



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 1, 2025 – 04:07 PM EDT

PDB ID : 9DR7 / pdb\_00009dr7  
Title : Product complex of DNA polymerase iota with 2 monophosphates  
Authors : Frevert, Z.; Reusch, D.; Freudenthal, B.; Washington, M.T.  
Deposited on : 2024-09-25  
Resolution : 2.45 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.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

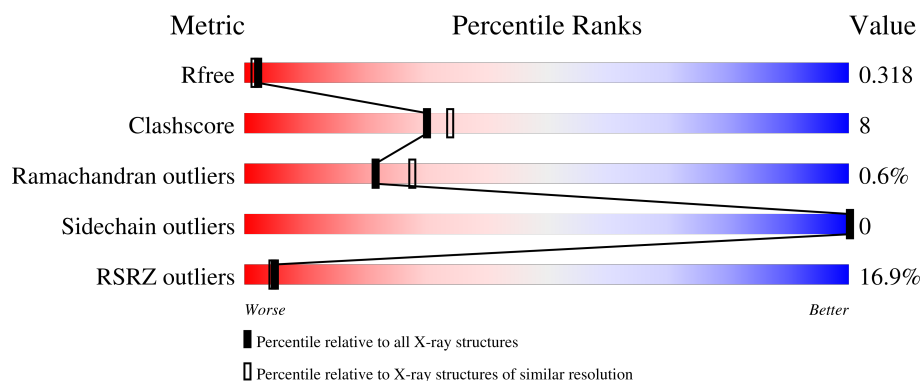
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)

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	420	<div> <div>15%</div> <div>74%</div> <div>13%</div> <div>13%</div> </div>
2	B	19	<div> <div>5%</div> <div>42%</div> <div>47%</div> <div>11%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6406 atoms, of which 3069 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 polymerase iota.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	367	5872	1825	2980	504	542	21	2	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(P\*AP\*AP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*AP\*GP\*GP\*AP\*CP\*CP\*CP\*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	B	17	438	165	89	66	101	17	0	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		

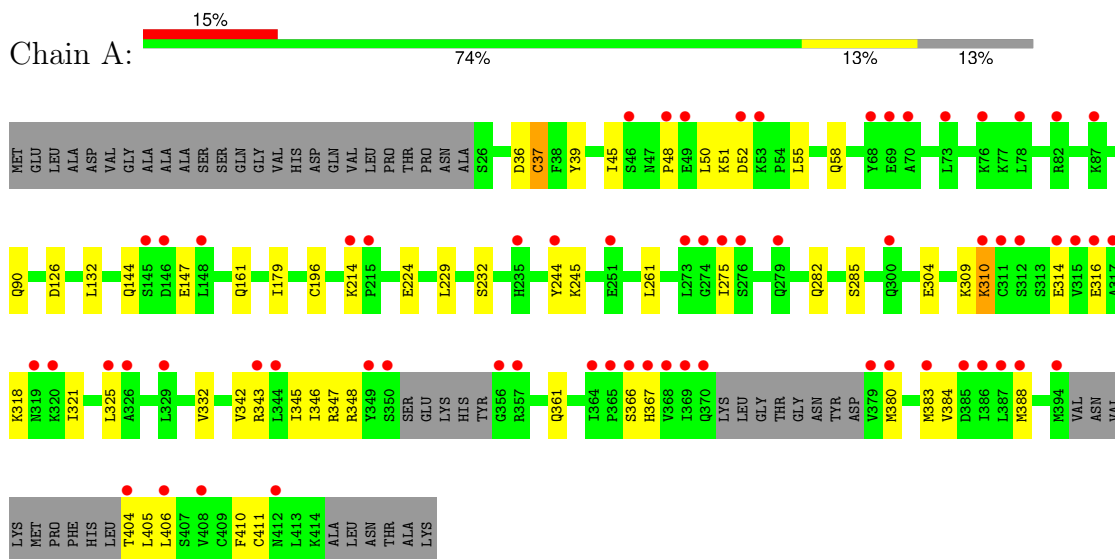
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	66	Total	O	0	0
			66	66		
5	B	17	Total	O	0	0
			17	17		

