



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2025 – 07:59 PM EDT

PDB ID : 1Z0S / pdb\_00001z0s  
Title : Crystal structure of an NAD kinase from *Archaeoglobus fulgidus* in complex with ATP  
Authors : Liu, J.; Lou, Y.; Yokota, H.; Adams, P.D.; Kim, R.; Kim, S.H.; Berkeley Structural Genomics Center (BSGC)  
Deposited on : 2005-03-02  
Resolution : 1.70 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	:	4.02b-467
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)	:	2.42

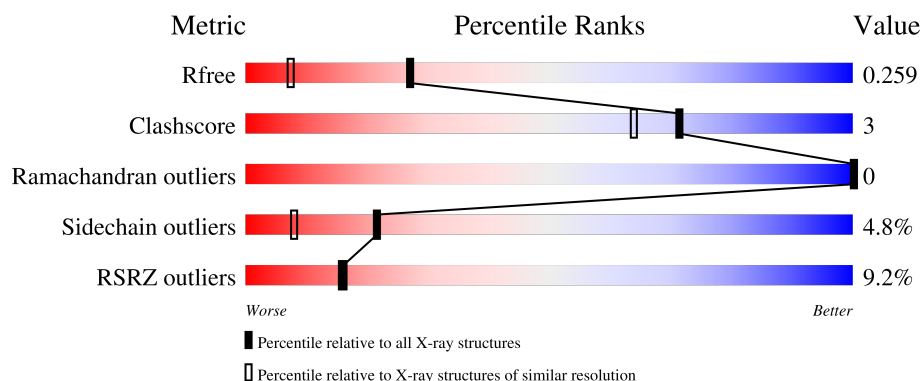
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

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	278	
1	B	278	
1	C	278	
1	D	278	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8423 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 Probable inorganic polyphosphate/ATP-NAD kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1963	1266	334	355	8			
1	B	249	Total	C	N	O	S	0	0	0
			1963	1266	334	355	8			
1	C	249	Total	C	N	O	S	0	0	0
			1963	1266	334	355	8			
1	D	249	Total	C	N	O	S	0	0	0
			1963	1266	334	355	8			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	cloning artifact	UNP O30297
A	-27	GLY	-	cloning artifact	UNP O30297
A	-26	SER	-	cloning artifact	UNP O30297
A	-25	SER	-	cloning artifact	UNP O30297
A	-24	HIS	-	cloning artifact	UNP O30297
A	-23	HIS	-	cloning artifact	UNP O30297
A	-22	HIS	-	cloning artifact	UNP O30297
A	-21	HIS	-	cloning artifact	UNP O30297
A	-20	HIS	-	cloning artifact	UNP O30297
A	-19	HIS	-	cloning artifact	UNP O30297
A	-18	ASP	-	cloning artifact	UNP O30297
A	-17	TYR	-	cloning artifact	UNP O30297
A	-16	ASP	-	cloning artifact	UNP O30297
A	-15	ILE	-	cloning artifact	UNP O30297
A	-14	PRO	-	cloning artifact	UNP O30297
A	-13	THR	-	cloning artifact	UNP O30297
A	-12	THR	-	cloning artifact	UNP O30297
A	-11	GLU	-	cloning artifact	UNP O30297
A	-10	ASN	-	cloning artifact	UNP O30297
A	-9	LEU	-	cloning artifact	UNP O30297
A	-8	TYR	-	cloning artifact	UNP O30297

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	PHE	-	cloning artifact	UNP O30297
A	-6	GLN	-	cloning artifact	UNP O30297
A	-5	GLY	-	cloning artifact	UNP O30297
A	-4	GLY	-	cloning artifact	UNP O30297
A	-3	GLY	-	cloning artifact	UNP O30297
A	-2	GLY	-	cloning artifact	UNP O30297
A	-1	GLY	-	cloning artifact	UNP O30297
A	0	GLY	-	cloning artifact	UNP O30297
B	-28	MET	-	cloning artifact	UNP O30297
B	-27	GLY	-	cloning artifact	UNP O30297
B	-26	SER	-	cloning artifact	UNP O30297
B	-25	SER	-	cloning artifact	UNP O30297
B	-24	HIS	-	cloning artifact	UNP O30297
B	-23	HIS	-	cloning artifact	UNP O30297
B	-22	HIS	-	cloning artifact	UNP O30297
B	-21	HIS	-	cloning artifact	UNP O30297
B	-20	HIS	-	cloning artifact	UNP O30297
B	-19	HIS	-	cloning artifact	UNP O30297
B	-18	ASP	-	cloning artifact	UNP O30297
B	-17	TYR	-	cloning artifact	UNP O30297
B	-16	ASP	-	cloning artifact	UNP O30297
B	-15	ILE	-	cloning artifact	UNP O30297
B	-14	PRO	-	cloning artifact	UNP O30297
B	-13	THR	-	cloning artifact	UNP O30297
B	-12	THR	-	cloning artifact	UNP O30297
B	-11	GLU	-	cloning artifact	UNP O30297
B	-10	ASN	-	cloning artifact	UNP O30297
B	-9	LEU	-	cloning artifact	UNP O30297
B	-8	TYR	-	cloning artifact	UNP O30297
B	-7	PHE	-	cloning artifact	UNP O30297
B	-6	GLN	-	cloning artifact	UNP O30297
B	-5	GLY	-	cloning artifact	UNP O30297
B	-4	GLY	-	cloning artifact	UNP O30297
B	-3	GLY	-	cloning artifact	UNP O30297
B	-2	GLY	-	cloning artifact	UNP O30297
B	-1	GLY	-	cloning artifact	UNP O30297
B	0	GLY	-	cloning artifact	UNP O30297
C	-28	MET	-	cloning artifact	UNP O30297
C	-27	GLY	-	cloning artifact	UNP O30297
C	-26	SER	-	cloning artifact	UNP O30297
C	-25	SER	-	cloning artifact	UNP O30297
C	-24	HIS	-	cloning artifact	UNP O30297

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-23	HIS	-	cloning artifact	UNP O30297
C	-22	HIS	-	cloning artifact	UNP O30297
C	-21	HIS	-	cloning artifact	UNP O30297
C	-20	HIS	-	cloning artifact	UNP O30297
C	-19	HIS	-	cloning artifact	UNP O30297
C	-18	ASP	-	cloning artifact	UNP O30297
C	-17	TYR	-	cloning artifact	UNP O30297
C	-16	ASP	-	cloning artifact	UNP O30297
C	-15	ILE	-	cloning artifact	UNP O30297
C	-14	PRO	-	cloning artifact	UNP O30297
C	-13	THR	-	cloning artifact	UNP O30297
C	-12	THR	-	cloning artifact	UNP O30297
C	-11	GLU	-	cloning artifact	UNP O30297
C	-10	ASN	-	cloning artifact	UNP O30297
C	-9	LEU	-	cloning artifact	UNP O30297
C	-8	TYR	-	cloning artifact	UNP O30297
C	-7	PHE	-	cloning artifact	UNP O30297
C	-6	GLN	-	cloning artifact	UNP O30297
C	-5	GLY	-	cloning artifact	UNP O30297
C	-4	GLY	-	cloning artifact	UNP O30297
C	-3	GLY	-	cloning artifact	UNP O30297
C	-2	GLY	-	cloning artifact	UNP O30297
C	-1	GLY	-	cloning artifact	UNP O30297
C	0	GLY	-	cloning artifact	UNP O30297
D	-28	MET	-	cloning artifact	UNP O30297
D	-27	GLY	-	cloning artifact	UNP O30297
D	-26	SER	-	cloning artifact	UNP O30297
D	-25	SER	-	cloning artifact	UNP O30297
D	-24	HIS	-	cloning artifact	UNP O30297
D	-23	HIS	-	cloning artifact	UNP O30297
D	-22	HIS	-	cloning artifact	UNP O30297
D	-21	HIS	-	cloning artifact	UNP O30297
D	-20	HIS	-	cloning artifact	UNP O30297
D	-19	HIS	-	cloning artifact	UNP O30297
D	-18	ASP	-	cloning artifact	UNP O30297
D	-17	TYR	-	cloning artifact	UNP O30297
D	-16	ASP	-	cloning artifact	UNP O30297
D	-15	ILE	-	cloning artifact	UNP O30297
D	-14	PRO	-	cloning artifact	UNP O30297
D	-13	THR	-	cloning artifact	UNP O30297
D	-12	THR	-	cloning artifact	UNP O30297
D	-11	GLU	-	cloning artifact	UNP O30297

