



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2021 – 07:33 PM JST

PDB ID : 5ZXM  
Title : Crystal Structure of GyraseB N-terminal at 1.93Å Resolution  
Authors : Tiwari, P.; Gupta, D.; Sachdeva, E.; Sharma, S.; Singh, T.P.; Ethayathulla, A.S.; Kaur, P.  
Deposited on : 2018-05-21  
Resolution : 1.94 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

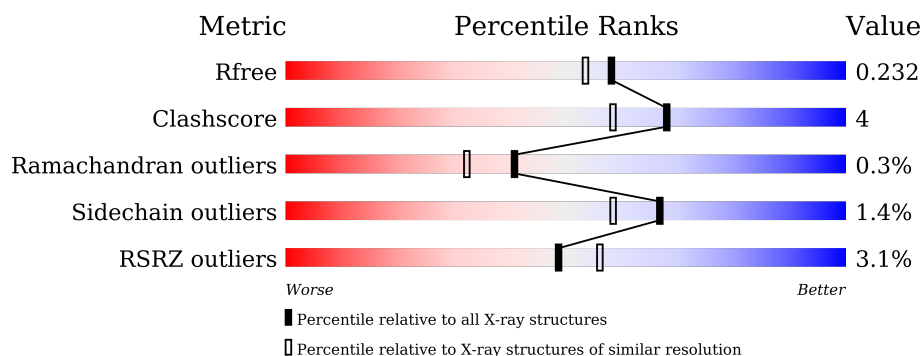
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	400	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div></div> </div> </div>
1	B	400	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div></div> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6710 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.

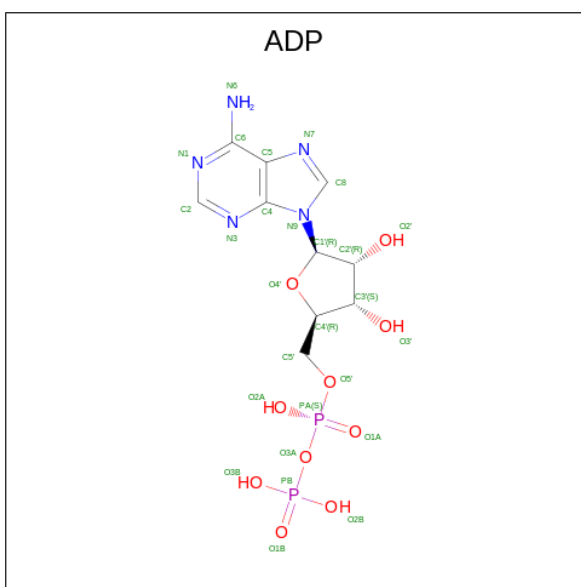
- Molecule 1 is a protein called DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	1	0
			3019	1887	535	587	10			
1	B	390	Total	C	N	O	S	0	3	0
			3033	1895	539	589	10			

There are 20 discrepancies between the modelled and reference sequences:

