



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:53 pm BST

PDB ID : 2Q28  
Title : Crystal structure of oxalyl-coA decarboxylase from Escherichia coli in complex with adenosine-5'-diphosphate  
Authors : Werther, T.; Zimmer, A.; Wille, G.; Hubner, G.; Weiss, M.S.; Konig, S.  
Deposited on : 2007-05-26  
Resolution : 1.74 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 : 2.11  
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) : 2.11

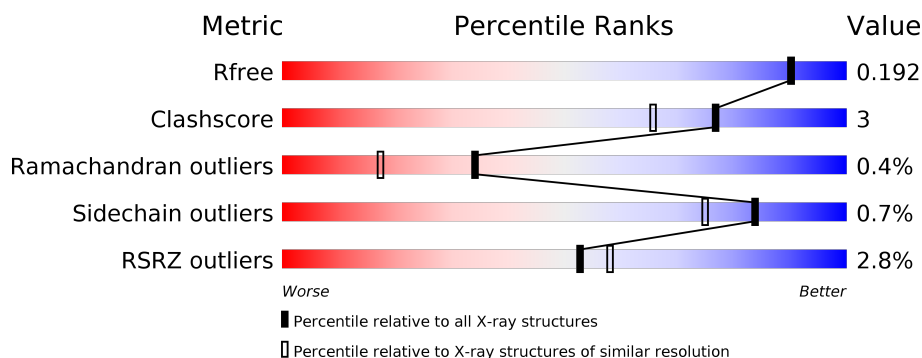
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	564	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div></div> </div> </div>
1	B	564	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div></div> </div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9344 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 oxalyl-CoA decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4147	2610	724	791	22			
1	B	550	Total	C	N	O	S	0	0	0
			4147	2610	724	791	22			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

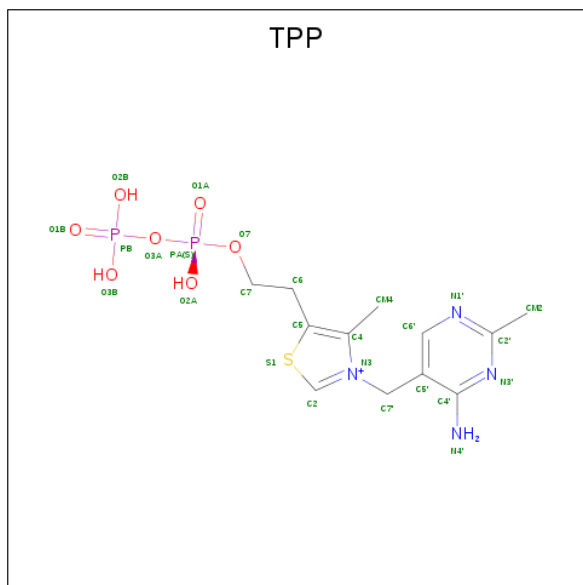
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula:  $C_{12}H_{19}N_4O_7P_2S$ ).



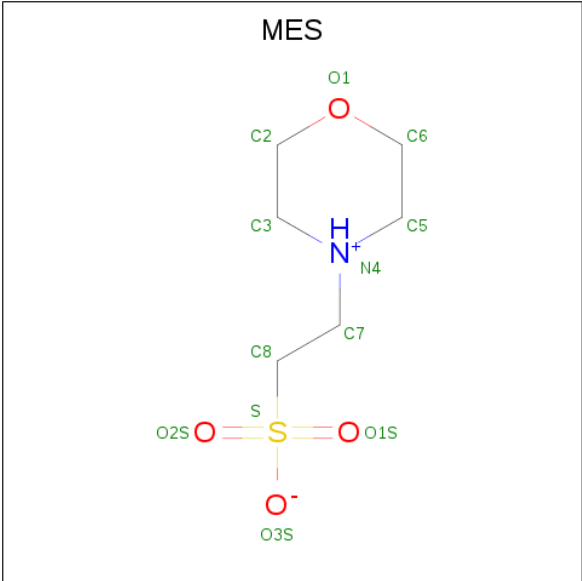
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 26 12 4 7 2 1	0	0
4	B	1	Total C N O P S 26 12 4 7 2 1	0	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

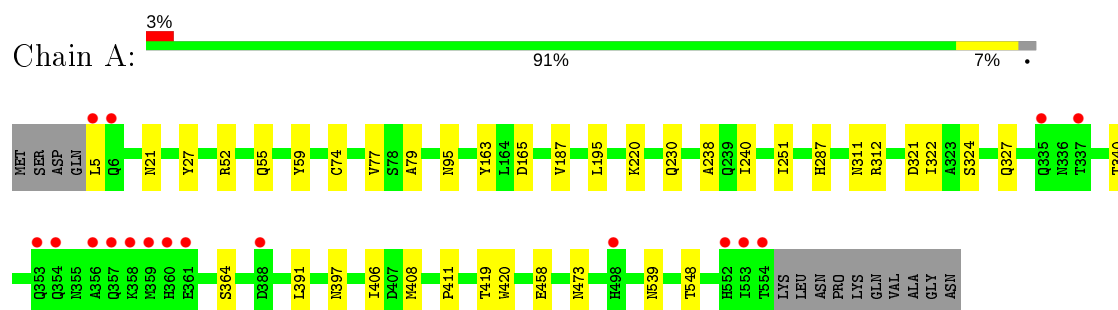
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	465	Total	O	0	0
			465	465		
8	B	427	Total	O	0	0
			427	427		

