



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:48 PM UTC

PDB ID : 8UZN / pdb_00008uzn
Title : Crystal Structure of Betaine aldehyde dehydrogenase (BetB) from *Klebsiella aerogenes* (AMP bound)
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2023-11-15
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

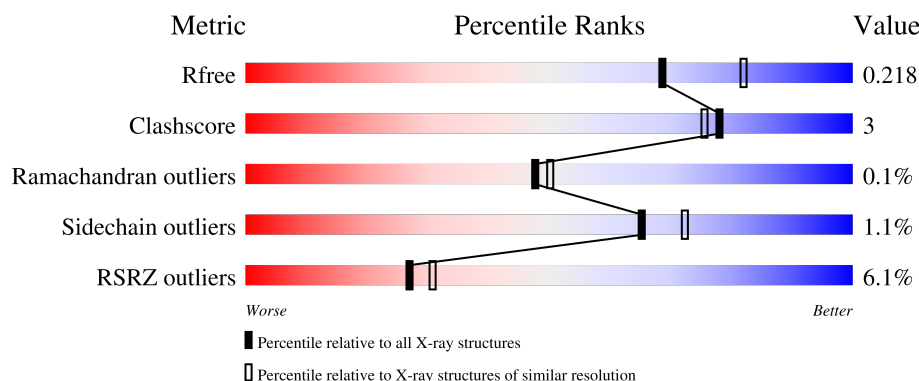
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	499	3% 91% 6%
1	B	499	2% 94% 4%
1	C	499	4% 90% 7%
1	D	499	14% 87% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15566 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 Betaine aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	10	0
			3755	2373	648	717	17			
1	B	488	Total	C	N	O	S	0	8	0
			3737	2363	644	712	18			
1	C	488	Total	C	N	O	S	0	8	0
			3738	2364	645	712	17			
1	D	486	Total	C	N	O	S	0	7	0
			3711	2349	639	707	16			

There are 44 discrepancies between the modelled and reference sequences:

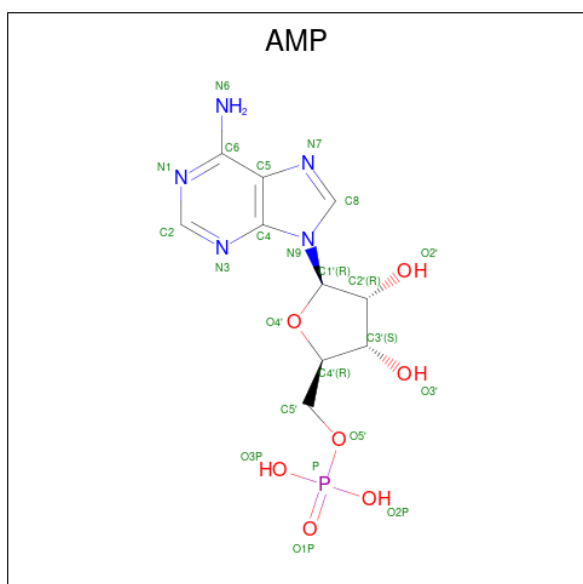
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP A0A447LC14
A	-7	ALA	-	expression tag	UNP A0A447LC14
A	-6	HIS	-	expression tag	UNP A0A447LC14
A	-5	HIS	-	expression tag	UNP A0A447LC14
A	-4	HIS	-	expression tag	UNP A0A447LC14
A	-3	HIS	-	expression tag	UNP A0A447LC14
A	-2	HIS	-	expression tag	UNP A0A447LC14
A	-1	HIS	-	expression tag	UNP A0A447LC14
A	0	HIS	-	expression tag	UNP A0A447LC14
A	62	ALA	VAL	engineered mutation	UNP A0A447LC14
A	485	PRO	GLN	engineered mutation	UNP A0A447LC14
B	-8	MET	-	expression tag	UNP A0A447LC14
B	-7	ALA	-	expression tag	UNP A0A447LC14
B	-6	HIS	-	expression tag	UNP A0A447LC14
B	-5	HIS	-	expression tag	UNP A0A447LC14
B	-4	HIS	-	expression tag	UNP A0A447LC14
B	-3	HIS	-	expression tag	UNP A0A447LC14
B	-2	HIS	-	expression tag	UNP A0A447LC14
B	-1	HIS	-	expression tag	UNP A0A447LC14
B	0	HIS	-	expression tag	UNP A0A447LC14
B	62	ALA	VAL	engineered mutation	UNP A0A447LC14

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Chain	Residue	Modelled	Actual	Comment	Reference
B	485	PRO	GLN	engineered mutation	UNP A0A447LC14
C	-8	MET	-	expression tag	UNP A0A447LC14
C	-7	ALA	-	expression tag	UNP A0A447LC14
C	-6	HIS	-	expression tag	UNP A0A447LC14
C	-5	HIS	-	expression tag	UNP A0A447LC14
C	-4	HIS	-	expression tag	UNP A0A447LC14
C	-3	HIS	-	expression tag	UNP A0A447LC14
C	-2	HIS	-	expression tag	UNP A0A447LC14
C	-1	HIS	-	expression tag	UNP A0A447LC14
C	0	HIS	-	expression tag	UNP A0A447LC14
C	62	ALA	VAL	engineered mutation	UNP A0A447LC14
C	485	PRO	GLN	engineered mutation	UNP A0A447LC14
D	-8	MET	-	expression tag	UNP A0A447LC14
D	-7	ALA	-	expression tag	UNP A0A447LC14
D	-6	HIS	-	expression tag	UNP A0A447LC14
D	-5	HIS	-	expression tag	UNP A0A447LC14
D	-4	HIS	-	expression tag	UNP A0A447LC14
D	-3	HIS	-	expression tag	UNP A0A447LC14
D	-2	HIS	-	expression tag	UNP A0A447LC14
D	-1	HIS	-	expression tag	UNP A0A447LC14
D	0	HIS	-	expression tag	UNP A0A447LC14
D	62	ALA	VAL	engineered mutation	UNP A0A447LC14
D	485	PRO	GLN	engineered mutation	UNP A0A447LC14

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



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		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