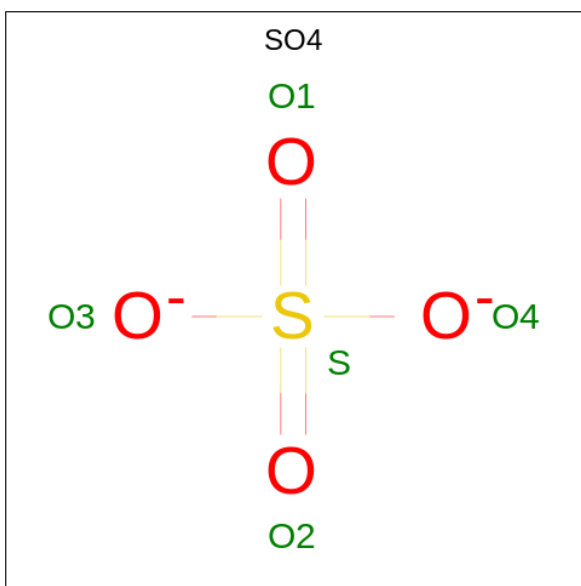
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ALA	VAL	engineered mutation	UNP A0A3R0U328
A	85	SER	GLU	engineered mutation	UNP A0A3R0U328
A	173	LYS	HIS	engineered mutation	UNP A0A3R0U328
A	174	SER	GLU	engineered mutation	UNP A0A3R0U328
A	395	HIS	-	expression tag	UNP A0A3R0U328
A	396	HIS	-	expression tag	UNP A0A3R0U328
A	397	HIS	-	expression tag	UNP A0A3R0U328
A	398	HIS	-	expression tag	UNP A0A3R0U328
A	399	HIS	-	expression tag	UNP A0A3R0U328
A	400	HIS	-	expression tag	UNP A0A3R0U328
B	40	ALA	VAL	engineered mutation	UNP A0A3R0U328
B	85	SER	GLU	engineered mutation	UNP A0A3R0U328
B	173	LYS	HIS	engineered mutation	UNP A0A3R0U328
B	174	SER	GLU	engineered mutation	UNP A0A3R0U328
B	395	HIS	-	expression tag	UNP A0A3R0U328
B	396	HIS	-	expression tag	UNP A0A3R0U328
B	397	HIS	-	expression tag	UNP A0A3R0U328
B	398	HIS	-	expression tag	UNP A0A3R0U328
B	399	HIS	-	expression tag	UNP A0A3R0U328
B	400	HIS	-	expression tag	UNP A0A3R0U328

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



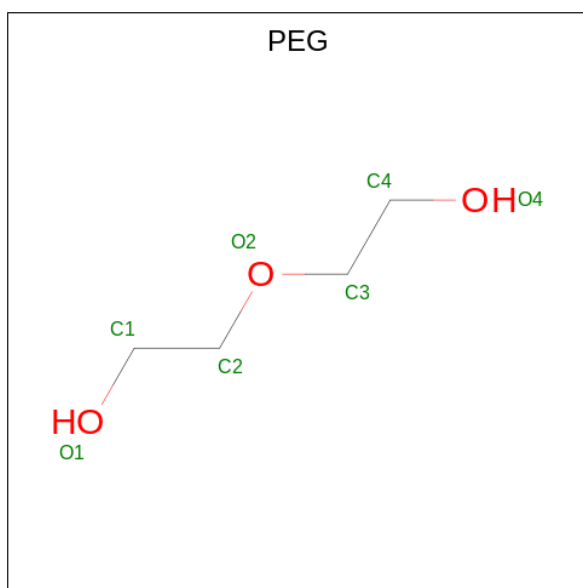
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

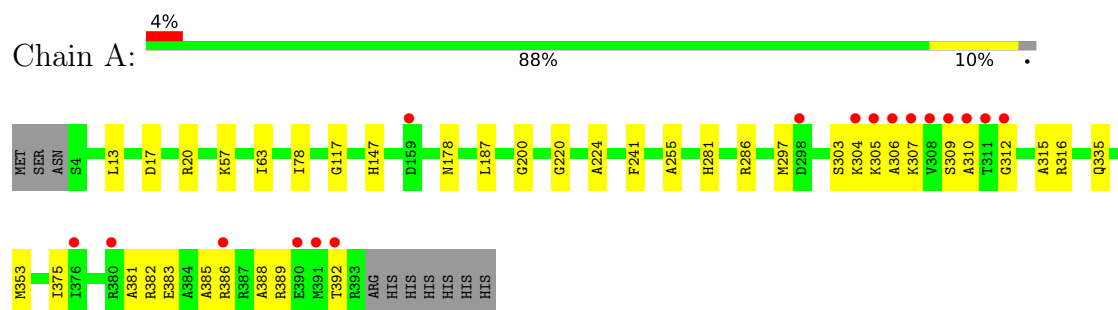
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	267	Total	O	0	0
			267	267		
7	B	293	Total	O	0	0
			293	293		