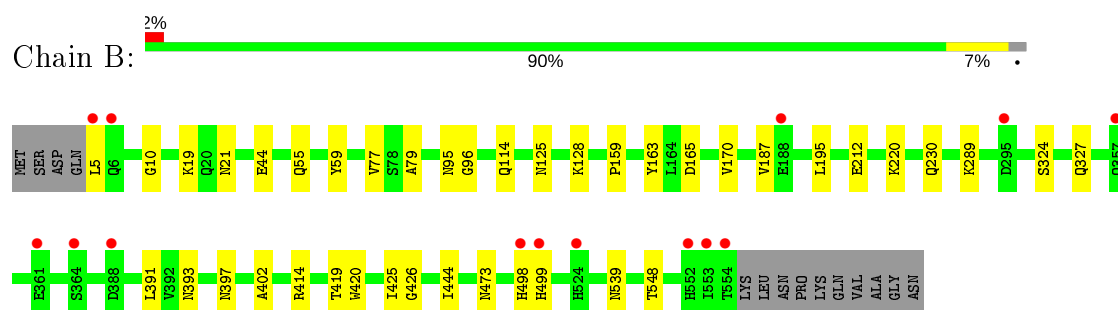
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: oxalyl-CoA decarboxylase



- Molecule 1: oxalyl-CoA decarboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.27Å 143.62Å 147.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.61 – 1.74 20.60 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.61-1.74) 99.6 (20.60-1.74)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 1.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.177 , 0.196 0.177 , 0.192	Depositor DCC
$R_{free}$ test set	1436 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9344	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: MG, ADP, EDO, SO4, MES, TPP

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	0.60	0/4223	0.67	0/5740
1	B	0.55	0/4223	0.63	0/5740
All	All	0.57	0/8446	0.65	0/11480

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

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	4147	0	4156	24	0
1	B	4147	0	4156	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	26	0	16	0	0
4	B	26	0	16	0	0
5	A	27	0	12	1	0
5	B	27	0	12	0	0
6	A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	12	0	12	0	0
7	A	8	0	12	0	0
7	B	8	0	12	0	0
8	A	465	0	0	1	0
8	B	427	0	0	4	0
All	All	9344	0	8416	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 3.

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:A:473:ASN:HD22	1:A:539:ASN:HD21	1.22	0.86
1:B:473:ASN:HD22	1:B:539:ASN:HD21	1.30	0.80
1:A:95:ASN:HD21	1:A:419:THR:H	1.34	0.76
1:A:21:ASN:HD21	1:A:187:VAL:H	1.36	0.74
1:B:128:LYS:HE3	8:B:5323:HOH:O	1.88	0.74
1:B:95:ASN:HD21	1:B:419:THR:H	1.35	0.73
1:B:397:ASN:HD21	1:B:548:THR:H	1.34	0.73
1:B:21:ASN:HD21	1:B:187:VAL:H	1.36	0.73
1:A:397:ASN:HD21	1:A:548:THR:H	1.37	0.72
1:B:212:GLU:HG2	8:B:5406:HOH:O	1.92	0.70
1:A:230:GLN:HE22	1:A:327:GLN:HG3	1.56	0.70
1:B:230:GLN:HE22	1:B:327:GLN:HG3	1.59	0.67
1:B:498:HIS:NE2	1:B:499:HIS:HD2	1.92	0.66
1:A:364:SER:HB2	8:A:4332:HOH:O	1.97	0.64
1:A:55:GLN:HG2	1:A:59:TYR:CE2	2.36	0.61
1:A:95:ASN:ND2	1:A:419:THR:H	2.03	0.55
1:B:397:ASN:ND2	1:B:548:THR:H	2.04	0.54
1:B:19:LYS:HD2	1:B:44:GLU:HB3	1.90	0.54
1:B:95:ASN:ND2	1:B:419:THR:H	2.03	0.53
1:B:393:ASN:HD22	1:B:414:ARG:HH22	1.57	0.53
1:A:397:ASN:ND2	1:A:548:THR:H	2.06	0.51
1:B:289:LYS:CE	8:B:5421:HOH:O	2.60	0.50
1:A:95:ASN:HD22	1:A:220:LYS:HE3	1.76	0.50
1:B:195:LEU:HG	1:B:324:SER:HB3	1.94	0.49
1:A:251:ILE:HA	1:A:411:PRO:HB3	1.93	0.48
1:B:163:TYR:CE2	1:B:165:ASP:HB2	2.49	0.47
1:A:27:TYR:O	1:A:74:CYS:HA	2.15	0.47
1:B:393:ASN:HD21	1:B:402:ALA:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:TYR:CE2	1:A:165:ASP:HB2	2.50	0.46
1:A:195:LEU:HG	1:A:324:SER:HB3	1.98	0.46
1:B:21:ASN:ND2	1:B:187:VAL:H	2.10	0.45
1:B:230:GLN:NE2	1:B:327:GLN:HG3	2.30	0.45
1:A:406:ILE:HG22	1:A:408:MET:CE	2.46	0.45
1:A:230:GLN:NE2	1:A:327:GLN:HG3	2.26	0.45
1:A:21:ASN:ND2	1:A:187:VAL:H	2.10	0.45
1:A:240:ILE:HA	1:A:340:THR:HG21	1.99	0.45
1:A:238:ALA:O	1:A:340:THR:HG23	2.17	0.44
1:B:55:GLN:HG2	1:B:59:TYR:CE2	2.53	0.44
1:B:96:GLY:HA2	1:B:159:PRO:O	2.18	0.43
1:A:391:LEU:HD22	1:A:408:MET:HE1	2.01	0.42
1:B:425:ILE:HD12	1:B:426:GLY:N	2.34	0.42
1:B:10:GLY:HA3	1:B:170:VAL:O	2.20	0.42
1:B:391:LEU:HD11	1:B:444:ILE:HD12	2.02	0.42
1:A:287:HIS:ND1	1:A:311:ASN:ND2	2.67	0.42
1:B:114:GLN:HG3	8:B:5418:HOH:O	2.21	0.41
1:A:312:ARG:HA	1:A:312:ARG:HD2	1.88	0.41
1:B:393:ASN:HD22	1:B:414:ARG:HH12	1.69	0.41
1:B:95:ASN:HD22	1:B:220:LYS:HE3	1.86	0.41
1:A:322:ILE:HG13	5:A:4003:ADP:C2	2.56	0.41
1:A:52:ARG:HD3	1:A:458:GLU:OE1	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	548/564 (97%)	533 (97%)	13 (2%)	2 (0%)	34	17
1	B	548/564 (97%)	530 (97%)	16 (3%)	2 (0%)	34	17
All	All	1096/1128 (97%)	1063 (97%)	29 (3%)	4 (0%)	34	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	ALA
1	B	79	ALA
1	A	77	VAL
1	B	77	VAL

