



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2021 – 04:03 PM EDT

PDB ID : 6WNN  
Title : Bacillus subtilis BioA in complex with amino donor L-Lys  
Authors : Souza, S.A.; Ng, H.L.  
Deposited on : 2020-04-22  
Resolution : 2.59 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 : 2.18  
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) : 2.18

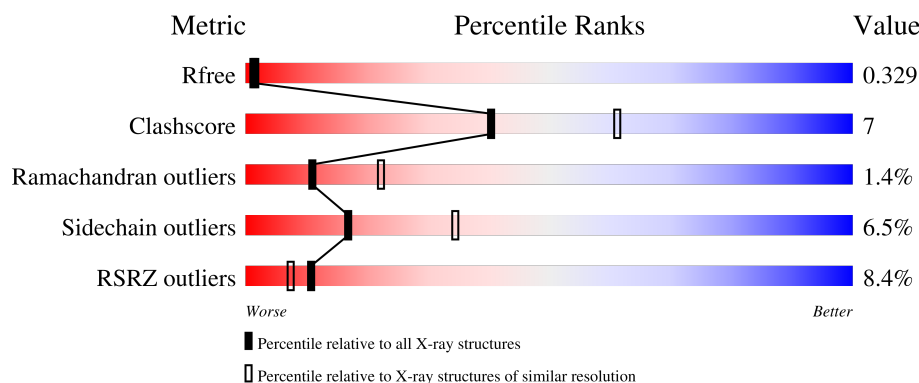
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	454	<div> <div>8%</div> <div>71%</div> <div>20%</div> <div>7%</div> </div>
1	B	454	<div> <div>8%</div> <div>73%</div> <div>17%</div> <div>8%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6618 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.

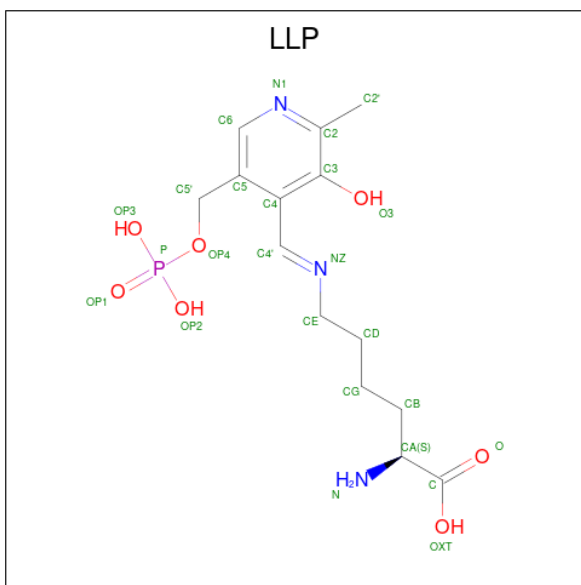
- Molecule 1 is a protein called Adenosylmethionine-8-amino-7-oxononanoate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3305	2108	548	627	22			
1	B	416	Total	C	N	O	S	0	0	0
			3272	2090	542	618	22			

There are 12 discrepancies between the modelled and reference sequences:

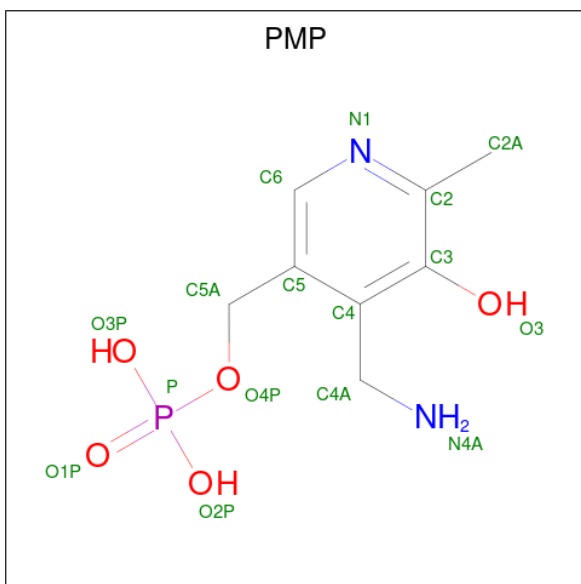
Chain	Residue	Modelled	Actual	Comment	Reference
A	449	HIS	-	expression tag	UNP A0A162RZA9
A	450	HIS	-	expression tag	UNP A0A162RZA9
A	451	HIS	-	expression tag	UNP A0A162RZA9
A	452	HIS	-	expression tag	UNP A0A162RZA9
A	453	HIS	-	expression tag	UNP A0A162RZA9
A	454	HIS	-	expression tag	UNP A0A162RZA9
B	449	HIS	-	expression tag	UNP A0A162RZA9
B	450	HIS	-	expression tag	UNP A0A162RZA9
B	451	HIS	-	expression tag	UNP A0A162RZA9
B	452	HIS	-	expression tag	UNP A0A162RZA9
B	453	HIS	-	expression tag	UNP A0A162RZA9
B	454	HIS	-	expression tag	UNP A0A162RZA9