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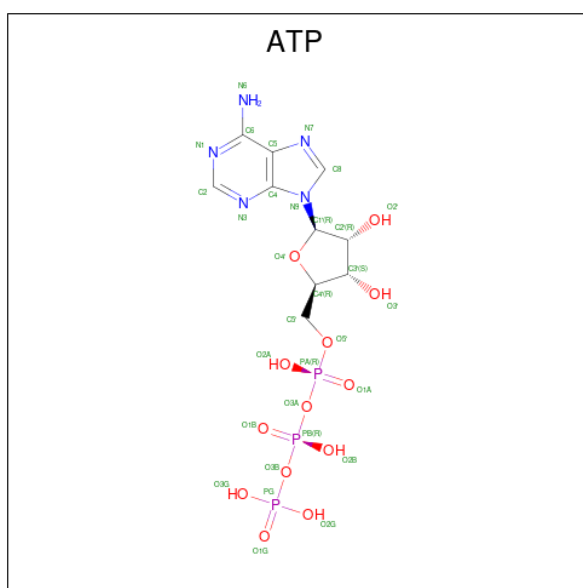
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	ASN	-	cloning artifact	UNP O30297
D	-9	LEU	-	cloning artifact	UNP O30297
D	-8	TYR	-	cloning artifact	UNP O30297
D	-7	PHE	-	cloning artifact	UNP O30297
D	-6	GLN	-	cloning artifact	UNP O30297
D	-5	GLY	-	cloning artifact	UNP O30297
D	-4	GLY	-	cloning artifact	UNP O30297
D	-3	GLY	-	cloning artifact	UNP O30297
D	-2	GLY	-	cloning artifact	UNP O30297
D	-1	GLY	-	cloning artifact	UNP O30297
D	0	GLY	-	cloning artifact	UNP O30297

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

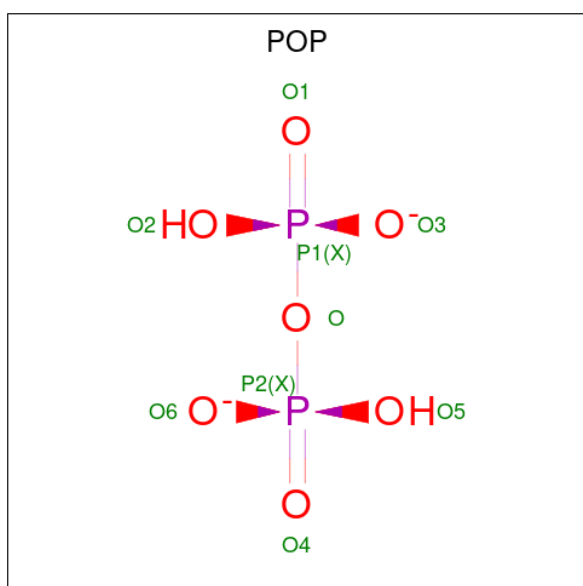
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is PYROPHOSPHATE 2- (CCD ID: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O P	0	0
			9 7 2			
4	B	1	Total	O P	0	0
			9 7 2			
4	C	1	Total	O P	0	0
			9 7 2			
4	D	1	Total	O P	0	0
			9 7 2			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total	O	0	0
			103 103			
5	B	90	Total	O	0	0
			90 90			

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	103	Total 103	O 103	0	0
5	D	111	Total 111	O 111	0	0

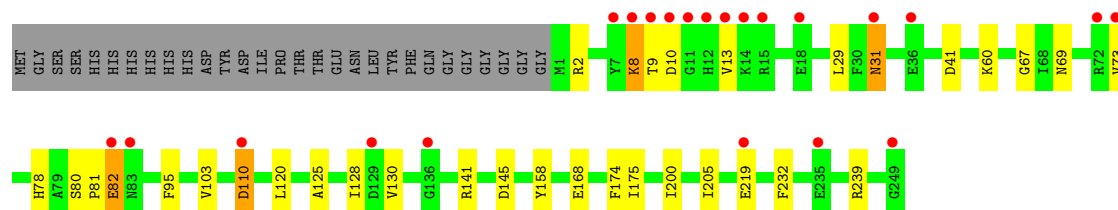


### 3 Residue-property plots [i](#)


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.

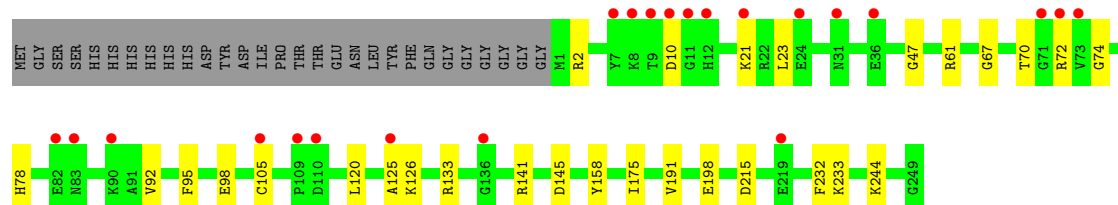
- Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase

Chain A: 




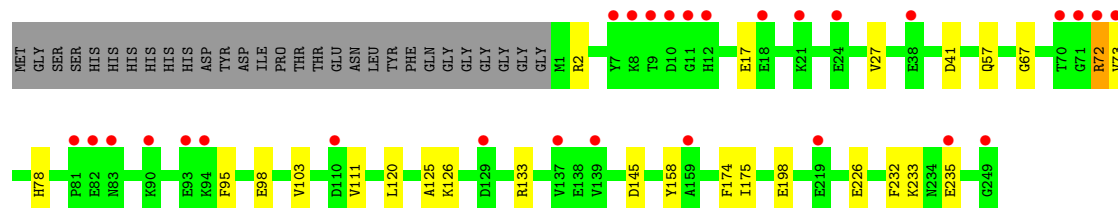
- Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase

Chain B: 




- Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase

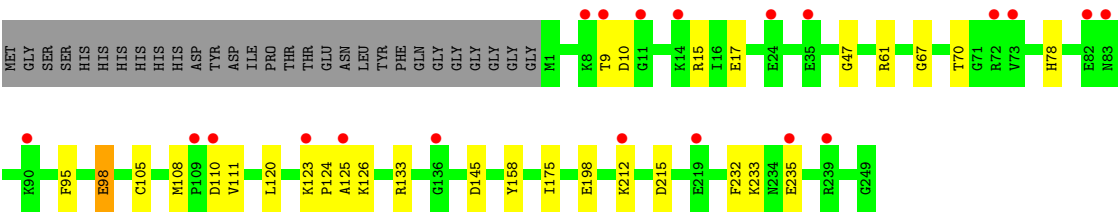
Chain C: 



- Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.25Å 69.73Å 76.29Å 106.35° 111.32° 101.30°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.70) 91.9 (20.00-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.200 , 0.231 0.232 , 0.259	Depositor DCC
$R_{free}$ test set	5111 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.3	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8423	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.07% 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: POP, ATP, MG

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	0.42	0/2001	0.70	4/2698 (0.1%)
1	B	0.41	0/2001	0.69	3/2698 (0.1%)
1	C	0.44	0/2001	0.72	4/2698 (0.1%)
1	D	0.44	0/2001	0.70	2/2698 (0.1%)
All	All	0.43	0/8004	0.70	13/10792 (0.1%)

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	C	1	0

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	ASP	CB-CG-OD2	7.10	124.69	118.30
1	C	145	ASP	CB-CG-OD2	6.45	124.10	118.30
1	B	215	ASP	CB-CG-OD2	6.08	123.77	118.30
1	D	215	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	145	ASP	CB-CG-OD2	5.85	123.57	118.30
1	C	72	ARG	N-CA-C	5.84	126.78	111.00
1	A	41	ASP	CB-CG-OD2	5.82	123.54	118.30
1	D	145	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	110	ASP	CB-CG-OD2	5.47	123.22	118.30
1	C	41	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	72	ARG	CB-CA-C	5.10	120.61	110.40
1	B	10	ASP	CB-CG-OD2	5.06	122.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ASP	CB-CG-OD2	5.00	122.80	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	72	ARG	CA

There are no planarity outliers.

## 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	1963	0	2015	19	0
1	B	1963	0	2015	13	0
1	C	1963	0	2015	12	0
1	D	1963	0	2015	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	9	0	0	1	0
4	B	9	0	0	0	0
4	C	9	0	0	0	0
4	D	9	0	0	0	0
5	A	103	0	0	2	0
5	B	90	0	0	0	1
5	C	103	0	0	0	1
5	D	111	0	0	0	0
All	All	8423	0	8108	52	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 3.

All (52) 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:111:VAL:HG21	1:D:212:LYS:HZ2	0.98	1.06
1:D:111:VAL:HG21	1:D:212:LYS:NZ	1.78	0.97
1:A:128:ILE:O	5:A:5098:HOH:O	1.92	0.87
1:A:125:ALA:HB2	1:D:120:LEU:HD11	1.71	0.71
1:A:120:LEU:HD11	1:D:125:ALA:HB2	1.74	0.69
1:B:120:LEU:HD11	1:C:125:ALA:HB2	1.75	0.68
1:C:78:HIS:HE1	1:C:232:PHE:O	1.77	0.67
1:D:108:MET:SD	1:D:212:LYS:NZ	2.63	0.66
1:B:125:ALA:HB2	1:C:120:LEU:HD11	1.79	0.65
1:B:78:HIS:HE1	1:B:232:PHE:O	1.79	0.64
1:D:78:HIS:HE1	1:D:232:PHE:O	1.81	0.63
1:A:78:HIS:HE1	1:A:232:PHE:O	1.82	0.63
1:B:120:LEU:CD1	1:C:125:ALA:HB2	2.31	0.60
1:C:57:GLN:HE22	1:C:111:VAL:HG13	1.68	0.57
1:A:8:LYS:HD2	1:A:9:THR:HG23	1.87	0.57
1:B:23:LEU:HD13	1:B:92:VAL:HG11	1.86	0.56
1:D:111:VAL:CG2	1:D:212:LYS:HZ2	1.93	0.56
1:B:175:ILE:HD12	1:B:175:ILE:N	2.22	0.54
1:A:200:ILE:HG13	1:A:219:GLU:HG2	1.89	0.53
1:B:125:ALA:HB2	1:C:120:LEU:CD1	2.40	0.52
1:A:67:GLY:H	1:A:78:HIS:CD2	2.29	0.51
1:D:67:GLY:H	1:D:78:HIS:CD2	2.29	0.51
1:B:133:ARG:HB2	1:B:198:GLU:HB2	1.93	0.50
1:C:175:ILE:HD12	1:C:175:ILE:N	2.27	0.50
1:A:130:VAL:HG23	5:A:5098:HOH:O	2.14	0.48
1:A:31:ASN:N	1:A:31:ASN:OD1	2.47	0.47
1:C:133:ARG:HB2	1:C:198:GLU:HB2	1.96	0.47
1:A:8:LYS:NZ	4:A:3953:POP:P1	2.88	0.47
1:A:80:SER:OG	1:A:82:GLU:CD	2.53	0.47
1:D:175:ILE:N	1:D:175:ILE:HD12	2.30	0.47
1:B:47:GLY:HA2	1:B:70:THR:OG1	2.15	0.47
1:D:133:ARG:HB2	1:D:198:GLU:HB2	1.98	0.46
1:C:17:GLU:HG3	1:C:27:VAL:HG11	1.99	0.44
1:A:67:GLY:H	1:A:78:HIS:HD2	1.66	0.44
1:B:98:GLU:HG3	1:B:233:LYS:HA	1.99	0.44
1:C:67:GLY:H	1:C:78:HIS:CD2	2.37	0.43
1:D:47:GLY:HA2	1:D:70:THR:OG1	2.18	0.42
1:D:108:MET:CG	1:D:212:LYS:HZ3	2.30	0.42
1:B:67:GLY:H	1:B:78:HIS:CD2	2.37	0.42
1:C:98:GLU:HG3	1:C:233:LYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ILE:HD12	1:A:175:ILE:N	2.35	0.42
1:D:108:MET:HB3	1:D:212:LYS:NZ	2.35	0.41
1:D:67:GLY:H	1:D:78:HIS:HD2	1.67	0.41
1:A:168:GLU:HG2	1:B:191:VAL:HA	2.01	0.41
1:B:74:GLY:O	1:B:244:LYS:NZ	2.40	0.41
1:A:200:ILE:CG1	1:A:219:GLU:HG2	2.49	0.41
1:A:205:ILE:HD11	1:D:124:PRO:HB2	2.03	0.41
1:A:69:ASN:O	1:A:81:PRO:HD3	2.21	0.40
1:D:98:GLU:CG	1:D:233:LYS:HA	2.51	0.40
1:A:103:VAL:HG11	1:A:174:PHE:HE2	1.87	0.40
1:C:103:VAL:HG11	1:C:174:PHE:HE2	1.86	0.40
1:A:13:VAL:CG1	1:A:29:LEU:HD22	2.50	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:B:5085:HOH:O	5:C:5096:HOH:O[1_554]	2.05	0.15

