



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:52 PM UTC

PDB ID : 5CE3 / pdb_00005ce3
Title : The Yersinia YopO - actin complex with MgADP
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Deposited on : 2015-07-06
Resolution : 2.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

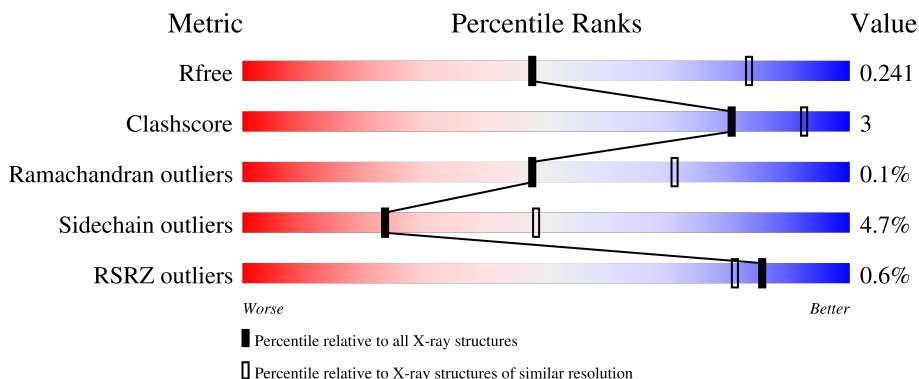
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	376	86% 9% • 5%
1	C	376	88% 6% • 5%
2	B	643	84% 9% 7%
2	D	643	83% 9% • 7%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 15121 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 Actin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	358	2786	1766	470	531	19	0	0	0
1	C	358	2786	1766	470	531	19	0	0	0

- Molecule 2 is a protein called Protein kinase YopO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	598	4710	2960	827	908	15	0	0	0
2	D	598	4710	2960	827	908	15	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	87	GLY	-	expression tag	UNP Q93KQ6
B	88	PRO	-	expression tag	UNP Q93KQ6
B	205	TYR	LYS	engineered mutation	UNP Q93KQ6
B	206	TYR	GLU	engineered mutation	UNP Q93KQ6
B	207	TYR	GLU	engineered mutation	UNP Q93KQ6
B	440	TYR	LYS	engineered mutation	UNP Q93KQ6
B	441	TYR	LYS	engineered mutation	UNP Q93KQ6
D	87	GLY	-	expression tag	UNP Q93KQ6
D	88	PRO	-	expression tag	UNP Q93KQ6
D	205	TYR	LYS	engineered mutation	UNP Q93KQ6
D	206	TYR	GLU	engineered mutation	UNP Q93KQ6
D	207	TYR	GLU	engineered mutation	UNP Q93KQ6
D	440	TYR	LYS	engineered mutation	UNP Q93KQ6
D	441	TYR	LYS	engineered mutation	UNP Q93KQ6

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	B	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		


- Molecule 7 is water.

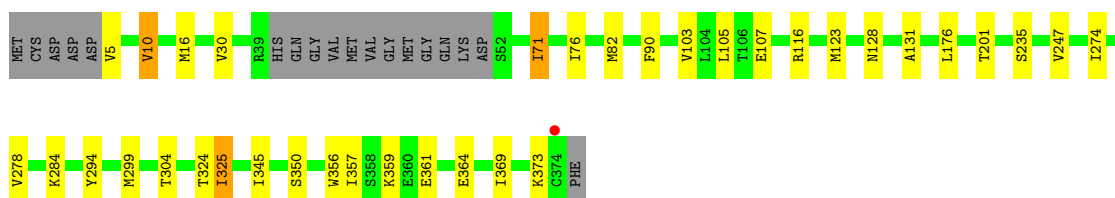
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	3	Total	O	0	0
			3	3		
7	B	3	Total	O	0	0
			3	3		
7	C	1	Total	O	0	0
			1	1		
7	D	2	Total	O	0	0
			2	2		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

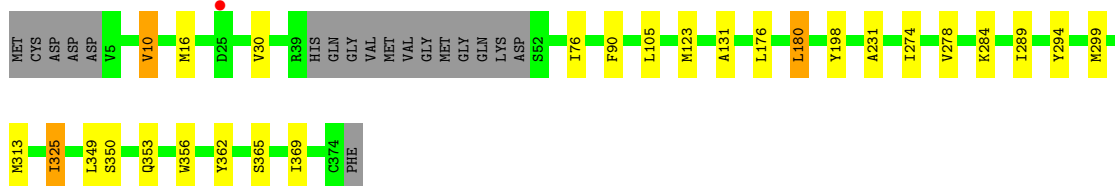
- Molecule 1: Actin

Chain A: 




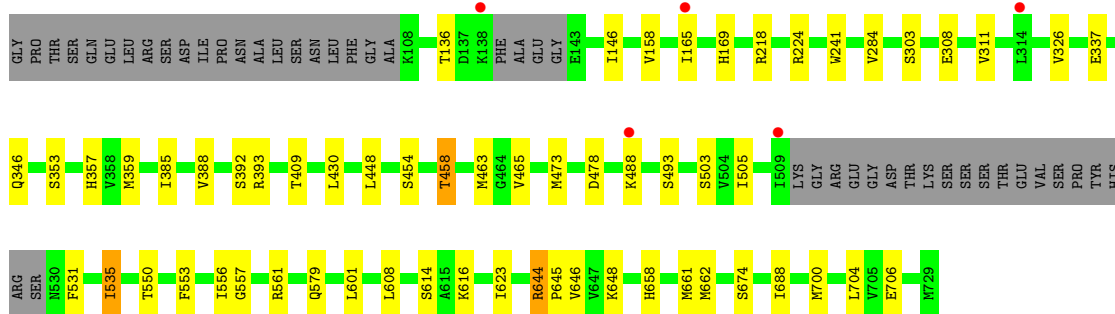
- Molecule 1: Actin

Chain C: 




