



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 10:25 PM BST

PDB ID : 4XYK  
Title : Crystal structure of human phosphofructokinase-1 in complex with ADP, Northeast Structural Genomics Consortium Target HR9275  
Authors : Forouhar, F.; Webb, B.A.; Szu, F.-E.; Seetharaman, J.; Barber, D.L.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2015-02-02  
Resolution : 3.40 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

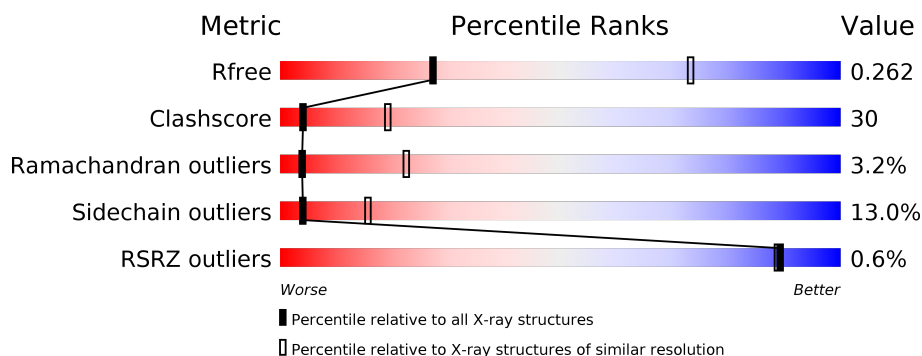
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	812	
1	B	812	
1	C	812	
1	D	812	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	803	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22897 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-dependent 6-phosphofructokinase, platelet type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	737	Total	C	N	O	S	0	0	0
			5640	3542	1000	1059	39			
1	B	749	Total	C	N	O	S	0	0	0
			5727	3595	1019	1074	39			
1	C	743	Total	C	N	O	S	0	0	0
			5681	3566	1008	1068	39			
1	D	743	Total	C	N	O	S	0	0	0
			5681	3566	1008	1068	39			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q01813
A	-26	SER	-	expression tag	UNP Q01813
A	-25	TYR	-	expression tag	UNP Q01813
A	-24	TYR	-	expression tag	UNP Q01813
A	-23	HIS	-	expression tag	UNP Q01813
A	-22	HIS	-	expression tag	UNP Q01813
A	-21	HIS	-	expression tag	UNP Q01813
A	-20	HIS	-	expression tag	UNP Q01813
A	-19	HIS	-	expression tag	UNP Q01813
A	-18	HIS	-	expression tag	UNP Q01813
A	-17	ASP	-	expression tag	UNP Q01813
A	-16	TYR	-	expression tag	UNP Q01813
A	-15	ASP	-	expression tag	UNP Q01813
A	-14	ILE	-	expression tag	UNP Q01813
A	-13	PRO	-	expression tag	UNP Q01813
A	-12	THR	-	expression tag	UNP Q01813
A	-11	THR	-	expression tag	UNP Q01813
A	-10	GLU	-	expression tag	UNP Q01813
A	-9	ASN	-	expression tag	UNP Q01813
A	-8	LEU	-	expression tag	UNP Q01813
A	-7	TYR	-	expression tag	UNP Q01813

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	PHE	-	expression tag	UNP Q01813
A	-5	GLN	-	expression tag	UNP Q01813
A	-4	GLY	-	expression tag	UNP Q01813
A	-3	ALA	-	expression tag	UNP Q01813
A	-2	MET	-	expression tag	UNP Q01813
A	-1	ASP	-	expression tag	UNP Q01813
A	0	PRO	-	expression tag	UNP Q01813
B	-27	MET	-	initiating methionine	UNP Q01813
B	-26	SER	-	expression tag	UNP Q01813
B	-25	TYR	-	expression tag	UNP Q01813
B	-24	TYR	-	expression tag	UNP Q01813
B	-23	HIS	-	expression tag	UNP Q01813
B	-22	HIS	-	expression tag	UNP Q01813
B	-21	HIS	-	expression tag	UNP Q01813
B	-20	HIS	-	expression tag	UNP Q01813
B	-19	HIS	-	expression tag	UNP Q01813
B	-18	HIS	-	expression tag	UNP Q01813
B	-17	ASP	-	expression tag	UNP Q01813
B	-16	TYR	-	expression tag	UNP Q01813
B	-15	ASP	-	expression tag	UNP Q01813
B	-14	ILE	-	expression tag	UNP Q01813
B	-13	PRO	-	expression tag	UNP Q01813
B	-12	THR	-	expression tag	UNP Q01813
B	-11	THR	-	expression tag	UNP Q01813
B	-10	GLU	-	expression tag	UNP Q01813
B	-9	ASN	-	expression tag	UNP Q01813
B	-8	LEU	-	expression tag	UNP Q01813
B	-7	TYR	-	expression tag	UNP Q01813
B	-6	PHE	-	expression tag	UNP Q01813
B	-5	GLN	-	expression tag	UNP Q01813
B	-4	GLY	-	expression tag	UNP Q01813
B	-3	ALA	-	expression tag	UNP Q01813
B	-2	MET	-	expression tag	UNP Q01813
B	-1	ASP	-	expression tag	UNP Q01813
B	0	PRO	-	expression tag	UNP Q01813
C	-27	MET	-	initiating methionine	UNP Q01813
C	-26	SER	-	expression tag	UNP Q01813
C	-25	TYR	-	expression tag	UNP Q01813
C	-24	TYR	-	expression tag	UNP Q01813
C	-23	HIS	-	expression tag	UNP Q01813
C	-22	HIS	-	expression tag	UNP Q01813
C	-21	HIS	-	expression tag	UNP Q01813

