



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:00 pm BST

PDB ID : 1W7I
Title : Crystal Structure Of Myosin V Motor Without nucleotide soaked in 10 mM MgADP
Authors : Coureux, P.-D.; Sweeney, H.L.; Houdusse, A.
Deposited on : 2004-09-03
Resolution : 3.00 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

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

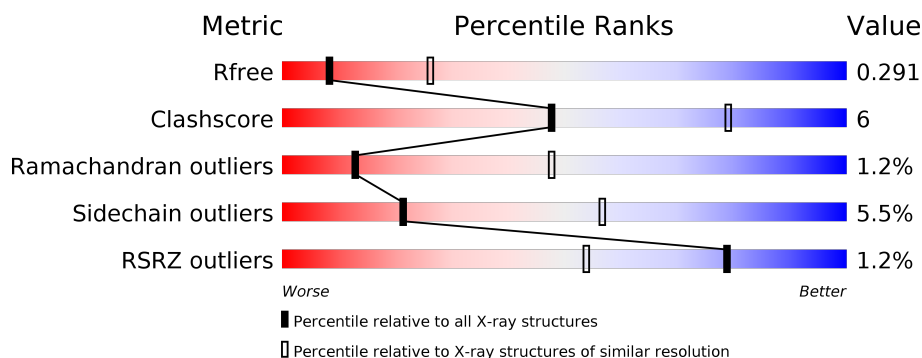
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 ≥ 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	795	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• 6%</div> </div> </div>
2	B	151	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6910 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.

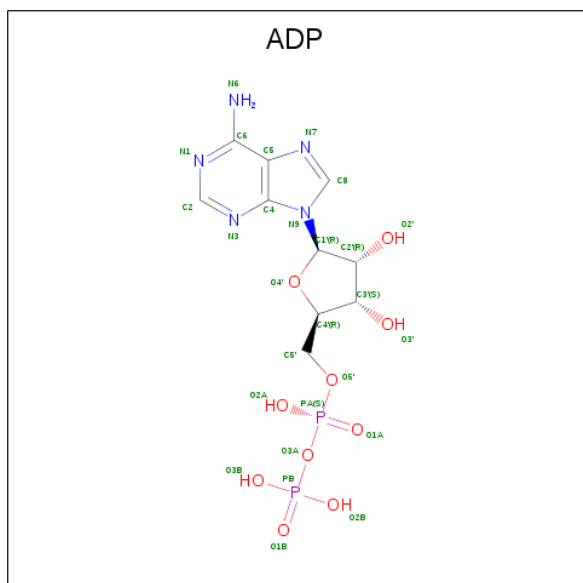
- Molecule 1 is a protein called MYOSIN VA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	750	5845	3736	986	1090	33	0	0	0

- Molecule 2 is a protein called MYOSIN LIGHT CHAIN 1, SLOW-TWITCH MUSCLE A ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	145	1027	646	174	202	5	0	0	0

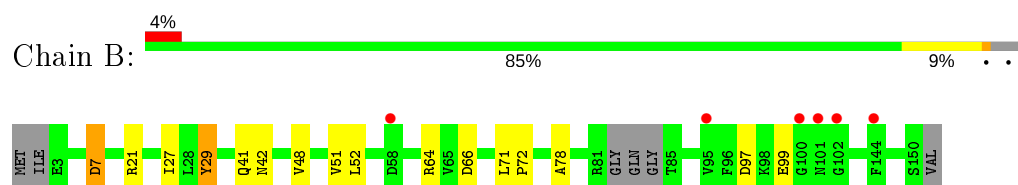
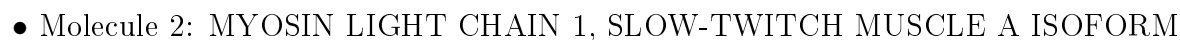
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		

- Molecule 1: MYOSIN VA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.93Å 99.25Å 112.51Å 90.00° 101.78° 90.00°	Depositor
Resolution (Å)	111.80 – 3.00 39.55 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (111.80-3.00) 97.3 (39.55-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.248 , 0.318 0.228 , 0.291	Depositor DCC
R_{free} test set	1176 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6910	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 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	0.55	0/5977	0.76	18/8109 (0.2%)
2	B	0.46	0/1042	0.70	2/1414 (0.1%)
All	All	0.54	0/7019	0.75	20/9523 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	510	ASP	CB-CG-OD2	8.87	126.28	118.30
1	A	674	ASP	CB-CG-OD2	8.04	125.53	118.30
1	A	95	ASP	CB-CG-OD2	7.01	124.61	118.30
1	A	507	ASP	CB-CG-OD2	6.68	124.32	118.30
1	A	30	ASP	CB-CG-OD2	6.05	123.74	118.30
1	A	47	ASP	CB-CG-OD2	5.93	123.63	118.30
1	A	17	ASP	CB-CG-OD2	5.87	123.59	118.30
1	A	355	ASP	CB-CG-OD2	5.82	123.53	118.30
2	B	97	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	488	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	66	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	301	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	229	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	401	ASP	CB-CG-OD2	5.46	123.22	118.30
2	B	7	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	794	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	719	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	570	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	134	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	520	ASP	CB-CG-OD2	5.03	122.83	118.30

