



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:55 am BST

PDB ID : 4EEI  
Title : Crystal Structure of Adenylosuccinate Lyase from *Francisella tularensis* Complexed with AMP and Succinate  
Authors : Maltseva, N.; Kim, Y.; Shatsman, S.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2012-03-28  
Resolution : 1.92 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

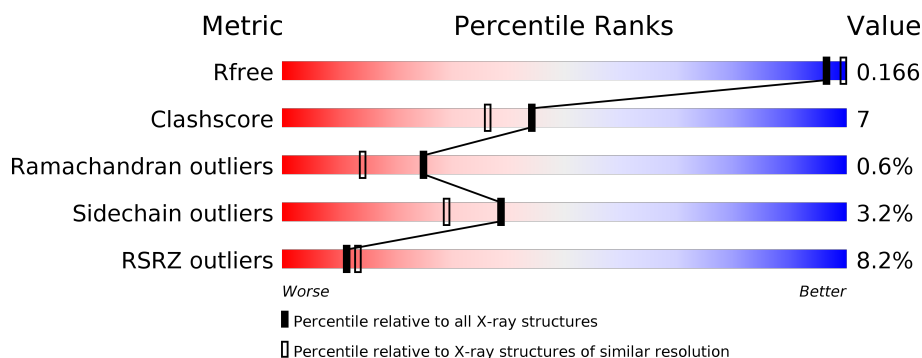
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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	438	<div> <div>8%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	438	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div></div> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7668 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 Adenylosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	7	12	0
			3435	2175	591	649	20			
1	B	423	Total	C	N	O	S	0	12	0
			3505	2220	600	665	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	433	ARG	-	EXPRESSION TAG	UNP Q5NIQ1
A	434	GLY	-	EXPRESSION TAG	UNP Q5NIQ1
A	435	GLU	-	EXPRESSION TAG	UNP Q5NIQ1
A	436	ASN	-	EXPRESSION TAG	UNP Q5NIQ1
A	437	LEU	-	EXPRESSION TAG	UNP Q5NIQ1
A	438	TYR	-	EXPRESSION TAG	UNP Q5NIQ1
B	433	ARG	-	EXPRESSION TAG	UNP Q5NIQ1
B	434	GLY	-	EXPRESSION TAG	UNP Q5NIQ1
B	435	GLU	-	EXPRESSION TAG	UNP Q5NIQ1
B	436	ASN	-	EXPRESSION TAG	UNP Q5NIQ1
B	437	LEU	-	EXPRESSION TAG	UNP Q5NIQ1
B	438	TYR	-	EXPRESSION TAG	UNP Q5NIQ1

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 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
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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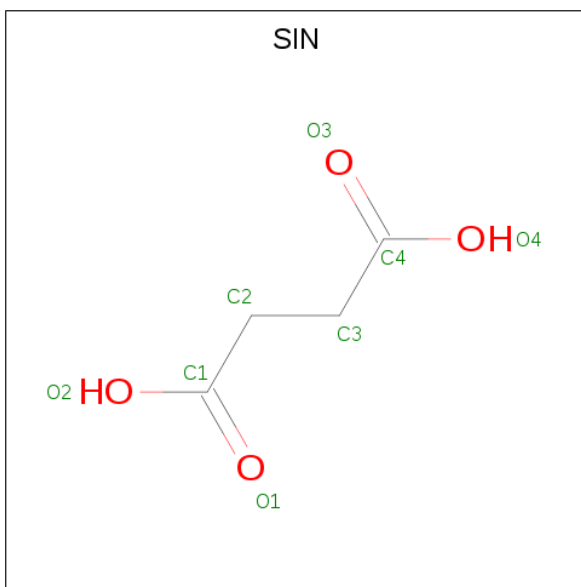
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is SUCCINIC ACID (three-letter code: SIN) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	4	4		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Cl	0	0
			2	2		

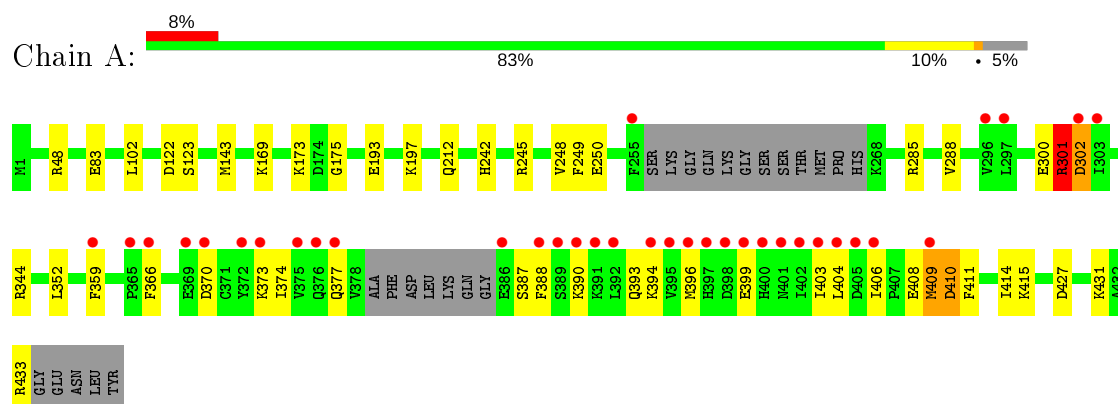
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	288	Total	O	0	0
			288	288		
7	B	313	Total	O	0	0
			313	313		