### 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	438/450 (97%)	435 (99%)	3 (1%)	84	75
1	B	438/450 (97%)	435 (99%)	3 (1%)	84	75
All	All	876/900 (97%)	870 (99%)	6 (1%)	84	75

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	321	ASP
1	A	420	TRP
1	B	5	LEU
1	B	125	ASN
1	B	420	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	21	ASN
1	A	55	GLN
1	A	95	ASN
1	A	226	GLN
1	A	230	GLN
1	A	239	GLN

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Mol	Chain	Res	Type
1	A	270	ASN
1	A	300	GLN
1	A	306	GLN
1	A	311	ASN
1	A	349	ASN
1	A	355	ASN
1	A	360	HIS
1	A	387	GLN
1	A	397	ASN
1	A	499	HIS
1	A	539	ASN
1	B	20	GLN
1	B	21	ASN
1	B	22	ASN
1	B	95	ASN
1	B	139	GLN
1	B	226	GLN
1	B	230	GLN
1	B	270	ASN
1	B	306	GLN
1	B	311	ASN
1	B	349	ASN
1	B	354	GLN
1	B	387	GLN
1	B	393	ASN
1	B	397	ASN
1	B	499	HIS
1	B	539	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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
7	EDO	A	3003	-	3,3,3	0.55	0	2,2,2	0.36	0
4	TPP	A	4001	2	22,27,27	1.68	7 (31%)	29,40,40	1.56	5 (17%)
7	EDO	B	3002	-	3,3,3	0.44	0	2,2,2	0.36	0
3	SO4	A	2001	-	4,4,4	0.15	0	6,6,6	0.38	0
5	ADP	A	4003	-	24,29,29	1.10	3 (12%)	29,45,45	1.30	3 (10%)
6	MES	A	4004	-	12,12,12	1.50	1 (8%)	14,16,16	3.00	5 (35%)
7	EDO	A	3001	-	3,3,3	0.54	0	2,2,2	0.33	0
3	SO4	B	2002	-	4,4,4	0.25	0	6,6,6	0.21	0
4	TPP	B	5001	2	22,27,27	1.37	5 (22%)	29,40,40	1.62	8 (27%)
7	EDO	B	3004	-	3,3,3	0.47	0	2,2,2	0.33	0
5	ADP	B	5003	-	24,29,29	0.98	2 (8%)	29,45,45	1.42	5 (17%)
6	MES	B	5004	-	12,12,12	1.49	1 (8%)	14,16,16	2.73	3 (21%)