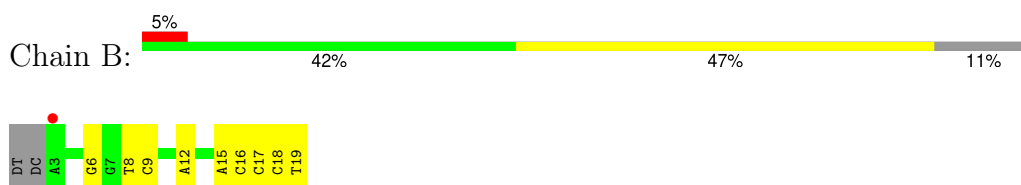
### 3 Residue-property plots [i](#)

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 polymerase iota



#### • Molecule 2: DNA (5'-D(P\*AP\*AP\*GP\*GP\*GP\*TP\*CP\*CP\*TP\*AP\*GP\*GP\*AP\*CP\*CP\*C P\*T)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.19Å 98.19Å 202.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.09 – 2.45 49.09 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.09-2.45) 99.7 (49.09-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.254 , 0.312 0.263 , 0.318	Depositor DCC
$R_{free}$ test set	1113 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 30.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6406	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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: MG, PO4

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	0.12	0/2931	0.31	0/3948
2	B	0.21	0/391	0.45	0/601
All	All	0.13	0/3322	0.33	0/4549

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	2892	2980	2980	42	0
2	B	349	89	191	13	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
4	A	3	0	0	0	0
5	A	66	0	0	9	1
5	B	17	0	0	3	1
All	All	3337	3069	3171	53	1

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 8.

All (53) 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)
2:B:16:DC:OP2	5:B:201:HOH:O	1.76	1.04
1:A:304:GLU:OE1	5:A:601:HOH:O	1.96	0.81
1:A:90:GLN:N	1:A:90:GLN:OE1	2.20	0.75
3:A:501:PO4:O4	5:A:602:HOH:O	2.05	0.75
2:B:19:DT:H3'	3:B:101:PO4:O4	1.88	0.74
1:A:347:ARG:O	1:A:404:THR:N	2.25	0.70
1:A:244:TYR:N	5:B:201:HOH:O	2.24	0.69
1:A:316:GLU:N	1:A:316:GLU:OE1	2.26	0.69
2:B:16:DC:H2''	2:B:17:DC:H5'	1.73	0.68
1:A:58:GLN:OE1	5:A:603:HOH:O	2.10	0.68
1:A:411:CYS:SG	5:A:657:HOH:O	2.51	0.67
1:A:404:THR:N	5:A:607:HOH:O	2.28	0.65
1:A:275:ILE:HD12	1:A:275:ILE:H	1.62	0.65
1:A:245:LYS:N	5:B:201:HOH:O	2.20	0.62
1:A:261:LEU:HD23	1:A:285:SER:HB3	1.83	0.61
1:A:367:HIS:ND1	5:A:606:HOH:O	2.31	0.60
1:A:126:ASP:OD1	5:A:604:HOH:O	2.15	0.60
1:A:50:LEU:HD22	1:A:55:LEU:HD12	1.87	0.57
1:A:161:GLN:NE2	1:A:224:GLU:OE1	2.35	0.56
5:A:604:HOH:O	2:B:18:DC:H2''	2.06	0.55
1:A:343:ARG:HD2	1:A:345:ILE:HD11	1.90	0.54
1:A:383:MET:HA	1:A:383:MET:HE3	1.89	0.53
1:A:39:TYR:CD2	2:B:19:DT:H2''	2.44	0.53
1:A:361:GLN:HG2	2:B:12:DA:OP2	2.09	0.53
2:B:16:DC:C2'	2:B:17:DC:H5'	2.38	0.52
1:A:39:TYR:CE2	2:B:19:DT:H2''	2.45	0.51
1:A:36:ASP:O	1:A:37:CYS:C	2.53	0.51
2:B:15:DA:H2'	2:B:16:DC:C6	2.47	0.50
1:A:229:LEU:O	1:A:232:SER:OG	2.28	0.49
1:A:318:LYS:HG2	1:A:388:MET:SD	2.52	0.49
1:A:309:LYS:O	1:A:310:LYS:C	2.55	0.49
1:A:405:LEU:O	1:A:406:LEU:HD23	2.13	0.48
1:A:144:GLN:N	1:A:147:GLU:OE1	2.42	0.47
1:A:325:LEU:HB2	1:A:380:MET:HE1	1.97	0.46
2:B:18:DC:H5''	2:B:18:DC:C6	2.50	0.46
1:A:366:SER:N	5:A:606:HOH:O	2.48	0.46
2:B:8:DT:H2''	2:B:9:DC:H5'	1.97	0.46
2:B:18:DC:H5''	2:B:18:DC:H6	1.80	0.46
1:A:384:VAL:O	1:A:388:MET:HG2	2.16	0.46
1:A:332:VAL:HG21	1:A:410:PHE:HD2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ILE:O	1:A:325:LEU:HD23	2.17	0.45
1:A:161:GLN:NE2	1:A:224:GLU:HB2	2.32	0.45
1:A:45:ILE:O	1:A:48:PRO:HD3	2.18	0.44
1:A:132:LEU:HD22	1:A:179:ILE:HG21	2.00	0.43
1:A:51:LYS:O	1:A:52:ASP:HB2	2.19	0.43
1:A:318:LYS:O	1:A:321:ILE:N	2.51	0.43
1:A:342:VAL:HG23	1:A:410:PHE:CE1	2.54	0.43
1:A:282:GLN:O	1:A:285:SER:OG	2.36	0.42
1:A:196:CYS:SG	1:A:214:LYS:O	2.77	0.42
1:A:314:GLU:HB3	1:A:316:GLU:OE1	2.20	0.41
1:A:161:GLN:HE22	1:A:224:GLU:HB2	1.85	0.41
1:A:346:ILE:HD11	1:A:348:ARG:HH11	1.86	0.41
2:B:6:DG:OP1	2:B:6:DG:H4'	2.19	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:601:HOH:O	5:B:208:HOH:O[10_665]	2.01	0.19