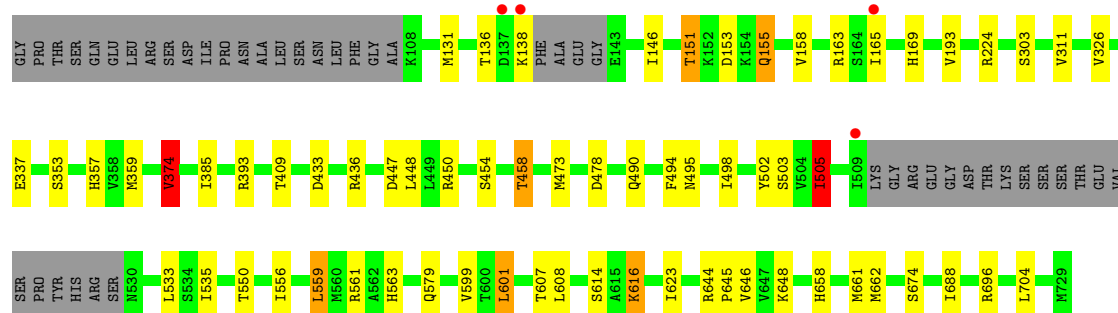
- Molecule 2: Protein kinase YopO

Chain B: 



- Molecule 2: Protein kinase YopO

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.73Å 121.75Å 118.58Å 90.00° 104.88° 90.00°	Depositor
Resolution (Å)	114.60 – 2.93 114.60 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.3 (114.60-2.93) 99.3 (114.60-2.93)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 5.8.0107, REFMAC 5.8.0107	Depositor
R, R_{free}	0.196 , 0.240 0.203 , 0.241	Depositor DCC
R_{free} test set	3230 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtrriage
Anisotropy	0.345	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15121	wwPDB-VP
Average B, all atoms (Å ²)	75.0	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 50.29 % 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 6.6078e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, MG, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.70	0/2846	0.92	1/3857 (0.0%)
1	C	0.69	0/2846	0.91	1/3857 (0.0%)
2	B	0.70	0/4796	0.94	1/6484 (0.0%)
2	D	0.71	0/4796	0.97	5/6484 (0.1%)
All	All	0.70	0/15284	0.94	8/20682 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	505	ILE	N-CA-C	-10.23	98.65	110.21
2	B	505	ILE	N-CA-C	5.85	116.32	110.23
2	D	155	GLN	N-CA-C	5.81	120.53	112.45
2	D	374	VAL	CB-CA-C	-5.56	101.18	111.18
1	A	369	ILE	N-CA-C	5.53	116.92	110.62
1	C	369	ILE	N-CA-C	5.12	116.46	110.62
2	D	155	GLN	CA-C-N	5.10	130.87	121.70
2	D	155	GLN	C-N-CA	5.10	130.87	121.70

There are no chirality outliers.

There are no planarity outliers.

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	2786	0	2762	17	0
1	C	2786	0	2762	15	0
2	B	4710	0	4701	26	0
2	D	4710	0	4701	24	0
3	A	31	0	12	0	0
3	C	31	0	12	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	B	27	0	12	1	0
5	D	27	0	12	2	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	3	0	0	0	0
7	B	3	0	0	0	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0
All	All	15121	0	14974	77	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 3.

All (77) 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)
2:B:556:ILE:HD11	2:B:608:LEU:HB3	1.71	0.71
1:A:16:MET:HE3	1:A:30:VAL:HG12	1.73	0.69
1:C:16:MET:HE3	1:C:30:VAL:HG12	1.75	0.68
2:D:658:HIS:CE1	2:D:662:MET:HE3	2.29	0.67
2:B:658:HIS:CE1	2:B:662:MET:HE3	2.29	0.67
1:A:10:VAL:HG22	1:A:105:LEU:HD23	1.80	0.64
1:A:176:LEU:HD21	1:A:284:LYS:HE3	1.80	0.64
1:C:176:LEU:HD21	1:C:284:LYS:HE3	1.81	0.63
1:C:10:VAL:HG22	1:C:105:LEU:HD23	1.81	0.63
2:B:388:VAL:HG22	2:B:392:SER:HB2	1.81	0.63
2:B:463:MET:HE2	2:B:463:MET:HA	1.82	0.60
2:B:326:VAL:HG21	2:B:385:ILE:HG21	1.82	0.59
2:D:494:PHE:O	2:D:498:ILE:HD12	2.01	0.59
2:D:326:VAL:HG21	2:D:385:ILE:HG21	1.83	0.59
2:B:224:ARG:HD3	2:B:337:GLU:OE2	2.02	0.58
2:D:224:ARG:HD3	2:D:337:GLU:OE2	2.03	0.58
2:B:645:PRO:HA	2:B:662:MET:HE2	1.85	0.58
1:A:247:VAL:HG11	2:B:644:ARG:NH2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ILE:O	1:C:278:VAL:HG23	2.03	0.58
1:A:103:VAL:HG11	1:A:123:MET:HE2	1.86	0.57
1:A:274:ILE:O	1:A:278:VAL:HG23	2.03	0.57
2:D:645:PRO:HA	2:D:662:MET:HE2	1.86	0.57
1:A:299:MET:HE3	1:A:304:THR:HB	1.87	0.56
1:C:231:ALA:O	2:D:696:ARG:NH1	2.39	0.55
2:D:556:ILE:HD11	2:D:608:LEU:HB3	1.89	0.55
1:C:294:TYR:CD2	1:C:325:ILE:HG21	2.45	0.52
1:C:362:TYR:O	1:C:365:SER:O	2.27	0.52
2:D:146:ILE:HD13	5:D:801:ADP:O4'	2.09	0.51
2:D:146:ILE:CD1	5:D:801:ADP:O4'	2.58	0.51
2:B:531:PHE:CZ	2:B:535:ILE:HD11	2.45	0.51
2:D:478:ASP:OD1	2:D:561:ARG:NH2	2.44	0.50
1:A:294:TYR:CD2	1:A:325:ILE:HG21	2.46	0.50
2:B:531:PHE:O	2:B:535:ILE:HD13	2.12	0.50
2:D:495:ASN:HA	2:D:498:ILE:HD13	1.94	0.49
1:A:107:GLU:OE2	1:A:116:ARG:NH1	2.45	0.49
2:B:557:GLY:HA2	2:B:700:MET:HE2	1.94	0.49
2:D:502:TYR:O	2:D:505:ILE:O	2.31	0.48
2:D:559:LEU:O	2:D:601:LEU:HD21	2.13	0.48
1:C:198:TYR:CD1	2:D:374:VAL:HG22	2.47	0.48
1:C:353:GLN:N	1:C:353:GLN:OE1	2.46	0.48
2:B:478:ASP:OD1	2:B:561:ARG:NH2	2.46	0.48
2:B:146:ILE:HG23	2:B:158:VAL:HG13	1.96	0.47
2:D:616:LYS:HG2	2:D:704:LEU:HD13	1.96	0.47
2:B:616:LYS:HG2	2:B:704:LEU:HD13	1.97	0.47
2:D:146:ILE:HG23	2:D:158:VAL:HG13	1.96	0.47
2:D:454:SER:O	2:D:458:THR:HG23	2.15	0.47
2:B:454:SER:O	2:B:458:THR:HG23	2.15	0.46
1:C:180:LEU:HD12	1:C:180:LEU:C	2.41	0.45
1:A:247:VAL:HG11	2:B:644:ARG:HH21	1.81	0.45
2:B:308:GLU:OE2	2:B:393:ARG:NH2	2.48	0.45
2:B:556:ILE:CD1	2:B:608:LEU:HB3	2.44	0.45
1:A:357:ILE:HG12	1:A:373:LYS:HD3	1.98	0.44
2:D:448:LEU:HD23	2:D:473:MET:HE1	1.99	0.44
2:B:658:HIS:CE1	2:B:662:MET:CE	2.97	0.44
2:D:658:HIS:CE1	2:D:662:MET:CE	2.97	0.44
1:A:131:ALA:HB1	1:A:356:TRP:HB3	1.98	0.44
2:D:131:MET:HG2	2:D:151:THR:HB	2.00	0.44
1:C:131:ALA:HB1	1:C:356:TRP:HB3	1.98	0.43
2:B:357:HIS:HE1	2:B:359:MET:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:CZ	1:A:123:MET:HE1	2.53	0.43
2:B:648:LYS:HE2	2:B:658:HIS:CE1	2.54	0.43
1:C:90:PHE:CZ	1:C:123:MET:HE1	2.53	0.43
2:B:448:LEU:HD23	2:B:473:MET:HE1	2.00	0.43
2:D:648:LYS:HE2	2:D:658:HIS:CE1	2.54	0.43
2:B:218:ARG:NH1	5:B:801:ADP:O3'	2.52	0.42
2:D:357:HIS:HE1	2:D:359:MET:HE2	1.84	0.42
1:C:299:MET:HE1	1:C:313:MET:HG3	2.01	0.42
2:B:388:VAL:O	2:B:393:ARG:NH1	2.53	0.41
1:A:201:THR:HG22	2:B:241:TRP:CE2	2.55	0.41
1:C:76:ILE:HD12	1:C:76:ILE:H	1.84	0.41
1:A:76:ILE:H	1:A:76:ILE:HD12	1.84	0.41
2:D:563:HIS:HB2	2:D:601:LEU:HD22	2.03	0.41
1:A:71:ILE:HD11	1:A:82:MET:CE	2.50	0.41
1:A:361:GLU:HA	1:A:364:GLU:HG2	2.03	0.41
2:B:553:PHE:O	2:B:556:ILE:HG12	2.20	0.40
1:C:349:LEU:O	1:C:353:GLN:OE1	2.39	0.40
2:D:447:ASP:OD1	2:D:450:ARG:NH1	2.53	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	354/376 (94%)	348 (98%)	6 (2%)	0	100	100
1	C	354/376 (94%)	347 (98%)	7 (2%)	0	100	100
2	B	592/643 (92%)	572 (97%)	19 (3%)	1 (0%)	43	65
2	D	592/643 (92%)	574 (97%)	17 (3%)	1 (0%)	43	65
All	All	1892/2038 (93%)	1841 (97%)	49 (3%)	2 (0%)	48	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	646	VAL
2	D	646	VAL

