



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 05:35 PM EDT

PDB ID : 4U1R  
Title : ATP-bound structure of human platelet phosphofructokinase in an R-state, crystal form II  
Authors : Kloos, M.; Straeter, N.  
Deposited on : 2014-07-16  
Resolution : 2.80 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>.

---

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	:	2.37.1
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)	:	2.37.1

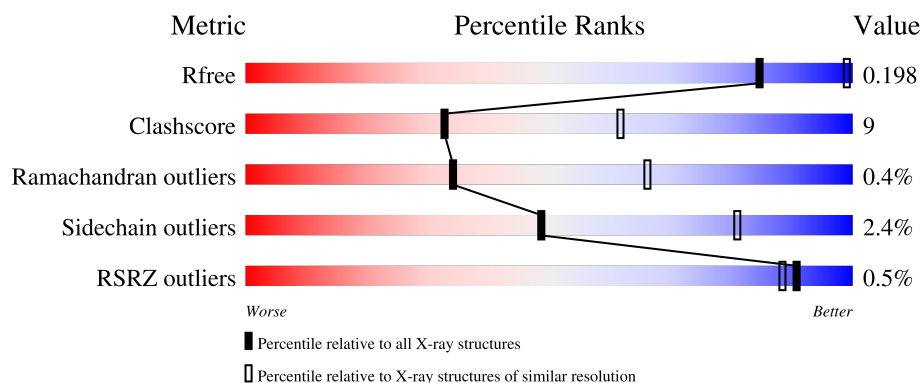
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	743	 82% 16% ..
1	B	743	 83% 15% ..
1	C	743	 80% 17% ..
1	D	743	 80% 18% ..

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	C	802	-	-	X	-
3	PO4	C	804	-	-	X	-
3	PO4	D	802	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22567 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	733	Total	C	N	O	S	0	0	0
			5604	3515	994	1056	39			
1	B	732	Total	C	N	O	S	0	0	0
			5593	3509	990	1055	39			
1	C	732	Total	C	N	O	S	0	0	0
			5593	3509	990	1055	39			
1	D	732	Total	C	N	O	S	0	0	0
			5593	3506	993	1055	39			

There are 24 discrepancies between the modelled and reference sequences:

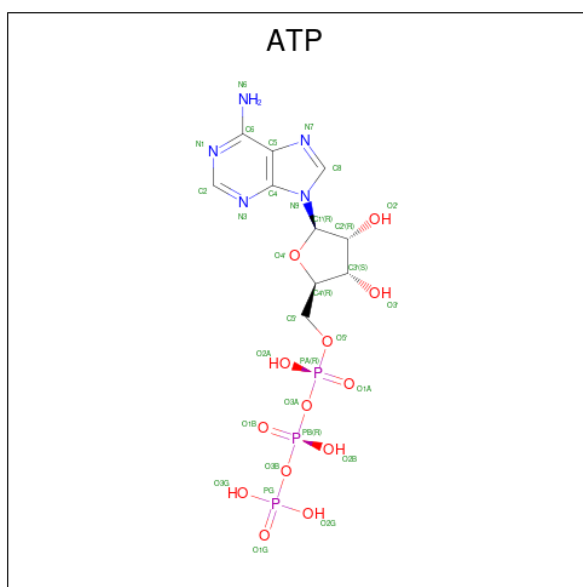
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	VAL	-	expression tag	UNP Q01813
A	21	PRO	-	expression tag	UNP Q01813
A	22	ASP	-	expression tag	UNP Q01813
A	23	PRO	-	expression tag	UNP Q01813
A	24	THR	-	expression tag	UNP Q01813
A	25	SER	-	expression tag	UNP Q01813
B	20	VAL	-	expression tag	UNP Q01813
B	21	PRO	-	expression tag	UNP Q01813
B	22	ASP	-	expression tag	UNP Q01813
B	23	PRO	-	expression tag	UNP Q01813
B	24	THR	-	expression tag	UNP Q01813
B	25	SER	-	expression tag	UNP Q01813
C	20	VAL	-	expression tag	UNP Q01813
C	21	PRO	-	expression tag	UNP Q01813
C	22	ASP	-	expression tag	UNP Q01813
C	23	PRO	-	expression tag	UNP Q01813
C	24	THR	-	expression tag	UNP Q01813
C	25	SER	-	expression tag	UNP Q01813
D	20	VAL	-	expression tag	UNP Q01813
D	21	PRO	-	expression tag	UNP Q01813
D	22	ASP	-	expression tag	UNP Q01813

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	23	PRO	-	expression tag	UNP Q01813
D	24	THR	-	expression tag	UNP Q01813
D	25	SER	-	expression tag	UNP Q01813

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

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

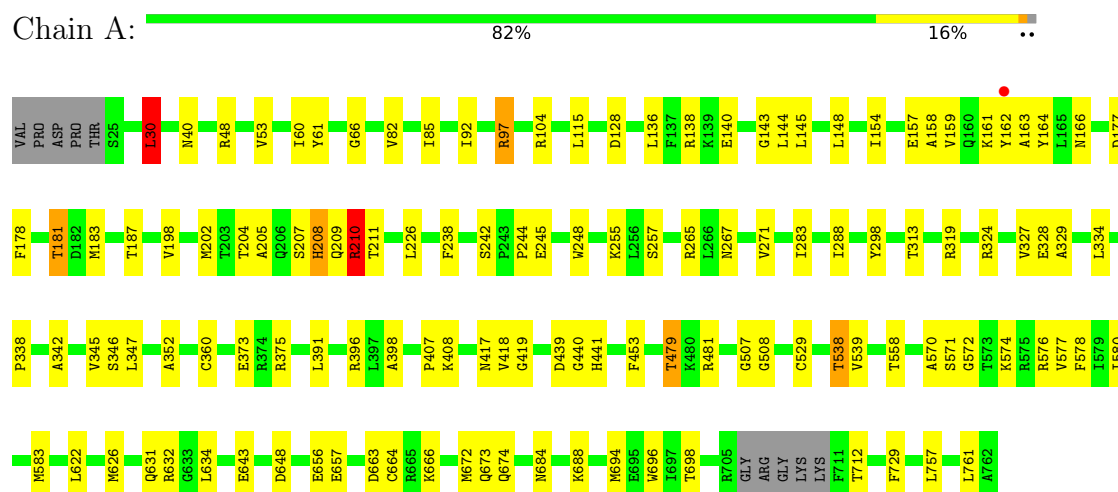


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total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

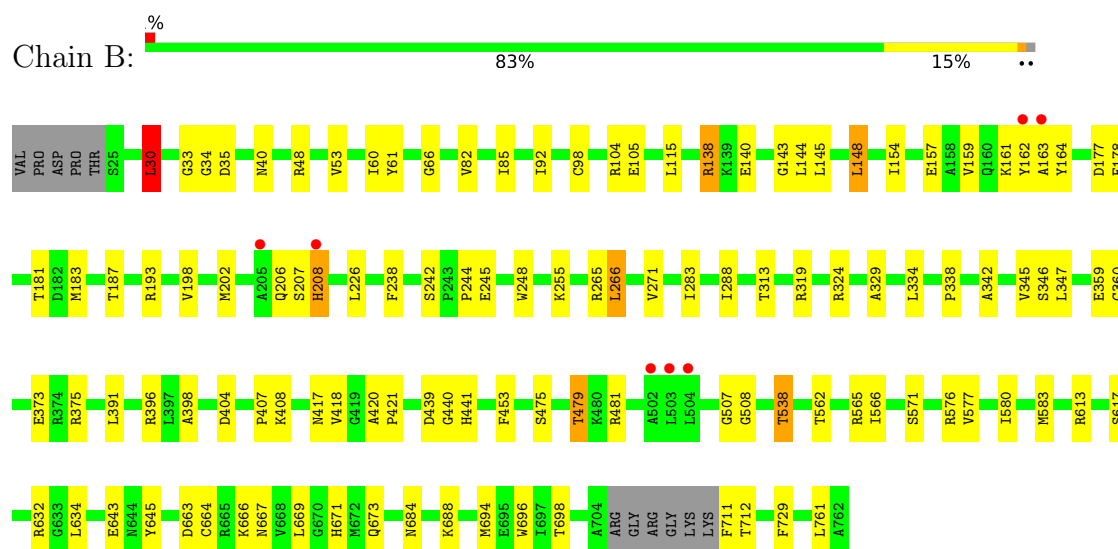
### 3 Residue-property plots

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.

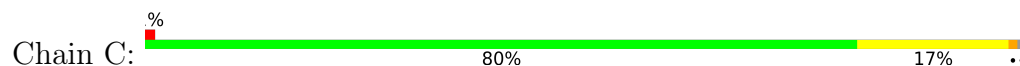
- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