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	5845	0	5504	75	0
2	B	1027	0	874	6	0
3	A	27	0	12	1	0
4	A	11	0	0	0	0
All	All	6910	0	6390	81	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 6.

All (81) 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:47:ASP:O	1:A:48:LEU:HB2	1.79	0.83
2:B:41:GLN:HE22	2:B:78:ALA:HA	1.55	0.69
1:A:198:ALA:O	1:A:201:PRO:HD2	1.94	0.67
1:A:47:ASP:O	1:A:48:LEU:CB	2.45	0.64
1:A:375:LEU:HA	1:A:576:GLN:HE21	1.61	0.64
1:A:660:ARG:HD2	1:A:685:CYS:SG	2.39	0.63
1:A:164:GLU:HG3	1:A:165:SER:N	2.14	0.63
1:A:165:SER:HB2	1:A:214:ASN:ND2	2.14	0.62
1:A:700:SER:HB2	1:A:751:PHE:HB2	1.82	0.62
1:A:246:LYS:NZ	1:A:639:GLN:HE22	1.99	0.61
1:A:186:SER:O	1:A:233:ARG:CZ	2.49	0.60
1:A:144:GLU:OE1	1:A:179:TYR:OH	2.13	0.59
1:A:375:LEU:HA	1:A:576:GLN:NE2	2.19	0.58
1:A:156:ASN:C	1:A:157:GLN:HE21	2.06	0.58
2:B:48:VAL:O	2:B:51:VAL:HG22	2.05	0.57
1:A:327:ARG:CB	1:A:586:PHE:HZ	2.19	0.56
1:A:246:LYS:NZ	1:A:570:ASP:OD2	2.37	0.56
1:A:715:MET:HG2	1:A:731:VAL:HG21	1.87	0.56
1:A:468:HIS:CD2	1:A:656:PRO:HD2	2.43	0.54
1:A:257:ARG:HB3	1:A:263:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ASN:HB3	1:A:424:HIS:NE2	2.23	0.53
1:A:649:GLU:O	1:A:650:THR:C	2.46	0.53
1:A:250:VAL:O	1:A:290:GLN:NE2	2.41	0.52
1:A:257:ARG:HB3	1:A:263:TYR:CZ	2.45	0.50
1:A:462:GLN:HG2	1:A:553:PHE:CD2	2.46	0.50
1:A:302:ALA:O	1:A:306:VAL:HG23	2.11	0.50
1:A:208:ASN:OD1	1:A:218:SER:HA	2.12	0.49
1:A:81:HIS:CE1	1:A:84:ALA:HB2	2.47	0.49
1:A:683:ARG:CG	1:A:688:LEU:HD12	2.42	0.49
1:A:438:ILE:HD13	1:A:461:LEU:HD11	1.93	0.49
1:A:681:GLN:O	1:A:685:CYS:HB2	2.13	0.48
1:A:85:VAL:HG21	1:A:691:ILE:HD13	1.95	0.48
1:A:40:LEU:HD12	1:A:50:TYR:HB2	1.96	0.48
1:A:157:GLN:HB2	1:A:433:ILE:HG12	1.96	0.48
1:A:741:LYS:HA	1:A:752:ARG:HG3	1.95	0.48
2:B:41:GLN:NE2	2:B:78:ALA:HA	2.28	0.47
1:A:200:ASN:O	1:A:204:GLU:HG3	2.15	0.46
2:B:29:TYR:CD2	2:B:52:LEU:HD22	2.51	0.46
1:A:158:SER:O	1:A:656:PRO:HA	2.16	0.46
1:A:465:PHE:HD1	1:A:658:TYR:CE2	2.34	0.46
