



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:06 pm BST

PDB ID : 2EWV  
Title : Crystal Structure of the Pilus Retraction Motor PilT and Bound ADP  
Authors : Satyshur, K.A.; Forest, K.T.  
Deposited on : 2005-11-07  
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 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 : 2.11  
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) : 2.11

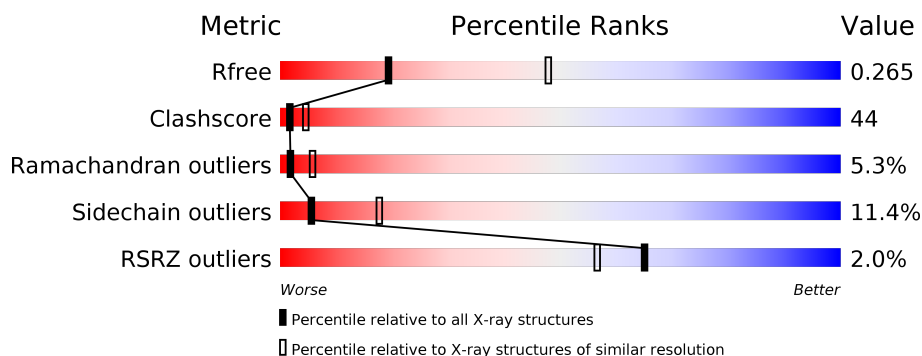
# 1 Overall quality at a glance

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	372	<div> <div>2%</div> <div> <div></div> <div>31%</div> <div>53%</div> <div>7%</div> <div>8%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2763 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.

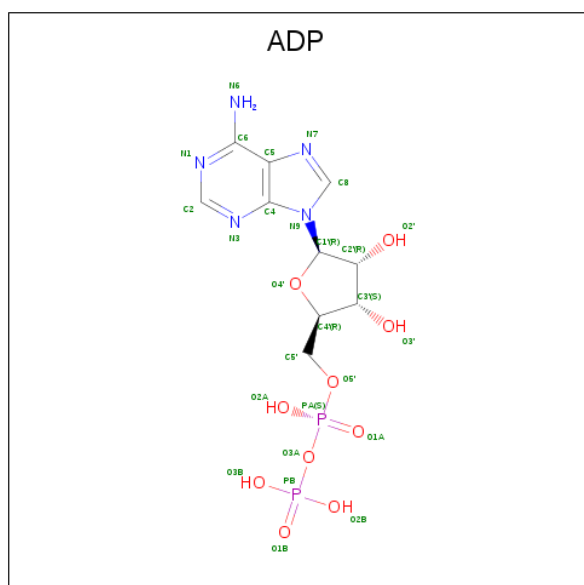
- Molecule 1 is a protein called twitching motility protein PilT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	343	2717	1731	471	505	10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	HIS	-	EXPRESSION TAG	GB 15606134
A	368	HIS	-	EXPRESSION TAG	GB 15606134
A	369	HIS	-	EXPRESSION TAG	GB 15606134
A	370	HIS	-	EXPRESSION TAG	GB 15606134
A	371	HIS	-	EXPRESSION TAG	GB 15606134
A	372	HIS	-	EXPRESSION TAG	GB 15606134

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.24Å 108.24Å 69.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 29.13 – 2.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 96.6 (29.13-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.40 (at 2.80Å)	Xtriage
Refinement program	CNS, TWIN_LSQ	Depositor
R, $R_{free}$	0.186 , 0.267 0.187 , 0.265	Depositor DCC
$R_{free}$ test set	552 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.4	Xtriage
Anisotropy	0.886	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 101.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.254 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2763	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.42	0/2761	0.74	3/3726 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	102	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	A	102	ARG	NE-CZ-NH2	5.11	122.85	120.30
1	A	49	LEU	CA-CB-CG	5.06	126.93	115.30

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	2717	0	2798	243	1
2	A	27	0	12	1	0
3	A	19	0	0	0	1
All	All	2763	0	2810	243	2

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 44.

