (43) 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)
2:A:502:ADP:O5'	2:A:502:ADP:PA	1.97	1.21
1:A:-1:HIS:CB	5:A:747:HOH:O	2.31	0.78
1:A:122:MET:HE3	1:A:127:VAL:HG21	1.76	0.68
2:A:502:ADP:PA	2:A:502:ADP:C5'	2.88	0.62
1:A:122:MET:HE1	1:A:273:MET:SD	2.45	0.57
1:A:122:MET:CE	1:A:273:MET:SD	2.94	0.55
1:A:276:ILE:HD11	2:A:501:ADP:H2'	1.90	0.54
1:A:443:HIS:O	1:A:446:VAL:HG22	2.10	0.52
1:A:5:VAL:HG23	1:A:26:ILE:HG21	1.93	0.50
1:A:205:PRO:HB2	1:A:276:ILE:HG23	1.95	0.49
2:A:502:ADP:H5'2	2:A:502:ADP:O1A	2.14	0.48
1:A:91:ALA:O	5:A:601:HOH:O	2.20	0.47
1:B:278:ASP:OD1	1:B:281:GLY:N	2.47	0.47
1:B:344:LYS:NZ	1:B:449:TYR:O	2.38	0.47
1:B:139:ASP:OD1	1:B:139:ASP:N	2.48	0.47
1:A:164:GLY:N	2:A:501:ADP:O1B	2.42	0.47
1:B:443:HIS:O	1:B:446:VAL:HG22	2.15	0.46
1:B:29:VAL:HG22	1:B:47:GLU:CG	2.46	0.46
1:A:297:PRO:O	1:A:301:MET:HG2	2.16	0.45
1:B:197:LEU:HD12	1:B:197:LEU:C	2.37	0.45
1:B:155:LEU:CD1	1:B:169:ILE:HG12	2.47	0.45
1:B:6:LEU:HD23	1:B:6:LEU:C	2.37	0.45
1:B:155:LEU:HA	1:B:155:LEU:HD12	1.89	0.44
1:B:297:PRO:O	1:B:301:MET:HG2	2.17	0.43
1:B:385:ILE:HG21	1:B:385:ILE:HD13	1.71	0.43
1:A:180:TYR:CE1	1:A:196:LEU:HD12	2.54	0.43
1:A:81:TYR:CZ	1:A:294:VAL:HG22	2.54	0.43
1:A:197:LEU:C	1:A:197:LEU:HD12	2.38	0.43
1:B:278:ASP:C	1:B:278:ASP:OD1	2.57	0.43
2:A:502:ADP:O3B	2:A:502:ADP:O2A	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD23	1:A:199:GLU:N	2.34	0.43
1:A:70:LEU:HD23	1:A:99:ILE:HD11	1.99	0.43
1:A:344:LYS:HE3	1:A:449:TYR:CE1	2.55	0.42
1:B:343:PRO:HG2	5:B:683:HOH:O	2.19	0.42
1:A:40:ARG:NH1	1:B:410:GLU:OE1	2.47	0.42
1:A:198:LEU:C	1:A:198:LEU:HD23	2.41	0.41
1:A:122:MET:HE1	1:A:273:MET:CE	2.51	0.41
1:B:116:ALA:HB1	1:B:135:GLY:HA2	2.03	0.41
1:B:88:GLU:CD	1:B:88:GLU:H	2.21	0.41
1:A:122:MET:HE2	1:A:273:MET:SD	2.61	0.41
1:A:231:GLN:O	1:A:440:LEU:HD12	2.21	0.41
1:B:296:HIS:N	1:B:297:PRO:CD	2.84	0.40
1:B:147:ALA:HB1	1:B:152:TYR:CZ	2.57	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	451/481 (94%)	442 (98%)	8 (2%)	1 (0%)	47	43
1	B	452/481 (94%)	437 (97%)	15 (3%)	0	100	100
All	All	903/962 (94%)	879 (97%)	23 (2%)	1 (0%)	51	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	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	352/402 (88%)	348 (99%)	4 (1%)	73	77
1	B	337/402 (84%)	333 (99%)	4 (1%)	71	75
All	All	689/804 (86%)	681 (99%)	8 (1%)	71	75

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	ARG
1	A	232	ARG
1	A	369	HIS
1	A	409	TYR
1	B	159	SER
1	B	232	ARG
1	B	369	HIS
1	B	409	TYR