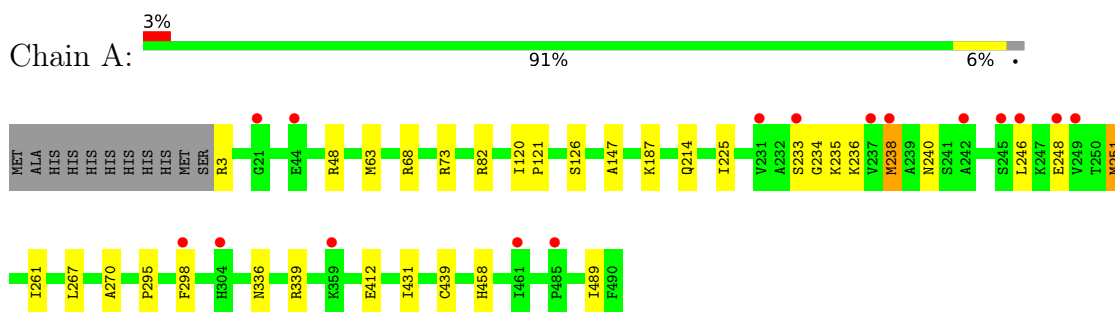
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	152	Total	O	0	0
			152	152		
4	B	149	Total	O	0	0
			149	149		
4	C	145	Total	O	0	0
			145	145		
4	D	83	Total	O	0	0
			83	83		

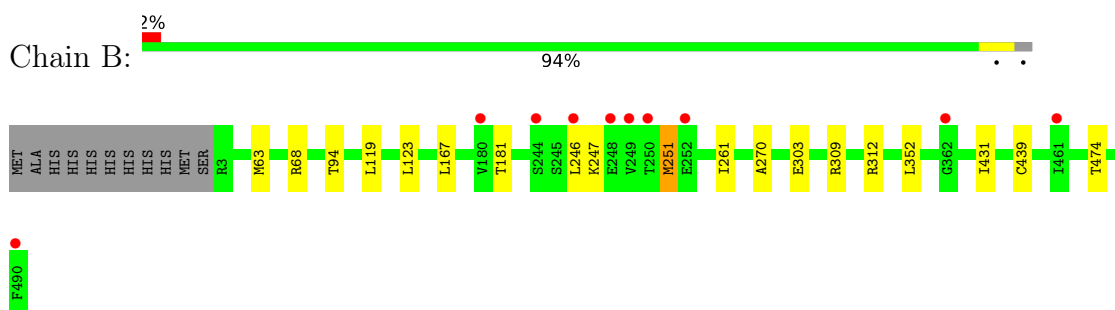
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

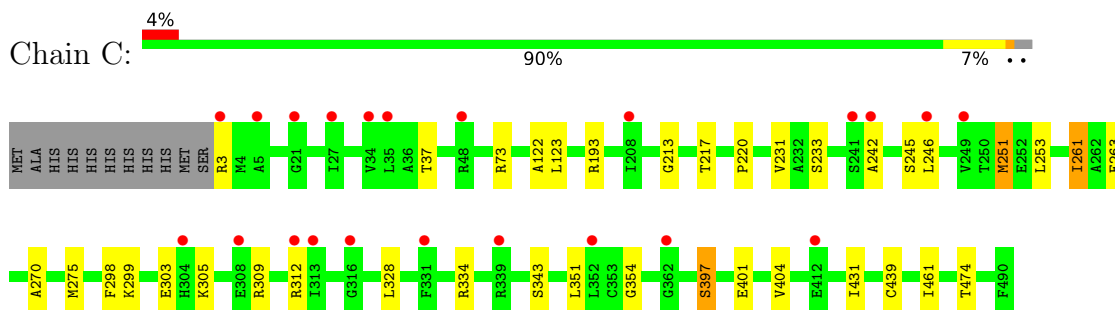
- Molecule 1: Betaine aldehyde dehydrogenase



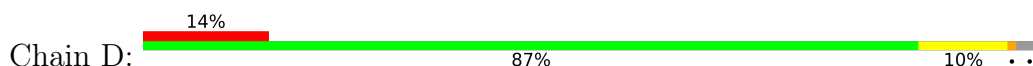
- Molecule 1: Betaine aldehyde dehydrogenase

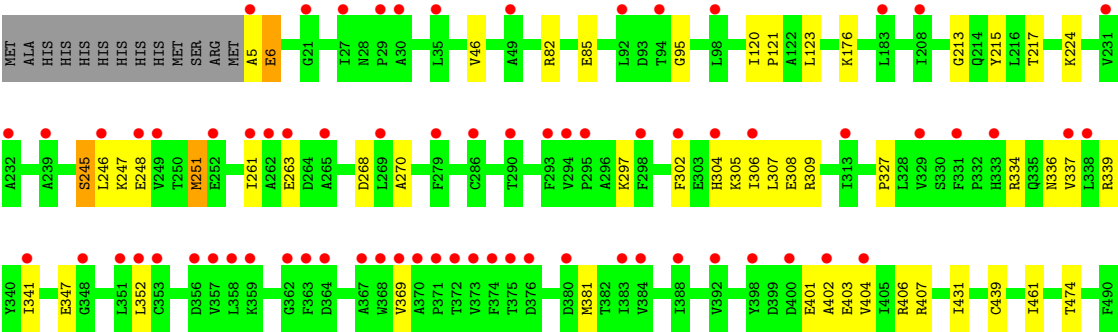


- Molecule 1: Betaine aldehyde dehydrogenase



- Molecule 1: Betaine aldehyde dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.88Å 100.50Å 123.72Å 90.00° 95.87° 90.00°	Depositor
Resolution (Å)	123.07 – 2.15 123.07 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.0 (123.07-2.15) 98.0 (123.07-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.186 , 0.214 0.190 , 0.218	Depositor DCC
R_{free} test set	5209 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15566	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: AMP, NA

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	0.19	0/3842	0.43	0/5209
1	B	0.18	0/3826	0.43	0/5185
1	C	0.17	0/3824	0.45	0/5184
1	D	0.23	0/3797	0.52	0/5149
All	All	0.20	0/15289	0.46	0/20727

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	A	0	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48	ARG	Sidechain
1	A	82	ARG	Sidechain
1	C	193	ARG	Sidechain