All (243) 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:A:331:ASN:HD22	1:A:358:LEU:HB2	1.21	1.04
1:A:166:TYR:O	1:A:184:SER:HB2	1.62	0.99
1:A:283:PRO:HA	1:A:288:GLY:O	1.64	0.97
1:A:259:LEU:HD23	1:A:259:LEU:H	1.35	0.91
1:A:284:LYS:HB2	1:A:290:VAL:HG23	1.54	0.89
1:A:61:GLN:HB2	1:A:105:VAL:HG21	1.57	0.85
1:A:71:LYS:NZ	1:A:71:LYS:HB2	1.95	0.82
1:A:358:LEU:HG	1:A:359:GLU:H	1.45	0.82
1:A:198:PHE:O	1:A:202:LEU:HB2	1.80	0.81
1:A:91:VAL:HG13	1:A:92:GLY:H	1.46	0.80
1:A:314:VAL:HA	1:A:317:LEU:HD23	1.63	0.78
1:A:331:ASN:ND2	1:A:358:LEU:HB2	1.98	0.77
1:A:12:GLU:HG3	1:A:13:LEU:H	1.49	0.76
1:A:49:LEU:HD12	1:A:49:LEU:O	1.85	0.75
1:A:23:ILE:CD1	1:A:91:VAL:HG11	2.15	0.75
1:A:21:GLU:O	1:A:25:LEU:HD12	1.86	0.74
1:A:355:PRO:HB2	1:A:356:LYS:NZ	2.03	0.74
1:A:254:VAL:HG11	1:A:266:ARG:HG3	1.69	0.74
1:A:138:LEU:HD22	1:A:140:LEU:HG	1.69	0.73
1:A:124:LEU:H	1:A:124:LEU:HD22	1.52	0.73
1:A:59:ASP:HB3	1:A:62:LYS:HG3	1.72	0.72
1:A:358:LEU:O	1:A:359:GLU:HG2	1.90	0.71
1:A:195:THR:O	1:A:196:LYS:HD2	1.91	0.71
1:A:65:TYR:C	1:A:67:VAL:H	1.94	0.71
1:A:273:LEU:HD11	1:A:276:ILE:HG13	1.73	0.70
1:A:302:ILE:HG12	1:A:314:VAL:HG13	1.74	0.70
1:A:88:VAL:HG12	1:A:90:GLY:H	1.57	0.70
1:A:310:LYS:HE2	1:A:313:GLN:HG3	1.74	0.70
1:A:269:LEU:HD11	1:A:273:LEU:HD23	1.75	0.69
1:A:299:ASN:ND2	1:A:301:ALA:H	1.91	0.69
1:A:269:LEU:O	1:A:273:LEU:HB2	1.91	0.68
1:A:15:ILE:HD11	1:A:109:LEU:HD11	1.74	0.68
1:A:158:ASP:O	1:A:162:GLN:HG3	1.94	0.67
1:A:341:GLY:C	1:A:342:LEU:HD12	2.14	0.67
1:A:302:ILE:O	1:A:306:ILE:HG13	1.94	0.67
1:A:69:SER:O	1:A:73:ARG:HG3	1.94	0.67
1:A:71:LYS:HZ3	1:A:71:LYS:HB2	1.59	0.67
1:A:21:GLU:OE1	1:A:49:LEU:HD13	1.94	0.67
1:A:358:LEU:HD11	1:A:361:MET:HB2	1.75	0.67
1:A:264:GLN:O	1:A:267:ILE:HB	1.95	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:LEU:HD11	1:A:353:PRO:HD2	1.76	0.66
1:A:68:MET:HB3	1:A:73:ARG:HG2	1.77	0.66
1:A:219:ARG:NH2	1:A:242:HIS:HB2	2.10	0.66
1:A:147:SER:HA	1:A:281:LEU:HG	1.76	0.66
1:A:110:ARG:HG2	1:A:111:SER:H	1.60	0.66
1:A:302:ILE:HG12	1:A:314:VAL:CG1	2.25	0.66
1:A:348:ALA:O	1:A:352:SER:HB2	1.94	0.66