## 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	359/420 (86%)	339 (94%)	18 (5%)	2 (1%)	22 28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	LYS
1	A	37	CYS

### 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	334/376 (89%)	334 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	128	ASN
1	A	141	GLN
1	A	160	ASN
1	A	189	ASN
1	A	319	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	PO4	B	101	-	4,4,4	1.02	0	6,6,6	0.42	0
3	PO4	A	501	4	4,4,4	1.01	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

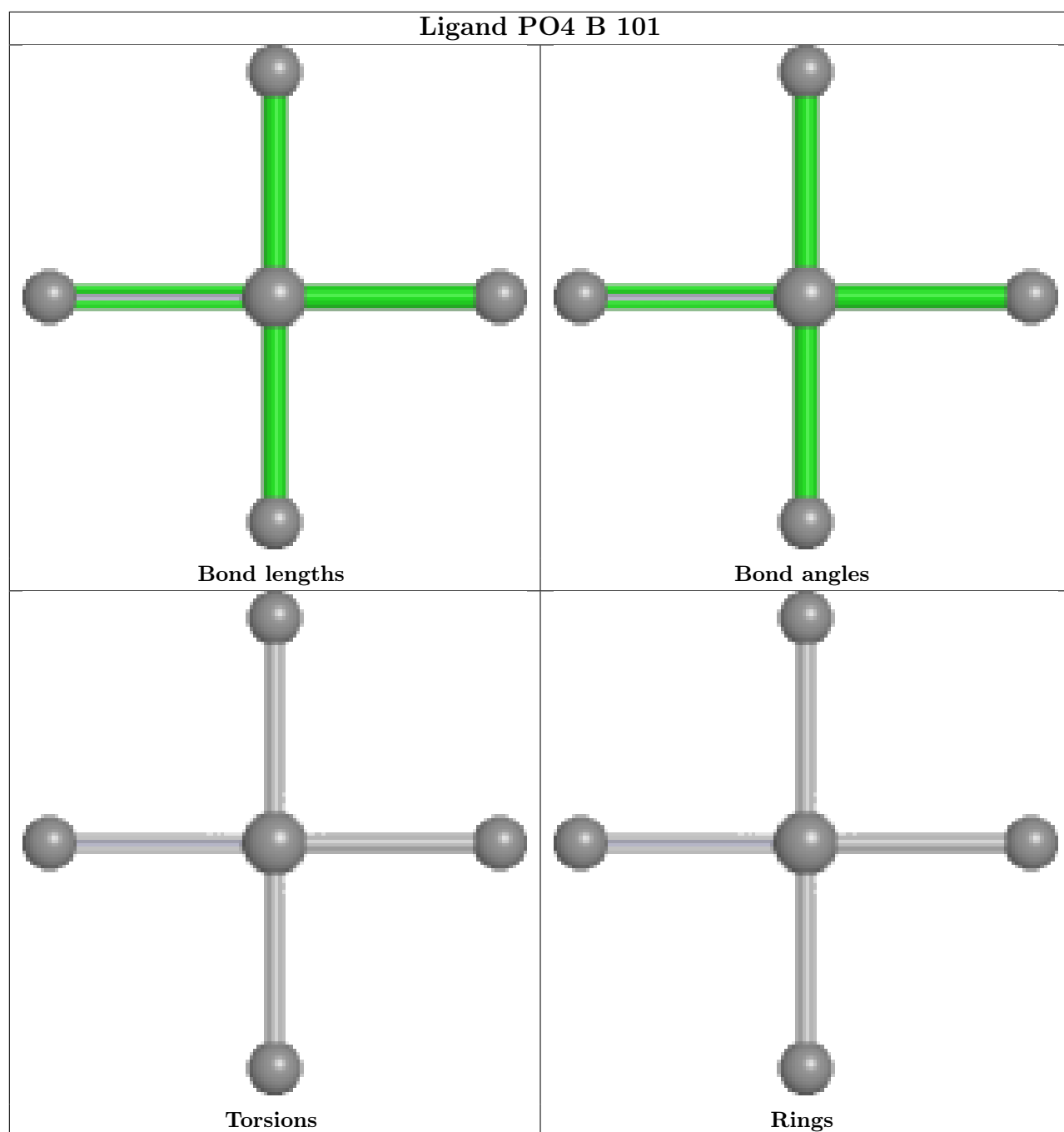
There are no torsion outliers.