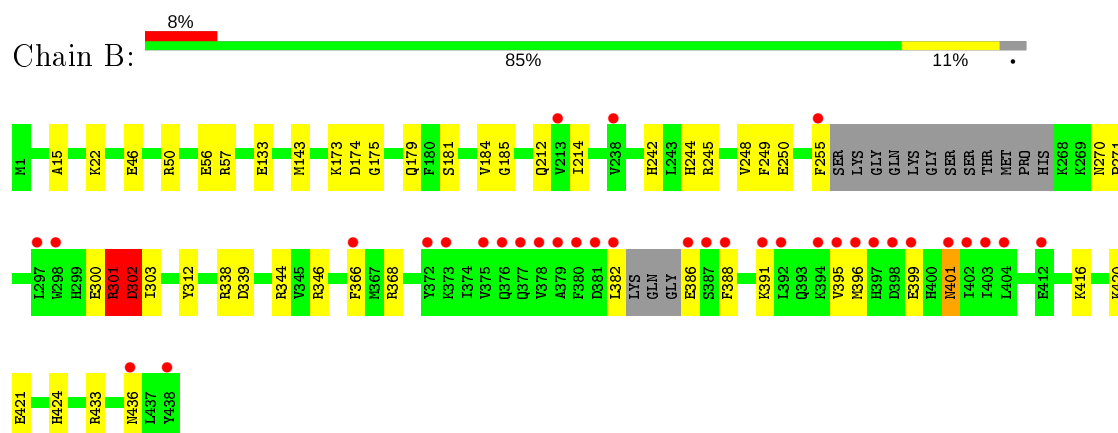
### 3 Residue-property plots [i](#)

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: Adenylosuccinate lyase



#### • Molecule 1: Adenylosuccinate lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.76 Å 88.76 Å 254.72 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.33 – 1.92 39.69 – 1.92	Depositor EDS
% Data completeness (in resolution range)	94.8 (39.33-1.92) 99.9 (39.69-1.92)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.89 (at 1.92 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_920)	Depositor
R, $R_{free}$	0.168 , 0.199 0.167 , 0.166	Depositor DCC
$R_{free}$ test set	3951 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7668	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, K, SIN, EDO, CL

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	0.37	0/3492	0.48	0/4695
1	B	0.37	0/3563	0.48	0/4793
All	All	0.37	0/7055	0.48	0/9488

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	302[B]	ASP	Mainchain

### 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	3435	0	3443	43	0
1	B	3505	0	3506	48	0
2	A	23	0	12	0	0
2	B	23	0	12	3	0
3	A	28	0	40	9	0
3	B	40	0	59	9	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	B	8	0	4	3	0
6	B	2	0	0	1	0
7	A	288	0	0	3	0
7	B	313	0	0	4	0
All	All	7668	0	7076	94	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 7.