1:A:336:LYS:HG3	1:A:339:LYS:HE2	1.78	0.65
1:A:284:LYS:HB2	1:A:290:VAL:CG2	2.26	0.65
1:A:219:ARG:HH22	1:A:242:HIS:HB2	1.62	0.65
1:A:170:THR:OG1	1:A:188:GLN:HG2	1.97	0.65
1:A:219:ARG:HB2	1:A:219:ARG:HH11	1.63	0.64
1:A:299:ASN:O	1:A:303:ARG:HG3	1.98	0.64
1:A:355:PRO:HB2	1:A:356:LYS:HZ3	1.63	0.64
1:A:57:PRO:C	1:A:59:ASP:H	2.02	0.63
1:A:279:GLN:HB3	1:A:291:LEU:HD11	1.81	0.63
1:A:56:THR:HG21	1:A:60:THR:HG22	1.78	0.63
1:A:222:GLU:O	1:A:225:GLU:HB3	1.99	0.63
1:A:52:PHE:H	1:A:53:PRO:HD2	1.64	0.63
1:A:91:VAL:HG13	1:A:92:GLY:N	2.14	0.62
1:A:110:ARG:CG	1:A:111:SER:H	2.12	0.62
1:A:334:LEU:HD11	1:A:352:SER:HA	1.81	0.62
1:A:156:MET:O	1:A:160:ILE:HG13	2.00	0.62
1:A:294:GLU:HB2	1:A:330:MET:HG2	1.82	0.61
1:A:198:PHE:HE1	1:A:217:GLU:H	1.46	0.61
1:A:23:ILE:HD11	1:A:91:VAL:HG11	1.81	0.61
1:A:195:THR:C	1:A:196:LYS:HD2	2.21	0.61
1:A:269:LEU:CD1	1:A:273:LEU:HD23	2.31	0.60
1:A:27:ALA:CB	1:A:40:VAL:HG13	2.31	0.60
1:A:270:SER:O	1:A:303:ARG:HD3	2.01	0.59
1:A:309:ASN:C	1:A:311:LEU:H	2.05	0.59
1:A:284:LYS:HE3	1:A:342:LEU:HD23	1.83	0.59
1:A:230:ALA:O	1:A:233:THR:HG22	2.02	0.59
1:A:15:ILE:O	1:A:19:ILE:HG13	2.01	0.59
1:A:36:ALA:HB1	1:A:37:PRO:HD2	1.85	0.59
1:A:259:LEU:CD2	1:A:259:LEU:H	2.14	0.58
1:A:358:LEU:CD1	1:A:361:MET:HB2	2.34	0.58
1:A:250:ILE:HG23	1:A:276:ILE:HD11	1.85	0.57
1:A:311:LEU:O	1:A:314:VAL:N	2.29	0.57
1:A:337:LEU:O	1:A:342:LEU:HD13	2.05	0.57
1:A:358:LEU:CG	1:A:359:GLU:H	2.17	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLY:HA3	1:A:274:GLN:HG2	1.87	0.56
1:A:218:MET:SD	1:A:239:GLY:HA3	2.44	0.56
1:A:34:ALA:O	1:A:56:THR:O	2.23	0.56
1:A:120:LYS:HG3	1:A:121:LYS:H	1.70	0.56
1:A:310:LYS:HG2	1:A:313:GLN:HB3	1.87	0.56
1:A:305:LEU:CG	1:A:314:VAL:HG22	2.36	0.56
1:A:302:ILE:HG23	1:A:314:VAL:HG11	1.87	0.56
1:A:71:LYS:HE3	1:A:72:HIS:CD2	2.41	0.55
1:A:12:GLU:HG3	1:A:13:LEU:HD22	1.87	0.55
1:A:309:ASN:O	1:A:311:LEU:HG	2.06	0.55
1:A:346:GLU:O	1:A:350:GLU:HG3	2.06	0.55
1:A:12:GLU:HG3	1:A:13:LEU:N	2.17	0.55
1:A:302:ILE:HA	1:A:305:LEU:HB2	1.87	0.55
1:A:23:ILE:HD13	1:A:91:VAL:HG21	1.88	0.55
1:A:64:ALA:O	1:A:68:MET:HG3	2.07	0.54