- Molecule 2 is (2S)-2-amino-6-[[3-hydroxy-2-methyl-5-(phosphonooxymethyl)pyridin-4-yl]methylideneamino]hexanoic acid (three-letter code: LLP) (formula: C<sub>14</sub>H<sub>22</sub>N<sub>3</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	14	3	7	1		

- Molecule 3 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula:  $C_8H_{13}N_2O_5P$ ).

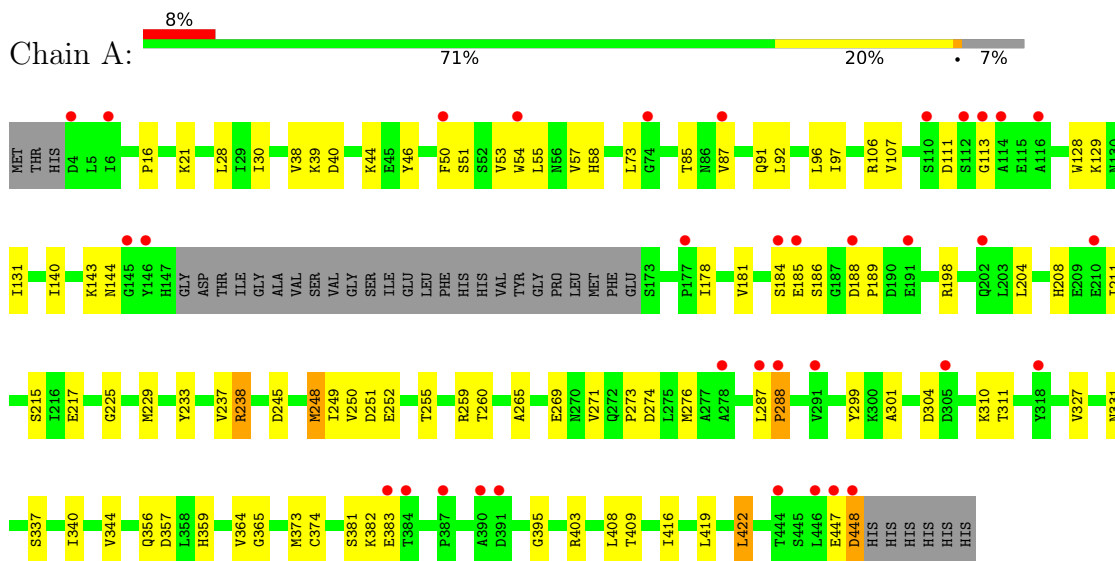


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

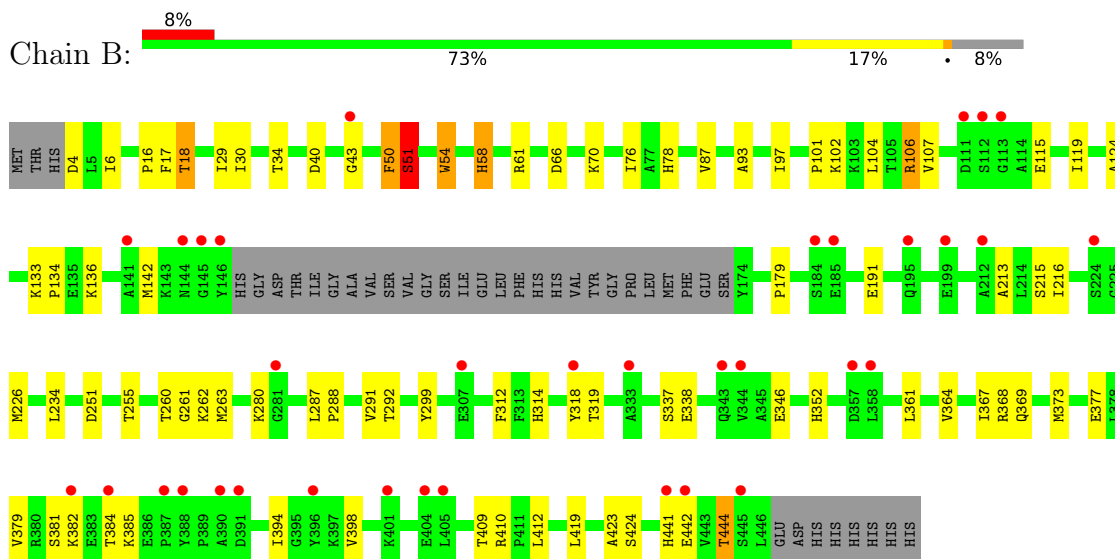
### 3 Residue-property plots [i](#)