All (94) 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:300[B]:GLU:O	1:B:301[B]:ARG:HB3	1.54	1.07
1:A:300[B]:GLU:O	1:A:301[B]:ARG:HB3	1.56	1.04
2:B:503:AMP:N6	5:B:507:SIN:H21	1.77	0.98
1:A:374:ILE:HD13	1:A:396:MET:HE1	1.48	0.96
1:B:395:VAL:HG13	1:B:399:GLU:HG3	1.46	0.94
1:B:300[A]:GLU:O	7:B:675:HOH:O	1.87	0.93
1:B:301[B]:ARG:C	1:B:301[B]:ARG:HD3	2.01	0.79
1:A:301[B]:ARG:HD3	1:A:301[B]:ARG:C	2.03	0.79
1:B:270[B]:ASN:HB2	1:B:271:PRO:HD2	1.66	0.78
1:A:300[A]:GLU:O	7:A:636:HOH:O	2.02	0.77
1:A:374:ILE:HD13	1:A:396:MET:CE	2.14	0.77
1:A:143:MET:HG3	1:B:270[B]:ASN:HB3	1.67	0.76
1:B:395:VAL:CG1	1:B:399:GLU:HG3	2.17	0.75
1:B:339:ASP:H	3:B:506:EDO:H21	1.52	0.74
1:B:301[B]:ARG:HD3	1:B:302[B]:ASP:N	2.03	0.73
1:A:390:LYS:O	1:A:394:LYS:HG3	1.93	0.68
1:B:300[B]:GLU:O	1:B:301[B]:ARG:CB	2.37	0.68
2:B:503:AMP:C6	5:B:507:SIN:H21	2.28	0.68
1:A:411:PHE:CE2	1:A:415:LYS:HE2	2.31	0.66
1:B:382:LEU:HD13	1:B:391:LYS:HZ2	1.60	0.65
1:A:300[B]:GLU:O	1:A:301[B]:ARG:CB	2.39	0.65
1:B:346:ARG:NH2	7:B:885:HOH:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:HB2	3:A:507:EDO:H11	1.80	0.62
1:A:408:GLU:OE1	1:A:408:GLU:HA	2.00	0.61
1:B:368:ARG:HD2	3:B:515:EDO:O2	2.01	0.60
1:B:270[B]:ASN:HB2	1:B:271:PRO:CD	2.31	0.59
1:A:344:ARG:HE	3:A:508:EDO:H12	1.67	0.59
1:A:285:ARG:O	1:A:288[A]:VAL:HG12	2.03	0.59
1:A:409:MET:O	1:A:414:ILE:HG13	2.04	0.57
3:A:509:EDO:O2	1:B:270[B]:ASN:ND2	2.37	0.57
3:A:509:EDO:HO2	1:B:270[B]:ASN:HD22	1.50	0.57
1:A:301[B]:ARG:HD3	1:A:302[B]:ASP:N	2.19	0.56
1:A:48:ARG:NH2	7:A:745:HOH:O	2.30	0.56
1:B:244:HIS:CE1	1:B:270[B]:ASN:HA	2.41	0.56
1:B:421:GLU:OE1	1:B:424:HIS:ND1	2.39	0.55
1:B:15:ALA:HB3	7:B:616:HOH:O	2.06	0.55
2:B:503:AMP:N6	5:B:507:SIN:C2	2.63	0.54
1:A:415:LYS:NZ	7:A:886:HOH:O	2.39	0.54
3:A:509:EDO:O2	1:B:270[A]:ASN:OD1	2.26	0.53
1:B:368:ARG:CD	3:B:515:EDO:O2	2.57	0.53
1:A:122:ASP:CB	3:A:507:EDO:H11	2.39	0.52
1:B:242:HIS:O	1:B:245:ARG:HG2	2.10	0.52
1:B:301[B]:ARG:HD3	1:B:302[B]:ASP:CA	2.40	0.52
1:A:123:SER:OG	3:A:507:EDO:H12	2.08	0.52
1:B:133:GLU:OE1	1:B:338:ARG:NH1	2.38	0.52
1:A:374:ILE:CD1	1:A:396:MET:HE1	2.29	0.52
1:B:248:VAL:HG12	1:B:250:GLU:HG3	1.92	0.51
1:B:401:ASN:O	1:B:401:ASN:ND2	2.38	0.51
1:A:374:ILE:HG21	1:A:396:MET:HE3	1.93	0.51
1:A:301[A]:ARG:HD3	1:A:301[A]:ARG:C	2.31	0.50
