



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:28 PM UTC

PDB ID : 4XYK / pdb_00004xyk
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

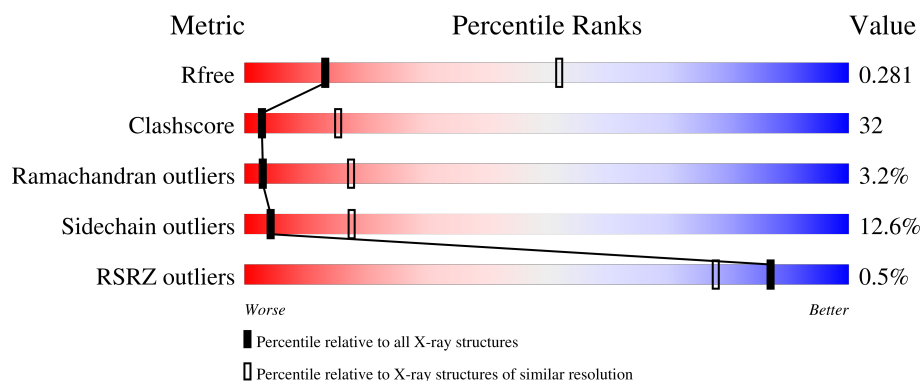
1 Overall quality at a glance

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 ≥ 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 criteria:

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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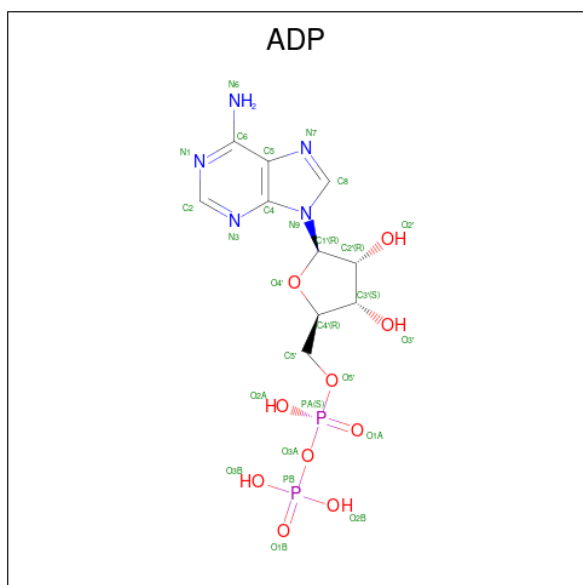
Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	HIS	-	expression tag	UNP Q01813
C	-19	HIS	-	expression tag	UNP Q01813
C	-18	HIS	-	expression tag	UNP Q01813
C	-17	ASP	-	expression tag	UNP Q01813
C	-16	TYR	-	expression tag	UNP Q01813
C	-15	ASP	-	expression tag	UNP Q01813
C	-14	ILE	-	expression tag	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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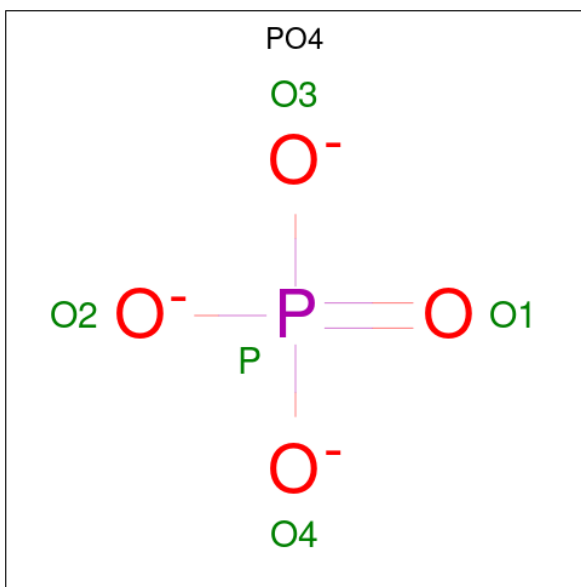
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	PHE	-	expression tag	UNP Q01813
D	-5	GLN	-	expression tag	UNP Q01813
D	-4	GLY	-	expression tag	UNP Q01813
D	-3	ALA	-	expression tag	UNP Q01813
D	-2	MET	-	expression tag	UNP Q01813
D	-1	ASP	-	expression tag	UNP Q01813
D	0	PRO	-	expression tag	UNP Q01813

