



# Full wwPDB X-ray Structure Validation Report

Jun 22, 2024 – 03:23 PM EDT

PDB ID : 5LVP  
Title : Human PDK1 Kinase Domain in Complex with an HM-Peptide Bound to the PIF-Pocket  
Authors : Schulze, J.O.; Saladino, G.; Busschots, K.; Neimanis, S.; Suess, E.; Odadzic, D.; Zeuzem, S.; Hindie, V.; Herbrand, A.K.; Lisa, M.N.; Alzari, P.M.; Gervasio, F.L.; Biondi, R.M.  
Deposited on : 2016-09-14  
Resolution : 2.50 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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

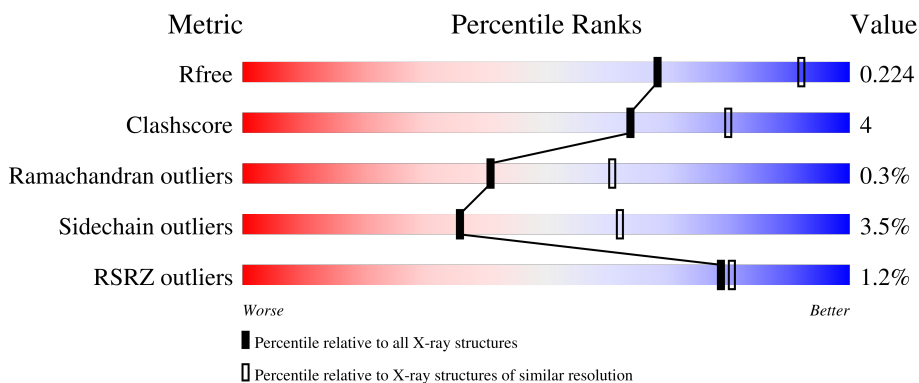
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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.



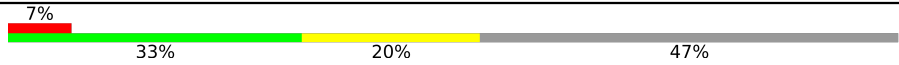
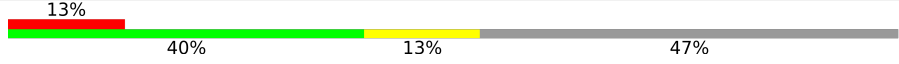

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	311	 78% 9% 11%
1	B	311	 79% 9% 11%
1	C	311	 79% 9% 11%
1	D	311	 75% 13% 11%
2	E	15	 7% 27% 20% 53%

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Mol	Chain	Length	Quality of chain
2	F	15	
2	G	15	
2	H	15	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9538 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 3-phosphoinositide-dependent protein kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	276	2209	1435	362	404	1	7	0	0	0
1	B	277	2222	1443	363	408	1	7	0	0	0
1	C	276	2213	1437	364	404	1	7	0	0	0
1	D	277	2235	1453	367	407	1	7	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	GLY	-	expression tag	UNP O15530
A	288	GLY	TYR	engineered mutation	UNP O15530
A	292	ALA	GLN	engineered mutation	UNP O15530
B	49	GLY	-	expression tag	UNP O15530
B	288	GLY	TYR	engineered mutation	UNP O15530
B	292	ALA	GLN	engineered mutation	UNP O15530
C	49	GLY	-	expression tag	UNP O15530
C	288	GLY	TYR	engineered mutation	UNP O15530
C	292	ALA	GLN	engineered mutation	UNP O15530
D	49	GLY	-	expression tag	UNP O15530
D	288	GLY	TYR	engineered mutation	UNP O15530
D	292	ALA	GLN	engineered mutation	UNP O15530

- Molecule 2 is a protein called hydrophobic-motif peptide of PKB/Akt.

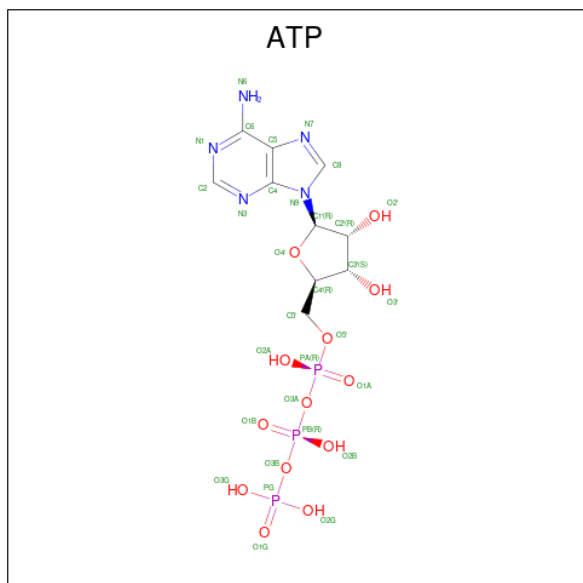
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	7	57	38	7	11	1	0	0	1
2	F	8	64	42	8	13	1	0	0	1

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	G	8	Total	C	N	O	P	0	0	1
			64	42	8	13	1			
2	H	7	Total	C	N	O	P	0	0	0
			62	41	7	13	1			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



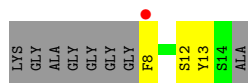
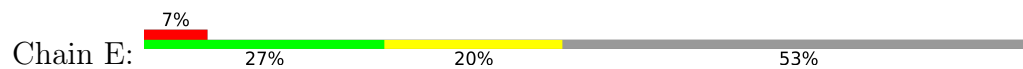
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	75	Total O 75 75	0	0
5	B	71	Total O 71 71	0	0
5	C	75	Total O 75 75	0	0
5	D	65	Total O 65 65	0	0



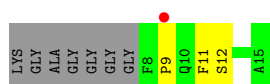




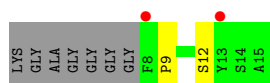
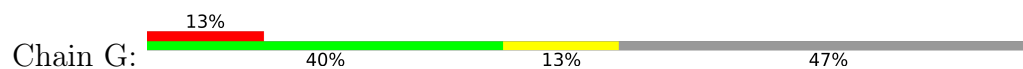
- Molecule 2: hydrophobic-motif peptide of PKB/Akt