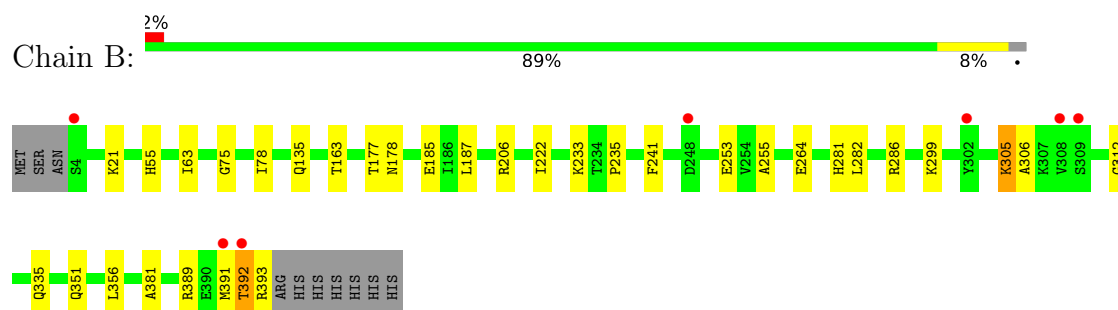
### 3 Residue-property plots [i](#)

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: DNA gyrase subunit B



#### • Molecule 1: DNA gyrase subunit B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.42Å 86.53Å 135.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.00 – 1.94 73.00 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.3 (73.00-1.94) 99.3 (73.00-1.94)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, $R_{free}$	0.181 , 0.226 0.194 , 0.232	Depositor DCC
$R_{free}$ test set	1458 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.5	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	6710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3190e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: SO4, MG, ADP, GOL, PEG

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	0.63	0/3076	0.69	0/4152
1	B	0.66	0/3093	0.68	0/4174
All	All	0.65	0/6169	0.68	0/8326

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	206[A]	ARG	Mainchain
1	B	206[B]	ARG	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	3019	0	2988	25	0
1	B	3033	0	3005	24	0
2	A	27	0	12	4	0
2	B	27	0	12	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	14	0	20	4	0
4	B	7	0	10	1	0
5	A	1	0	0	0	0
6	B	12	0	16	4	0
7	A	267	0	0	1	0
7	B	293	0	0	2	0
All	All	6710	0	6063	46	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 4.