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



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

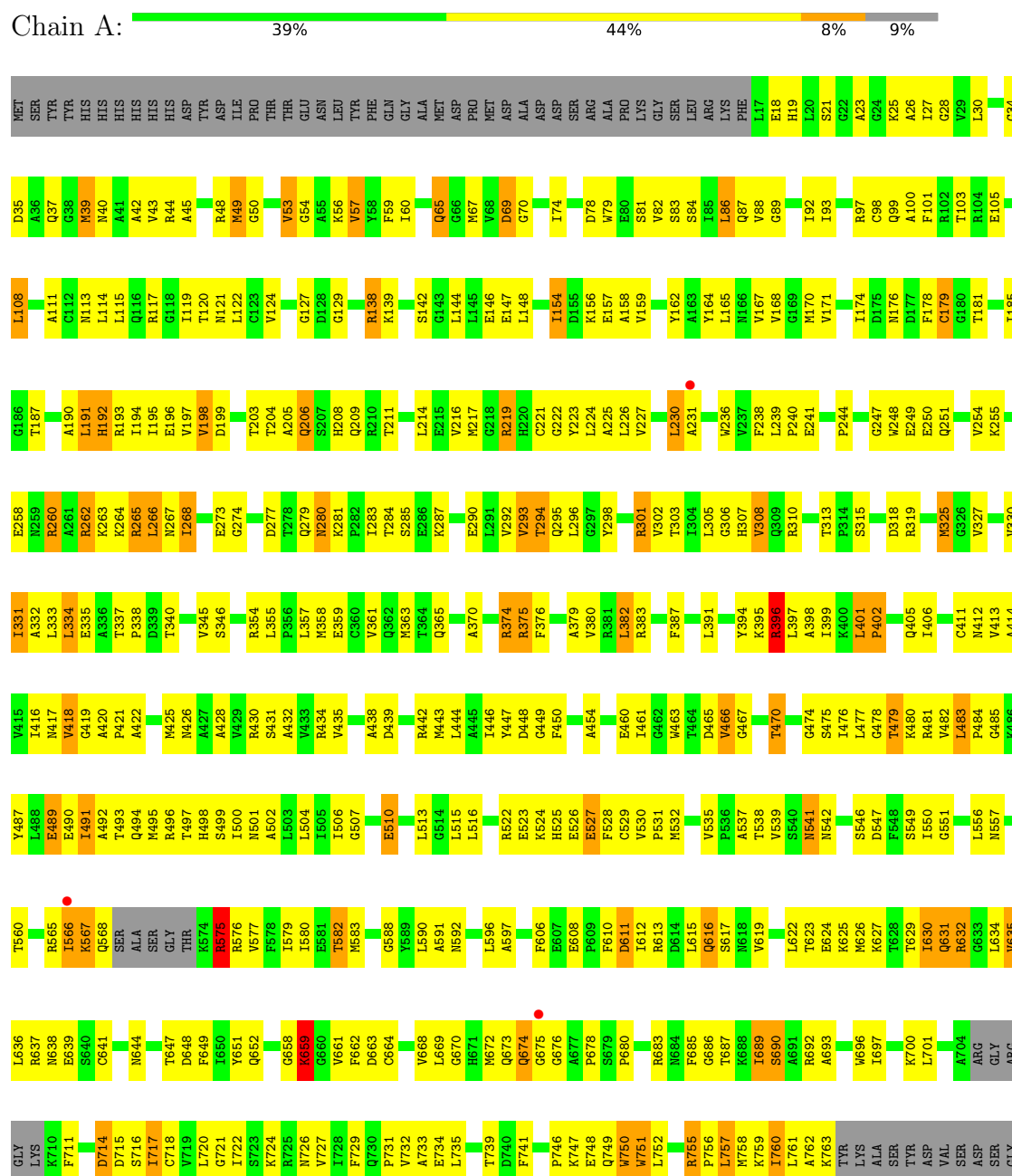


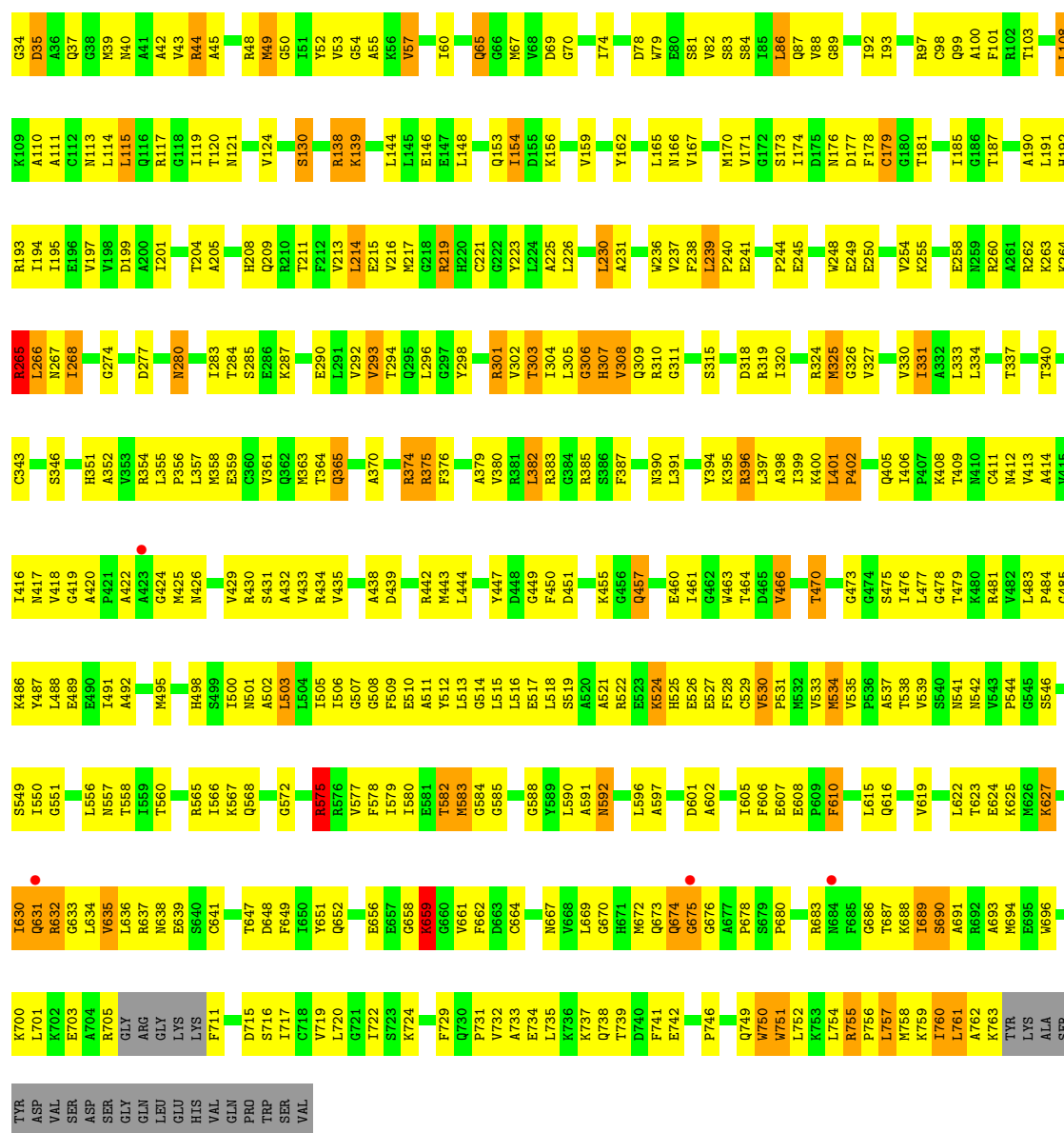
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total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