1:A:393:GLN:HB2	1:A:406:ILE:HD12	1.94	0.49
1:B:143:MET:HB2	3:B:502:EDO:H22	1.93	0.49
1:A:302[B]:ASP:C	1:A:302[B]:ASP:OD1	2.51	0.48
1:A:431:LYS:HG3	3:A:506:EDO:H12	1.95	0.48
1:A:427:ASP:OD1	1:A:433:ARG:NE	2.39	0.48
1:B:46:GLU:OE2	1:B:50:ARG:NH1	2.46	0.48
1:A:242:HIS:O	1:A:245:ARG:HG2	2.13	0.48
1:B:181:SER:HB2	1:B:185:GLY:HA2	1.96	0.48
1:B:395:VAL:O	1:B:399:GLU:N	2.44	0.47
1:A:102:LEU:HD22	3:A:504:EDO:H12	1.97	0.46
1:A:301[A]:ARG:HD3	1:A:302[A]:ASP:N	2.31	0.46
1:B:270[B]:ASN:CB	1:B:271:PRO:CD	2.93	0.46
1:A:301[A]:ARG:HD3	1:A:302[A]:ASP:CA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302[B]:ASP:OD2	1:B:302[B]:ASP:C	2.54	0.45
1:A:374:ILE:HG21	1:A:396:MET:CE	2.47	0.45
3:B:512:EDO:O2	7:B:875:HOH:O	2.21	0.45
1:B:433:ARG:NH1	6:B:509:CL:CL	2.63	0.45
1:A:387:SER:HB3	1:A:390:LYS:HB2	1.99	0.45
1:A:352:LEU:HD22	1:A:409:MET:HG3	1.99	0.45
1:B:184:VAL:HB	1:B:300[A]:GLU:HG2	1.99	0.44
1:B:386:GLU:HB3	1:B:391:LYS:HE3	2.00	0.44
1:B:344:ARG:HE	3:B:514:EDO:C2	2.31	0.44
1:B:301[A]:ARG:C	1:B:301[A]:ARG:HD3	2.37	0.43
1:B:56[B]:GLU:HG2	1:B:57:ARG:N	2.33	0.43
1:B:173:LYS:O	3:B:511:EDO:H22	2.17	0.43
1:A:370:ASP:O	1:A:373:LYS:HG2	2.19	0.43
1:A:169:LYS:O	1:A:173:LYS:HG3	2.18	0.43
1:A:193:GLU:HG2	1:A:197:LYS:HE3	1.99	0.43
1:A:409:MET:O	1:A:414:ILE:CD1	2.67	0.43
1:B:179:GLN:HG2	1:B:214:ILE:HG13	2.01	0.43
1:B:401:ASN:HD22	1:B:401:ASN:C	2.22	0.43
1:A:366:PHE:CD1	1:A:366:PHE:N	2.87	0.42
1:A:212:GLN:OE1	1:A:301[A]:ARG:HG2	2.18	0.42
1:B:368:ARG:NE	3:B:515:EDO:O2	2.52	0.42
1:B:420:LYS:HE2	1:B:421:GLU:HG2	2.02	0.42
1:A:248:VAL:HG12	1:A:250:GLU:HG3	2.00	0.42
1:A:359:PHE:CE2	1:A:406:ILE:HG12	2.56	0.41
1:B:212:GLN:OE1	1:B:301[A]:ARG:HG2	2.19	0.41
1:B:133:GLU:HB3	3:B:512:EDO:O1	2.20	0.41
1:A:408:GLU:HG3	1:A:410:ASP:H	1.86	0.41
1:B:301[A]:ARG:HD3	1:B:302[A]:ASP:N	2.36	0.41
1:B:301[B]:ARG:CD	1:B:301[B]:ARG:C	2.74	0.41
1:B:386:GLU:OE1	1:B:391:LYS:HE3	2.21	0.41
1:A:301[B]:ARG:C	1:A:301[B]:ARG:CD	2.75	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	420/438 (96%)	404 (96%)	12 (3%)	4 (1%)	15	6
1	B	429/438 (98%)	411 (96%)	15 (4%)	3 (1%)	22	11
All	All	849/876 (97%)	815 (96%)	27 (3%)	7 (1%)	25	9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301[A]	ARG
1	A	301[B]	ARG
1	B	301[A]	ARG
1	B	301[B]	ARG
1	A	175	GLY
1	B	175	GLY
1	A	410	ASP