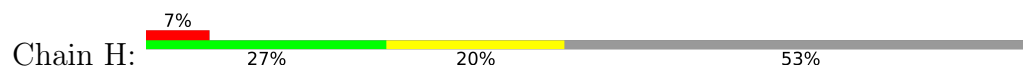
- Molecule 2: hydrophobic-motif peptide of PKB/Akt



- Molecule 2: hydrophobic-motif peptide of PKB/Akt



- Molecule 2: hydrophobic-motif peptide of PKB/Akt



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.83Å 168.51Å 94.88Å 90.00° 93.06° 90.00°	Depositor
Resolution (Å)	94.75 – 2.50 94.74 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (94.75-2.50) 99.7 (94.74-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.174 , 0.226 0.176 , 0.224	Depositor DCC
$R_{free}$ test set	2580 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtrriage
Anisotropy	0.583	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9538	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8499e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, CL, SEP

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	0.40	0/2250	0.56	0/3036
1	B	0.41	0/2265	0.56	0/3058
1	C	0.40	0/2254	0.55	0/3041
1	D	0.40	0/2278	0.57	0/3071
2	E	0.40	0/49	0.48	0/65
2	F	0.48	0/56	0.62	0/74
2	G	0.34	0/56	0.44	0/74
2	H	0.43	0/54	0.60	0/71
All	All	0.40	0/9262	0.56	0/12490

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	2209	0	2198	18	0
1	B	2222	0	2212	19	0
1	C	2213	0	2203	13	0
1	D	2235	0	2238	26	0
2	E	57	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	64	0	45	1	0
2	G	64	0	45	0	0
2	H	62	0	44	2	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	2	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	75	0	0	3	0
5	B	71	0	0	1	0
5	C	75	0	0	1	0
5	D	65	0	0	1	0
All	All	9538	0	9072	76	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 4.

All (76) 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:B:139:HIS:HD2	1:B:141:PHE:H	1.30	0.80
1:D:139:HIS:HD2	1:D:141:PHE:H	1.30	0.77
1:D:255:THR:HG22	1:D:256:GLU:HG3	1.68	0.75
1:C:139:HIS:HD2	1:C:141:PHE:H	1.34	0.73
1:A:118:ILE:HD13	1:A:127:VAL:HG21	1.74	0.69
1:B:118:ILE:HD13	1:B:127:VAL:HG21	1.78	0.66
1:D:118:ILE:HD13	1:D:127:VAL:HG21	1.78	0.66
1:D:123:LYS:HG3	1:D:126:TYR:HB3	1.80	0.63
1:B:139:HIS:CD2	1:B:141:PHE:H	2.14	0.63
1:C:255:THR:HG22	1:C:256:GLU:HG3	1.81	0.62
1:C:139:HIS:CD2	1:C:141:PHE:H	2.18	0.61
1:D:139:HIS:CD2	1:D:141:PHE:H	2.18	0.59
1:C:118:ILE:HD13	1:C:127:VAL:HG21	1.85	0.58
1:B:118:ILE:HG23	1:B:123:LYS:HB2	1.85	0.57
1:B:173:LYS:HG3	5:C:518:HOH:O	2.05	0.56
1:B:254:LEU:HD13	1:B:295:ILE:HD13	1.88	0.56
1:D:284:ALA:HB3	1:D:290:ILE:HG13	1.89	0.54
1:A:202:ILE:HD11	1:A:230:LEU:HD21	1.88	0.54
1:D:148:THR:OG1	2:H:13:TYR:HB3	2.08	0.53
1:A:197:HIS:HB3	1:A:261:LYS:HD3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:N	5:A:603:HOH:O	2.41	0.53
1:D:262:SER:OG	1:D:324:ARG:HD2	2.10	0.52
1:C:348:GLU:O	1:D:105:SER:OG	2.26	0.51
1:A:113:LEU:HD13	1:A:118:ILE:HD11	1.92	0.50
1:D:139:HIS:HE1	5:D:642:HOH:O	1.95	0.50
1:C:144:LYS:HD3	1:C:146:TYR:CE2	2.47	0.50
1:A:246:ALA:O	1:A:249:VAL:HG12	2.12	0.49
1:A:163:LYS:HD3	1:A:215:GLU:HG3	1.93	0.49
1:D:174:ILE:HD11	1:D:177:PHE:CD1	2.47	0.49
1:B:295:ILE:H	1:B:295:ILE:HG12	1.40	0.48
1:D:148:THR:HB	2:H:11:PHE:CE2	2.49	0.48
1:A:260:CYS:HB2	5:A:623:HOH:O	2.13	0.48
1:D:289:LEU:O	1:D:293:LYS:HG3	2.14	0.47
1:B:113:LEU:HD13	1:B:118:ILE:HD11	1.96	0.47
1:A:284:ALA:HB3	1:A:290:ILE:HG13	1.97	0.47
1:D:295:ILE:H	1:D:295:ILE:HG12	1.54	0.47
1:B:144:LYS:HD3	1:B:146:TYR:CE2	2.50	0.47
1:C:197:HIS:HB3	1:C:261:LYS:HD3	1.95	0.47
3:D:500:ATP:O1B	3:D:500:ATP:H5'2	2.14	0.47
1:A:349:ASN:O	1:A:353:GLN:HG3	2.15	0.47
1:D:78:ARG:NH2	1:D:80:GLU:HG3	2.30	0.47
1:A:154:LYS:HD3	1:A:156:TYR:OH	2.15	0.46
1:A:148:THR:HB	2:F:11:PHE:CE2	2.51	0.46
1:D:89:GLY:HA3	3:D:500:ATP:H4'	1.96	0.46
1:D:168:LEU:HD22	1:D:209:GLU:HG2	1.96	0.46
1:D:281:PRO:HG2	1:D:282:PHE:CD2	2.51	0.46
1:D:358:LEU:HD23	1:D:358:LEU:HA	1.77	0.46
1:A:204:ARG:NH1	1:A:241:SEP:O2P	2.44	0.45
1:A:351:HIS:HD2	5:A:603:HOH:O	2.00	0.45
1:B:281:PRO:HG2	1:B:282:PHE:CD2	2.51	0.45
1:D:118:ILE:HG23	1:D:123:LYS:HB3	1.98	0.45
1:B:111:LYS:HB3	1:B:157:PHE:HB2	1.98	0.45
1:D:311:ASP:OD2	1:D:339:HIS:NE2	2.42	0.43
1:D:359:THR:OXT	1:D:359:THR:OG1	2.30	0.43
1:C:111:LYS:HB3	1:C:157:PHE:HB2	2.00	0.43
1:B:275:LEU:HD23	1:B:275:LEU:HA	1.86	0.43
1:A:80:GLU:CD	1:A:80:GLU:H	2.20	0.43
1:B:146:TYR:HE1	1:B:160:SER:HB3	1.84	0.42
1:B:104:THR:O	1:B:105:SER:HB2	2.19	0.42
1:B:216:ASP:O	1:B:217:MET:HB2	2.19	0.42
5:B:540:HOH:O	1:C:173:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:LEU:O	1:D:220:GLN:N	2.48	0.42
1:A:77:LYS:HB2	1:A:149:PHE:CD2	2.55	0.42
1:B:80:GLU:CD	1:B:80:GLU:H	2.22	0.42
1:D:129:ARG:O	1:D:133:VAL:HG23	2.20	0.41
1:B:144:LYS:HD3	1:B:146:TYR:CZ	2.54	0.41
1:D:177:PHE:CD2	1:D:275:LEU:HD22	2.56	0.41
1:B:268:LEU:O	1:B:272:ILE:HG13	2.20	0.41
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.88	0.41
1:A:187:ALA:HB1	1:A:350:LEU:HD11	2.02	0.41
1:B:291:PHE:O	1:B:295:ILE:HG12	2.21	0.41
1:C:124:VAL:HG22	2:E:8:PHE:CE2	2.56	0.40
1:C:161:TYR:CZ	1:C:163:LYS:HA	2.56	0.40
1:C:202:ILE:HD11	1:C:230:LEU:HD21	2.03	0.40
1:D:279:LEU:HB3	1:D:283:ARG:HD3	2.03	0.40
1:C:281:PRO:HG2	1:C:282:PHE:CD2	2.57	0.40