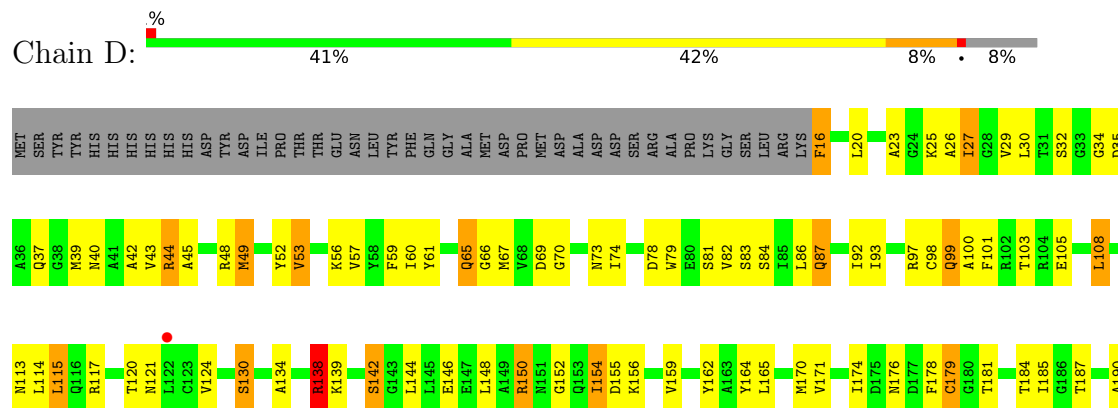
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type



