



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:27 PM UTC

PDB ID : 4XW6 / pdb_00004xw6
Title : X-ray structure of PKAc with ADP, free phosphate ion, CP20, magnesium ions
Authors : Gerlits, O.; Tian, J.; Das, A.; Taylor, S.; Langan, P.; Heller, T.W.; Kovalevsky, A.
Deposited on : 2015-01-28
Resolution : 1.90 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 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

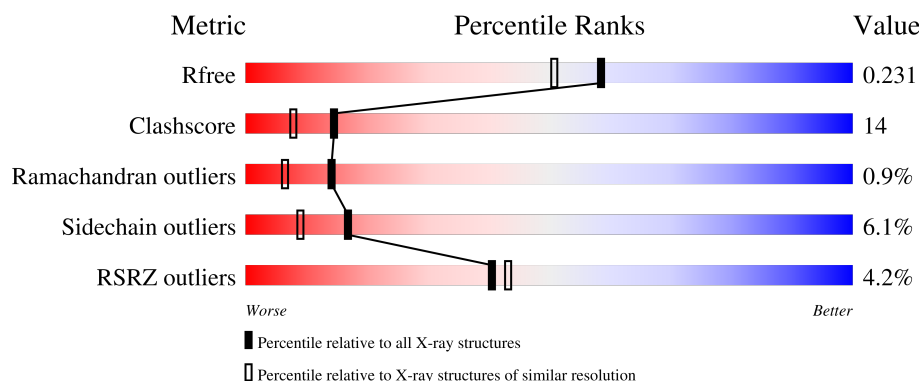
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

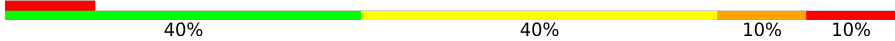
The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	356	 4% 72% 18% • • 5%
2	B	20	 10% 40% 40% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	404	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3399 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 cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	P	S	0	3	0
			2809	1819	470	509	3	8			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P05132
A	-4	HIS	-	expression tag	UNP P05132
A	-3	HIS	-	expression tag	UNP P05132
A	-2	HIS	-	expression tag	UNP P05132
A	-1	HIS	-	expression tag	UNP P05132
A	0	HIS	-	expression tag	UNP P05132
A	1	GLY	-	expression tag	UNP P05132
A	2	ASN	-	expression tag	UNP P05132
A	3	ALA	-	expression tag	UNP P05132
A	4	ALA	-	expression tag	UNP P05132
A	5	ALA	-	expression tag	UNP P05132
A	6	ALA	-	expression tag	UNP P05132
A	7	LYS	-	expression tag	UNP P05132
A	8	LYS	-	expression tag	UNP P05132
A	9	GLY	-	expression tag	UNP P05132
A	10	SER	-	expression tag	UNP P05132
A	11	GLU	-	expression tag	UNP P05132
A	12	GLN	-	expression tag	UNP P05132
A	13	GLU	-	expression tag	UNP P05132

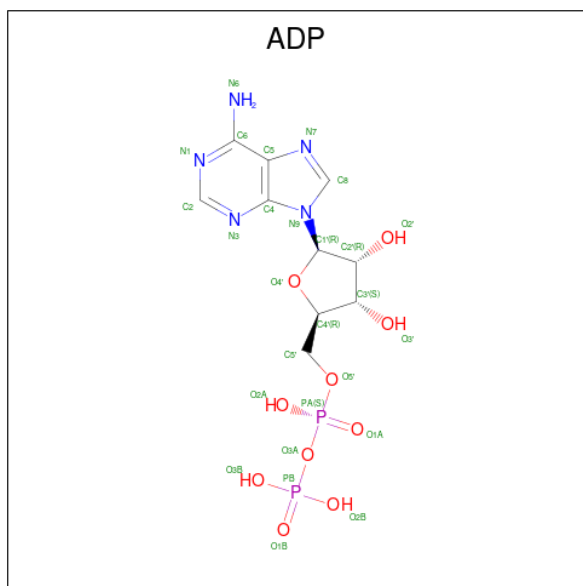
- Molecule 2 is a protein called cAMP-dependent protein kinase inhibitor alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	20	Total	C	N	O	S	0	3	0
			179	108	36	33	2			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