### 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	379/386 (98%)	366 (97%)	13 (3%)	37	27
1	B	386/386 (100%)	369 (96%)	17 (4%)	28	18
All	All	765/772 (99%)	735 (96%)	30 (4%)	39	22

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83[A]	GLU
1	A	83[B]	GLU
1	A	249	PHE
1	A	301[A]	ARG
1	A	301[B]	ARG
1	A	302[A]	ASP

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Mol	Chain	Res	Type
1	A	302[B]	ASP
1	A	377	GLN
1	A	388	PHE
1	A	399	GLU
1	A	403	ILE
1	A	404	LEU
1	A	409	MET
1	B	22	LYS
1	B	174[A]	ASP
1	B	174[B]	ASP
1	B	249	PHE
1	B	255	PHE
1	B	301[A]	ARG
1	B	301[B]	ARG
1	B	302[A]	ASP
1	B	302[B]	ASP
1	B	303	ILE
1	B	312	TYR
1	B	366	PHE
1	B	388	PHE
1	B	396	MET
1	B	401	ASN
1	B	416	LYS
1	B	436	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 5 are monoatomic - leaving 20 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
3	EDO	A	502	-	3,3,3	0.46	0	2,2,2	0.34	0
3	EDO	B	502	-	3,3,3	0.47	0	2,2,2	0.46	0
3	EDO	A	508	4	3,3,3	0.49	0	2,2,2	0.22	0
3	EDO	A	506	4	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	B	506	-	3,3,3	0.54	0	2,2,2	0.24	0
3	EDO	A	509	-	3,3,3	0.44	0	2,2,2	0.32	0
3	EDO	B	501	-	3,3,3	0.48	0	2,2,2	0.21	0
3	EDO	B	512	-	3,3,3	0.41	0	2,2,2	0.52	0
5	SIN	B	507	-	1,7,7	0.13	0	2,8,8	1.84	1 (50%)
3	EDO	A	507	-	3,3,3	0.41	0	2,2,2	0.31	0
3	EDO	B	505	-	3,3,3	0.41	0	2,2,2	0.48	0
2	AMP	A	501	-	22,25,25	0.98	1 (4%)	25,38,38	1.26	2 (8%)
3	EDO	B	515	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	B	513	-	3,3,3	0.48	0	2,2,2	0.34	0
3	EDO	A	504	-	3,3,3	0.46	0	2,2,2	0.45	0
3	EDO	A	505	-	3,3,3	0.47	0	2,2,2	0.28	0
3	EDO	B	514	4	3,3,3	0.53	0	2,2,2	0.21	0
3	EDO	B	504	-	3,3,3	0.53	0	2,2,2	0.31	0
2	AMP	B	503	-	22,25,25	0.97	1 (4%)	25,38,38	1.29	2 (8%)
3	EDO	B	511	-	3,3,3	0.51	0	2,2,2	0.17	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
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	A	508	4	-	0/1/1/1	-
3	EDO	A	506	4	-	1/1/1/1	-
3	EDO	B	506	-	-	1/1/1/1	-
3	EDO	A	509	-	-	1/1/1/1	-
3	EDO	B	501	-	-	1/1/1/1	-
3	EDO	B	512	-	-	1/1/1/1	-
5	SIN	B	507	-	-	0/1/5/5	-
3	EDO	A	507	-	-	1/1/1/1	-
3	EDO	B	505	-	-	1/1/1/1	-
2	AMP	A	501	-	-	1/6/26/26	0/3/3/3
3	EDO	B	515	-	-	0/1/1/1	-
3	EDO	B	513	-	-	0/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	A	505	-	-	1/1/1/1	-
3	EDO	B	514	4	-	0/1/1/1	-
3	EDO	B	504	-	-	0/1/1/1	-
2	AMP	B	503	-	-	1/6/26/26	0/3/3/3
3	EDO	B	511	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	503	AMP	C5-C4	2.43	1.47	1.40
2	A	501	AMP	C5-C4	2.42	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	AMP	N3-C2-N1	-3.21	123.66	128.68
2	B	503	AMP	N3-C2-N1	-3.19	123.69	128.68
2	B	503	AMP	C4-C5-N7	-2.69	106.60	109.40
2	A	501	AMP	C4-C5-N7	-2.67	106.61	109.40
5	B	507	SIN	C2-C3-C4	-2.03	109.27	112.67

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	EDO	O1-C1-C2-O2
3	B	506	EDO	O1-C1-C2-O2

