



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 02:11 PM BST

PDB ID : 1Z7N  
Title : ATP Phosphoribosyl transferase (HisZG ATP-PRTase) from *Lactococcus lactis* with bound PRPP substrate  
Authors : Champagne, K.S.; Sissler, M.; Larrabee, Y.; Doublié, S.; Francklyn, C.S.  
Deposited on : 2005-03-25  
Resolution : 3.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.13.1  
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) : 2.13.1

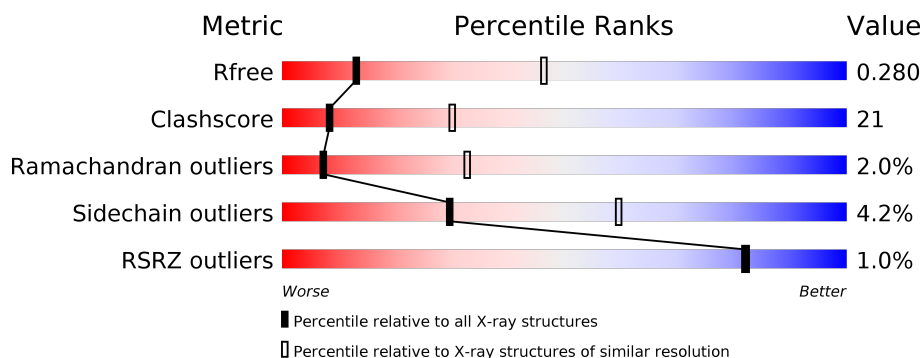
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	344	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>28%</div> <div>5%</div> <div>9%</div> </div> </div>
1	B	344	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>33%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	344	<div> <div></div> <div> <div>55%</div> <div>30%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	344	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>30%</div> <div>•</div> <div>9%</div> </div> </div>
2	E	208	<div> <div></div> <div> <div>54%</div> <div>42%</div> <div>••</div> </div> </div>
2	F	208	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>38%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	208	<div> <div>%</div> <div> </div> <div>53%41%..</div> </div>
2	H	208	<div> <div>%</div> <div> </div> <div>55%39%..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	G	1001	-	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16750 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 ATP phosphoribosyltransferase regulatory subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	21	0	0
			2547	1636	415	485	11			
1	B	318	Total	C	N	O	S	12	0	0
			2584	1657	424	492	11			
1	C	304	Total	C	N	O	S	10	0	0
			2472	1591	399	471	11			
1	D	312	Total	C	N	O	S	5	0	0
			2541	1633	416	481	11			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	cloning artifact	UNP Q02147
A	-14	ARG	-	cloning artifact	UNP Q02147
A	-13	GLY	-	cloning artifact	UNP Q02147
A	-12	SER	-	cloning artifact	UNP Q02147
A	-11	HIS	-	expression tag	UNP Q02147
A	-10	HIS	-	expression tag	UNP Q02147
A	-9	HIS	-	expression tag	UNP Q02147
A	-8	HIS	-	expression tag	UNP Q02147
A	-7	HIS	-	expression tag	UNP Q02147
A	-6	HIS	-	expression tag	UNP Q02147
A	-5	GLY	-	cloning artifact	UNP Q02147
A	-4	SER	-	cloning artifact	UNP Q02147
A	-3	ILE	-	cloning artifact	UNP Q02147
A	-2	GLU	-	cloning artifact	UNP Q02147
A	-1	GLY	-	cloning artifact	UNP Q02147
A	0	ARG	-	cloning artifact	UNP Q02147
B	-15	MET	-	cloning artifact	UNP Q02147
B	-14	ARG	-	cloning artifact	UNP Q02147
B	-13	GLY	-	cloning artifact	UNP Q02147
B	-12	SER	-	cloning artifact	UNP Q02147
B	-11	HIS	-	expression tag	UNP Q02147

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP Q02147
B	-9	HIS	-	expression tag	UNP Q02147
B	-8	HIS	-	expression tag	UNP Q02147
B	-7	HIS	-	expression tag	UNP Q02147
B	-6	HIS	-	expression tag	UNP Q02147
B	-5	GLY	-	cloning artifact	UNP Q02147
B	-4	SER	-	cloning artifact	UNP Q02147
B	-3	ILE	-	cloning artifact	UNP Q02147
B	-2	GLU	-	cloning artifact	UNP Q02147
B	-1	GLY	-	cloning artifact	UNP Q02147
B	0	ARG	-	cloning artifact	UNP Q02147
C	-15	MET	-	cloning artifact	UNP Q02147
C	-14	ARG	-	cloning artifact	UNP Q02147
C	-13	GLY	-	cloning artifact	UNP Q02147
C	-12	SER	-	cloning artifact	UNP Q02147
C	-11	HIS	-	expression tag	UNP Q02147
C	-10	HIS	-	expression tag	UNP Q02147
C	-9	HIS	-	expression tag	UNP Q02147
C	-8	HIS	-	expression tag	UNP Q02147
C	-7	HIS	-	expression tag	UNP Q02147
C	-6	HIS	-	expression tag	UNP Q02147
C	-5	GLY	-	cloning artifact	UNP Q02147
C	-4	SER	-	cloning artifact	UNP Q02147
C	-3	ILE	-	cloning artifact	UNP Q02147
C	-2	GLU	-	cloning artifact	UNP Q02147
C	-1	GLY	-	cloning artifact	UNP Q02147
C	0	ARG	-	cloning artifact	UNP Q02147
D	-15	MET	-	cloning artifact	UNP Q02147
D	-14	ARG	-	cloning artifact	UNP Q02147
D	-13	GLY	-	cloning artifact	UNP Q02147
D	-12	SER	-	cloning artifact	UNP Q02147
D	-11	HIS	-	expression tag	UNP Q02147
D	-10	HIS	-	expression tag	UNP Q02147
D	-9	HIS	-	expression tag	UNP Q02147
D	-8	HIS	-	expression tag	UNP Q02147
D	-7	HIS	-	expression tag	UNP Q02147
D	-6	HIS	-	expression tag	UNP Q02147
D	-5	GLY	-	cloning artifact	UNP Q02147
D	-4	SER	-	cloning artifact	UNP Q02147
D	-3	ILE	-	cloning artifact	UNP Q02147
D	-2	GLU	-	cloning artifact	UNP Q02147
D	-1	GLY	-	cloning artifact	UNP Q02147