## 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	247/278 (89%)	243 (98%)	4 (2%)	0	100	100
1	B	247/278 (89%)	242 (98%)	5 (2%)	0	100	100
1	C	247/278 (89%)	243 (98%)	4 (2%)	0	100	100
1	D	247/278 (89%)	243 (98%)	4 (2%)	0	100	100
All	All	988/1112 (89%)	971 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	213/235 (91%)	202 (95%)	11 (5%)	19	7
1	B	213/235 (91%)	204 (96%)	9 (4%)	25	10
1	C	213/235 (91%)	205 (96%)	8 (4%)	28	12
1	D	213/235 (91%)	200 (94%)	13 (6%)	15	4
All	All	852/940 (91%)	811 (95%)	41 (5%)	21	8

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	8	LYS
1	A	31	ASN
1	A	60	LYS
1	A	73	VAL
1	A	82	GLU
1	A	95	PHE
1	A	110	ASP
1	A	141	ARG
1	A	158	TYR
1	A	239	ARG
1	B	2	ARG
1	B	21	LYS
1	B	61	ARG
1	B	72	ARG
1	B	95	PHE
1	B	105	CYS
1	B	126	LYS
1	B	141	ARG
1	B	158	TYR
1	C	2	ARG
1	C	72	ARG
1	C	73	VAL
1	C	95	PHE

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Mol	Chain	Res	Type
1	C	126	LYS
1	C	158	TYR
1	C	226	GLU
1	C	235	GLU
1	D	9	THR
1	D	10	ASP
1	D	15	ARG
1	D	17	GLU
1	D	61	ARG
1	D	95	PHE
1	D	98	GLU
1	D	105	CYS
1	D	110	ASP
1	D	123	LYS
1	D	126	LYS
1	D	158	TYR
1	D	235	GLU

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	78	HIS
1	B	78	HIS
1	C	57	GLN
1	C	78	HIS
1	D	78	HIS

### 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

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
4	POP	B	3954	2	6,8,8	0.47	0	12,13,13	1.04	1 (8%)
3	ATP	B	738	2	28,33,33	1.23	3 (10%)	34,52,52	1.59	3 (8%)
3	ATP	D	740	2	28,33,33	1.07	2 (7%)	34,52,52	1.67	4 (11%)
4	POP	C	3955	2	6,8,8	0.35	0	12,13,13	0.97	0
3	ATP	A	737	2	28,33,33	1.13	2 (7%)	34,52,52	1.72	5 (14%)
4	POP	A	3953	2	6,8,8	0.45	0	12,13,13	0.92	0
3	ATP	C	739	2	28,33,33	1.28	2 (7%)	34,52,52	1.61	4 (11%)
4	POP	D	3956	2	6,8,8	0.42	0	12,13,13	0.98	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
4	POP	B	3954	2	-	3/6/6/6	-
3	ATP	B	738	2	-	3/18/38/38	0/3/3/3
3	ATP	D	740	2	-	2/18/38/38	0/3/3/3
4	POP	C	3955	2	-	4/6/6/6	-
3	ATP	A	737	2	-	3/18/38/38	0/3/3/3
4	POP	A	3953	2	-	3/6/6/6	-
3	ATP	C	739	2	-	1/18/38/38	0/3/3/3
4	POP	D	3956	2	-	1/6/6/6	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	739	ATP	C2-N3	4.41	1.38	1.32
3	D	740	ATP	C2-N3	4.23	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	737	ATP	C2-N3	4.10	1.38	1.32
3	B	738	ATP	C2-N3	3.95	1.38	1.32
3	B	738	ATP	PB-O3B	2.71	1.62	1.59
3	B	738	ATP	C2-N1	2.62	1.38	1.33
3	C	739	ATP	C2-N1	2.46	1.38	1.33
3	D	740	ATP	C2-N1	2.12	1.37	1.33
3	A	737	ATP	C2-N1	2.05	1.37	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	740	ATP	N3-C2-N1	-7.01	119.16	128.67
3	A	737	ATP	N3-C2-N1	-6.78	119.47	128.67
3	B	738	ATP	N3-C2-N1	-6.46	119.91	128.67
3	C	739	ATP	N3-C2-N1	-6.34	120.06	128.67
3	A	737	ATP	O4'-C1'-N9	4.23	114.36	108.75
3	C	739	ATP	C4'-O4'-C1'	-3.91	106.34	109.92
3	C	739	ATP	O4'-C1'-N9	3.72	113.68	108.75
3	D	740	ATP	C4'-O4'-C1'	-3.54	106.69	109.92
3	D	740	ATP	O4'-C1'-N9	3.53	113.42	108.75
3	B	738	ATP	O4'-C1'-N9	3.52	113.41	108.75
3	A	737	ATP	C4'-O4'-C1'	-3.27	106.93	109.92
3	B	738	ATP	C4'-O4'-C1'	-3.22	106.97	109.92
3	D	740	ATP	O3B-PB-O1B	2.61	118.55	110.70
3	C	739	ATP	O3A-PA-O1A	-2.26	103.90	110.70
3	A	737	ATP	C5-C6-N6	2.12	123.54	120.31
3	A	737	ATP	O2A-PA-O3A	2.10	112.95	107.27
4	B	3954	POP	O2-P1-O	2.07	111.56	104.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3954	POP	P1-O-P2-O6
4	A	3953	POP	P2-O-P1-O1
4	C	3955	POP	P2-O-P1-O1
4	C	3955	POP	P1-O-P2-O4
4	A	3953	POP	P1-O-P2-O6
4	B	3954	POP	P2-O-P1-O2
4	B	3954	POP	P2-O-P1-O3
4	D	3956	POP	P1-O-P2-O6
3	C	739	ATP	PB-O3A-PA-O2A