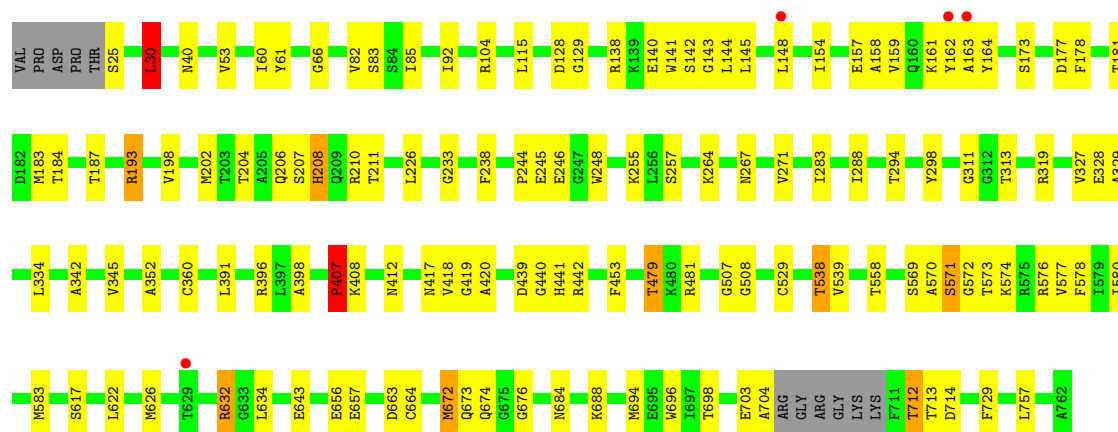


- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type



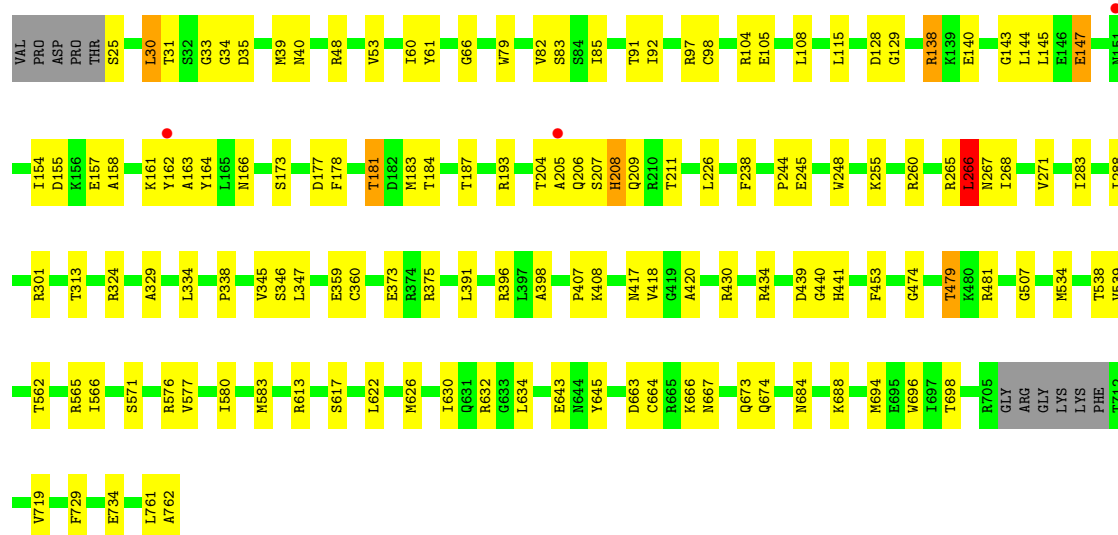
- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type





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

Chain D: 80% 18% ::





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.90Å 132.90Å 399.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.01 – 2.80 47.01 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.01-2.80) 99.7 (47.01-2.80)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.162 , 0.198 0.162 , 0.198	Depositor DCC
$R_{free}$ test set	5065 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.9	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 15.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.427 for -h,-k,l	Xtriage
Reported twinning fraction	0.444 for H, K, L 0.556 for -h,-k,l	Depositor
Outliers	0 of 101291 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22567	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 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	0.56	0/5694	0.75	5/7691 (0.1%)
1	B	0.56	0/5683	0.74	3/7677 (0.0%)
1	C	0.53	0/5683	0.74	7/7677 (0.1%)
1	D	0.56	0/5682	0.74	1/7675 (0.0%)
All	All	0.55	0/22742	0.74	16/30720 (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	A	0	1
1	C	0	3
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	210	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	D	266	LEU	CB-CG-CD1	6.62	122.25	111.00
1	A	210	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	148	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	97	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	246	GLU	CB-CA-C	5.84	122.07	110.40
1	C	407	PRO	CB-CA-C	-5.57	98.08	112.00
1	B	138	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	648	ASP	CB-CG-OD2	5.36	123.12	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	632	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	C	193	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	30	LEU	CA-CB-CG	5.23	127.34	115.30
1	B	30	LEU	CA-CB-CG	5.20	127.25	115.30
1	C	632	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	676	GLY	N-CA-C	-5.12	100.29	113.10
1	C	30	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	571	SER	Peptide
1	C	141	TRP	Peptide
1	C	142	SER	Peptide
1	C	712	THR	Peptide
1	D	25	SER	Peptide

## 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	5604	0	5628	92	0
1	B	5593	0	5615	91	0
1	C	5593	0	5615	100	1
1	D	5593	0	5619	124	1
2	A	31	0	12	1	0
2	B	31	0	12	2	0
2	C	31	0	12	4	0
2	D	31	0	12	6	0
3	A	20	0	0	1	0
3	B	10	0	0	1	0
3	C	20	0	0	5	0
3	D	10	0	0	4	0
All	All	22567	0	22525	391	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 9.