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	271/311 (87%)	262 (97%)	9 (3%)	0	100	100
1	B	273/311 (88%)	260 (95%)	12 (4%)	1 (0%)	34	54
1	C	271/311 (87%)	260 (96%)	11 (4%)	0	100	100
1	D	272/311 (88%)	258 (95%)	14 (5%)	0	100	100
2	E	4/15 (27%)	3 (75%)	1 (25%)	0	100	100
2	F	5/15 (33%)	4 (80%)	0	1 (20%)	0	0
2	G	5/15 (33%)	3 (60%)	1 (20%)	1 (20%)	0	0
2	H	4/15 (27%)	3 (75%)	1 (25%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1105/1304 (85%)	1053 (95%)	49 (4%)	3 (0%)	41 61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	9	PRO
2	G	9	PRO
1	B	223	ASP

### 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	233/266 (88%)	227 (97%)	6 (3%)	46 72
1	B	235/266 (88%)	227 (97%)	8 (3%)	37 63
1	C	233/266 (88%)	226 (97%)	7 (3%)	41 68
1	D	238/266 (90%)	226 (95%)	12 (5%)	24 46
2	E	4/7 (57%)	3 (75%)	1 (25%)	0 1
2	F	5/7 (71%)	5 (100%)	0	100 100
2	G	5/7 (71%)	5 (100%)	0	100 100
2	H	5/7 (71%)	5 (100%)	0	100 100
All	All	958/1092 (88%)	924 (96%)	34 (4%)	36 62

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	154	LYS
1	A	253	LEU
1	A	254	LEU
1	A	295	ILE
1	A	354	THR
1	B	80	GLU

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Mol	Chain	Res	Type
1	B	134	MET
1	B	209	GLU
1	B	254	LEU
1	B	276	VAL
1	B	286	ASN
1	B	295	ILE
1	B	330	MET
1	C	80	GLU
1	C	97	VAL
1	C	183	ARG
1	C	254	LEU
1	C	276	VAL
1	C	295	ILE
1	C	346	THR
1	D	80	GLU
1	D	105	SER
1	D	106	ARG
1	D	123	LYS
1	D	160	SER
1	D	209	GLU
1	D	243	VAL
1	D	253	LEU
1	D	254	LEU
1	D	295	ILE
1	D	303	GLU
1	D	354	THR
2	E	13	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	B	139	HIS
1	C	139	HIS
1	C	353	GLN
1	D	139	HIS
1	D	351	HIS

### 5.3.3 RNA

There are no RNA molecules in this entry.



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

8 non-standard protein/DNA/RNA residues 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
2	SEP	G	12	2	8,9,10	1.59	1 (12%)	8,12,14	1.53	1 (12%)
1	SEP	A	241	1	8,9,10	1.58	1 (12%)	8,12,14	1.87	2 (25%)
2	SEP	H	12	2	8,9,10	1.65	1 (12%)	8,12,14	1.67	2 (25%)
1	SEP	C	241	1	8,9,10	1.59	1 (12%)	8,12,14	1.80	2 (25%)
1	SEP	D	241	1	8,9,10	1.57	1 (12%)	8,12,14	1.54	2 (25%)
2	SEP	E	12	2	8,9,10	1.60	1 (12%)	8,12,14	1.48	2 (25%)
2	SEP	F	12	2	8,9,10	1.60	1 (12%)	8,12,14	1.63	1 (12%)
1	SEP	B	241	1	8,9,10	1.64	1 (12%)	8,12,14	1.67	2 (25%)