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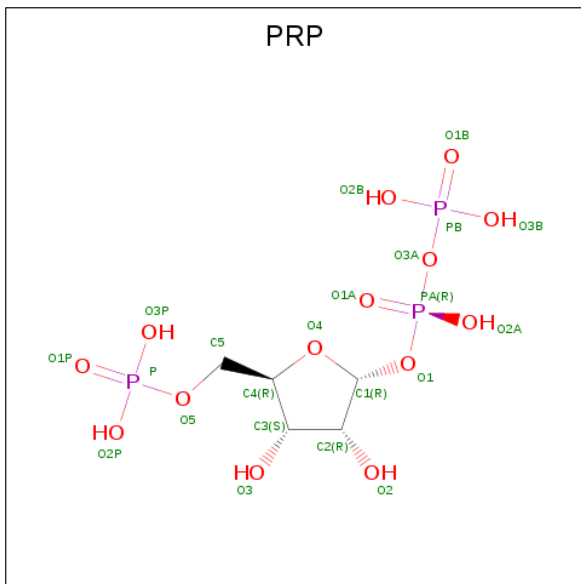
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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	ARG	-	cloning artifact	UNP Q02147

- Molecule 2 is a protein called ATP phosphoribosyltransferase.

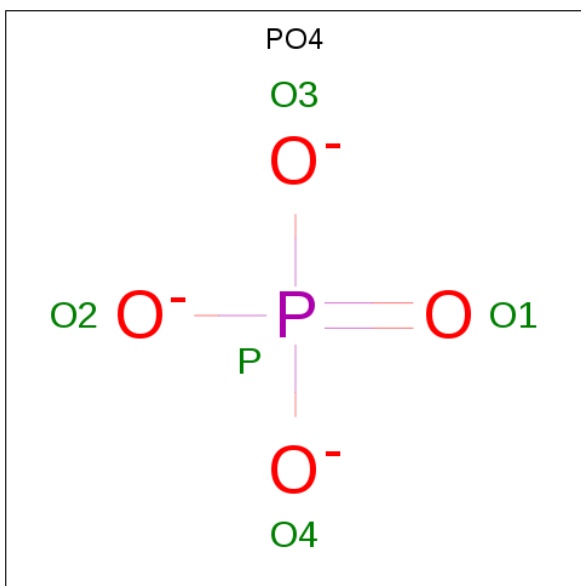
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	203	Total	C	N	O	S	9	0	0
			1630	1048	266	312	4			
2	F	205	Total	C	N	O	S	0	0	0
			1643	1055	269	315	4			
2	G	203	Total	C	N	O	S	4	0	0
			1632	1048	267	313	4			
2	H	200	Total	C	N	O	S	0	0	0
			1603	1030	261	308	4			

- Molecule 3 is 1-O-pyrophosphono-5-O-phosphono-alpha-D-ribofuranose (three-letter code: PRP) (formula:  $C_5H_{13}O_{14}P_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	O	P	0	0
			22	5	14	3		
3	F	1	Total	C	O	P	0	0
			22	5	14	3		
3	G	1	Total	C	O	P	0	0
			22	5	14	3		
3	H	1	Total	C	O	P	0	0
			22	5	14	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).

