



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:44 pm BST

PDB ID : 3Q10  
Title : Pantoate-beta-alanine ligase from Yersinia pestis  
Authors : Osipiuk, J.; Maltseva, N.; Kwon, K.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2010-12-16  
Resolution : 1.83 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

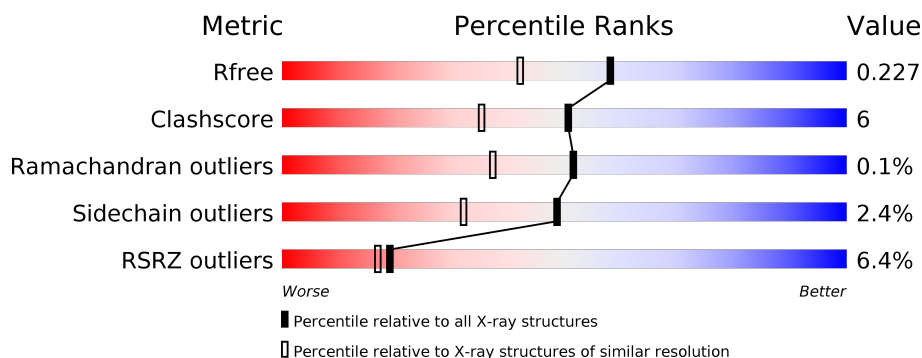
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	287	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	287	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>..</div> </div> </div>
1	C	287	<div> <div>13%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>
1	D	287	<div> <div>7%</div> <div> <div></div> <div>61%</div> <div>8%</div> <div>.</div> <div>31%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9440 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.

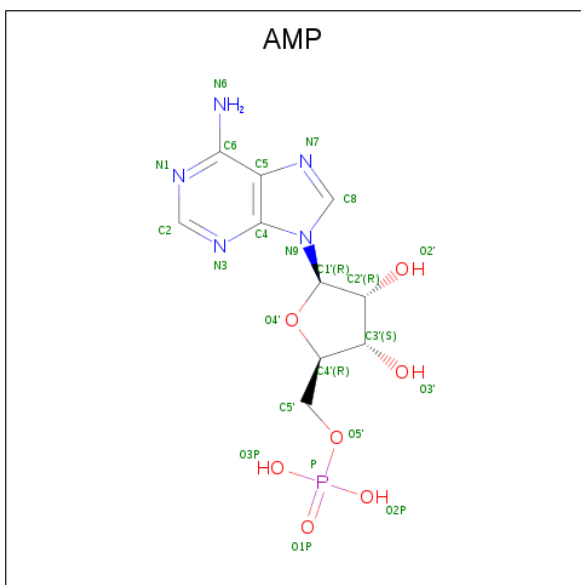
- Molecule 1 is a protein called Pantoate--beta-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	20	0
			2361	1504	410	437	10			
1	B	285	Total	C	N	O	S	0	15	0
			2320	1479	400	431	10			
1	C	284	Total	C	N	O	S	0	19	0
			2343	1498	405	429	11			
1	D	198	Total	C	N	O	S	0	5	0
			1590	1015	278	289	8			

There are 12 discrepancies between the modelled and reference sequences:

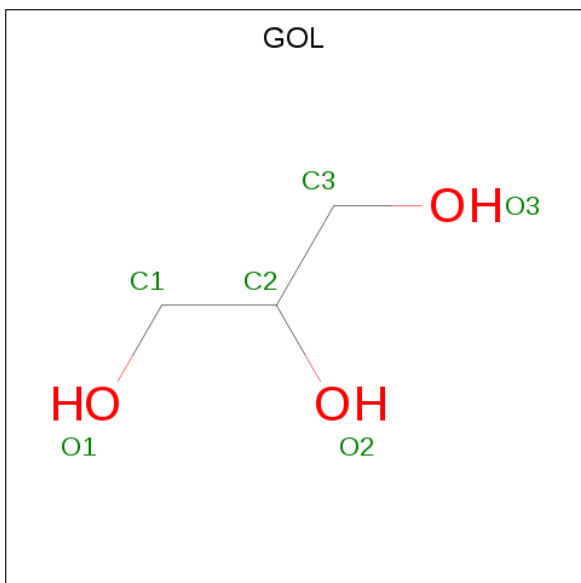
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q8ZBK7
A	-1	ASN	-	EXPRESSION TAG	UNP Q8ZBK7
A	0	ALA	-	EXPRESSION TAG	UNP Q8ZBK7
B	-2	SER	-	EXPRESSION TAG	UNP Q8ZBK7
B	-1	ASN	-	EXPRESSION TAG	UNP Q8ZBK7
B	0	ALA	-	EXPRESSION TAG	UNP Q8ZBK7
C	-2	SER	-	EXPRESSION TAG	UNP Q8ZBK7
C	-1	ASN	-	EXPRESSION TAG	UNP Q8ZBK7
C	0	ALA	-	EXPRESSION TAG	UNP Q8ZBK7
D	-2	SER	-	EXPRESSION TAG	UNP Q8ZBK7
D	-1	ASN	-	EXPRESSION TAG	UNP Q8ZBK7
D	0	ALA	-	EXPRESSION TAG	UNP Q8ZBK7

- 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).



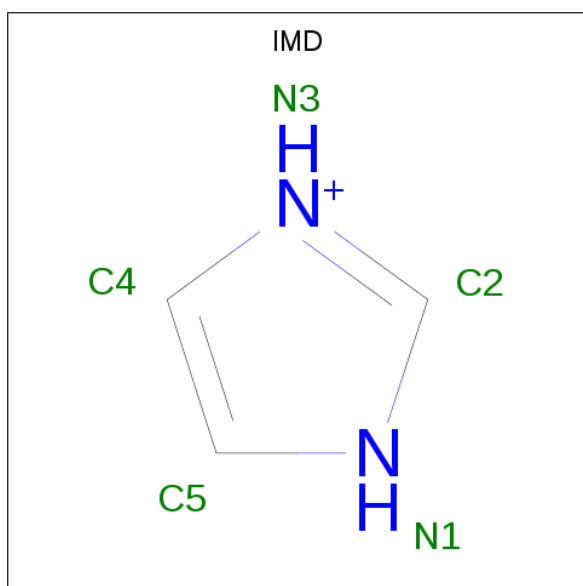
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula:  $Cl$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

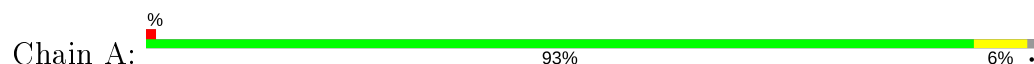
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	292	Total 292	O 292	0	4
6	B	163	Total 163	O 163	0	0
6	C	196	Total 196	O 196	0	2
6	D	47	Total 47	O 47	0	0

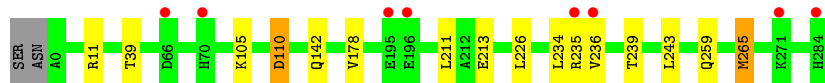
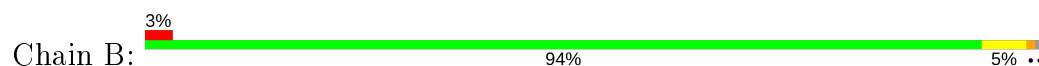
### 3 Residue-property plots [i](#)

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.