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	301/316 (95%)	291 (97%)	10 (3%)	33	58
1	C	301/316 (95%)	296 (98%)	5 (2%)	53	73
2	B	517/554 (93%)	491 (95%)	26 (5%)	22	46
2	D	517/554 (93%)	481 (93%)	36 (7%)	14	32
All	All	1636/1740 (94%)	1559 (95%)	77 (5%)	23	48

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	10	VAL
1	A	71	ILE
1	A	128	ASN
1	A	235	SER
1	A	324	THR
1	A	325	ILE
1	A	345	ILE
1	A	350	SER
1	A	359	LYS
2	B	136	THR
2	B	165	ILE
2	B	169	HIS
2	B	284	VAL
2	B	303	SER
2	B	311	VAL
2	B	346	GLN
2	B	353	SER
2	B	409	THR
2	B	430	LEU

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Mol	Chain	Res	Type
2	B	458	THR
2	B	465	VAL
2	B	488	LYS
2	B	493	SER
2	B	503	SER
2	B	535	ILE
2	B	550	THR
2	B	579	GLN
2	B	601	LEU
2	B	614	SER
2	B	623	ILE
2	B	644	ARG
2	B	661	MET
2	B	674	SER
2	B	688	ILE
2	B	706	GLU
1	C	10	VAL
1	C	180	LEU
1	C	289	ILE
1	C	325	ILE
1	C	350	SER
2	D	136	THR
2	D	138	LYS
2	D	151	THR
2	D	153	ASP
2	D	155	GLN
2	D	163	ARG
2	D	165	ILE
2	D	169	HIS
2	D	193	VAL
2	D	303	SER
2	D	311	VAL
2	D	353	SER
2	D	374	VAL
2	D	393	ARG
2	D	409	THR
2	D	433	ASP
2	D	436	ARG
2	D	458	THR
2	D	490	GLN
2	D	503	SER
2	D	505	ILE

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Mol	Chain	Res	Type
2	D	533	LEU
2	D	535	ILE
2	D	550	THR
2	D	559	LEU
2	D	579	GLN
2	D	599	VAL
2	D	601	LEU
2	D	607	THR
2	D	614	SER
2	D	616	LYS
2	D	623	ILE
2	D	644	ARG
2	D	661	MET
2	D	674	SER
2	D	688	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	92	ASN
1	A	225	GLN
1	A	275	HIS
2	B	145	HIS
2	B	232	GLN
2	B	256	ASN
2	B	357	HIS
2	B	397	ASN
2	B	490	GLN
2	B	563	HIS
2	B	592	ASN
2	B	635	GLN
2	B	682	ASN
1	C	59	GLN
1	C	92	ASN
1	C	225	GLN
1	C	275	HIS
2	D	155	GLN
2	D	232	GLN
2	D	346	GLN
2	D	460	GLN
2	D	592	ASN

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Mol	Chain	Res	Type
2	D	635	GLN
2	D	682	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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
5	ADP	B	801	6	28,29,29	1.46	6 (21%)	43,45,45	1.77	11 (25%)
5	ADP	D	801	6	28,29,29	1.50	6 (21%)	43,45,45	1.89	12 (27%)
3	ATP	A	401	4	32,33,33	1.43	6 (18%)	48,52,52	1.71	9 (18%)
3	ATP	C	401	4	32,33,33	1.45	6 (18%)	48,52,52	1.75	10 (20%)