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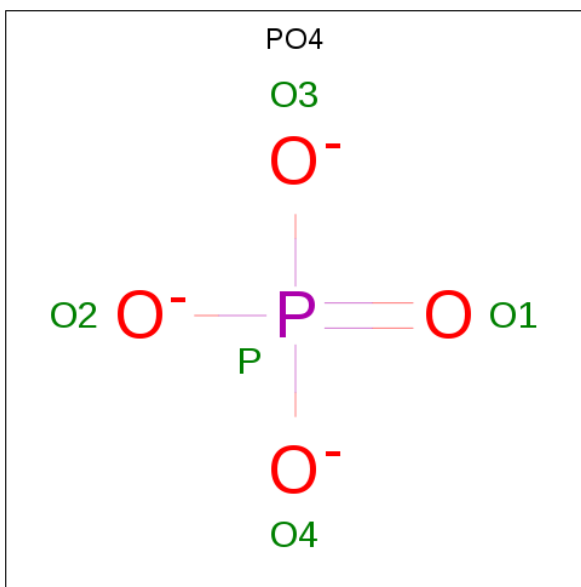
Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	HIS	-	expression tag	UNP Q01813
C	-19	HIS	-	expression tag	UNP Q01813
C	-18	HIS	-	expression tag	UNP Q01813
C	-17	ASP	-	expression tag	UNP Q01813
C	-16	TYR	-	expression tag	UNP Q01813
C	-15	ASP	-	expression tag	UNP Q01813
C	-14	ILE	-	expression tag	UNP Q01813
C	-13	PRO	-	expression tag	UNP Q01813
C	-12	THR	-	expression tag	UNP Q01813
C	-11	THR	-	expression tag	UNP Q01813
C	-10	GLU	-	expression tag	UNP Q01813
C	-9	ASN	-	expression tag	UNP Q01813
C	-8	LEU	-	expression tag	UNP Q01813
C	-7	TYR	-	expression tag	UNP Q01813
C	-6	PHE	-	expression tag	UNP Q01813
C	-5	GLN	-	expression tag	UNP Q01813
C	-4	GLY	-	expression tag	UNP Q01813
C	-3	ALA	-	expression tag	UNP Q01813
C	-2	MET	-	expression tag	UNP Q01813
C	-1	ASP	-	expression tag	UNP Q01813
C	0	PRO	-	expression tag	UNP Q01813
D	-27	MET	-	initiating methionine	UNP Q01813
D	-26	SER	-	expression tag	UNP Q01813
D	-25	TYR	-	expression tag	UNP Q01813
D	-24	TYR	-	expression tag	UNP Q01813
D	-23	HIS	-	expression tag	UNP Q01813
D	-22	HIS	-	expression tag	UNP Q01813
D	-21	HIS	-	expression tag	UNP Q01813
D	-20	HIS	-	expression tag	UNP Q01813
D	-19	HIS	-	expression tag	UNP Q01813
D	-18	HIS	-	expression tag	UNP Q01813
D	-17	ASP	-	expression tag	UNP Q01813
D	-16	TYR	-	expression tag	UNP Q01813
D	-15	ASP	-	expression tag	UNP Q01813
D	-14	ILE	-	expression tag	UNP Q01813
D	-13	PRO	-	expression tag	UNP Q01813
D	-12	THR	-	expression tag	UNP Q01813
D	-11	THR	-	expression tag	UNP Q01813
D	-10	GLU	-	expression tag	UNP Q01813
D	-9	ASN	-	expression tag	UNP Q01813
D	-8	LEU	-	expression tag	UNP Q01813
D	-7	TYR	-	expression tag	UNP Q01813

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	PHE	-	expression tag	UNP Q01813
D	-5	GLN	-	expression tag	UNP Q01813
D	-4	GLY	-	expression tag	UNP Q01813
D	-3	ALA	-	expression tag	UNP Q01813
D	-2	MET	-	expression tag	UNP Q01813
D	-1	ASP	-	expression tag	UNP Q01813
D	0	PRO	-	expression tag	UNP Q01813

- # ADP

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



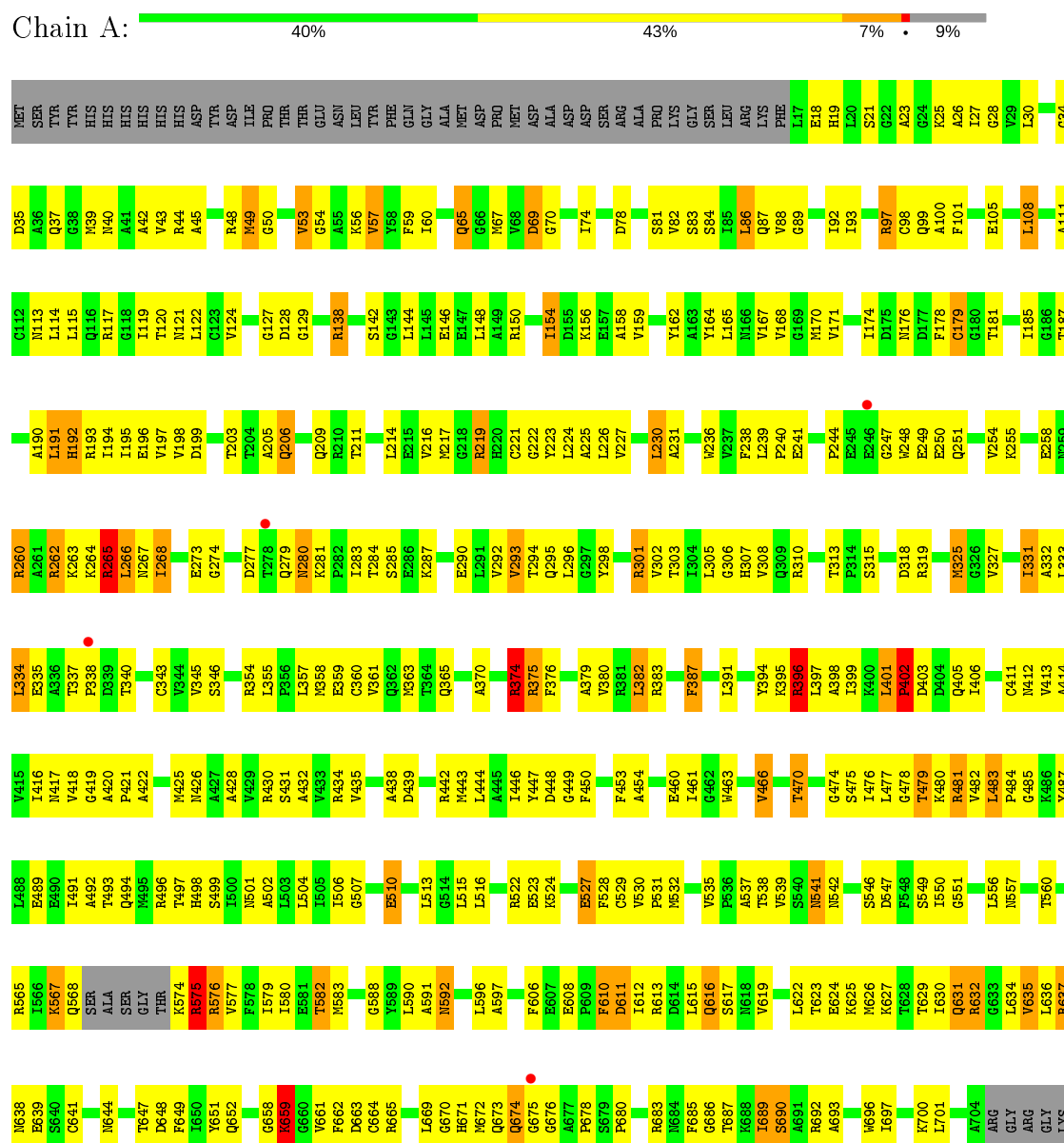
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total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