1:A:199:ALA:O	1:A:203:ARG:HB2	2.07	0.54
1:A:334:LEU:CD1	1:A:352:SER:HA	2.38	0.54
1:A:147:SER:O	1:A:279:GLN:NE2	2.38	0.54
1:A:213:ILE:HB	1:A:237:VAL:HG22	1.89	0.54
1:A:241:LEU:HD21	1:A:253:ILE:HG23	1.89	0.54
1:A:21:GLU:OE1	1:A:51:ASP:HB2	2.09	0.53
1:A:54:ARG:O	1:A:55:LEU:C	2.46	0.53
1:A:68:MET:HE3	1:A:82:VAL:HG21	1.90	0.53
1:A:91:VAL:HG22	1:A:92:GLY:N	2.23	0.53
1:A:349:MET:SD	1:A:355:PRO:HA	2.48	0.53
1:A:312:GLN:CD	1:A:312:GLN:H	2.12	0.53
1:A:65:TYR:C	1:A:67:VAL:N	2.62	0.53
1:A:173:ASP:HB2	1:A:191:VAL:HB	1.91	0.53
1:A:55:LEU:H	1:A:55:LEU:HD12	1.74	0.52
1:A:135:LYS:HD3	1:A:135:LYS:N	2.24	0.52
1:A:27:ALA:HB2	1:A:40:VAL:HG13	1.91	0.52
1:A:124:LEU:HB3	1:A:128:VAL:HG21	1.91	0.52
1:A:301:ALA:C	1:A:305:LEU:HD23	2.30	0.52
1:A:120:LYS:HG3	1:A:121:LYS:N	2.25	0.52
1:A:267:ILE:HG12	1:A:307:ARG:HG3	1.92	0.52
1:A:241:LEU:HD21	1:A:253:ILE:CG2	2.40	0.51
1:A:311:LEU:O	1:A:314:VAL:HG23	2.09	0.51
1:A:37:PRO:O	1:A:38:PRO:C	2.46	0.51
1:A:199:ALA:C	1:A:201:ALA:H	2.13	0.51
1:A:41:ARG:NH2	1:A:46:ILE:HD11	2.25	0.51
1:A:104:SER:O	1:A:105:VAL:HG13	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:MET:HA	1:A:352:SER:HB3	1.93	0.51
1:A:33:THR:O	1:A:60:THR:HG21	2.11	0.51
1:A:334:LEU:O	1:A:343:ILE:HD11	2.11	0.51
1:A:153:ILE:O	1:A:157:ILE:HG12	2.11	0.51
1:A:338:TYR:C	1:A:340:GLN:H	2.12	0.51
1:A:170:THR:HB	1:A:214:PHE:HD2	1.76	0.50
1:A:99:PHE:CE2	1:A:106:ALA:HB3	2.46	0.50
1:A:261:GLN:HB3	1:A:264:GLN:NE2	2.26	0.50
1:A:264:GLN:HA	1:A:267:ILE:HD12	1.94	0.50
1:A:71:LYS:HZ2	1:A:71:LYS:HB2	1.74	0.50
1:A:231:ALA:O	1:A:272:ILE:HD11	2.11	0.50
1:A:247:ILE:O	1:A:251:HIS:HB2	2.12	0.50
1:A:290:VAL:HG12	1:A:291:LEU:N	2.27	0.50
1:A:299:ASN:O	1:A:303:ARG:CG	2.59	0.50
1:A:250:ILE:HG23	1:A:276:ILE:CD1	2.42	0.50
1:A:56:THR:CG2	1:A:60:THR:HG22	2.42	0.50
1:A:110:ARG:HG2	1:A:111:SER:N	2.24	0.49
1:A:27:ALA:HB2	1:A:40:VAL:CG1	2.41	0.49
1:A:41:ARG:HA	1:A:45:TYR:O	2.12	0.49
1:A:331:ASN:C	1:A:333:THR:N	2.65	0.49
1:A:118:GLU:HB2	1:A:121:LYS:HE3	1.94	0.49
1:A:342:LEU:HD12	1:A:342:LEU:N	2.27	0.49
1:A:142:THR:HG22	1:A:241:LEU:HB2	1.95	0.49