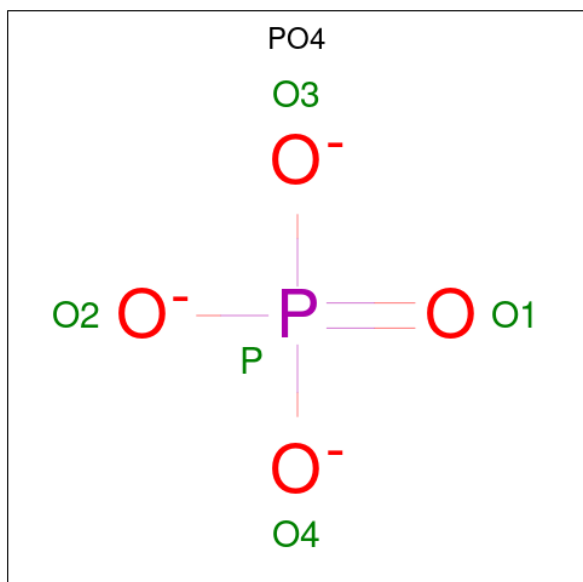
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	346	Total	O	0	0
			346	346		
6	B	31	Total	O	0	0
			31	31		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.30Å 79.23Å 97.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.9 (20.00-1.90) 87.8 (20.00-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 1.91Å)	Xtriage
Refinement program	SHELX, SHELXL-97	Depositor
R, R_{free}	0.186 , 0.265 (Not available) , 0.231	Depositor DCC
R_{free} test set	1597 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 77.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3399	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, SEP, MG, ADP, TPO

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	0.96	13/2850 (0.5%)	1.33	21/3834 (0.5%)
2	B	1.78	6/182 (3.3%)	1.10	2/243 (0.8%)
All	All	1.03	19/3032 (0.6%)	1.31	23/4077 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	5
All	All	0	6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217[A]	LYS	CA-C	9.01	1.65	1.52
1	A	217[B]	LYS	CA-C	9.01	1.65	1.52
1	A	217[A]	LYS	N-CA	-7.63	1.36	1.46
1	A	217[B]	LYS	N-CA	-7.63	1.36	1.46
2	B	617	GLY	C-O	-6.93	1.17	1.23
2	B	608	ALA	C-O	-6.34	1.16	1.24
1	A	134	ARG	C-O	-6.14	1.17	1.24
1	A	217[A]	LYS	C-O	-6.14	1.16	1.24
1	A	217[B]	LYS	C-O	-6.14	1.16	1.24
1	A	245	GLN	C-O	-6.00	1.17	1.24
1	A	270	ARG	C-O	-6.00	1.16	1.24
1	A	241	ASP	C-O	-5.98	1.16	1.24
1	A	101	PRO	N-CD	5.89	1.55	1.47
2	B	614	GLY	C-O	-5.73	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	GLU	C-O	-5.68	1.17	1.24
2	B	611	ILE	C-O	-5.61	1.17	1.24
2	B	609	ASP	C-O	-5.41	1.17	1.24
2	B	615	ARG	C-O	-5.26	1.17	1.24
1	A	81	LYS	C-O	-5.09	1.17	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217[A]	LYS	N-CA-C	11.75	127.62	112.34
1	A	217[B]	LYS	N-CA-C	11.75	127.62	112.34
1	A	321[A]	PRO	CA-C-N	9.26	139.49	122.83
1	A	321[A]	PRO	C-N-CA	9.26	139.49	122.83
1	A	321[B]	PRO	CA-C-N	9.26	139.49	122.83
1	A	321[B]	PRO	C-N-CA	9.26	139.49	122.83
1	A	217[A]	LYS	CA-C-O	8.52	129.84	119.10
1	A	217[B]	LYS	CA-C-O	8.52	129.84	119.10
1	A	144	ARG	CD-NE-CZ	8.49	136.29	124.40
2	B	620	ALA	O-C-N	-6.83	115.00	122.79
1	A	144	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	A	335	ILE	CA-C-N	6.28	129.75	120.90
1	A	335	ILE	C-N-CA	6.28	129.75	120.90
1	A	213	LYS	N-CA-C	6.02	118.80	111.82
1	A	336	ARG	N-CA-C	5.96	118.64	110.24
1	A	138	PHE	CA-CB-CG	5.34	119.14	113.80
2	B	620	ALA	CA-C-O	-5.30	115.73	121.87
1	A	44	ASP	CA-C-N	5.18	129.24	121.72
1	A	44	ASP	C-N-CA	5.18	129.24	121.72
1	A	174	ILE	O-C-N	-5.18	117.28	123.03
1	A	144	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	A	174	ILE	CA-C-N	-5.05	113.22	122.12
1	A	174	ILE	C-N-CA	-5.05	113.22	122.12