TRP	V719	T647	L491	V418	R339	K264	L191
SER	L720	Q652	A492	G419	T340	R265	H192
VAL	G721	Q652	A420	A421	C343	L266	R193
	I722	S655	M495	P421	C343	N267	I194
	S723	S656	R496	A422	V344	I268	I195
	K724	E657	T497	A423	V345	E196	E196
	R725	E657	H498	G424	S346	V197	
	N726	G658	S499	M425	A352	A200	
	V727	R575	T500	M426	V353	M202	
	L669	R576	N501	V429	R354	I201	
	E734	G660	A502	R430	L355	T278	
	L735	F578	L503	S431	M358	Q279	
	K736	F662	L504	A432	E359	T204	
	Q737	D663	L505	V433	T364	M280	
	P731	C664	E581	R434	Q365	A205	
	V732		F582	V435	A370	Q206	
	A733	L669	E510	D439	R374	S207	
	E734	G670	A511	R442	R375	I283	
	L735	M671	Y512	L444	V291	Q209	
	K736	M672	Y512	L444	V292	H208	
	Q737	Q673	L515	R447	V293	Q210	
	T738	Q674	L516	Y447	T294	T211	
	T739	G675	L517	D448	V295	L214	
	D740	G676	F528	L448	R381	E215	
		G677	C529	Y449	R382	M216	
	H743	A677	V530	D449	R383	M217	
		P678	P531	D449	G384	G218	
	P746	S679	H621	F450	R385	H219	
	K747	P680	L622	F450	V380	H220	
	E748	R683	E624	A454	L392	C221	
	Q749	M684	E625	A454	R393	Q222	
	W750	F685	H626	T470	G384	Q222	
	W751	G686	K627	T470	R384	Y223	
	L752	T687	L615	T470	R385	L224	
		K688	V619	T470	S386	A225	
	R755	L689	E620	T470	F387	L226	
	P756	S690	H621	T470	N390	L230	
	L757	M694	L622	T470	L391	A231	
	M758	E695	E624	T470	Y394	W236	
	K759	W696	E625	T470	K395	V237	
	I760	I697	K625	T470	Q309	F238	
	L761	K700	K626	T470	R396	L239	
	A762	L701	K627	T470	L397	P240	
	K763	K702	T630	T470	A398		
TYR	LYS	R705	V639	T470	I399	P244	
LYS	ALA	GLY	S540	T470	K400		
LYS	SER	ARG	N541	T470	R401	W248	
ASP	TYR	GLY	P544	T470	P402	R319	
VAL	VAL	GLY	G545	T470	D403	I320	
SER	SER	LYS	S546	T470	D404	E250	
ASP	ASP	LYS	D547	T470	Q405	Q251	
SER	SER	LYS	F711	T470	V327	V254	
GLY	GLY	LYS	T712	T470	M325	K255	
GLN	GLN	LYS	F548	T470	G326		
LEU	LEU	LYS	S549	T470	V327		
GLU	GLU	LYS	I550	T470	I331	E258	
HIS	HIS	ASP	C641	T470	A332	W259	
VAL	VAL	ASP	N644	T470	L333	R260	
GLN	GLN	ASP		T470	L334	A261	
PRO	PRO	ASP		T470	T337	R262	
		ASP		T470	P338	K263	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.40Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.256 , 0.290 0.269 , 0.281	Depositor DCC
R_{free} test set	3943 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	69.6	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ADP, 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	0.70	0/5730	0.95	5/7735 (0.1%)
1	B	0.68	0/5819	0.97	20/7854 (0.3%)
1	C	0.69	1/5773 (0.0%)	0.96	12/7795 (0.2%)
1	D	0.68	1/5773 (0.0%)	1.00	21/7795 (0.3%)
All	All	0.68	2/23095 (0.0%)	0.97	58/31179 (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	D	134	ALA	CA-CB	-5.33	1.44	1.53
1	C	55	ALA	CA-CB	-5.15	1.46	1.53

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	374	ARG	NE-CZ-NH2	12.98	130.88	119.20
1	D	374	ARG	NE-CZ-NH1	-11.79	109.71	121.50
1	B	665	ARG	NE-CZ-NH1	-11.40	110.10	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	ARG	NE-CZ-NH2	-11.07	109.24	119.20
1	B	665	ARG	NE-CZ-NH2	10.87	128.98	119.20

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 [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	5640	0	5674	365	0
1	B	5727	0	5764	371	0
1	C	5681	0	5709	382	0
1	D	5681	0	5709	408	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	1487	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 32.

The worst 5 of 1487 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:512:TYR:HA	1:D:534:MET:HE1	1.36	1.06
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

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%)	2	16
1	B	745/812 (92%)	631 (85%)	87 (12%)	27 (4%)	2	16
1	C	739/812 (91%)	620 (84%)	97 (13%)	22 (3%)	3	18
1	D	739/812 (91%)	618 (84%)	101 (14%)	20 (3%)	4	20
All	All	2954/3248 (91%)	2479 (84%)	380 (13%)	95 (3%)	3	17

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%)	517 (87%)	77 (13%)	4	16
1	B	602/658 (92%)	531 (88%)	71 (12%)	5	20
1	C	598/658 (91%)	523 (88%)	75 (12%)	4	18
1	D	598/658 (91%)	520 (87%)	78 (13%)	4	16
All	All	2392/2632 (91%)	2091 (87%)	301 (13%)	4	18

5 of 301 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	65	GLN
1	D	624	GLU
1	D	115	LEU
1	D	325	MET
1	D	763	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	206	GLN
1	D	730	GLN
1	D	280	ASN
1	D	541	ASN
1	B	135	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	C	803	-	4,4,4	1.62	0	6,6,6	0.54	0
3	PO4	A	803	-	4,4,4	1.44	0	6,6,6	0.43	0
3	PO4	B	802	-	4,4,4	1.57	1 (25%)	6,6,6	0.44	0
3	PO4	D	804	-	4,4,4	1.61	0	6,6,6	0.49	0
3	PO4	B	803	-	4,4,4	1.57	0	6,6,6	0.47	0
3	PO4	A	802	-	4,4,4	1.69	0	6,6,6	0.48	0
3	PO4	D	803	-	4,4,4	1.66	1 (25%)	6,6,6	0.45	0
2	ADP	C	801	-	28,29,29	1.87	4 (14%)	43,45,45	0.95	2 (4%)
2	ADP	B	801	-	28,29,29	2.21	4 (14%)	43,45,45	1.11	5 (11%)
3	PO4	C	805	-	4,4,4	1.61	1 (25%)	6,6,6	0.44	0
2	ADP	D	802	-	28,29,29	2.42	6 (21%)	43,45,45	1.24	5 (11%)
3	PO4	A	804	-	4,4,4	1.69	1 (25%)	6,6,6	0.49	0
3	PO4	C	804	-	4,4,4	1.52	0	6,6,6	0.46	0
3	PO4	C	802	-	4,4,4	1.70	1 (25%)	6,6,6	0.43	0
3	PO4	D	801	-	4,4,4	1.59	1 (25%)	6,6,6	0.50	0
2	ADP	A	801	-	28,29,29	1.73	3 (10%)	43,45,45	1.11	3 (6%)