1:A:242:HIS:O	1:A:243:THR:O	2.31	0.49
1:A:331:ASN:C	1:A:333:THR:H	2.16	0.49
1:A:284:LYS:C	1:A:286:GLY:H	2.16	0.49
1:A:310:LYS:HE2	1:A:313:GLN:CG	2.41	0.49
1:A:167:HIS:HA	1:A:185:ILE:HG23	1.94	0.48
1:A:284:LYS:N	1:A:288:GLY:O	2.46	0.48
1:A:343:ILE:O	1:A:343:ILE:HG13	2.14	0.48
1:A:358:LEU:O	1:A:359:GLU:CG	2.61	0.48
1:A:57:PRO:C	1:A:59:ASP:N	2.66	0.48
1:A:305:LEU:HG	1:A:314:VAL:HG22	1.95	0.48
1:A:305:LEU:HB3	1:A:314:VAL:HG22	1.95	0.47
1:A:148:GLY:HA2	2:A:500:ADP:C8	2.49	0.47
1:A:338:TYR:CD2	1:A:338:TYR:O	2.68	0.47
1:A:230:ALA:HA	1:A:233:THR:HG22	1.96	0.47
1:A:279:GLN:HB3	1:A:291:LEU:CD1	2.43	0.47
1:A:74:GLN:HB3	1:A:74:GLN:HE21	1.56	0.47
1:A:202:LEU:HD12	1:A:215:VAL:HG11	1.96	0.47
1:A:209:ASP:N	1:A:210:PRO:CD	2.78	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:TYR:O	1:A:67:VAL:N	2.47	0.47
1:A:168:ILE:HG23	1:A:212:VAL:HB	1.96	0.46
1:A:219:ARG:CB	1:A:219:ARG:HH11	2.26	0.46
1:A:358:LEU:C	1:A:360:ARG:H	2.17	0.46
1:A:113:PRO:HB2	1:A:177:TYR:CE1	2.51	0.46
1:A:334:LEU:CD1	1:A:353:PRO:HD2	2.42	0.46
1:A:39:ALA:O	1:A:40:VAL:HG23	2.15	0.46
1:A:57:PRO:O	1:A:59:ASP:N	2.49	0.46
1:A:76:LEU:O	1:A:76:LEU:HG	2.16	0.46
1:A:216:GLY:O	1:A:240:THR:OG1	2.34	0.46
1:A:122:LEU:HD11	1:A:151:THR:HG22	1.98	0.45
1:A:349:MET:HE1	1:A:355:PRO:HA	1.97	0.45
1:A:52:PHE:HB3	1:A:53:PRO:CD	2.47	0.45
1:A:294:GLU:OE2	1:A:330:MET:HB2	2.17	0.45
1:A:116:ILE:HA	1:A:117:PRO:HD3	1.80	0.45
1:A:142:THR:O	1:A:278:SER:HA	2.17	0.45
1:A:57:PRO:O	1:A:60:THR:HG23	2.17	0.45
1:A:179:PHE:HD1	1:A:188:GLN:CD	2.20	0.45
1:A:219:ARG:HB2	1:A:219:ARG:NH1	2.28	0.45
1:A:189:ARG:NH1	1:A:195:THR:HG23	2.32	0.45
1:A:272:ILE:HD12	1:A:272:ILE:HA	1.84	0.45
1:A:40:VAL:HG12	1:A:42:ILE:HG13	1.98	0.44
1:A:40:VAL:HG21	1:A:49:LEU:HD23	1.99	0.44
1:A:71:LYS:HE3	1:A:72:HIS:NE2	2.32	0.44
1:A:12:GLU:CG	1:A:13:LEU:HD22	2.45	0.44
1:A:276:ILE:HD12	1:A:296:LEU:HD23	1.99	0.44
1:A:204:ALA:O	1:A:208:GLU:HG3	2.17	0.44
1:A:338:TYR:C	1:A:340:GLN:N	2.71	0.44
1:A:353:PRO:O	1:A:354:ASP:HB2	2.17	0.44
1:A:219:ARG:HA	1:A:219:ARG:HD3	1.80	0.44
1:A:349:MET:CE	1:A:355:PRO:HA	2.47	0.44