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

Mol	Chain	Res	Type
1	A	219	ASN
1	B	231	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	ADP	A	502	-	24,29,29	2.79	7 (29%)	29,45,45	2.15	12 (41%)
2	ADP	B	502	3	24,29,29	2.10	7 (29%)	29,45,45	2.09	6 (20%)
2	ADP	B	501	-	24,29,29	2.35	10 (41%)	29,45,45	2.24	10 (34%)
2	ADP	A	501	3	24,29,29	1.76	3 (12%)	29,45,45	2.13	7 (24%)
4	BCT	A	504	-	0,3,3	0.00	-	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	502	-	-	7/12/32/32	0/3/3/3
2	ADP	B	502	3	-	5/12/32/32	0/3/3/3
2	ADP	B	501	-	-	4/12/32/32	0/3/3/3
2	ADP	A	501	3	-	3/12/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	ADP	PA-O5'	9.49	1.97	1.59
2	A	501	ADP	PA-O5'	7.12	1.88	1.59
2	B	502	ADP	PA-O5'	6.69	1.86	1.59
2	B	501	ADP	PA-O5'	6.29	1.84	1.59
2	B	501	ADP	O4'-C4'	-4.38	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	ADP	C3'-C4'	4.31	1.64	1.53
2	A	502	ADP	O3'-C3'	-4.24	1.33	1.43
2	A	502	ADP	O4'-C1'	-3.92	1.35	1.41
2	B	501	ADP	O4'-C1'	-3.76	1.35	1.41
2	B	502	ADP	O4'-C4'	-3.53	1.37	1.45
2	B	501	ADP	O2'-C2'	-3.36	1.35	1.43
2	B	501	ADP	C2-N3	3.24	1.37	1.32
2	A	502	ADP	O2'-C2'	-3.19	1.35	1.43
2	B	502	ADP	C2-N1	3.13	1.39	1.33
2	B	502	ADP	O3'-C3'	-3.01	1.35	1.43
2	B	501	ADP	C3'-C4'	2.97	1.60	1.53
2	B	501	ADP	O3'-C3'	-2.85	1.36	1.43
2	A	502	ADP	C2-N1	2.78	1.39	1.33
2	A	502	ADP	C2-N3	2.54	1.36	1.32
2	B	501	ADP	C4-N3	2.44	1.39	1.35
2	B	502	ADP	C8-N7	2.36	1.38	1.34
2	B	501	ADP	C5'-C4'	-2.33	1.44	1.51
2	A	501	ADP	O2'-C2'	2.28	1.48	1.43
2	B	501	ADP	C2-N1	2.25	1.38	1.33
2	B	502	ADP	O4'-C1'	2.12	1.44	1.41
2	B	502	ADP	C5-C4	2.07	1.46	1.40
2	A	501	ADP	C2'-C1'	-2.05	1.50	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ADP	PA-O3A-PB	-6.17	111.66	132.83
2	B	502	ADP	PA-O3A-PB	-6.02	112.17	132.83
2	B	501	ADP	C3'-C2'-C1'	-5.33	92.96	100.98
2	A	502	ADP	PA-O3A-PB	-4.78	116.41	132.83
2	B	502	ADP	C5'-C4'-C3'	-4.64	97.80	115.18
2	B	501	ADP	PA-O3A-PB	-4.41	117.68	132.83
2	B	501	ADP	O3B-PB-O3A	-4.18	90.62	104.64
2	A	501	ADP	O2B-PB-O1B	4.06	126.57	110.68
2	B	502	ADP	O5'-PA-O1A	-3.80	94.20	109.07
2	B	502	ADP	O2B-PB-O1B	3.65	124.99	110.68
2	A	502	ADP	C5'-C4'-C3'	-3.58	101.77	115.18
2	B	501	ADP	O2B-PB-O1B	3.58	124.68	110.68
2	A	501	ADP	O5'-PA-O1A	-3.55	95.21	109.07
2	B	501	ADP	C5'-C4'-C3'	-3.54	101.93	115.18
2	A	502	ADP	C2'-C3'-C4'	-3.23	96.37	102.64
2	A	502	ADP	O5'-PA-O1A	-3.08	97.04	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ADP	O2A-PA-O5'	-3.05	93.59	107.75
2	A	502	ADP	C3'-C2'-C1'	-2.82	96.74	100.98
2	A	502	ADP	O2B-PB-O1B	2.79	121.61	110.68
2	A	502	ADP	O2B-PB-O3A	-2.77	95.34	104.64
2	A	501	ADP	O3B-PB-O3A	-2.66	95.72	104.64
2	B	502	ADP	O3B-PB-O3A	-2.65	95.76	104.64
2	A	502	ADP	O2A-PA-O5'	-2.52	96.03	107.75
2	B	501	ADP	C2-N1-C6	-2.51	114.46	118.75
2	B	502	ADP	O4'-C1'-C2'	2.50	110.58	106.93
2	A	501	ADP	C2-N1-C6	-2.49	114.50	118.75
2	A	502	ADP	O3B-PB-O3A	-2.45	96.42	104.64
2	B	501	ADP	O5'-PA-O1A	-2.41	99.63	109.07
2	B	501	ADP	C4-C5-N7	2.35	111.84	109.40
2	B	501	ADP	O2A-PA-O1A	2.28	123.49	112.24
2	A	502	ADP	O2A-PA-O1A	2.27	123.45	112.24
2	B	501	ADP	O3'-C3'-C4'	-2.26	104.51	111.05
2	A	501	ADP	C2'-C3'-C4'	-2.25	98.27	102.64
2	A	502	ADP	C2-N1-C6	-2.22	114.96	118.75
2	A	502	ADP	O4'-C4'-C3'	2.22	109.50	105.11

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	ADP	PA-O3A-PB-O3B
2	B	502	ADP	O4'-C4'-C5'-O5'
2	A	502	ADP	O4'-C4'-C5'-O5'
2	A	502	ADP	C3'-C4'-C5'-O5'
2	B	501	ADP	O4'-C4'-C5'-O5'
2	B	502	ADP	C3'-C4'-C5'-O5'
2	B	501	ADP	C3'-C4'-C5'-O5'
2	B	502	ADP	PB-O3A-PA-O1A
2	A	502	ADP	PB-O3A-PA-O5'
2	B	502	ADP	PA-O3A-PB-O2B
2	A	502	ADP	PA-O3A-PB-O2B
2	B	501	ADP	PA-O3A-PB-O3B
2	A	502	ADP	C5'-O5'-PA-O3A
2	A	501	ADP	C5'-O5'-PA-O3A
2	A	501	ADP	C5'-O5'-PA-O1A
2	A	501	ADP	C5'-O5'-PA-O2A
2	B	502	ADP	PB-O3A-PA-O2A
2	B	501	ADP	PA-O3A-PB-O2B