All (391) 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:534:MET:HE2	1:D:719:VAL:HG22	1.39	1.01
1:D:128:ASP:CB	2:D:801:ATP:O2G	2.16	0.94
1:A:574:LYS:HB3	1:A:631:GLN:O	1.68	0.93
1:D:534:MET:CE	1:D:719:VAL:HG22	1.99	0.93
1:B:583:MET:HE3	1:B:671:HIS:HA	1.51	0.91
1:D:266:LEU:HG	1:D:267:ASN:N	1.88	0.88
1:D:128:ASP:HB2	2:D:801:ATP:O2G	1.75	0.87
1:D:31:THR:HG21	1:D:91:THR:HG21	1.58	0.84
1:D:108:LEU:HD22	1:D:147:GLU:OE1	1.77	0.84
1:A:115:LEU:HD11	1:A:144:LEU:HD22	1.61	0.83
1:C:115:LEU:HD11	1:C:144:LEU:HD22	1.61	0.82
1:C:684:ASN:O	1:C:688:LYS:HG3	1.80	0.82
1:B:115:LEU:HD11	1:B:144:LEU:HD22	1.61	0.82
1:D:128:ASP:HB3	2:D:801:ATP:O2G	1.79	0.81
1:D:684:ASN:O	1:D:688:LYS:HG3	1.81	0.81
1:D:205:ALA:CB	1:D:266:LEU:HD13	2.12	0.80
1:A:684:ASN:O	1:A:688:LYS:HG3	1.83	0.79
1:B:684:ASN:O	1:B:688:LYS:HG3	1.81	0.79
1:B:98:CYS:H	2:B:801:ATP:HO3'	1.30	0.78
1:C:407:PRO:O	1:C:407:PRO:HG2	1.83	0.77
1:B:669:LEU:HB3	1:B:673:GLN:CG	2.15	0.77
1:A:205:ALA:O	1:A:209:GLN:O	2.03	0.77
1:C:632:ARG:NH2	3:C:804:PO4:O4	2.19	0.75
1:B:669:LEU:HD13	1:B:673:GLN:HE21	1.52	0.74
1:D:40:ASN:HB3	1:D:85:ILE:HG23	1.67	0.74
1:D:430:ARG:NH2	3:D:802:PO4:O2	2.19	0.74
1:B:162:TYR:O	1:B:164:TYR:N	2.21	0.73
1:D:209:GLN:OE1	1:D:260:ARG:HD2	1.89	0.72
1:B:669:LEU:HD13	1:B:673:GLN:NE2	2.04	0.71
1:C:40:ASN:HB3	1:C:85:ILE:HG23	1.72	0.71
1:A:529:CYS:HB3	1:A:712:THR:HG21	1.72	0.71
1:B:40:ASN:HB3	1:B:85:ILE:HG23	1.72	0.71
1:A:40:ASN:HB3	1:A:85:ILE:HG23	1.72	0.70
1:D:566:ILE:HD13	1:D:580:ILE:HD11	1.73	0.70
1:B:439:ASP:OD2	1:B:698:THR:HG21	1.92	0.70
1:B:566:ILE:HD13	1:B:580:ILE:HD11	1.73	0.69
1:D:439:ASP:OD2	1:D:698:THR:HG21	1.93	0.69
1:D:583:MET:SD	1:D:673:GLN:NE2	2.66	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:CYS:N	2:D:801:ATP:O3'	2.23	0.69
1:C:439:ASP:OD2	1:C:698:THR:HG21	1.93	0.68
1:A:529:CYS:CB	1:A:712:THR:HG21	2.22	0.68
1:B:583:MET:HE3	1:B:671:HIS:CA	2.22	0.68
1:D:162:TYR:O	1:D:164:TYR:N	2.26	0.68
1:B:183:MET:HE1	1:B:187:THR:HB	1.76	0.68
1:D:138:ARG:HD3	1:D:138:ARG:O	1.93	0.68
1:D:31:THR:CG2	1:D:39:MET:SD	2.82	0.68
1:A:439:ASP:OD2	1:A:698:THR:HG21	1.94	0.67
1:B:162:TYR:C	1:B:164:TYR:H	1.98	0.67
1:B:98:CYS:N	2:B:801:ATP:O3'	2.22	0.67
1:A:183:MET:HE1	1:A:187:THR:HB	1.76	0.67
1:D:129:GLY:N	2:D:801:ATP:O2B	2.25	0.66
1:C:162:TYR:O	1:C:164:TYR:N	2.28	0.66
1:B:613:ARG:NH2	1:C:657:GLU:OE1	2.28	0.66
1:C:183:MET:HE1	1:C:187:THR:HB	1.77	0.66
1:A:162:TYR:O	1:A:164:TYR:N	2.28	0.66
1:A:85:ILE:HD11	1:A:92:ILE:HG21	1.78	0.65
1:A:244:PRO:HB2	1:A:248:TRP:CD1	2.31	0.65
1:B:162:TYR:C	1:B:164:TYR:N	2.50	0.65
1:D:183:MET:HE1	1:D:187:THR:HB	1.79	0.65
1:C:408:LYS:HB2	1:C:440:GLY:HA3	1.79	0.65
1:D:31:THR:HG21	1:D:39:MET:SD	2.37	0.65
1:D:79:TRP:CZ3	1:D:630:ILE:HD13	2.32	0.64
1:D:31:THR:HG21	1:D:91:THR:CG2	2.27	0.64
1:D:82:VAL:HA	1:D:85:ILE:HD12	1.79	0.63
1:C:82:VAL:HA	1:C:85:ILE:HD12	1.81	0.63
1:C:173:SER:HB3	1:C:184:THR:HG21	1.80	0.63
1:B:669:LEU:HB3	1:B:673:GLN:HG3	1.79	0.63
1:A:283:ILE:HG22	1:A:288:ILE:HD11	1.81	0.63
1:B:244:PRO:HB2	1:B:248:TRP:CD1	2.33	0.63
1:C:85:ILE:HD11	1:C:92:ILE:HG21	1.80	0.63
1:D:85:ILE:HD11	1:D:92:ILE:HG21	1.80	0.62
1:D:162:TYR:C	1:D:164:TYR:N	2.50	0.62
1:B:82:VAL:HA	1:B:85:ILE:HD12	1.80	0.62
1:D:162:TYR:C	1:D:164:TYR:H	2.02	0.62
1:B:85:ILE:HD11	1:B:92:ILE:HG21	1.81	0.62
1:B:159:VAL:HA	1:B:162:TYR:HD1	1.64	0.62
1:A:204:THR:HG23	1:B:35:ASP:OD1	2.00	0.61
1:C:162:TYR:C	1:C:164:TYR:N	2.52	0.61
1:D:434:ARG:NH1	3:D:802:PO4:O2	2.31	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ALA:HB2	1:B:421:PRO:HG2	1.82	0.61
1:C:703:GLU:CG	1:C:703:GLU:O	2.47	0.61
1:A:136:LEU:HD23	1:A:136:LEU:C	2.21	0.61
1:D:79:TRP:HZ2	1:D:762:ALA:O	1.83	0.61
1:A:53:VAL:HG11	1:A:334:LEU:CD1	2.30	0.61
1:A:162:TYR:C	1:A:164:TYR:N	2.53	0.61
1:C:162:TYR:C	1:C:164:TYR:H	2.03	0.61
1:D:173:SER:HB3	1:D:184:THR:HG21	1.82	0.61
1:C:159:VAL:HA	1:C:162:TYR:HD1	1.65	0.61
1:A:159:VAL:HA	1:A:162:TYR:HD1	1.66	0.60
1:C:53:VAL:HG11	1:C:334:LEU:CD1	2.31	0.60
1:A:82:VAL:HA	1:A:85:ILE:HD12	1.84	0.60
1:A:162:TYR:C	1:A:164:TYR:H	2.04	0.60
1:A:209:GLN:HA	1:A:265:ARG:O	2.01	0.60
1:C:283:ILE:HG22	1:C:288:ILE:HD11	1.83	0.60
1:D:244:PRO:HB2	1:D:248:TRP:CD1	2.36	0.59
1:C:703:GLU:O	1:C:703:GLU:HG3	2.02	0.59
1:C:244:PRO:HB2	1:C:248:TRP:CD1	2.37	0.59
1:D:283:ILE:HG22	1:D:288:ILE:HD11	1.84	0.59
1:A:529:CYS:CA	1:A:712:THR:HG21	2.33	0.59
1:D:266:LEU:HD21	1:D:268:ILE:HG13	1.85	0.59
1:B:138:ARG:HD3	1:B:342:ALA:HB2	1.85	0.58
1:C:204:THR:HG23	1:D:35:ASP:OD1	2.03	0.58
1:B:283:ILE:HG22	1:B:288:ILE:HD11	1.85	0.58
1:B:645:TYR:CE2	1:C:656:GLU:HG2	2.39	0.58
1:B:53:VAL:HG11	1:B:334:LEU:CD1	2.34	0.58
1:A:97:ARG:HA	2:A:801:ATP:O3'	2.04	0.58
1:A:164:TYR:CD1	1:A:338:PRO:HA	2.39	0.58
1:A:244:PRO:O	1:A:245:GLU:HB2	2.04	0.57
1:B:164:TYR:CD1	1:B:338:PRO:HB3	2.39	0.57
1:D:31:THR:CG2	1:D:91:THR:HG21	2.33	0.57
1:B:669:LEU:HD13	1:B:673:GLN:HG3	1.87	0.57
1:D:173:SER:O	1:D:184:THR:HG22	2.05	0.57
1:B:266:LEU:O	1:B:266:LEU:HD12	2.04	0.57
1:A:209:GLN:O	1:A:210:ARG:HB2	2.05	0.57
1:B:669:LEU:HB3	1:B:673:GLN:HG2	1.85	0.57
1:D:40:ASN:HB3	1:D:85:ILE:CG2	2.34	0.56
1:A:85:ILE:CD1	1:A:92:ILE:HG21	2.35	0.56
1:B:244:PRO:O	1:B:245:GLU:HB2	2.05	0.56
1:D:244:PRO:O	1:D:245:GLU:HB2	2.05	0.56
1:A:417:ASN:HB3	1:A:479:THR:HG23	1.88	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ALA:HB1	1:D:266:LEU:HD13	1.86	0.56
1:B:632:ARG:NH2	3:B:803:PO4:O4	2.38	0.55
1:D:53:VAL:HG11	1:D:334:LEU:CD1	2.37	0.55
1:D:85:ILE:CD1	1:D:92:ILE:HG21	2.37	0.55
1:D:408:LYS:HG3	1:D:440:GLY:HA3	1.89	0.55
1:C:417:ASN:HB3	1:C:479:THR:HG23	1.88	0.55
1:A:558:THR:OG1	1:B:565:ARG:NH1	2.35	0.55
1:C:570:ALA:HB1	1:C:573:THR:OG1	2.06	0.55
1:C:244:PRO:O	1:C:245:GLU:HB2	2.06	0.55
1:D:40:ASN:CB	1:D:85:ILE:HG23	2.37	0.55