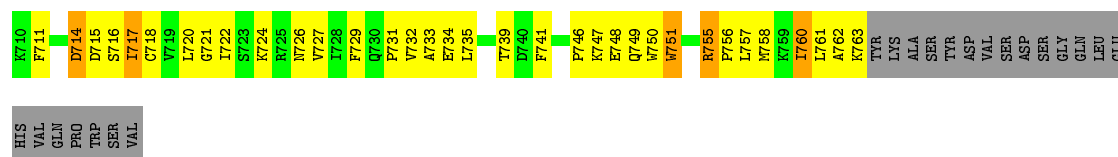


### 3 Residue-property plots

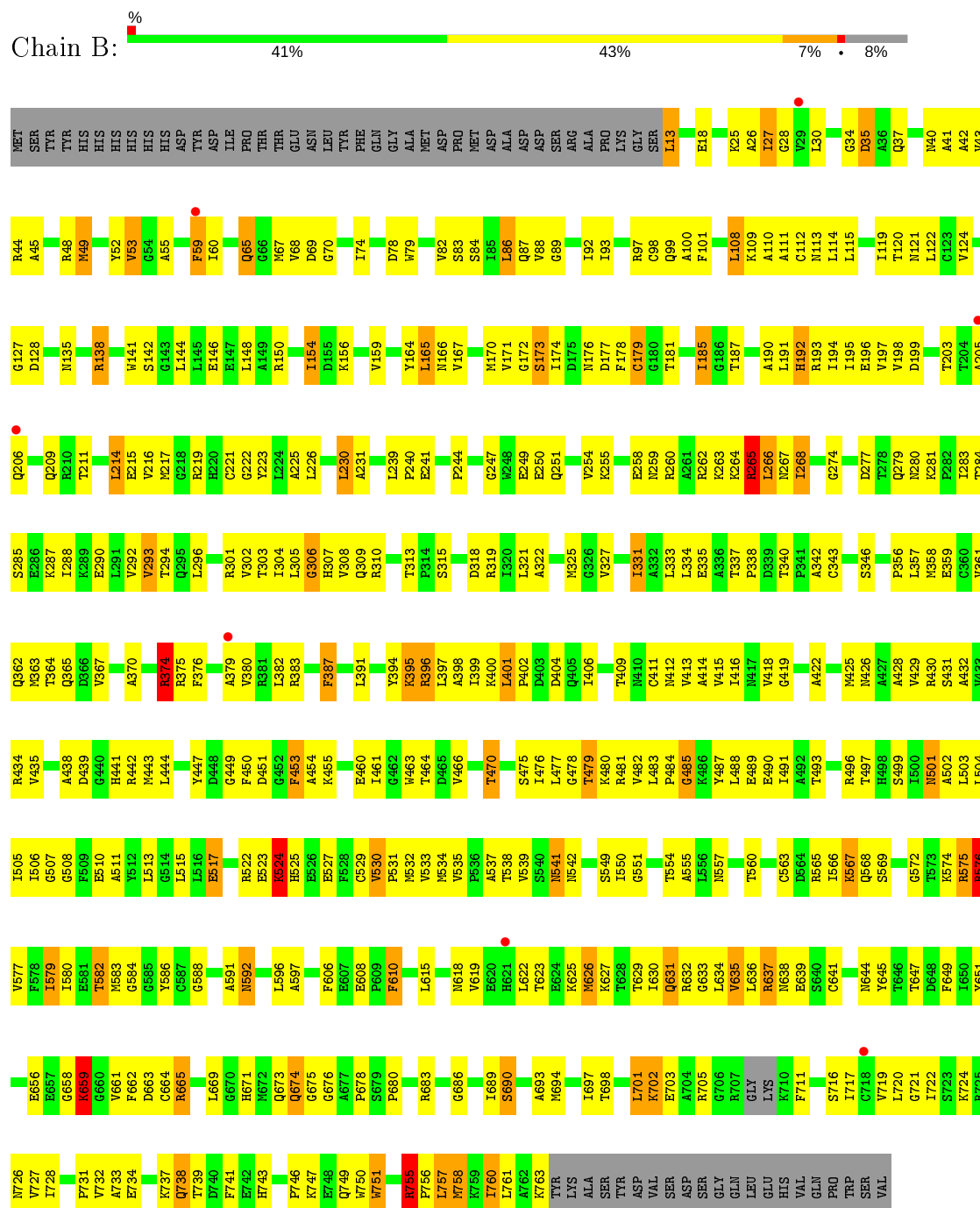
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-dependent 6-phosphofructokinase, platelet type