1:A:245:THR:HG23	1:A:248:ASP:H	1.82	0.44
1:A:27:ALA:HB1	1:A:40:VAL:HG13	2.00	0.44
1:A:292:ALA:O	1:A:293:TYR:HB3	2.17	0.43
1:A:264:GLN:O	1:A:268:VAL:HG23	2.18	0.43
1:A:68:MET:CE	1:A:82:VAL:HG21	2.48	0.43
1:A:203:ARG:O	1:A:206:LEU:HB2	2.18	0.43
1:A:261:GLN:HB2	1:A:264:GLN:CD	2.38	0.43
1:A:104:SER:C	1:A:105:VAL:HG22	2.37	0.43
1:A:124:LEU:H	1:A:124:LEU:CD2	2.25	0.43
1:A:127:LYS:HG3	1:A:327:MET:HE2	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:VAL:CG2	1:A:153:ILE:HD11	2.48	0.43
1:A:137:GLY:HA3	1:A:274:GLN:CG	2.48	0.43
1:A:124:LEU:N	1:A:124:LEU:HD22	2.26	0.42
1:A:270:SER:O	1:A:303:ARG:CD	2.65	0.42
1:A:313:GLN:O	1:A:317:LEU:HD22	2.19	0.42
1:A:356:LYS:HA	1:A:359:GLU:OE1	2.20	0.42
1:A:141:VAL:HG21	1:A:153:ILE:HD11	2.00	0.42
1:A:330:MET:CB	1:A:353:PRO:HG3	2.49	0.42
1:A:191:VAL:HG21	1:A:198:PHE:CD2	2.54	0.42
1:A:247:ILE:HG13	1:A:248:ASP:N	2.35	0.42
1:A:252:ARG:HH11	1:A:252:ARG:HG2	1.83	0.42
1:A:305:LEU:CD1	1:A:310:LYS:HB3	2.49	0.42
1:A:309:ASN:C	1:A:311:LEU:N	2.72	0.42
1:A:330:MET:O	1:A:334:LEU:HG	2.20	0.42
1:A:124:LEU:HB3	1:A:125:PRO:HD2	2.01	0.42
1:A:134:ARG:HG3	1:A:274:GLN:OE1	2.20	0.42
1:A:141:VAL:HG21	1:A:153:ILE:CD1	2.50	0.42
1:A:296:LEU:O	1:A:298:PRO:HD3	2.19	0.42
1:A:285:ILE:HG22	1:A:285:ILE:O	2.20	0.42
1:A:52:PHE:N	1:A:53:PRO:HD2	2.31	0.42
1:A:82:VAL:O	1:A:97:ASN:HA	2.20	0.42
1:A:347:ASP:C	1:A:349:MET:H	2.22	0.41
1:A:142:THR:CG2	1:A:241:LEU:HB2	2.51	0.41
1:A:57:PRO:HG2	1:A:59:ASP:HB2	2.02	0.41
1:A:334:LEU:HD13	1:A:352:SER:CB	2.50	0.41
1:A:284:LYS:HE3	1:A:342:LEU:CD2	2.49	0.41
1:A:56:THR:HG23	1:A:57:PRO:HD2	2.02	0.41
1:A:102:ARG:CG	1:A:102:ARG:O	2.68	0.41
1:A:132:CYS:HB3	1:A:160:ILE:HG12	2.01	0.41
1:A:263:GLU:O	1:A:267:ILE:HG13	2.21	0.41
1:A:310:LYS:HG2	1:A:313:GLN:CB	2.50	0.41
1:A:273:LEU:HD11	1:A:276:ILE:CG1	2.46	0.40
1:A:305:LEU:HB3	1:A:314:VAL:CG2	2.51	0.40
1:A:305:LEU:HD12	1:A:314:VAL:HG22	2.03	0.40
1:A:261:GLN:CB	1:A:264:GLN:NE2	2.84	0.40
1:A:250:ILE:CG2	1:A:276:ILE:HD11	2.50	0.40
1:A:311:LEU:O	1:A:312:GLN:C	2.60	0.40
1:A:330:MET:HB3	1:A:353:PRO:HG3	2.03	0.40
1:A:70:GLU:C	1:A:72:HIS:H	2.24	0.40