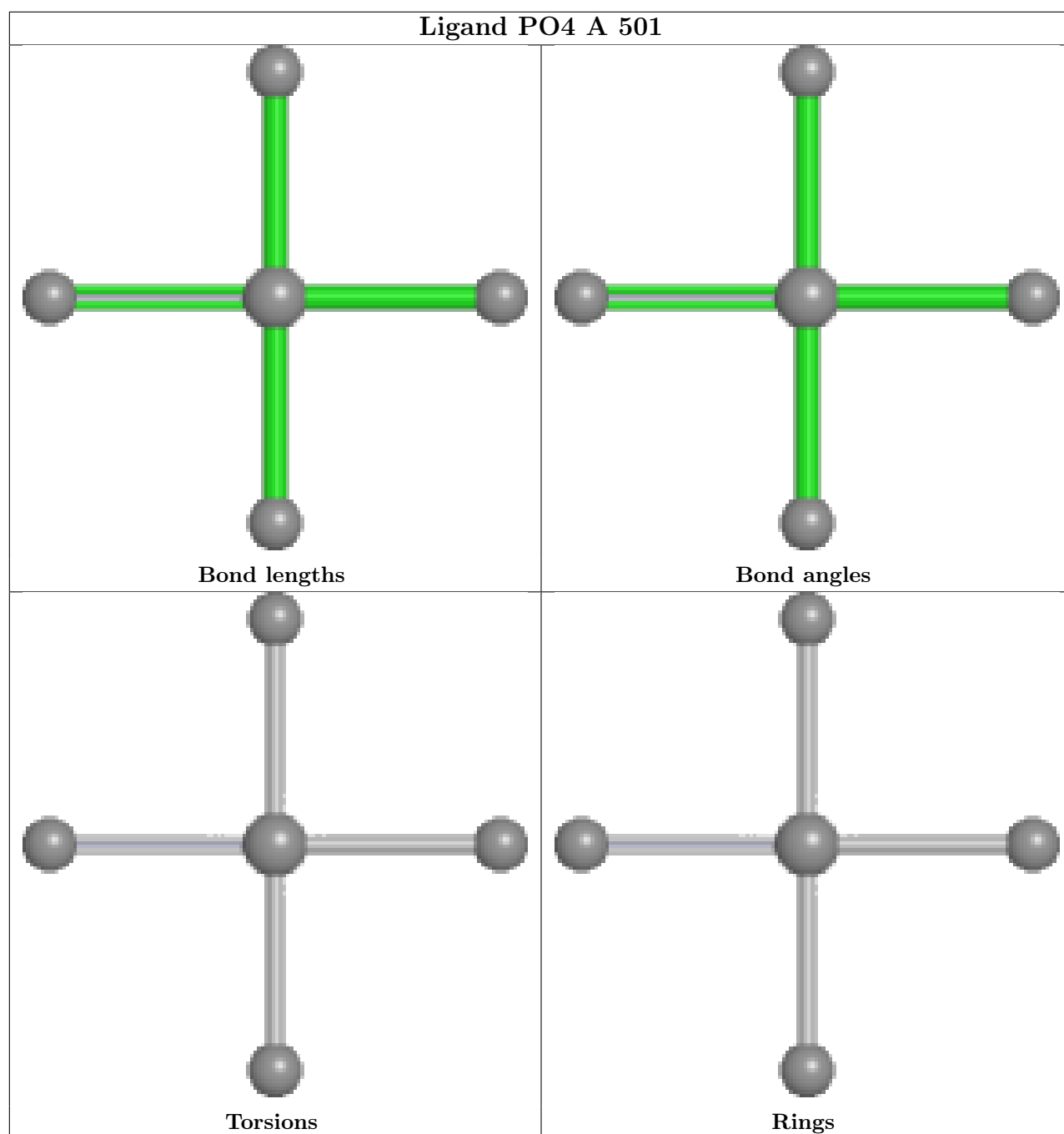
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	101	PO4	1	0
3	A	501	PO4	1	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	367/420 (87%)	0.82	64 (17%) <b>5</b> <b>4</b>	32, 54, 83, 98	0
2	B	17/19 (89%)	0.14	1 (5%) 29 29	34, 42, 52, 79	0
All	All	384/439 (87%)	0.79	65 (16%) <b>5</b> <b>4</b>	32, 52, 83, 98	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	LYS	5.6
1	A	386	ILE	4.2
1	A	312	SER	3.9
1	A	368	VAL	3.7
1	A	367	HIS	3.7
1	A	379	VAL	3.6
1	A	385	ASP	3.5
1	A	311	CYS	3.5
1	A	394	MET	3.4
1	A	370	GLN	3.4
1	A	364	ILE	3.4
1	A	310	LYS	3.3
1	A	315	VAL	3.3
1	A	326	ALA	3.2
1	A	380	MET	3.2
1	A	325	LEU	3.0
1	A	148	LEU	2.9
1	A	316	GLU	2.9
1	A	388	MET	2.9
1	A	76	LYS	2.9
1	A	329	LEU	2.9
1	A	369	ILE	2.8
1	A	274	GLY	2.8