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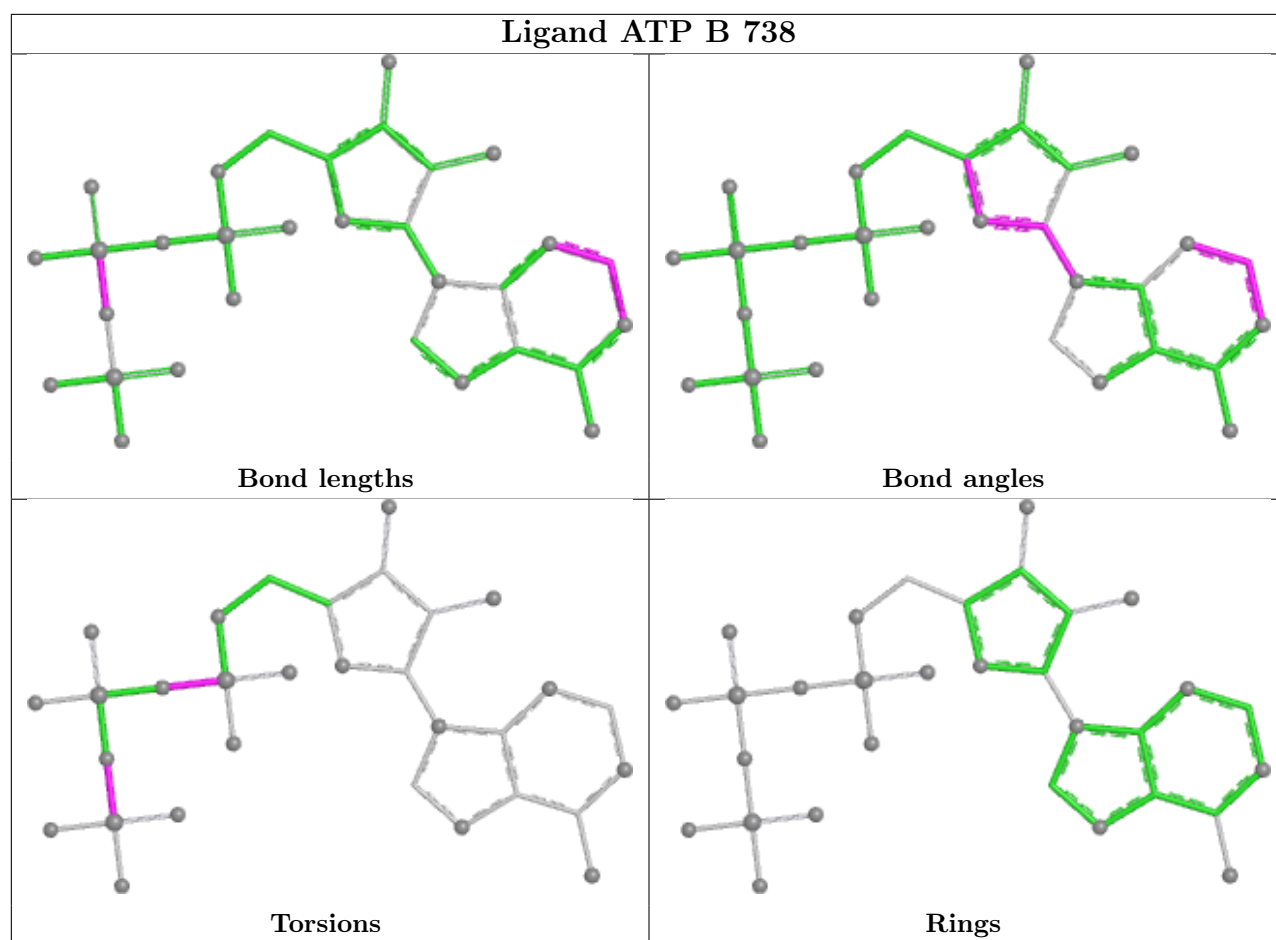
Mol	Chain	Res	Type	Atoms
3	B	738	ATP	PB-O3A-PA-O2A
3	A	737	ATP	PB-O3B-PG-O3G
3	B	738	ATP	PB-O3B-PG-O3G
3	D	740	ATP	PB-O3B-PG-O2G
4	A	3953	POP	P2-O-P1-O2
4	C	3955	POP	P1-O-P2-O5
4	C	3955	POP	P1-O-P2-O6
3	A	737	ATP	PB-O3A-PA-O1A
3	A	737	ATP	PB-O3A-PA-O2A
3	B	738	ATP	PB-O3A-PA-O1A
3	D	740	ATP	PB-O3A-PA-O1A

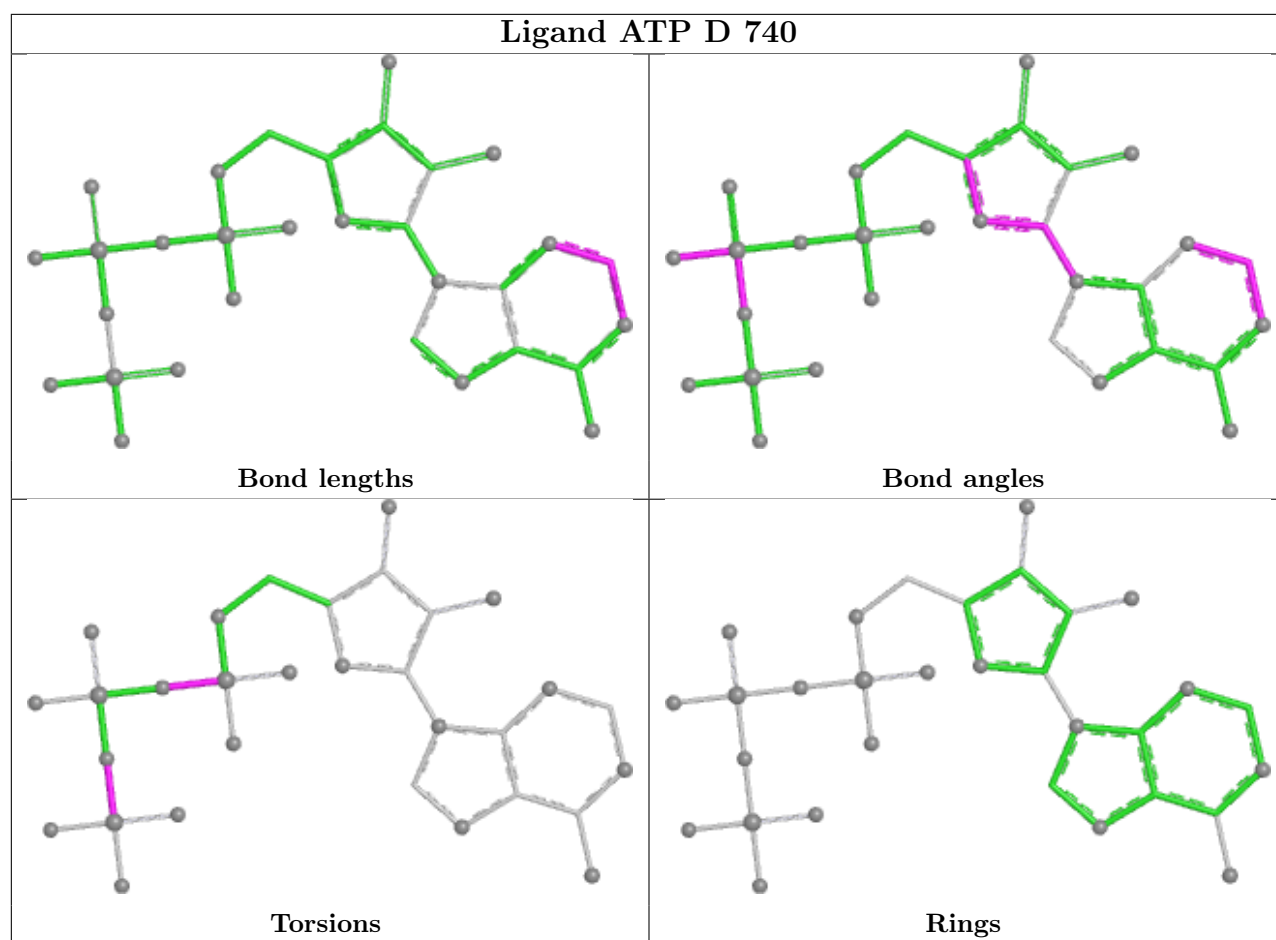
There are no ring outliers.