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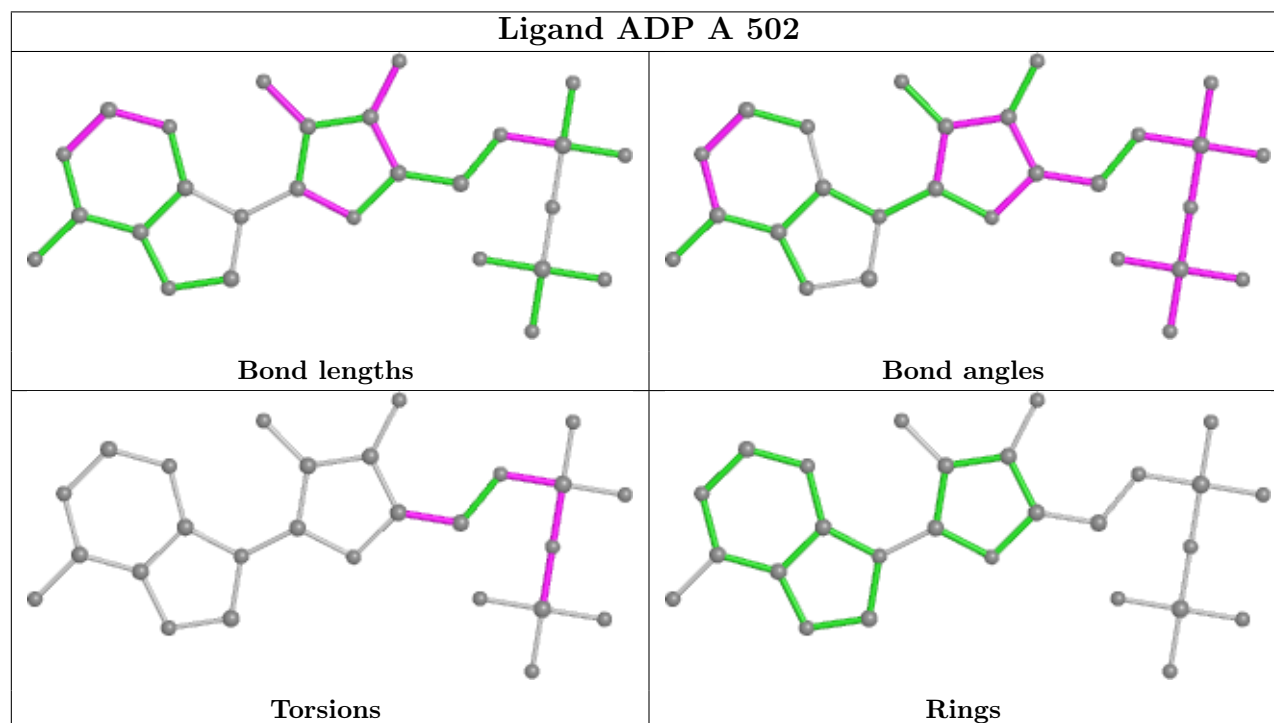
Mol	Chain	Res	Type	Atoms
2	A	502	ADP	C5'-O5'-PA-O2A