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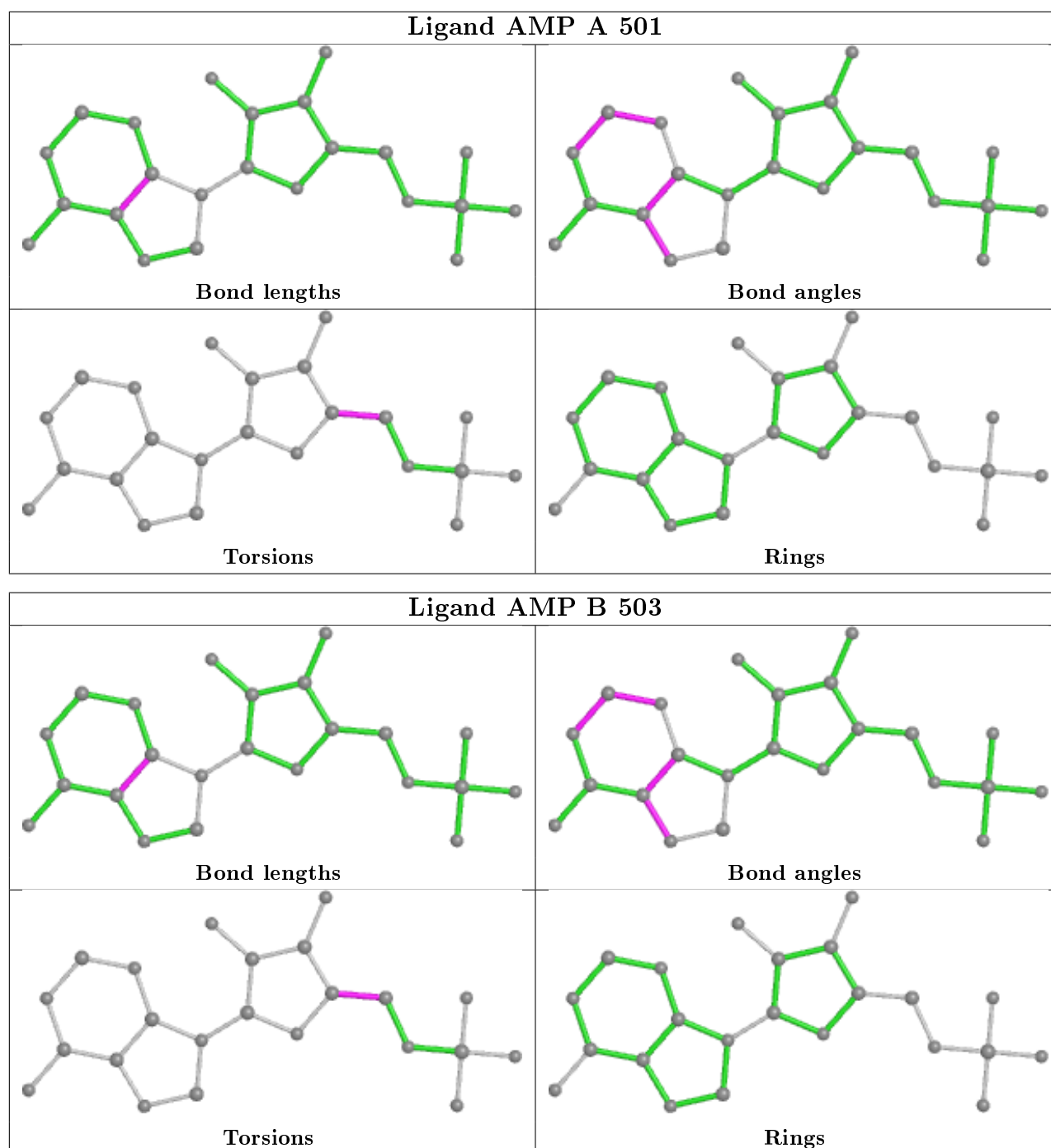
Mol	Chain	Res	Type	Atoms
3	A	506	EDO	O1-C1-C2-O2
3	A	505	EDO	O1-C1-C2-O2
3	A	507	EDO	O1-C1-C2-O2
2	B	503	AMP	O4'-C4'-C5'-O5'
3	B	512	EDO	O1-C1-C2-O2
3	B	501	EDO	O1-C1-C2-O2
3	B	505	EDO	O1-C1-C2-O2
2	A	501	AMP	O4'-C4'-C5'-O5'
3	A	509	EDO	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	EDO	1	0
3	A	508	EDO	1	0
3	A	506	EDO	1	0
3	B	506	EDO	1	0
3	A	509	EDO	3	0
3	B	512	EDO	2	0
5	B	507	SIN	3	0
3	A	507	EDO	3	0
3	B	515	EDO	3	0
3	A	504	EDO	1	0
3	B	514	EDO	1	0
2	B	503	AMP	3	0
3	B	511	EDO	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	414/438 (94%)	0.26	35 (8%) 10 12	18, 29, 83, 105	3 (0%)
1	B	423/438 (96%)	0.19	34 (8%) 12 14	17, 29, 77, 97	7 (1%)
All	All	837/876 (95%)	0.22	69 (8%) 11 13	17, 29, 80, 105	10 (1%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	380	PHE	11.1
1	A	394	LYS	7.5
1	A	255	PHE	6.5
1	A	398	ASP	6.2
1	A	395	VAL	5.8
1	A	392	LEU	5.2
1	A	373	LYS	5.2
1	B	366	PHE	4.9
1	A	399	GLU	4.7
1	B	394	LYS	4.7
1	B	391	LYS	4.6
1	A	397	HIS	4.6
1	A	376	GLN	4.4
1	A	388	PHE	4.4
1	B	382	LEU	4.4
1	B	438	TYR	4.3
1	A	366	PHE	4.2
1	B	379	ALA	4.2
1	A	396	MET	4.1
1	A	391	LYS	4.1
1	A	377	GLN	3.8
1	A	404	LEU	3.8
1	B	396	MET	3.7
1	A	402	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	401	ASN	3.6
1	B	395	VAL	3.6
1	B	403	ILE	3.5
1	B	378	VAL	3.5
1	A	401	ASN	3.5
1	B	377	GLN	3.4
1	B	404	LEU	3.3
1	A	372	TYR	3.2
1	B	373	LYS	3.2
1	B	255	PHE	3.2
1	B	375	VAL	3.2
1	A	302[A]	ASP	3.1
1	B	388	PHE	3.1
1	B	397	HIS	3.1
1	A	386	GLU	3.0
1	B	412	GLU	3.0
1	B	436	ASN	3.0
1	B	376	GLN	3.0
1	A	406	ILE	3.0
1	B	399	GLU	3.0
1	A	400	HIS	2.9
1	B	381	ASP	2.9
1	A	369	GLU	2.7
1	A	405	ASP	2.6
1	A	403	ILE	2.6
1	A	375	VAL	2.5
1	B	402	ILE	2.5
1	B	386	GLU	2.5
1	B	297	LEU	2.4
1	B	392	LEU	2.4
1	A	296	VAL	2.4
1	A	297	LEU	2.4
1	B	372	TYR	2.4
1	B	298	TRP	2.4
1	A	370	ASP	2.4
1	B	213	VAL	2.3
1	B	387	SER	2.3
1	A	365	PRO	2.3
1	A	389	SER	2.2
1	A	303	ILE	2.2
1	A	409	MET	2.2
1	B	398	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	390	LYS	2.1
1	A	359	PHE	2.0
1	B	238	VAL	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.