1:B:30:LEU:HB3	1:B:60:ILE:HB	1.89	0.54
1:C:173:SER:O	1:C:184:THR:HG22	2.06	0.54
1:B:85:ILE:CD1	1:B:92:ILE:HG21	2.37	0.54
1:B:408:LYS:HG3	1:B:440:GLY:HA3	1.89	0.54
1:C:30:LEU:HB3	1:C:60:ILE:HB	1.88	0.54
1:B:417:ASN:HB3	1:B:479:THR:HG23	1.88	0.54
1:C:148:LEU:HD11	1:C:158:ALA:CB	2.38	0.54
1:A:30:LEU:HB3	1:A:60:ILE:HB	1.90	0.54
1:A:408:LYS:HB2	1:A:440:GLY:HA3	1.88	0.54
1:C:85:ILE:CD1	1:C:92:ILE:HG21	2.37	0.54
1:B:40:ASN:HB3	1:B:85:ILE:CG2	2.38	0.54
1:A:672:MET:HE3	1:B:562:THR:HG23	1.89	0.54
1:C:481:ARG:NE	3:C:805:PO4:O4	2.39	0.54
1:C:572:GLY:HA2	1:C:574:LYS:HE2	1.90	0.54
1:A:207:SER:O	1:A:208:HIS:HB2	2.08	0.53
1:A:40:ASN:HB3	1:A:85:ILE:CG2	2.39	0.53
1:B:408:LYS:HB2	1:B:440:GLY:HA3	1.90	0.53
1:D:408:LYS:HB2	1:D:440:GLY:HA3	1.91	0.53
1:D:539:VAL:HG11	1:D:674:GLN:HG2	1.90	0.53
1:D:583:MET:HG3	1:D:673:GLN:OE1	2.09	0.53
1:A:148:LEU:HD11	1:A:158:ALA:CB	2.39	0.53
1:C:558:THR:OG1	1:D:565:ARG:NH1	2.36	0.53
1:D:164:TYR:CD1	1:D:338:PRO:HA	2.43	0.53
1:A:408:LYS:HG3	1:A:440:GLY:HA3	1.90	0.53
1:B:140:GLU:O	1:B:143:GLY:N	2.39	0.53
1:B:61:TYR:O	1:B:66:GLY:HA3	2.09	0.53
1:D:30:LEU:HB3	1:D:60:ILE:HB	1.90	0.53
1:A:61:TYR:O	1:A:66:GLY:HA3	2.09	0.53
1:A:656:GLU:HG2	1:D:645:TYR:CE2	2.44	0.53
1:B:207:SER:O	1:B:208:HIS:HB2	2.08	0.53
1:C:408:LYS:HG3	1:C:440:GLY:HA3	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:ASN:CB	1:B:479:THR:HG23	2.39	0.52
1:D:61:TYR:O	1:D:66:GLY:HA3	2.10	0.52
1:C:164:TYR:O	1:C:164:TYR:CD1	2.62	0.52
1:D:207:SER:O	1:D:208:HIS:HB2	2.09	0.52
1:C:128:ASP:CB	2:C:801:ATP:O1G	2.57	0.52
1:C:713:THR:HG22	1:C:714:ASP:N	2.25	0.52
1:D:417:ASN:HB3	1:D:479:THR:HG23	1.91	0.52
1:D:140:GLU:O	1:D:143:GLY:N	2.41	0.52
1:B:40:ASN:CB	1:B:85:ILE:HG23	2.39	0.51
1:C:264:LYS:NZ	3:C:802:PO4:O2	2.43	0.51
1:B:226:LEU:HD11	1:B:391:LEU:HA	1.93	0.51
1:A:657:GLU:OE1	1:D:613:ARG:NH2	2.43	0.51
1:D:79:TRP:CZ2	1:D:762:ALA:O	2.63	0.51
1:A:417:ASN:CB	1:A:479:THR:HG23	2.40	0.51
1:A:164:TYR:CE2	1:A:166:ASN:HB2	2.46	0.51
1:D:183:MET:CE	1:D:187:THR:HB	2.40	0.51
1:A:40:ASN:CB	1:A:85:ILE:HG23	2.41	0.51
1:C:61:TYR:O	1:C:66:GLY:HA3	2.10	0.51
1:C:206:GLN:O	1:C:208:HIS:O	2.28	0.51
1:D:583:MET:SD	1:D:673:GLN:CD	2.89	0.51
1:C:138:ARG:HD3	1:C:342:ALA:HB2	1.92	0.51
1:B:154:ILE:HB	1:B:157:GLU:HG2	1.94	0.50
1:C:183:MET:CE	1:C:187:THR:HB	2.42	0.50
1:D:417:ASN:CB	1:D:479:THR:HG23	2.40	0.50
1:D:566:ILE:HD13	1:D:580:ILE:CD1	2.42	0.50
1:A:138:ARG:HD3	1:A:342:ALA:HB2	1.94	0.50
1:A:140:GLU:O	1:A:143:GLY:N	2.43	0.50
1:C:40:ASN:HB3	1:C:85:ILE:CG2	2.39	0.50
1:B:566:ILE:HG21	1:B:580:ILE:HD11	1.94	0.50
1:C:417:ASN:CB	1:C:479:THR:HG23	2.41	0.50
1:A:183:MET:CE	1:A:187:THR:HB	2.42	0.50
1:D:164:TYR:CE2	1:D:166:ASN:HB2	2.47	0.50
1:B:669:LEU:CB	1:B:673:GLN:HG3	2.42	0.49
1:D:266:LEU:HD21	1:D:268:ILE:CG1	2.41	0.49
1:D:396:ARG:NH2	1:D:439:ASP:OD1	2.44	0.49
1:D:226:LEU:HD11	1:D:391:LEU:HA	1.93	0.49
1:A:226:LEU:HD11	1:A:391:LEU:HA	1.94	0.49
1:C:226:LEU:HD11	1:C:391:LEU:HA	1.93	0.49
1:B:666:LYS:C	1:B:667:ASN:HD22	2.15	0.49
1:D:566:ILE:HG21	1:D:580:ILE:HD11	1.94	0.49
1:A:178:PHE:CE2	1:A:360:CYS:HB3	2.48	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:HB	1:A:157:GLU:HG2	1.94	0.49
1:C:672:MET:HE3	1:D:562:THR:HG23	1.95	0.49
1:C:207:SER:O	1:C:208:HIS:HB2	2.13	0.48
1:A:207:SER:O	1:A:208:HIS:CB	2.60	0.48
1:B:396:ARG:NH2	1:B:439:ASP:OD1	2.45	0.48
1:C:407:PRO:O	1:C:407:PRO:CG	2.40	0.48
1:A:164:TYR:CE1	1:A:338:PRO:HA	2.49	0.48
1:D:430:ARG:HH21	3:D:802:PO4:P	2.33	0.48
1:C:53:VAL:O	1:C:53:VAL:HG12	2.14	0.48
1:C:569:SER:O	1:C:570:ALA:C	2.50	0.48
1:C:583:MET:HG3	1:C:673:GLN:OE1	2.14	0.48
1:A:529:CYS:HA	1:A:712:THR:HG21	1.95	0.48
1:C:154:ILE:HB	1:C:157:GLU:HG2	1.94	0.48
1:C:178:PHE:CE2	1:C:360:CYS:HB3	2.49	0.48
1:D:205:ALA:HB2	1:D:266:LEU:HD13	1.92	0.48
1:B:183:MET:CE	1:B:187:THR:HB	2.42	0.48
1:C:713:THR:CG2	1:C:714:ASP:N	2.77	0.48
1:D:206:GLN:O	1:D:265:ARG:NH2	2.38	0.48
1:C:40:ASN:CB	1:C:85:ILE:HG23	2.41	0.48
1:D:154:ILE:HB	1:D:157:GLU:HG2	1.96	0.48
1:C:128:ASP:HB3	2:C:801:ATP:O1G	2.14	0.48
1:A:570:ALA:CB	1:B:421:PRO:HG2	2.43	0.48
1:D:183:MET:HE2	1:D:183:MET:HB3	1.69	0.47
1:B:571:SER:OG	1:B:632:ARG:HD3	2.14	0.47
1:C:207:SER:O	1:C:208:HIS:CB	2.62	0.47
1:A:255:LYS:NZ	1:A:398:ALA:O	2.47	0.47
1:B:53:VAL:HG12	1:B:53:VAL:O	2.15	0.47
1:D:97:ARG:HA	2:D:801:ATP:O3'	2.14	0.47
1:A:583:MET:HG3	1:A:673:GLN:OE1	2.14	0.47
1:C:420:ALA:HB2	1:C:481:ARG:NH2	2.30	0.47
1:C:576:ARG:HD2	1:C:578:PHE:CZ	2.49	0.47
1:A:53:VAL:HG12	1:A:53:VAL:O	2.15	0.47
1:A:164:TYR:CZ	1:A:166:ASN:HB2	2.50	0.47
1:A:313:THR:CG2	1:A:319:ARG:HH21	2.28	0.47
1:B:694:MET:O	1:B:698:THR:HG23	2.15	0.47
1:C:408:LYS:CB	1:C:440:GLY:HA3	2.45	0.47
1:A:209:GLN:O	1:A:210:ARG:CB	2.63	0.47
1:A:576:ARG:HD2	1:A:578:PHE:CZ	2.51	0.46
1:B:313:THR:CG2	1:B:319:ARG:HH21	2.28	0.46
1:A:238:PHE:HD2	1:A:271:VAL:HG22	1.79	0.46
1:B:324:ARG:CZ	1:B:347:LEU:HD21	2.46	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:ILE:HD12	1:B:634:LEU:CD1	2.46	0.46
1:C:255:LYS:NZ	1:C:398:ALA:O	2.45	0.46
1:C:703:GLU:O	1:C:704:ALA:HB2	2.16	0.46
1:D:583:MET:HG3	1:D:673:GLN:CD	2.35	0.46
1:A:441:HIS:NE2	1:A:698:THR:HG22	2.30	0.46
1:D:441:HIS:NE2	1:D:698:THR:HG22	2.31	0.46
1:D:580:ILE:HD12	1:D:634:LEU:CD1	2.46	0.46
1:D:694:MET:O	1:D:698:THR:HG23	2.15	0.46
1:B:441:HIS:NE2	1:B:698:THR:HG22	2.31	0.46
1:D:255:LYS:NZ	1:D:398:ALA:O	2.48	0.46
1:D:571:SER:OG	1:D:632:ARG:HD3	2.15	0.46
1:C:313:THR:CG2	1:C:319:ARG:HH21	2.29	0.46
1:C:694:MET:O	1:C:698:THR:HG23	2.15	0.46
1:D:144:LEU:HD13	1:D:158:ALA:HA	1.96	0.46
1:A:539:VAL:HG11	1:A:674:GLN:HA	1.97	0.46
1:D:138:ARG:HD3	1:D:138:ARG:C	2.37	0.46
1:D:164:TYR:CE1	1:D:338:PRO:HA	2.51	0.46
1:C:140:GLU:O	1:C:143:GLY:N	2.46	0.46
1:A:283:ILE:CG2	1:A:288:ILE:HD11	2.47	0.45