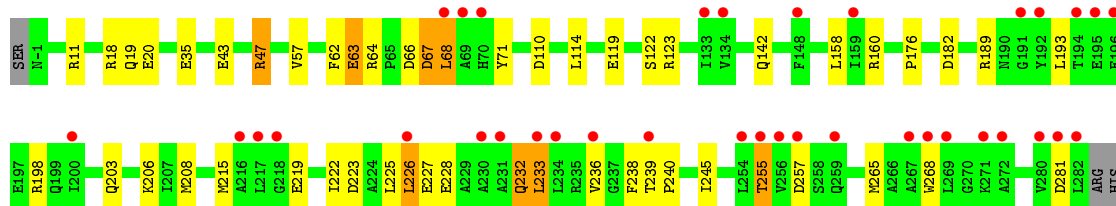
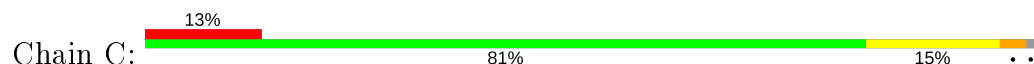
- Molecule 1: Pantoate--beta-alanine ligase



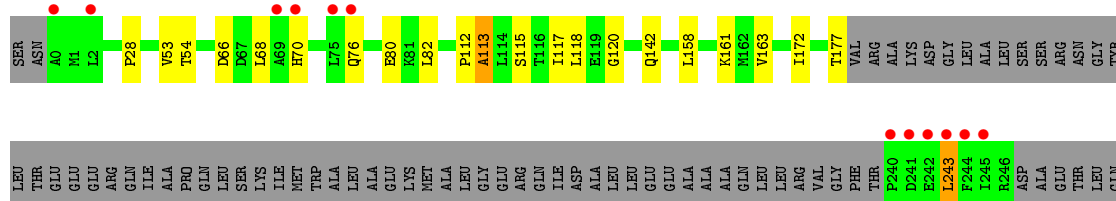
- Molecule 1: Pantoate--beta-alanine ligase



- Molecule 1: Pantoate--beta-alanine ligase



- Molecule 1: Pantoate--beta-alanine ligase



PRO	LEU	THR	VAL	ASP	SER	GLN	GLN	ALA	V262	I263	I264	I265	I266	I267	TRP	LEU	GLY	LYS	A272	A273	I274	I275	I276	I277	Q278	LEU	VAL	ASP	LEU	ARG	HIS



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.81Å 77.24Å 98.46Å 101.33° 94.91° 94.37°	Depositor
Resolution (Å)	33.10 – 1.83 33.12 – 1.83	Depositor EDS
% Data completeness (in resolution range)	96.4 (33.10-1.83) 96.4 (33.12-1.83)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.174 , 0.211 0.188 , 0.227	Depositor DCC
$R_{free}$ test set	5527 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.3	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	9440	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 4.56% 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: GOL, CL, IMD, AMP

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	0.97	2/2461 (0.1%)	0.87	4/3331 (0.1%)
1	B	0.73	0/2404	0.76	4/3260 (0.1%)
1	C	0.84	0/2439	0.85	3/3306 (0.1%)
1	D	0.61	0/1633	0.69	0/2212
All	All	0.82	2/8937 (0.0%)	0.80	11/12109 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35[A]	GLU	CD-OE1	5.25	1.31	1.25
1	A	35[B]	GLU	CD-OE1	5.25	1.31	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	LEU	CA-CB-CG	6.00	129.11	115.30
1	B	110[A]	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	110[B]	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	110[A]	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	B	110[B]	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	A	73[A]	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	A	73[B]	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	A	11[A]	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	11[B]	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	47	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	67	ASP	CB-CG-OD1	5.02	122.82	118.30

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	2361	0	2445	13	0
1	B	2320	0	2399	15	0
1	C	2343	0	2442	53	0
1	D	1590	0	1627	18	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	1	0
2	D	23	0	12	0	0
3	A	6	0	7	0	0
3	B	12	0	16	2	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	5	0	5	0	0
5	A	1	0	0	0	0
6	A	292	0	0	3	0
6	B	163	0	0	6	0
6	C	196	0	0	6	0
6	D	47	0	0	1	0
All	All	9440	0	9005	101	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 6.