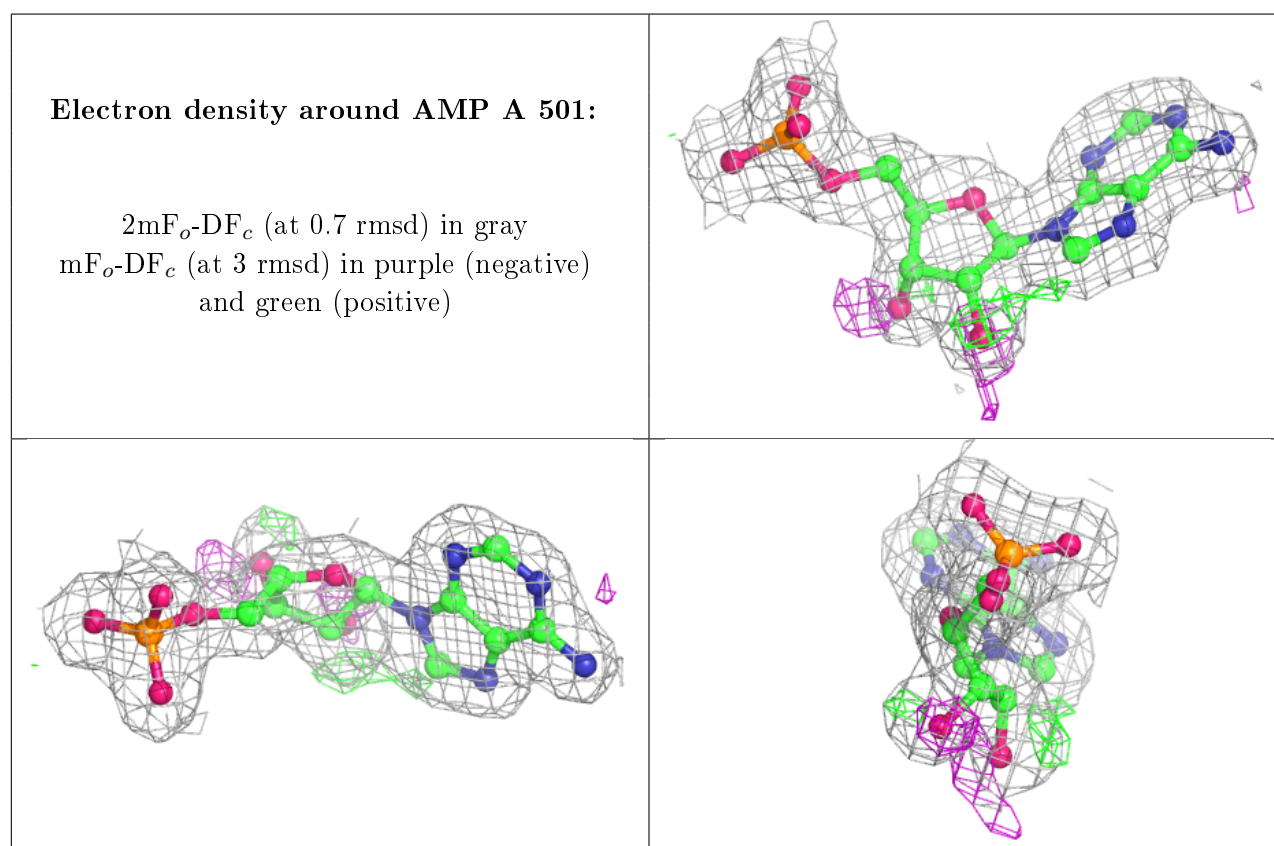
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	B	514	4/4	0.51	0.40	58,61,67,71	0
4	K	A	503	1/1	0.52	0.21	100,100,100,100	0
3	EDO	B	512	4/4	0.55	0.34	78,79,79,79	0
4	K	A	510	1/1	0.64	0.17	64,64,64,64	0
3	EDO	B	511	4/4	0.65	0.38	58,58,59,59	0
3	EDO	A	506	4/4	0.69	0.17	83,83,83,84	0
3	EDO	B	515	4/4	0.70	0.23	63,63,63,66	0
3	EDO	B	506	4/4	0.71	0.32	41,47,50,53	0
5	SIN	B	507	8/8	0.74	0.30	48,51,56,58	8
3	EDO	B	513	4/4	0.77	0.29	79,80,80,81	0
3	EDO	A	508	4/4	0.78	0.26	59,60,62,62	0
4	K	B	510	1/1	0.82	0.20	58,58,58,58	0
3	EDO	A	502	4/4	0.82	0.24	38,39,46,55	0
3	EDO	B	502	4/4	0.86	0.23	37,43,49,53	4
3	EDO	A	507	4/4	0.86	0.36	56,57,58,58	0
3	EDO	A	505	4/4	0.87	0.23	69,70,71,72	0
3	EDO	B	501	4/4	0.87	0.30	61,61,61,62	0
3	EDO	B	505	4/4	0.88	0.29	38,42,42,44	2
3	EDO	B	504	4/4	0.90	0.15	31,39,42,43	0
3	EDO	A	509	4/4	0.91	0.17	40,40,45,49	1