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
5	ADP	B	801	6	-	2/16/32/32	0/3/3/3
5	ADP	D	801	6	-	2/16/32/32	0/3/3/3
3	ATP	A	401	4	-	1/22/38/38	0/3/3/3
3	ATP	C	401	4	-	3/22/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	801	ADP	C5-C4	4.62	1.47	1.39
5	D	801	ADP	C5-C4	4.57	1.47	1.39
3	C	401	ATP	C5-C4	4.50	1.47	1.39
3	A	401	ATP	C5-C4	4.48	1.47	1.39
3	C	401	ATP	PB-O3B	3.24	1.63	1.59
5	D	801	ADP	PA-O3A	3.05	1.62	1.59
5	D	801	ADP	C5-C6	2.96	1.49	1.41
5	B	801	ADP	C5-C6	2.69	1.48	1.41
5	B	801	ADP	C4-N9	-2.61	1.32	1.37
3	C	401	ATP	C8-N7	2.60	1.36	1.31
3	A	401	ATP	C4-N9	-2.57	1.32	1.37
3	C	401	ATP	C5-N7	-2.54	1.34	1.39
3	A	401	ATP	C8-N7	2.54	1.36	1.31
3	C	401	ATP	C4-N9	-2.51	1.32	1.37
3	A	401	ATP	C5-C6	2.49	1.47	1.41
5	B	801	ADP	C8-N7	2.47	1.36	1.31
5	D	801	ADP	C8-N7	2.45	1.36	1.31
3	A	401	ATP	C5-N7	-2.44	1.34	1.39
3	C	401	ATP	C5-C6	2.44	1.47	1.41
3	A	401	ATP	PB-O3B	2.29	1.62	1.59
5	B	801	ADP	C5-N7	-2.23	1.35	1.39
5	D	801	ADP	C4-N9	-2.20	1.33	1.37
5	D	801	ADP	C5-N7	-2.06	1.35	1.39
5	B	801	ADP	PA-O3A	2.03	1.61	1.59

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ATP	C5-C4-N3	-5.52	119.11	126.72
3	C	401	ATP	C5-C4-N3	-5.40	119.28	126.72
5	D	801	ADP	C5-C4-N3	-5.31	119.41	126.72
5	B	801	ADP	C5-C4-N3	-4.51	120.50	126.72
3	A	401	ATP	N3-C4-N9	4.20	134.31	127.17
3	C	401	ATP	N3-C4-N9	4.00	133.97	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	801	ADP	N3-C2-N1	-3.86	122.75	128.58
5	D	801	ADP	C2-N3-C4	3.85	121.22	111.83
5	D	801	ADP	C4-C5-N7	-3.82	106.21	110.58
5	B	801	ADP	N3-C2-N1	-3.81	122.82	128.58
5	D	801	ADP	N3-C4-N9	3.79	133.61	127.17
3	C	401	ATP	C4-C5-N7	-3.67	106.39	110.58
3	A	401	ATP	C4-C5-N7	-3.61	106.45	110.58
5	B	801	ADP	N3-C4-N9	3.59	133.28	127.17
3	A	401	ATP	C2-N3-C4	3.58	120.57	111.83
3	C	401	ATP	C2-N3-C4	3.51	120.41	111.83
5	B	801	ADP	C2-N3-C4	3.51	120.41	111.83
3	C	401	ATP	N3-C2-N1	-3.34	123.53	128.58
3	A	401	ATP	N3-C2-N1	-3.31	123.57	128.58
5	B	801	ADP	C4-N9-C8	3.19	109.09	105.74
3	A	401	ATP	C4-N9-C8	3.14	109.03	105.74
5	B	801	ADP	C4-C5-N7	-3.13	107.00	110.58
3	C	401	ATP	C4-N9-C8	2.89	108.78	105.74
5	D	801	ADP	C6-C5-N7	2.76	137.41	132.09
3	C	401	ATP	C6-C5-N7	2.64	137.17	132.09
5	D	801	ADP	C5-N7-C8	2.63	107.59	103.45
3	C	401	ATP	C5-N7-C8	2.60	107.54	103.45
3	A	401	ATP	C5-N7-C8	2.58	107.51	103.45
3	A	401	ATP	C6-C5-N7	2.54	136.98	132.09
5	D	801	ADP	C4-N9-C8	2.53	108.40	105.74
5	B	801	ADP	C6-C5-N7	2.50	136.91	132.09
3	A	401	ATP	N9-C8-N7	-2.47	110.43	113.94
3	C	401	ATP	N9-C8-N7	-2.40	110.54	113.94
5	B	801	ADP	C2-N1-C6	2.35	122.59	118.73
3	C	401	ATP	O4'-C1'-N9	2.29	112.48	108.09
5	B	801	ADP	N9-C8-N7	-2.28	110.70	113.94
5	B	801	ADP	C5-N7-C8	2.24	106.98	103.45
5	D	801	ADP	C2-N1-C6	2.20	122.34	118.73
5	D	801	ADP	N9-C8-N7	-2.20	110.82	113.94
5	D	801	ADP	O2A-PA-O1A	2.09	122.17	112.44
5	B	801	ADP	C4-N9-C1'	-2.09	121.75	126.63
5	D	801	ADP	C4-N9-C1'	-2.03	121.88	126.63