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VAL	VAL	Q631	S546	P484	I416	V345	I267	R193	G112	G34	MET
SER	SER	R632	S549	G485	I417	S346	I268	I194	N113	D85	SER
ASP	ASP	G633	S549	K486	V418	S347	I269	I195	L114	D86	ASP
GLY	GLY	L634	I550	Y487	G419	G274	G274	E196	L115	Q37	TYR
GLN	GLN	V635	G551	L488	A420	E351	D277	V197	Q116	N40	HIS
LEU	LEU	L636	I556	E490	P421	R354	D277	V198	R117	N41	HIS
GLY	GLY	R637	I557	I491	A422	L355	N280	D199	G118	A41	HIS
LYS	LYS	N638	I557	A492	A423	L356	I283	A200	T119	A42	HIS
LYS	LYS	E639	I560	A492	A424	L357	I284	I201	T120	V43	HIS
VAL	VAL	S640	T560	M495	M425	L357	I284	A205	N121	R44	HIS
GLN	GLN	C641	T560	M495	M426	L357	I284	A205	N121	R44	ASP
PRO	PRO	D642	B565	H498	V429	C360	S285	H208	V124	R43	TYR
TRP	TRP	D643	B566	S499	R430	C361	S286	Q209	D128	R43	ASP
SER	SER	P649	B567	S499	S431	V361	K287	Q209	D128	M49	ILE
VAL	VAL	I650	Q568	N501	A432	V362	E290	R210	G129	G50	PRO
		G572	G572	A502	V433	T364	E290	T211	S130	I51	THR
		Q652	G572	L503	R434	T364	L291	F212	V52	Y52	THR
			R575	L504	V435	Q365	V292	V213	V53	V53	GLU
			R576	L505		A370	V293	L214	G54	G54	ASN
			R577	I506	A438	R374	T294	E215			LEU
			R578	I506	D439	R375	T294	E216			TYR
			R579	G507	D439	R376	T294	V216			PHE
			R580	G508		F376	T294	M217			GLN
			R581	F509			T294	G218			GLY
			R582	E510			T294	G218			ALA
			R583	E511			T294	G218			MET
			R584	E511			T294	G218			ASP
			R585	E511			T294	G218			ALA
			R586	E511			T294	G218			ASP
			R587	E511			T294	G218			ASP
			R588	E511			T294	G218			ASP
			R589	E511			T294	G218			ASP
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			R705	E511			T294	G218			ASP
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			R708	E511			T294	G218			ASP
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			R711	E511			T294	G218			ASP
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			R713	E511			T294	G218			ASP
			R714	E511			T294	G218			ASP
			R715	E511			T294	G218			ASP
			R716	E511			T294	G218			ASP
			R717	E511			T294	G218			ASP
			R718	E511			T294	G218			ASP
			R719	E511			T294	G218			ASP
			R720	E511			T294	G218			ASP
			R721	E511			T294				



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.34Å 168.37Å 133.27Å 90.00° 103.78° 90.00°	Depositor
Resolution (Å)	45.37 – 3.40 45.37 – 3.40	Depositor EDS
% Data completeness (in resolution range)	74.2 (45.37-3.40) 84.5 (45.37-3.40)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 3.40Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.256 , 0.290 0.250 , 0.262	Depositor DCC
$R_{free}$ test set	3943 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.6	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 14.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	22897	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, ADP

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	0.57	1/5730 (0.0%)	0.75	15/7735 (0.2%)
1	B	0.55	0/5819	0.85	18/7854 (0.2%)
1	C	0.54	1/5773 (0.0%)	0.81	16/7795 (0.2%)
1	D	0.53	0/5773	0.89	16/7795 (0.2%)
All	All	0.55	2/23095 (0.0%)	0.83	65/31179 (0.2%)

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	5
1	B	0	4
1	C	0	4
1	D	0	2
All	All	0	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	664	CYS	CB-SG	-6.17	1.71	1.82
1	A	360	CYS	CB-SG	-5.68	1.72	1.81

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	ARG	NE-CZ-NH2	-22.12	109.24	120.30
1	D	374	ARG	NE-CZ-NH1	-21.17	109.71	120.30
1	D	374	ARG	NE-CZ-NH2	21.17	130.88	120.30

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*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	665	ARG	NE-CZ-NH1	-20.40	110.10	120.30
1	C	97	ARG	NE-CZ-NH1	19.91	130.25	120.30

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	ARG	Sidechain
1	A	262	ARG	Sidechain
1	A	301	ARG	Sidechain
1	A	632	ARG	Sidechain
1	A	692	ARG	Sidechain

## 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	5640	0	5674	340	0
1	B	5727	0	5764	340	0
1	C	5681	0	5709	358	0
1	D	5681	0	5709	376	0
2	A	27	0	12	2	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	0	0
3	A	15	0	0	2	0
3	B	10	0	0	0	0
3	C	20	0	0	1	0
3	D	15	0	0	1	0
All	All	22897	0	22904	1376	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 30.