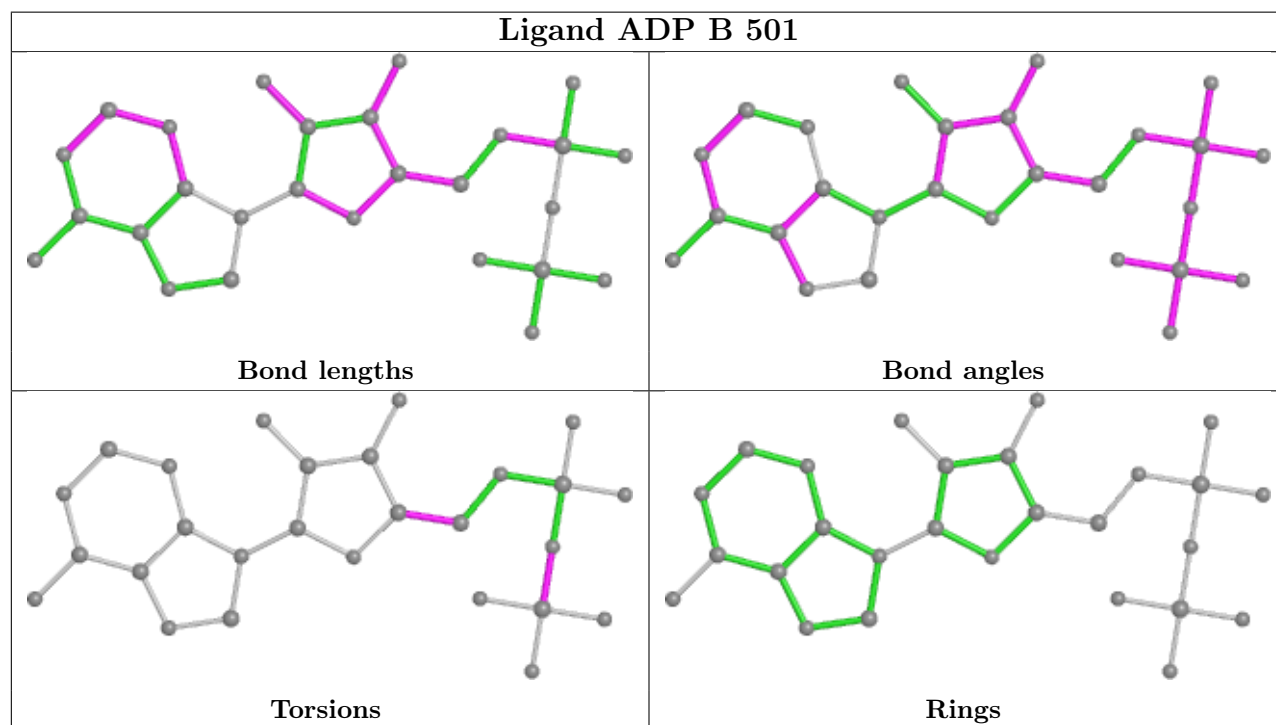
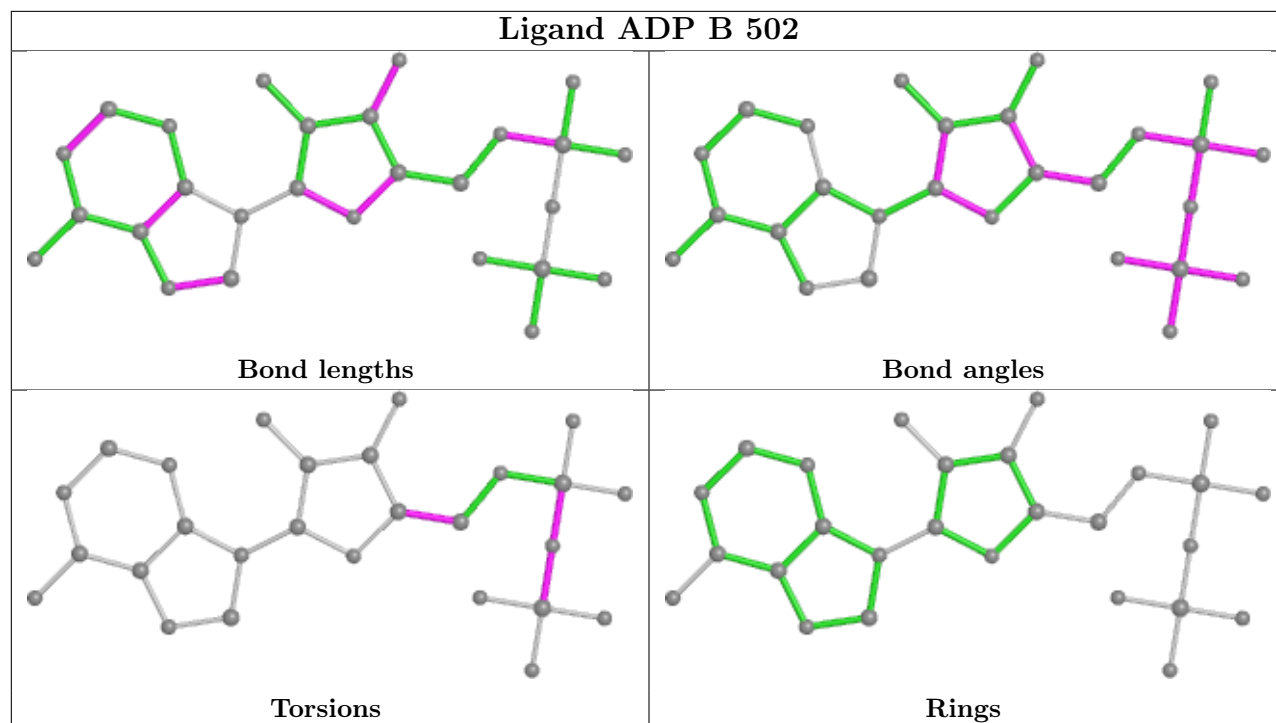
There are no ring outliers.

2 monomers are involved in 6 short contacts:

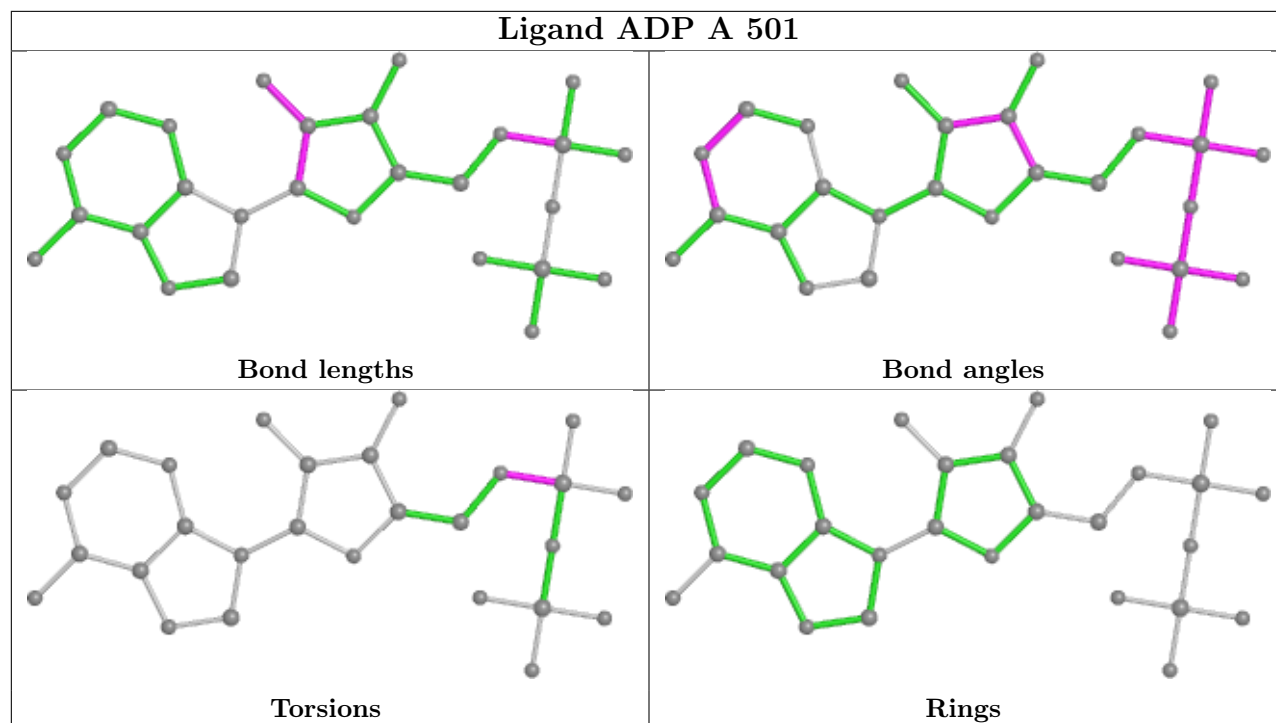
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	ADP	4	0
2	A	501	ADP	2	0