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	SEP	G	12	2	-	2/5/8/10	-
1	SEP	A	241	1	-	1/5/8/10	-
2	SEP	H	12	2	-	0/5/8/10	-
1	SEP	C	241	1	-	2/5/8/10	-
1	SEP	D	241	1	-	2/5/8/10	-
2	SEP	E	12	2	-	4/5/8/10	-
2	SEP	F	12	2	-	1/5/8/10	-
1	SEP	B	241	1	-	0/5/8/10	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	241	SEP	P-O1P	3.53	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	12	SEP	P-O1P	3.47	1.61	1.50
2	G	12	SEP	P-O1P	3.43	1.61	1.50
1	A	241	SEP	P-O1P	3.41	1.61	1.50
2	H	12	SEP	P-O1P	3.40	1.61	1.50
1	C	241	SEP	P-O1P	3.37	1.61	1.50
1	D	241	SEP	P-O1P	3.35	1.61	1.50
2	E	12	SEP	P-O1P	3.34	1.61	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	SEP	OG-CB-CA	4.12	112.15	108.14
1	C	241	SEP	OG-CB-CA	3.99	112.02	108.14
1	B	241	SEP	OG-CB-CA	3.42	111.47	108.14
2	H	12	SEP	OG-CB-CA	3.39	111.44	108.14
2	F	12	SEP	OG-CB-CA	3.18	111.24	108.14
1	D	241	SEP	OG-CB-CA	3.12	111.19	108.14
2	G	12	SEP	OG-CB-CA	3.06	111.12	108.14
2	E	12	SEP	OG-CB-CA	3.04	111.10	108.14
1	B	241	SEP	P-OG-CB	-2.68	110.91	118.30
1	A	241	SEP	P-OG-CB	-2.36	111.81	118.30
1	C	241	SEP	P-OG-CB	-2.34	111.84	118.30
1	D	241	SEP	P-OG-CB	-2.32	111.91	118.30
2	E	12	SEP	O3P-P-OG	2.17	112.52	106.73
2	H	12	SEP	O3P-P-OG	2.09	112.30	106.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	12	SEP	CA-CB-OG-P
2	E	12	SEP	CB-OG-P-O1P
2	E	12	SEP	CB-OG-P-O2P
2	G	12	SEP	CA-CB-OG-P
2	G	12	SEP	CB-OG-P-O1P
1	C	241	SEP	CB-OG-P-O3P
1	D	241	SEP	CB-OG-P-O3P
1	A	241	SEP	CA-CB-OG-P
1	C	241	SEP	CA-CB-OG-P
1	D	241	SEP	CA-CB-OG-P
2	F	12	SEP	CA-CB-OG-P
2	E	12	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	241	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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$
3	ATP	B	401	-	26,33,33	0.95	2 (7%)	31,52,52	1.52	6 (19%)
3	ATP	C	401	-	26,33,33	0.98	2 (7%)	31,52,52	1.50	7 (22%)
3	ATP	A	500	-	26,33,33	0.91	2 (7%)	31,52,52	1.49	5 (16%)
3	ATP	D	500	-	26,33,33	0.92	1 (3%)	31,52,52	1.55	6 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	401	-	-	2/18/38/38	0/3/3/3
3	ATP	C	401	-	-	3/18/38/38	0/3/3/3
3	ATP	A	500	-	-	1/18/38/38	0/3/3/3
3	ATP	D	500	-	-	7/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	500	ATP	C5-C4	2.40	1.47	1.40
3	C	401	ATP	C5-C4	2.36	1.47	1.40
3	A	500	ATP	C5-C4	2.35	1.47	1.40
3	C	401	ATP	O4'-C1'	2.31	1.44	1.41
3	B	401	ATP	C5-C4	2.27	1.46	1.40
3	B	401	ATP	C2-N3	2.16	1.35	1.32
3	A	500	ATP	C2-N3	2.05	1.35	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	500	ATP	N3-C2-N1	-3.77	122.79	128.68
3	B	401	ATP	N3-C2-N1	-3.75	122.82	128.68
3	C	401	ATP	N3-C2-N1	-3.63	123.00	128.68
3	A	500	ATP	N3-C2-N1	-3.53	123.17	128.68
3	B	401	ATP	C3'-C2'-C1'	3.32	105.97	100.98
3	A	500	ATP	PB-O3B-PG	-3.31	121.48	132.83
3	C	401	ATP	PA-O3A-PB	-3.28	121.57	132.83
3	B	401	ATP	PB-O3B-PG	-3.08	122.26	132.83
3	D	500	ATP	N6-C6-N1	2.95	124.70	118.57
3	D	500	ATP	O3'-C3'-C2'	-2.94	102.32	111.82
3	A	500	ATP	PA-O3A-PB	-2.86	123.03	132.83
3	C	401	ATP	C4-C5-N7	-2.80	106.48	109.40
3	D	500	ATP	PA-O3A-PB	-2.77	123.33	132.83
3	C	401	ATP	PB-O3B-PG	-2.57	124.02	132.83
3	A	500	ATP	C3'-C2'-C1'	2.37	104.55	100.98
3	D	500	ATP	C5-C6-N6	-2.27	116.90	120.35
3	B	401	ATP	PA-O3A-PB	-2.20	125.28	132.83
3	A	500	ATP	C4-C5-N7	-2.20	107.11	109.40
3	C	401	ATP	O2B-PB-O1B	2.18	123.01	112.24
3	B	401	ATP	O3G-PG-O2G	2.15	115.84	107.64
3	D	500	ATP	PB-O3B-PG	-2.14	125.49	132.83
3	C	401	ATP	C3'-C2'-C1'	2.13	104.19	100.98
3	C	401	ATP	C2-N1-C6	2.09	122.33	118.75
3	B	401	ATP	N6-C6-N1	2.02	122.77	118.57

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	401	ATP	C5'-O5'-PA-O1A
3	C	401	ATP	C5'-O5'-PA-O2A