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	401	ATP	PB-O3B-PG-O3G

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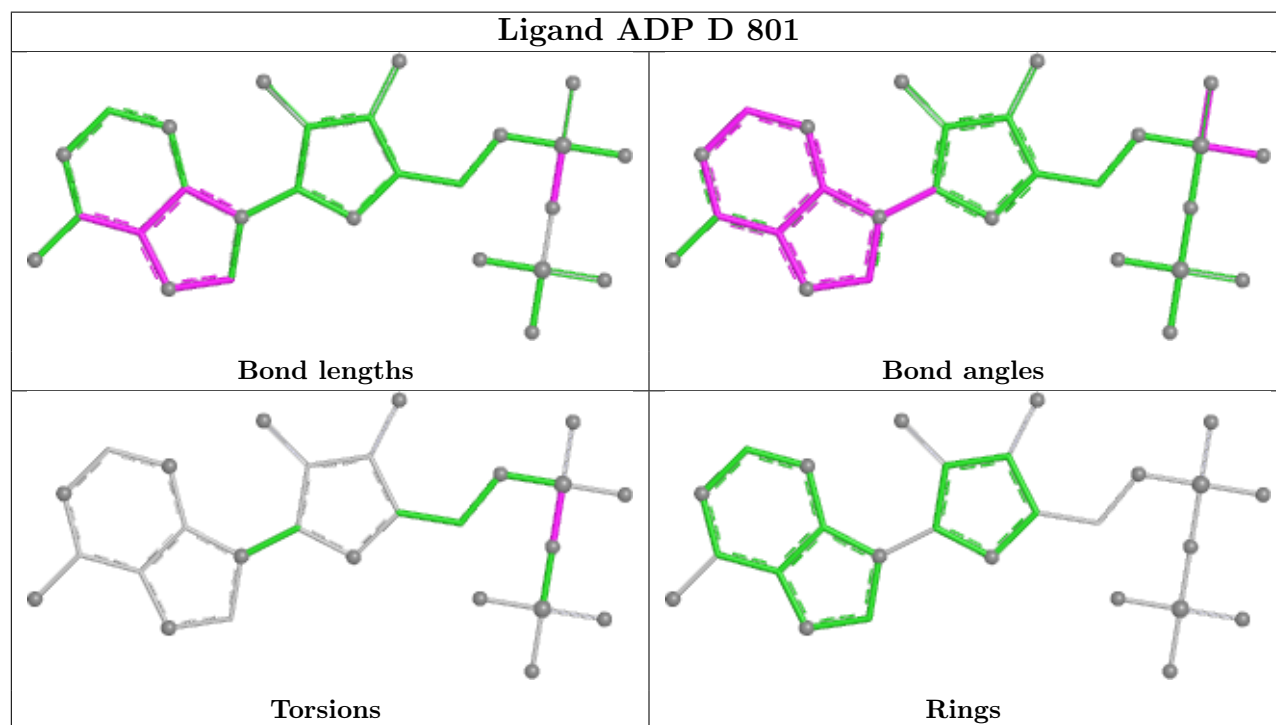
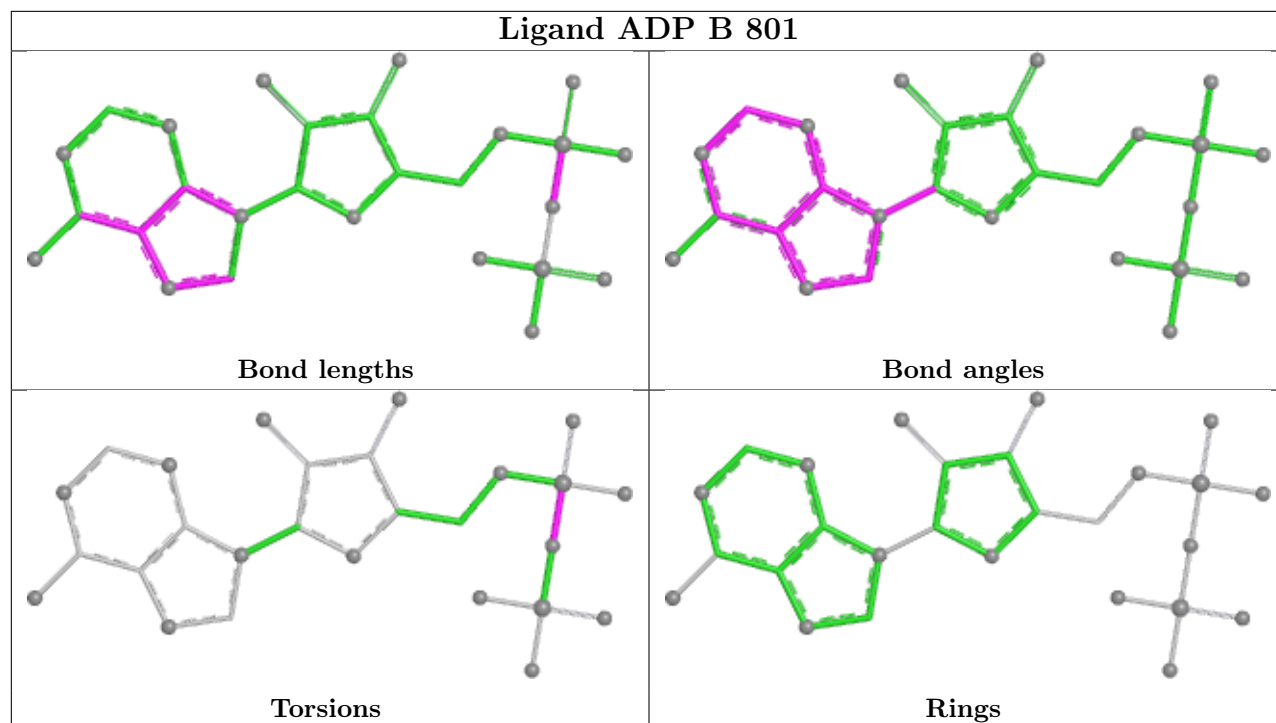
Mol	Chain	Res	Type	Atoms
3	C	401	ATP	PB-O3B-PG-O2G
5	B	801	ADP	PB-O3A-PA-O2A
5	D	801	ADP	PB-O3A-PA-O2A
3	C	401	ATP	PB-O3B-PG-O1G
3	A	401	ATP	PB-O3B-PG-O2G
5	B	801	ADP	PB-O3A-PA-O1A
5	D	801	ADP	PB-O3A-PA-O1A