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	C	801	-	-	3/16/32/32	0/3/3/3
2	ADP	A	801	-	-	3/16/32/32	0/3/3/3
2	ADP	B	801	-	-	0/16/32/32	0/3/3/3
2	ADP	D	802	-	-	0/16/32/32	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	802	ADP	PA-O3A	-8.98	1.49	1.59
2	B	801	ADP	PA-O3A	-7.67	1.51	1.59
2	A	801	ADP	PA-O3A	-6.87	1.52	1.59
2	D	802	ADP	PB-O1B	6.66	1.71	1.50
2	C	801	ADP	PA-O3A	-6.62	1.52	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	802	ADP	O4'-C1'-N9	3.46	114.73	108.09
2	A	801	ADP	O2B-PB-O3A	3.38	115.98	104.64
2	D	802	ADP	O5'-C5'-C4'	3.21	119.92	108.99
2	A	801	ADP	O4'-C1'-N9	2.93	113.72	108.09
2	C	801	ADP	O2B-PB-O3A	2.80	114.03	104.64

There are no chirality outliers.

5 of 6 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

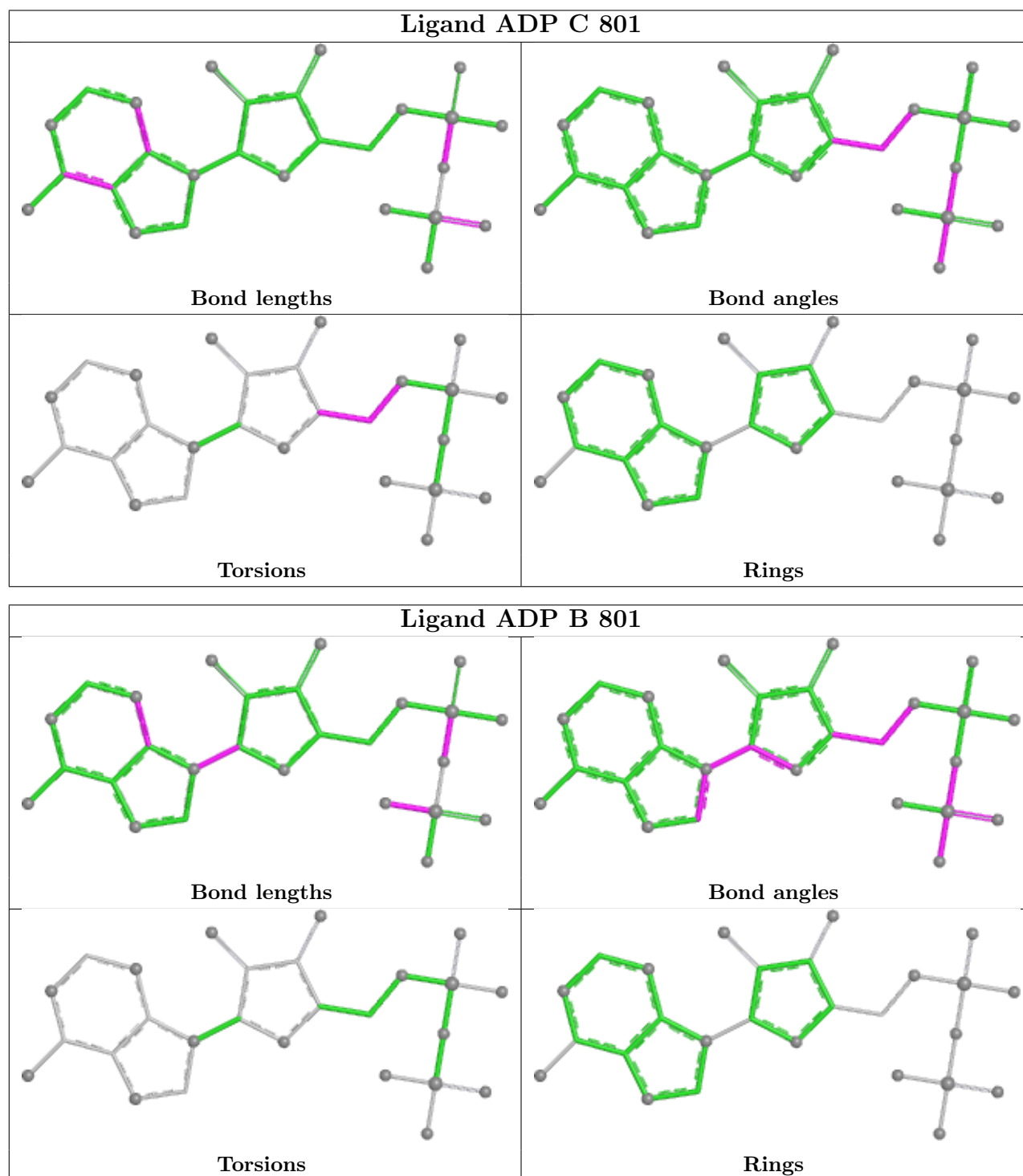
There are no ring outliers.