1	A	244	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	344	LEU	2.7
1	A	275	ILE	2.7
1	A	365	PRO	2.7
1	A	314	GLU	2.7
1	A	406	LEU	2.6
1	A	350	SER	2.6
1	A	52	ASP	2.6
1	A	78	LEU	2.5
1	A	317	ALA	2.5
1	A	387	LEU	2.4
1	A	215	PRO	2.4
1	A	319	ASN	2.4
1	A	383	MET	2.4
1	A	251	GLU	2.4
1	A	343	ARG	2.4
1	A	87	LYS	2.3
1	A	320	LYS	2.3
1	A	69	GLU	2.3
1	A	273	LEU	2.3
2	B	3	DA	2.3
1	A	48	PRO	2.3
1	A	68	TYR	2.3
1	A	408	VAL	2.3
1	A	276	SER	2.2
1	A	357	ARG	2.2
1	A	46	SER	2.2
1	A	146	ASP	2.2
1	A	53	LYS	2.2
1	A	70	ALA	2.2
1	A	82	ARG	2.1
1	A	49	GLU	2.1
1	A	279	GLN	2.1
1	A	300	GLN	2.1
1	A	349	TYR	2.1
1	A	356	GLY	2.1
1	A	145	SER	2.1
1	A	412	ASN	2.1
1	A	235	HIS	2.1
1	A	73	LEU	2.1
1	A	366	SER	2.0
1	A	404	THR	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, 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.