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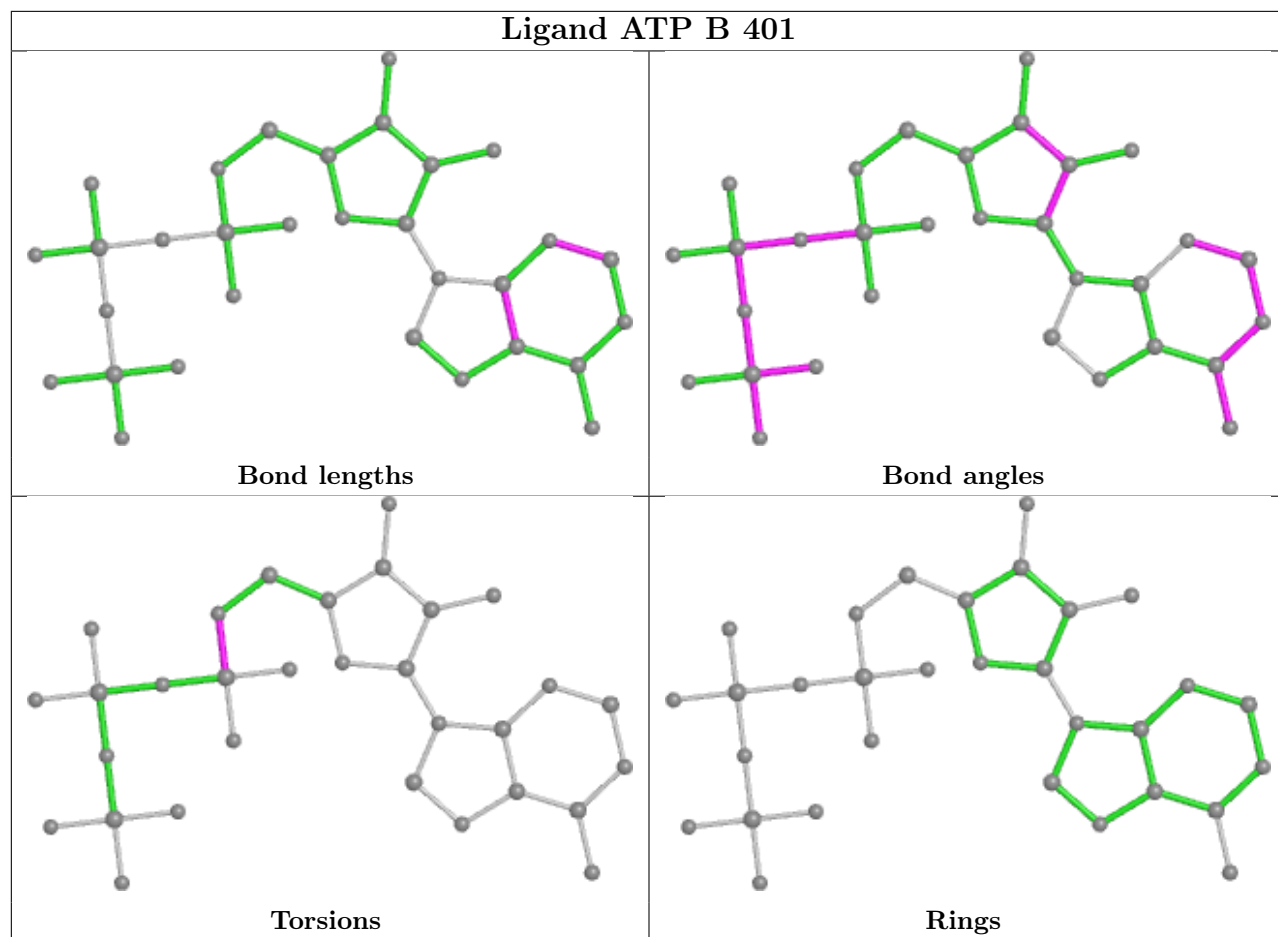
Mol	Chain	Res	Type	Atoms
3	C	401	ATP	C5'-O5'-PA-O3A
3	D	500	ATP	C5'-O5'-PA-O2A
3	D	500	ATP	C5'-O5'-PA-O3A
3	D	500	ATP	O4'-C4'-C5'-O5'
3	D	500	ATP	C3'-C4'-C5'-O5'
3	B	401	ATP	C5'-O5'-PA-O3A
3	D	500	ATP	PG-O3B-PB-O2B
3	D	500	ATP	C5'-O5'-PA-O1A
3	D	500	ATP	PG-O3B-PB-O1B
3	A	500	ATP	C5'-O5'-PA-O1A
3	B	401	ATP	C5'-O5'-PA-O1A

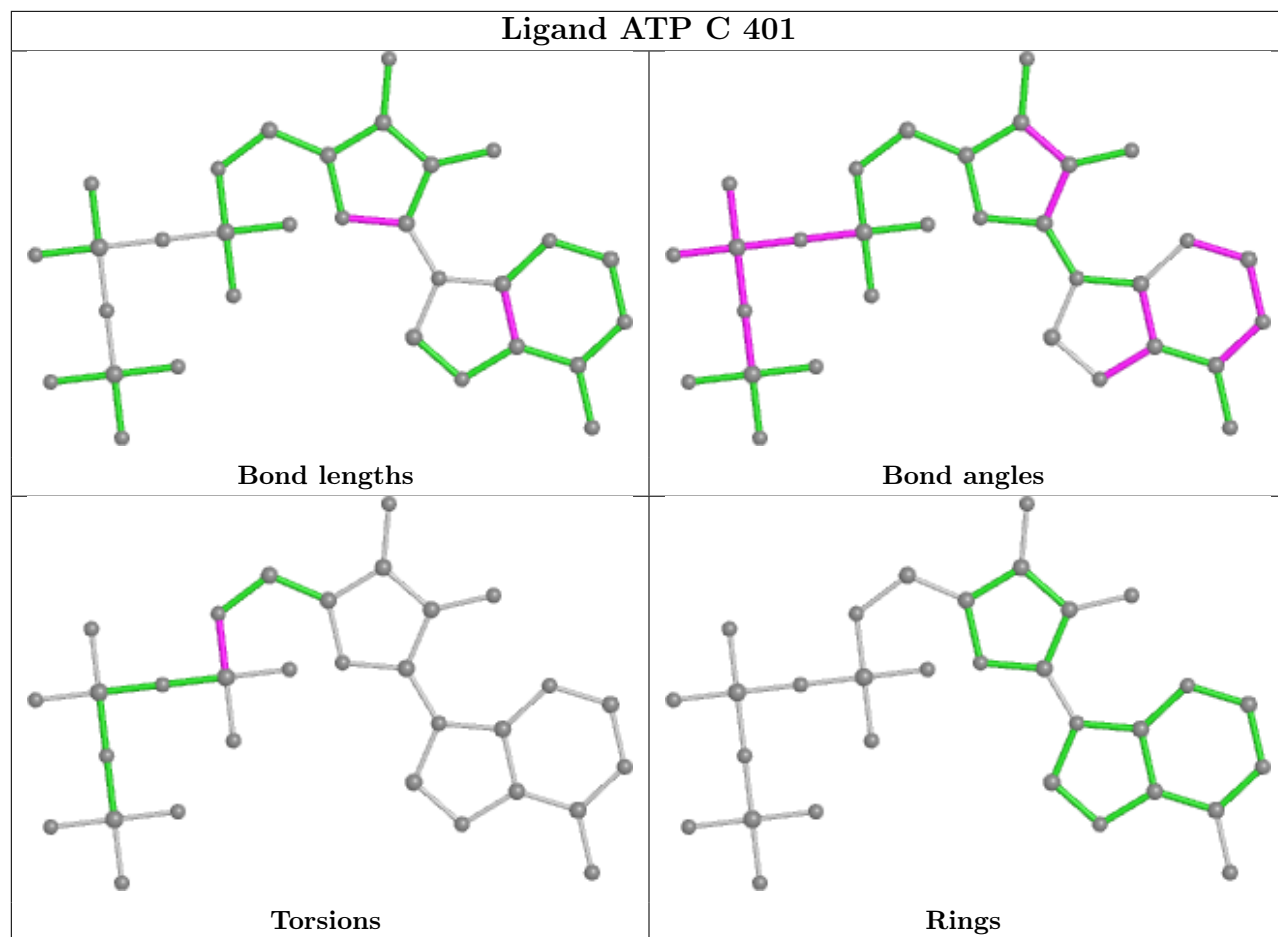
There are no ring outliers.