2:B:71:LEU:HB3	2:B:72:PRO:HD3	1.98	0.46
1:A:712:ARG:HA	1:A:715:MET:SD	2.55	0.46
1:A:157:GLN:O	1:A:433:ILE:HA	2.16	0.46
1:A:570:ASP:OD2	1:A:639:GLN:NE2	2.47	0.45
1:A:74:LEU:HD12	1:A:103:CYS:HB2	1.99	0.45
1:A:222:LYS:O	1:A:436:LEU:HD12	2.16	0.45
1:A:683:ARG:HG2	1:A:688:LEU:HD12	1.98	0.45
1:A:375:LEU:HD23	1:A:576:GLN:NE2	2.32	0.44
1:A:251:PHE:C	1:A:251:PHE:CD2	2.90	0.44
1:A:278:ARG:O	1:A:334:HIS:NE2	2.50	0.44
1:A:285:PHE:HA	1:A:337:ASN:HD21	1.83	0.44
1:A:73:ASP:OD1	1:A:75:THR:OG1	2.36	0.44
2:B:27:ILE:O	2:B:64:ARG:HA	2.18	0.44
1:A:177:MET:O	1:A:178:ARG:C	2.56	0.43
1:A:414:TRP:CZ2	1:A:418:HIS:CE1	3.07	0.43
1:A:700:SER:CB	1:A:751:PHE:HB2	2.48	0.43
1:A:192:VAL:O	1:A:193:GLU:C	2.56	0.43
1:A:271:LEU:HB3	1:A:273:GLU:OE1	2.19	0.43
1:A:163:GLY:N	1:A:169:LYS:HD3	2.33	0.43
1:A:737:LEU:O	1:A:738:ASP:C	2.56	0.43
1:A:223:TYR:HB3	1:A:240:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:PRO:HD2	1:A:547:ALA:O	2.19	0.42
1:A:158:SER:HA	1:A:434:GLY:O	2.20	0.42
1:A:226:ILE:O	1:A:432:PHE:HA	2.20	0.42
1:A:772:ILE:HA	1:A:775:GLN:OE1	2.19	0.42
1:A:45:GLY:O	1:A:47:ASP:OD1	2.38	0.42
1:A:555:ASP:CG	1:A:556:LYS:H	2.23	0.42
1:A:163:GLY:O	1:A:169:LYS:NZ	2.35	0.41
1:A:204:GLU:O	1:A:208:ASN:HB2	2.19	0.41
1:A:205:SER:HA	1:A:260:HIS:HB2	2.01	0.41
1:A:170:THR:HB	3:A:1796:ADP:O1B	2.21	0.41
1:A:224:ILE:HD13	1:A:239:MET:HG3	2.02	0.41
1:A:179:TYR:O	1:A:183:VAL:HG22	2.20	0.41
1:A:683:ARG:HG3	1:A:688:LEU:HD12	2.03	0.41
1:A:700:SER:O	1:A:701:ARG:HG3	2.20	0.41
1:A:9:LYS:O	1:A:10:TYR:HB2	2.20	0.41
1:A:438:ILE:HG12	1:A:439:TYR:N	2.35	0.41
1:A:463:GLN:HE21	1:A:463:GLN:HB3	1.65	0.41
1:A:60:PRO:HA	1:A:61:PRO:HD3	1.98	0.41
1:A:570:ASP:HB2	1:A:636:VAL:HG23	2.04	0.40
1:A:187:ALA:HB3	1:A:190:ALA:HB3	2.04	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	744/795 (94%)	660 (89%)	74 (10%)	10 (1%)	12	45
2	B	141/151 (93%)	127 (90%)	13 (9%)	1 (1%)	22	60
All	All	885/946 (94%)	787 (89%)	87 (10%)	11 (1%)	13	48