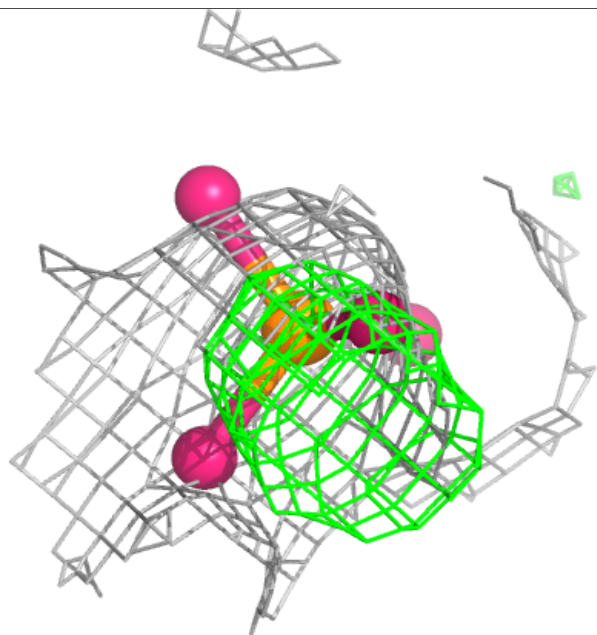
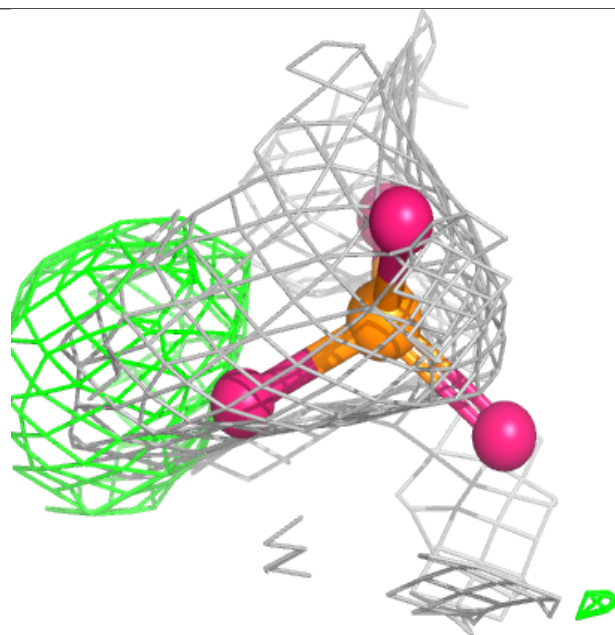
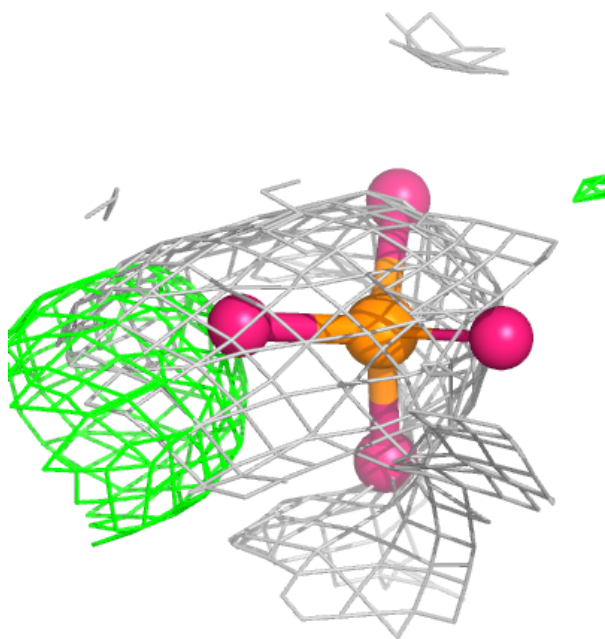
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	B	101	5/5	0.59	0.24	46,47,51,53	5
4	MG	A	502	1/1	0.76	0.15	51,51,51,51	0
4	MG	A	504	1/1	0.92	0.07	43,43,43,43	0
4	MG	A	503	1/1	0.93	0.09	38,38,38,38	0
3	PO4	A	501	5/5	0.94	0.07	48,51,63,64	0

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.