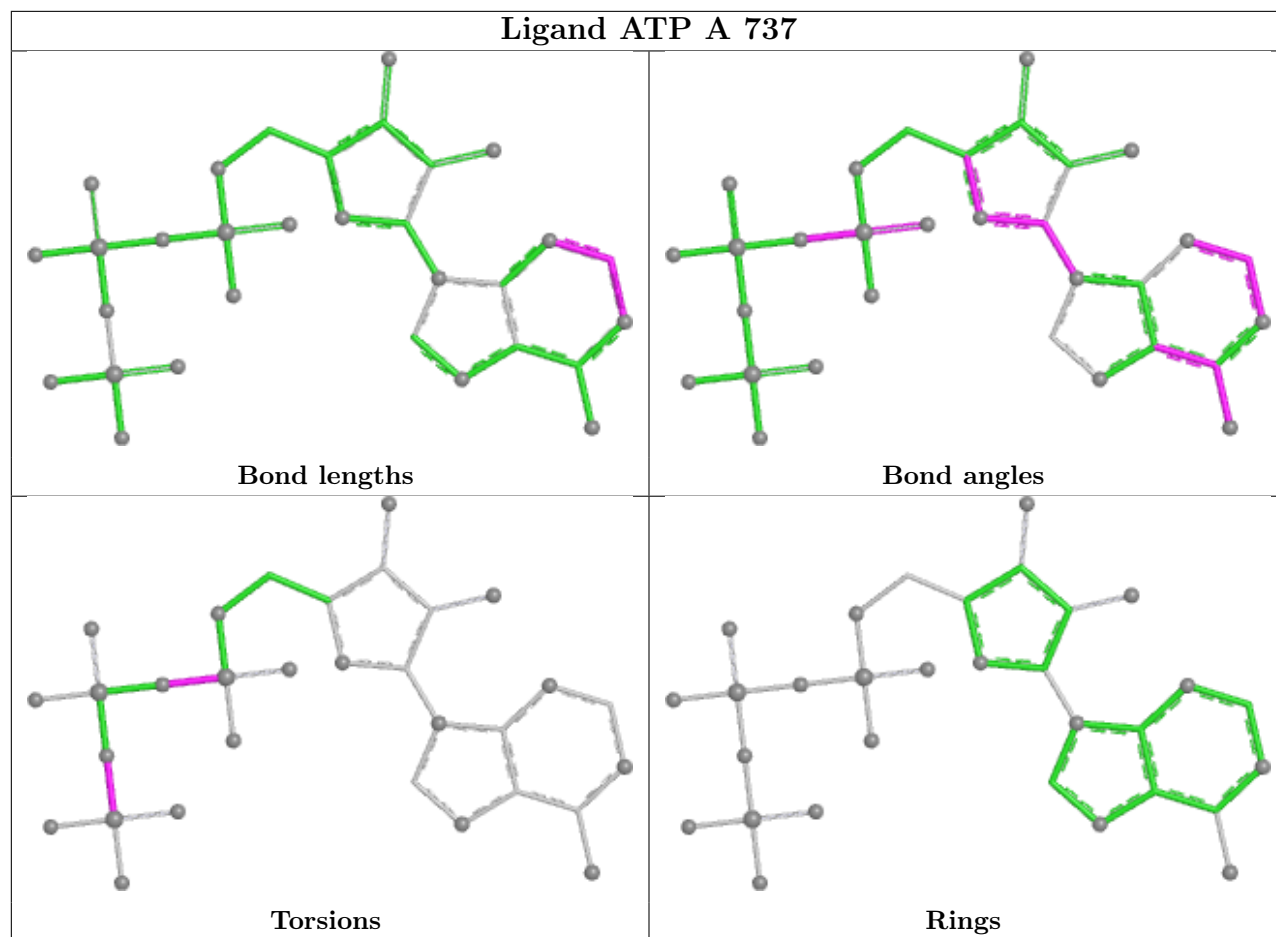
1 monomer is involved in 1 short contact:

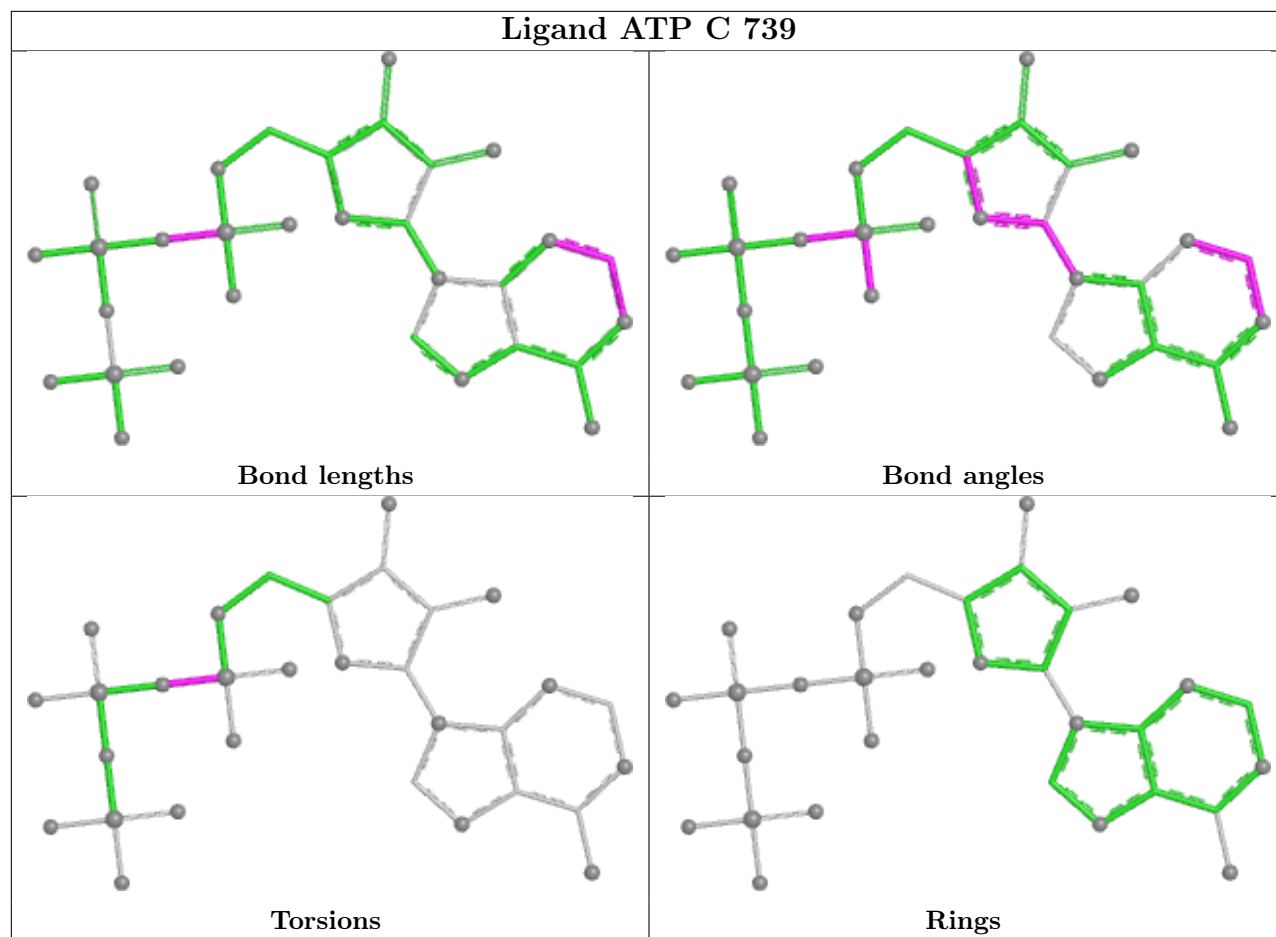
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3953	POP	1	0