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	3755	0	3740	26	0
1	B	3737	0	3739	11	0
1	C	3738	0	3735	28	0
1	D	3711	0	3711	29	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	152	0	0	1	0
4	B	149	0	0	0	0
4	C	145	0	0	0	0
4	D	83	0	0	0	0
All	All	15566	0	14973	83	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 (83) 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:235:LYS:HA	1:A:238:MET:HE2	1.41	1.03
1:A:235:LYS:HA	1:A:238:MET:CE	2.21	0.70
1:C:309:ARG:HG3	1:C:312:ARG:HH21	1.57	0.69
1:A:238:MET:SD	1:C:246:LEU:CD1	2.84	0.66
1:C:261[A]:ILE:HG12	1:C:270:ALA:HB1	1.77	0.65
1:C:309:ARG:HG3	1:C:312:ARG:NH2	2.12	0.65
1:B:251:MET:HE2	1:D:246:LEU:HD11	1.81	0.63
1:D:268:ASP:HA	1:D:309:ARG:HH21	1.64	0.62
1:A:147:ALA:HB3	1:A:225:ILE:HD13	1.83	0.61
1:A:238:MET:SD	1:C:246:LEU:HD11	2.43	0.59
1:A:238:MET:HE3	1:C:242:ALA:HB1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:ILE:HD12	1:B:439:CYS:HB3	1.87	0.57
1:D:46:VAL:HG21	1:D:215:TYR:HB2	1.88	0.55
1:D:305:LYS:O	1:D:309:ARG:HG2	2.07	0.54
1:A:248:GLU:HG2	1:C:461[A]:ILE:HG23	1.90	0.54
1:A:336:ASN:OD1	1:A:339:ARG:NH2	2.38	0.53
1:C:3:ARG:NH2	1:C:37:THR:OG1	2.41	0.53
1:C:261[B]:ILE:HD12	1:C:270:ALA:HB1	1.90	0.53
1:C:305:LYS:O	1:C:309:ARG:HD3	2.08	0.53
1:B:63:MET:O	1:B:68:ARG:NH1	2.43	0.52
1:C:431:ILE:HD12	1:C:439:CYS:HB3	1.91	0.52
1:D:347:GLU:O	1:D:381:MET:HE2	2.10	0.52
1:A:295:PRO:HB2	1:A:298:PHE:HD2	1.75	0.51
1:B:246:LEU:HD11	1:D:251:MET:HE2	1.92	0.51
1:A:261[B]:ILE:HD12	1:A:270:ALA:HB1	1.93	0.50
1:A:458:HIS:NE2	1:C:245:SER:HB2	2.25	0.50
1:D:431:ILE:HD12	1:D:439:CYS:HB3	1.94	0.50
1:B:123:LEU:HD21	1:B:474:THR:HG21	1.94	0.50
1:C:328:LEU:HD12	1:C:334:ARG:HA	1.93	0.50
1:B:309:ARG:HG2	1:B:312:ARG:HH21	1.78	0.49
1:D:336:ASN:OD1	1:D:339:ARG:NH1	2.46	0.49
1:B:94:THR:HG22	1:B:181:THR:HG21	1.95	0.48
1:B:247:LYS:O	1:D:461[B]:ILE:HD11	2.14	0.48
1:A:214:GLN:HG3	1:A:240:ASN:HD22	1.79	0.47
1:D:5:ALA:O	1:D:6:GLU:C	2.58	0.47
1:D:123:LEU:HD21	1:D:474:THR:HG21	1.97	0.47
1:D:213:GLY:O	1:D:217:THR:HG23	2.15	0.46
1:A:63:MET:O	1:A:68:ARG:NH1	2.48	0.46
1:A:234:GLY:HA3	1:A:251:MET:HE1	1.96	0.46
1:A:240:ASN:N	1:A:240:ASN:OD1	2.46	0.46
1:B:261[B]:ILE:HD12	1:B:270:ALA:HB1	1.97	0.46
1:D:403:GLU:HG2	1:D:407:ARG:HD3	1.97	0.46
1:D:334:ARG:HG3	1:D:369:VAL:CG2	2.46	0.46
1:A:187:LYS:NZ	4:A:607:HOH:O	2.48	0.45
1:A:246:LEU:HD11	1:C:251:MET:HE2	1.98	0.45
1:D:261[B]:ILE:HD12	1:D:270:ALA:HB1	1.97	0.45
1:C:299:LYS:NZ	1:C:303:GLU:OE2	2.50	0.45
1:D:402:ALA:O	1:D:406:ARG:HG3	2.16	0.45
1:A:412:GLU:OE1	1:A:458:HIS:ND1	2.50	0.45
1:D:304:HIS:O	1:D:308:GLU:HG3	2.18	0.44
1:A:431:ILE:HD12	1:A:439:CYS:HB3	2.00	0.43
1:C:231:VAL:HA	1:C:253:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ILE:HB	1:D:121:PRO:HD3	2.00	0.43
1:B:119:LEU:HD21	1:C:122:ALA:HB2	1.99	0.43
1:C:123:LEU:HD21	1:C:474:THR:HG21	2.00	0.43
1:D:224:LYS:HA	1:D:248:GLU:O	2.19	0.43
1:A:238:MET:HE2	1:A:238:MET:HB2	1.78	0.42
1:C:275:MET:HG3	1:C:309:ARG:HB3	2.00	0.42
1:A:238:MET:HE3	1:C:242:ALA:CB	2.48	0.42
1:D:95:GLY:O	1:D:327:PRO:HD2	2.20	0.42
1:C:299:LYS:HD2	1:C:397:SER:HB2	2.02	0.42
1:C:309:ARG:CG	1:C:312:ARG:HH21	2.29	0.42
1:C:401:GLU:O	1:C:404:VAL:HG12	2.20	0.42
1:D:307:LEU:HD21	1:D:352:LEU:HG	2.01	0.42
1:A:251:MET:HE3	1:A:251:MET:HB3	1.77	0.41
1:C:263:GLU:O	1:C:298:PHE:HE2	2.04	0.41
1:D:268:ASP:HA	1:D:309:ARG:NH2	2.33	0.41
1:C:220:PRO:HA	1:C:245:SER:HB3	2.02	0.41
1:D:302:PHE:CZ	1:D:306:ILE:HD11	2.55	0.41
1:B:303:GLU:HB3	1:B:352:LEU:HD21	2.03	0.41
1:D:82[B]:ARG:NH2	1:D:85:GLU:OE2	2.54	0.41
1:D:245:SER:OG	1:D:247:LYS:NZ	2.49	0.41
1:D:401:GLU:O	1:D:404:VAL:HG12	2.20	0.41
1:D:406:ARG:HE	1:D:406:ARG:HB2	1.64	0.41
1:D:403:GLU:OE2	1:D:407:ARG:NH1	2.51	0.41
1:A:267:LEU:HD11	1:A:298:PHE:HB3	2.03	0.40
1:C:213:GLY:O	1:C:217:THR:HG23	2.21	0.40
1:C:351:LEU:HD21	1:C:354:GLY:O	2.21	0.40
1:D:337:VAL:O	1:D:341:ILE:HG13	2.21	0.40
1:A:120:ILE:HB	1:A:121:PRO:HD3	2.03	0.40
1:A:233:SER:HA	1:A:236:LYS:NZ	2.36	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	496/499 (99%)	485 (98%)	11 (2%)	0	100	100
1	B	494/499 (99%)	484 (98%)	10 (2%)	0	100	100
1	C	494/499 (99%)	482 (98%)	12 (2%)	0	100	100
1	D	491/499 (98%)	480 (98%)	10 (2%)	1 (0%)	43	44
All	All	1975/1996 (99%)	1931 (98%)	43 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	6	GLU