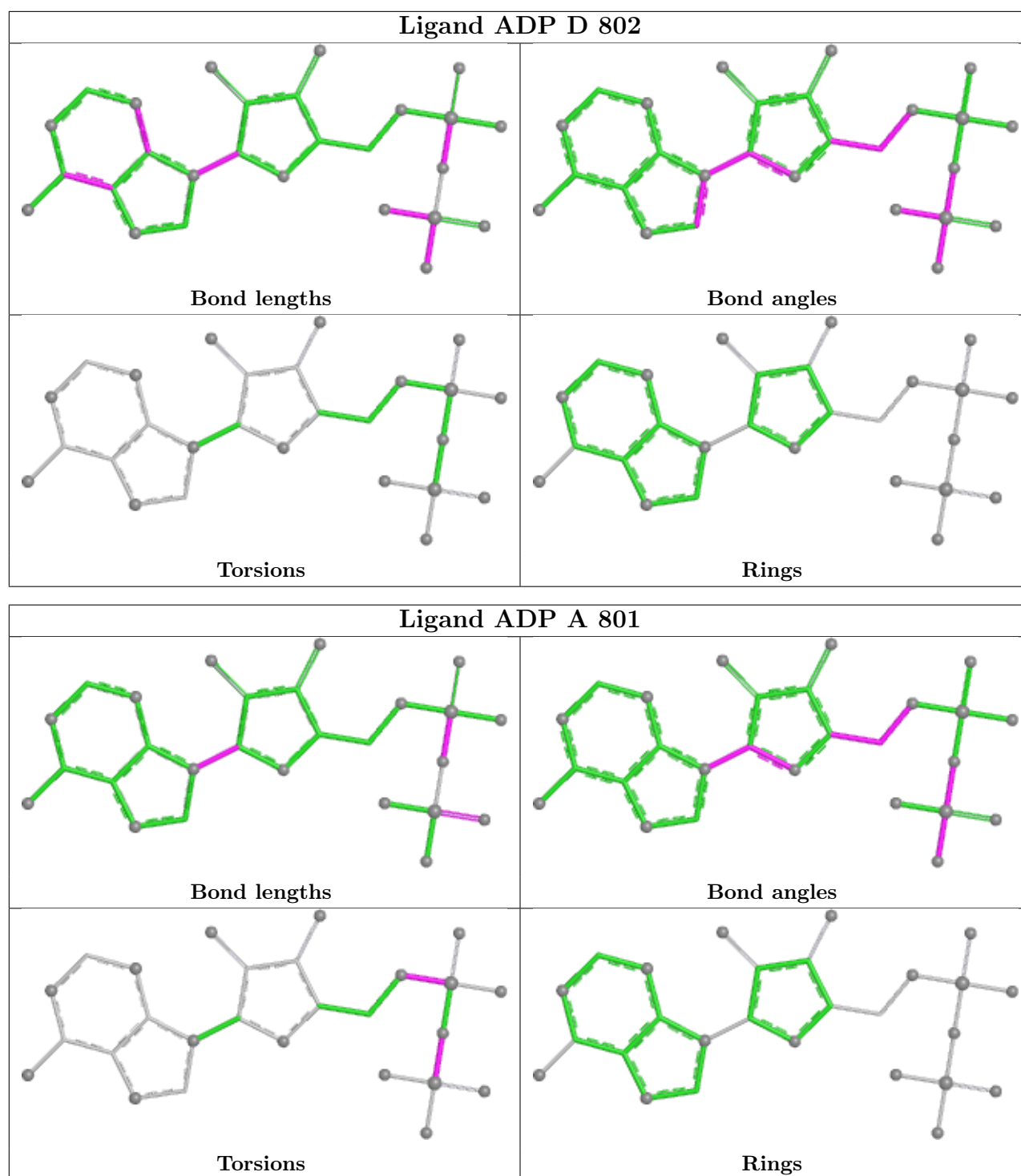
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	PO4	2	0
2	C	801	ADP	1	0
2	B	801	ADP	1	0
3	C	805	PO4	1	0
3	D	801	PO4	1	0
2	A	801	ADP	2	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, 95th 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 ²)	Q<0.9
1	A	737/812 (90%)	-0.06	3 (0%) 88 81	27, 73, 113, 162	0
1	B	749/812 (92%)	-0.06	3 (0%) 88 81	25, 75, 114, 162	0
1	C	743/812 (91%)	-0.13	4 (0%) 87 78	26, 73, 112, 161	0
1	D	743/812 (91%)	-0.12	6 (0%) 82 71	28, 74, 113, 162	0
All	All	2972/3248 (91%)	-0.09	16 (0%) 87 78	25, 74, 113, 162	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	ALA	3.3
1	D	435	VAL	3.0
1	B	204	THR	3.0
1	D	122	LEU	2.7
1	D	344	VAL	2.7

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](#)