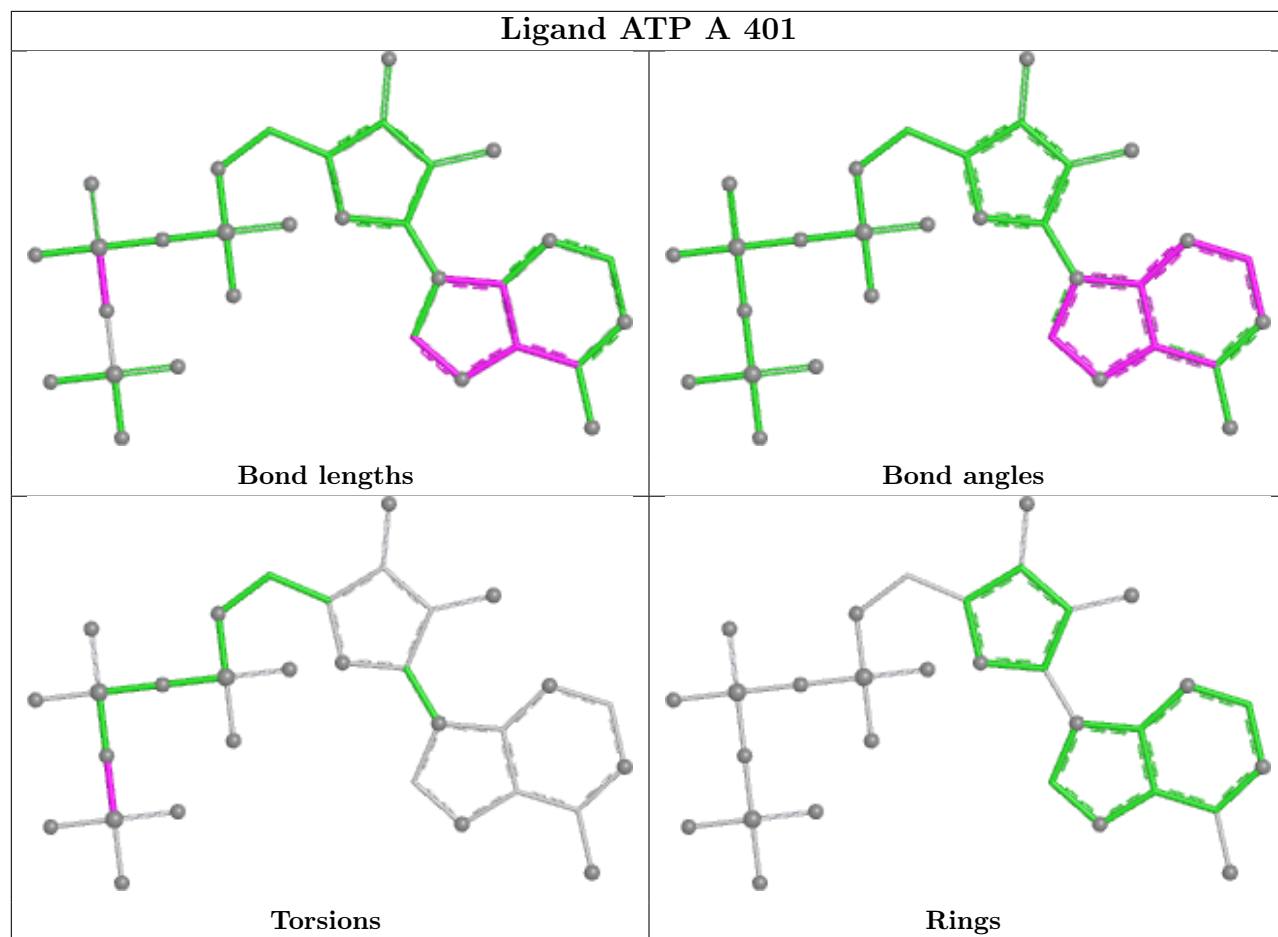
There are no ring outliers.

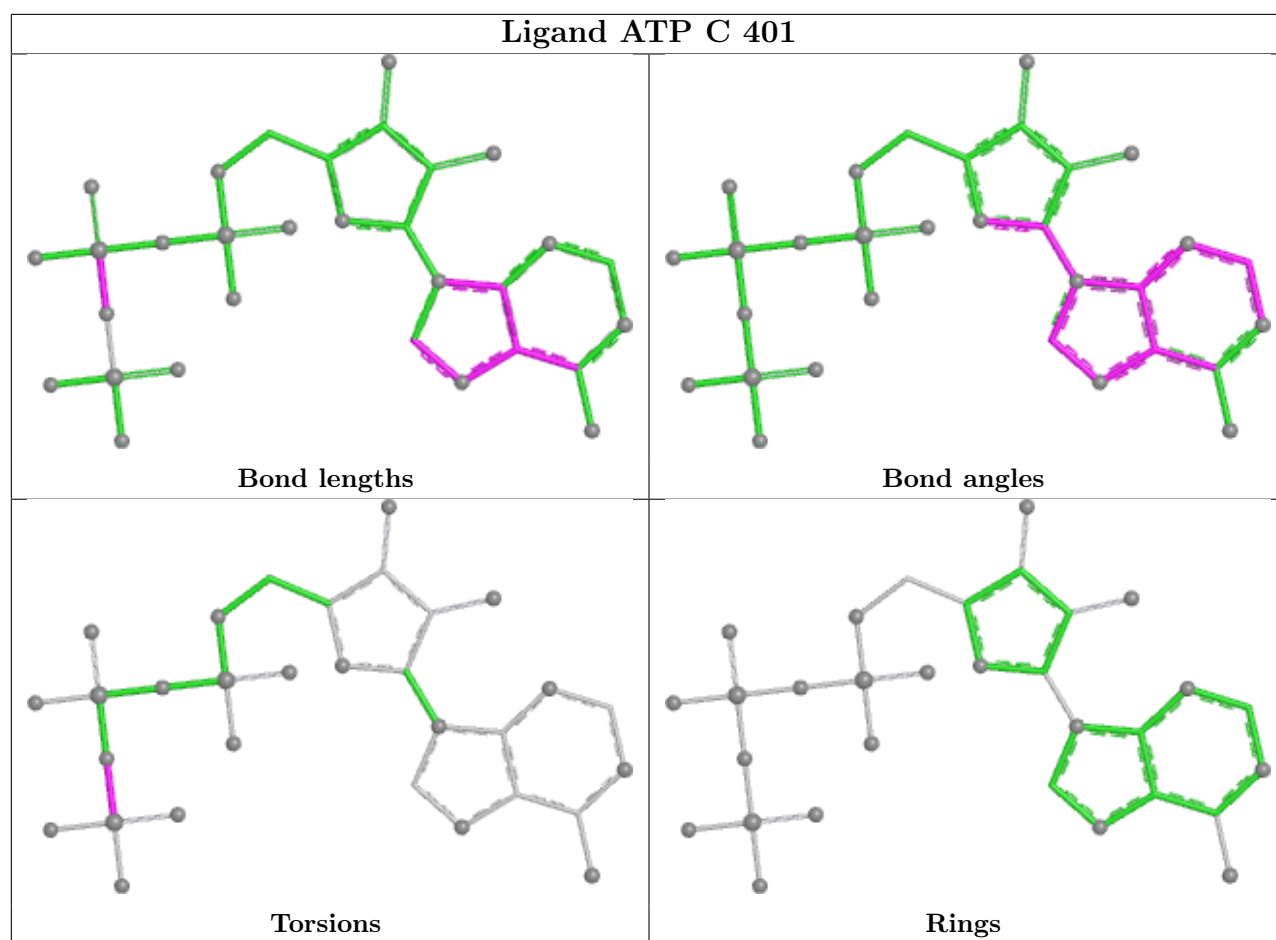
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	801	ADP	1	0
5	D	801	ADP	2	0