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	392/394 (100%)	386 (98%)	6 (2%)	57	64
1	B	391/394 (99%)	389 (100%)	2 (0%)	81	87
1	C	390/394 (99%)	384 (98%)	6 (2%)	57	64
1	D	387/394 (98%)	382 (99%)	5 (1%)	61	68
All	All	1560/1576 (99%)	1541 (99%)	19 (1%)	65	70

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	126[A]	SER
1	A	126[B]	SER
1	A	238	MET
1	A	251	MET
1	A	489	ILE
1	B	167	LEU
1	B	251	MET
1	C	233	SER
1	C	251	MET

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Mol	Chain	Res	Type
1	C	261[A]	ILE
1	C	261[B]	ILE
1	C	343	SER
1	C	397	SER
1	D	176	LYS
1	D	245	SER
1	D	251	MET
1	D	263	GLU
1	D	297	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	B	127	GLN
1	C	8	GLN
1	C	54	GLN
1	D	284	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	AMP	C	501	-	25,25,25	0.35	0	37,38,38	0.44	0
2	AMP	D	501	-	25,25,25	0.35	0	37,38,38	0.45	0
2	AMP	B	501	-	25,25,25	0.37	0	37,38,38	0.47	0
2	AMP	A	501	-	25,25,25	0.38	0	37,38,38	0.46	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
2	AMP	C	501	-	-	2/10/26/26	0/3/3/3
2	AMP	D	501	-	-	6/10/26/26	0/3/3/3
2	AMP	B	501	-	-	4/10/26/26	0/3/3/3
2	AMP	A	501	-	-	1/10/26/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

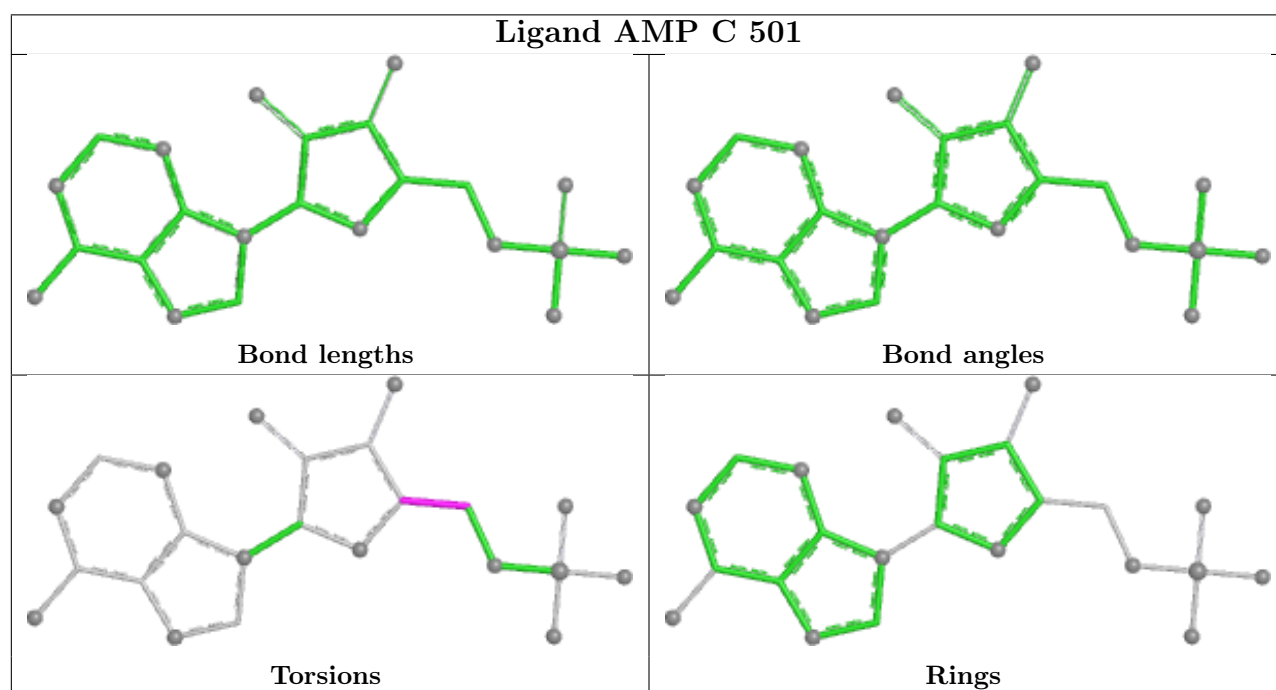
All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	AMP	C5'-O5'-P-O3P
2	D	501	AMP	C5'-O5'-P-O1P
2	D	501	AMP	C5'-O5'-P-O3P
2	B	501	AMP	O4'-C4'-C5'-O5'
2	C	501	AMP	O4'-C4'-C5'-O5'
2	D	501	AMP	O4'-C4'-C5'-O5'
2	C	501	AMP	C3'-C4'-C5'-O5'
2	B	501	AMP	C3'-C4'-C5'-O5'
2	D	501	AMP	C3'-C4'-C5'-O5'
2	D	501	AMP	C5'-O5'-P-O2P
2	A	501	AMP	C2'-C1'-N9-C8
2	B	501	AMP	C2'-C1'-N9-C8
2	D	501	AMP	C2'-C1'-N9-C8