All (101) 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:C:215[A]:MET:HE1	1:C:245:ILE:HD13	1.23	1.14
1:B:243:LEU:HD22	1:B:265:MET:HE2	1.36	1.06
1:C:11[B]:ARG:NH1	1:C:11[B]:ARG:HG2	1.58	1.05
1:C:11[B]:ARG:HH11	1:C:11[B]:ARG:HG2	0.89	1.02
1:C:63[B]:GLU:OE1	1:C:64[B]:ARG:NH2	1.91	1.02
1:C:11[B]:ARG:CG	1:C:11[B]:ARG:HH11	1.77	0.97
1:C:203:GLN:HE21	1:C:236:VAL:HG11	1.35	0.91
1:C:215[A]:MET:CE	1:C:245:ILE:HD13	2.03	0.88
2:C:501:AMP:C2	6:C:603:HOH:O	2.29	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:GLN:NE2	1:C:236:VAL:HG11	1.91	0.85
1:C:226:LEU:HD11	1:C:245:ILE:HG13	1.63	0.80
1:C:255:THR:HG22	1:C:257:ASP:H	1.46	0.79
1:C:223:ASP:O	1:C:227:GLU:HG3	1.89	0.73
1:C:18[A]:ARG:HD2	1:C:142:GLN:NE2	2.04	0.72
1:B:243:LEU:HD22	1:B:265:MET:CE	2.16	0.72
1:C:233:LEU:HD23	1:C:238:PHE:HB2	1.74	0.70
1:C:62[B]:PHE:HE2	1:C:68[B]:LEU:CG	2.05	0.70
3:B:605:GOL:H2	6:B:343:HOH:O	1.91	0.69
1:A:195[B]:GLU:HG2	6:A:656:HOH:O	1.93	0.69
1:C:62[B]:PHE:CD2	1:C:68[B]:LEU:HB2	2.30	0.67
1:C:62[B]:PHE:HE2	1:C:68[B]:LEU:CB	2.07	0.67
1:C:62[B]:PHE:CE2	1:C:68[B]:LEU:HB2	2.28	0.67
1:C:57:VAL:CG1	1:C:62[B]:PHE:HZ	2.06	0.67
1:C:57:VAL:HG12	1:C:62[B]:PHE:HZ	1.59	0.65
1:C:62[B]:PHE:CE2	1:C:68[B]:LEU:CB	2.79	0.65
1:B:142:GLN:NE2	6:B:560:HOH:O	2.27	0.65
1:D:112:PRO:O	1:D:113:ALA:HB3	1.98	0.64
1:A:195[B]:GLU:HG3	1:A:196[B]:GLU:OE2	1.98	0.63
1:C:233:LEU:HD22	1:C:240:PRO:HB3	1.80	0.62
1:C:62[B]:PHE:HE2	1:C:68[B]:LEU:HG	1.66	0.60
1:B:213:GLU:OE1	6:B:697:HOH:O	2.15	0.59
1:C:226:LEU:HD11	1:C:245:ILE:CG1	2.32	0.58
1:D:163:VAL:HG21	1:D:172:ILE:HD11	1.86	0.58
1:A:112:PRO:HD2	6:C:366:HOH:O	2.02	0.57
1:A:39[B]:THR:HG21	1:A:178:VAL:HG21	1.86	0.57
1:A:71:TYR:O	1:A:73[B]:ARG:HD3	2.05	0.57
1:B:265:MET:CE	1:B:265:MET:HA	2.34	0.56
1:C:43[A]:GLU:OE2	1:C:47:ARG:NE	2.29	0.56
1:B:105:LYS:O	1:D:161:LYS:NZ	2.37	0.56
1:C:63[B]:GLU:OE1	1:C:64[B]:ARG:HG3	2.07	0.55
1:A:16[B]:ARG:NE	1:A:20:GLU:OE2	2.41	0.54
1:C:18[A]:ARG:CD	1:C:142:GLN:NE2	2.71	0.54
1:C:226:LEU:HD11	1:C:245:ILE:CD1	2.39	0.53
1:C:215[A]:MET:HE1	1:C:245:ILE:CD1	2.16	0.52
1:D:117:ILE:CG1	1:D:118:LEU:HD13	2.39	0.52
1:C:19:GLN:NE2	6:C:465:HOH:O	2.40	0.52
1:A:226:LEU:HD21	1:A:245:ILE:HG13	1.93	0.51
1:C:215[A]:MET:HE2	1:C:222:ILE:CD1	2.41	0.50
1:C:57:VAL:HG12	1:C:62[B]:PHE:CZ	2.42	0.50
1:D:117:ILE:HD12	1:D:118:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39[A]:THR:HG21	6:B:527:HOH:O	2.11	0.49
1:D:277:ASN:O	1:D:278:GLN:HB2	2.12	0.49
1:C:215[A]:MET:HE3	1:C:225:LEU:HD13	1.95	0.48
1:C:226:LEU:CD1	1:C:245:ILE:CD1	2.92	0.48
1:C:236:VAL:O	1:C:236:VAL:HG12	2.14	0.48
1:D:118:LEU:HD12	1:D:118:LEU:N	2.28	0.48
1:D:112:PRO:O	1:D:113:ALA:CB	2.62	0.47
1:A:96:ALA:O	1:A:100:PRO:HA	2.15	0.47
1:D:117:ILE:HG13	1:D:118:LEU:HD13	1.97	0.47
1:C:11[B]:ARG:NH1	1:C:11[B]:ARG:CG	2.44	0.46
1:B:39[B]:THR:HG21	1:B:178:VAL:HG21	1.96	0.46
1:B:243:LEU:HD13	1:B:265:MET:HE1	1.98	0.46
1:C:35:GLU:OE2	6:C:639:HOH:O	2.20	0.46
1:D:142:GLN:NE2	6:D:305:HOH:O	2.49	0.46
1:B:265:MET:HE3	1:B:265:MET:HA	1.97	0.46
1:C:208:MET:HA	1:C:265:MET:CE	2.46	0.45
1:C:255:THR:HG22	1:C:257:ASP:N	2.23	0.45
1:C:225:LEU:O	1:C:228:GLU:HB2	2.17	0.44
1:C:182:ASP:OD2	1:C:198:ARG:NH1	2.33	0.44
1:C:219:GLU:HG2	1:C:225:LEU:HD21	1.99	0.44
1:C:160:ARG:NE	6:C:479:HOH:O	2.44	0.43
1:C:71:TYR:OH	6:C:520:HOH:O	2.20	0.43
1:D:117:ILE:CD1	1:D:118:LEU:HD13	2.48	0.43
1:C:239:THR:HB	1:C:268:TRP:HB2	1.98	0.43
1:B:11:ARG:HH12	1:B:142:GLN:HE21	1.65	0.43
1:B:39[A]:THR:HG23	6:B:511:HOH:O	2.19	0.43
1:D:68:LEU:C	1:D:68:LEU:HD23	2.39	0.43
1:A:19[A]:GLN:OE1	6:A:572:HOH:O	2.21	0.42
1:C:63[A]:GLU:H	1:C:63[A]:GLU:CD	2.23	0.42
1:A:201:ALA:N	1:A:202:PRO:CD	2.82	0.42
3:B:605:GOL:H31	6:B:664:HOH:O	2.19	0.42
1:D:115:SER:O	1:D:120:GLY:HA3	2.19	0.42
1:D:76:GLN:O	1:D:80[A]:GLU:HG3	2.20	0.42
1:C:208:MET:HG3	1:C:265:MET:HE2	2.01	0.42
1:C:62[A]:PHE:HD1	1:C:67:ASP:HB2	1.85	0.42
1:D:53:VAL:HG21	1:D:82:LEU:HD22	2.02	0.42
1:B:235[B]:ARG:HG2	1:B:236:VAL:HG13	2.02	0.42
1:C:114[B]:LEU:HD13	1:C:158:LEU:HA	2.02	0.41
1:D:243:LEU:HD12	1:D:243:LEU:N	2.35	0.41
1:B:211:LEU:HD11	1:B:226:LEU:HD23	2.02	0.41
1:C:119[B]:GLU:OE2	1:C:123:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39[B]:THR:HG21	6:A:346:HOH:O	2.21	0.41
1:B:259[B]:GLN:HA	1:B:259[B]:GLN:NE2	2.36	0.41
1:C:62[B]:PHE:CE2	1:C:68[B]:LEU:HA	2.56	0.41
1:D:28:PRO:HA	1:D:54:THR:OG1	2.20	0.41
1:A:39[B]:THR:CG2	1:A:178:VAL:HG21	2.50	0.40
1:C:233:LEU:HD23	1:C:238:PHE:CB	2.47	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	302/287 (105%)	297 (98%)	5 (2%)	0	100	100
1	B	298/287 (104%)	293 (98%)	5 (2%)	0	100	100
1	C	301/287 (105%)	294 (98%)	7 (2%)	0	100	100
1	D	195/287 (68%)	190 (97%)	4 (2%)	1 (0%)	29	15
All	All	1096/1148 (96%)	1074 (98%)	21 (2%)	1 (0%)	51	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	113	ALA