All (2) 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:A:159:TYR:OH	1:A:159:TYR:OH[4_565]	1.97	0.23
3:A:622:HOH:O	3:A:622:HOH:O[4_565]	2.08	0.12

## 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	339/372 (91%)	266 (78%)	55 (16%)	18 (5%)	<b>2</b> <b>6</b>

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	SER
1	A	243	THR
1	A	261	GLN
1	A	311	LEU
1	A	90	GLY
1	A	91	VAL
1	A	105	VAL
1	A	119	PHE
1	A	52	PHE
1	A	58	GLU
1	A	66	SER
1	A	256	ILE
1	A	312	GLN
1	A	298	PRO
1	A	249	THR
1	A	67	VAL
1	A	285	ILE
1	A	209	ASP

### 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	297/321 (92%)	263 (89%)	34 (11%)	5 18

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

Mol	Chain	Res	Type
1	A	30	ILE
1	A	47	LYS
1	A	71	LYS
1	A	74	GLN
1	A	79	ASN
1	A	81	GLN
1	A	82	VAL
1	A	95	ARG
1	A	105	VAL
1	A	135	LYS
1	A	138	LEU
1	A	145	THR
1	A	174	PRO
1	A	182	LYS
1	A	193	GLU
1	A	195	THR
1	A	207	ARG
1	A	215	VAL
1	A	219	ARG
1	A	229	ARG
1	A	252	ARG
1	A	259	LEU
1	A	261	GLN
1	A	262	GLN
1	A	263	GLU
1	A	271	PHE
1	A	273	LEU
1	A	289	ARG
1	A	293	TYR
1	A	295	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	298	PRO
1	A	315	TYR
1	A	330	MET
1	A	335	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	81	GLN
1	A	133	HIS
1	A	187	ASN
1	A	260	ASN
1	A	264	GLN
1	A	304	ASN
1	A	312	GLN
1	A	331	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	ADP	A	500	-	24,29,29	1.31	4 (16%)	29,45,45	1.69	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	500	-	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	ADP	O4'-C1'	3.90	1.46	1.41
2	A	500	ADP	PB-O2B	2.07	1.62	1.54
2	A	500	ADP	C2-N3	2.04	1.35	1.32
2	A	500	ADP	C8-N7	-2.02	1.31	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	ADP	PA-O3A-PB	-5.55	113.77	132.83
2	A	500	ADP	N3-C2-N1	-4.53	121.59	128.68
2	A	500	ADP	PA-O5'-C5'	-2.26	108.45	121.68
2	A	500	ADP	C3'-C2'-C1'	2.21	104.30	100.98
2	A	500	ADP	C4-C5-N7	-2.01	107.31	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

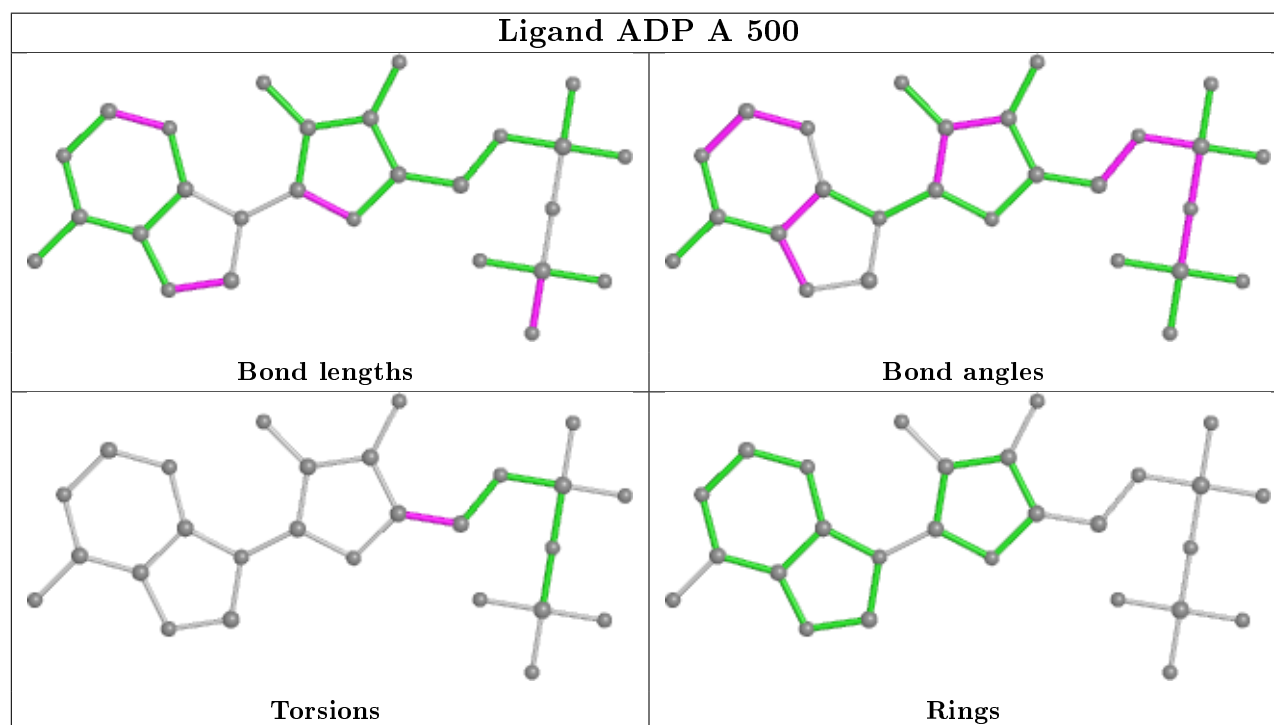
Mol	Chain	Res	Type	Atoms
2	A	500	ADP	O4'-C4'-C5'-O5'
2	A	500	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	ADP	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	343/372 (92%)	0.09	7 (2%) 65 56	33, 73, 113, 129	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	ALA	4.8
1	A	353	PRO	3.1
1	A	302	ILE	2.8
1	A	361	MET	2.4
1	A	254	VAL	2.3
1	A	231	ALA	2.1
1	A	348	ALA	2.1