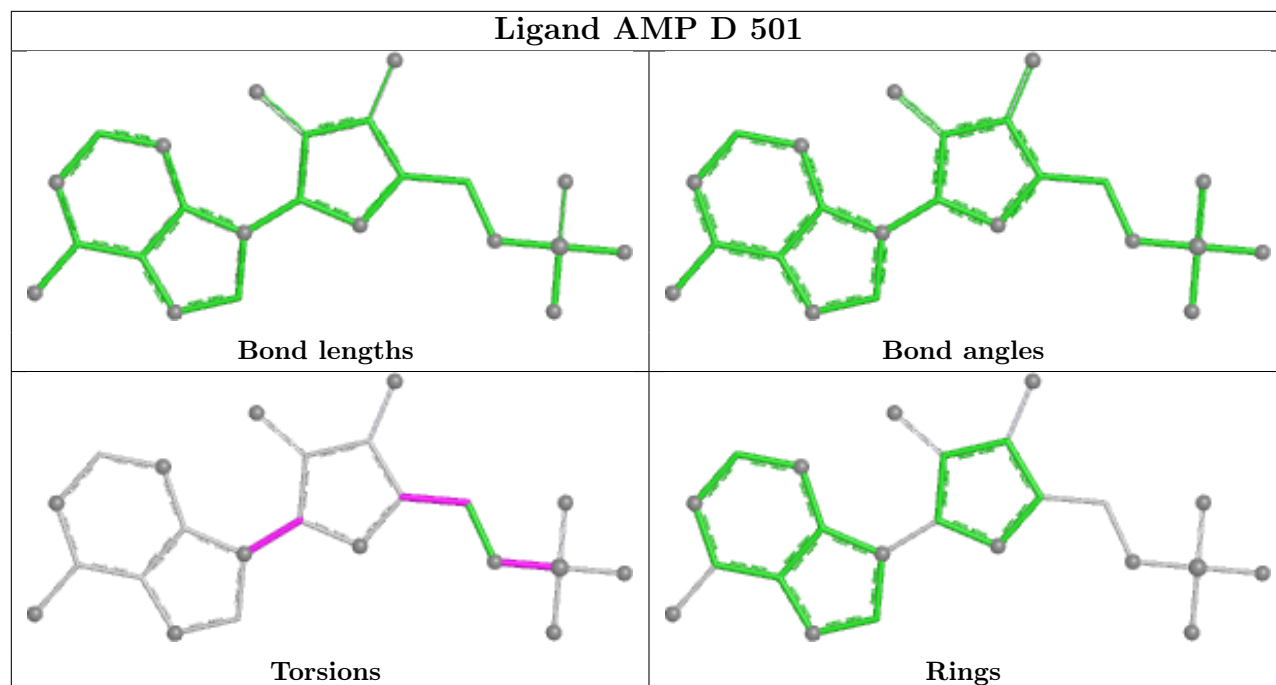
There are no ring outliers.

No monomer is involved in short contacts.

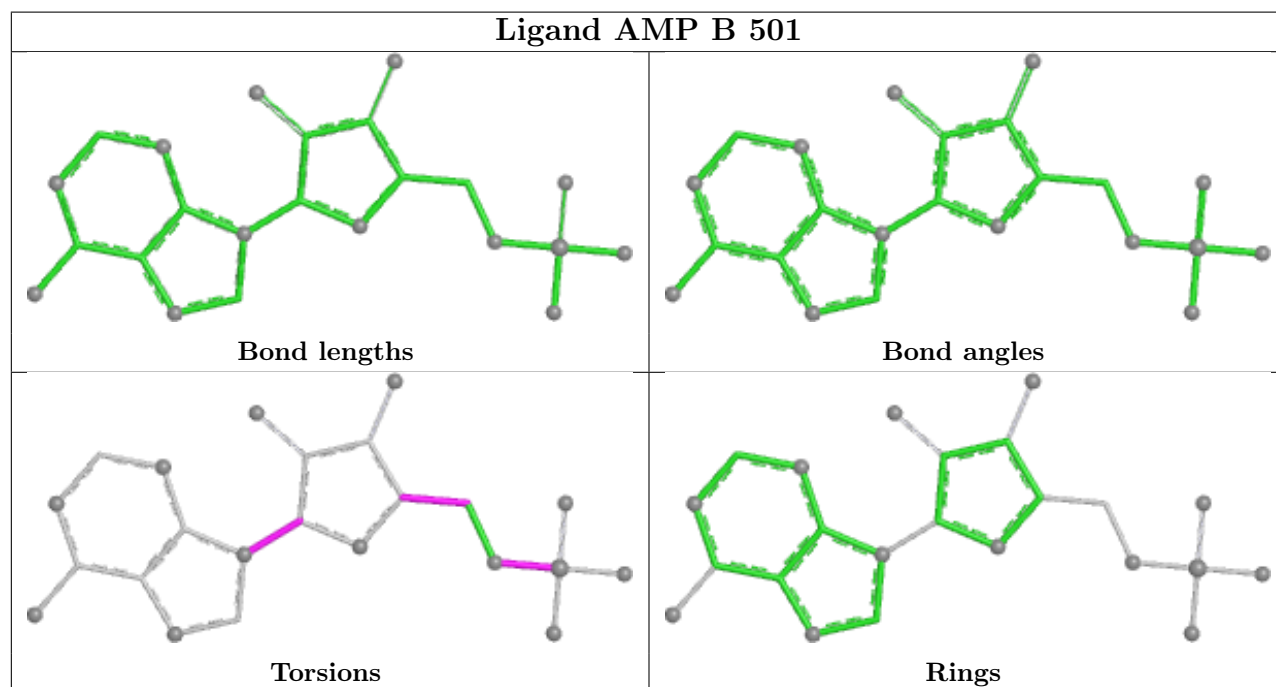
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