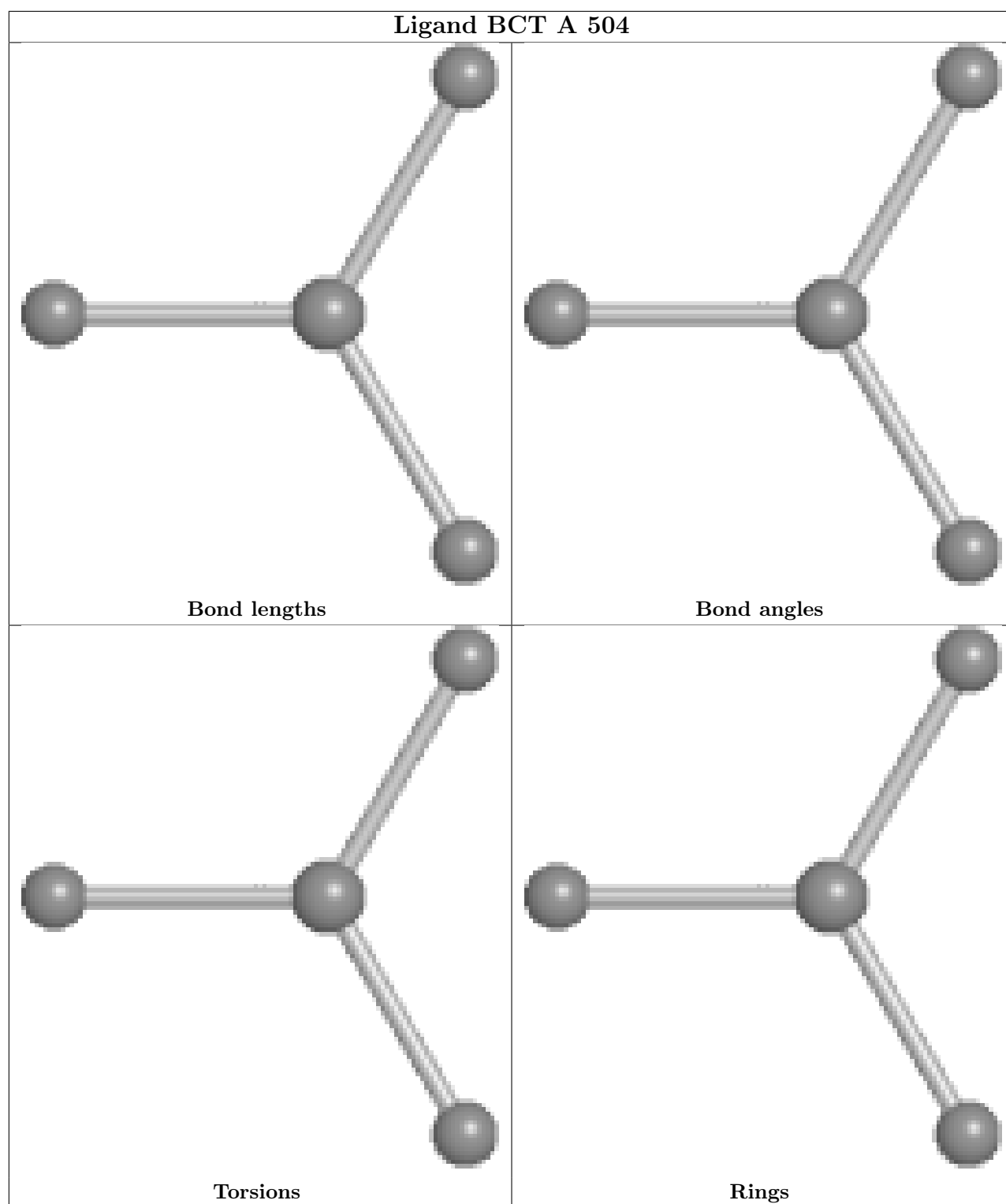
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	453/481 (94%)	0.02	15 (3%) 46 46	22, 36, 59, 71	0
1	B	453/481 (94%)	0.30	37 (8%) 11 11	23, 37, 89, 116	0
All	All	906/962 (94%)	0.16	52 (5%) 23 23	22, 36, 67, 116	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	LEU	8.3
1	B	176	LEU	8.3
1	B	183	ALA	7.3
1	B	140	VAL	6.7
1	B	184	TYR	5.9
1	B	194	GLY	5.9
1	B	143	ALA	5.7
1	B	191	PHE	5.1
1	B	180	TYR	4.9
1	B	182	ASN	4.7
1	B	150	ILE	4.2
1	A	180	TYR	4.2
1	B	179	ASN	4.2
1	B	177	VAL	4.0
1	A	146	ILE	4.0
1	A	0	GLN	4.0
1	B	146	ILE	3.9
1	B	139	ASP	3.9
1	B	169	ILE	3.7
1	B	156	LEU	3.6
1	A	184	TYR	3.6
1	A	177	VAL	3.5
1	B	175	GLU	3.4
1	A	190	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	193	ARG	3.3
1	B	186	GLU	3.3
1	B	147	ALA	3.2
1	B	192	GLY	3.1
1	A	150	ILE	3.0
1	A	140	VAL	2.9
1	A	143	ALA	2.8
1	B	142	GLU	2.7
1	B	170	CYS	2.6
1	B	198	LEU	2.5
1	B	171	ARG	2.5
1	B	351	ILE	2.5
1	B	151	GLY	2.5
1	A	187	ALA	2.4
1	B	197	LEU	2.4
1	B	172	ASN	2.3
1	B	181	GLU	2.3
1	A	195	ASP	2.2
1	B	174	GLU	2.2
1	A	176	LEU	2.2
1	B	188	VAL	2.2
1	B	163	GLY	2.1
1	B	136	ILE	2.1
1	B	141	GLU	2.1
1	A	194	GLY	2.1
1	A	319	ARG	2.1
1	B	-1	HIS	2.1
1	A	217	TYR	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.