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







5.7 Other polymers [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	358/376 (95%)	-0.10	1 (0%) 90 88	49, 67, 102, 118	0
1	C	358/376 (95%)	-0.09	1 (0%) 90 88	48, 68, 98, 112	0
2	B	598/643 (93%)	-0.03	5 (0%) 82 77	50, 76, 113, 147	0
2	D	598/643 (93%)	0.00	4 (0%) 84 79	48, 76, 113, 138	0
All	All	1912/2038 (93%)	-0.04	11 (0%) 85 81	48, 72, 108, 147	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	509	ILE	4.5
2	B	138	LYS	3.1
2	B	165	ILE	2.8
2	D	137	ASP	2.7
2	D	165	ILE	2.6
2	B	314	LEU	2.6
1	A	374	CYS	2.5
1	C	25	ASP	2.3
2	D	509	ILE	2.3
2	D	138	LYS	2.2
2	B	488	LYS	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 [i](#)

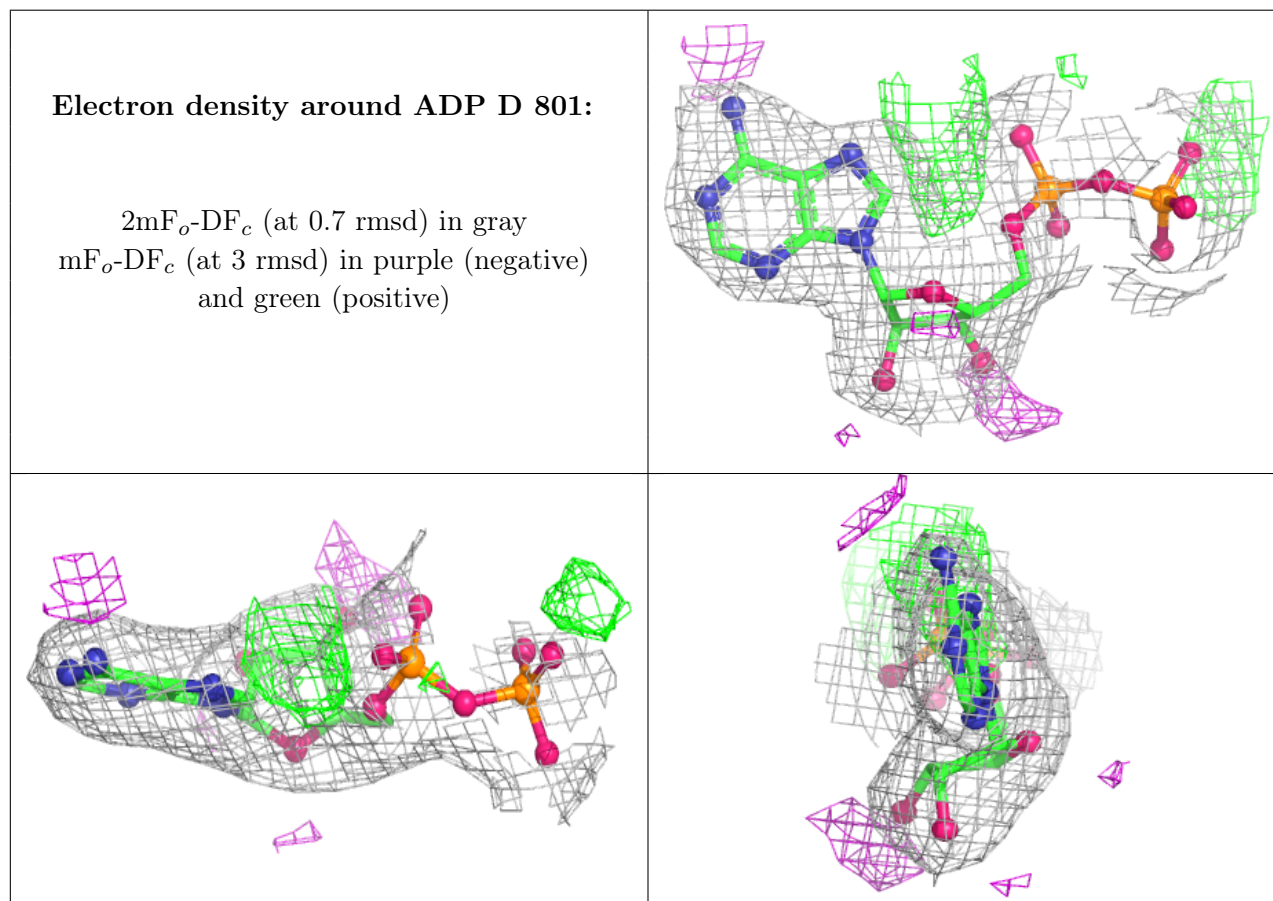
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