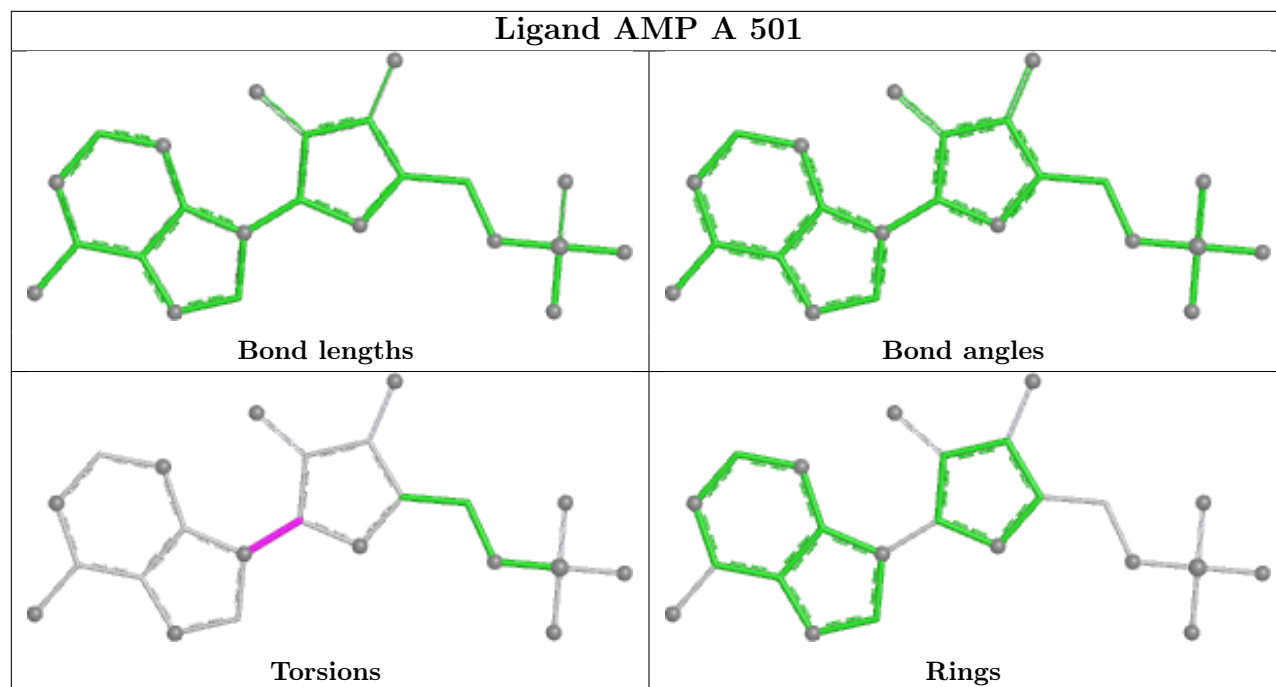


Ligand AMP D 501



Ligand AMP B 501





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, 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	488/499 (97%)	0.22	16 (3%)	49	53	18, 42, 70, 84	10 (2%)
1	B	488/499 (97%)	0.19	10 (2%)	65	69	18, 42, 67, 99	8 (1%)
1	C	488/499 (97%)	0.43	22 (4%)	38	43	20, 52, 82, 110	8 (1%)
1	D	486/499 (97%)	0.97	71 (14%)	6	6	21, 67, 110, 141	7 (1%)
All	All	1950/1996 (97%)	0.45	119 (6%)	27	31	18, 48, 92, 141	33 (1%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	398	TYR	4.5
1	D	338	LEU	3.9
1	D	368	TRP	3.8
1	A	461[A]	ILE	3.8
1	D	5	ALA	3.8
1	A	304[A]	HIS	3.6
1	D	341	ILE	3.6
1	D	295	PRO	3.5
1	D	30	ALA	3.5
1	C	35	LEU	3.5
1	C	242	ALA	3.4
1	A	231	VAL	3.4
1	B	490	PHE	3.3
1	D	358	LEU	3.2
1	D	208	ILE	3.2
1	D	374	PHE	3.2
1	D	367	ALA	3.1
1	D	384	VAL	3.1
1	D	402	ALA	3.1
1	D	337	VAL	3.1
1	D	27	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	331	PHE	3.1
1	D	373	VAL	3.0
1	D	98	LEU	3.0
1	D	279	PHE	3.0
1	D	252	GLU	2.9
1	B	246	LEU	2.9
1	D	246	LEU	2.9
1	B	250	THR	2.9
1	D	265	ALA	2.9
1	D	304	HIS	2.9
1	D	329	VAL	2.8
1	C	304	HIS	2.8
1	D	362	GLY	2.8
1	D	370	ALA	2.8
1	D	383	ILE	2.8
1	D	293	PHE	2.8
1	D	248	GLU	2.8
1	D	232	ALA	2.7
1	D	351	LEU	2.7
1	A	237	VAL	2.7
1	C	241	SER	2.7
1	D	35	LEU	2.7
1	D	294	VAL	2.7
1	C	308	GLU	2.6
1	C	5	ALA	2.6
1	D	375	THR	2.6
1	C	246	LEU	2.6
1	D	302	PHE	2.6
1	D	352	LEU	2.6
1	B	180	VAL	2.6
1	D	357	VAL	2.6
1	D	356	ASP	2.6
1	B	244	SER	2.6
1	D	249	VAL	2.5
1	C	362	GLY	2.5
1	C	27	ILE	2.5
1	C	3	ARG	2.5
1	D	313	ILE	2.5
1	D	369	VAL	2.4
1	D	92	LEU	2.4
1	D	231	VAL	2.4
1	A	298	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	363	PHE	2.4
1	C	208	ILE	2.4
1	C	249	VAL	2.4
1	D	371	PRO	2.4
1	D	400	ASP	2.3
1	D	388	ILE	2.3
1	D	392	VAL	2.3
1	A	485	PRO	2.3
1	D	333	HIS	2.3
1	A	238	MET	2.3
1	B	252	GLU	2.3
1	D	261[A]	ILE	2.3
1	A	249	VAL	2.3
1	C	339	ARG	2.3
1	D	353	CYS	2.3
1	A	242	ALA	2.3
1	D	21	GLY	2.3
1	D	359	LYS	2.2
1	D	49	ALA	2.2
1	A	248	GLU	2.2
1	D	298	PHE	2.2
1	D	290	THR	2.2
1	C	34	VAL	2.2
1	A	44	GLU	2.2
1	D	183	LEU	2.2
1	C	48	ARG	2.2
1	C	312	ARG	2.2
1	D	29	PRO	2.2
1	A	21	GLY	2.2
1	D	262	ALA	2.2
1	C	412	GLU	2.1
1	C	316	GLY	2.1
1	D	348	GLY	2.1
1	D	286	CYS	2.1
1	A	359	LYS	2.1
1	D	376	ASP	2.1
1	D	404	VAL	2.1
1	C	352	LEU	2.1
1	D	269	LEU	2.1
1	D	364	ASP	2.1
1	D	94	THR	2.1
1	B	461	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	313	ILE	2.1
1	A	245	SER	2.1
1	A	246	LEU	2.0
1	D	380	ASP	2.0
1	B	362	GLY	2.0
1	D	306	ILE	2.0
1	B	248	GLU	2.0
1	B	249	VAL	2.0
1	C	331	PHE	2.0
1	D	263	GLU	2.0
1	A	233	SER	2.0
1	D	239	ALA	2.0
1	D	372	THR	2.0
1	C	21	GLY	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](#)