The worst 5 of 1376 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:D:480:LYS:HB3	1:D:482:VAL:HG23	1.29	1.05
1:B:522:ARG:HH12	1:B:529:CYS:HA	1.25	1.00
1:D:532:MET:HB2	1:D:717:ILE:HG22	1.41	1.00
1:A:539:VAL:HG11	1:A:674:GLN:HB3	1.43	0.99
1:A:121:ASN:HB3	1:A:333:LEU:HD22	1.46	0.97

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	731/812 (90%)	610 (83%)	95 (13%)	26 (4%)	3	21
1	B	745/812 (92%)	631 (85%)	87 (12%)	27 (4%)	3	21
1	C	739/812 (91%)	620 (84%)	97 (13%)	22 (3%)	4	23
1	D	739/812 (91%)	618 (84%)	101 (14%)	20 (3%)	5	26
All	All	2954/3248 (91%)	2479 (84%)	380 (13%)	95 (3%)	4	22

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ASP
1	A	724	LYS
1	B	724	LYS
1	C	19	HIS
1	C	724	LYS

### 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	594/658 (90%)	516 (87%)	78 (13%)	4	15
1	B	602/658 (92%)	529 (88%)	73 (12%)	5	18
1	C	598/658 (91%)	518 (87%)	80 (13%)	4	15
1	D	598/658 (91%)	517 (86%)	81 (14%)	4	14
All	All	2392/2632 (91%)	2080 (87%)	312 (13%)	4	16

5 of 312 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	671	HIS
1	C	230	LEU
1	D	519	SER
1	B	702	LYS
1	C	59	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	65	GLN
1	C	295	GLN
1	D	541	ASN
1	C	73	ASN
1	C	116	GLN

### 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

16 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	PO4	A	804	-	4,4,4	1.64	1 (25%)	6,6,6	0.46	0
3	PO4	D	804	-	4,4,4	1.56	0	6,6,6	0.45	0
3	PO4	C	804	-	4,4,4	1.47	0	6,6,6	0.42	0
3	PO4	A	803	-	4,4,4	1.39	0	6,6,6	0.40	0
3	PO4	D	801	-	4,4,4	1.54	0	6,6,6	0.46	0
3	PO4	C	803	-	4,4,4	1.57	0	6,6,6	0.51	0
3	PO4	C	802	-	4,4,4	1.64	1 (25%)	6,6,6	0.40	0
2	ADP	A	801	-	24,29,29	1.33	2 (8%)	29,45,45	1.26	4 (13%)
3	PO4	A	802	-	4,4,4	1.64	0	6,6,6	0.45	0
2	ADP	C	801	-	24,29,29	1.51	3 (12%)	29,45,45	1.18	3 (10%)
3	PO4	B	802	-	4,4,4	1.51	0	6,6,6	0.41	0
2	ADP	B	801	-	24,29,29	1.67	4 (16%)	29,45,45	1.25	4 (13%)
2	ADP	D	802	-	24,29,29	1.84	5 (20%)	29,45,45	1.37	4 (13%)
3	PO4	B	803	-	4,4,4	1.52	0	6,6,6	0.44	0
3	PO4	C	805	-	4,4,4	1.56	0	6,6,6	0.41	0
3	PO4	D	803	-	4,4,4	1.61	1 (25%)	6,6,6	0.42	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	801	-	-	4/12/32/32	0/3/3/3
2	ADP	C	801	-	-	3/12/32/32	0/3/3/3
2	ADP	B	801	-	-	0/12/32/32	0/3/3/3
2	ADP	D	802	-	-	1/12/32/32	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	802	ADP	PB-O1B	6.40	1.71	1.50
2	B	801	ADP	PB-O1B	5.95	1.69	1.50
2	C	801	ADP	PB-O3B	3.85	1.69	1.54
2	A	801	ADP	PB-O3B	3.54	1.68	1.54
2	D	802	ADP	O4'-C1'	3.47	1.45	1.41

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ADP	O2B-PB-O3A	3.38	115.98	104.64
2	C	801	ADP	C5-C6-N6	3.25	125.29	120.35
2	D	802	ADP	O5'-C5'-C4'	3.18	119.92	108.99
2	D	802	ADP	C5-C6-N6	3.16	125.16	120.35
2	C	801	ADP	O2B-PB-O3A	2.80	114.03	104.64

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ADP	PA-O3A-PB-O2B
2	A	801	ADP	C5'-O5'-PA-O1A
2	C	801	ADP	C3'-C4'-C5'-O5'
2	C	801	ADP	O4'-C4'-C5'-O5'
2	C	801	ADP	C4'-C5'-O5'-PA