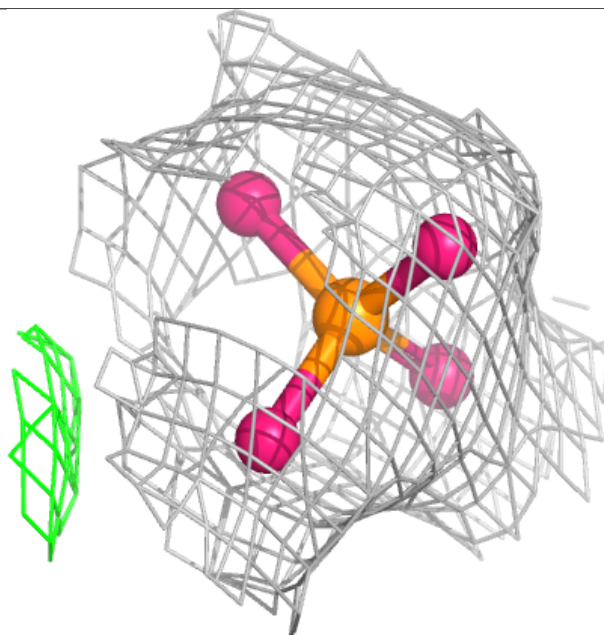
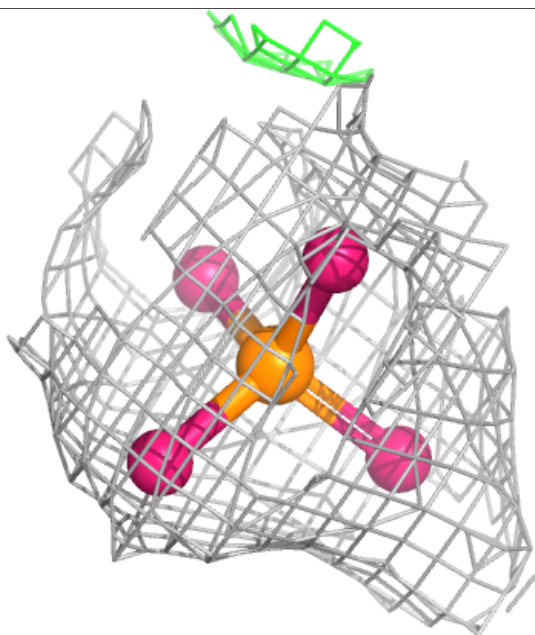
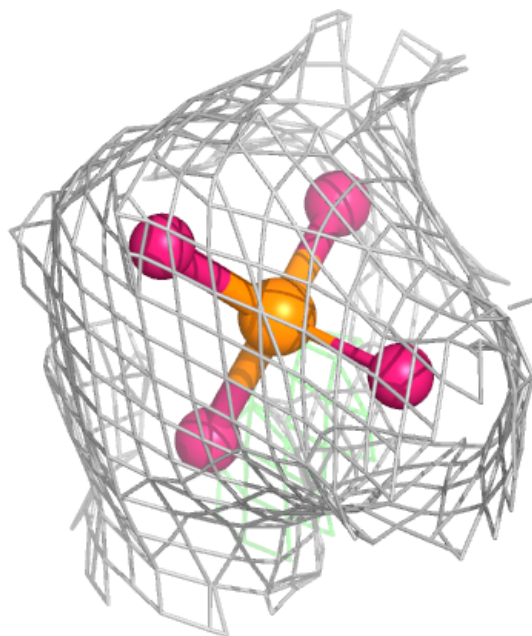
**Electron density around PO4 B 101:**

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



**Electron density around PO4 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.