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
7	EDO	A	3003	-	-	0/1/1/1	-
4	TPP	A	4001	2	-	4/16/17/17	0/2/2/2
7	EDO	B	3002	-	-	0/1/1/1	-
5	ADP	A	4003	-	-	1/12/32/32	0/3/3/3
6	MES	A	4004	-	-	1/6/14/14	0/1/1/1
7	EDO	A	3001	-	-	0/1/1/1	-
4	TPP	B	5001	2	-	2/16/17/17	0/2/2/2
7	EDO	B	3004	-	-	0/1/1/1	-
5	ADP	B	5003	-	-	2/12/32/32	0/3/3/3
6	MES	B	5004	-	-	3/6/14/14	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	5004	MES	C8-S	-4.85	1.70	1.77
6	A	4004	MES	C8-S	-4.83	1.70	1.77
4	A	4001	TPP	C4'-N3'	3.76	1.40	1.35
4	A	4001	TPP	C6-C5	3.07	1.52	1.50
4	A	4001	TPP	C2'-N1'	2.72	1.38	1.34
4	B	5001	TPP	C4'-N3'	2.64	1.38	1.35
4	B	5001	TPP	C4-N3	-2.59	1.37	1.39
5	A	4003	ADP	O4'-C1'	2.58	1.44	1.41
4	B	5001	TPP	C2'-N3'	2.57	1.38	1.34
5	A	4003	ADP	C5-C4	2.50	1.47	1.40
4	B	5001	TPP	C6'-N1'	2.47	1.39	1.34
4	B	5001	TPP	C2'-N1'	2.46	1.38	1.34
5	B	5003	ADP	O4'-C1'	2.46	1.44	1.41
4	A	4001	TPP	C6'-N1'	2.38	1.39	1.34
4	A	4001	TPP	C2'-N3'	2.26	1.38	1.34
4	A	4001	TPP	C4-N3	-2.17	1.37	1.39
4	A	4001	TPP	C2-N3	2.07	1.40	1.36
5	B	5003	ADP	C5-C4	2.05	1.46	1.40
5	A	4003	ADP	C2-N3	2.02	1.35	1.32

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	5004	MES	C5-N4-C3	6.95	124.48	108.83
6	A	4004	MES	C5-N4-C3	6.45	123.35	108.83
6	A	4004	MES	O1S-S-C8	6.45	114.68	106.92
6	B	5004	MES	O1S-S-C8	5.66	113.73	106.92
6	A	4004	MES	C7-N4-C3	4.12	121.76	111.23
5	B	5003	ADP	N3-C2-N1	-3.59	123.06	128.68
4	A	4001	TPP	CM2-C2'-N1'	3.52	121.01	117.14
6	B	5004	MES	C7-N4-C5	3.39	119.91	111.23
4	A	4001	TPP	N1'-C2'-N3'	-3.38	119.72	125.54
4	B	5001	TPP	CM4-C4-N3	3.22	126.64	122.53
6	A	4004	MES	O2S-S-C8	3.14	110.69	106.92
4	B	5001	TPP	N1'-C2'-N3'	-3.05	120.29	125.54
4	B	5001	TPP	C6'-N1'-C2'	2.96	121.00	115.96
4	A	4001	TPP	C6'-N1'-C2'	2.82	120.76	115.96
5	A	4003	ADP	N3-C2-N1	-2.81	124.29	128.68
5	A	4003	ADP	O4'-C1'-C2'	-2.74	102.92	106.93
4	B	5001	TPP	C5'-C6'-N1'	-2.74	119.26	123.82
4	A	4001	TPP	PA-O3A-PB	-2.59	123.95	132.83
5	B	5003	ADP	C4-C5-N7	-2.58	106.71	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	5003	ADP	O4'-C1'-C2'	-2.58	103.16	106.93
4	B	5001	TPP	C6'-C5'-C4'	2.50	119.12	115.72
5	B	5003	ADP	C1'-N9-C4	-2.48	122.29	126.64
6	A	4004	MES	C6-C5-N4	2.29	113.57	110.10
5	A	4003	ADP	C1'-N9-C4	-2.25	122.69	126.64
4	B	5001	TPP	C5'-C7'-N3	-2.24	109.55	113.28
4	B	5001	TPP	CM2-C2'-N1'	2.17	119.53	117.14
4	B	5001	TPP	PA-O3A-PB	-2.03	125.86	132.83
4	A	4001	TPP	C5-C4-N3	2.02	111.61	107.57
5	B	5003	ADP	PA-O3A-PB	-2.01	125.93	132.83

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4001	TPP	C4-C5-C6-C7
4	A	4001	TPP	PA-O3A-PB-O3B
6	A	4004	MES	C8-C7-N4-C3
4	B	5001	TPP	C4-C5-C6-C7
4	B	5001	TPP	PA-O3A-PB-O2B
5	B	5003	ADP	O4'-C4'-C5'-O5'
5	B	5003	ADP	C3'-C4'-C5'-O5'
6	B	5004	MES	C8-C7-N4-C3
6	B	5004	MES	C7-C8-S-O3S
6	B	5004	MES	C7-C8-S-O2S
5	A	4003	ADP	O4'-C4'-C5'-O5'
4	A	4001	TPP	PA-O3A-PB-O2B
4	A	4001	TPP	PA-O3A-PB-O1B

There are no ring outliers.