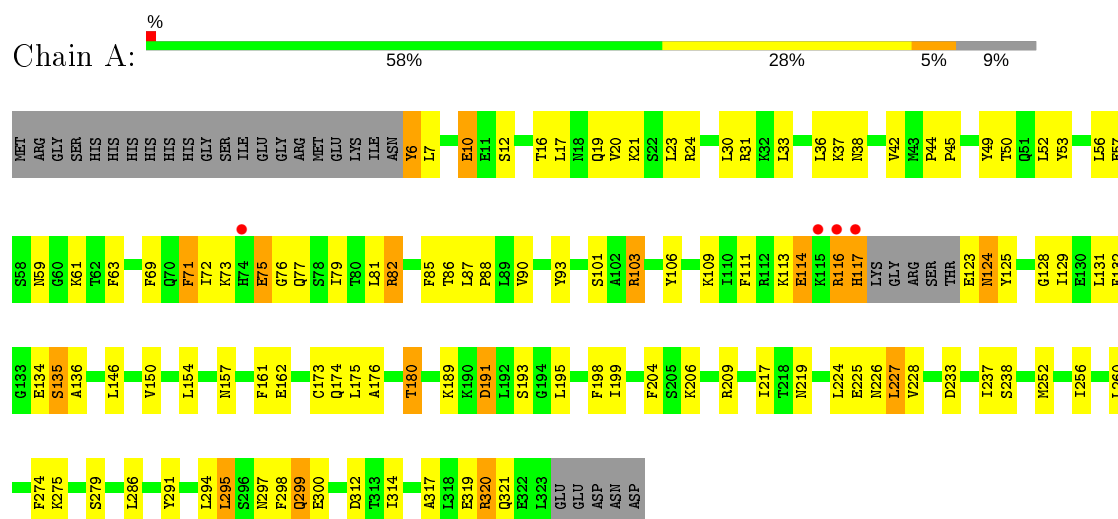


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		

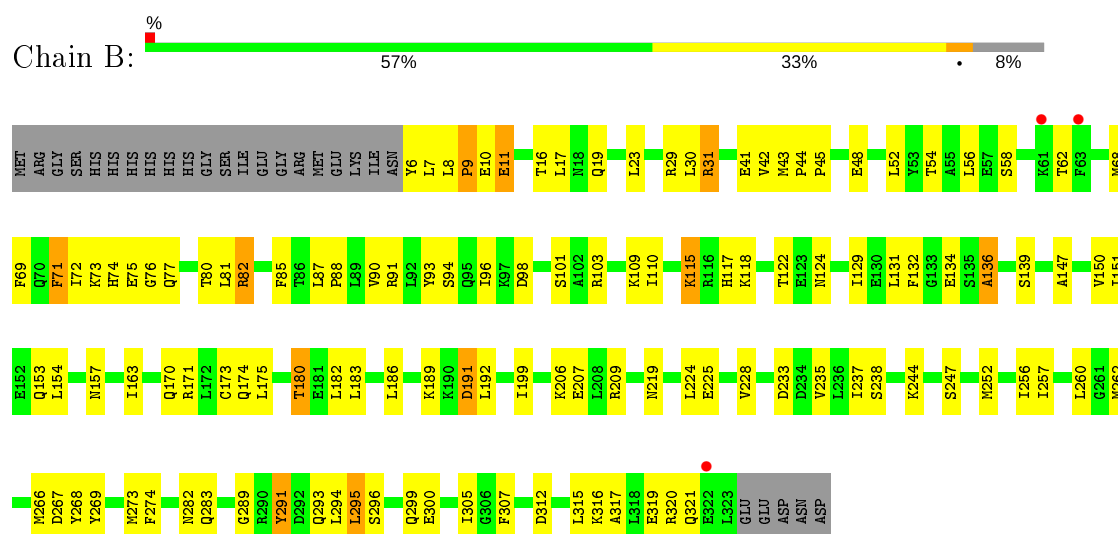
### 3 Residue-property plots

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: ATP phosphoribosyltransferase regulatory subunit



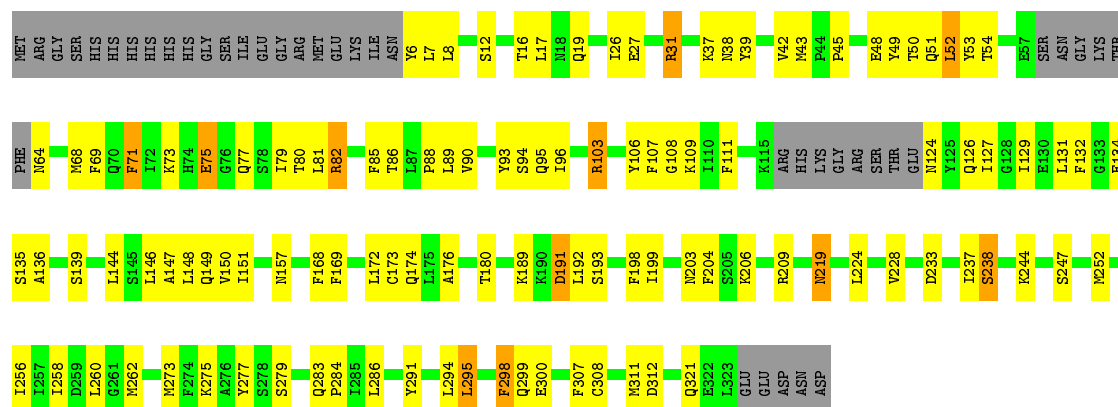
- Molecule 1: ATP phosphoribosyltransferase regulatory subunit



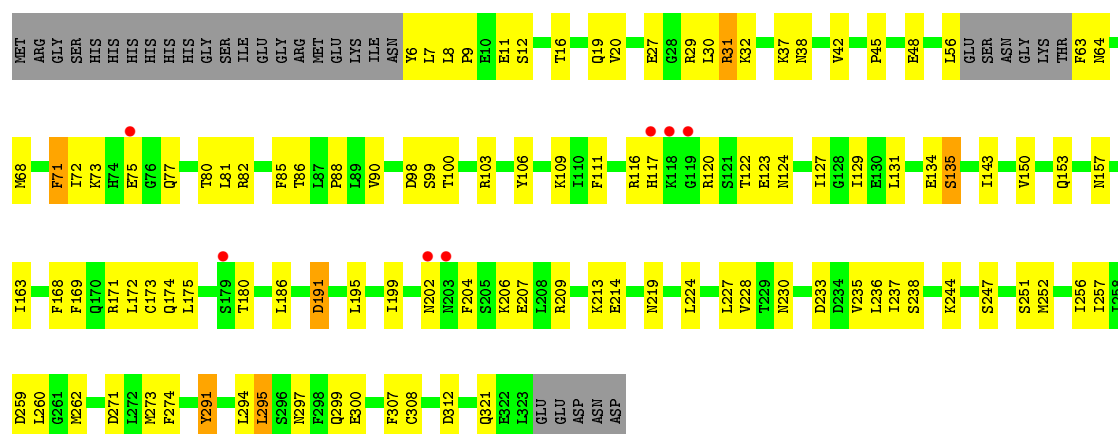
- Molecule 1: ATP phosphoribosyltransferase regulatory subunit



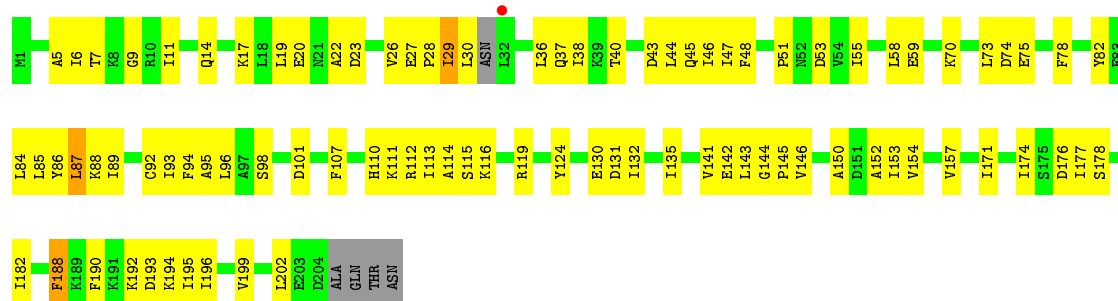




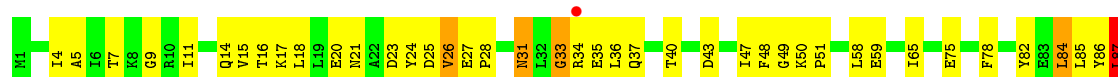
- Molecule 1: ATP phosphoribosyltransferase regulatory subunit