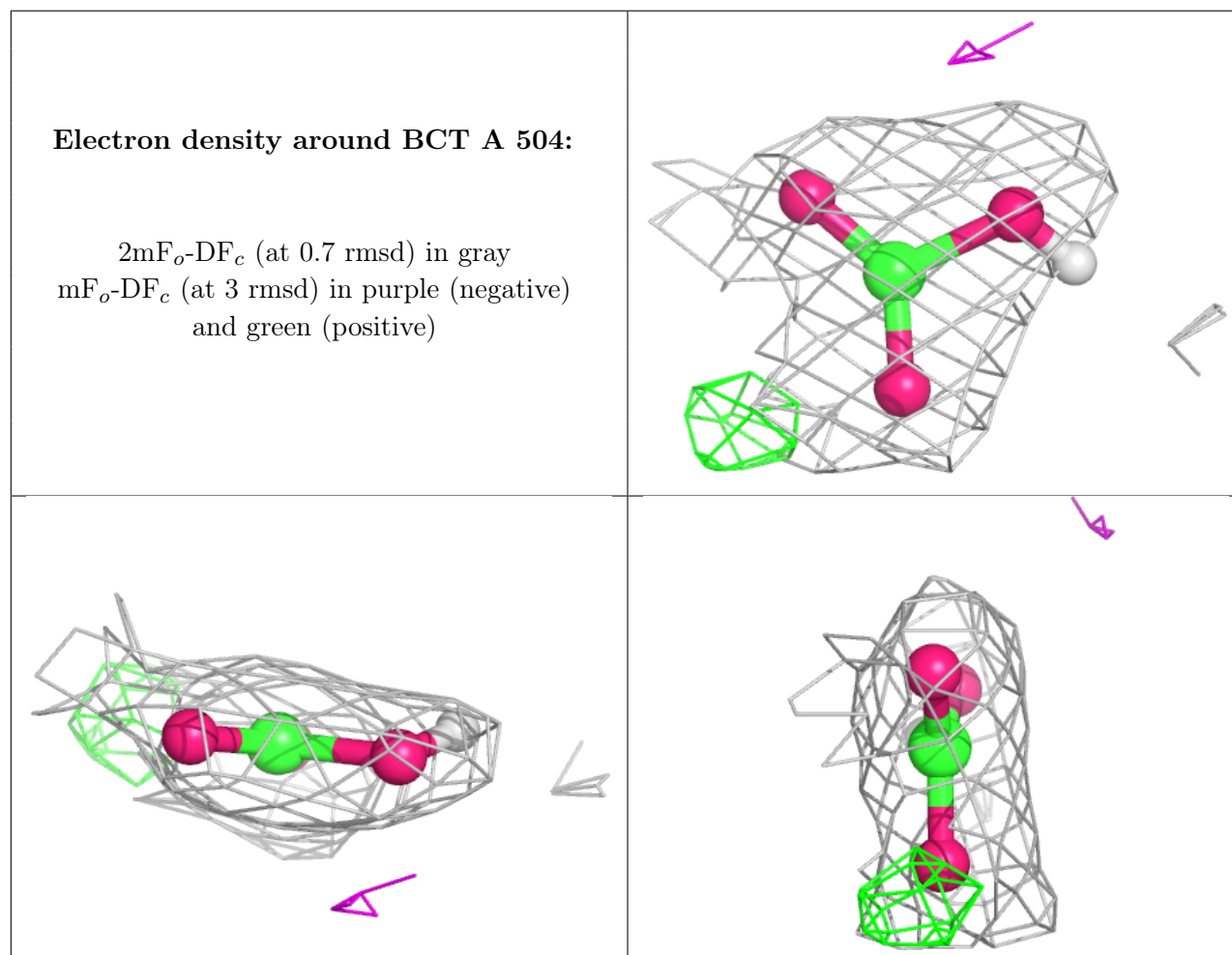
## 6.4 Ligands [i](#)

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.