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	LEU	Mainchain
2	B	620	ALA	Mainchain
2	B	623[A]	HIS	Peptide,Mainchain
2	B	623[B]	HIS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2809	0	2798	72	0
2	B	179	0	166	21	0
3	A	2	0	0	0	0
4	A	27	0	12	2	0
5	A	5	0	0	2	0
6	A	346	0	0	24	0
6	B	31	0	0	2	0
All	All	3399	0	2976	84	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 14.

All (84) 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:285[B]:LYS:HE3	1:A:285[B]:LYS:H	0.99	1.06
1:A:87:HIS:CE1	2:B:623[B]:HIS:CE1	2.43	1.05
2:B:622[B]:ILE:HG22	2:B:624:ASP:HB2	1.32	1.05
1:A:87:HIS:CE1	2:B:623[B]:HIS:HE1	1.75	1.05
1:A:87:HIS:HE1	2:B:623[B]:HIS:CE1	1.78	1.00
2:B:622[B]:ILE:CG2	2:B:624:ASP:HB2	1.92	0.99
1:A:285[B]:LYS:HE3	1:A:285[B]:LYS:N	1.82	0.94
5:A:404:PO4:O1	2:B:621[A]:CYS:HB3	1.74	0.88
1:A:253:GLY:O	6:A:818:HOH:O	1.98	0.81
1:A:336:ARG:HG2	6:A:766:HOH:O	1.81	0.79
1:A:336:ARG:CG	6:A:766:HOH:O	2.33	0.76
2:B:622[B]:ILE:HG22	2:B:623[B]:HIS:H	1.50	0.76
1:A:139:SEP:O2P	1:A:142:HIS:HB2	1.86	0.76
1:A:285[A]:LYS:HD2	1:A:285[A]:LYS:N	2.01	0.75
1:A:21:LYS:HG3	6:A:780:HOH:O	1.87	0.74
2:B:622[B]:ILE:HG22	2:B:623[B]:HIS:N	2.03	0.74
2:B:622[B]:ILE:CD1	6:B:726:HOH:O	2.37	0.72
1:A:336:ARG:NH1	6:A:766:HOH:O	2.23	0.72
1:A:303:ILE:O	1:A:307:GLN:HG3	1.91	0.71
1:A:163:ILE:HG12	1:A:217[A]:LYS:HG2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:O	2:B:623[B]:HIS:HA	1.95	0.67
1:A:244:ILE:HG13	6:A:775:HOH:O	1.95	0.67
1:A:217[A]:LYS:HG3	6:A:811:HOH:O	1.93	0.67
1:A:336:ARG:CZ	6:A:766:HOH:O	2.43	0.66
1:A:52:GLY:HA3	4:A:403:ADP:O2B	1.95	0.66
1:A:192:LYS:HB2	6:A:507:HOH:O	1.98	0.64
1:A:14:SER:OG	1:A:17:GLU:HB2	1.98	0.64
2:B:622[B]:ILE:CG2	2:B:624:ASP:CB	2.74	0.62
1:A:285[A]:LYS:HD2	1:A:285[A]:LYS:H	1.66	0.61
1:A:336:ARG:HH12	1:A:338:SEP:HB3	1.68	0.58
2:B:622[B]:ILE:HD11	6:B:726:HOH:O	2.02	0.58
1:A:336:ARG:N	6:A:767:HOH:O	2.39	0.55
1:A:333:GLU:HA	1:A:333:GLU:OE2	2.07	0.53
1:A:126:GLY:HA2	1:A:327:PHE:CZ	2.44	0.53
1:A:284:LEU:HB3	1:A:285[B]:LYS:CE	2.40	0.52
1:A:81:LYS:NZ	6:A:503:HOH:O	2.43	0.52
1:A:158:HIS:HD2	6:A:774:HOH:O	1.93	0.52
2:B:622[B]:ILE:HG22	2:B:624:ASP:CB	2.22	0.51
1:A:45:ARG:HA	1:A:60:VAL:HG12	1.91	0.50