### 5.3.2 Protein sidechains [i](#)

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	258/240 (108%)	258 (100%)	0	100	100
1	B	253/240 (105%)	248 (98%)	5 (2%)	55	40
1	C	256/240 (107%)	239 (93%)	17 (7%)	16	4
1	D	173/240 (72%)	168 (97%)	5 (3%)	42	25
All	All	940/960 (98%)	913 (97%)	27 (3%)	49	25

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	110[A]	ASP
1	B	110[B]	ASP
1	B	234	LEU
1	B	239	THR
1	B	265	MET
1	C	63[A]	GLU
1	C	63[B]	GLU
1	C	66	ASP
1	C	68[A]	LEU
1	C	68[B]	LEU
1	C	110[A]	ASP
1	C	110[B]	ASP
1	C	122	SER
1	C	176	PRO
1	C	189	ARG
1	C	193	LEU
1	C	206	LYS
1	C	226	LEU
1	C	232[A]	GLN
1	C	232[B]	GLN
1	C	255	THR
1	C	281	ASP
1	D	66[A]	ASP
1	D	66[B]	ASP
1	D	158	LEU
1	D	177	THR
1	D	243	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	A	199	GLN
1	B	13	GLN
1	B	142	GLN
1	B	260	GLN
1	C	19	GLN
1	C	142	GLN
1	C	199	GLN
1	C	203	GLN
1	D	19	GLN
1	D	32	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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	GOL	D	604	-	5,5,5	0.36	0	5,5,5	0.60	0
2	AMP	A	501	-	22,25,25	1.21	3 (13%)	25,38,38	1.36	4 (16%)
3	GOL	C	602	-	5,5,5	0.37	0	5,5,5	0.79	0
3	GOL	B	605	-	5,5,5	0.47	0	5,5,5	0.52	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	601	-	5,5,5	0.97	0	5,5,5	1.20	0
2	AMP	D	501	-	22,25,25	0.95	1 (4%)	25,38,38	1.44	3 (12%)
4	IMD	A	606	-	3,5,5	0.41	0	4,5,5	0.58	0
2	AMP	B	501	-	22,25,25	0.86	0	25,38,38	1.41	5 (20%)
2	AMP	C	501	-	22,25,25	1.16	2 (9%)	25,38,38	1.50	3 (12%)
3	GOL	B	603	-	5,5,5	0.57	0	5,5,5	1.00	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	GOL	D	604	-	-	2/4/4/4	-
2	AMP	A	501	-	-	0/6/26/26	0/3/3/3
3	GOL	C	602	-	-	0/4/4/4	-
3	GOL	B	605	-	-	2/4/4/4	-
3	GOL	A	601	-	-	2/4/4/4	-
2	AMP	D	501	-	-	3/6/26/26	0/3/3/3
4	IMD	A	606	-	-	-	0/1/1/1
2	AMP	B	501	-	-	2/6/26/26	0/3/3/3
2	AMP	C	501	-	-	2/6/26/26	0/3/3/3
3	GOL	B	603	-	-	4/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	AMP	C2-N3	2.66	1.36	1.32
2	A	501	AMP	O4'-C1'	2.48	1.44	1.41
2	C	501	AMP	C5-C4	2.37	1.47	1.40
2	D	501	AMP	C5-C4	2.26	1.46	1.40
2	A	501	AMP	C2-N3	2.15	1.35	1.32
2	A	501	AMP	C2-N1	2.07	1.37	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	AMP	N3-C2-N1	-4.31	121.94	128.68
2	A	501	AMP	N3-C2-N1	-3.65	122.97	128.68
2	B	501	AMP	N3-C2-N1	-3.56	123.12	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	AMP	N3-C2-N1	-3.45	123.28	128.68
2	C	501	AMP	C4-C5-N7	-3.36	105.90	109.40
2	A	501	AMP	C1'-N9-C4	-2.87	121.60	126.64
2	A	501	AMP	N6-C6-N1	2.51	123.79	118.57
2	D	501	AMP	C4-C5-N7	-2.40	106.89	109.40
2	D	501	AMP	C2-N1-C6	2.40	122.85	118.75
2	B	501	AMP	N6-C6-N1	2.32	123.39	118.57
2	A	501	AMP	C5-C6-N6	-2.24	116.95	120.35
2	B	501	AMP	O4'-C1'-C2'	-2.23	103.66	106.93
2	B	501	AMP	C2-N1-C6	2.08	122.32	118.75
2	C	501	AMP	P-O5'-C5'	2.06	123.98	118.30
2	B	501	AMP	C1'-N9-C4	-2.03	123.08	126.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