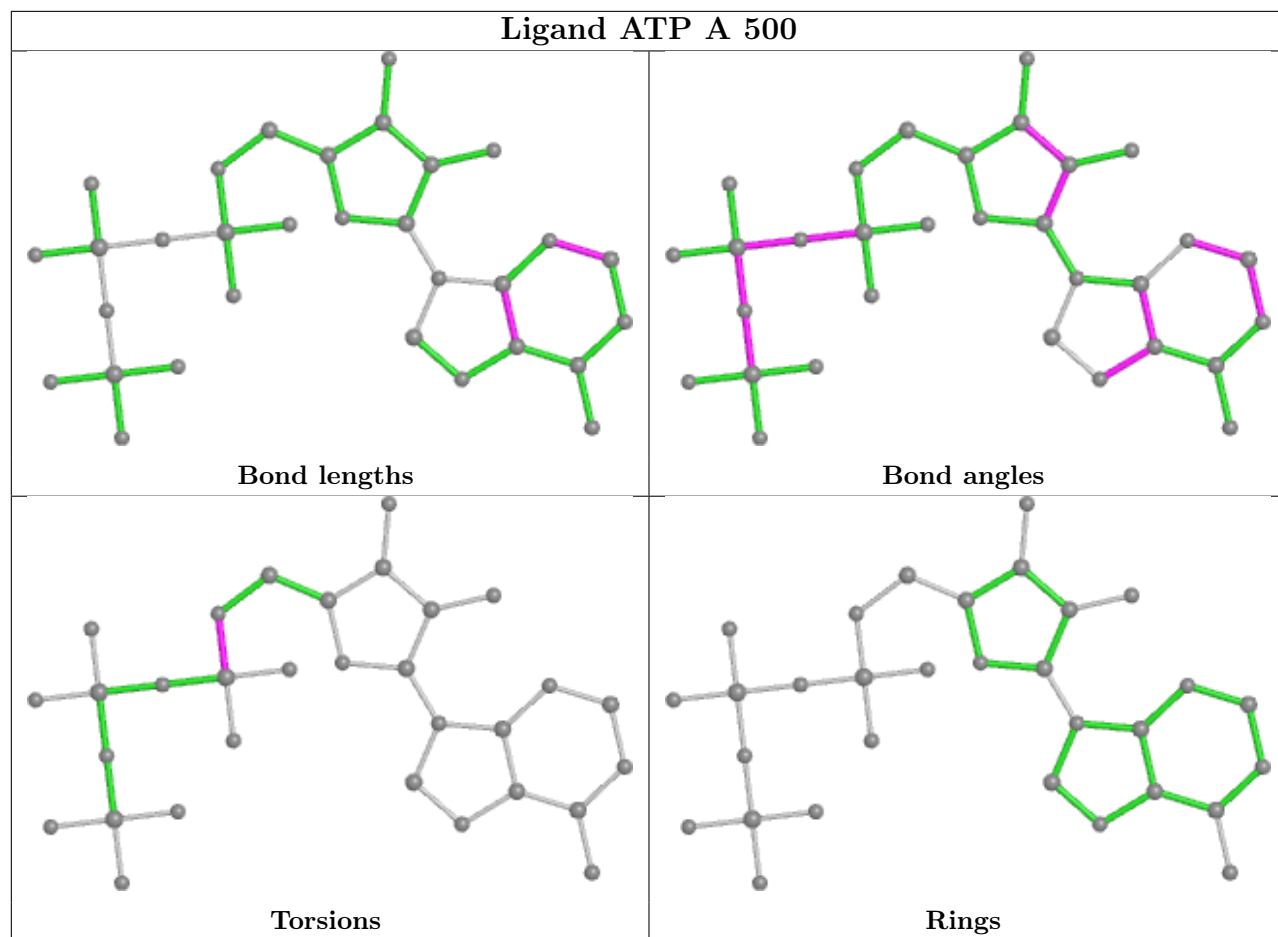
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	500	ATP	2	0