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

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

### 6.3 Carbohydrates [i](#)

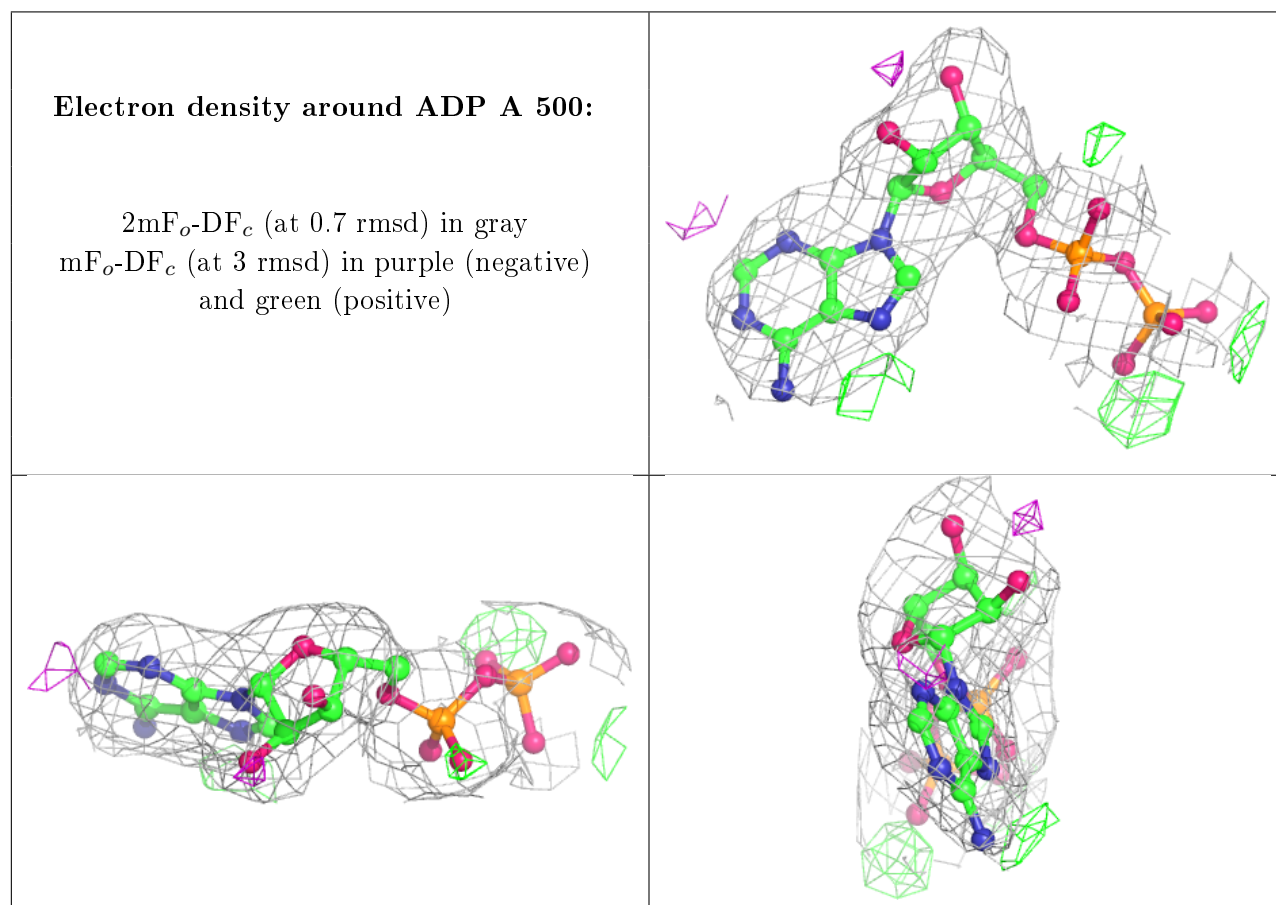
There are no carbohydrates in this entry.

### 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
2	ADP	A	500	27/27	0.93	0.16	58,62,66,66	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.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.