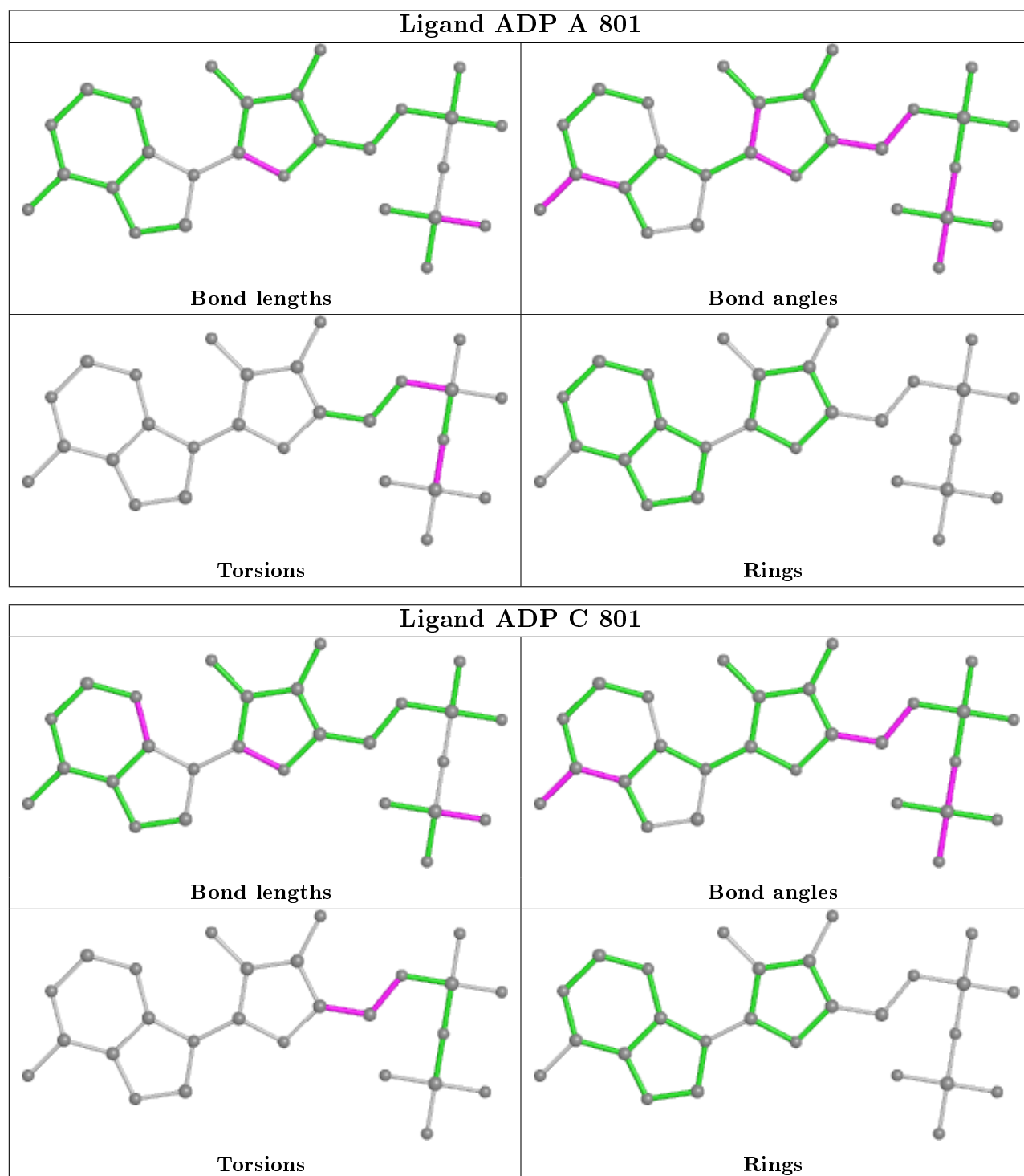
There are no ring outliers.

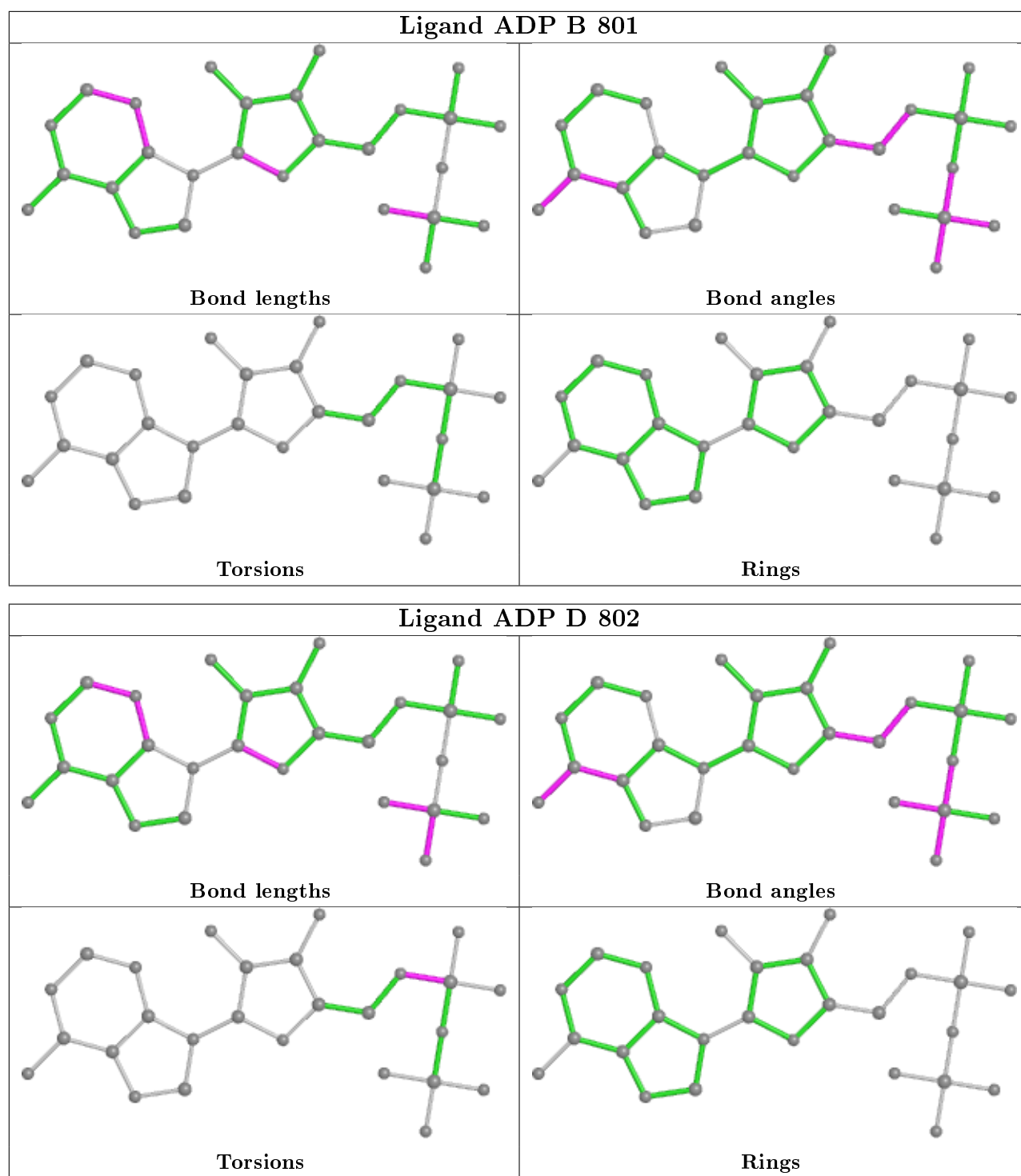
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	PO4	2	0
3	D	801	PO4	1	0
2	A	801	ADP	2	0
2	C	801	ADP	1	0
2	B	801	ADP	1	0
3	C	805	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 ⓘ