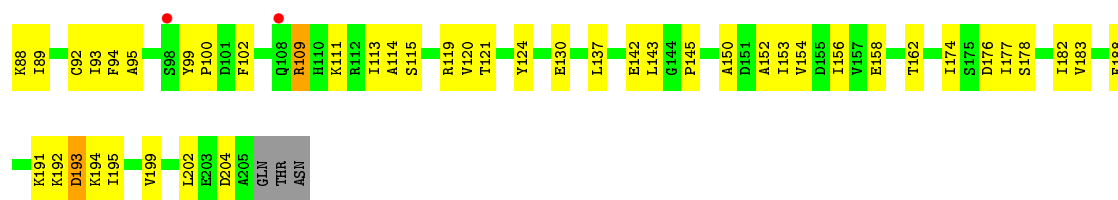


- Molecule 2: ATP phosphoribosyltransferase

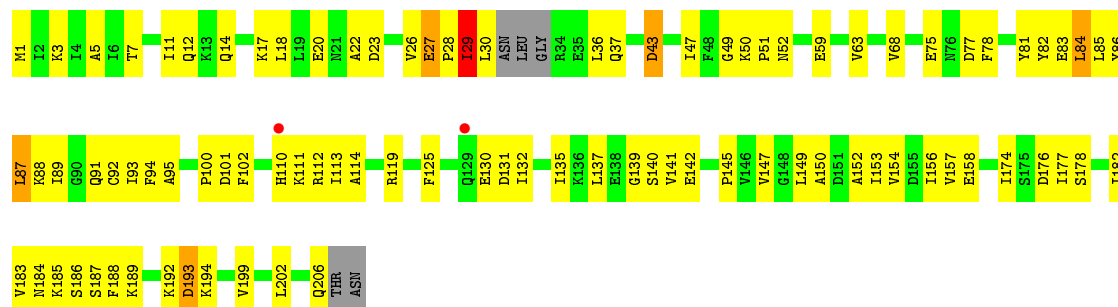


- Molecule 2: ATP phosphoribosyltransferase

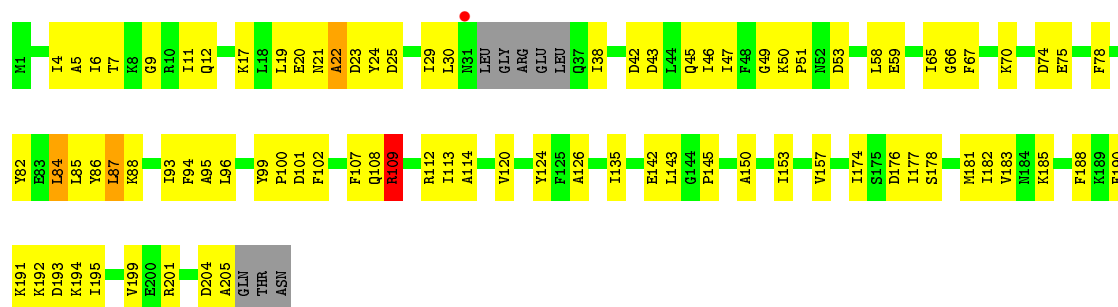




• Molecule 2: ATP phosphoribosyltransferase



• Molecule 2: ATP phosphoribosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.68 Å   222.94 Å   86.38 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.00 – 3.25 28.71 – 3.26	Depositor EDS
% Data completeness (in resolution range)	85.7 (29.00-3.25) 86.0 (28.71-3.26)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 3.24 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.247   ,   0.301 0.229   ,   0.280	Depositor DCC
$R_{free}$ test set	1981 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.3	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	16750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: PO4, PRP

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	0.53	1/2589 (0.0%)	0.67	3/3475 (0.1%)
1	B	0.47	0/2627	0.63	0/3526
1	C	0.47	0/2511	0.66	0/3370
1	D	0.43	0/2583	0.60	0/3466
2	E	0.57	1/1652 (0.1%)	0.73	5/2220 (0.2%)
2	F	0.43	0/1666	0.63	1/2241 (0.0%)
2	G	0.44	0/1654	0.66	1/2223 (0.0%)
2	H	0.46	0/1625	0.68	1/2185 (0.0%)
All	All	0.48	2/16907 (0.0%)	0.65	11/22706 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	E	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	29	ILE	C-N	-13.02	1.04	1.34
1	A	114	GLU	C-N	-5.85	1.20	1.34

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	GLU	C-N-CA	-7.37	103.27	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	29	ILE	CA-C-N	-7.03	101.73	117.20
2	E	188	PHE	CB-CG-CD1	6.77	125.54	120.80
2	E	188	PHE	CB-CG-CD2	-6.28	116.41	120.80
2	G	29	ILE	N-CA-C	-6.03	94.72	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	GLU	Mainchain
2	E	26	VAL	Mainchain
2	E	29	ILE	Mainchain

## 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	2547	0	2573	112	0
1	B	2584	0	2616	110	0
1	C	2472	0	2504	117	0
1	D	2541	0	2575	100	0
2	E	1630	0	1679	86	0
2	F	1643	0	1692	83	0
2	G	1632	0	1679	80	0
2	H	1603	0	1647	79	0
3	E	22	0	8	0	0
3	F	22	0	8	1	0
3	G	22	0	8	1	0
3	H	22	0	8	0	0
4	F	5	0	0	0	0
4	G	5	0	0	2	0
All	All	16750	0	16997	704	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 21.