All (46) 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:389:ARG:O	1:B:392:THR:HG22	1.79	0.81
1:B:312:GLY:H	6:B:505:GOL:H2	1.50	0.77
1:A:17:ASP:HB3	4:A:503:PEG:H31	1.72	0.70
1:A:303:SER:O	1:A:307:LYS:HG2	1.99	0.62
1:A:385:ALA:HB2	1:B:389:ARG:HG3	1.87	0.56
1:B:312:GLY:N	6:B:505:GOL:H2	2.19	0.55
1:A:13:LEU:HD22	4:A:503:PEG:H42	1.90	0.54
7:A:783:HOH:O	1:B:178:ASN:HB2	2.07	0.54
1:A:63:ILE:HD11	1:A:187:LEU:HD12	1.90	0.53
1:A:381:ALA:HA	1:B:392:THR:HG21	1.89	0.53
1:A:383:GLU:HG3	1:A:386:ARG:HH11	1.73	0.53
1:A:382:ARG:HH21	1:A:382:ARG:HG2	1.74	0.52
1:A:388:ALA:O	1:A:392:THR:HG23	2.09	0.52
1:B:389:ARG:NE	7:B:609:HOH:O	2.41	0.51
1:A:117:GLY:HA2	2:A:501:ADP:O3A	2.12	0.50
1:A:315:ALA:HA	1:A:375:ILE:HG12	1.94	0.49
1:A:20:ARG:NE	4:A:504:PEG:H22	2.28	0.49
1:B:305:LYS:NZ	1:B:306:ALA:HB2	2.29	0.48
1:B:177:THR:O	1:B:178:ASN:HB3	2.13	0.48
1:A:220:GLY:HA3	1:A:224:ALA:HB2	1.96	0.48
1:B:235:PRO:O	4:B:503:PEG:H42	2.14	0.48
1:A:117:GLY:N	2:A:501:ADP:O3B	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:MET:O	1:B:393:ARG:N	2.47	0.47
1:B:282:LEU:HD21	1:B:286:ARG:NH2	2.31	0.46
1:A:147:HIS:O	4:A:504:PEG:H42	2.16	0.46
1:A:286:ARG:HD3	1:A:316:ARG:CZ	2.46	0.45
1:B:21:LYS:HB2	6:B:504:GOL:H2	1.98	0.45
1:B:222:ILE:HD11	1:B:253:GLU:HG2	1.99	0.45
1:A:306:ALA:O	1:A:309:SER:HB2	2.17	0.45
1:A:312:GLY:O	1:A:316:ARG:HG3	2.18	0.44
1:B:63:ILE:HD11	1:B:187:LEU:HD12	1.99	0.44
1:B:78:ILE:HG12	2:B:501:ADP:C4	2.52	0.43
1:A:117:GLY:HA2	2:A:501:ADP:PB	2.58	0.43
1:A:304:LYS:HG3	1:A:305:LYS:N	2.33	0.43
1:B:241:PHE:O	1:B:255:ALA:HA	2.19	0.43
1:B:233:LYS:HB3	7:B:617:HOH:O	2.19	0.42
1:B:356:LEU:HD23	1:B:356:LEU:HA	1.91	0.41
1:A:78:ILE:HG12	2:A:501:ADP:C4	2.55	0.41
1:A:241:PHE:O	1:A:255:ALA:HA	2.20	0.41
1:B:135:GLN:O	1:B:163:THR:HA	2.20	0.41
1:B:264:GLU:OE1	1:B:286:ARG:NH1	2.52	0.41
1:A:297:MET:HE1	1:A:310:ALA:HB3	2.01	0.41
1:B:312:GLY:HA3	6:B:505:GOL:H2	2.03	0.41
1:A:57:LYS:HD2	1:A:200:GLY:O	2.20	0.41
1:A:389:ARG:HG2	1:B:381:ALA:HB1	2.03	0.40