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	737/812 (90%)	-0.17	4 (0%) 91 90	27, 73, 113, 162	0
1	B	749/812 (92%)	-0.11	7 (0%) 84 83	25, 75, 114, 162	0
1	C	743/812 (91%)	-0.16	2 (0%) 94 93	26, 73, 112, 161	0
1	D	743/812 (91%)	-0.14	4 (0%) 91 90	29, 74, 113, 162	0
All	All	2972/3248 (91%)	-0.14	17 (0%) 89 89	25, 74, 113, 162	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	PRO	3.2
1	D	343	CYS	2.9
1	B	59	PHE	2.8
1	B	205	ALA	2.8
1	B	206	GLN	2.5

### 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](#)

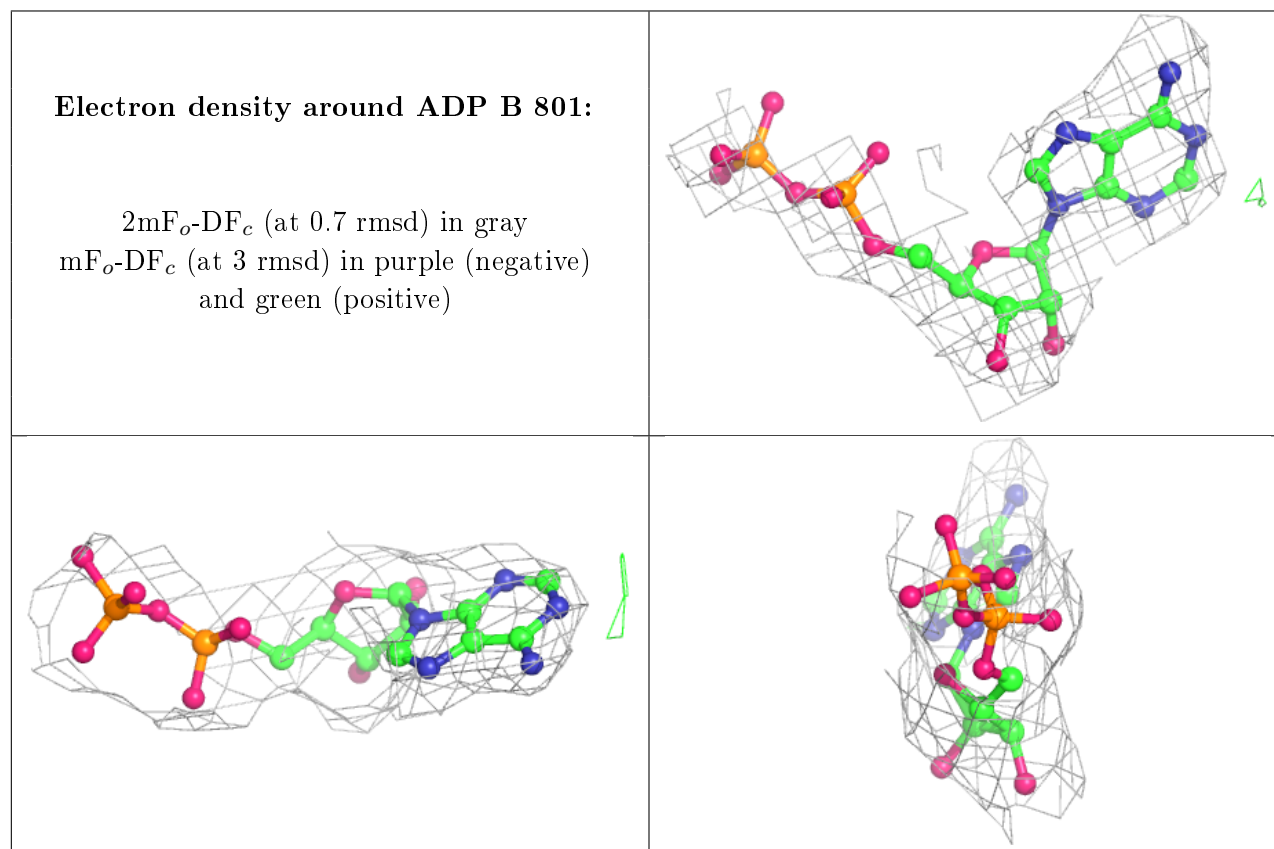
There are no monosaccharides in this entry.

### 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
3	PO4	C	804	5/5	0.90	0.19	6,89,105,127	0
3	PO4	A	803	5/5	0.91	0.17	17,29,126,144	0
3	PO4	C	805	5/5	0.91	0.12	65,81,155,163	0
2	ADP	B	801	27/27	0.92	0.17	21,98,154,163	0
2	ADP	C	801	27/27	0.94	0.17	35,98,135,151	0
3	PO4	C	803	5/5	0.94	0.15	1,20,85,87	0
2	ADP	D	802	27/27	0.94	0.21	1,91,129,134	0
2	ADP	A	801	27/27	0.94	0.19	1,73,118,137	0
3	PO4	B	803	5/5	0.95	0.16	7,34,89,107	0
3	PO4	B	802	5/5	0.95	0.12	16,71,134,135	0
3	PO4	D	801	5/5	0.96	0.14	14,27,57,97	0
3	PO4	C	802	5/5	0.97	0.12	1,66,70,97	0
3	PO4	A	802	5/5	0.97	0.13	1,67,103,108	0
3	PO4	D	803	5/5	0.97	0.10	31,32,74,82	0
3	PO4	D	804	5/5	0.98	0.13	18,41,68,78	0
3	PO4	A	804	5/5	0.99	0.13	4,10,57,70	0