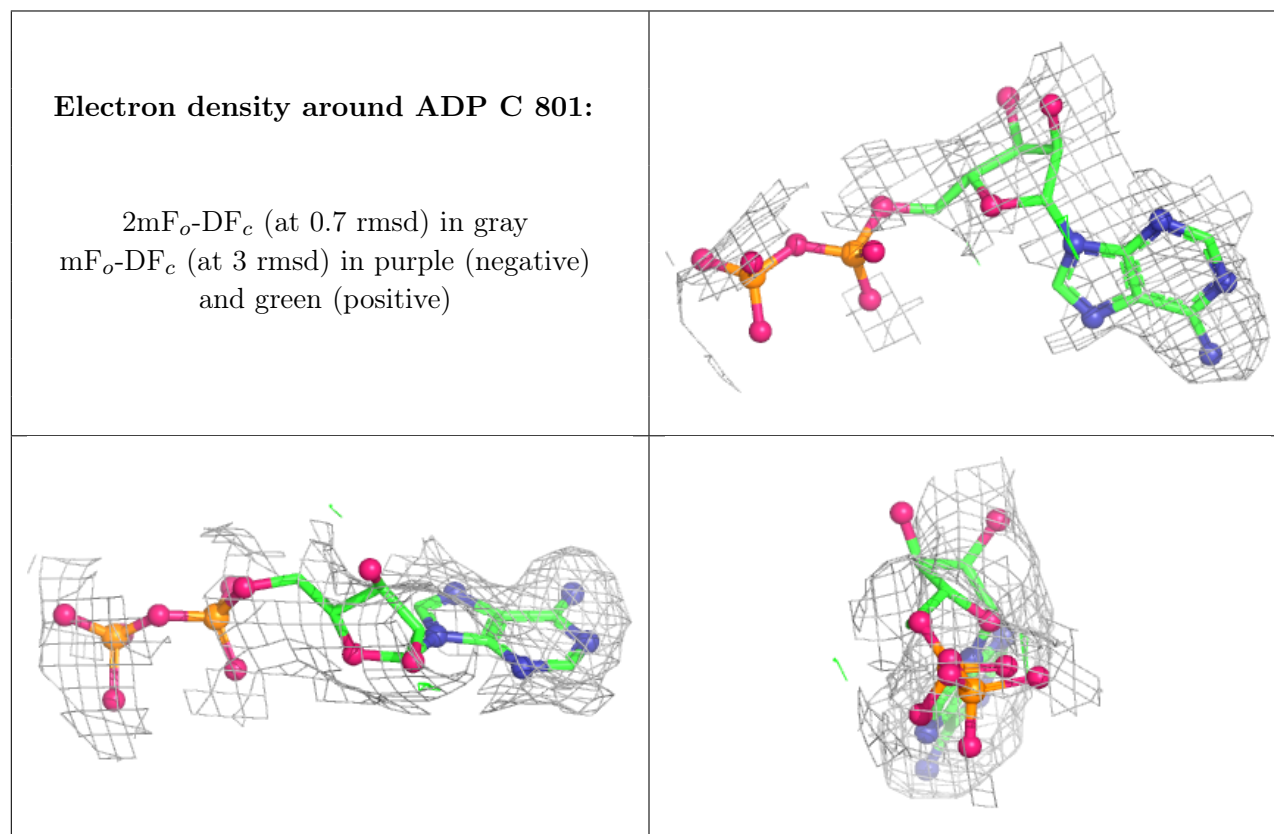
There are no oligosaccharides in this entry.

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, 95th 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.

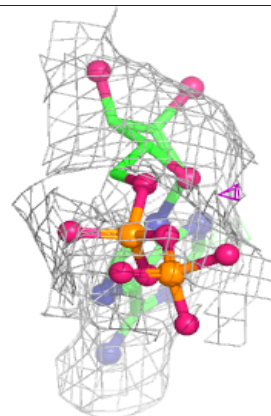
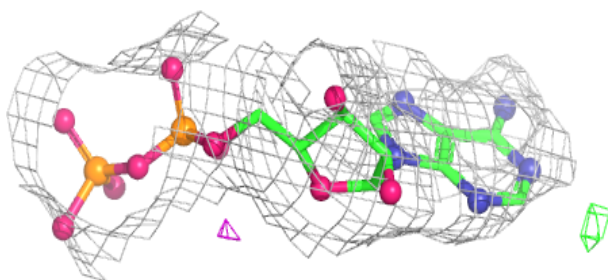
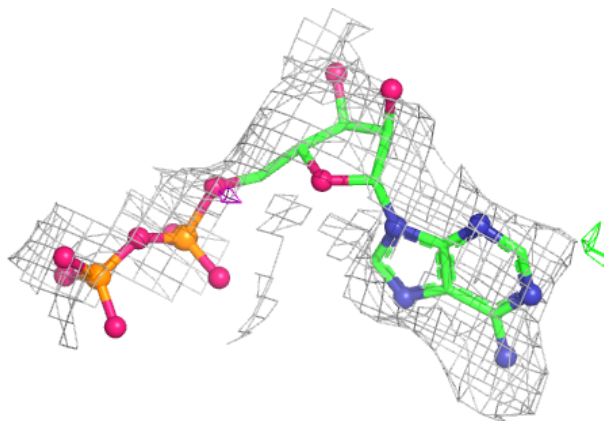
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	C	804	5/5	0.79	0.11	6,89,105,127	0
2	ADP	C	801	27/27	0.87	0.09	35,98,135,151	0
2	ADP	B	801	27/27	0.87	0.09	21,98,154,163	0
3	PO4	B	802	5/5	0.88	0.09	16,71,134,135	0
2	ADP	A	801	27/27	0.88	0.09	1,73,118,137	0
3	PO4	D	803	5/5	0.88	0.09	31,32,74,82	0
3	PO4	D	801	5/5	0.89	0.07	14,27,57,97	0
3	PO4	C	805	5/5	0.91	0.06	65,81,155,163	0
3	PO4	A	802	5/5	0.92	0.08	1,67,103,108	0
3	PO4	A	803	5/5	0.93	0.10	17,29,126,144	0
3	PO4	C	803	5/5	0.93	0.07	1,20,85,87	0
3	PO4	C	802	5/5	0.94	0.05	1,66,70,97	0
2	ADP	D	802	27/27	0.94	0.08	1,91,129,134	0
3	PO4	B	803	5/5	0.94	0.07	7,34,89,107	0
3	PO4	D	804	5/5	0.96	0.06	18,41,68,78	0
3	PO4	A	804	5/5	0.97	0.04	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.