The worst 5 of 704 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ARG:O	1:A:117:HIS:CD2	1.76	1.37
2:E:27:GLU:O	2:E:30:LEU:HG	1.24	1.28
1:A:116:ARG:C	1:A:117:HIS:CD2	2.08	1.25
1:A:116:ARG:O	1:A:117:HIS:CG	1.91	1.22
2:H:19:LEU:O	2:H:22:ALA:O	1.63	1.15

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	309/344 (90%)	272 (88%)	32 (10%)	5 (2%)	9	37
1	B	316/344 (92%)	275 (87%)	37 (12%)	4 (1%)	12	41
1	C	298/344 (87%)	265 (89%)	29 (10%)	4 (1%)	12	41
1	D	308/344 (90%)	285 (92%)	20 (6%)	3 (1%)	15	47
2	E	199/208 (96%)	165 (83%)	31 (16%)	3 (2%)	10	39
2	F	203/208 (98%)	170 (84%)	25 (12%)	8 (4%)	3	18
2	G	199/208 (96%)	167 (84%)	24 (12%)	8 (4%)	3	17
2	H	196/208 (94%)	162 (83%)	29 (15%)	5 (3%)	5	27
All	All	2028/2208 (92%)	1761 (87%)	227 (11%)	40 (2%)	7	33

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	84	LEU
2	G	84	LEU
2	G	140	SER
1	A	191	ASP
1	B	115	LYS

### 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	284/311 (91%)	267 (94%)	17 (6%)	19	49
1	B	288/311 (93%)	273 (95%)	15 (5%)	23	53
1	C	276/311 (89%)	263 (95%)	13 (5%)	26	57
1	D	283/311 (91%)	268 (95%)	15 (5%)	22	53
2	E	182/186 (98%)	178 (98%)	4 (2%)	52	74
2	F	183/186 (98%)	177 (97%)	6 (3%)	38	65
2	G	182/186 (98%)	178 (98%)	4 (2%)	52	74
2	H	179/186 (96%)	175 (98%)	4 (2%)	52	74
All	All	1857/1988 (93%)	1779 (96%)	78 (4%)	30	59

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	71	PHE
1	C	295	LEU
2	G	87	LEU
1	C	75	GLU
1	C	174	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	310	HIS
2	F	14	GLN
2	H	21	ASN
2	E	21	ASN
2	F	21	ASN

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	PRP	F	4008	-	19,22,22	0.98	1 (5%)	33,35,35	1.00	2 (6%)
3	PRP	H	4010	-	19,22,22	1.02	1 (5%)	33,35,35	0.99	1 (3%)
4	PO4	G	1001	-	4,4,4	1.53	0	6,6,6	0.42	0
4	PO4	F	1002	-	4,4,4	1.54	0	6,6,6	0.42	0
3	PRP	G	4009	-	19,22,22	0.99	1 (5%)	33,35,35	1.01	1 (3%)
3	PRP	E	4007	-	19,22,22	1.23	2 (10%)	33,35,35	1.07	1 (3%)

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	PRP	H	4010	-	-	1/16/33/33	0/1/1/1
3	PRP	F	4008	-	-	3/16/33/33	0/1/1/1
3	PRP	G	4009	-	-	6/16/33/33	0/1/1/1
3	PRP	E	4007	-	-	4/16/33/33	0/1/1/1

All (5) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4007	PRP	O4-C4	3.22	1.52	1.45
3	E	4007	PRP	C1-C2	2.72	1.56	1.52
3	H	4010	PRP	O4-C4	2.62	1.50	1.45
3	F	4008	PRP	O4-C4	2.54	1.50	1.45
3	G	4009	PRP	O4-C4	2.48	1.50	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4009	PRP	P-O5-C5	2.43	124.98	118.30
3	E	4007	PRP	P-O5-C5	2.39	124.87	118.30
3	H	4010	PRP	P-O5-C5	2.18	124.30	118.30
3	F	4008	PRP	O3P-P-O5	-2.09	101.18	106.73
3	F	4008	PRP	P-O5-C5	2.06	123.97	118.30

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	4008	PRP	C5-O5-P-O1P
3	E	4007	PRP	PA-O3A-PB-O2B
3	E	4007	PRP	C3-C4-C5-O5
3	E	4007	PRP	O4-C4-C5-O5
3	G	4009	PRP	C3-C4-C5-O5

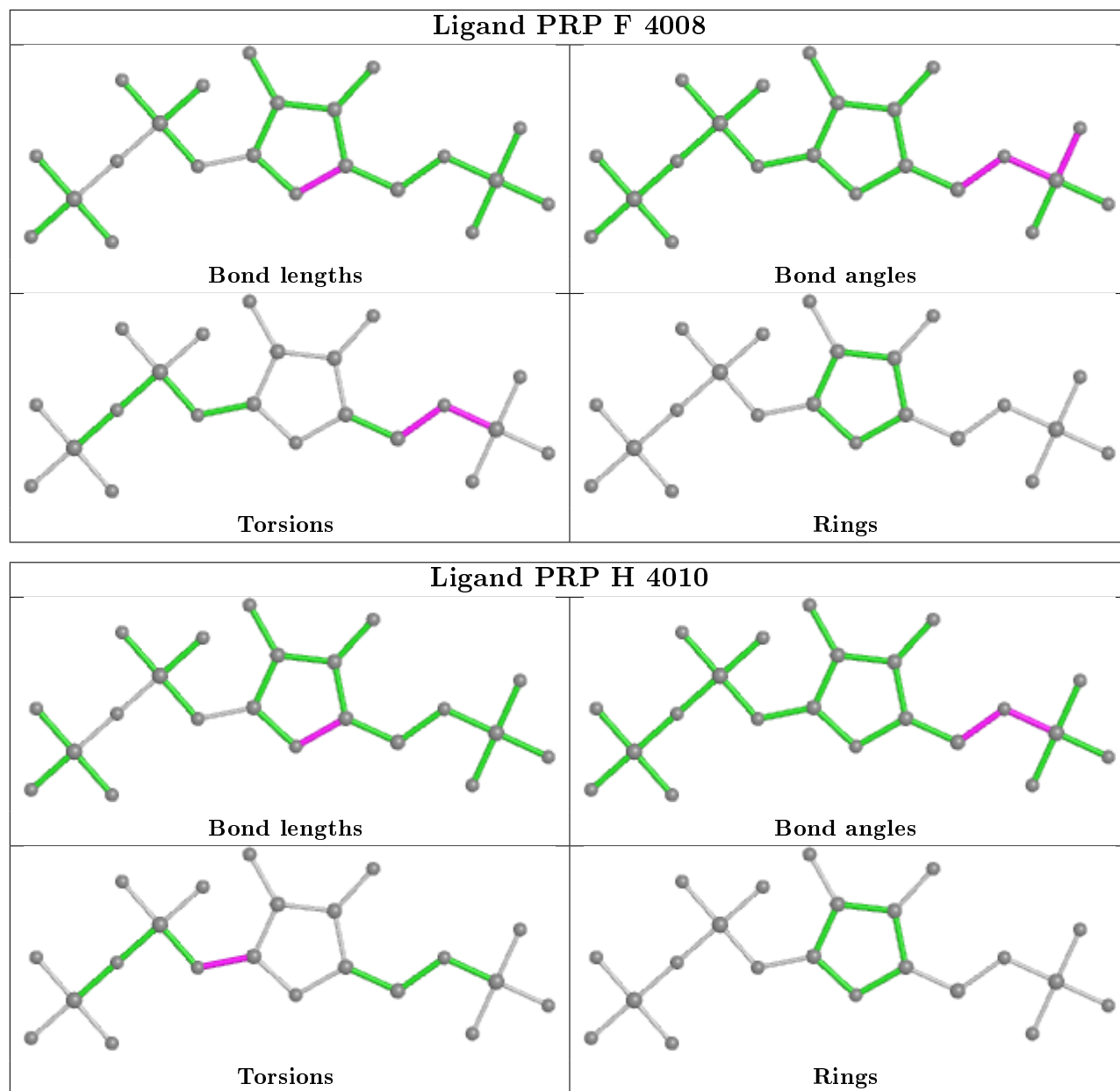
There are no ring outliers.