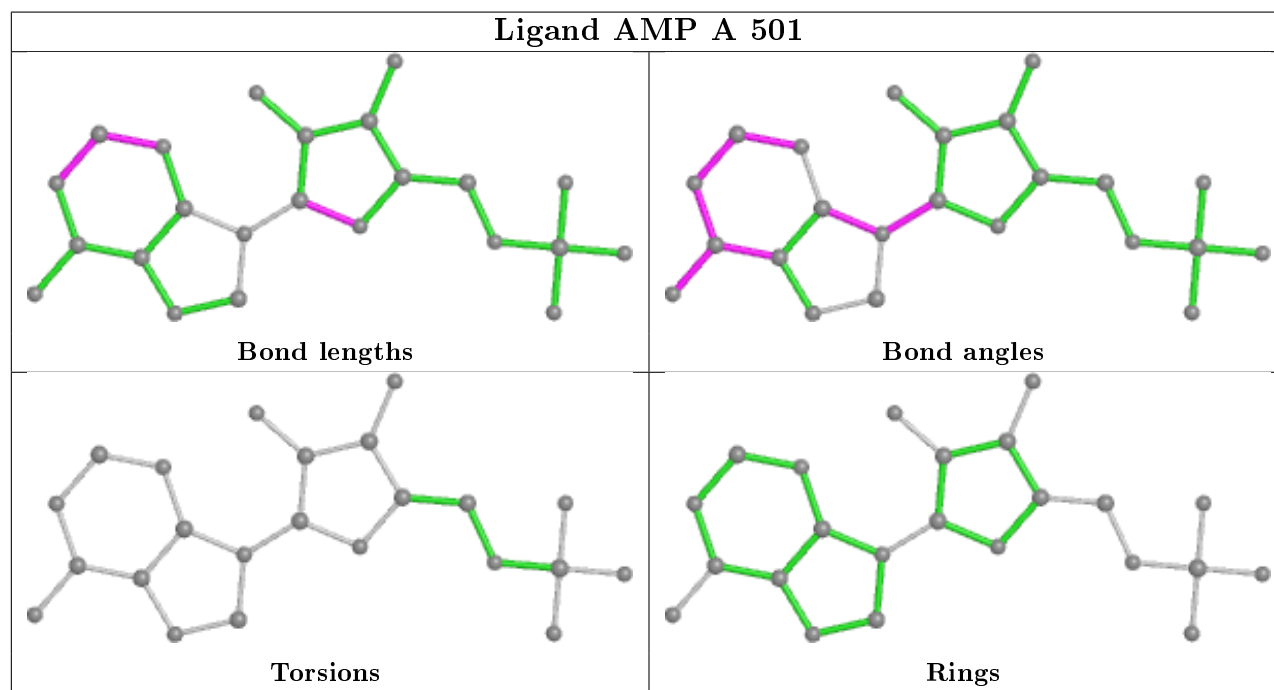
Mol	Chain	Res	Type	Atoms
3	D	604	GOL	C1-C2-C3-O3
3	D	604	GOL	O2-C2-C3-O3
3	B	605	GOL	O1-C1-C2-C3
2	D	501	AMP	C5'-O5'-P-O1P
2	D	501	AMP	C5'-O5'-P-O2P
2	D	501	AMP	C5'-O5'-P-O3P
2	C	501	AMP	C5'-O5'-P-O1P
3	B	603	GOL	O1-C1-C2-C3
3	B	603	GOL	C1-C2-C3-O3
3	A	601	GOL	C1-C2-C3-O3
3	B	605	GOL	O1-C1-C2-O2
3	B	603	GOL	O1-C1-C2-O2
2	B	501	AMP	C5'-O5'-P-O1P
3	B	603	GOL	O2-C2-C3-O3
3	A	601	GOL	O2-C2-C3-O3
2	B	501	AMP	C5'-O5'-P-O2P
2	C	501	AMP	C5'-O5'-P-O2P

There are no ring outliers.

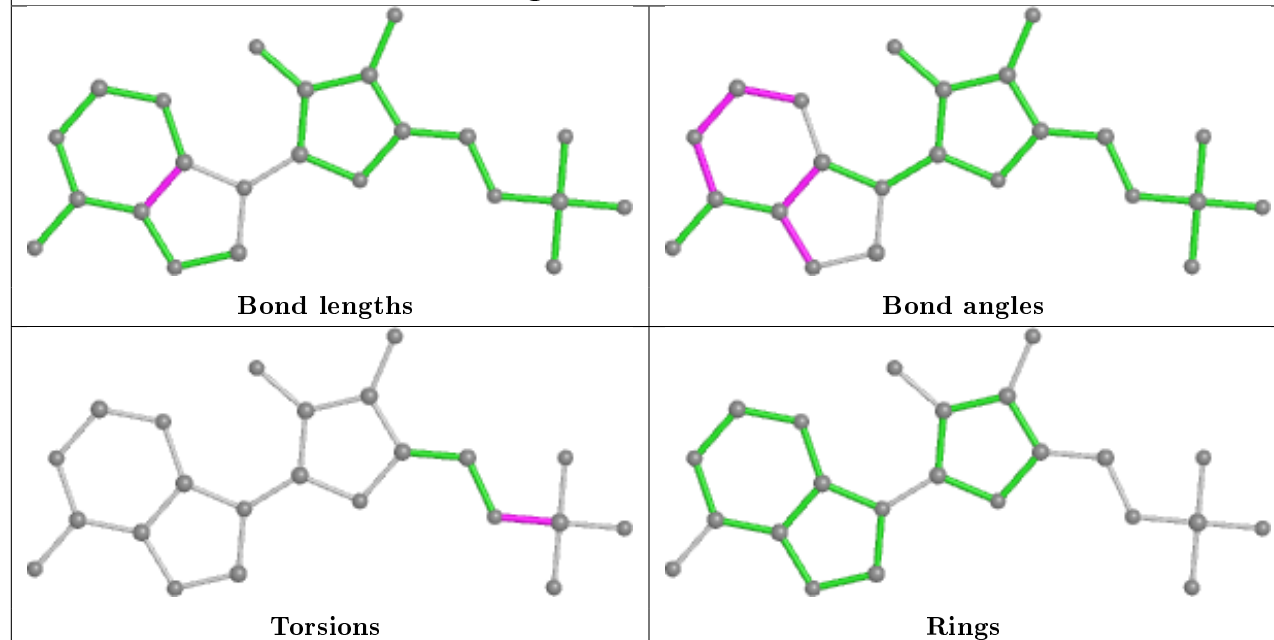
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	605	GOL	2	0
2	C	501	AMP	1	0