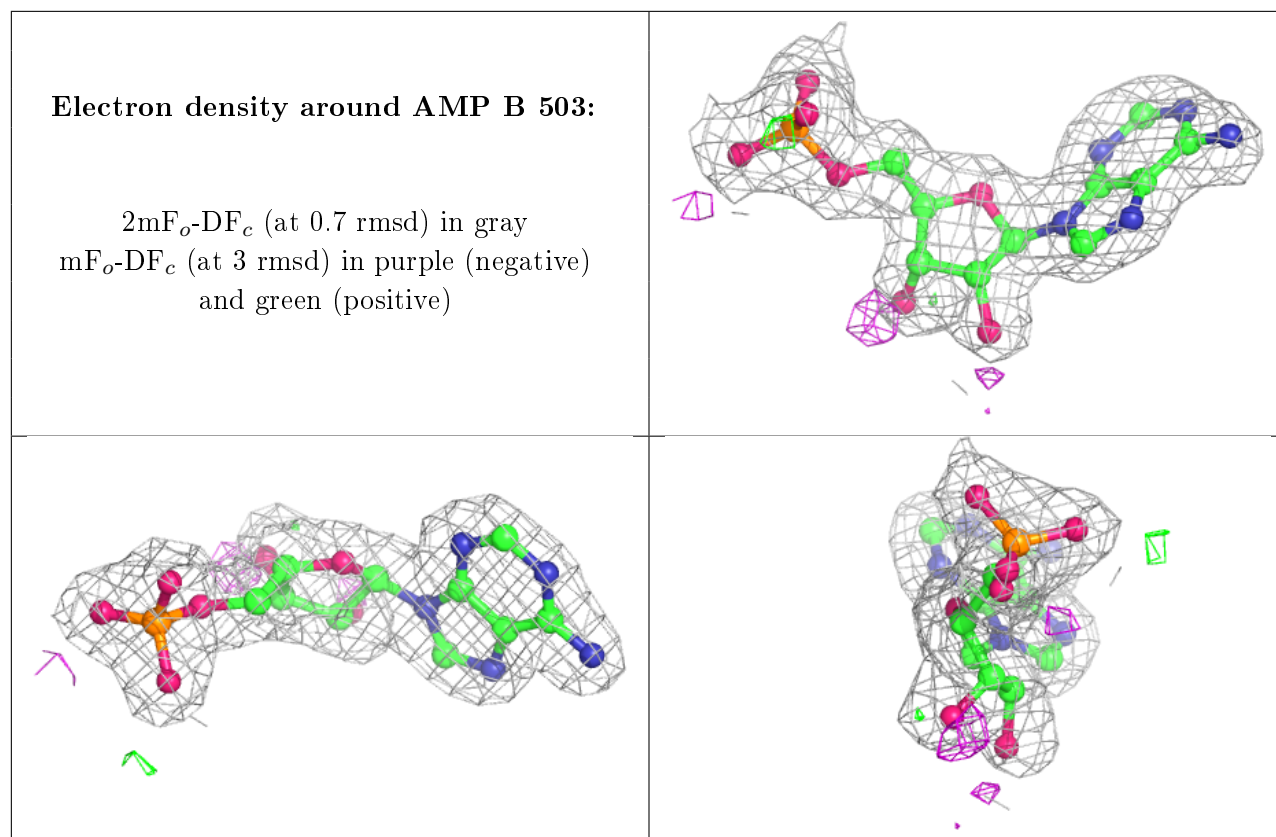
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	504	4/4	0.93	0.23	42,49,55,60	0
6	CL	B	509	1/1	0.94	0.34	56,56,56,56	0
2	AMP	A	501	23/23	0.96	0.13	22,26,28,30	0
2	AMP	B	503	23/23	0.96	0.10	27,33,38,41	0
6	CL	B	508	1/1	0.97	0.19	54,54,54,54	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.