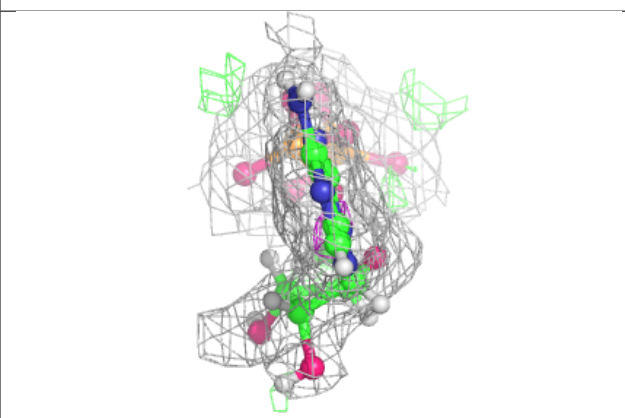
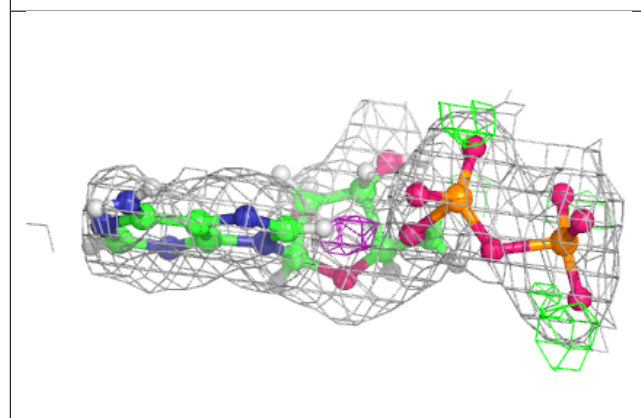
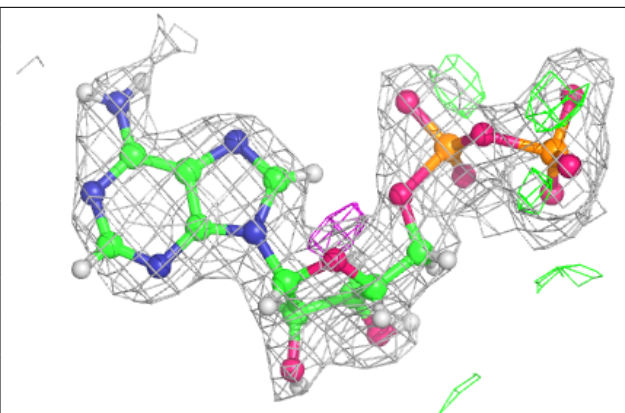
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BCT	A	504	4/4	0.86	0.23	54,55,60,66	0
3	MG	B	503	1/1	0.89	0.09	48,48,48,48	0
2	ADP	B	502	27/27	0.90	0.13	42,51,60,62	0
2	ADP	A	501	27/27	0.93	0.11	32,41,53,55	0
2	ADP	A	502	27/27	0.94	0.12	35,49,66,67	0
2	ADP	B	501	27/27	0.95	0.13	31,45,60,72	0
3	MG	A	503	1/1	0.96	0.09	47,47,47,47	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.

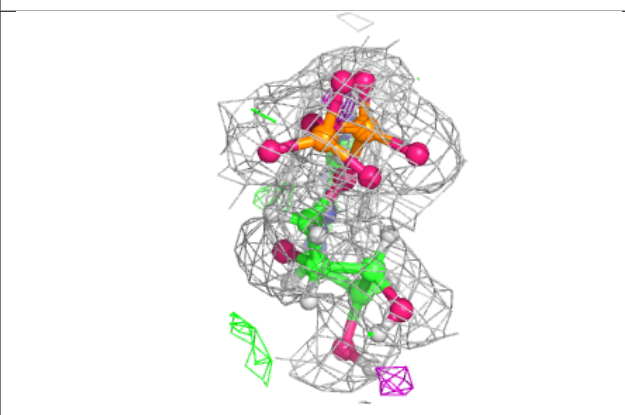
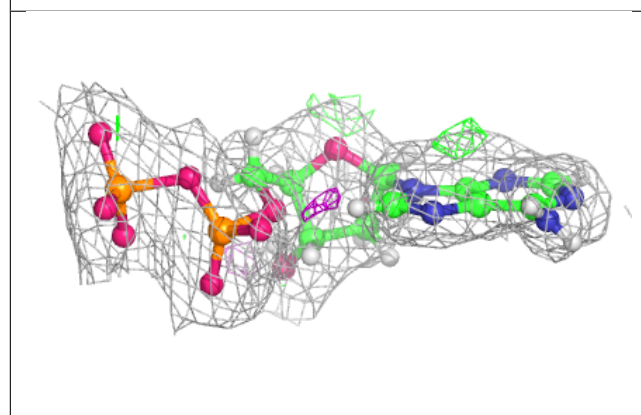
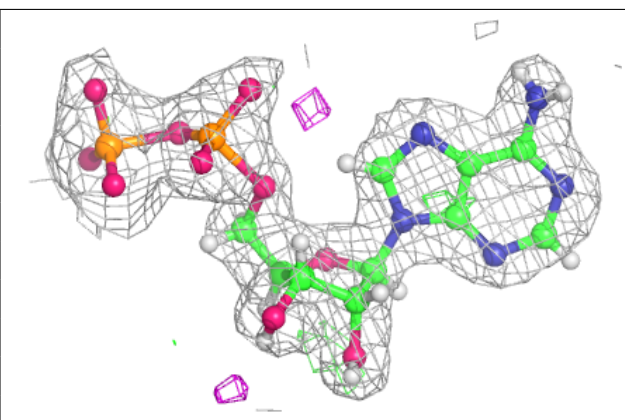