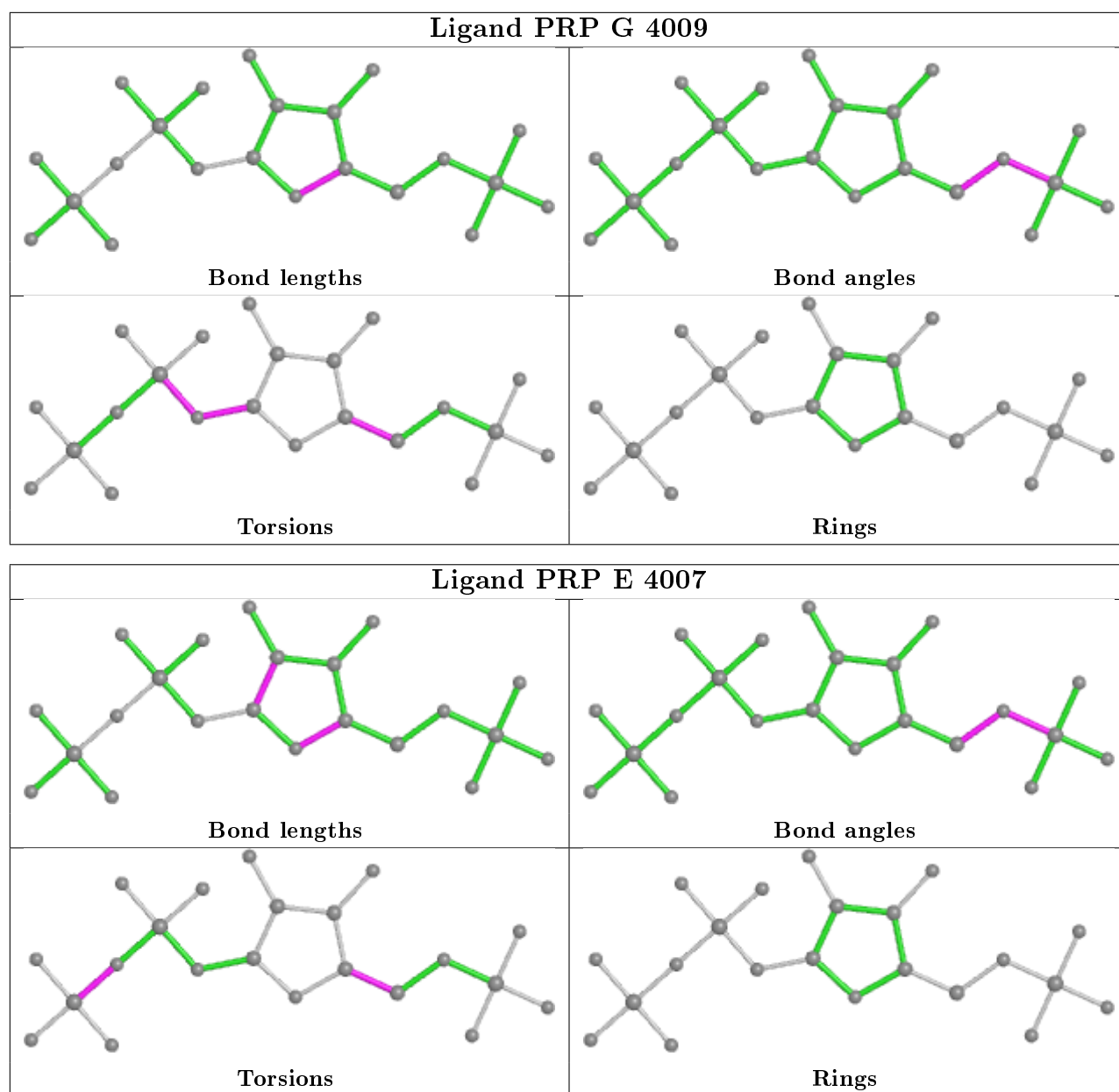
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4008	PRP	1	0
4	G	1001	PO4	2	0
3	G	4009	PRP	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	29:ILE	C	30:LEU	N	1.04