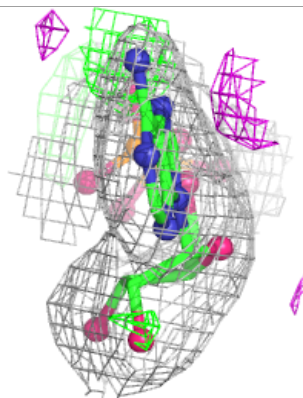
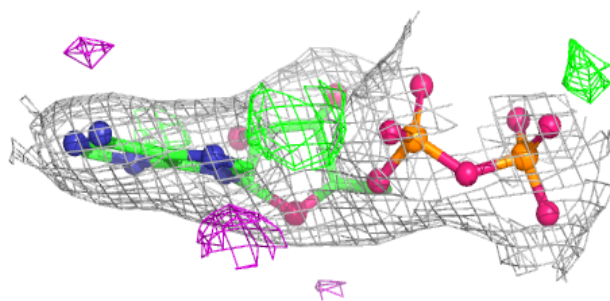
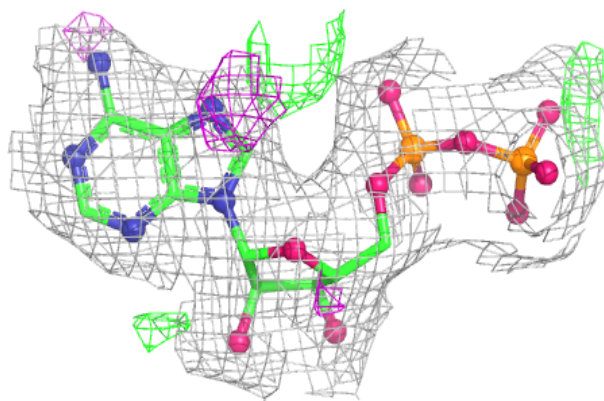
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	C	402	1/1	0.95	0.13	66,66,66,66	0
5	ADP	D	801	27/27	0.95	0.07	52,57,66,71	0
5	ADP	B	801	27/27	0.96	0.07	51,56,66,68	0
3	ATP	C	401	31/31	0.98	0.05	47,52,56,59	0
3	ATP	A	401	31/31	0.98	0.06	48,54,59,62	0
6	MG	D	802	1/1	0.98	0.07	51,51,51,51	0
6	MG	B	802	1/1	0.99	0.02	59,59,59,59	0
4	CA	A	402	1/1	0.99	0.05	59,59,59,59	0

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

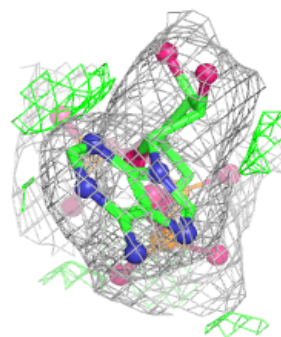
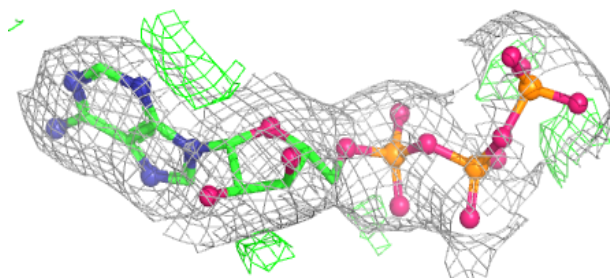
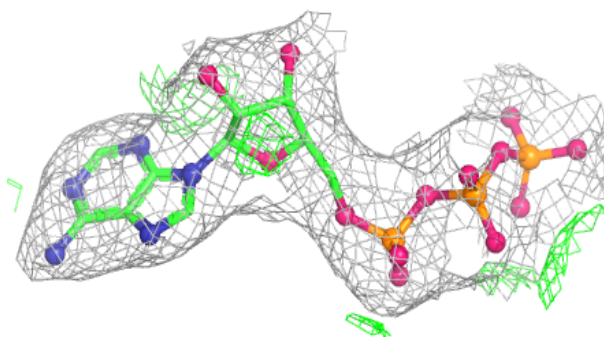


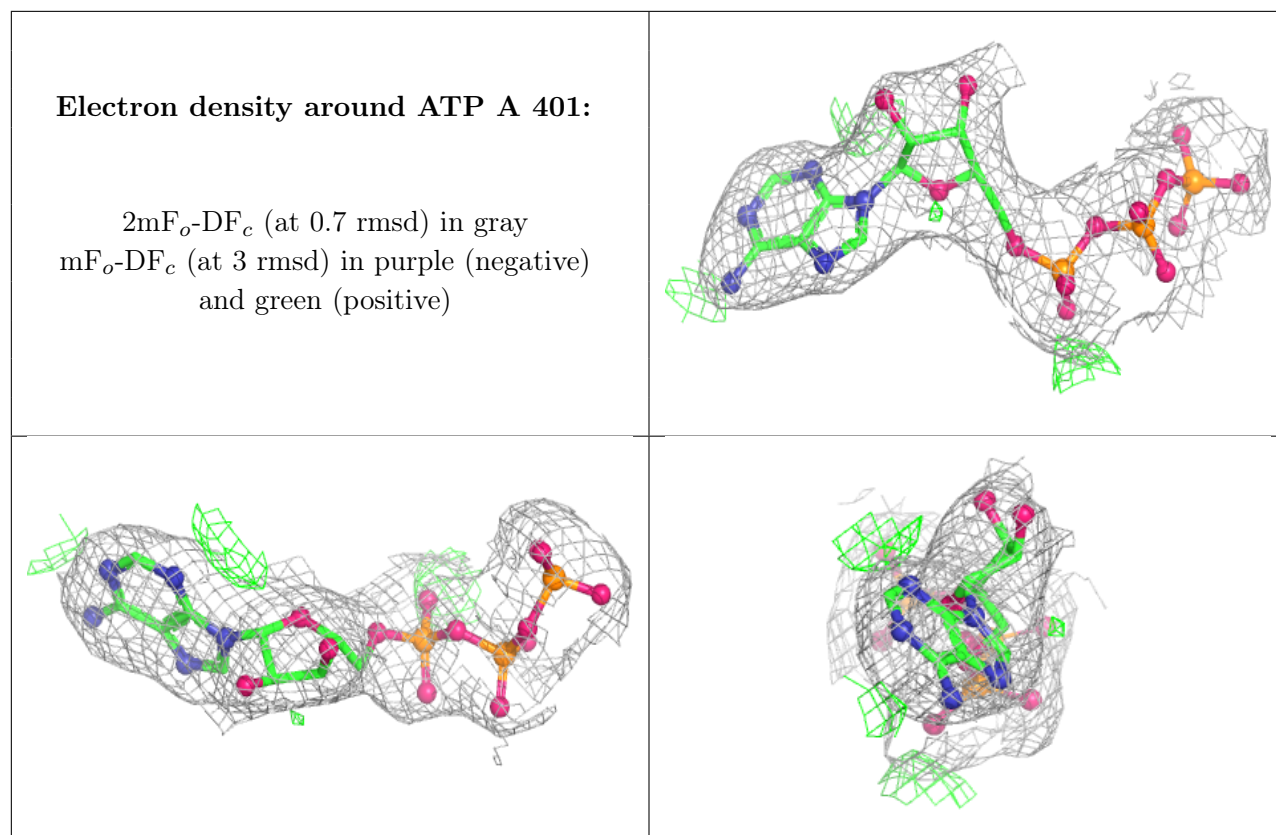
Electron density around ADP B 801:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.