1:A:158:HIS:HE1	1:A:220:ASP:OD2	1.94	0.50
1:A:335:ILE:HD13	1:A:335:ILE:O	2.10	0.50
2:B:622[B]:ILE:CG2	2:B:623[B]:HIS:H	2.16	0.50
1:A:21:LYS:HD2	1:A:21:LYS:C	2.37	0.50
1:A:278:THR:HG22	1:A:279:LYS:HG3	1.93	0.49
1:A:146:TYR:HB3	1:A:180:ILE:HD11	1.93	0.49
1:A:284:LEU:CB	1:A:285[A]:LYS:HD2	2.43	0.49
1:A:52:GLY:HA3	4:A:403:ADP:PB	2.53	0.48
1:A:146:TYR:HB3	1:A:180:ILE:CD1	2.44	0.48
1:A:158:HIS:HB3	1:A:217[B]:LYS:HE3	1.96	0.48
1:A:87:HIS:ND1	2:B:623[B]:HIS:HE1	2.08	0.48
1:A:194:ARG:HD2	1:A:214:GLY:HA3	1.96	0.47
1:A:81:LYS:NZ	6:A:504:HOH:O	2.48	0.47
1:A:168:LYS:HZ3	5:A:404:PO4:P	2.38	0.46
1:A:99:ASN:HD22	1:A:105:LYS:NZ	2.13	0.46
1:A:186:GLY:HA3	6:A:713:HOH:O	2.15	0.46
1:A:270:ARG:HD3	6:A:842:HOH:O	2.16	0.46
1:A:286:ASN:O	1:A:289:ASN:HB2	2.16	0.46
1:A:284:LEU:HB2	1:A:285[A]:LYS:HD2	1.97	0.46
1:A:78:LYS:HE3	6:A:805:HOH:O	2.15	0.45
2:B:622[B]:ILE:HG21	2:B:624:ASP:HB2	1.93	0.45
1:A:78:LYS:HG2	6:A:769:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASP:HA	1:A:217[A]:LYS:HE2	2.00	0.44
1:A:284:LEU:HB3	1:A:285[B]:LYS:CD	2.47	0.44
1:A:95:LEU:HG	1:A:106:LEU:HB2	1.99	0.44
1:A:244:ILE:CD1	6:A:775:HOH:O	2.65	0.44
1:A:202:PRO:HD3	2:B:622[B]:ILE:HG12	1.99	0.44
1:A:315:ILE:HD11	6:A:747:HOH:O	2.18	0.43
1:A:339:ILE:HG12	6:A:501:HOH:O	2.17	0.43
1:A:317:LYS:HE2	6:A:783:HOH:O	2.18	0.43
1:A:84:GLN:HE22	2:B:623[B]:HIS:CE1	2.36	0.43
1:A:55:GLY:N	6:A:686:HOH:O	2.51	0.43
1:A:111:LYS:NZ	1:A:350:PHE:O	2.50	0.42
1:A:239:PHE:O	1:A:249:LYS:HE3	2.18	0.42
1:A:341:GLU:HG2	6:A:748:HOH:O	2.19	0.42
2:B:607:TYR:CZ	2:B:611:ILE:HG13	2.54	0.42
1:A:87:HIS:ND1	2:B:623[B]:HIS:CE1	2.85	0.41
1:A:197:TPO:HG22	2:B:623[B]:HIS:NE2	2.36	0.41
1:A:284:LEU:HB3	1:A:285[B]:LYS:HD2	2.02	0.41
1:A:21:LYS:C	1:A:21:LYS:CD	2.93	0.41
1:A:215:TYR:CD2	1:A:219:VAL:HG11	2.55	0.41
1:A:21:LYS:HD2	1:A:21:LYS:O	2.21	0.40
1:A:244:ILE:CG1	6:A:775:HOH:O	2.63	0.40
1:A:292:LYS:HA	1:A:302:TRP:CZ2	2.57	0.40
1:A:107:GLU:N	1:A:119:VAL:O	2.50	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	335/356 (94%)	323 (96%)	10 (3%)	2 (1%)	21	13
2	B	21/20 (105%)	17 (81%)	0	4 (19%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	356/376 (95%)	340 (96%)	10 (3%)	6 (2%)	14	2