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	249/278 (89%)	0.58	22 (8%)	17 17	4, 12, 19, 25	0
1	B	249/278 (89%)	0.60	22 (8%)	17 17	5, 12, 19, 25	0
1	C	249/278 (89%)	0.69	28 (11%)	11 10	5, 12, 19, 25	0
1	D	249/278 (89%)	0.49	20 (8%)	20 20	4, 12, 19, 26	0
All	All	996/1112 (89%)	0.59	92 (9%)	16 16	4, 12, 19, 26	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	GLY	4.6
1	D	72	ARG	4.5
1	A	31	ASN	4.4
1	B	73	VAL	4.2
1	C	9	THR	4.2
1	C	73	VAL	4.1
1	C	72	ARG	4.1
1	A	73	VAL	3.8
1	C	11	GLY	3.7
1	A	9	THR	3.7
1	A	110	ASP	3.6
1	B	8	LYS	3.6
1	B	9	THR	3.6
1	A	8	LYS	3.6
1	D	73	VAL	3.6
1	A	82	GLU	3.5
1	C	235	GLU	3.4
1	A	11	GLY	3.4
1	A	249	GLY	3.3
1	D	9	THR	3.3
1	B	72	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	24	GLU	3.2
1	D	235	GLU	3.1
1	A	72	ARG	3.1
1	B	7	TYR	3.1
1	C	8	LYS	3.1
1	D	125	ALA	3.0
1	D	110	ASP	3.0
1	C	21	LYS	3.0
1	B	83	ASN	3.0
1	B	136	GLY	3.0
1	D	212	LYS	2.9
1	C	83	ASN	2.9
1	C	12	HIS	2.9
1	D	219	GLU	2.9
1	C	139	VAL	2.9
1	C	18	GLU	2.8
1	B	125	ALA	2.8
1	D	83	ASN	2.8
1	A	13	VAL	2.8
1	C	137	VAL	2.7
1	D	11	GLY	2.7
1	C	24	GLU	2.7
1	A	10	ASP	2.7
1	A	36	GLU	2.7
1	A	18	GLU	2.6
1	C	82	GLU	2.6
1	D	82	GLU	2.6
1	B	11	GLY	2.6
1	A	235	GLU	2.5
1	D	90	LYS	2.5
1	C	219	GLU	2.5
1	B	10	ASP	2.5
1	C	110	ASP	2.5
1	D	239	ARG	2.5
1	A	129	ASP	2.4
1	A	83	ASN	2.4
1	C	71	GLY	2.4
1	A	7	TYR	2.4
1	C	129	ASP	2.4
1	D	109	PRO	2.4
1	A	12	HIS	2.4
1	B	109	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	36	GLU	2.3
1	A	14	LYS	2.3
1	D	136	GLY	2.3
1	C	70	THR	2.3
1	B	105	CYS	2.3
1	C	10	ASP	2.3
1	C	7	TYR	2.3
1	A	136	GLY	2.2
1	B	82	GLU	2.2
1	B	219	GLU	2.2
1	C	38	GLU	2.2
1	B	71	GLY	2.2
1	C	159	ALA	2.2
1	A	15	ARG	2.1
1	B	90	LYS	2.1
1	D	8	LYS	2.1
1	D	14	LYS	2.1
1	A	219	GLU	2.1
1	B	31	ASN	2.1
1	C	94	LYS	2.1
1	D	123	LYS	2.1
1	D	24	GLU	2.1
1	D	35	GLU	2.1
1	B	110	ASP	2.1
1	C	93	GLU	2.1
1	B	12	HIS	2.1
1	C	81	PRO	2.1
1	B	21	LYS	2.0
1	C	90	LYS	2.0

## 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

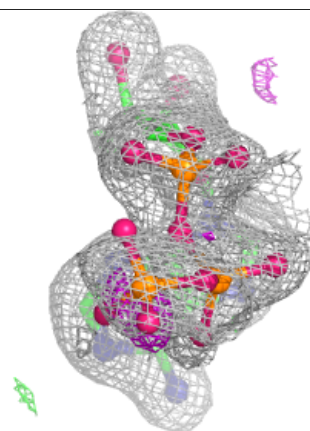
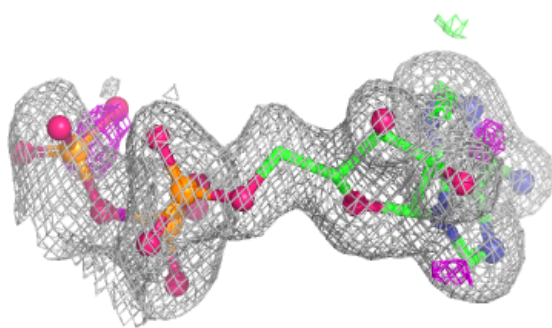
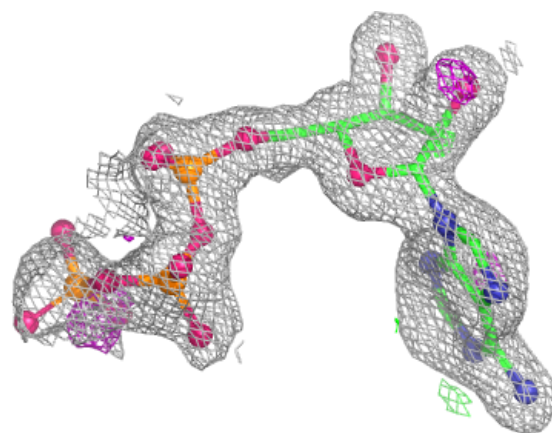
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	5002	1/1	0.77	0.12	42,42,42,42	0
4	POP	C	3955	9/9	0.77	0.20	62,63,63,64	0
4	POP	B	3954	9/9	0.82	0.15	38,41,43,43	0
2	MG	C	5003	1/1	0.83	0.12	37,37,37,37	0
4	POP	D	3956	9/9	0.87	0.13	29,34,36,37	0
4	POP	A	3953	9/9	0.88	0.14	34,37,39,39	0
2	MG	A	5001	1/1	0.88	0.08	32,32,32,32	0
2	MG	D	5004	1/1	0.89	0.09	29,29,29,29	0
3	ATP	B	738	31/31	0.89	0.11	18,20,47,47	0
3	ATP	C	739	31/31	0.90	0.10	16,21,48,48	0
3	ATP	A	737	31/31	0.93	0.10	14,17,35,37	0
3	ATP	D	740	31/31	0.93	0.10	15,16,36,37	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.