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: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase



- Molecule 1: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.30Å 60.54Å 62.72Å 96.15° 106.04° 99.23°	Depositor
Resolution (Å)	59.51 – 2.59 38.90 – 2.59	Depositor EDS
% Data completeness (in resolution range)	91.8 (59.51-2.59) 91.8 (38.90-2.59)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.232 , 0.333 0.237 , 0.329	Depositor DCC
$R_{free}$ test set	1157 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.0	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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: LLP, PMP

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	0/3373	0.77	0/4550
1	B	0.60	0/3339	0.78	0/4504
All	All	0.60	0/6712	0.78	0/9054

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	3305	0	3291	56	0
1	B	3272	0	3269	45	0
2	A	25	0	18	3	0
3	B	16	0	10	2	0
All	All	6618	0	6588	95	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 (95) 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:381:SER:HB3	1:B:384:THR:OG1	1.65	0.95
1:A:238:ARG:HG2	1:A:248:MET:SD	2.11	0.91
1:A:238:ARG:HG3	1:A:271:VAL:HG13	1.54	0.89
1:A:364:VAL:O	1:A:382:LYS:HD2	1.72	0.88
2:A:501:LLP:H5'1	2:A:501:LLP:NZ	1.97	0.78
1:A:381:SER:OG	1:A:383:GLU:HG2	1.85	0.76
1:A:238:ARG:O	1:A:238:ARG:HD3	1.89	0.73
1:A:140:ILE:HD11	1:A:211:ILE:HD13	1.74	0.70
1:B:16:PRO:O	1:B:18:THR:HG22	1.99	0.63
1:B:381:SER:CB	1:B:384:THR:OG1	2.45	0.62
1:B:361:LEU:O	1:B:382:LYS:NZ	2.32	0.62
1:B:106:ARG:HG3	1:B:299:TYR:CD1	2.35	0.60
1:A:204:LEU:O	1:A:208:HIS:HB3	2.03	0.58
1:A:28:LEU:HD22	1:A:403:ARG:HD3	1.85	0.57
1:A:259:ARG:HG3	1:A:373:MET:HG3	1.86	0.57
1:A:340:ILE:O	1:A:344:VAL:HG23	2.03	0.57
1:B:337:SER:OG	1:B:338:GLU:N	2.37	0.56
1:B:58:HIS:HA	1:B:423:ALA:HB2	1.88	0.56
1:A:255:THR:HG22	1:A:373:MET:SD	2.46	0.55
1:A:87:VAL:HG12	1:A:91:GLN:OE1	2.06	0.55
1:A:288:PRO:HG2	1:B:288:PRO:HG2	1.89	0.55
1:A:128:TRP:CE3	1:A:131:ILE:HD11	2.42	0.54
1:A:106:ARG:HG3	1:A:299:TYR:HB2	1.89	0.54
1:A:92:LEU:HG	1:A:96:LEU:HD12	1.91	0.53
1:A:51:SER:OG	1:A:419:LEU:O	2.21	0.53
1:A:403:ARG:HG2	1:A:408:LEU:HD23	1.91	0.53
1:A:259:ARG:HG3	1:A:373:MET:CG	2.39	0.53
1:B:107:VAL:HG13	1:B:291:VAL:HG13	1.91	0.51
1:A:58:HIS:NE2	1:A:331:ASN:OD1	2.44	0.51
1:B:441:HIS:HA	1:B:444:THR:HG22	1.91	0.51
1:B:364:VAL:CG1	1:B:367:ILE:HD11	2.41	0.51
1:A:238:ARG:NH2	1:A:274:ASP:OD2	2.44	0.50
1:A:448:ASP:N	1:A:448:ASP:OD1	2.45	0.50
1:B:115:GLU:O	1:B:119:ILE:HD12	2.11	0.50
1:B:381:SER:O	1:B:385:LYS:N	2.44	0.50
1:A:233:TYR:O	1:A:237:VAL:HG23	2.11	0.50
1:B:255:THR:HG22	1:B:373:MET:SD	2.52	0.49
1:B:54:TRP:CD1	1:B:54:TRP:N	2.81	0.49
3:B:501:PMP:O3	3:B:501:PMP:N4A	2.46	0.49