**Electron density around ADP B 502:**

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

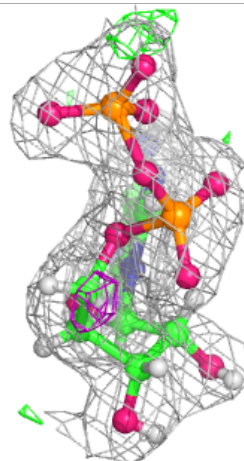
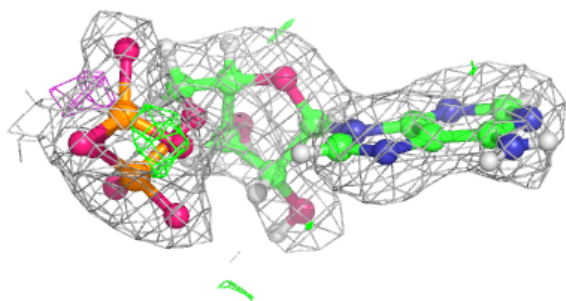
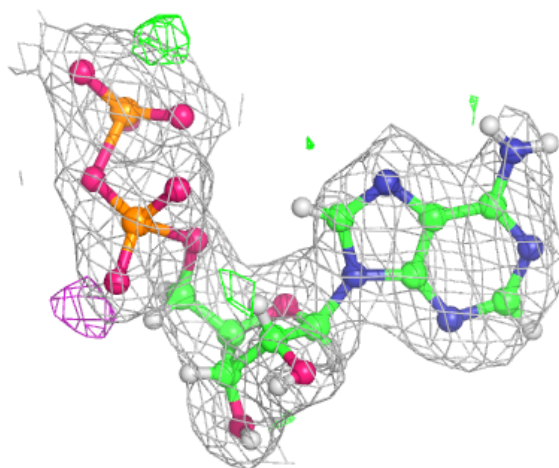
**Electron density around ADP A 501:**

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

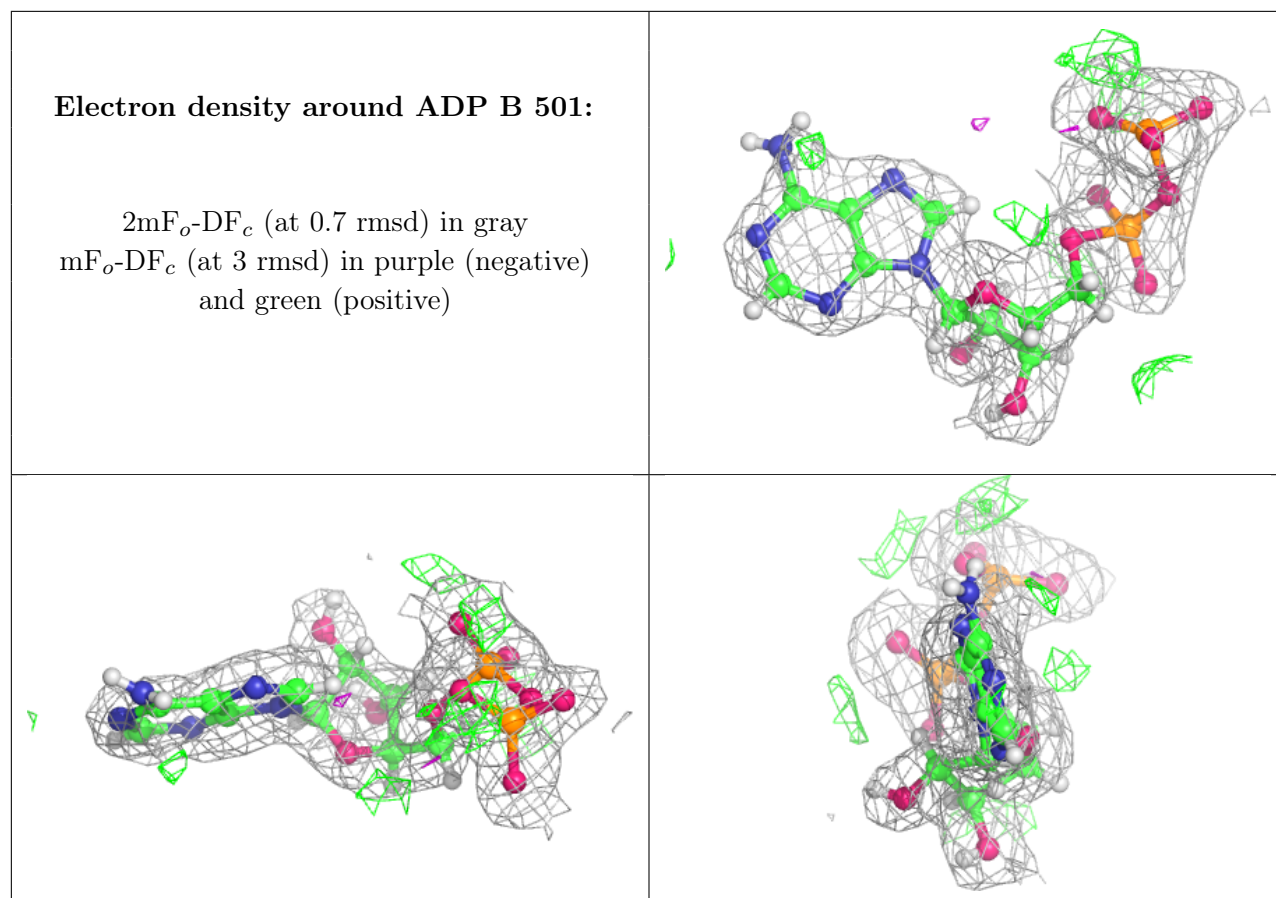


**Electron density around ADP A 502:**

$2mF_o-DF_c$  (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.