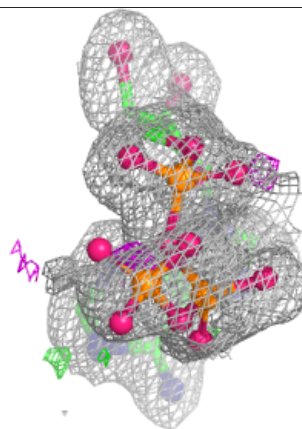
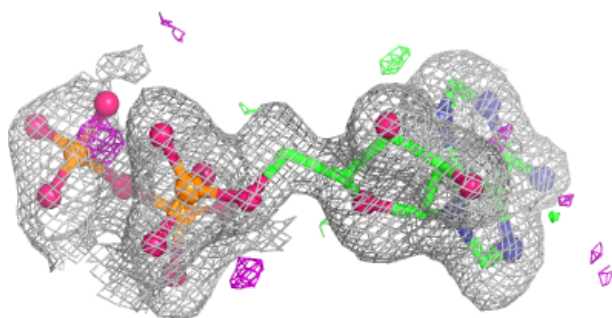
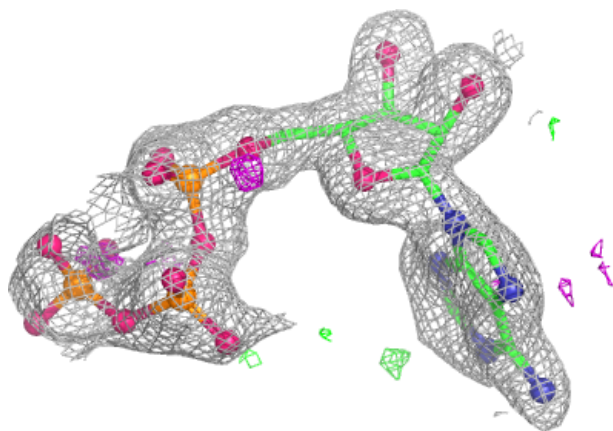
**Electron density around ATP B 738:**

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



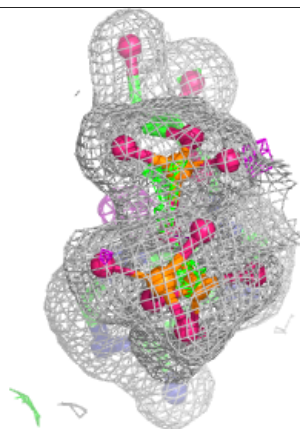
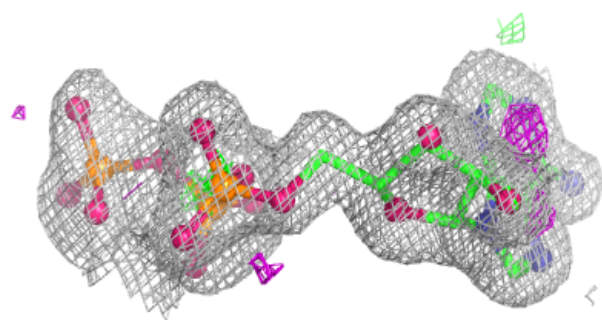
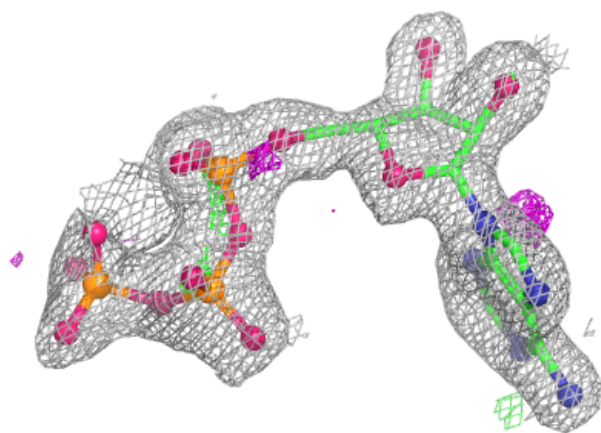
**Electron density around ATP C 739:**

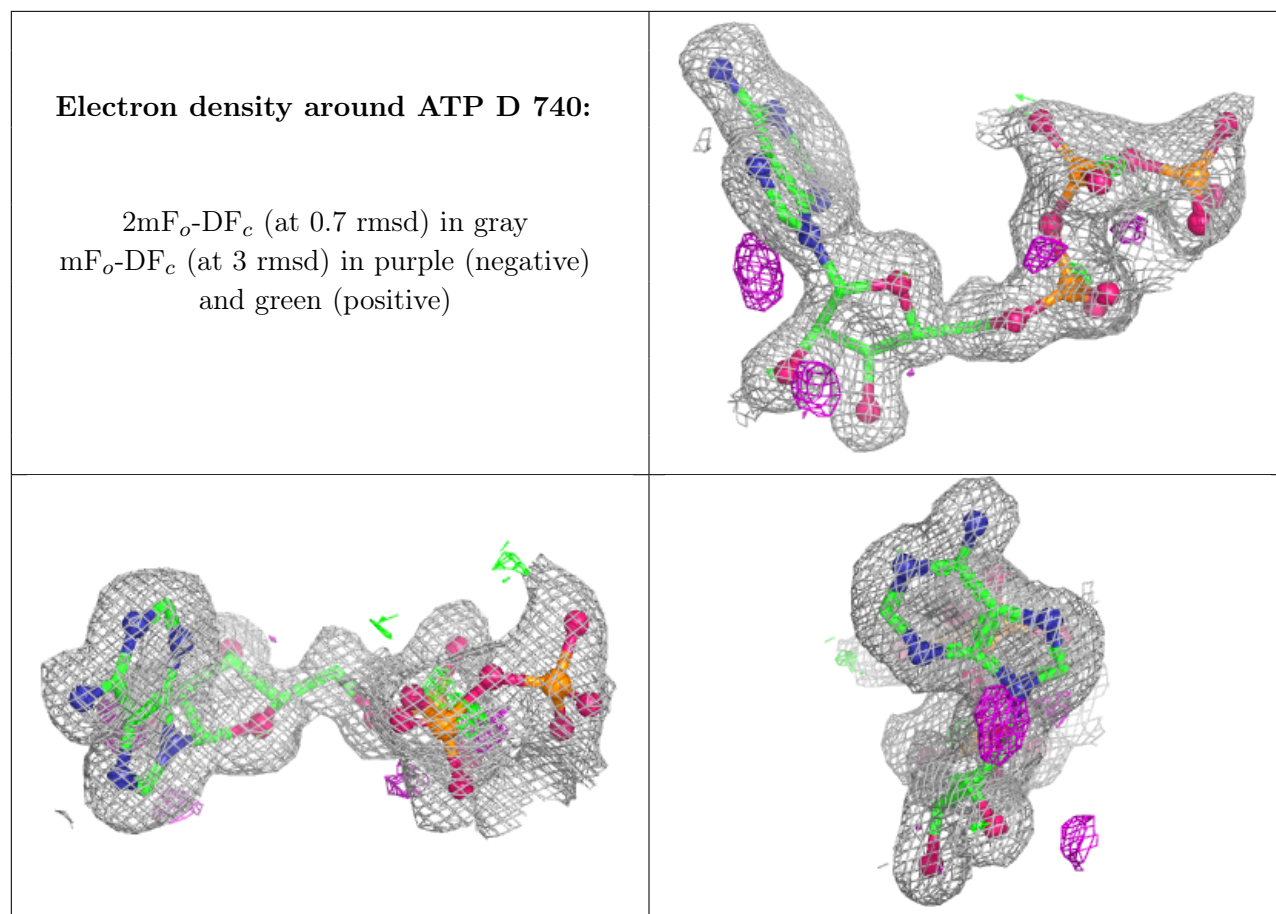
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ATP A 737:**

$2mF_o - DF_c$  (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.