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285[A]	LYS
1	A	285[B]	LYS
2	B	622[A]	ILE
2	B	622[B]	ILE
2	B	623[A]	HIS
2	B	623[B]	HIS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/308 (97%)	278 (93%)	20 (7%)	15	7
2	B	18/15 (120%)	16 (89%)	2 (11%)	6	2
All	All	316/323 (98%)	294 (93%)	22 (7%)	17	7

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	17	GLU
1	A	21	LYS
1	A	28	LYS
1	A	244	ILE
1	A	255	VAL
1	A	268	LEU
1	A	278	THR
1	A	284	LEU
1	A	285[A]	LYS
1	A	285[B]	LYS
1	A	286	ASN

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Mol	Chain	Res	Type
1	A	295	LYS
1	A	309	LYS
1	A	321[A]	PRO
1	A	321[B]	PRO
1	A	331	GLU
1	A	333	GLU
1	A	335	ILE
1	A	345	LYS
2	B	622[A]	ILE
2	B	622[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	84	GLN
1	A	99	ASN
1	A	113	ASN
1	A	158	HIS
1	A	176	GLN
1	A	242	GLN
1	A	271	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 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
1	SEP	A	338	1	8,9,10	1.24	0	7,12,14	1.67	1 (14%)
1	TPO	A	197	1	8,10,11	1.43	1 (12%)	10,14,16	2.14	1 (10%)
1	SEP	A	139	1	8,9,10	1.73	2 (25%)	7,12,14	1.50	1 (14%)

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
1	SEP	A	338	1	-	5/6/8/10	-
1	TPO	A	197	1	-	1/9/11/13	-
1	SEP	A	139	1	-	3/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	SEP	P-O1P	3.95	1.62	1.50
1	A	197	TPO	P-O1P	3.23	1.60	1.50
1	A	139	SEP	P-O3P	2.03	1.62	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	TPO	P-OG1-CB	-6.16	106.59	123.33
1	A	338	SEP	OG-CB-CA	4.15	112.18	108.14
1	A	139	SEP	OG-CB-CA	2.70	110.77	108.14

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	139	SEP	C-CA-CB-OG
1	A	139	SEP	CB-OG-P-O1P
1	A	338	SEP	C-CA-CB-OG
1	A	338	SEP	CA-CB-OG-P
1	A	338	SEP	CB-OG-P-O2P
1	A	338	SEP	CB-OG-P-O3P
1	A	139	SEP	CB-OG-P-O2P
1	A	338	SEP	N-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
1	A	197	TPO	C-CA-CB-CG2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	338	SEP	1	0
1	A	197	TPO	1	0
1	A	139	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	PO4	A	404	3	4,4,4	2.15	2 (50%)	6,6,6	0.82	0
4	ADP	A	403	3	28,29,29	1.79	8 (28%)	43,45,45	1.84	10 (23%)

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
4	ADP	A	403	3	-	0/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	ADP	C5-C4	4.44	1.47	1.39
4	A	403	ADP	C5-N7	-3.63	1.32	1.39
4	A	403	ADP	C4-N9	-3.15	1.31	1.37
4	A	403	ADP	C8-N9	-2.99	1.32	1.37
5	A	404	PO4	P-O3	-2.70	1.46	1.54
4	A	403	ADP	C5-C6	2.38	1.47	1.41
4	A	403	ADP	PA-O1A	-2.15	1.43	1.50
5	A	404	PO4	P-O1	2.10	1.55	1.50
4	A	403	ADP	PB-O3B	-2.05	1.47	1.54
4	A	403	ADP	PA-O2A	-2.02	1.46	1.55

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	ADP	C5-C4-N3	-6.25	118.11	126.72
4	A	403	ADP	N3-C4-N9	5.08	135.80	127.17
4	A	403	ADP	C4-C5-N7	-3.59	106.47	110.58
4	A	403	ADP	C2-N3-C4	3.55	120.51	111.83
4	A	403	ADP	C2-N1-C6	2.51	122.85	118.73
4	A	403	ADP	N3-C2-N1	-2.39	124.96	128.58
4	A	403	ADP	C5-N7-C8	2.20	106.91	103.45
4	A	403	ADP	C4-N9-C8	2.19	108.04	105.74
4	A	403	ADP	C6-C5-N7	2.15	136.24	132.09
4	A	403	ADP	N6-C6-N1	2.01	122.84	118.38

There are no chirality outliers.