1:A:40:ASP:OD1	1:A:40:ASP:C	2.52	0.48
1:A:403:ARG:HG2	1:A:408:LEU:CD2	2.43	0.48
1:A:252:GLU:HG3	1:A:276:MET:SD	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLY:N	2:A:501:LLP:OP1	2.45	0.48
1:B:381:SER:HB3	1:B:384:THR:HG1	1.77	0.48
1:B:106:ARG:HA	1:B:106:ARG:HD2	1.68	0.48
1:A:178:ILE:HD11	1:A:229:MET:HE2	1.97	0.47
1:A:181:VAL:O	1:A:184:SER:OG	2.21	0.47
1:B:101:PRO:HD2	1:B:104:LEU:HD12	1.96	0.47
1:A:186:SER:C	1:A:188:ASP:H	2.18	0.47
1:A:106:ARG:NH1	1:A:299:TYR:CE2	2.84	0.46
1:A:250:VAL:CG2	1:A:273:PRO:HB3	2.46	0.46
1:A:16:PRO:HG3	1:B:319:THR:HG21	1.98	0.46
1:A:215:SER:HA	1:A:249:ILE:HB	1.98	0.46
1:A:250:VAL:HG21	1:A:273:PRO:HB3	1.98	0.45
1:B:368:ARG:NH2	1:B:377:GLU:OE1	2.49	0.45
1:B:379:VAL:HG11	1:B:385:LYS:HA	1.98	0.45
1:A:54:TRP:N	1:A:54:TRP:CD1	2.85	0.45
1:B:261:GLY:O	1:B:262:LYS:HG2	2.17	0.44
1:B:6:ILE:HA	1:B:29:ILE:HD11	1.99	0.44
1:A:73:LEU:HD22	1:B:66:ASP:OD1	2.18	0.44
1:B:312:PHE:CE2	1:B:314:HIS:HB3	2.52	0.44
1:A:395:GLY:HA2	1:A:416:ILE:HD11	1.99	0.44
1:B:379:VAL:HG13	1:B:381:SER:H	1.82	0.44
1:A:39:LYS:HA	1:A:44:LYS:O	2.18	0.44
1:A:85:THR:CG2	1:B:29:ILE:HG12	2.48	0.44
1:A:251:ASP:OD1	2:A:501:LLP:H2'2	2.18	0.44
1:B:142:MET:HG3	1:B:216:ILE:HD12	2.00	0.44
1:B:50:PHE:O	1:B:51:SER:C	2.57	0.43
1:A:57:VAL:HG13	1:A:422:LEU:HD22	2.00	0.43
1:B:226:MET:SD	1:B:419:LEU:HD11	2.58	0.43
1:B:133:LYS:N	1:B:134:PRO:HD3	2.32	0.43
1:A:30:ILE:O	1:B:87:VAL:HG23	2.18	0.43
1:B:379:VAL:CG1	1:B:381:SER:O	2.66	0.43
1:A:44:LYS:HD3	1:A:46:TYR:CZ	2.54	0.43
1:A:87:VAL:HG23	1:B:30:ILE:O	2.19	0.42
1:B:106:ARG:O	1:B:107:VAL:HG23	2.19	0.42
1:B:251:ASP:OD2	3:B:501:PMP:C2A	2.68	0.42
1:B:394:ILE:O	1:B:398:VAL:HG23	2.20	0.42
1:B:352:HIS:HA	1:B:369:GLN:OE1	2.19	0.42
1:A:287:LEU:HD12	1:A:327:VAL:HG11	2.02	0.41
1:B:124:ALA:HB1	1:B:213:ALA:HB2	2.03	0.41
1:B:66:ASP:O	1:B:70:LYS:HG3	2.20	0.41
1:A:44:LYS:HD3	1:A:46:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:SER:HG	1:A:383:GLU:HG2	1.84	0.41
1:B:17:PHE:O	1:B:410:ARG:NH2	2.54	0.41
1:A:55:LEU:HD22	1:B:318:TYR:CZ	2.55	0.41
1:A:97:ILE:HD11	1:A:107:VAL:HG23	2.02	0.41
1:A:287:LEU:HD22	1:B:287:LEU:HD22	2.02	0.41
1:A:381:SER:OG	1:A:383:GLU:CG	2.61	0.41
1:B:78:HIS:CE1	1:B:318:TYR:HA	2.56	0.41
1:B:93:ALA:O	1:B:97:ILE:HG12	2.20	0.41
1:A:381:SER:HG	1:A:383:GLU:CD	2.24	0.41
1:A:143:LYS:HG2	1:A:144:ASN:ND2	2.35	0.40
1:A:260:THR:HG21	1:A:265:ALA:HB2	2.03	0.40
1:A:365:GLY:HA2	1:A:382:LYS:HG3	2.03	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	416/454 (92%)	372 (89%)	38 (9%)	6 (1%)	11	22
1	B	412/454 (91%)	366 (89%)	40 (10%)	6 (2%)	10	21
All	All	828/908 (91%)	738 (89%)	78 (9%)	12 (1%)	11	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	GLY
1	A	337	SER
1	B	43	GLY
1	B	51	SER
1	B	280	LYS
1	A	301	ALA