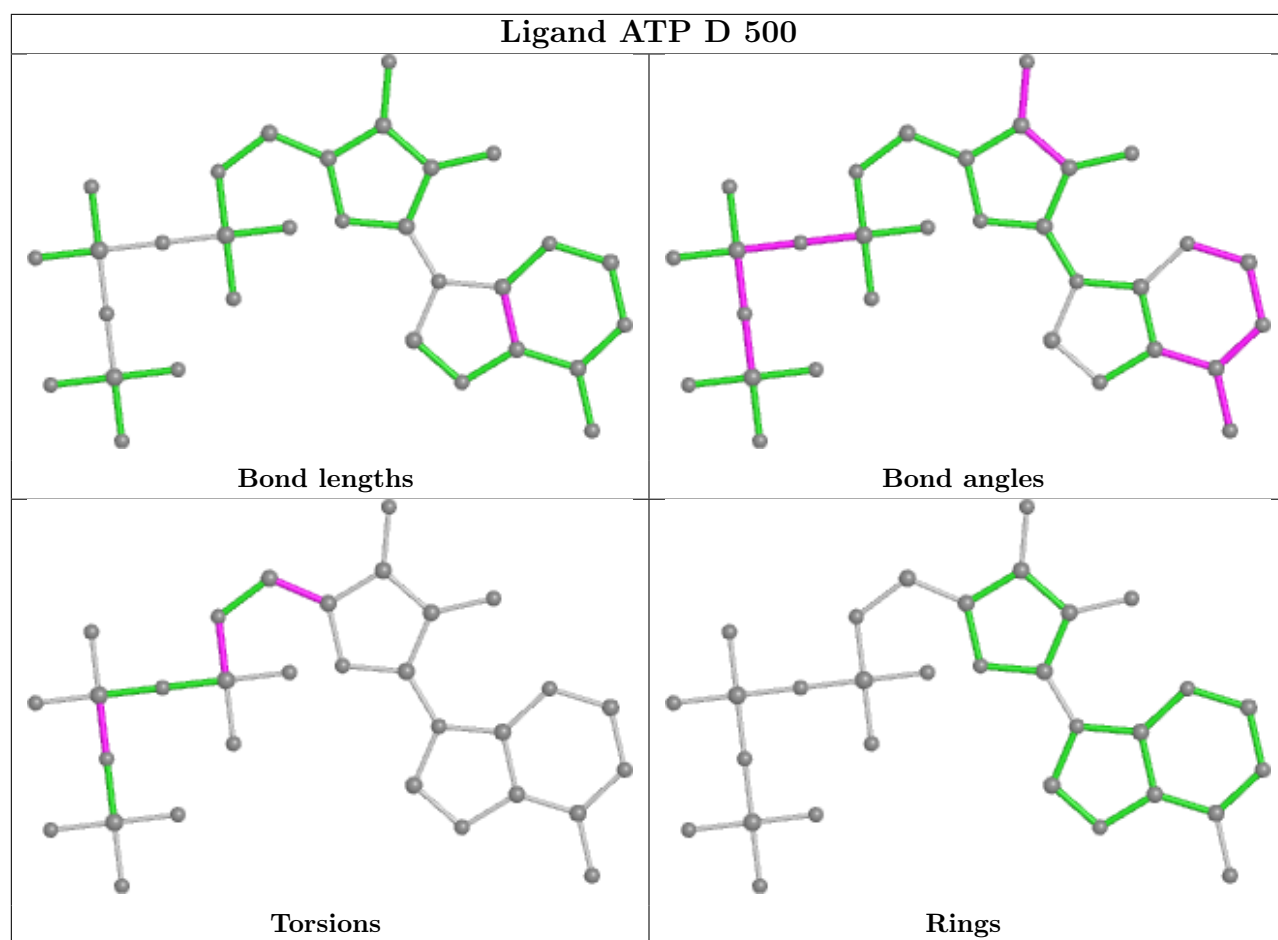
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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	275/311 (88%)	-0.13	2 (0%) 87 89	23, 40, 89, 117	0
1	B	276/311 (88%)	-0.02	3 (1%) 80 82	22, 44, 89, 110	0
1	C	275/311 (88%)	-0.07	3 (1%) 80 82	22, 43, 84, 130	0
1	D	276/311 (88%)	-0.09	1 (0%) 92 93	23, 41, 87, 123	0
2	E	6/15 (40%)	0.65	1 (16%) 1 1	76, 83, 90, 93	0
2	F	7/15 (46%)	1.27	1 (14%) 2 2	67, 80, 91, 122	0
2	G	7/15 (46%)	1.63	2 (28%) 0 0	71, 86, 112, 133	0
2	H	6/15 (40%)	0.84	1 (16%) 1 1	70, 87, 91, 97	0
All	All	1128/1304 (86%)	-0.05	14 (1%) 79 80	22, 43, 90, 133	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	9	PRO	4.4
1	C	122	ASN	3.3
1	B	125	PRO	3.0
1	C	93	PHE	2.6
1	D	126	TYR	2.5
1	B	122	ASN	2.5
1	C	125	PRO	2.4
2	G	13	TYR	2.3
2	H	13	TYR	2.3
2	E	8	PHE	2.3
1	A	92	SER	2.3
1	A	122	ASN	2.1
1	B	124	VAL	2.1
2	G	8	PHE	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SEP	H	12	10/11	0.80	0.27	76,94,121,123	0
1	SEP	B	241	10/11	0.81	0.17	91,100,110,112	0
1	SEP	D	241	10/11	0.85	0.16	104,115,121,124	0
2	SEP	F	12	10/11	0.86	0.25	82,95,124,125	0
2	SEP	E	12	10/11	0.87	0.26	81,99,117,118	0
2	SEP	G	12	10/11	0.88	0.18	88,101,123,124	0
1	SEP	A	241	10/11	0.89	0.17	93,99,106,107	0
1	SEP	C	241	10/11	0.93	0.17	84,100,108,112	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

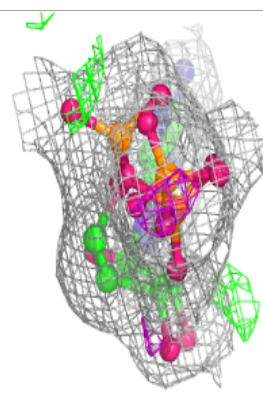
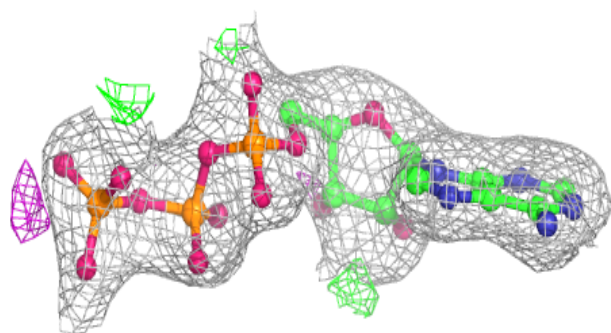
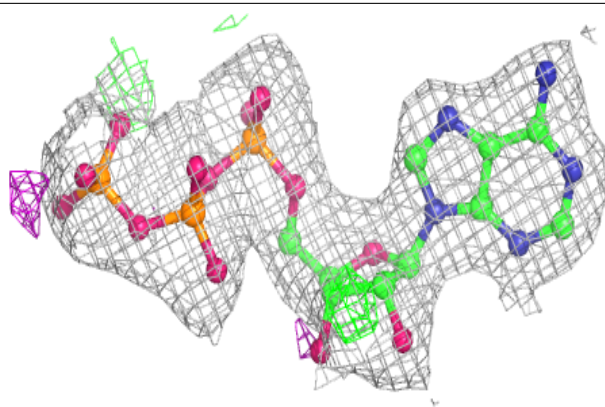
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ATP	B	401	31/31	0.95	0.14	25,50,77,87	2
3	ATP	C	401	31/31	0.95	0.14	25,50,79,87	3
3	ATP	D	500	31/31	0.95	0.14	23,58,96,98	3
3	ATP	A	500	31/31	0.96	0.12	24,52,93,99	2
4	CL	B	402	1/1	0.97	0.14	76,76,76,76	0
4	CL	C	402	1/1	0.97	0.13	64,64,64,64	0