1:B:55:HIS:O	1:B:75:GLY:HA2	2.21	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	389/400 (97%)	383 (98%)	5 (1%)	1 (0%)	41 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	391/400 (98%)	381 (97%)	9 (2%)	1 (0%)	41	32
All	All	780/800 (98%)	764 (98%)	14 (2%)	2 (0%)	41	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	392	THR
1	A	178	ASN

### 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	326/335 (97%)	323 (99%)	3 (1%)	78	75
1	B	328/335 (98%)	322 (98%)	6 (2%)	59	47
All	All	654/670 (98%)	645 (99%)	9 (1%)	67	58

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	HIS
1	A	335	GLN
1	A	353	MET
1	B	185	GLU
1	B	281	HIS
1	B	299	LYS
1	B	305	LYS
1	B	335	GLN
1	B	351	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	SO4	B	502	-	4,4,4	0.16	0	6,6,6	0.10	0
3	SO4	A	502	-	4,4,4	0.62	0	6,6,6	0.74	0
2	ADP	A	501	5	24,29,29	0.97	2 (8%)	29,45,45	1.48	5 (17%)
4	PEG	A	503	-	6,6,6	0.54	0	5,5,5	0.87	0
6	GOL	B	504	-	5,5,5	0.72	0	5,5,5	0.91	0
6	GOL	B	505	-	5,5,5	0.47	0	5,5,5	0.74	0
4	PEG	A	504	-	6,6,6	0.58	0	5,5,5	0.52	0
2	ADP	B	501	-	24,29,29	1.90	6 (25%)	29,45,45	1.21	3 (10%)
4	PEG	B	503	-	6,6,6	0.29	0	5,5,5	0.60	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	ADP	A	501	5	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	503	-	-	3/4/4/4	-
6	GOL	B	504	-	-	4/4/4/4	-
6	GOL	B	505	-	-	0/4/4/4	-
4	PEG	A	504	-	-	1/4/4/4	-
2	ADP	B	501	-	-	1/12/32/32	0/3/3/3
4	PEG	B	503	-	-	1/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ADP	PB-O3B	-3.83	1.40	1.54
2	B	501	ADP	PB-O2B	-3.52	1.41	1.54
2	B	501	ADP	PA-O2A	-2.96	1.41	1.55
2	B	501	ADP	PB-O1B	-2.89	1.41	1.50
2	B	501	ADP	O4'-C4'	-2.79	1.38	1.45
2	A	501	ADP	C5-C4	2.66	1.48	1.40
2	B	501	ADP	C5-N7	-2.31	1.31	1.39
2	A	501	ADP	C2-N3	2.31	1.35	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ADP	O2'-C2'-C3'	-3.97	98.97	111.82
2	B	501	ADP	C4-C5-N7	-2.90	106.38	109.40
2	A	501	ADP	N3-C2-N1	-2.78	124.34	128.68
2	A	501	ADP	O2A-PA-O1A	2.58	124.99	112.24
2	B	501	ADP	N3-C2-N1	-2.56	124.68	128.68
2	B	501	ADP	C2-N1-C6	2.21	122.54	118.75
2	A	501	ADP	N6-C6-N1	2.06	122.86	118.57
2	A	501	ADP	C4-C5-N7	-2.05	107.26	109.40