1:C:207:SER:HB3	1:D:91:THR:H	1.81	0.45
1:D:79:TRP:HZ3	1:D:630:ILE:HD13	1.80	0.45
1:B:115:LEU:HD22	1:B:161:LYS:HB3	1.98	0.45
1:B:238:PHE:HD2	1:B:271:VAL:HG22	1.80	0.45
1:C:441:HIS:NE2	1:C:698:THR:HG22	2.31	0.45
1:C:238:PHE:HD2	1:C:271:VAL:HG22	1.81	0.45
1:D:583:MET:HB2	1:D:673:GLN:HE22	1.82	0.45
1:C:396:ARG:NH2	1:C:439:ASP:OD1	2.47	0.45
1:D:238:PHE:HD2	1:D:271:VAL:HG22	1.81	0.45
1:A:694:MET:O	1:A:698:THR:HG23	2.17	0.45
1:D:30:LEU:C	1:D:30:LEU:HD22	2.37	0.45
1:D:420:ALA:HB2	1:D:481:ARG:NH2	2.32	0.45
1:A:529:CYS:HB3	1:A:712:THR:CG2	2.46	0.45
1:B:33:GLY:O	1:B:34:GLY:C	2.55	0.45
1:B:566:ILE:HD13	1:B:580:ILE:CD1	2.42	0.45
1:B:669:LEU:CD1	1:B:673:GLN:HG3	2.47	0.45
1:C:529:CYS:SG	1:C:712:THR:CG2	3.05	0.45
1:D:164:TYR:CZ	1:D:166:ASN:HB2	2.51	0.45
1:C:283:ILE:CG2	1:C:288:ILE:HD11	2.47	0.44
1:D:583:MET:HB2	1:D:673:GLN:NE2	2.31	0.44
1:A:576:ARG:HG3	1:A:663:ASP:OD1	2.17	0.44
1:B:183:MET:HE2	1:B:183:MET:HB3	1.68	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:ALA:HB2	1:B:481:ARG:NH2	2.32	0.44
1:A:396:ARG:NH2	1:A:439:ASP:OD1	2.47	0.44
1:A:580:ILE:HD12	1:A:634:LEU:CD1	2.48	0.44
1:C:128:ASP:HB2	2:C:801:ATP:O1G	2.18	0.44
1:D:178:PHE:CE2	1:D:360:CYS:HB3	2.53	0.44
1:D:329:ALA:HA	1:D:345:VAL:HG21	2.00	0.44
1:A:572:GLY:HA3	1:B:475:SER:O	2.18	0.44
1:D:583:MET:SD	1:D:673:GLN:CG	3.06	0.44
1:A:183:MET:HB3	1:A:183:MET:HE2	1.72	0.44
1:B:576:ARG:HG3	1:B:663:ASP:OD1	2.17	0.44
1:C:412:ASN:OD1	1:C:442:ARG:NH1	2.50	0.44
1:C:419:GLY:O	1:C:479:THR:HB	2.17	0.44
1:D:577:VAL:O	1:D:664:CYS:HA	2.17	0.44
1:A:211:THR:HG23	1:A:267:ASN:HB2	2.00	0.44
1:A:408:LYS:CB	1:A:440:GLY:HA3	2.48	0.44
1:A:577:VAL:O	1:A:664:CYS:HA	2.17	0.44
1:B:255:LYS:NZ	1:B:398:ALA:O	2.47	0.44
1:C:193:ARG:NH2	1:C:313:THR:O	2.50	0.44
1:C:193:ARG:HA	1:C:193:ARG:HD3	1.84	0.44
1:C:311:GLY:HA2	1:D:204:THR:CG2	2.48	0.44
1:D:53:VAL:HG12	1:D:53:VAL:O	2.18	0.44
1:D:283:ILE:CG2	1:D:288:ILE:HD11	2.48	0.44
1:D:115:LEU:HD22	1:D:161:LYS:HB3	2.00	0.43
1:A:329:ALA:HA	1:A:345:VAL:HG21	2.01	0.43
1:D:83:SER:HB2	3:D:803:PO4:O4	2.18	0.43
1:B:178:PHE:CE2	1:B:360:CYS:HB3	2.54	0.43
1:B:329:ALA:HA	1:B:345:VAL:HG21	2.00	0.43
1:C:329:ALA:HA	1:C:345:VAL:HG21	2.01	0.43
1:C:577:VAL:O	1:C:664:CYS:HA	2.19	0.43
1:C:183:MET:HE2	1:C:183:MET:HB3	1.71	0.43
1:D:666:LYS:C	1:D:667:ASN:HD22	2.22	0.43
1:B:283:ILE:CG2	1:B:288:ILE:HD11	2.48	0.43
1:B:711:PHE:C	1:B:712:THR:HG23	2.38	0.43
1:C:211:THR:HG23	1:C:267:ASN:HB2	2.01	0.43
1:D:205:ALA:HB1	1:D:266:LEU:CD1	2.49	0.43
1:D:418:VAL:O	1:D:507:GLY:HA3	2.19	0.43
1:A:48:ARG:NH1	1:A:761:LEU:O	2.52	0.42
1:D:33:GLY:O	1:D:34:GLY:C	2.57	0.42
1:A:696:TRP:HB2	1:A:729:PHE:CZ	2.54	0.42
1:B:508:GLY:HA3	1:B:538:THR:HG23	2.02	0.42
1:D:30:LEU:C	1:D:30:LEU:CD2	2.87	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:ARG:NH2	1:D:313:THR:O	2.52	0.42
1:A:481:ARG:NH2	3:A:805:PO4:O2	2.50	0.42
1:C:53:VAL:O	1:C:53:VAL:CG1	2.68	0.42
1:C:83:SER:HB3	3:C:804:PO4:O1	2.20	0.42
1:B:266:LEU:CD1	1:B:266:LEU:C	2.88	0.42
1:B:418:VAL:O	1:B:507:GLY:HA3	2.19	0.42
1:D:576:ARG:HG3	1:D:663:ASP:OD1	2.20	0.42
1:B:696:TRP:HB2	1:B:729:PHE:CZ	2.54	0.42
1:B:181:THR:HG22	1:B:346:SER:OG	2.20	0.42
1:D:181:THR:HG22	1:D:346:SER:OG	2.20	0.42
1:D:622:LEU:O	1:D:626:MET:HG2	2.19	0.42
1:B:198:VAL:O	1:B:202:MET:HG3	2.20	0.42
1:C:539:VAL:HG11	1:C:674:GLN:HA	2.02	0.42
1:B:193:ARG:NH2	1:B:313:THR:O	2.53	0.42
1:B:408:LYS:CB	1:B:440:GLY:HA3	2.49	0.42
1:B:577:VAL:O	1:B:664:CYS:HA	2.20	0.42
1:C:580:ILE:HD12	1:C:634:LEU:CD1	2.49	0.42
1:D:266:LEU:HG	1:D:267:ASN:H	1.80	0.42
1:A:508:GLY:HA3	1:A:538:THR:HG23	2.01	0.41
1:D:193:ARG:HA	1:D:193:ARG:HD3	1.85	0.41
1:A:328:GLU:HG2	1:A:352:ALA:HB1	2.02	0.41
1:B:53:VAL:O	1:B:53:VAL:CG1	2.68	0.41
1:C:198:VAL:O	1:C:202:MET:HG3	2.21	0.41
1:C:328:GLU:HG2	1:C:352:ALA:HB1	2.02	0.41
1:A:181:THR:HG22	1:A:346:SER:OG	2.21	0.41
1:A:257:SER:HA	1:A:298:TYR:OH	2.20	0.41
1:A:419:GLY:O	1:A:479:THR:HB	2.21	0.41
1:B:206:GLN:O	1:B:265:ARG:NH2	2.43	0.41
1:D:53:VAL:O	1:D:53:VAL:CG1	2.68	0.41
1:C:696:TRP:HB2	1:C:729:PHE:CZ	2.56	0.41
1:D:408:LYS:CB	1:D:440:GLY:HA3	2.50	0.41
1:D:696:TRP:HB2	1:D:729:PHE:CZ	2.55	0.41
1:A:418:VAL:O	1:A:507:GLY:HA3	2.20	0.41
1:D:30:LEU:HD22	1:D:30:LEU:O	2.21	0.41
1:D:324:ARG:CZ	1:D:347:LEU:HD21	2.50	0.41
1:B:159:VAL:O	1:B:162:TYR:HB2	2.20	0.41
1:C:576:ARG:HG3	1:C:663:ASP:OD1	2.20	0.41
1:A:327:VAL:HG21	1:A:757:LEU:HD22	2.03	0.41
1:B:48:ARG:NH1	1:B:761:LEU:O	2.54	0.41
1:C:327:VAL:HG21	1:C:757:LEU:HD22	2.03	0.41
1:C:622:LEU:O	1:C:626:MET:HG2	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:GLU:OE1	1:B:375:ARG:NH1	2.54	0.41
1:C:129:GLY:HA3	2:C:801:ATP:O1A	2.21	0.41
1:C:148:LEU:HD11	1:C:158:ALA:HB2	2.03	0.41
1:C:257:SER:HA	1:C:298:TYR:OH	2.21	0.41
1:D:108:LEU:CD2	1:D:147:GLU:OE1	2.61	0.41
1:A:198:VAL:O	1:A:202:MET:HG3	2.21	0.41
1:A:324:ARG:CZ	1:A:347:LEU:HD21	2.50	0.41
1:D:301:ARG:HA	1:D:301:ARG:HD3	1.97	0.41
1:A:373:GLU:OE1	1:A:375:ARG:NH1	2.55	0.40
1:A:622:LEU:O	1:A:626:MET:HG2	2.21	0.40
1:C:115:LEU:HD22	1:C:161:LYS:HB3	2.02	0.40
1:C:418:VAL:O	1:C:507:GLY:HA3	2.21	0.40
1:C:571:SER:H	1:D:474:GLY:HA3	1.86	0.40
1:D:211:THR:HG23	1:D:267:ASN:HB2	2.03	0.40
1:D:583:MET:CG	1:D:673:GLN:CD	2.89	0.40
1:A:30:LEU:HD22	1:A:30:LEU:C	2.42	0.40
1:C:233:GLY:O	3:C:802:PO4:O4	2.38	0.40
1:D:31:THR:HG22	1:D:39:MET:SD	2.61	0.40
1:C:30:LEU:HD22	1:C:30:LEU:C	2.42	0.40
1:D:48:ARG:NH1	1:D:761:LEU:O	2.52	0.40
1:A:53:VAL:O	1:A:53:VAL:CG1	2.69	0.40
1:A:115:LEU:HD22	1:A:161:LYS:HB3	2.03	0.40
1:B:30:LEU:O	1:B:30:LEU:HD22	2.22	0.40
1:C:508:GLY:HA3	1:C:538:THR:HG23	2.03	0.40
1:D:373:GLU:OE1	1:D:375:ARG:NH1	2.55	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)
1:C:294:THR:O	1:D:734:GLU:OE1[5_7107]	1.81	0.39