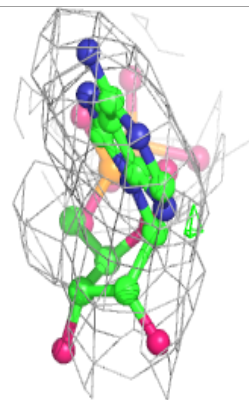
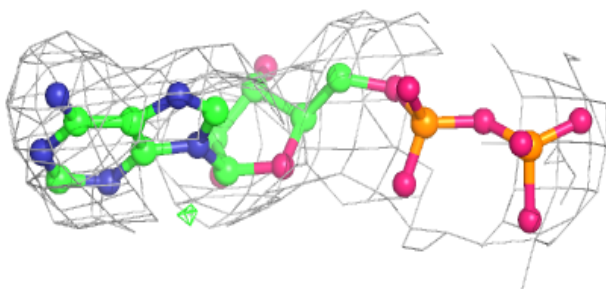
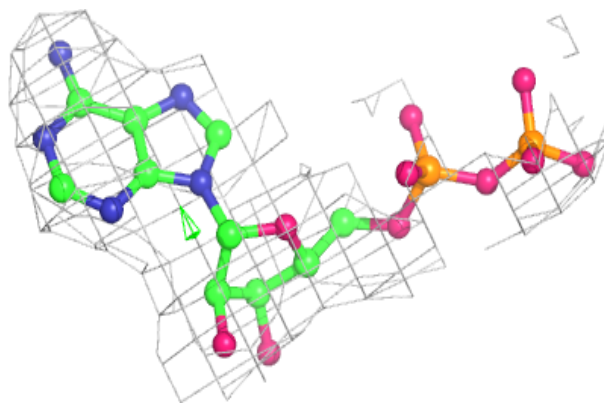
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



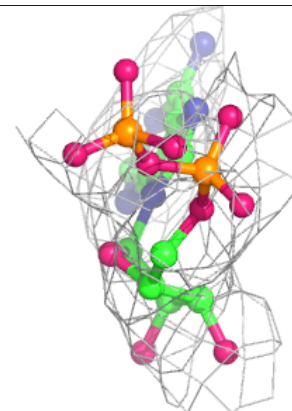
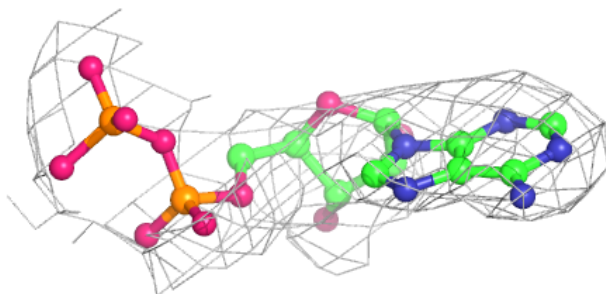
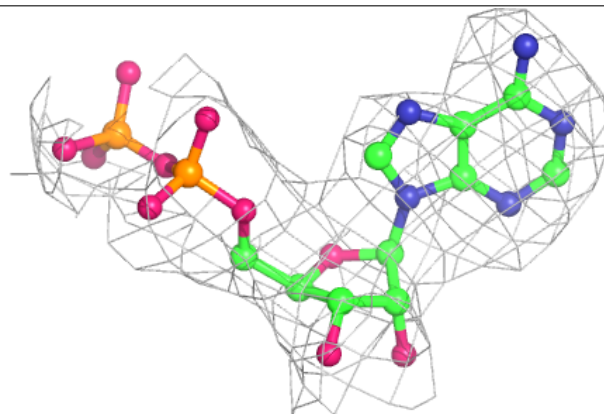


**Electron density around ADP C 801:**

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

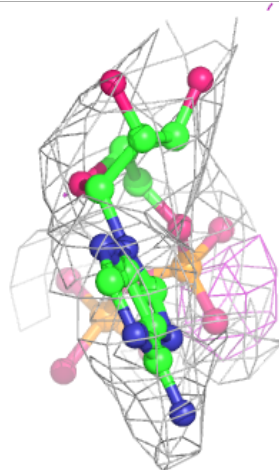
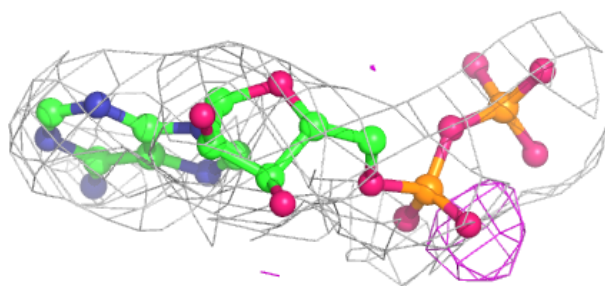
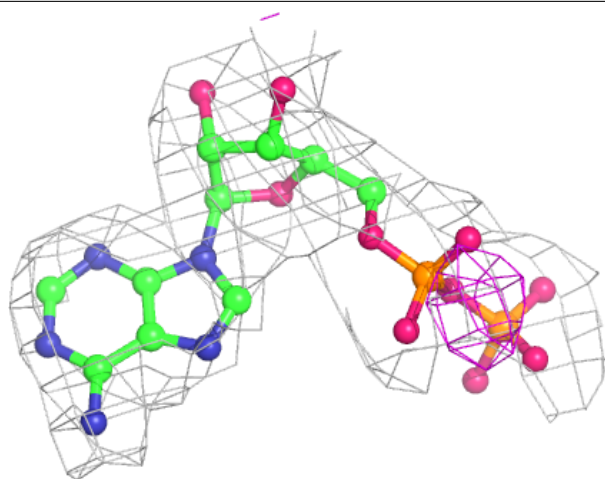
**Electron density around ADP D 802:**

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



**Electron density around ADP A 801:**

$2mF_o-DF_c$  (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.