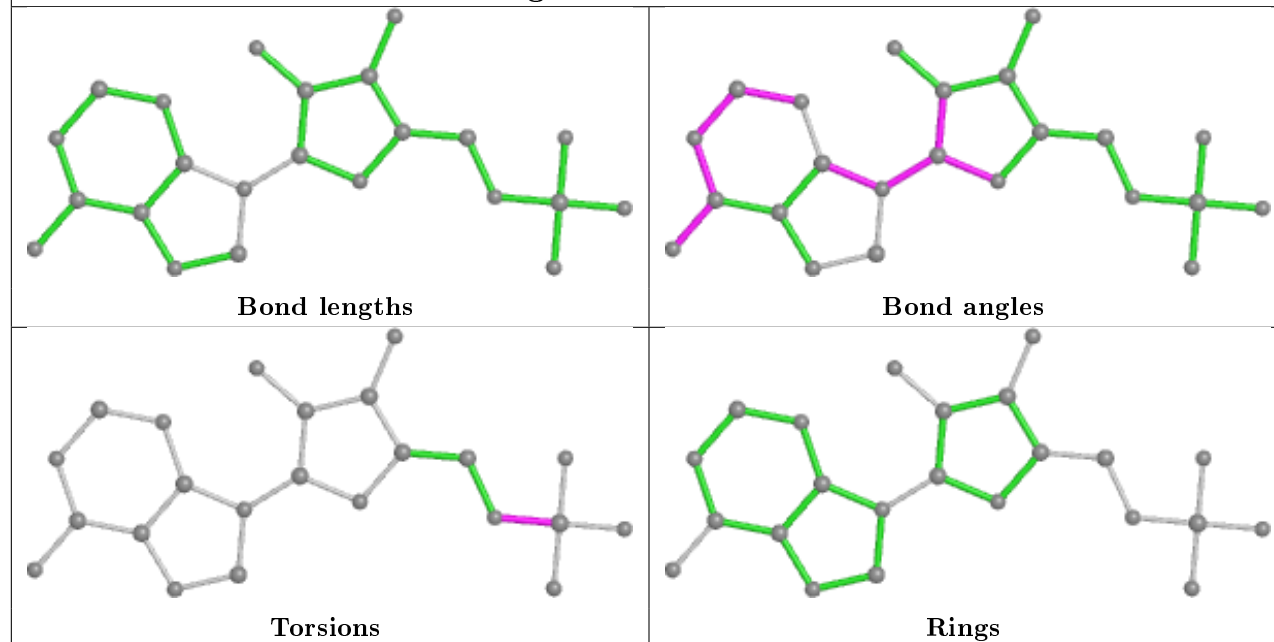
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