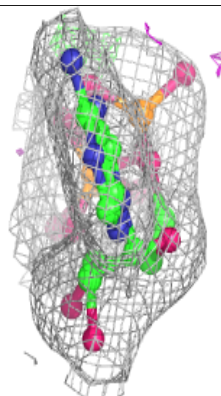
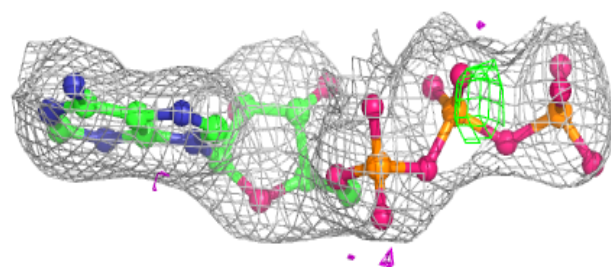
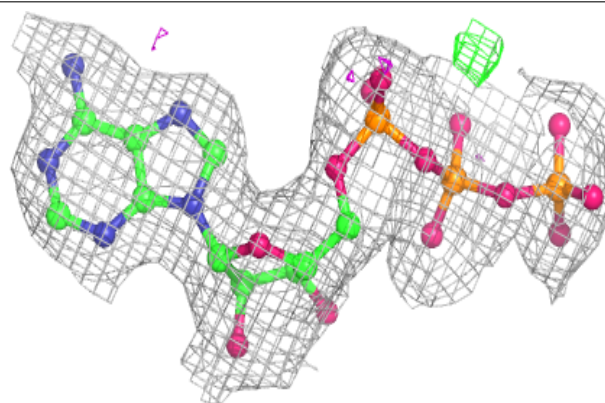
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP B 401:**

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

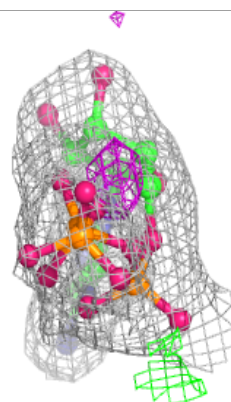
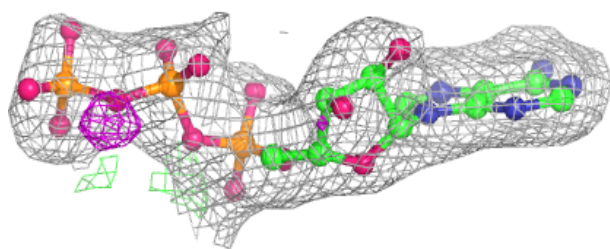
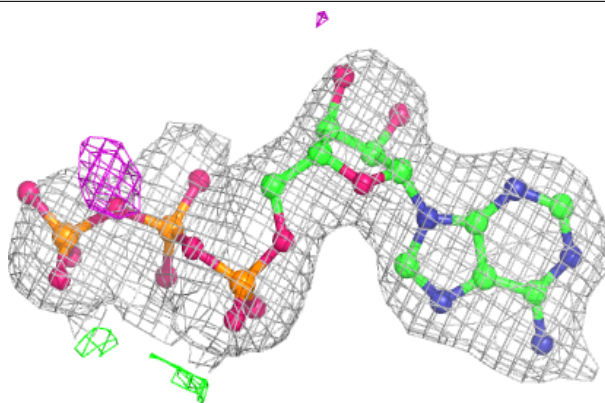
**Electron density around ATP C 401:**

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

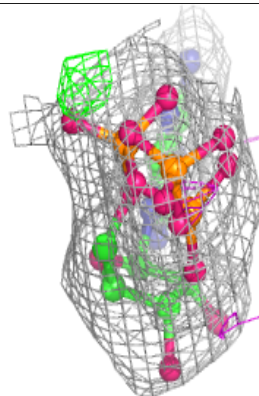
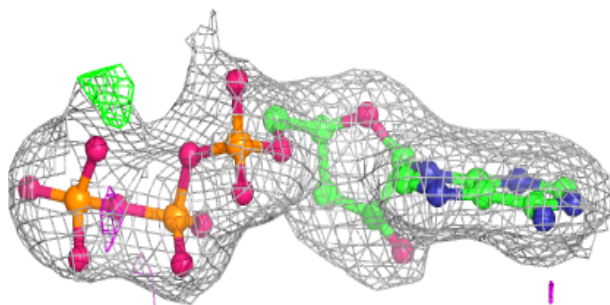
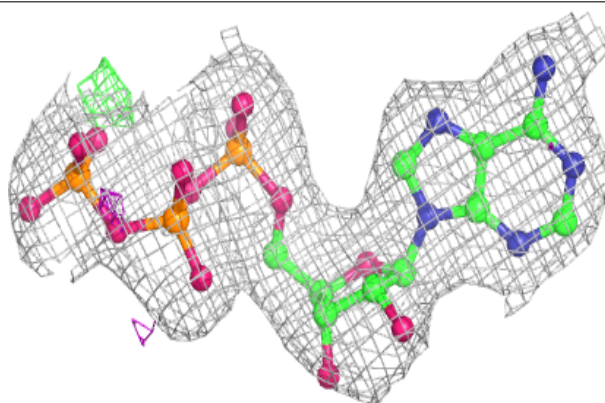


**Electron density around ATP D 500:**

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

**Electron density around ATP A 500:**

$2mF_o-DF_c$  (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.