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ADP	PA-O3A-PB-O2B
2	A	501	ADP	PA-O3A-PB-O3B
6	B	504	GOL	O1-C1-C2-O2
6	B	504	GOL	O1-C1-C2-C3
6	B	504	GOL	O2-C2-C3-O3
4	A	503	PEG	O2-C3-C4-O4

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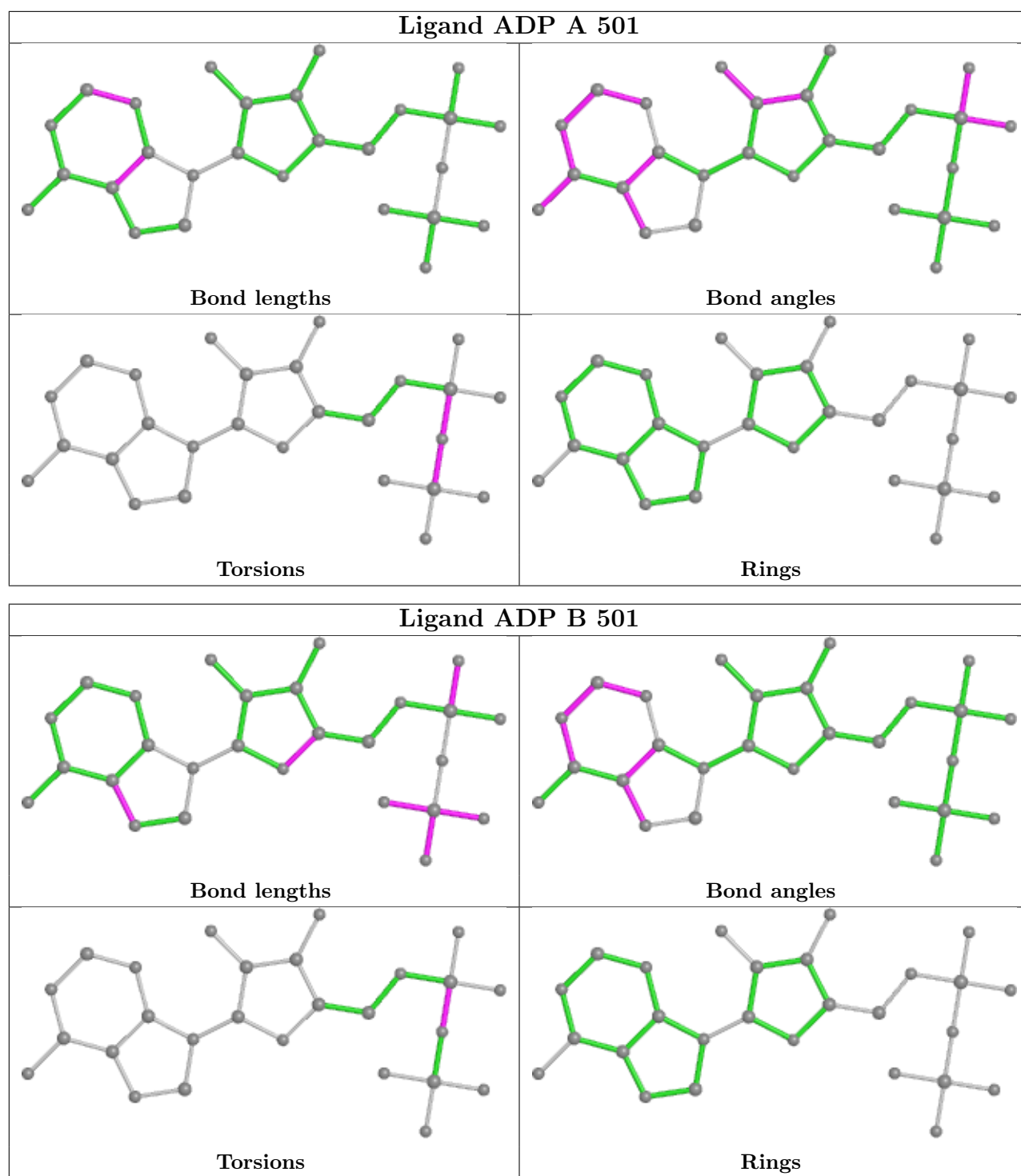
Mol	Chain	Res	Type	Atoms
6	B	504	GOL	C1-C2-C3-O3
4	A	503	PEG	O1-C1-C2-O2
2	A	501	ADP	PB-O3A-PA-O5'
2	B	501	ADP	PB-O3A-PA-O5'
4	A	504	PEG	O1-C1-C2-O2
4	A	503	PEG	C4-C3-O2-C2
4	B	503	PEG	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ADP	4	0
4	A	503	PEG	2	0
6	B	504	GOL	1	0
6	B	505	GOL	3	0
4	A	504	PEG	2	0
2	B	501	ADP	1	0
4	B	503	PEG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	390/400 (97%)	0.42	17 (4%) 34 41	19, 29, 67, 97	0
1	B	390/400 (97%)	0.32	7 (1%) 68 74	19, 29, 60, 87	0
All	All	780/800 (97%)	0.37	24 (3%) 49 56	19, 29, 63, 97	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	VAL	8.2
1	A	306	ALA	6.9
1	A	307	LYS	5.4
1	A	305	LYS	3.8
1	A	298	ASP	3.8
1	A	309	SER	3.4
1	A	311	THR	3.4
1	A	304	LYS	3.3
1	A	376	ILE	3.2
1	B	391	MET	3.1
1	A	391	MET	3.0
1	A	380	ARG	2.9
1	A	392	THR	2.9
1	B	309	SER	2.8
1	B	308	VAL	2.8
1	A	390	GLU	2.7
1	A	312	GLY	2.7
1	B	4	SER	2.6
1	B	302	TYR	2.5
1	A	159	ASP	2.3
1	A	386	ARG	2.3
1	B	248	ASP	2.3
1	B	392	THR	2.2
1	A	310	ALA	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