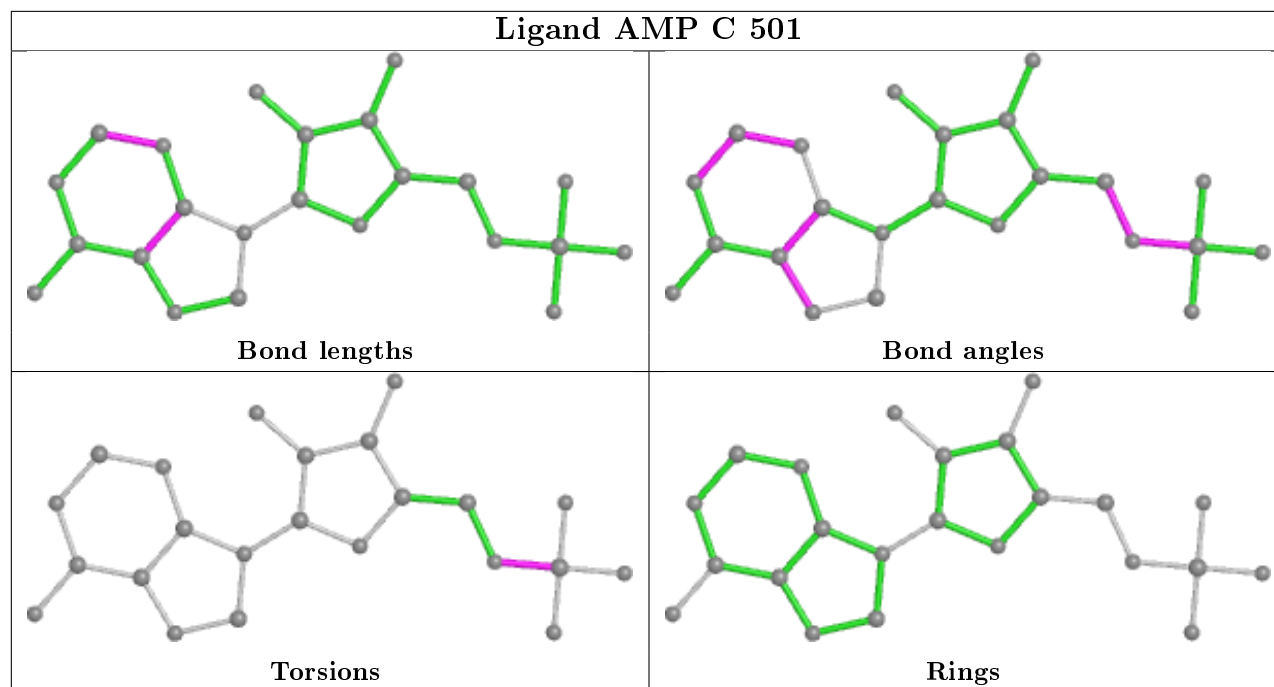


## Ligand AMP D 501



## 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, 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	285/287 (99%)	-0.28	2 (0%) 87 87	14, 23, 38, 47	0
1	B	285/287 (99%)	-0.04	8 (2%) 53 51	22, 37, 59, 71	0
1	C	284/287 (98%)	0.54	36 (12%) 3 3	13, 33, 71, 83	0
1	D	198/287 (68%)	0.53	21 (10%) 6 5	24, 47, 95, 113	0
All	All	1052/1148 (91%)	0.16	67 (6%) 19 17	13, 33, 68, 113	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	245	ILE	6.8
1	D	263	ILE	6.8
1	C	192	TYR	6.7
1	D	274	LEU	6.3
1	D	272	ALA	5.9
1	C	234	LEU	5.0
1	C	256	VAL	4.9
1	D	267	ALA	4.5
1	D	278	GLN	4.4
1	C	239	THR	4.4
1	C	271	LYS	4.4
1	C	217	LEU	4.1
1	D	243	LEU	4.1
1	D	240	PRO	4.0
1	C	269	LEU	3.8
1	C	194	THR	3.7
1	D	265	MET	3.6
1	B	236	VAL	3.6
1	D	70[A]	HIS	3.6
1	C	268	TRP	3.6
1	C	191	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	282	LEU	3.5
1	C	69	ALA	3.5
1	D	76	GLN	3.5
1	D	273	ARG	3.4
1	C	272	ALA	3.4
1	C	231	ALA	3.4
1	C	195	GLU	3.3
1	D	2	LEU	3.3
1	C	267	ALA	3.2
1	A	0	ALA	3.1
1	C	70	HIS	3.1
1	D	69	ALA	3.1
1	D	0	ALA	3.1
1	C	200	ILE	3.0
1	C	281	ASP	2.9
1	B	70	HIS	2.9
1	C	218	GLY	2.9
1	C	257	ASP	2.9
1	B	66	ASP	2.9
1	B	271	LYS	2.9
1	B	284	HIS	2.8
1	C	236	VAL	2.8
1	D	244	PHE	2.7
1	C	196	GLU	2.7
1	C	134	VAL	2.7
1	C	233	LEU	2.5
1	D	266	ALA	2.5
1	C	255	THR	2.4
1	C	259	GLN	2.4
1	C	226	LEU	2.4
1	B	195[A]	GLU	2.4
1	C	280	VAL	2.4
1	C	230	ALA	2.3
1	B	196	GLU	2.3
1	C	216	ALA	2.3
1	C	159	ILE	2.3
1	C	68[A]	LEU	2.3
1	D	75	LEU	2.3
1	C	148	PHE	2.2
1	B	235[A]	ARG	2.1
1	D	275	ILE	2.1
1	D	241	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	133	ILE	2.0
1	C	254	LEU	2.0
1	A	284[A]	HIS	2.0
1	D	242	GLU	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.

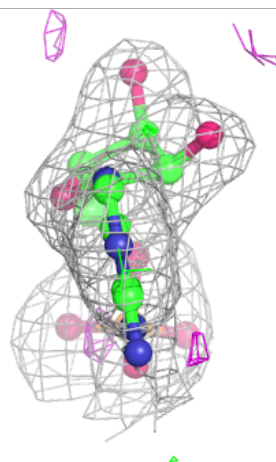
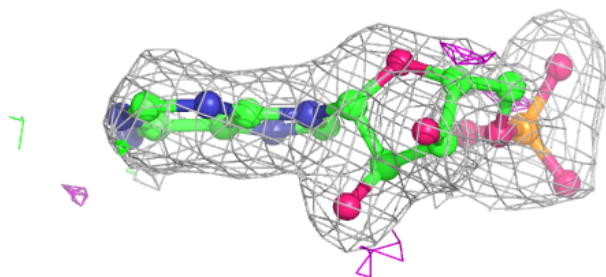
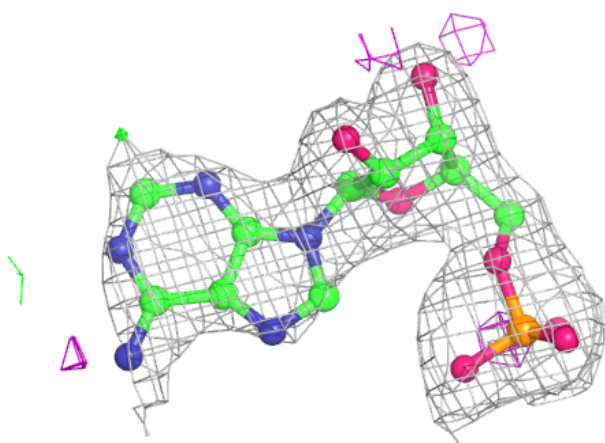
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	605	6/6	0.73	0.16	72,74,74,74	0
2	AMP	D	501	23/23	0.87	0.14	56,67,72,75	0
2	AMP	C	501	23/23	0.87	0.14	25,40,47,48	0
3	GOL	D	604	6/6	0.88	0.25	50,65,69,70	0
3	GOL	B	603	6/6	0.88	0.29	52,53,55,58	0
4	IMD	A	606	5/5	0.91	0.14	70,70,71,71	0
3	GOL	C	602	6/6	0.94	0.23	25,36,38,43	0
3	GOL	A	601	6/6	0.96	0.17	25,35,39,45	0
2	AMP	A	501	23/23	0.97	0.12	14,21,27,28	0
2	AMP	B	501	23/23	0.97	0.12	29,36,46,50	0
5	CL	A	607	1/1	0.99	0.16	32,32,32,32	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.



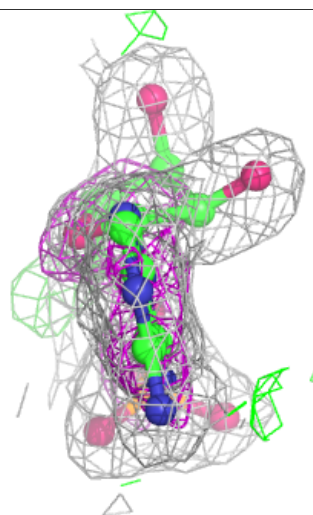
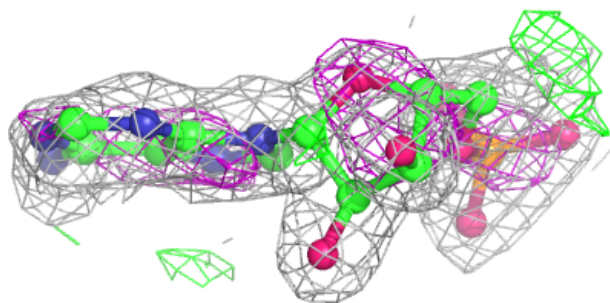
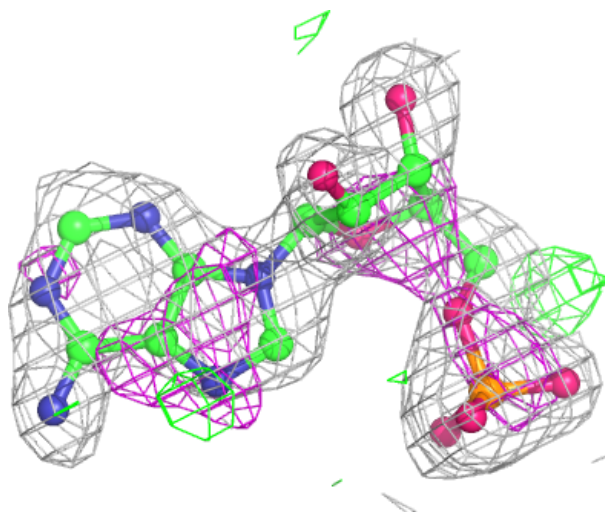
**Electron density around AMP D 501:**