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Mol	Chain	Res	Type
1	B	424	SER
1	B	179	PRO
1	A	53	VAL
1	A	189	PRO
1	B	76	ILE
1	A	288	PRO

### 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	355/384 (92%)	332 (94%)	23 (6%)	17	34
1	B	351/384 (91%)	328 (93%)	23 (7%)	16	33
All	All	706/768 (92%)	660 (94%)	46 (6%)	17	34

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	38	VAL
1	A	50	PHE
1	A	111	ASP
1	A	129	LYS
1	A	185	GLU
1	A	198	ARG
1	A	217	GLU
1	A	238	ARG
1	A	245	ASP
1	A	248	MET
1	A	269	GLU
1	A	304	ASP
1	A	310	LYS
1	A	311	THR
1	A	356	GLN
1	A	357	ASP

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Mol	Chain	Res	Type
1	A	359	HIS
1	A	374	CYS
1	A	409	THR
1	A	422	LEU
1	A	447	GLU
1	A	448	ASP
1	B	4	ASP
1	B	18	THR
1	B	34	THR
1	B	40	ASP
1	B	50	PHE
1	B	51	SER
1	B	54	TRP
1	B	58	HIS
1	B	61	ARG
1	B	102	LYS
1	B	106	ARG
1	B	136	LYS
1	B	191	GLU
1	B	215	SER
1	B	234	LEU
1	B	260	THR
1	B	263	MET
1	B	292	THR
1	B	346	GLU
1	B	409	THR
1	B	412	LEU
1	B	442	GLU
1	B	444	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	137	GLN
1	B	207	HIS
1	B	321	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	PMP	B	501	-	16,16,16	3.14	4 (25%)	21,23,23	1.78	6 (28%)
2	LLP	A	501	-	21,25,25	2.43	3 (14%)	26,34,34	1.32	3 (11%)

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	PMP	B	501	-	-	2/8/8/8	0/1/1/1
2	LLP	A	501	-	-	3/15/19/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	PMP	C3-C2	8.12	1.49	1.40
2	A	501	LLP	C3-C2	8.03	1.48	1.40
3	B	501	PMP	C5-C4	6.82	1.50	1.40
3	B	501	PMP	C3-C4	5.77	1.48	1.40
2	A	501	LLP	C4-C5	5.35	1.48	1.42
2	A	501	LLP	C4-C3	5.06	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	PMP	C2-N1	2.04	1.37	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	LLP	C4-C3-C2	-4.35	117.50	120.19
3	B	501	PMP	C2A-C2-C3	-3.68	116.34	120.89
3	B	501	PMP	C2A-C2-N1	2.87	123.27	117.67
3	B	501	PMP	O3P-P-O4P	-2.76	99.40	106.73
3	B	501	PMP	O4P-C5A-C5	2.45	114.02	109.35
2	A	501	LLP	CD-CE-NZ	-2.42	105.00	110.93
2	A	501	LLP	C6-N1-C2	2.29	123.42	119.17
3	B	501	PMP	C6-C5-C4	2.16	119.65	118.12
3	B	501	PMP	C6-N1-C2	2.10	123.06	119.17