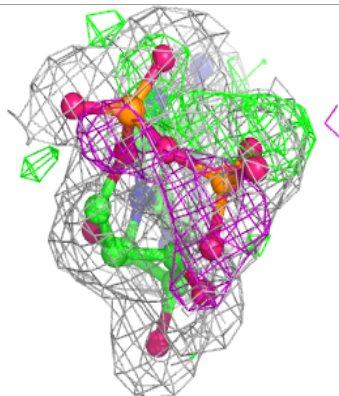
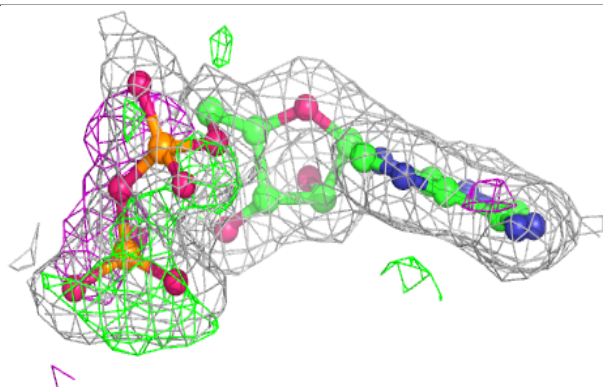
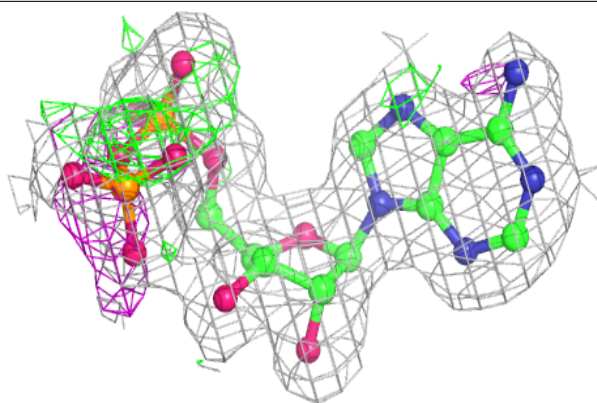
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
6	GOL	B	505	6/6	0.61	0.22	51,62,64,64	0
4	PEG	A	504	7/7	0.76	0.29	26,30,41,47	7
5	MG	A	505	1/1	0.80	0.28	36,36,36,36	1
3	SO4	A	502	5/5	0.81	0.21	23,39,45,48	5
4	PEG	B	503	7/7	0.81	0.14	35,43,47,57	0
6	GOL	B	504	6/6	0.88	0.19	28,37,42,46	0
4	PEG	A	503	7/7	0.89	0.24	22,43,50,54	0
2	ADP	A	501	27/27	0.92	0.15	16,19,21,23	0
3	SO4	B	502	5/5	0.95	0.18	50,56,61,63	0
2	ADP	B	501	27/27	0.98	0.10	18,19,22,22	0

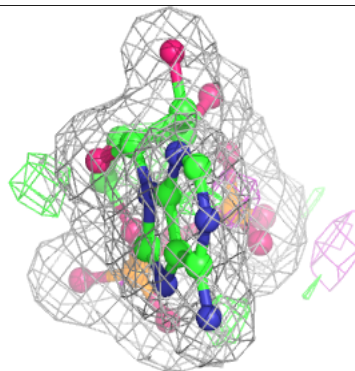
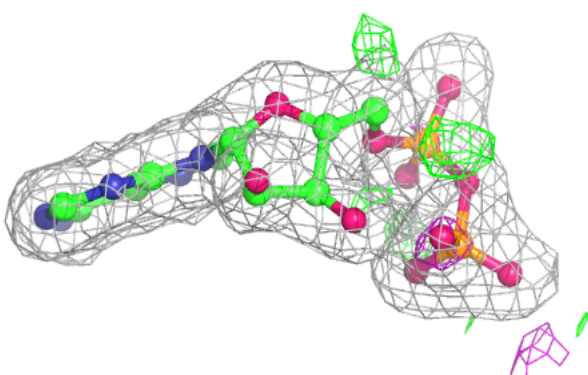
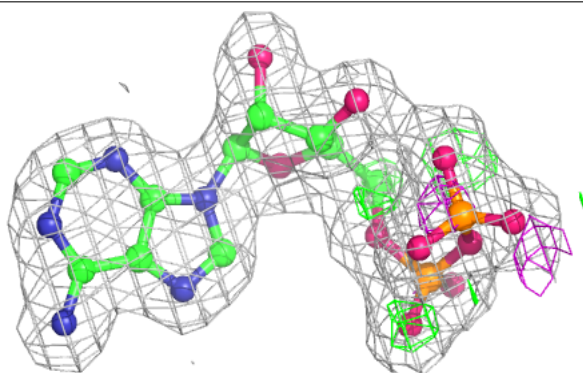
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around ADP 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)

**Electron density around ADP 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.