There are no torsion outliers.

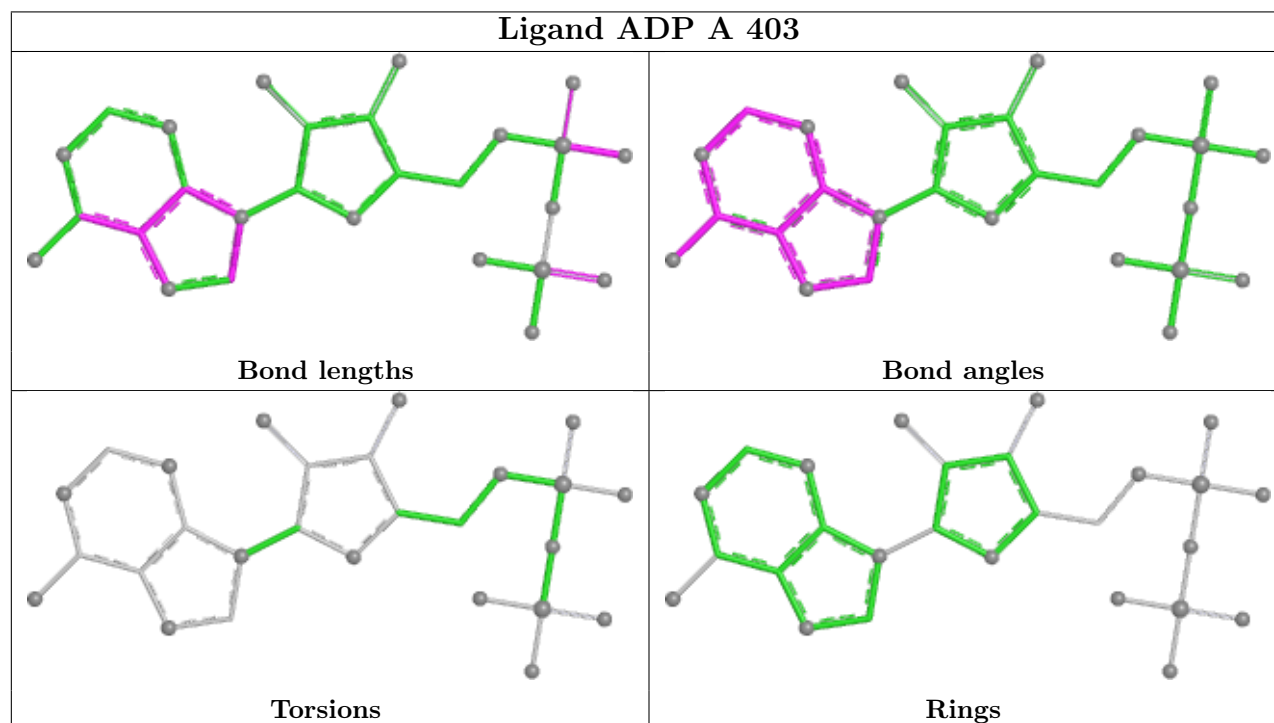
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	404	PO4	2	0
4	A	403	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	334/356 (93%)	-0.11	13 (3%) 43 46	11, 21, 55, 87	3 (0%)
2	B	20/20 (100%)	0.07	2 (10%) 12 13	15, 19, 28, 113	3 (15%)
All	All	354/376 (94%)	-0.10	15 (4%) 40 43	11, 21, 55, 113	6 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	PHE	4.8
2	B	623[A]	HIS	4.3
1	A	335	ILE	3.5
2	B	624	ASP	3.4
1	A	55	GLY	3.1
1	A	53	SER	3.0
1	A	321[A]	PRO	3.0
1	A	15	VAL	2.8
1	A	336	ARG	2.5
1	A	253	GLY	2.5
1	A	337	VAL	2.5
1	A	54	PHE	2.4
1	A	319	LYS	2.2
1	A	316	PRO	2.2
1	A	193	GLY	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, 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($\text{\AA}^2$)	Q<0.9
1	SEP	A	139	10/11	0.92	0.16	13,22,88,113	0
1	SEP	A	338	10/11	0.95	0.08	19,29,33,34	0
1	TPO	A	197	11/12	0.98	0.05	14,17,23,28	0