## 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	729/743 (98%)	700 (96%)	25 (3%)	4 (0%)	29	61
1	B	728/743 (98%)	700 (96%)	25 (3%)	3 (0%)	34	66
1	C	728/743 (98%)	698 (96%)	27 (4%)	3 (0%)	34	66
1	D	728/743 (98%)	699 (96%)	26 (4%)	3 (0%)	34	66
All	All	2913/2972 (98%)	2797 (96%)	103 (4%)	13 (0%)	34	66

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	ALA
1	A	407	PRO
1	B	163	ALA
1	B	407	PRO
1	C	163	ALA
1	D	163	ALA
1	D	407	PRO
1	C	208	HIS
1	C	407	PRO
1	A	208	HIS
1	A	210	ARG
1	B	208	HIS
1	D	208	HIS

### 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	591/599 (99%)	579 (98%)	12 (2%)	55	84
1	B	590/599 (98%)	575 (98%)	15 (2%)	47	80
1	C	590/599 (98%)	577 (98%)	13 (2%)	52	83
1	D	590/599 (98%)	574 (97%)	16 (3%)	44	78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2361/2396 (98%)	2305 (98%)	56 (2%)	49 81

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	104	ARG
1	A	128	ASP
1	A	145	LEU
1	A	177	ASP
1	A	181	THR
1	A	242	SER
1	A	453	PHE
1	A	479	THR
1	A	538	THR
1	A	643	GLU
1	A	666	LYS
1	B	30	LEU
1	B	104	ARG
1	B	105	GLU
1	B	145	LEU
1	B	148	LEU
1	B	177	ASP
1	B	242	SER
1	B	266	LEU
1	B	359	GLU
1	B	404	ASP
1	B	453	PHE
1	B	479	THR
1	B	538	THR
1	B	617	SER
1	B	643	GLU
1	C	25	SER
1	C	30	LEU
1	C	104	ARG
1	C	145	LEU
1	C	177	ASP
1	C	181	THR
1	C	453	PHE
1	C	479	THR
1	C	538	THR
1	C	571	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	617	SER
1	C	643	GLU
1	C	672	MET
1	D	30	LEU
1	D	104	ARG
1	D	105	GLU
1	D	138	ARG
1	D	145	LEU
1	D	147	GLU
1	D	155	ASP
1	D	177	ASP
1	D	181	THR
1	D	266	LEU
1	D	359	GLU
1	D	453	PHE
1	D	479	THR
1	D	538	THR
1	D	617	SER
1	D	643	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	644	ASN
1	A	667	ASN
1	B	65	GLN
1	B	644	ASN
1	B	652	GLN
1	B	673	GLN
1	C	151	ASN
1	C	644	ASN
1	C	667	ASN
1	D	644	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 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	803	-	4,4,4	0.57	0	6,6,6	1.54	2 (33%)
2	ATP	A	801	-	26,33,33	0.98	1 (3%)	31,52,52	1.29	5 (16%)
2	ATP	B	801	-	26,33,33	0.98	0	31,52,52	1.68	9 (29%)
3	PO4	A	802	-	4,4,4	1.29	0	6,6,6	2.17	2 (33%)
3	PO4	B	802	-	4,4,4	0.71	0	6,6,6	0.39	0
3	PO4	C	803	-	4,4,4	0.60	0	6,6,6	1.09	0
3	PO4	A	804	-	4,4,4	0.77	0	6,6,6	0.84	0
3	PO4	C	804	-	4,4,4	0.90	0	6,6,6	1.41	1 (16%)
2	ATP	C	801	-	26,33,33	1.15	3 (11%)	31,52,52	1.64	7 (22%)
3	PO4	A	805	-	4,4,4	0.40	0	6,6,6	0.45	0
3	PO4	C	802	-	4,4,4	0.91	0	6,6,6	0.74	0
3	PO4	C	805	-	4,4,4	0.89	0	6,6,6	0.42	0
3	PO4	D	802	-	4,4,4	1.02	0	6,6,6	1.02	0
3	PO4	D	803	-	4,4,4	1.62	1 (25%)	6,6,6	0.86	0
2	ATP	D	801	-	26,33,33	0.98	1 (3%)	31,52,52	1.59	7 (22%)
3	PO4	B	803	-	4,4,4	1.12	0	6,6,6	1.42	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	ATP	A	801	-	-	4/18/38/38	0/3/3/3
2	ATP	D	801	-	-	6/18/38/38	0/3/3/3
2	ATP	B	801	-	-	4/18/38/38	0/3/3/3
2	ATP	C	801	-	-	2/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ATP	C2'-C1'	-2.69	1.49	1.53
2	D	801	ATP	C5-C4	2.60	1.47	1.40
2	C	801	ATP	C5-C4	2.39	1.47	1.40
2	C	801	ATP	O4'-C1'	2.32	1.44	1.41
2	A	801	ATP	C5-C4	2.30	1.47	1.40
3	D	803	PO4	P-O1	2.07	1.55	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	ATP	N3-C2-N1	-4.00	122.43	128.68
2	B	801	ATP	N3-C2-N1	-3.90	122.58	128.68
2	D	801	ATP	N3-C2-N1	-3.83	122.70	128.68
3	A	802	PO4	O4-P-O1	-3.70	97.35	110.89
2	C	801	ATP	O2A-PA-O1A	3.14	127.78	112.24
2	A	801	ATP	N3-C2-N1	-3.04	123.93	128.68
2	B	801	ATP	C3'-C2'-C1'	3.01	105.52	100.98
3	A	802	PO4	O4-P-O3	2.94	117.41	107.97
2	D	801	ATP	PB-O3B-PG	-2.91	122.84	132.83
2	A	801	ATP	O3G-PG-O2G	2.70	117.97	107.64
2	D	801	ATP	C5'-C4'-C3'	-2.54	105.64	115.18
2	B	801	ATP	O3B-PG-O1G	-2.48	97.46	111.19
2	C	801	ATP	O3'-C3'-C4'	2.47	118.20	111.05
2	A	801	ATP	PA-O3A-PB	-2.47	124.35	132.83
3	A	803	PO4	O2-P-O1	-2.38	102.19	110.89
2	D	801	ATP	C3'-C2'-C1'	2.38	104.56	100.98
2	A	801	ATP	O2B-PB-O1B	2.35	123.87	112.24
2	C	801	ATP	PB-O3B-PG	-2.35	124.77	132.83
2	B	801	ATP	C4-C5-N7	-2.33	106.97	109.40
2	C	801	ATP	C2-N1-C6	2.30	122.68	118.75
2	C	801	ATP	N6-C6-N1	2.29	123.33	118.57
2	B	801	ATP	O2G-PG-O3B	2.28	112.29	104.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	ATP	C5'-C4'-C3'	-2.27	106.68	115.18
2	B	801	ATP	C2-N1-C6	2.21	122.54	118.75
3	A	803	PO4	O4-P-O2	2.21	115.07	107.97
2	B	801	ATP	PA-O5'-C5'	-2.15	109.05	121.68
2	D	801	ATP	C2-N1-C6	2.15	122.43	118.75
2	A	801	ATP	C4-C5-N7	-2.12	107.19	109.40
2	C	801	ATP	O3B-PG-O1G	-2.07	99.71	111.19
2	D	801	ATP	O2'-C2'-C3'	-2.06	105.16	111.82
2	B	801	ATP	O4'-C4'-C3'	2.03	109.13	105.11
3	C	804	PO4	O4-P-O2	2.01	114.41	107.97
2	D	801	ATP	C4-C5-N7	-2.00	107.31	109.40

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	ATP	C5'-O5'-PA-O3A
2	C	801	ATP	PB-O3B-PG-O2G
2	D	801	ATP	C5'-O5'-PA-O2A
2	D	801	ATP	C5'-O5'-PA-O3A
2	B	801	ATP	C3'-C4'-C5'-O5'
2	C	801	ATP	PB-O3B-PG-O1G
2	A	801	ATP	PB-O3A-PA-O1A
2	B	801	ATP	O4'-C4'-C5'-O5'
2	A	801	ATP	PB-O3A-PA-O2A
2	D	801	ATP	PA-O3A-PB-O2B
2	B	801	ATP	C5'-O5'-PA-O1A
2	D	801	ATP	C3'-C4'-C5'-O5'
2	D	801	ATP	O4'-C4'-C5'-O5'
2	A	801	ATP	PG-O3B-PB-O1B
2	D	801	ATP	PA-O3A-PB-O1B
2	A	801	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

11 monomers are involved in 24 short contacts:

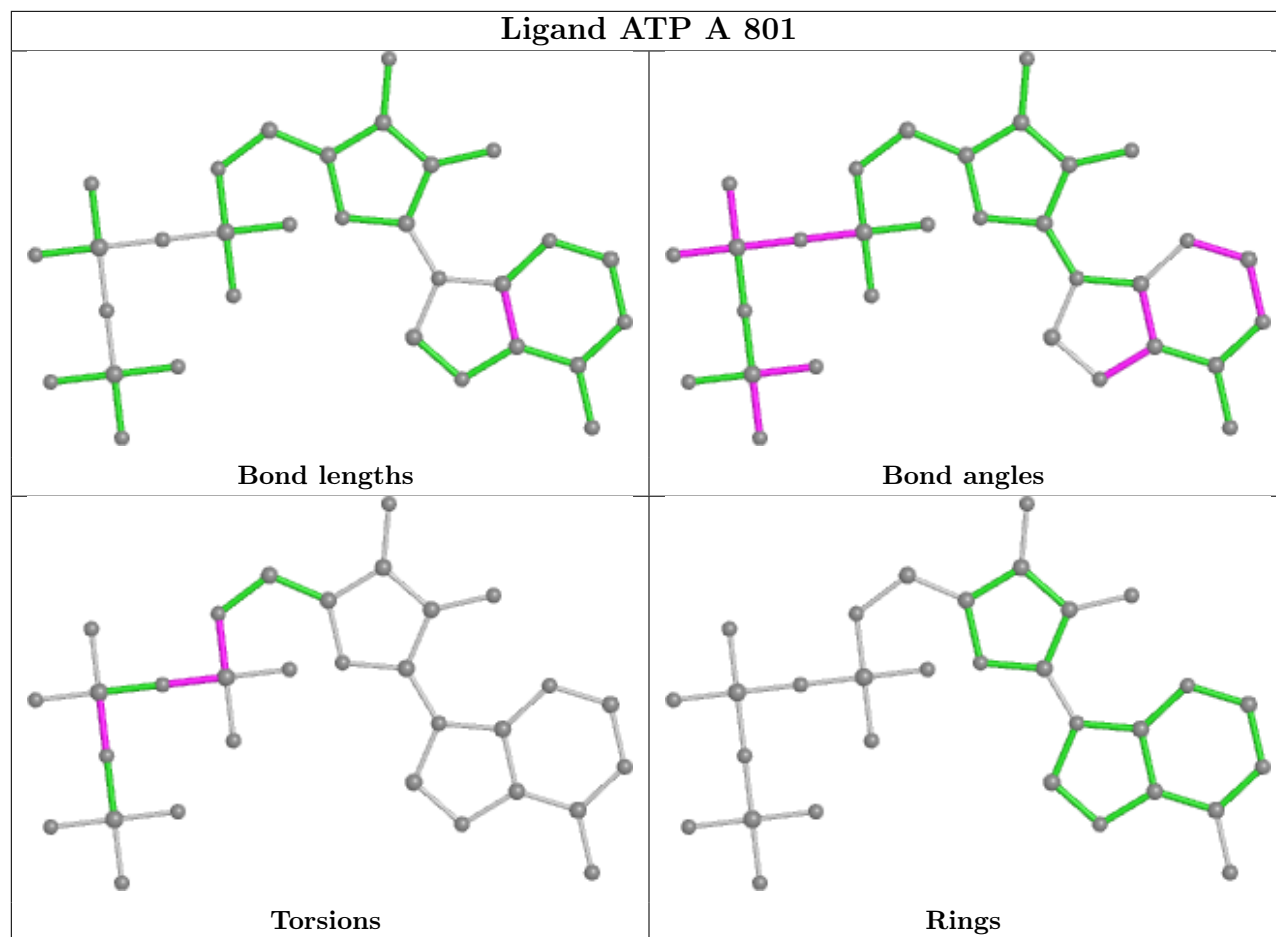
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ATP	1	0
2	B	801	ATP	2	0
3	C	804	PO4	2	0
2	C	801	ATP	4	0