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	48	LEU
1	A	149	GLN
1	A	671	PHE
1	A	188	SER
2	B	99	GLU
1	A	180	PHE
1	A	346	ASP
1	A	650	THR
1	A	186	SER
1	A	351	PRO

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	589/696 (85%)	557 (95%)	32 (5%)	22	57
2	B	88/129 (68%)	83 (94%)	5 (6%)	20	56
All	All	677/825 (82%)	640 (94%)	37 (6%)	21	57

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	A	81	HIS
1	A	96	SER
1	A	99	ILE
1	A	158	SER
1	A	164	GLU
1	A	186	SER
1	A	188	SER
1	A	212	THR
1	A	233	ARG
1	A	273	GLU
1	A	297	ASP
1	A	310	GLN

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Mol	Chain	Res	Type
1	A	319	ASP
1	A	321	TYR
1	A	344	ASP
1	A	346	ASP
1	A	430	HIS
1	A	439	TYR
1	A	463	GLN
1	A	487	ILE
1	A	534	LYS
1	A	562	GLU
1	A	586	PHE
1	A	641	ARG
1	A	646	LEU
1	A	655	THR
1	A	672	THR
1	A	676	LYS
1	A	679	VAL
1	A	747	THR
1	A	776	LYS
2	B	7	ASP
2	B	21	ARG
2	B	29	TYR
2	B	42	ASN
2	B	66	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	157	GLN
1	A	310	GLN
1	A	337	ASN
1	A	458	ASN
1	A	463	GLN
1	A	464	GLN
1	A	468	HIS
1	A	493	GLN
1	A	497	ASN
1	A	576	GLN
1	A	639	GLN
2	B	41	GLN
2	B	42	ASN

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Mol	Chain	Res	Type
2	B	75	GLN

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	$\# Z > 2$
3	ADP	A	1796	-	24,29,29	1.37	2 (8%)	29,45,45	1.90	8 (27%)

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	ADP	A	1796	-	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1796	ADP	C2-N3	4.15	1.38	1.32
3	A	1796	ADP	C2-N1	3.23	1.39	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1796	ADP	PA-O3A-PB	-4.72	116.62	132.83
3	A	1796	ADP	N3-C2-N1	-4.69	121.35	128.68
3	A	1796	ADP	C3'-C2'-C1'	3.79	106.69	100.98
3	A	1796	ADP	O3B-PB-O1B	-3.00	98.94	110.68
3	A	1796	ADP	O2B-PB-O3A	2.67	113.59	104.64
3	A	1796	ADP	C4-C5-N7	-2.49	106.81	109.40
3	A	1796	ADP	O3B-PB-O3A	2.21	112.06	104.64
3	A	1796	ADP	O2B-PB-O1B	2.17	119.19	110.68

There are no chirality outliers.

All (3) torsion outliers are listed below:

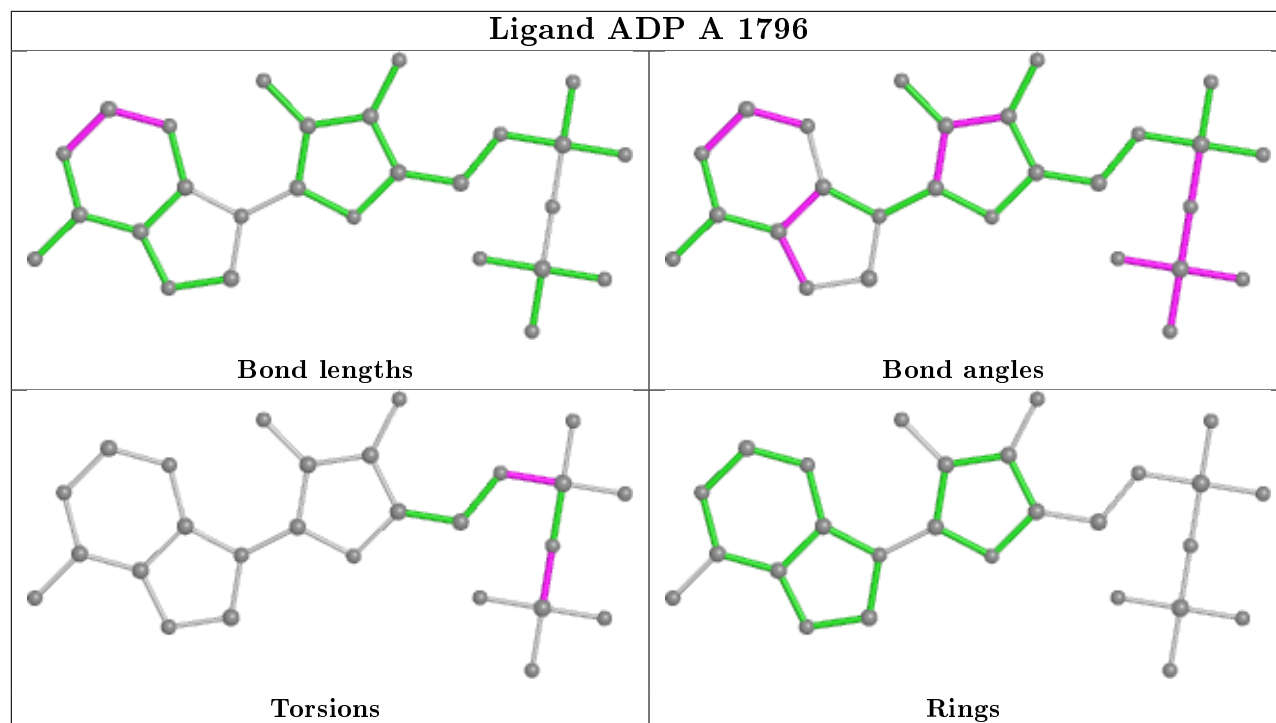
Mol	Chain	Res	Type	Atoms
3	A	1796	ADP	PA-O3A-PB-O2B
3	A	1796	ADP	PA-O3A-PB-O1B
3	A	1796	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1796	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, 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	750/795 (94%)	-0.27	5 (0%) 87 69	22, 57, 82, 94	0
2	B	145/151 (96%)	0.09	6 (4%) 37 14	67, 83, 98, 100	0
All	All	895/946 (94%)	-0.21	11 (1%) 79 54	22, 63, 92, 100	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	101	ASN	4.2
1	A	381	ALA	3.8
2	B	100	GLY	3.5
2	B	144	PHE	3.0
1	A	235	ILE	2.6
2	B	58	ASP	2.6
1	A	218	SER	2.5
2	B	95	VAL	2.4
1	A	236	GLY	2.4
1	A	345	SER	2.3
2	B	102	GLY	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](#)