6.3 Carbohydrates [i](#)

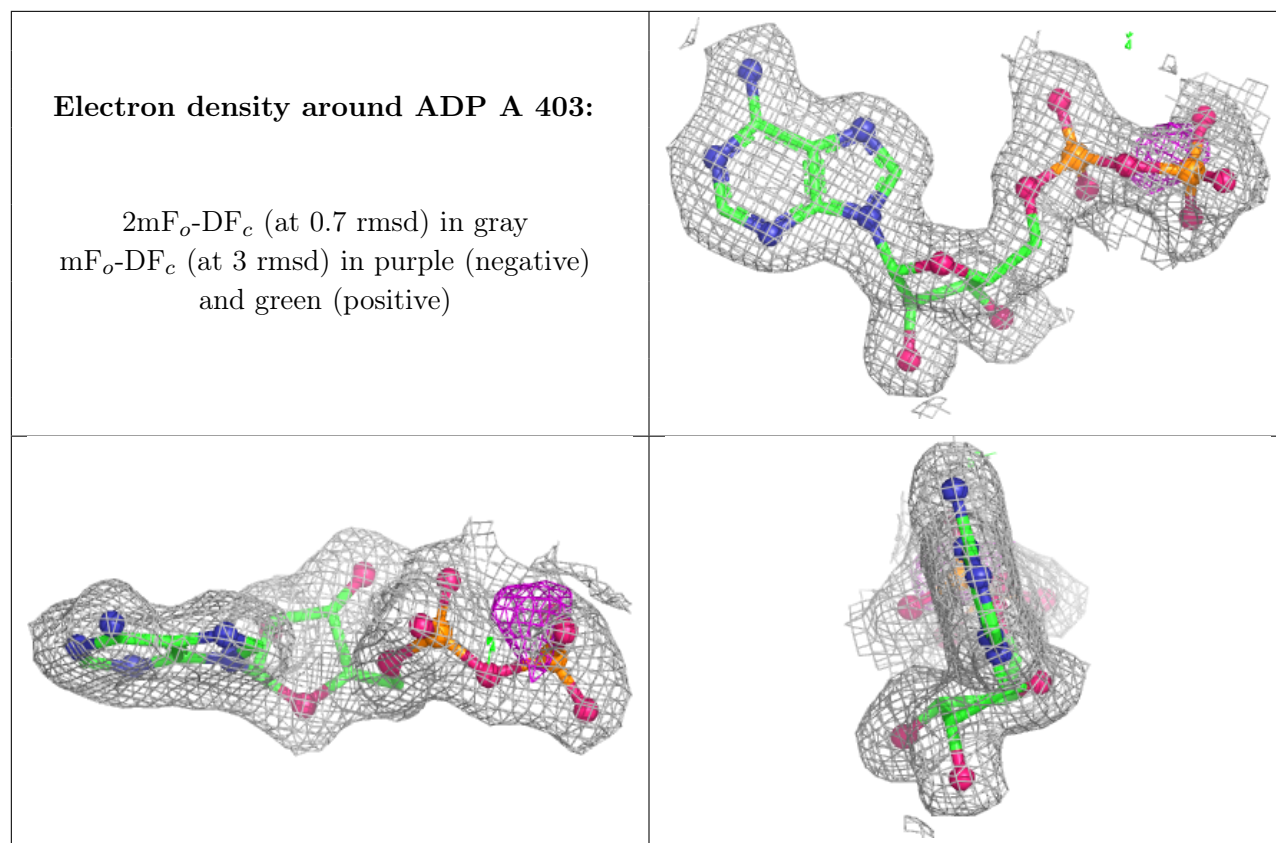
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	MG	A	401	1/1	0.90	0.08	43,43,43,43	0
3	MG	A	402	1/1	0.90	0.06	33,33,33,33	0
5	PO4	A	404	5/5	0.91	0.14	15,24,32,49	5
4	ADP	A	403	27/27	0.96	0.06	15,19,44,52	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.