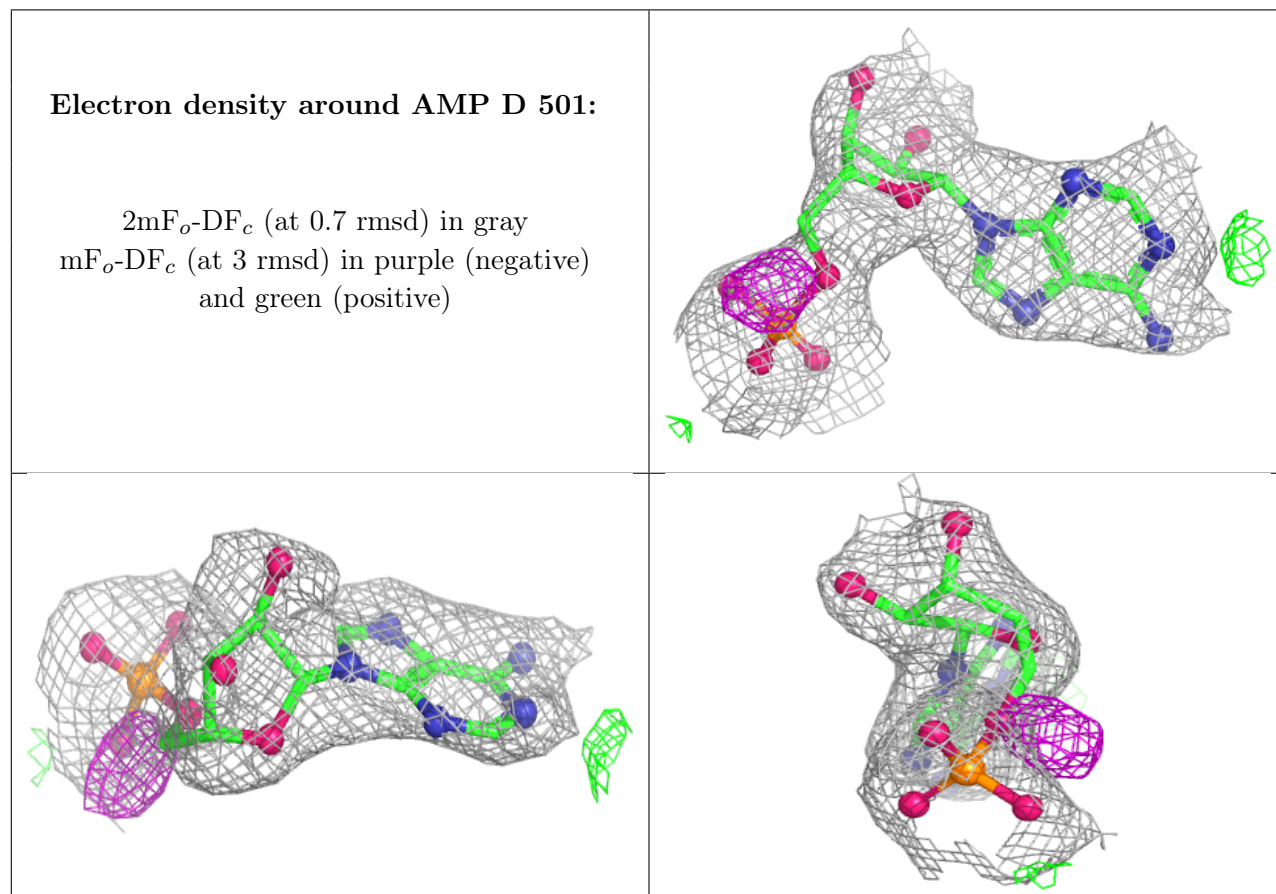
There are no oligosaccharides in this entry.

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.