## 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	311/344 (90%)	-0.44	4 (1%) 77 75	14, 43, 117, 169	2 (0%)
1	B	316/344 (91%)	-0.35	3 (0%) 84 84	17, 55, 119, 176	0
1	C	304/344 (88%)	-0.36	0 100 100	17, 50, 109, 182	3 (0%)
1	D	312/344 (90%)	-0.22	7 (2%) 62 59	22, 70, 126, 166	1 (0%)
2	E	202/208 (97%)	-0.41	1 (0%) 91 90	25, 61, 120, 166	0
2	F	205/208 (98%)	-0.25	3 (1%) 73 71	26, 71, 126, 162	0
2	G	202/208 (97%)	-0.33	2 (0%) 82 82	25, 62, 119, 164	0
2	H	200/208 (96%)	-0.32	1 (0%) 91 90	27, 65, 129, 168	0
All	All	2052/2208 (92%)	-0.34	21 (1%) 82 82	14, 59, 123, 182	6 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	31	ASN	3.5
2	F	108	GLN	3.5
1	B	61	LYS	3.4
1	A	117	HIS	3.2
2	F	98	SER	3.0

### 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 ⓘ

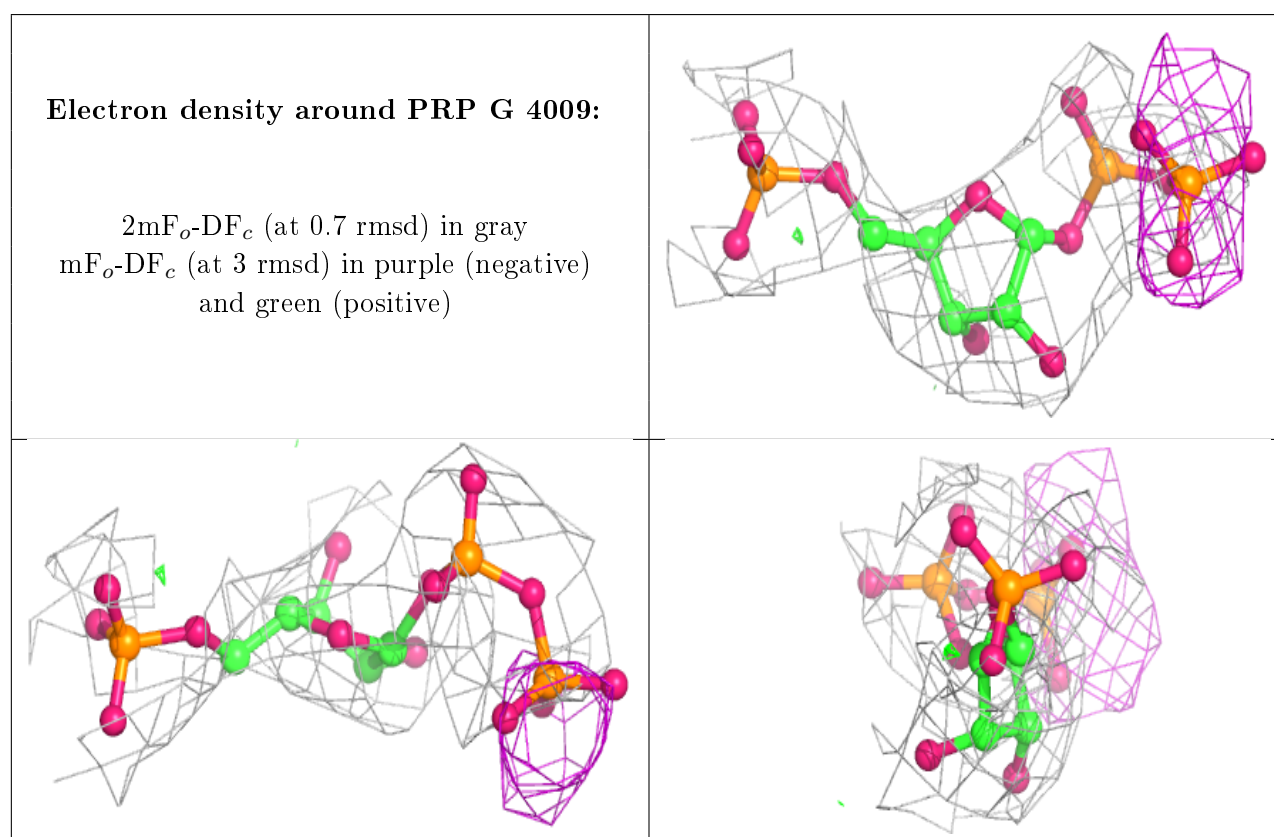
There are no monosaccharides in this entry.

## 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.

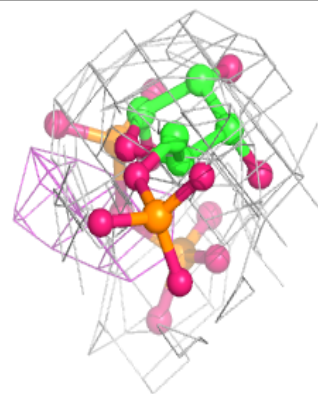
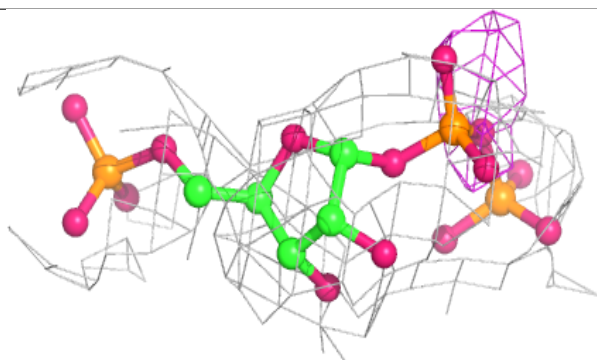
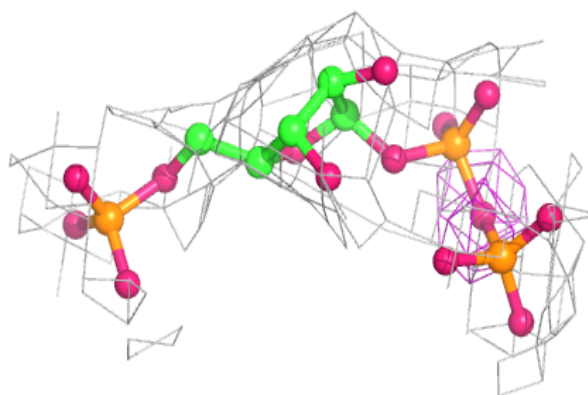
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	PO4	G	1001	5/5	0.68	0.44	127,127,127,127	0
3	PRP	G	4009	22/22	0.78	0.27	118,118,118,118	0
3	PRP	F	4008	22/22	0.81	0.22	117,117,117,117	0
3	PRP	H	4010	22/22	0.81	0.25	138,138,138,138	0
3	PRP	E	4007	22/22	0.84	0.22	113,113,113,113	0
4	PO4	F	1002	5/5	0.87	0.34	111,111,111,111	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.