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LLP	CG-CD-CE-NZ
3	B	501	PMP	C5-C4-C4A-N4A
3	B	501	PMP	C3-C4-C4A-N4A
2	A	501	LLP	CA-CB-CG-CD
2	A	501	LLP	CD-CE-NZ-C4'

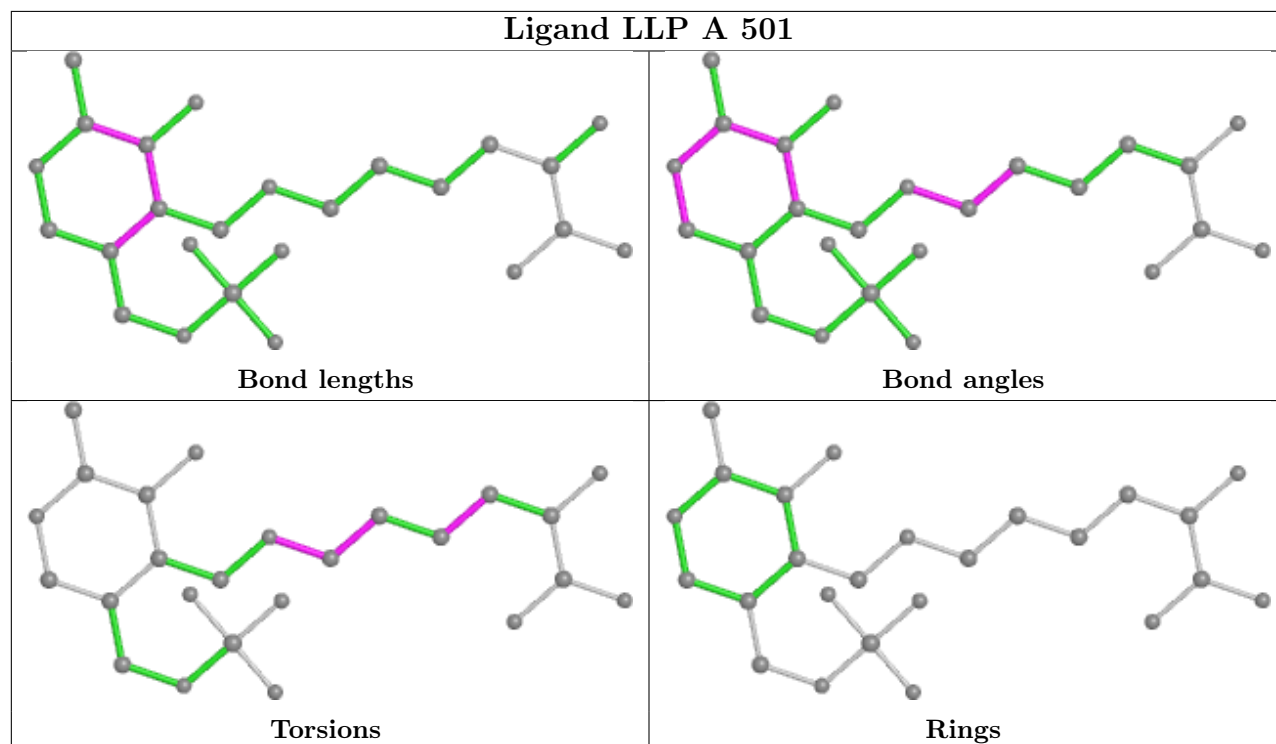
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	PMP	2	0
2	A	501	LLP	3	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	420/454 (92%)	0.67	35 (8%)	11 8	18, 42, 68, 93	0
1	B	416/454 (91%)	0.72	35 (8%)	11 7	18, 47, 72, 90	0
All	All	836/908 (92%)	0.70	70 (8%)	11 7	18, 45, 71, 93	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	SER	6.0
1	B	391	ASP	5.6
1	A	185	GLU	5.4
1	B	384	THR	5.1
1	B	185	GLU	4.3
1	B	144	ASN	4.1
1	A	145	GLY	3.9
1	A	446	LEU	3.8
1	B	333	ALA	3.7
1	A	74	GLY	3.6
1	A	202	GLN	3.5
1	B	445	SER	3.4
1	B	441	HIS	3.4
1	A	191	GLU	3.3
1	B	390	ALA	3.2
1	B	195	GLN	3.2
1	A	112	SER	3.2
1	A	177	PRO	3.2
1	A	110	SER	3.1
1	B	401	LYS	3.0
1	A	383	GLU	3.0
1	A	448	ASP	3.0
1	B	184	SER	2.9
1	A	113	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	358	LEU	2.9
1	B	224	SER	2.9
1	B	442	GLU	2.7
1	A	4	ASP	2.7
1	B	357	ASP	2.7
1	A	287	LEU	2.6
1	B	388	TYR	2.6
1	B	318	TYR	2.6
1	B	404	GLU	2.6
1	B	387	PRO	2.6
1	A	447	GLU	2.6
1	A	384	THR	2.6
1	B	145	GLY	2.6
1	A	146	TYR	2.6
1	B	112	SER	2.5
1	A	391	ASP	2.4
1	B	146	TYR	2.4
1	A	390	ALA	2.4
1	A	444	THR	2.4
1	B	343	GLN	2.3
1	A	87	VAL	2.3
1	A	50	PHE	2.2
1	B	43	GLY	2.2
1	A	318	TYR	2.2
1	B	113	GLY	2.2
1	A	116	ALA	2.2
1	B	212	ALA	2.2
1	B	396	TYR	2.2
1	B	199	GLU	2.2
1	A	114	ALA	2.1
1	B	405	LEU	2.1
1	B	344	VAL	2.1
1	A	288	PRO	2.1
1	B	111	ASP	2.1
1	A	188	ASP	2.1
1	B	141	ALA	2.1
1	A	210	GLU	2.1
1	A	291	VAL	2.1
1	B	307	GLU	2.1
1	A	305	ASP	2.1
1	A	387	PRO	2.0
1	A	54	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	278	ALA	2.0
1	B	382	LYS	2.0
1	B	281	GLY	2.0
1	A	6	ILE	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