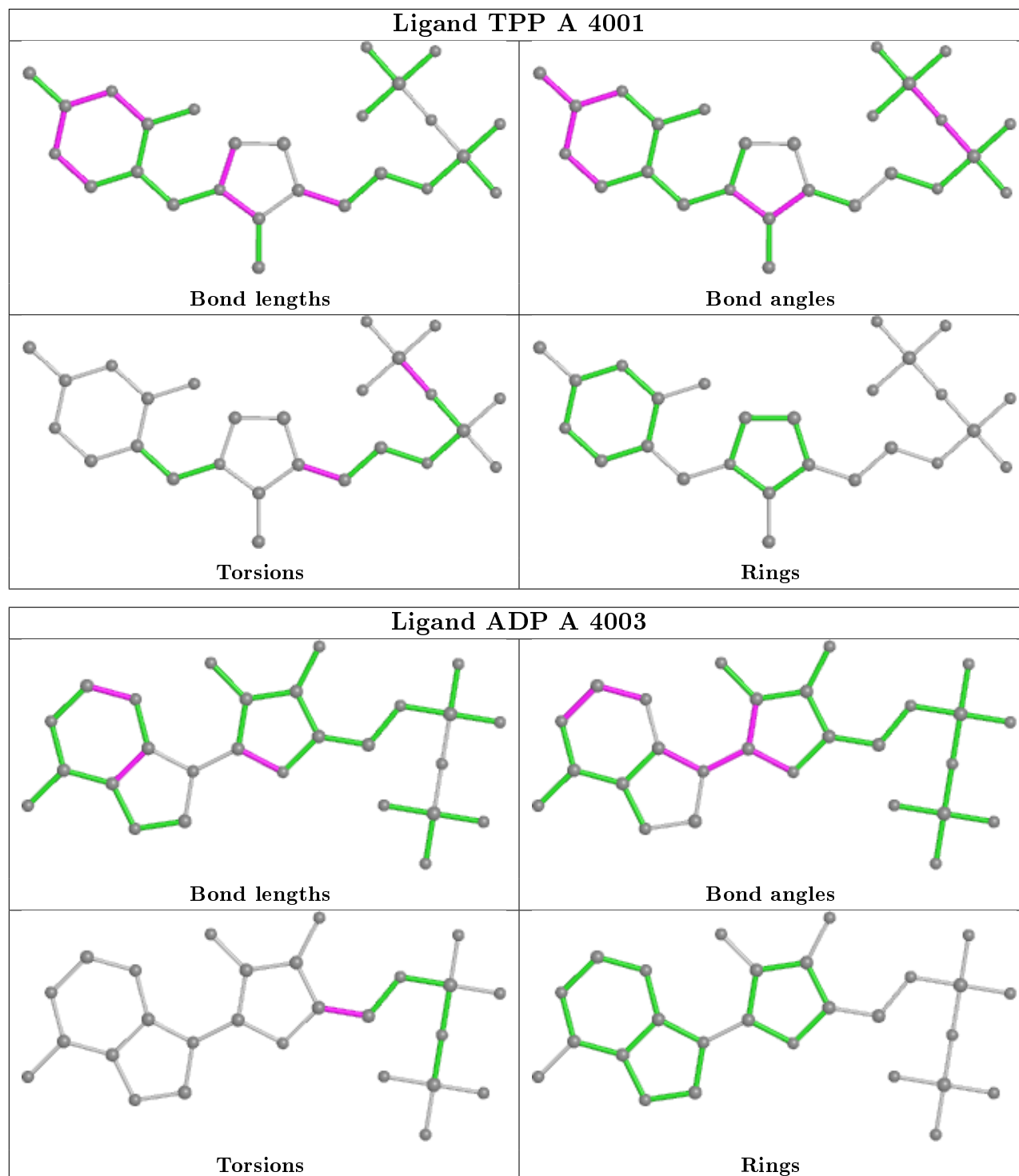
1 monomer is involved in 1 short contact:

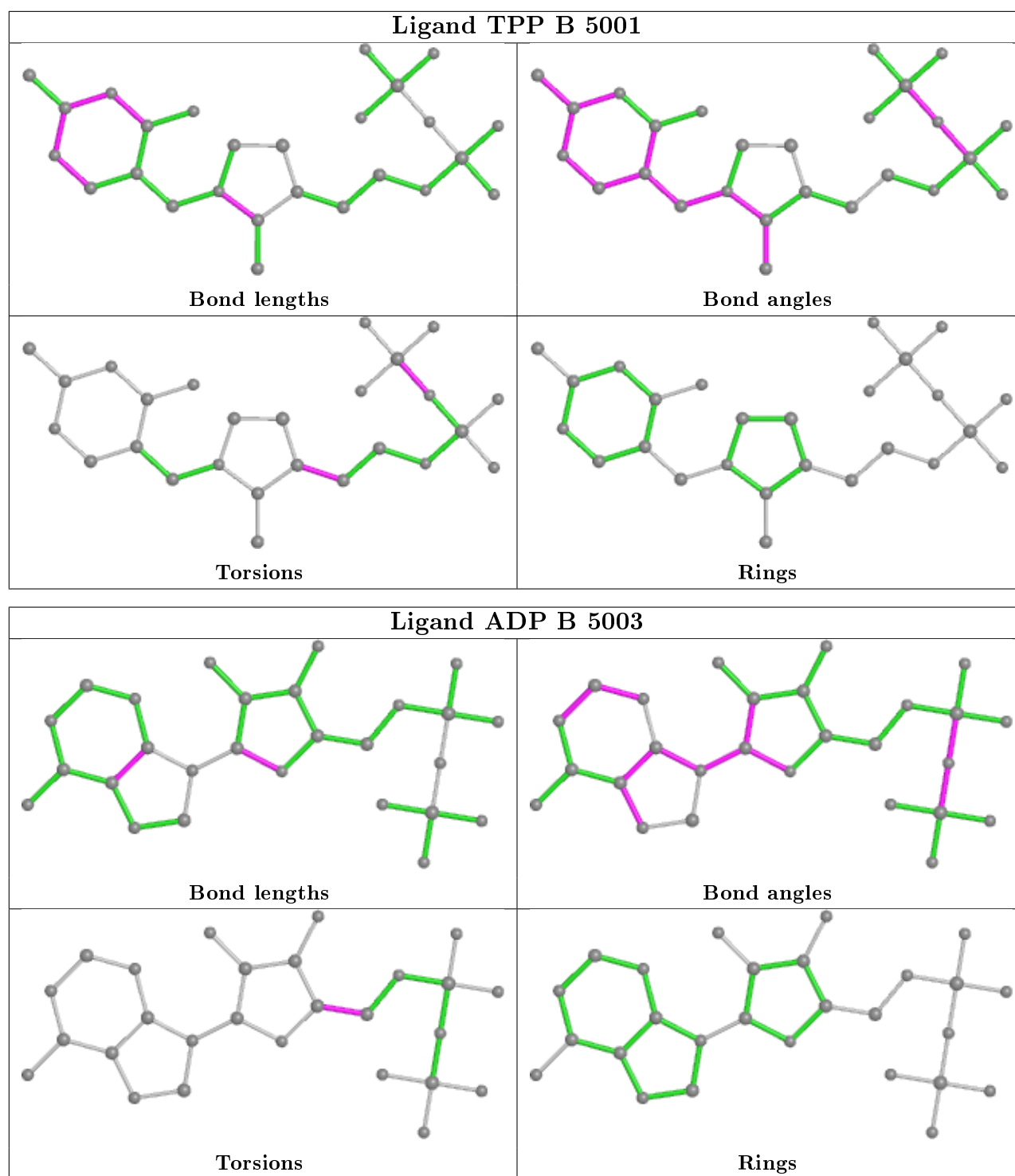
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	4003	ADP	1	0

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 ⓘ

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	550/564 (97%)	-0.23	17 (3%)	49 55	11, 15, 28, 48	0
1	B	550/564 (97%)	-0.07	14 (2%)	57 63	12, 20, 30, 52	0
All	All	1100/1128 (97%)	-0.15	31 (2%)	53 58	11, 18, 30, 52	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	553	ILE	7.7
1	B	5	LEU	7.5
1	B	554	THR	7.2
1	A	5	LEU	6.8
1	A	357	GLN	6.1
1	A	553	ILE	6.0
1	A	554	THR	5.5
1	B	552	HIS	5.0
1	A	360	HIS	4.5
1	B	295	ASP	3.8
1	A	552	HIS	3.7
1	B	6	GLN	3.6
1	B	498	HIS	3.2
1	A	358	LYS	3.1
1	A	388	ASP	3.0
1	A	353	GLN	3.0
1	A	354	GLN	2.9
1	A	6	GLN	2.9
1	A	361	GLU	2.8
1	A	359	MET	2.6
1	B	364	SER	2.6
1	A	356	ALA	2.5
1	B	388	ASP	2.5
1	B	361	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	335	GLN	2.3
1	B	524	HIS	2.3
1	B	188	GLU	2.2
1	A	498	HIS	2.1
1	B	499	HIS	2.1
1	A	337	THR	2.0
1	B	357	GLN	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 carbohydrates in this entry.