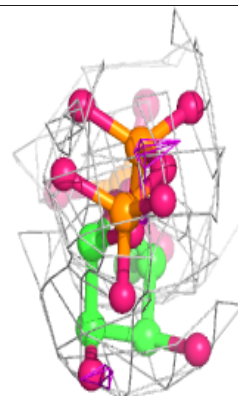
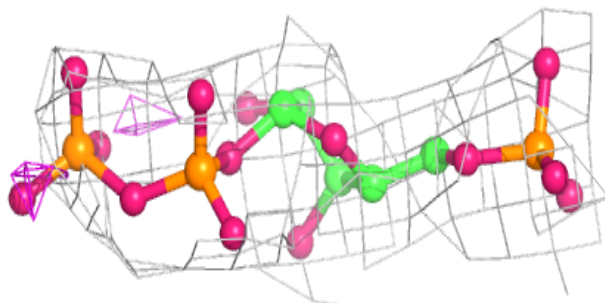
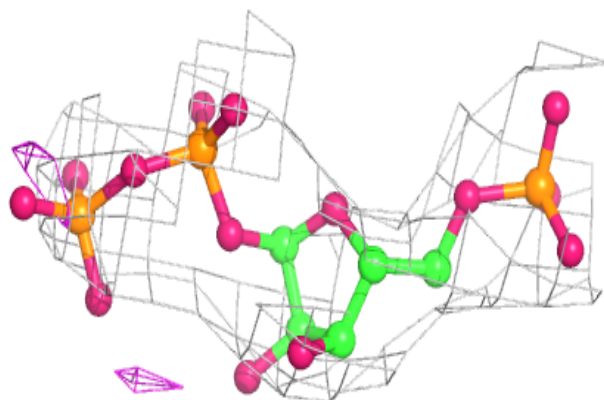


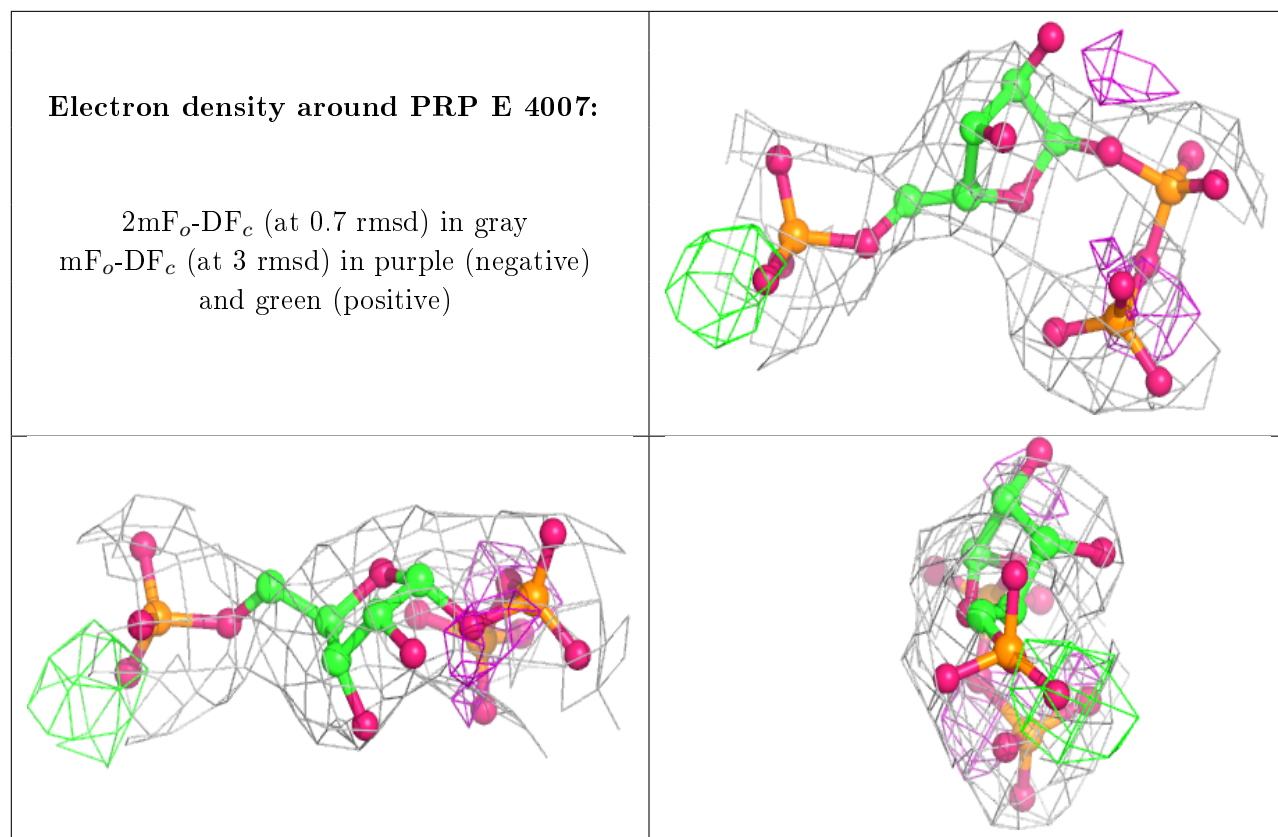
**Electron density around PRP F 4008:**

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

**Electron density around PRP H 4010:**

$2mF_o-DF_c$  (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.