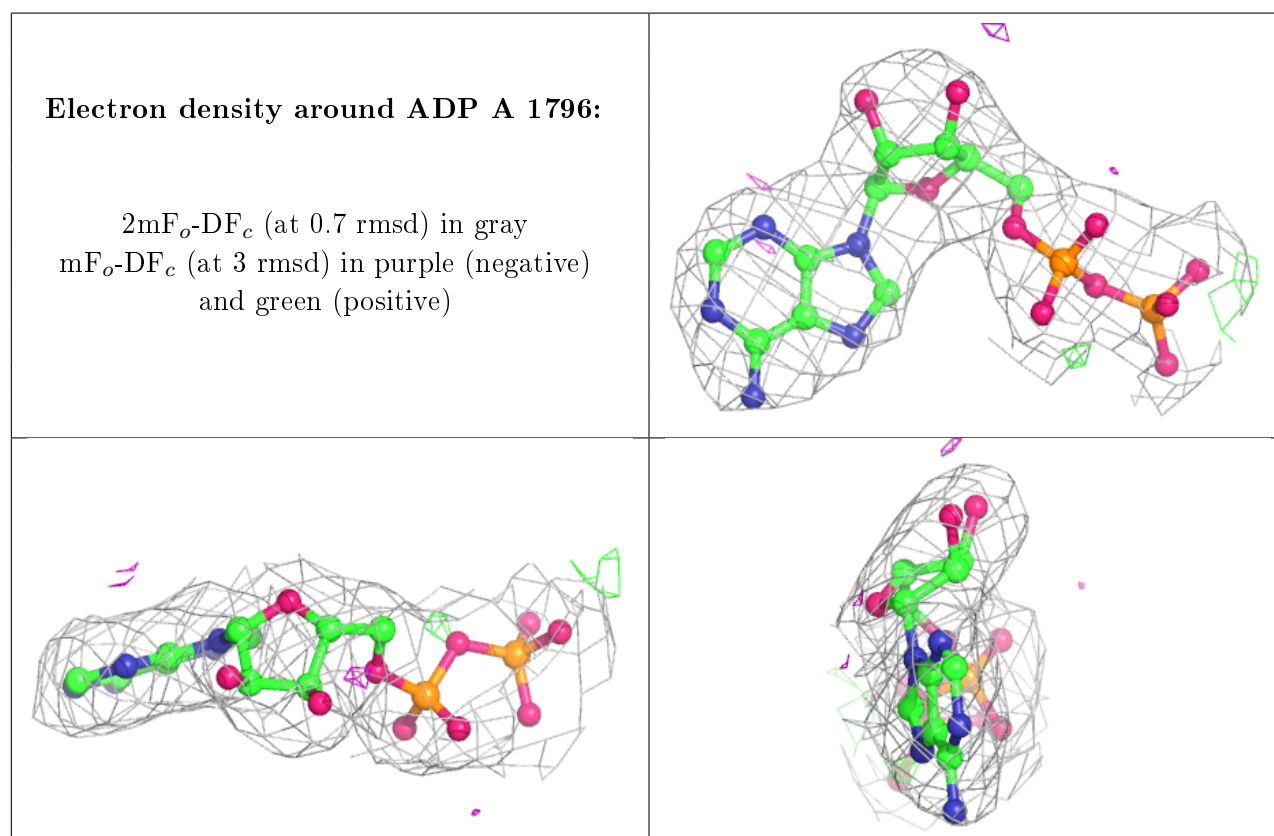
There are no carbohydrates in this entry.

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, 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
3	ADP	A	1796	27/27	0.94	0.20	30,39,42,42	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 [i](#)

There are no such residues in this entry.