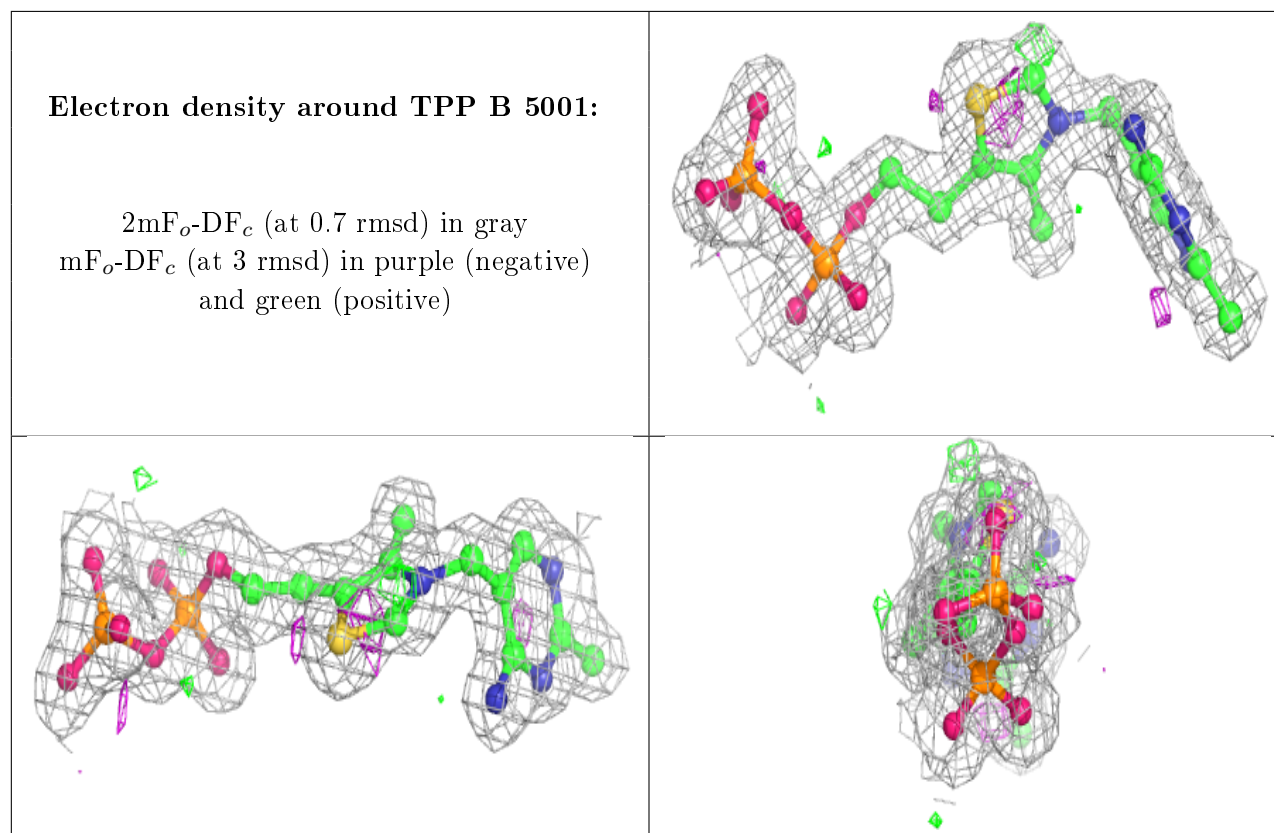
## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	EDO	B	3002	4/4	0.96	0.07	18,19,20,20	0
7	EDO	A	3001	4/4	0.96	0.08	16,17,19,19	0
7	EDO	B	3004	4/4	0.96	0.08	22,26,27,30	0
3	SO4	B	2002	5/5	0.97	0.18	31,32,32,32	0
6	MES	A	4004	12/12	0.97	0.10	21,23,27,29	0
7	EDO	A	3003	4/4	0.97	0.06	20,20,22,22	0
6	MES	B	5004	12/12	0.97	0.11	23,29,30,31	0
4	TPP	B	5001	26/26	0.98	0.06	16,18,20,21	0
5	ADP	B	5003	27/27	0.98	0.06	14,15,16,18	0
2	MG	B	1002	1/1	0.98	0.08	23,23,23,23	0
2	MG	A	1001	1/1	0.99	0.08	13,13,13,13	0
3	SO4	A	2001	5/5	0.99	0.15	25,25,27,27	0
5	ADP	A	4003	27/27	0.99	0.06	11,13,14,15	0
4	TPP	A	4001	26/26	0.99	0.07	10,12,14,15	0

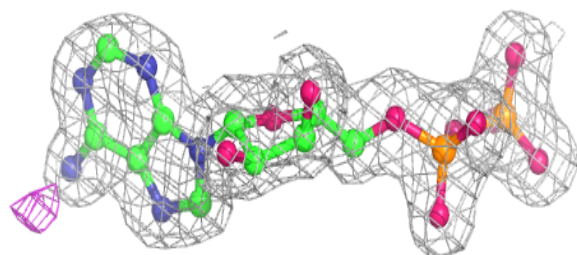
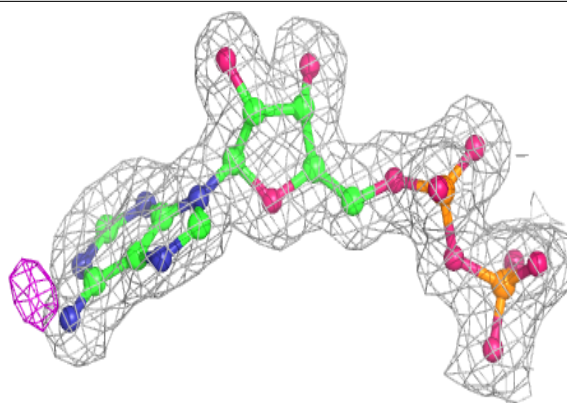
The following is a graphical depiction of the model fit to experimental electron density of all

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.