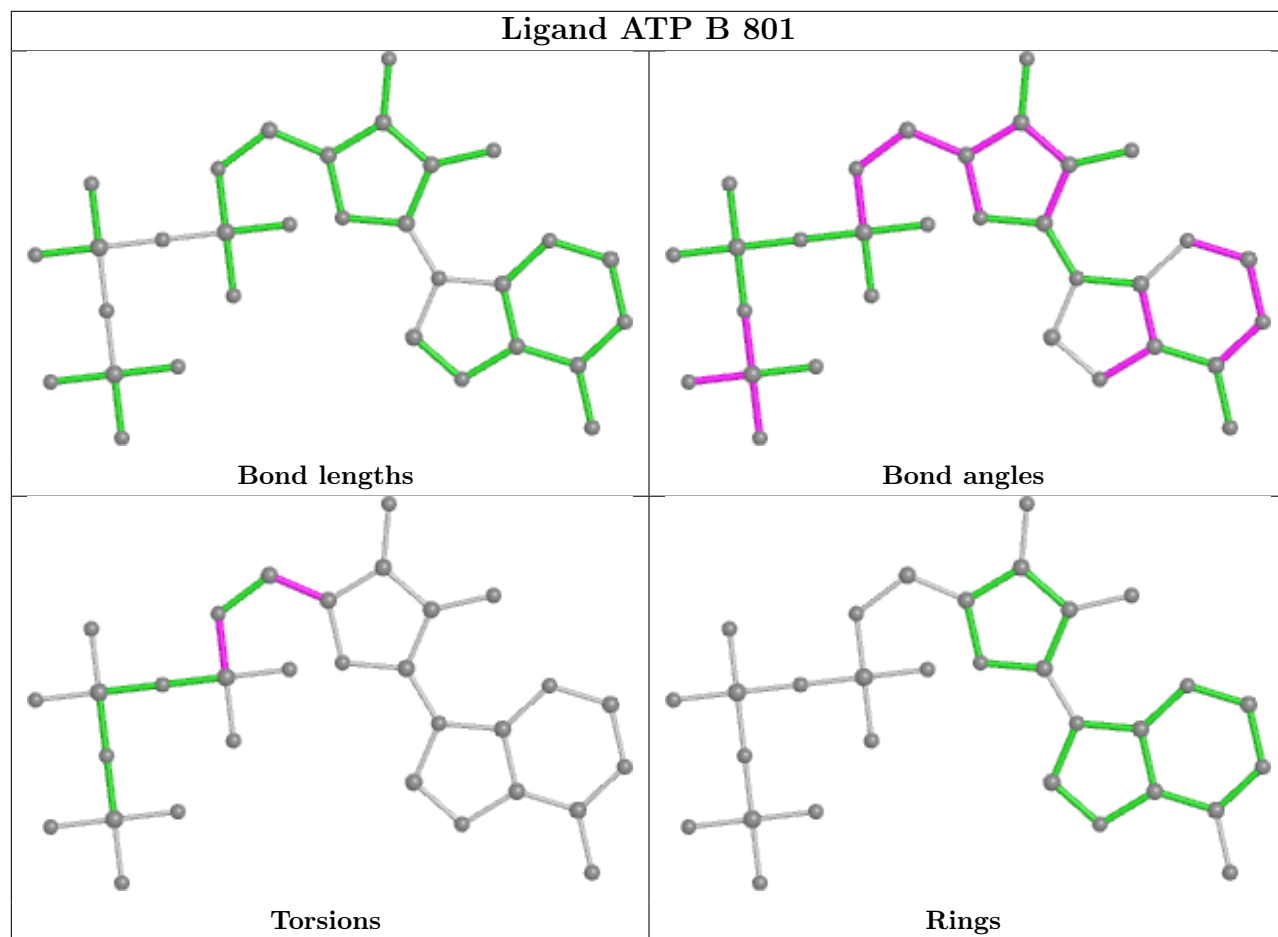
*Continued on next page...*

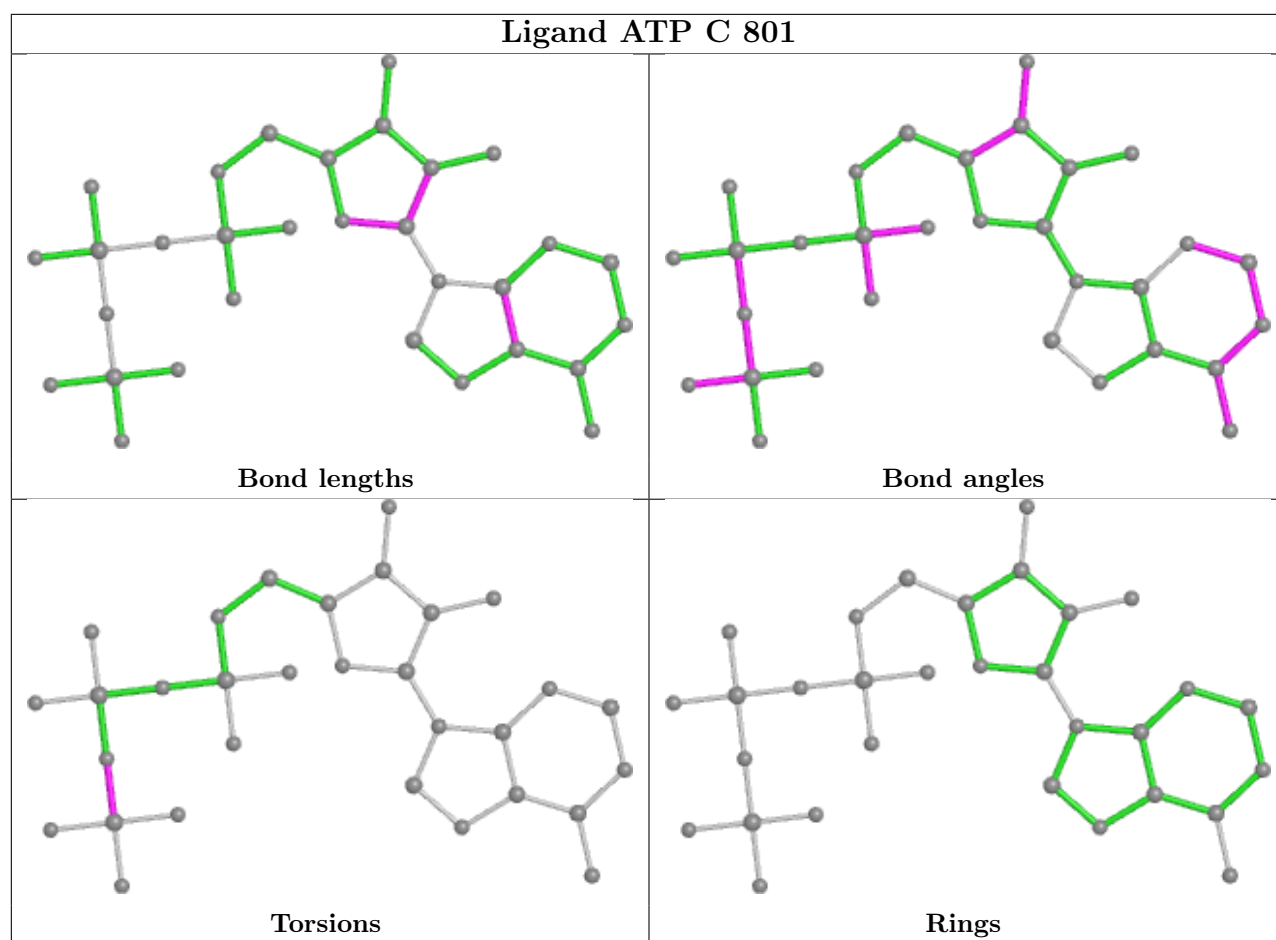
*Continued from previous page...*

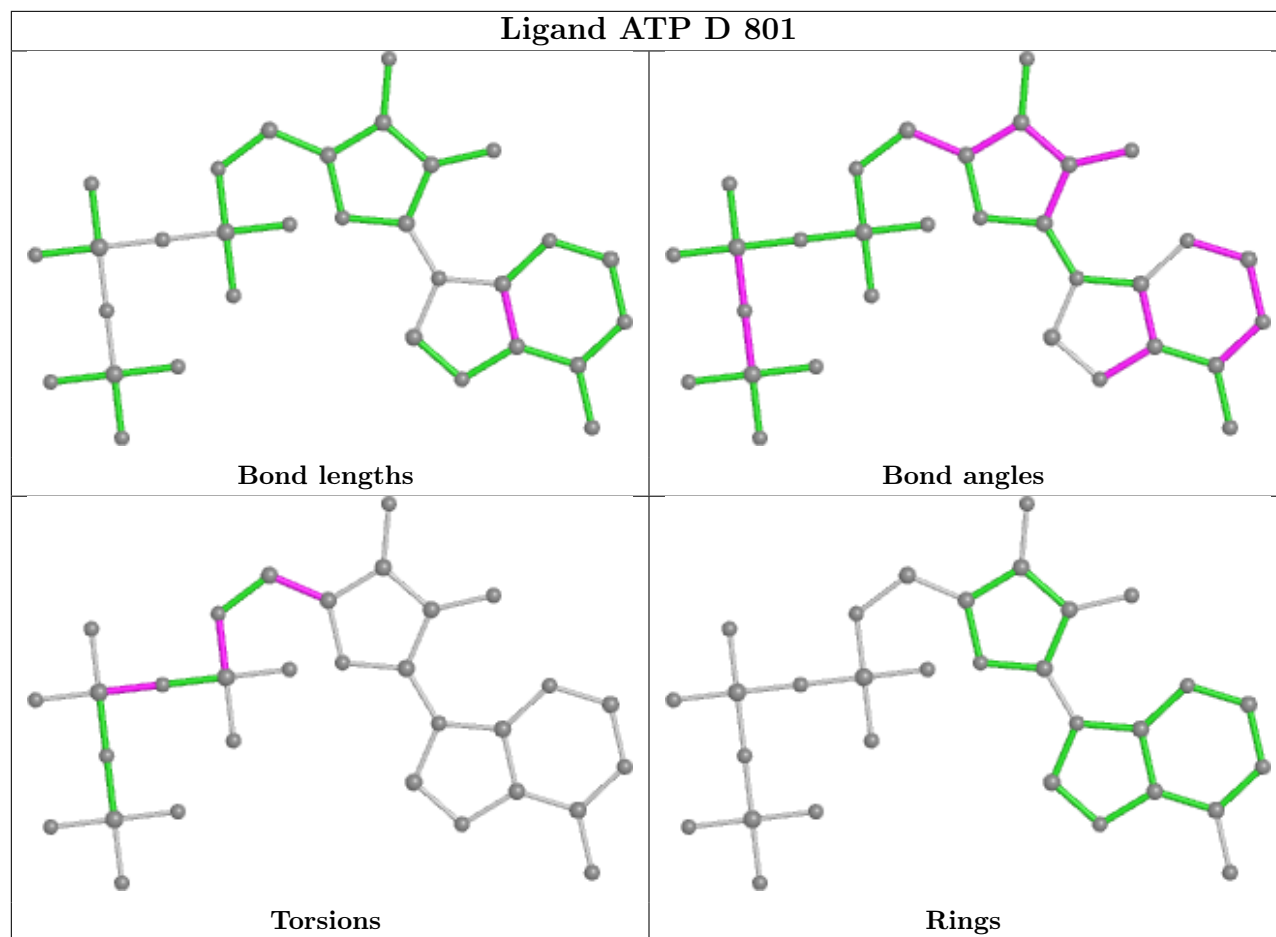
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	805	PO4	1	0
3	C	802	PO4	2	0
3	C	805	PO4	1	0
3	D	802	PO4	3	0
3	D	803	PO4	1	0
2	D	801	ATP	6	0
3	B	803	PO4	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data [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	733/743 (98%)	-0.47	1 (0%) 95 95	31, 54, 90, 129	0
1	B	732/743 (98%)	-0.42	7 (0%) 82 77	30, 57, 102, 151	0
1	C	732/743 (98%)	-0.45	4 (0%) 91 88	35, 62, 95, 135	0
1	D	732/743 (98%)	-0.39	3 (0%) 92 91	33, 60, 107, 155	0
All	All	2929/2972 (98%)	-0.43	15 (0%) 91 88	30, 59, 101, 155	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	ALA	5.3
1	B	503	LEU	4.1
1	C	162	TYR	3.6
1	B	162	TYR	3.5
1	D	162	TYR	3.0
1	D	205	ALA	2.5
1	C	629	THR	2.4
1	B	502	ALA	2.2
1	B	504	LEU	2.2
1	B	208	HIS	2.2
1	B	163	ALA	2.2
1	D	151	ASN	2.1
1	C	163	ALA	2.1
1	C	148	LEU	2.1
1	A	162	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