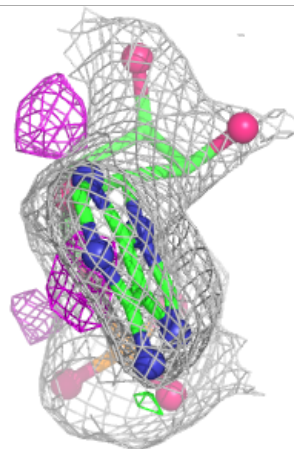
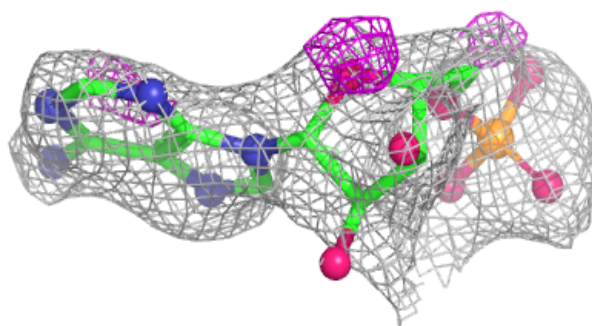
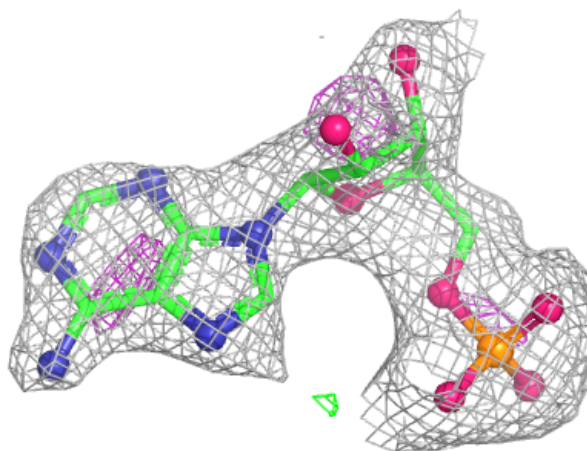
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	D	502	1/1	0.73	0.19	78,78,78,78	0
2	AMP	D	501	23/23	0.84	0.12	61,76,84,87	0
2	AMP	C	501	23/23	0.84	0.11	62,73,80,84	0
3	NA	C	502	1/1	0.85	0.12	63,63,63,63	0
2	AMP	B	501	23/23	0.90	0.09	48,59,66,67	0
3	NA	B	502	1/1	0.93	0.06	48,48,48,48	0
2	AMP	A	501	23/23	0.94	0.08	41,54,64,65	0
3	NA	A	502	1/1	0.95	0.08	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.



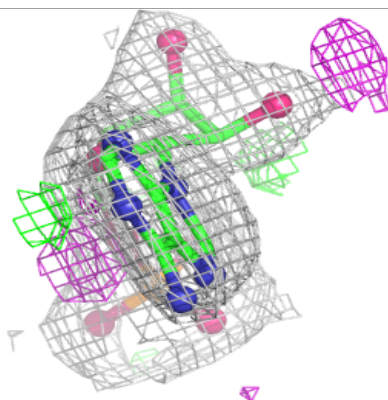
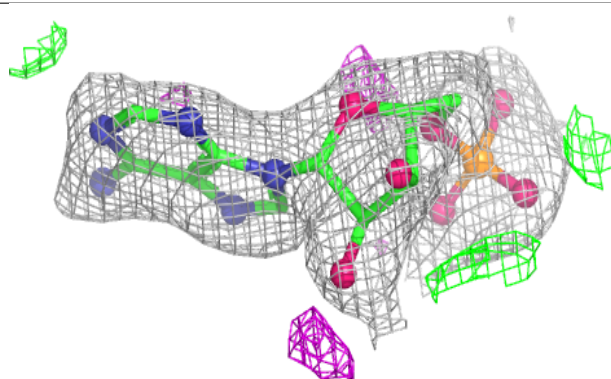
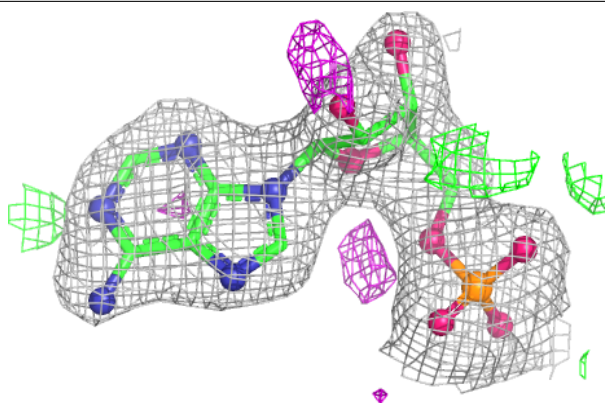
Electron density around AMP C 501:

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

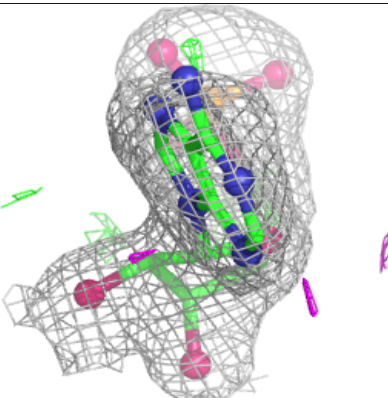
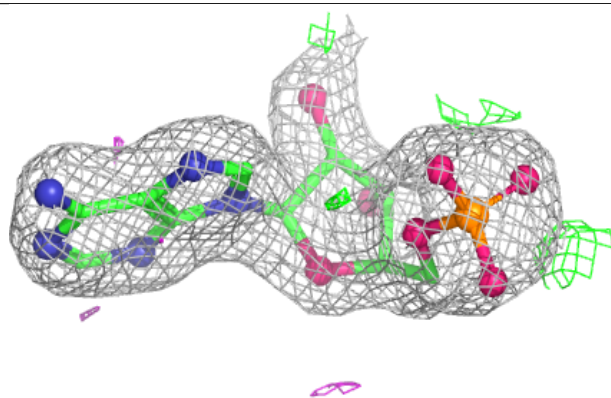
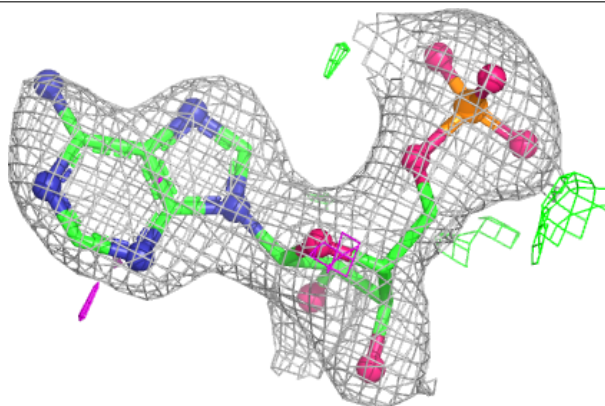


Electron density around AMP B 501:

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

**Electron density around AMP 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 [i](#)

There are no such residues in this entry.