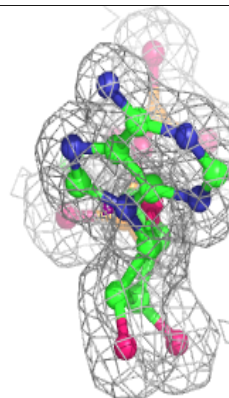
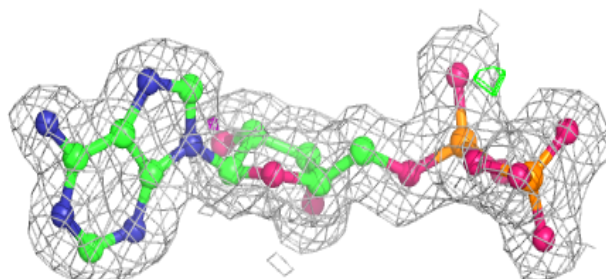
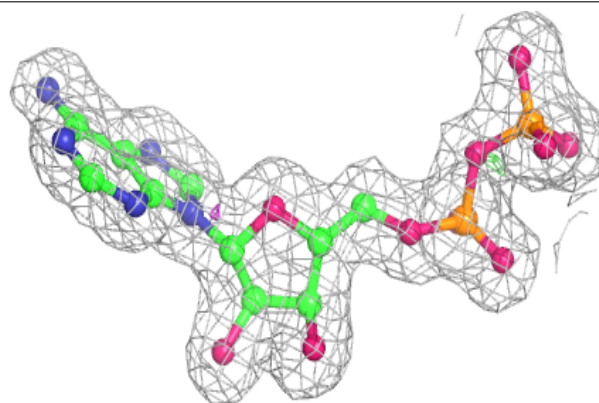


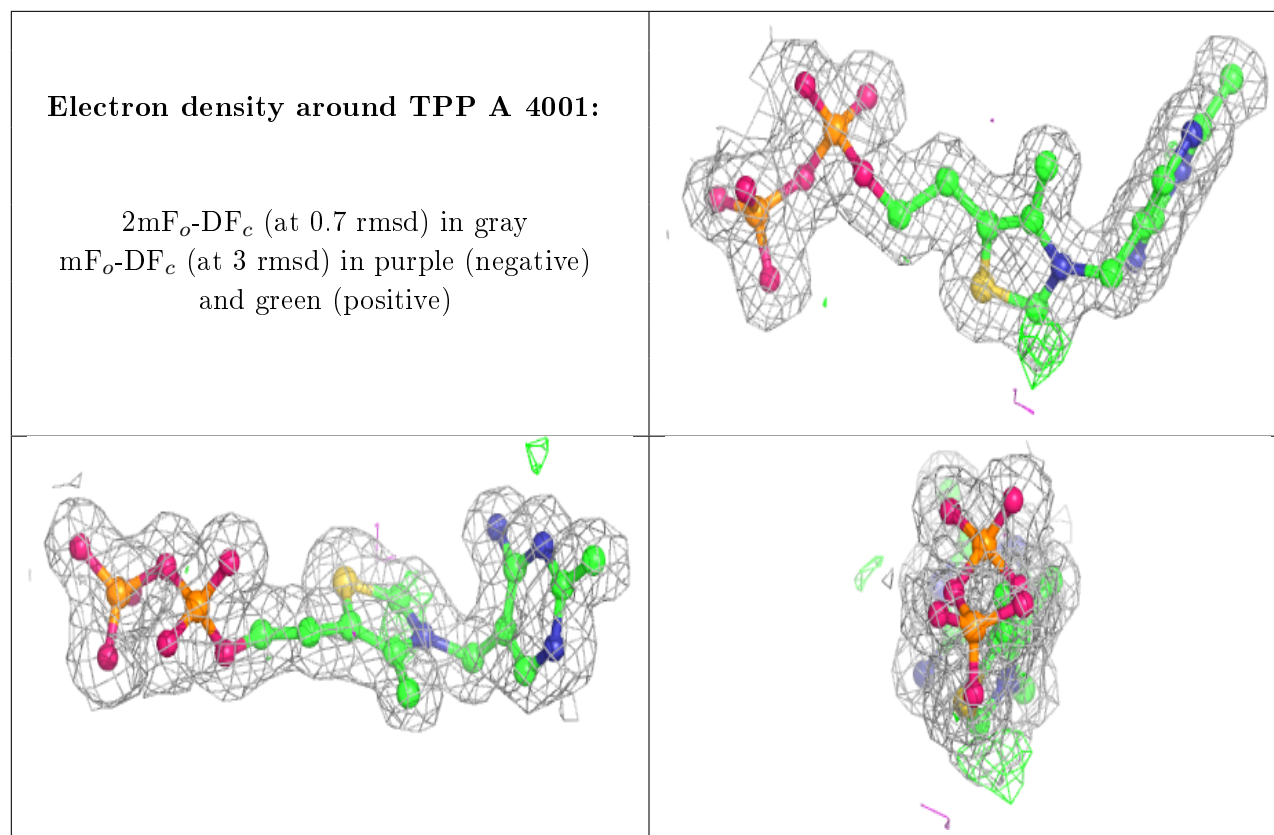
**Electron density around ADP B 5003:**

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

**Electron density around ADP A 4003:**

$2mF_o-DF_c$  (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.