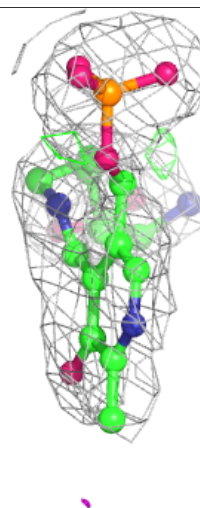
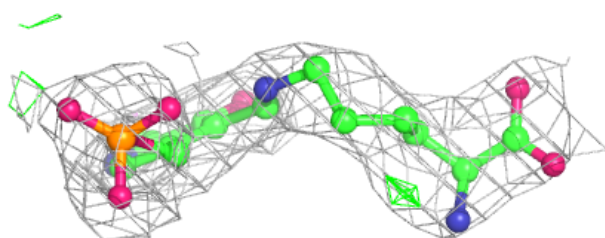
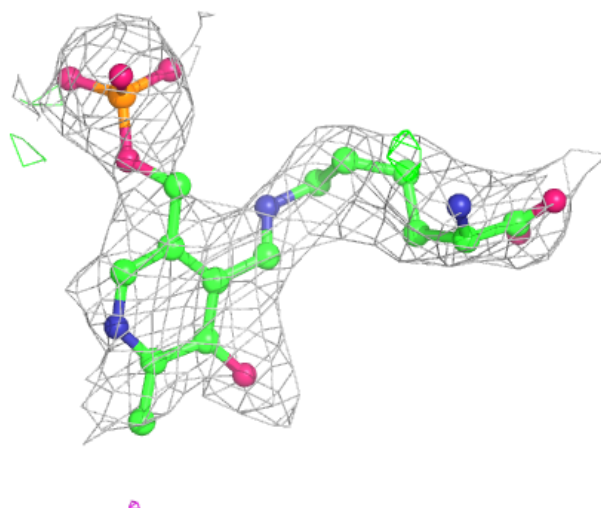
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LLP	A	501	25/25	0.89	0.28	56,64,66,68	0
3	PMP	B	501	16/16	0.94	0.24	46,67,74,77	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 LLP 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.