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



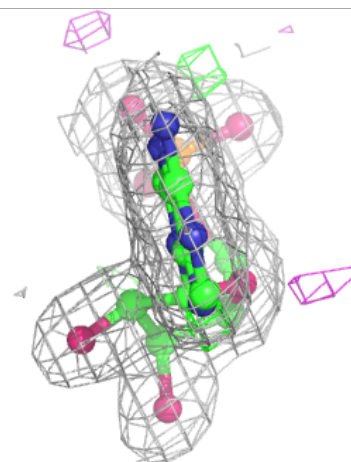
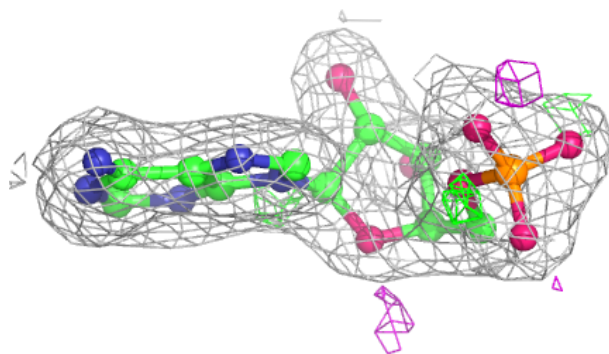
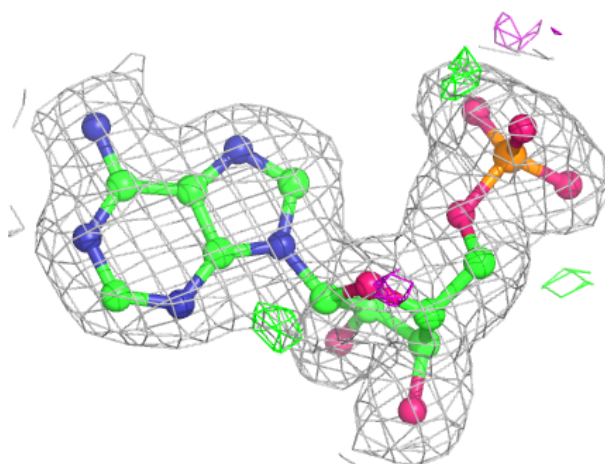
**Electron density around AMP C 501:**

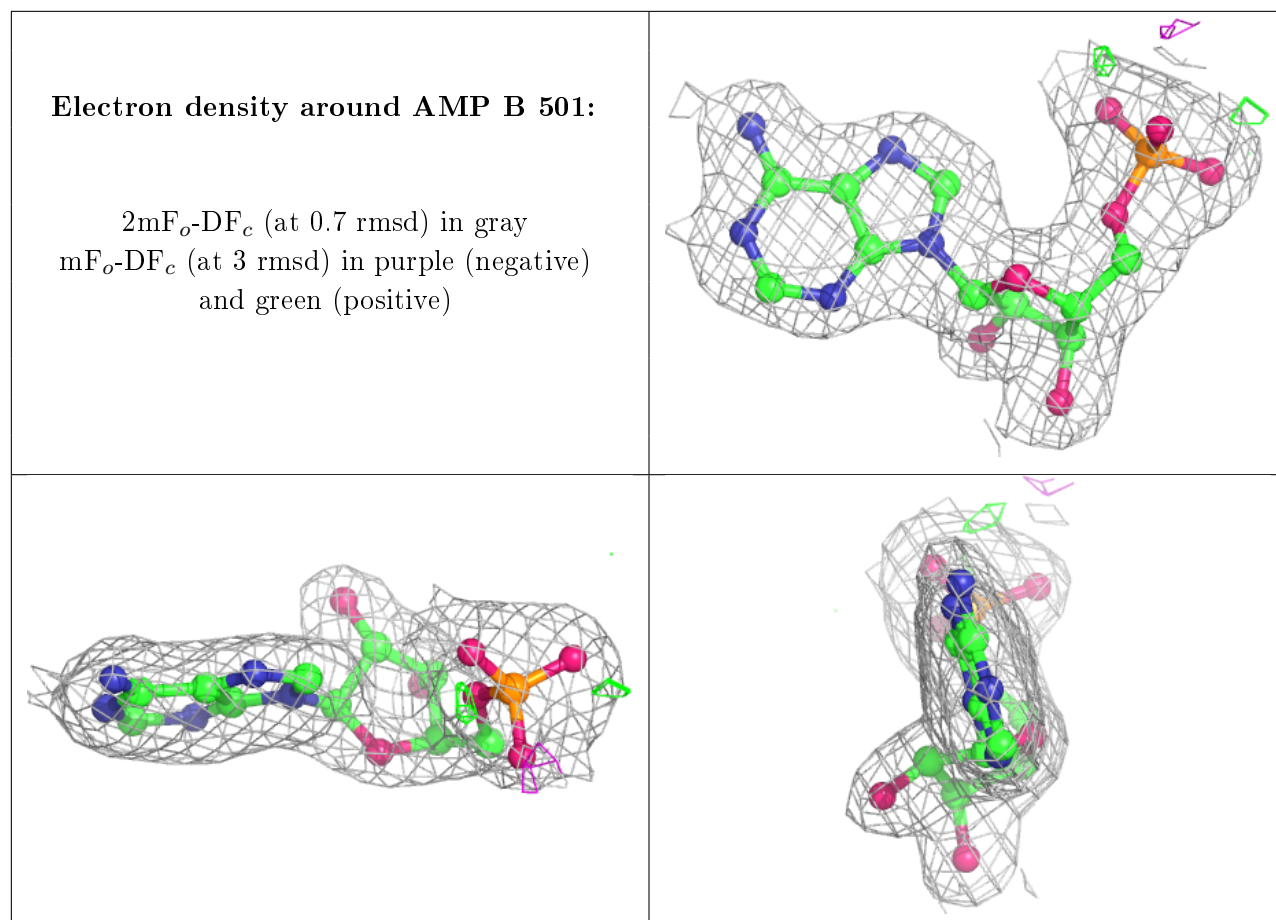
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around AMP A 501:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.