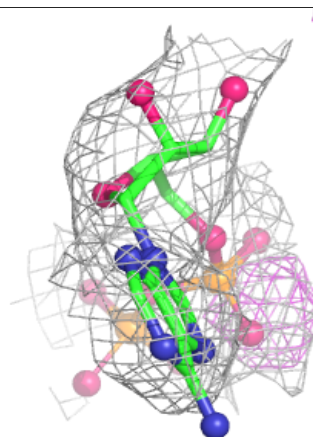
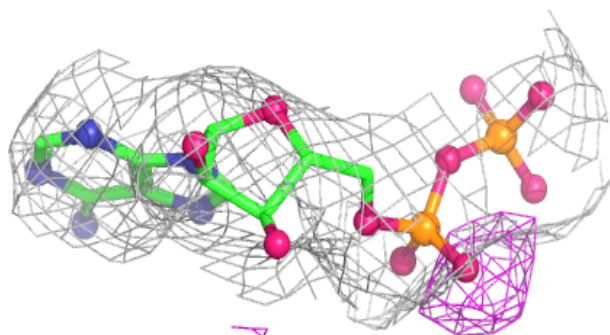
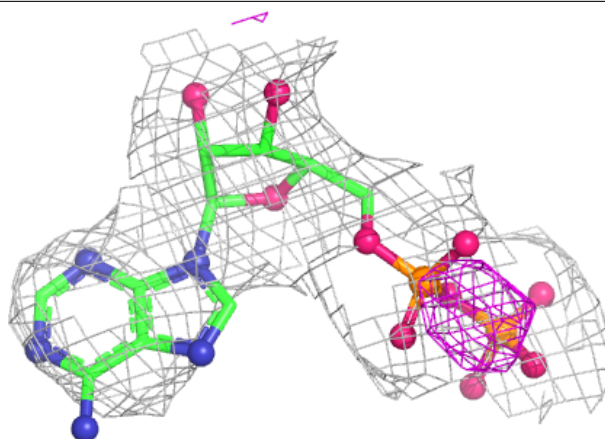
Electron density around ADP B 801:

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

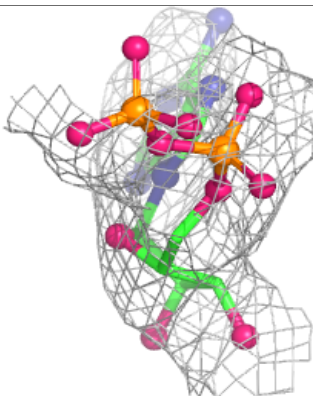
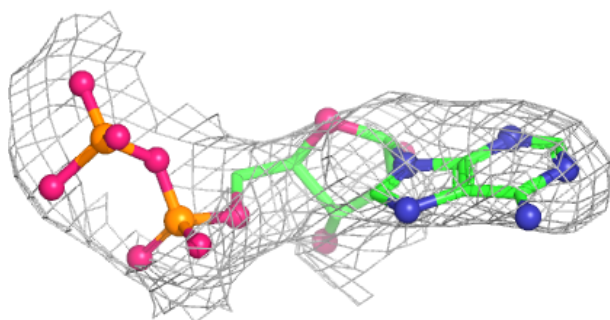
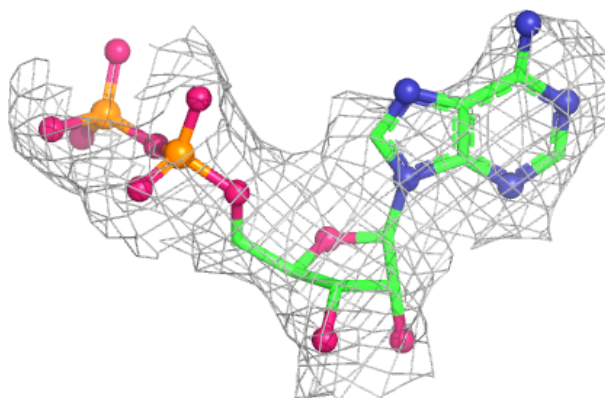


Electron density around ADP A 801:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.