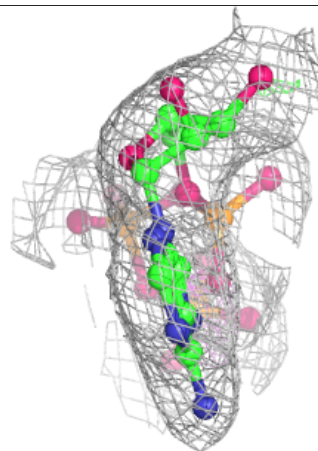
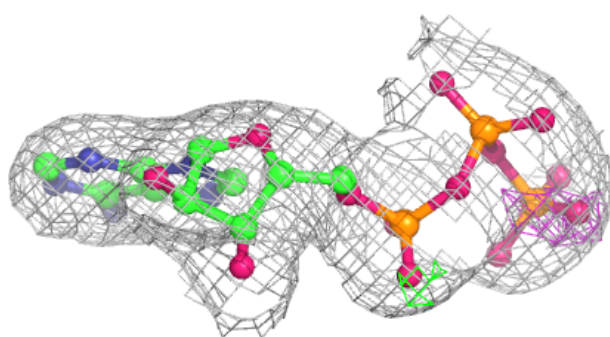
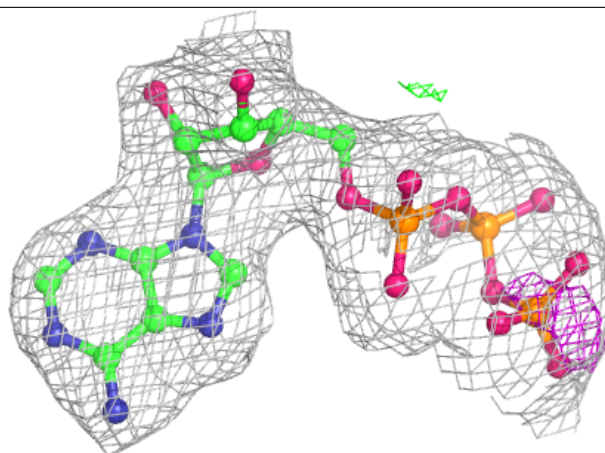
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PO4	A	804	5/5	0.94	0.12	55,58,66,70	5
3	PO4	C	803	5/5	0.95	0.13	65,69,72,78	0
3	PO4	C	804	5/5	0.95	0.17	59,65,70,71	5
3	PO4	A	803	5/5	0.97	0.14	57,61,69,70	0
2	ATP	C	801	31/31	0.97	0.12	51,55,87,93	0
2	ATP	B	801	31/31	0.98	0.12	38,47,59,64	0
2	ATP	A	801	31/31	0.98	0.12	53,60,86,88	0
2	ATP	D	801	31/31	0.98	0.11	45,47,59,67	0
3	PO4	A	802	5/5	0.98	0.15	26,26,27,29	5
3	PO4	C	805	5/5	0.98	0.11	57,58,61,63	0
3	PO4	D	802	5/5	0.98	0.15	52,55,56,56	5
3	PO4	A	805	5/5	0.99	0.08	50,57,60,60	0
3	PO4	B	802	5/5	0.99	0.12	41,42,44,44	5
3	PO4	B	803	5/5	0.99	0.18	22,22,23,24	5
3	PO4	C	802	5/5	0.99	0.13	34,34,36,36	5
3	PO4	D	803	5/5	0.99	0.20	28,30,30,30	5

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.

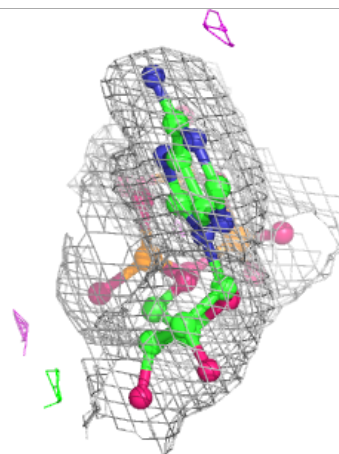
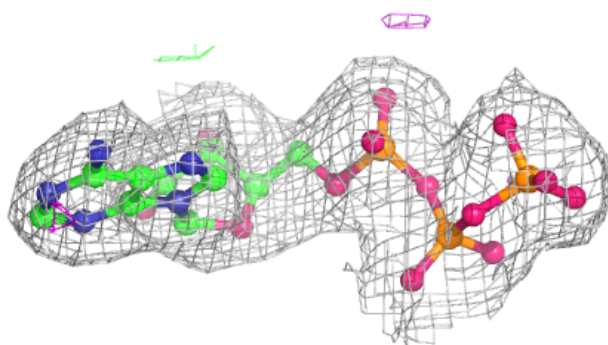
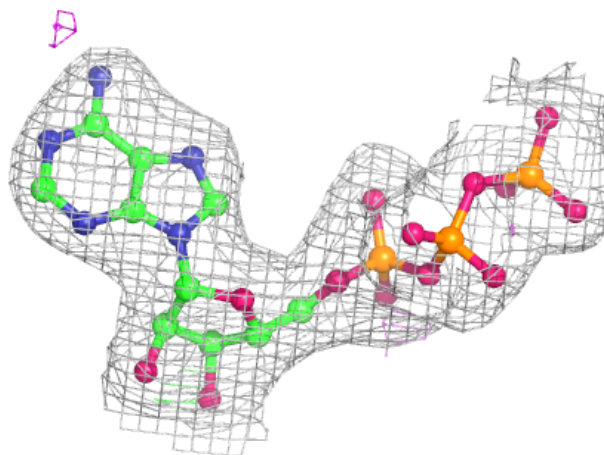
**Electron density around ATP C 801:**

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



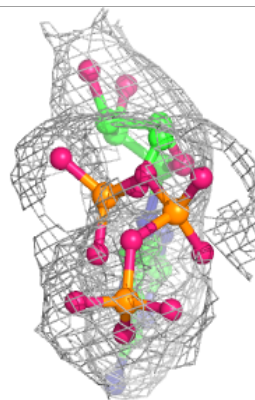
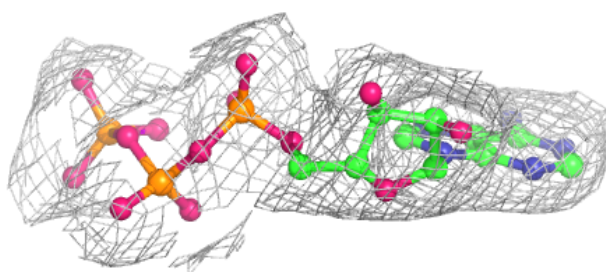
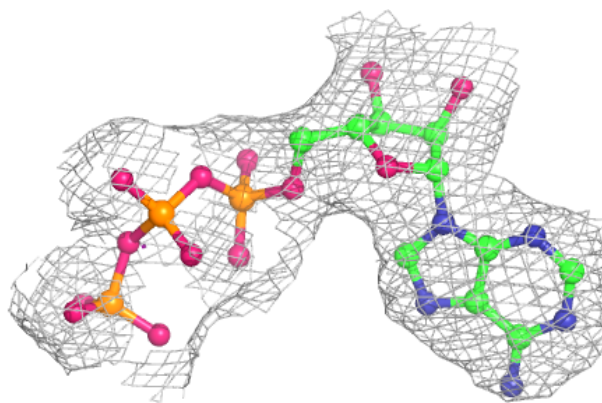
**Electron density around ATP B 801:**

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

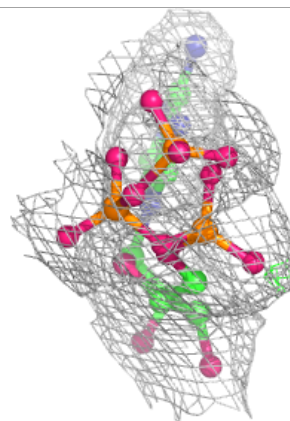
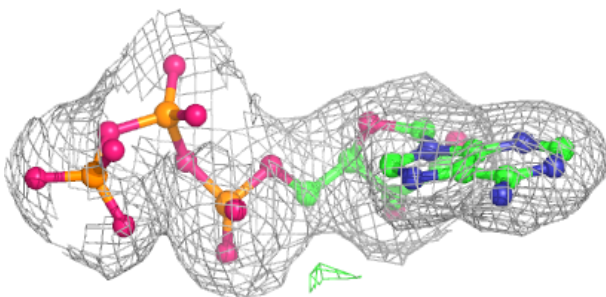
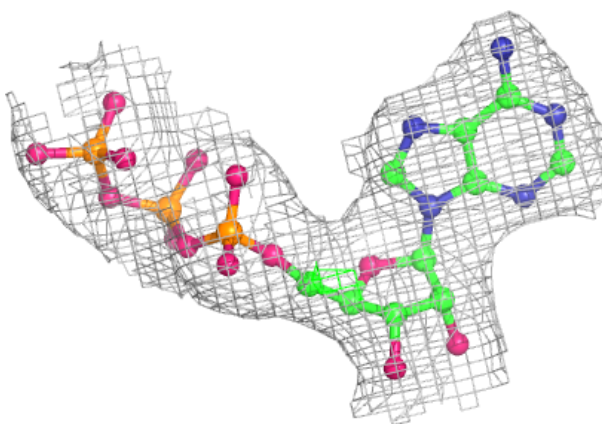


**Electron density around ATP A 801:**

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

**Electron density around ATP D 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.